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X-ray Analysis of Excited-State Structures in the Crystals of the Diplatinum Complex Anion

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Photo-excited structure change of Ptpop compound 40

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Chapter 1

General introduction

1.1 Single crystal X-ray analysis

1.1.1 Start of the X-ray analysis

In 1895, W. C. Röntgen discovered X-ray, and the first X-ray diffraction from $CuSO_4 \cdot 5H_2O$ crystal was reported in 1912 by Laue et al. [1,2] W. H. Bragg and W. L. Bragg succeeded the first structure determination of NaCl [3] and diamond [4] in 1913, and the X-ray crystallography started since then. Until 2004, the number of reported organic and metal organic crystal structures exceeds over 270000 [5], and the crystal structures of proteins, determined by X-ray analysis, also reported more than 20000 since 1971. [6] The number of molecular structures determined by single crystal X-ray analysis increases explosively.

The advantage of single crystal X-ray analysis is to obtain the molecular structure with high accuracy. This feature makes the single crystal X-ray analysis more powerful than other methods such as spectroscopy, theoretical calculation and so on. However the weak points of this powerful method have been the phase problem and the long data collection time. Recently these weak points have been almost overcome by the development of equipments.

1.1.2 Development of X-ray analysis

In order to solve the above two weak points, many ideas have been proposed, and at the present day, most of the crystal structures can be determined by single crystal X-ray analysis in a short time. The progress of technology plays the important role in the large development of this method.

The X-ray film was used as the detector in the early days of X-ray analysis, and all diffraction intensities on these films had to be read by eyes

and the density distribution map must be calculated by hand or calculator. At that time, many years were required to determine only one crystal structure. In 1960's the four-circle diffractmeter was developed and the data collection time decreased to a few days. In 1990's the two-dimensional detectors such as imaging-plate (IP) and CCD were developed to obtain the data within one day. At present the diffractmeters with IP or CCD as a detector are widely used for the crystal structure determination. For near future, the new generation diffractometer with various detectors, e.g. the pixel array detector [7,8] and micro-strip-gas-chamber (MSGC), [9] will be developed and these will make it possible to collect the intensity data within 1 second. The progresses of equipments are summarized in Table 1.1.

The X-ray sources have also been developed for a hundred years. The sealed tube has been used for a long time. The rotating anode X-ray generator is several times stronger than sealed tube and reduced the data collection time to several hours using the two-dimensional diffractometer. The newly developed light source, synchrotron radiation, brought the new field of X-ray analysis. The brightness is a few tens times stronger than that of the rotating anode. The data collection time became shorter, and the sub-micrometer-sized single crystal can be analyzed using synchrotron radiation. [10]

In addition to the developments of the X-ray source and diffractometer, the developments of the computer and the software programs for the structure solution and refinement or graphical user interface (GUI) have caused significant changes in the X-ray method. The developments of X-ray sources and diffractometer shorten the data collection time, while the developments of computer and software programs shorten the time for

Table 1.1 Relationship between development of diffractometer and measurement time.

Year	Tolal measurement time	Measurement equipment(s)
~ 1960	5000 ~ 10000 hrs	X-ray film
1960 ~ 1980	100 ~ 150 hrs	Four-circle diffractometer & Sealed tube
1980 ~ 1990	50 ~ 100 hrs	Four-circle diffractometer & Rotating anode
1990 ~ 2000	3 ~ 10 hrs	IP, CCD
2000 ~	< 10 sec	MSGC & Rotating anode
	1 μsec	MSGC & Synchrotron radiation

structure analysis after the measurement. Although the process of solving and refining the structure became a black box, it is true that many researchers can use X-ray analysis for their study without the knowledge of crystallography. However shorter the time for data collection and the structure analysis become, the time for the interpretation of the phenomenon in the crystal may not change so short.

Moreover the structure analyses under extreme conditions, e.g. under high temperature, [11,12] high pressure, [13] magnetic field [14] and so on, have been reported recently. Especially the low temperature measurements are the most effective and widely used. The advantages of low temperature measurement are well understood, [15] and the cooling equipment has also been improved. New gas-flow methods, which use nitrogen gas separated from air to cool the samples to 77 K and helium gas to cool the sample to less than 20 K, [16,17] have been developed.

The compounds, whose melting point is below room temperature, have been analyzed using the *in situ* crystallization technique. [18,19,20,21,22] The low temperature measurement, which is called cryotrapping method, [23] has brought not only the precise structure of the stable molecules but also the structure of unstable or metastable molecules.

1.1.3 Analysis of the metastable species

The improvement of the equipment, e.g. diffractometer, X-ray sources and low temperature equipment, enables to determine the structure of reactant molecules and small amount of product molecules generated in the crystal lattice directly.

Our group has reported a variety of crystalline-state reactions such as photo-racemization [24, 25] and photo-isomerization of cobaloxime

complexes, [26,27] the cyclization reactions [28] and the oxygen insertion reaction, [29] in which the reactant molecules are completely changed to the product molecules with retention of the single crystal form. Among these reactions, unstable intermediate structures were observed by X-ray analysis. [30] This indicates that the structures of the reaction intermediates as well as the reactant and product molecules can be observed by X-ray analysis in the crystalline-state reactions.

Recently several structures of unstable species such as unstable structures of photochromic crystals, [31,32] intermediate of nitrosyl-metal complexes, [33] and photoproduced radical pairs, [34,35] triplet carbenes, [23] and triplet nitrenes [36,37] have been observed using the single crystal X-ray analysis. These structure analyses suggest that the unstable structures can be observed by X-ray analysis at low temperatures less than 100 K, although the produced unstable species were less than 5-10% concentration in the original crystal.

1.2 Study of the excited state molecule

1.2.1 Time-resolved measurement and excited state molecules

As the measurement techniques developed, single crystal X-ray analysis of the excited state or much faster chemical reactions have been attracted recent years. The excited molecules have been studied by the spectroscopy for the long time, because the lifetimes, e.g. platinum poly-ynes, ranges typically from μs to ps. [38,39,40,41] Indeed a lot of studies on the excited state species has been reported by spectroscopy. Therefore one can prepare the compounds in order to study the emissive properties of various kinds of the metal and ligand type compounds by spectroscopy. However, the observed

transient spectroscopic band in the UV/vis range are normally very broad, and this research requires knowledge about the nature of excited state that is responsible for the emission. This is a very significant problem, since this emissive state is usually a mixture of various types of low energy excited states. [42] It is possible to obtain a certain level of information indirectly through UV/vis spectroscopic measurements, by comparing the different emission wavelengths, lifetimes and quantum yields for a series of complexes, and such inferences can be supported by theoretical calculations.

Although the recent developments in time-resolved infrared spectroscopy [43,44,45] can be obtained the more direct information, it cannot cover the whole frequency range necessary for a complete structure determination. [46] Moreover, experimental results in ultra fast spectroscopy also raise the question whether ultra fast structure change on the excited state can be described within the Born-Oppenheimer approximation or whether one has to go beyond.

In contrast to spectroscopy, advantage of the diffraction analysis is obtainable the structure information directory. Time-resolved powder X-ray diffraction has been carried out to investigate the structure dynamics. [47] Recently, Techert et al. reported the pico-second transient structure change of *N*, *N*-dimethylaminobenzonitrile ($C_9H_{10}N_2$) by time-resolved powder X-ray diffraction.[48] Such works undoubtedly provide invaluable information.

In order to investigate both direct and quantitative information of the excited-state structure, the stroboscopic pump-probe technique has been developed for time-resolved single-crystal X-ray diffraction. The techniques were applied to the photo-induced crystal structures exist for μs

to ns timescale. [49,50]

The stroboscopic pump-probe techniques was mainly carried out using a combination of pulse laser beam and polychromatic synchrotron radiation (Laue diffraction method [51,52,53]) or monochromic pulse synchrotron radiation. [54,55,56] The former was used frequently in the field of the protein crystals, investigating the reaction processes of protein molecules with light. [57,58,59,60,61] Because Laue method use the polychromatic X-ray (white X-ray), it is possible to cover the most of reciprocal space at once. However it occurred many overlap of diffraction, and the resolution of the resulting structure is significantly obscure compared with an analogous experiment used monochromatic X-ray and oscillatory scans.

The latter was used for the metastable small molecules. [62,63] Although the data collection time of the method using the monochromatic X-ray will increase compared with that of Laue method, the analyzed structure has much higher resolution.

If these time-resolved analyses with micro- and nano-second level will be applied to the single crystal of small molecules, e.g. photo-induced excited molecule, it will afford the key information of the physical and chemical properties, such as fluorescent and phosphorescent, reaction mechanism and so on.

K. Moffat pointed out the two experimental differences between the crystals of macromolecule and small-molecule in regard to this crystallography. [60] First point is the environment around a molecule. Macromolecular crystals contain a large volume of liquid, e.g. water, and the strength of intermolecular interactions that stabilize the crystal lattice are weak. Since the environment of the molecules in a macromolecular crystal more resembles that in a concentrated solution, the conformational

changes accompanied by biological processes in the crystal lattice often proceed via the same chemical pathway as in solution, with similar rate constants, and with retention of the original crystal lattice. In contrast, crystals of small organic and inorganic molecules generally do not contain liquid and the stabilizing interactions are strong. Since the each molecule is packed closely, conformational changes are restricted and reactivity in the solid state differs qualitatively from that in solution. Therefore reaction is often accompanied by degradation of crystallinity and/or a phase change. As a rule of thumb, the fewer the number of atoms involved in a conformational change, the more rapidly it occurs. Hence time-resolved studies in small-molecule chemical crystallography and materials science may require the very highest time resolution.

Second point is the generation of heat. At a more practical level, initiation of conformational changes of molecules in a crystal deposits energy in the crystal and this leads to temperature rise that may itself influence the nature and rate of the conformational change and at worst brings a disorder to the crystal. That is, all experiments cause temperature-jump unavoidably. This effect may be quite large and differs significantly in magnitude between crystals of macromolecules and small molecules.

Considering a structural change that is initiated by light, the temperature rise in the crystal (ΔT) is derived to be proportional to the concentration of molecules in the crystal. The concentration of macromolecular crystals might range from 5 mM to 100 mM, and ΔT is estimated at the range between 0.2 and 4.3 °C for the macromolecular crystals. [64] Moreover since the rate of heat transfer from the interior of the crystal to its surface from which the heat is dissipated may be quite slow, the time necessary to the

thermal equilibration is milliseconds or longer for typical crystals. [65,66]

For the crystals of small molecules, since the concentration for such crystals can easily attain 1-50 M, ΔT become two or three orders of magnitude greater than that of crystals of macromolecules. Thus, in most cases, the temperature rise may be unavoidable even if effective cooling system were used. It is experimentally probable to induce a very large temperature jump in such crystals. It is therefore no surprise that the pioneering nanosecond time-resolved crystallographic experiments [67] involved laser-induced melting and subsequent recrystallization of the surface of silicon crystals. To avoid temperature rise, stroboscopic or other repetitive signal-averaging techniques are applied to measure the very small changes in the X-ray diffraction amplitudes accurately. [54,68]

The above discussions are based on the usage of laser beam as excitation light. In regard to this points, the continuous light irradiation using but Xe lamp not laser beam overcome the difficulties for small molecule crystals as well as stroboscopic technique. Using the laser beam with the wavelength at the absorption maximum caused the excitation only on crystal surface and increased the temperature locally. In contrast, the Xe lamp has the wide wavelength distribution and the light with longer wavelength can penetrate into the crystal since the absorption may be low. [69] Although the continuous excitation of the molecules may occur in a whole crystal and create the equilibrium crystal lattice, the temperature rise at the equilibrium state should be small.

1.2.2 History of diplatinum complex, $[Pt_2(P_2O_5H_2)_4]^{4-}$

Diplatinum complex, $[Pt_2(pop)_4]^{4-}$ ($pop=P_2O_5H_2^{2-}$), is well known as an anion showing a lot of unusual spectroscopic properties. This complex was

reported first at 1977. [70] At that time, the authors considered this complex was $Pt(OP(OH)_2)_2(P(OH)_3)_2$, reported in 1961. [71] This compound was synthesized in the reaction of potassium tetrachloro platinate with phosphorous acid. It shows an intense green luminescence by photo-irradiation. Within ten years, the complex was known as $[Pt_2(pop)_4]^{4-}$, and a lot of unusual properties have been reported. Because of the intense luminescence, the early studies were mainly carried out by spectroscopic method. [72,73,74] Soon after the complex was discovered, [75] the intense luminescence was suggested to be a transition in the process of the Pt-Pt bond formation.

The absorption spectra are shown in Fig. 1.1. [76] The complex anion of $[Pt_2(pop)_4]^{4-}$, abbreviated to "Ptpop", has a strong absorption band at 367 nm and a weak absorption band at 440 nm. The first attempt to interpret the absorbance and emission data was carried out using the orbital scheme [77] for Ptpop compounds. [78] Simplified MO energy level scheme and schematic energy-level diagram are shown in Fig. 1.2. [79] Platinum atom has eight 5d electrons and forms a square-planar moiety, PtP_4, with four phosphorus atoms. The HOMO of the PtP_4 moiety is $a_{1g}(d_z^2)$ and two PtP_4 moieties form the diplatimum complex, Pt_2P_8 , which is the model of the Ptpop complex. The orbitals perpendicular to the molecular plane, d_z^2 and p_z, interact strongly, and yielding $d\sigma/\sigma^*$ and $p\sigma/\sigma^*$ orbital. At the ground state, Pt_2P_8 complex occupies $1a_{1g}$ and $1a_{2u}$ orbital, and it is equal $d\sigma$ and $d\sigma^*$ orbital, respectively. Therefore, the binuclear d^8-d^8 ion, $[Pt_2(pop)_4]^{4-}$, with orbital $(d\sigma)^2(d\sigma^*)^2$ has a formal bond order of zero.

As the result, the strong absorption peak was found as the electron transition from ground state to singlet excited state ($1a_{2u} \rightarrow 2a_{1g}$; $^1A_{1g} \rightarrow {}^1A_{2u}$) that have a weak fluorescence at 400 nm. The weak absorption

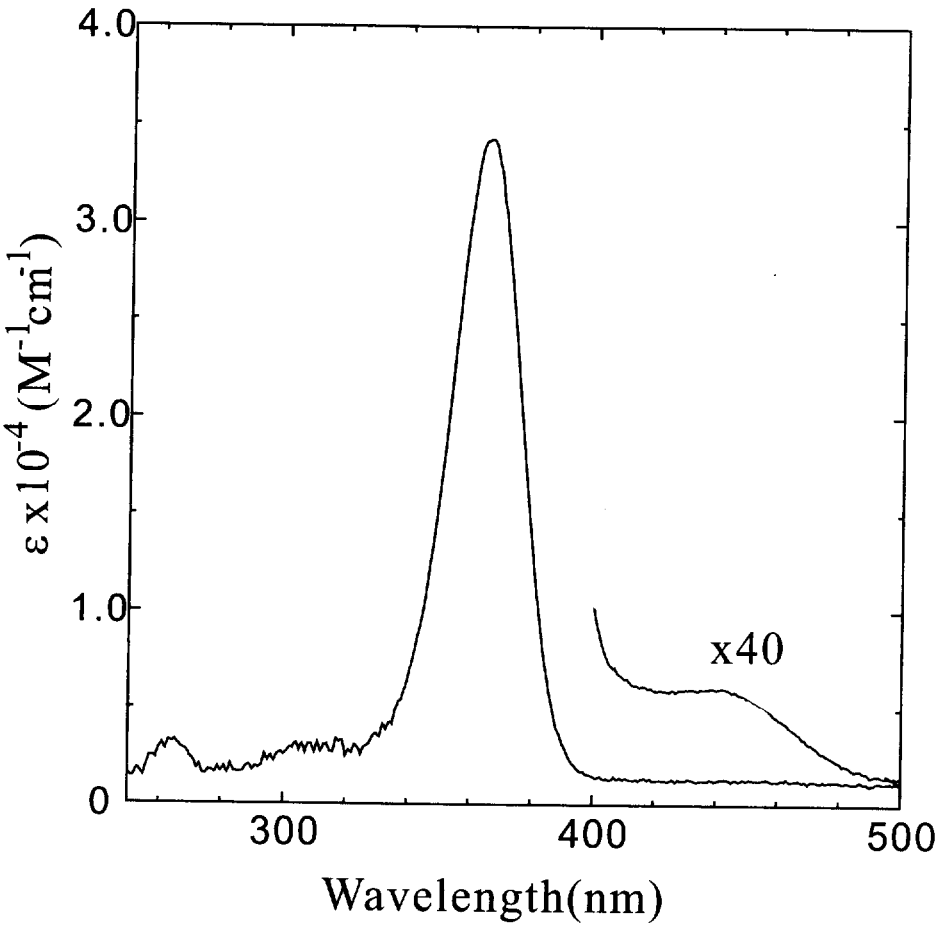

Fig. 1.1 Absorption spectra of the aqueous $[Pt_2(pop)_4]^{4-}$ anion. The large absorption spectra (367 nm) was assigned as the singlet transition and the small peak (440 nm) is the absorption caused by the triplet transition.

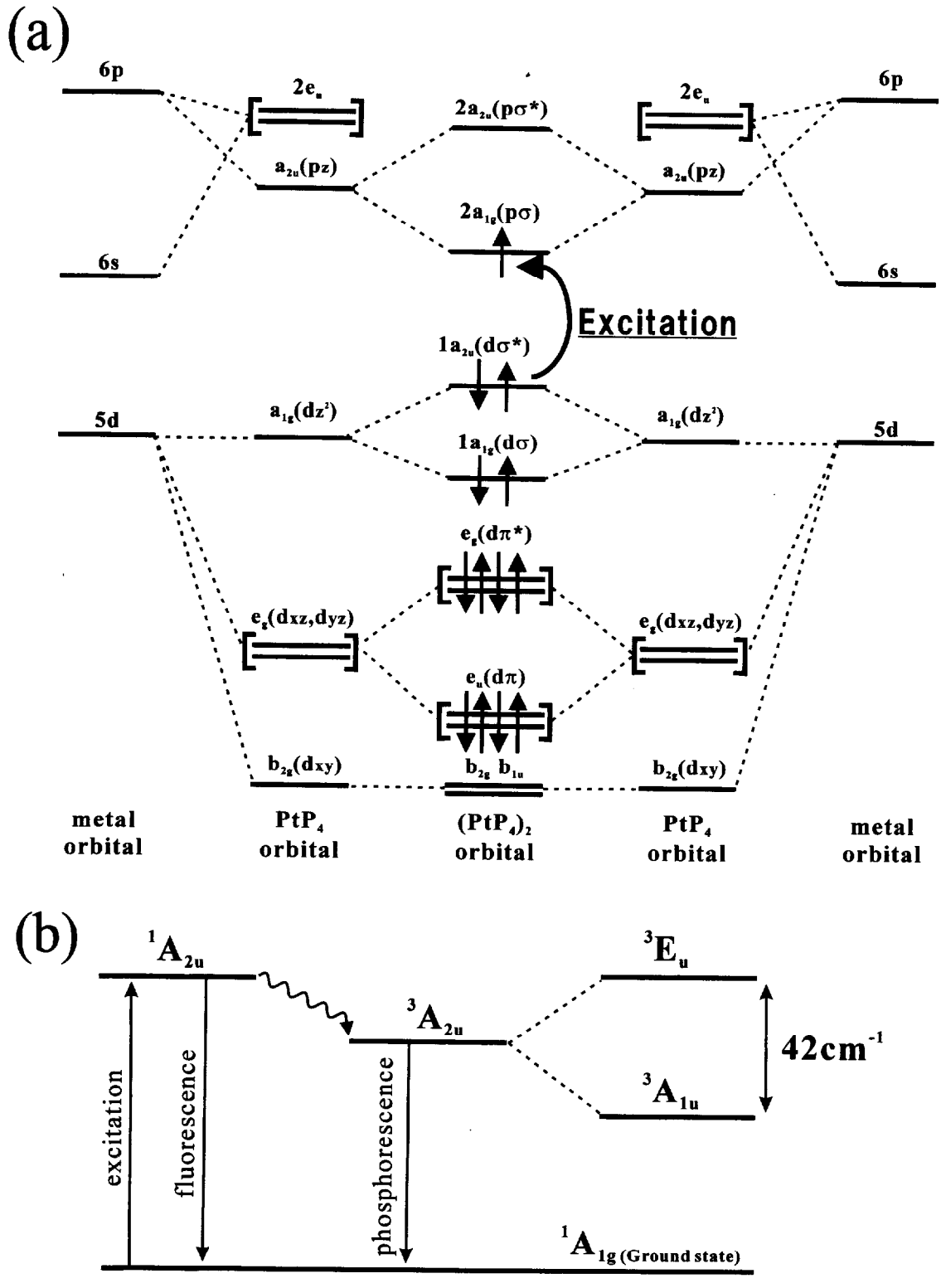

Fig. 1.2
(a) Simplified MO energy level.
(b) Schematic energy-level diagram of the Ptpop complex.

peak was the transition from the ground state to the triplet excited state ($1a_{2u} \rightarrow 2a_{1g}$; $^1A_{1g} \rightarrow {}^3A_{2u}$), that have a strong phosphorescence and longer lifetime than singlet excited state and can undergo many different chemical reactions. [80,81,82] The excited state $^3A_{2u}$ is split into ^3E_u and $^3A_{1u}$ levels, with a spacing of only about 42 cm^{-1}, [83,84,85] and lower $^3A_{1u}$ level has much longer lifetime (6.06 msec) than the ^3E_u level (4.2 μsec). [83] It is interesting that $[Pt_2(pcp)_4]^{4-}$ complex ($pcp=CH_2P_2O_4H_2$) shows no fluorescence corresponding to Ptpop, and the lifetime of the triplet excited state on aqueous solution is much shorter (0.055 μsec) than that of Ptpop (9.8 μsec) at r.t. [86] and the lifetime is 10 μsec for both compounds at 77 K. [77,87,88] The energy of the triplet excited state, estimated by spectroscopy, was 58.1 and 59.7 kcal/mol for Ptpop and Ptpcp complex, respectively. [89]

A number of studies have been carried out to elucidate the spectroscopy, photophysics and photochemistry associated with the excited electronic states of $[Pt_2(pop)_4]^{4-}$ in the 300-450 nm region. [90] It was found from the vibronically resolved absorption and emission spectra of low-temperature crystalline of $[N(C_4H_9)_4]_4[Pt_2(pop)_4]$ that the Pt-Pt bond distance for the $^3A_{2u}$ state becomes shorter by about 0.21 Å than the $^1A_{1g}$ ground state [84] and the similarity of the bandwidths and excited state vibrational wavenumbers for the $^1A_{2u}$ and $^3A_{2u}$ states suggest that they have almost the same structure. [91] This contraction can be interpreted that the orbital of d^8 electron change by excitation from non-bonding orbital, $(d\sigma)^2(d\sigma^*)^2$, to bonding orbital, $(d\sigma)^2(d\sigma^*)(p\sigma)$, and metal-metal single bond was formed between the Pt-Pt centers in the excited state.

From the combination of the EXAFS method with rapid-flow laser spectroscopy in an aqueous solution with glycerol, it was estimated that the $^3A_{2u}$ state with a lifetime of about 4 μs undergoes a contraction in the Pt-Pt

distance of 0.52 ± 0.13 Å and in the Pt-P distance of 0.047 ± 0.011 Å relative to the $^1A_{1g}$ ground state. [92] Recently it was reported from a resonance Raman intensity analysis of the $^1A_{1g} \rightarrow {}^1A_{2u}$ transition of $[N(C_4H_9)_4]_4$ $[Pt_2(pop)_4]$ in acetonitrile solution at room temperature that the Pt-Pt bond distance contraction was estimated to be about 0.225 Å in the initially excited $^1A_{2u}$ state relative to the $^1A_{1g}$ ground state. [93]

The ground and excited states of the $[Pt_2(pop)_4]^{4-}$ anion were investigated using density functional theory. [94] Calculations with different functional employing quasi-relativistic Pauli and ZORA formalisms predict a Pt-Pt shortening of 0.18-0.51 Å and a Pt-P lengthening of 0.01-0.05 Å.

In contrast to these spectroscopic or theoretical studies, the first determination of molecular structure of Ptpop anion was reported in 1980 by X-ray analysis and NMR study, [75,95] although this structure was the ground state structure. Two platinum atoms were bridging the four-diphosphite ligands as shown in Fig. 1.3. In contrast to a lot of spectroscopic studies, the crystal structures were determined only the ground state molecules for a long time, and nobody tried to measure the photo-excited structure of the Ptpop complex. Because it has been believed for a long time that X-ray analysis is applicable to only the stable structures in the crystalline state, and it is impossible to determine the unstable species such as the excited structure.

However, the development of the measurement technique, such as a combination of pulse laser beam and synchrotron radiation, and measurement equipments, such as two-dimensional detector, low-temperature equipment, pulse and continuous-wave (CW) laser, synchrotron radiation and so on, were made possible to detect a variety of unstable or small amount species in crystalline state described above. Even

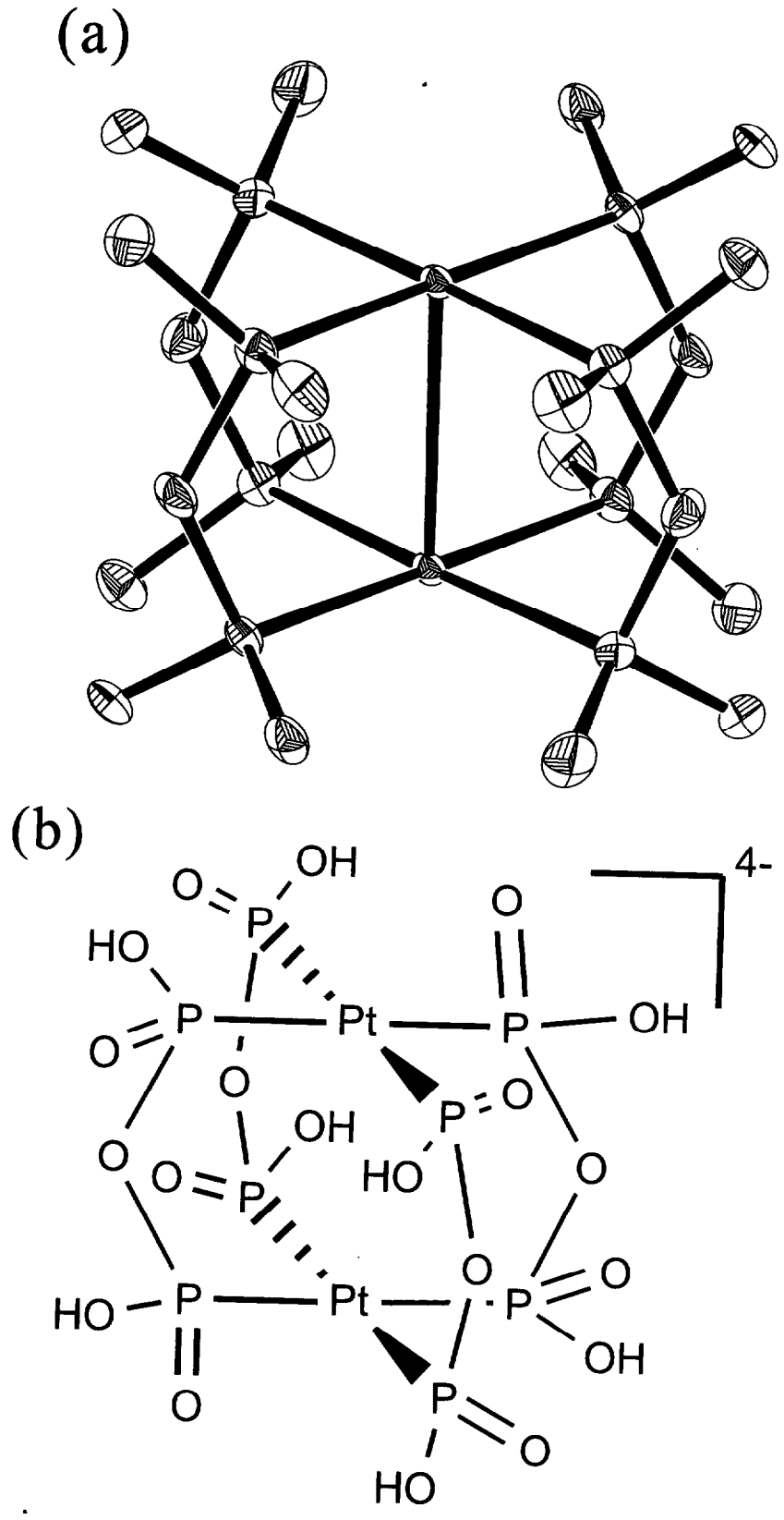

Fig. 1.3
(a) The structure of Ptpop anion. Hydrogen atoms were omitted for clearly.
(b) Schematic figure of $[Pt_2(pop)_4]^{4-}$ anion.

the excited-state molecule is considered to be able to detect using the single crystal X-ray diffraction method.

Kaizu et al. reported that the powder pattern of the Ptpop complex, $[N(C_4H_9)_4]_4[Pt_2(pop)_4]$, shifted reversibly to its higher diffraction angle when the powdered sample was irradiated with the xenon lamp at room temperature as shown in Fig. 1.4.[96] This peak shift indicated the cell-parameter and the cell-volume decrease, and estimated to be caused by the contraction of the Pt-Pt distance. This is the first report suggested that the observation of excited-state Ptpop complex can be analyzed by X-ray diffraction method, and such an observation of the reversible lattice change at constant temperature is very useful to check the possibility whether the excited structure can be observed by X-ray analysis or not.

In 2002 the first excited-state structure of a platinum complex anion, $[Pt_2(Hpop)(pop)_3]^{3-}$, was reported by Coppens et al. [97] They proposed the stroboscopic technique, in which the molecules in a crystal were repeatedly excited by pulsed laser and the structural change was probed for a period of microseconds immediately after the excitation by pulsed monochromatic X-ray of synchrotron radiation. This time-resolved diffraction technique is very useful method to analyze the transient irreversible structural change.

Ozawa et al. also reported excited-state structure change of platinum complex anion, $[N(C_4H_9)_4]_2[Pt_2(Hpop)_2(pop)_2]$. [98] They used synchrotron radiation at SPring-8, CW-laser beam and low-temperature vacuum camera.

In either case they used synchrotron radiation and laser beam as excitation light. However the measurement of the excited state Ptpop complex will be able to analyze in laboratory systems because of the result from Kaizu et al. It is attractive to confirm that the excited state structures

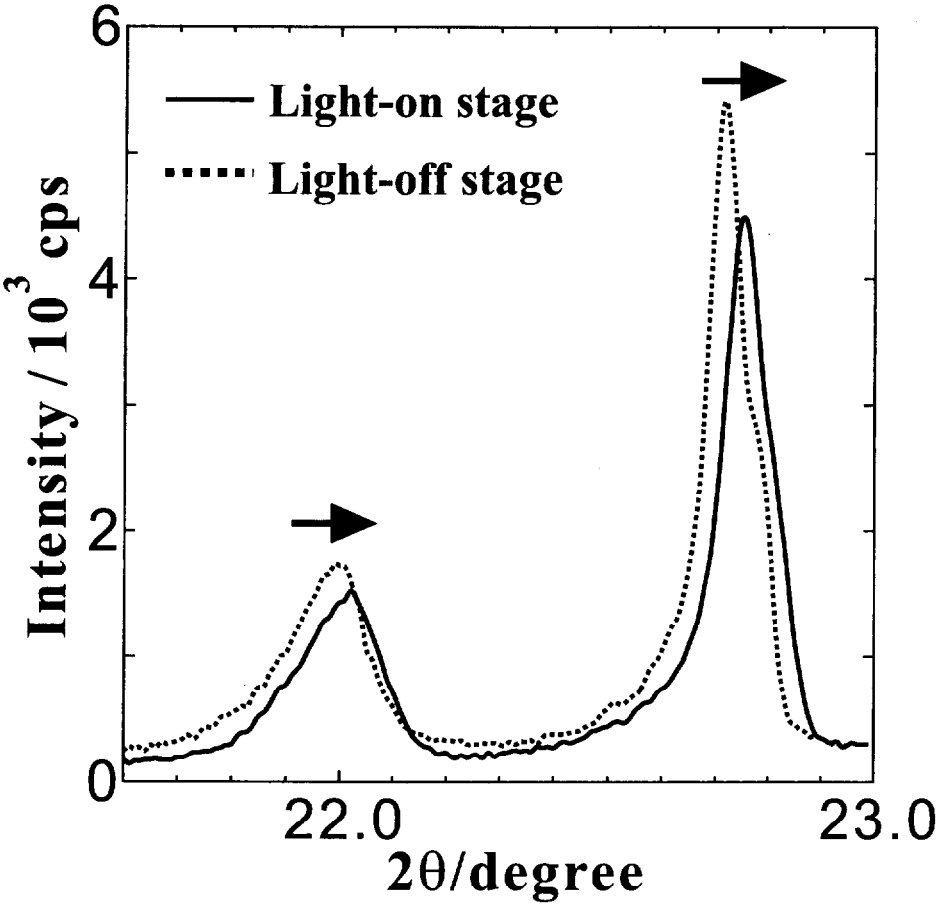

Fig. 1.4 Powder X-ray diffraction pattern of $[Bu_4N]_4[Pt_2(pop)_4]$ reported by Kaizu et al. The dotted and solid lines are light-off and light-on stages, respectively. Diffraction peak shifted to higher angle by photo-irradiation.

can be analyzed by X-ray analysis in laboratory systems without synchrotron radiation. Because the summation of the diffraction by X-ray pulses is essentially the same as the structure analysis by continuous monochromatic X-ray diffraction if we can assume that the excited structure does not change to the other transient ones and there are only two structures composed of the ground and the excited states in the irradiated crystal. The diffraction should be brought about by the periodic structure composed of the equilibrium structure between the ground-state and excited-state molecules. If the concentration of the excited molecules exceeds the threshold value in the equilibrium structure, the structure change of the excited molecule can be analyzed using the diffraction data at light-on stage (during irradiation).

The author intended to develop the conventional method utilizing the photo-irradiation with continuous wavelengths and the X-ray with monochromatic wavelength to observe the excited molecule. The crystal would be in the equilibrium state between the ground state and excited state when it was photo-irradiated and kept at low temperatures. The light with longer wavelengths than the absorption maximum was selected to penetrate the excitation light effectively into the crystal. If the concentration of the excited molecules exceeds the threshold value (≈5%) at the equilibrium condition, the reversible structural change, how quickly it occurs, should be observed by the single crystal X-ray analysis.

1.3 Purpose of this thesis

1.3.1 Purpose of this thesis

From many spectroscopic and X-ray analyses, the Ptpop complex is a

suitable target to observe the photo-excited state structure.

The observation of the photo-excited structure change at laboratory system would enable to expand the research field of X-ray diffraction analysis to study the excited-state molecule.

In contrast to the laboratory system, the application of the synchrotron radiation may enable to observe the change just like a movie. This is completely different from the stroboscopic technique that clips the structure change in the process of the reaction, and this will become the next development of single crystal X-ray analysis.

Therefore the purpose of this thesis is not only the observation of the photo-excited structure of the Ptpop complex at the laboratory system, but also the time-resolved analysis of the Ptpop complex in order to observe the photo-excitation process using a combination the synchrotron radiation and a new generation of detector called "micro-strip-gas chamber (MSGC)".

1.3.2 Outline of this thesis

This thesis consists of the two studies. One is the study about "the determination of the photo-excited structure of Ptpop complexes in laboratory system", described in chapter 3. The three dimensional structural change of the photo-excited Ptpop complex was analyzed by the single crystal X-ray method. The feature of this study is the structure analyses of a series of Ptpop compounds at the equilibrium state of the ground and excited states using the conventional single crystal X-ray diffraction technique.

Another study is "the time-resolved analysis of the photo-excitation process using the combination of synchrotron radiation and MSGC",

described in chapter 4. In order to investigate the time-resolved photo-excitation process of Ptpop compound, the movement of one diffraction peak was measured using micro-strip-gas-chamber (MSGC), which was originally developed for the rapid data measurement. This analysis can give the information about the behaviors of the molecules in the crystal at the initial stage of photo-irradiation.

In addition, the general experiment, including the synthesis of the platinum complex and the condition of photo-irradiation, are described in chapter 2. The general discussion and summary are in chapter 5.

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Chapter 2

General experiment

2.1 Preparations of Ptpop crystal

2.1.1 Synthesis

The Ptpop complex with $N(C_4H_9)_4^+$ was synthesized in a way reported previously. [1] All compounds were prepared in minor modified ways to obtain the compound with high yield.

In order to avoid the side reactions with oxygen, all solvents were bubbled nitrogen gas before use and all reactions proceeded in the nitrogen gas atmosphere. The synthetic equipment is shown in Fig. 2.1.

K_2PtCl_4 (0.8 g; 1.93 mmol) and H_3PO_3 (3.0 g; 36.59 mmol) in water (about 10ml) were refluxed for 3 hours at 105-110 °C. A brown solution gradually changed to a pale yellow solution. After refluxing, reflux condenser was removed then the solvent water evaporated to dryness at 105-110 °C for a few hours with a stream nitrogen gas. Yellow solid, $K_4[Pt_2(pop)_4]\cdot 2H_2O$ was obtained, [2] and other color solid, e.g. green or purple, were partially oxide compounds. [3,4] The yellow solid was washed a few times with methanol and acetone to remove unreacted H_3PO_3.

In order to synthesize the $[Pt_2(pop)_4]^{4-}$ complex with ammonium cation (R_4N^+), the solids of $K_4[Pt_2(pop)_4]\cdot 2H_2O$ were solved in water (10-15 ml) and a large amount of ammonium chloride (R_4NCl) was added in the solution until a yellowish green solid precipitated. To improve the yield, the solution was cooled in the refrigerator and filtered and then washed with diethyl ether to remove excess ammonium chloride. Obtained solids were dried in air and preserved in the refrigerator. The crude product was obtained up to about 90 % yield.

2.1.2 Crystallization

In order to obtain the crystals of Ptpop complex suitable for X-ray

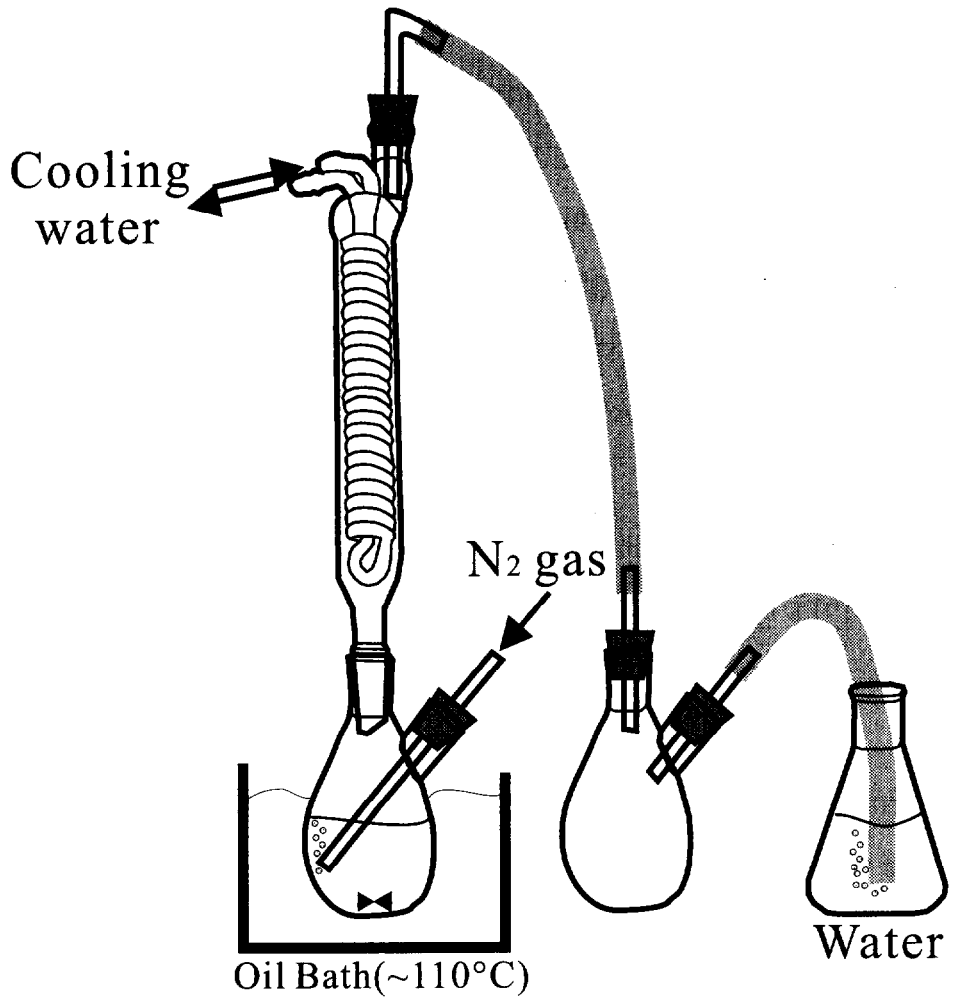

Fig. 2.1 The synthetic equipment of Ptpop compounds. The condenser was removed after the reflux.

measurement, the crude Ptpop compound (ca. 0.3 g) were dissolved in methanol (ca. 10 ml) and the saturated solution was prepared. The saturated solution was filtered with 0.2μm syringe filter and separated a few small beakers, then stored in refrigerator under diethyl ether atmosphere for a few days. The obtained crystals were stored in solution and picked up before use for X-ray measurement. Five crystals, suitable for single X-ray analysis, were obtained from the compounds with tetrabutylammonium (Bu), tetrapentylammonium (Pn), benzyltriethylammonium (Bzte), benzyltributylammonium (Bztbu) and benzyldimethylphenylammonium (Bzdmp) as counter cations. The structures of each ammnonium cations are shown in Fig. 2.2

The block and needle crystals were obtained for the Bu compound. Needle and plate crystals were obtained for the Pn and Bzte compounds respectively, and block crystals were obtained for the Bztbu and Bzdmp compounds.

The preliminary X-ray analyses indicated that the polymorphic crystals were found for the Bu, Pn and Bzte complexes in the same batch. The structural differences in polymorphic crystals for each compound will be described in chapter 3.3.2. For the Bu complex, the block and needlelike crystals, named Bu1 and Bu2 respectively, were distinguished using the microscope. However it is difficult to distinguish the two polymorphic forms under the microscope for the Pn (Pn1 and Pn2) and Bzte (Bzte1 and Bzte2) complexes because the appearances of the two crystal forms are very similar to each other. Therefore the crystal form was distinguished from the difference in unit-cell dimensions determined by X-ray measurement.

For the Bzte compound, one crystal form (Bzte1) has a twin structure, but

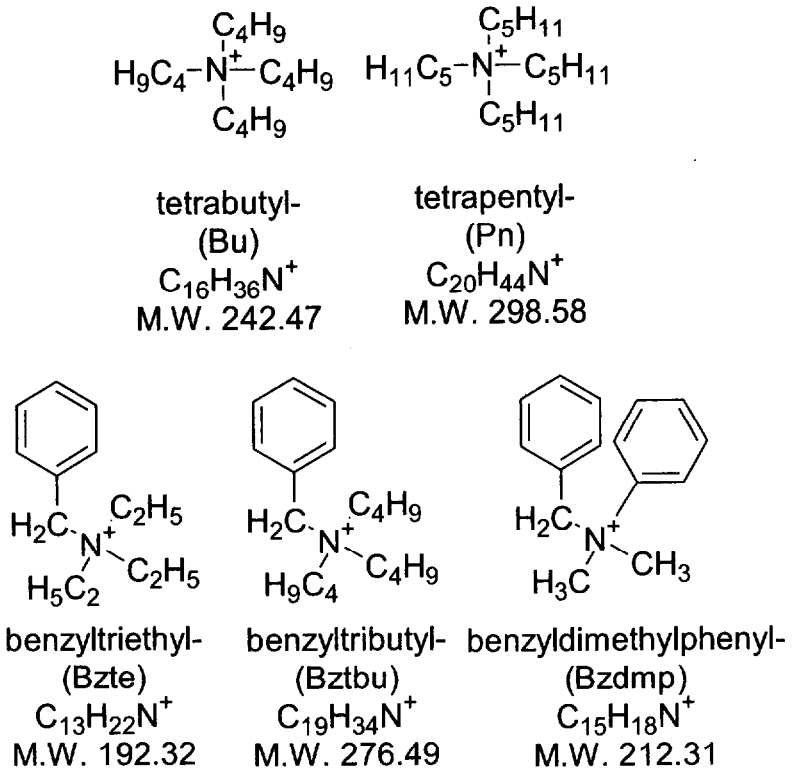

Fig. 2.2 Five ammonium cations used in this thesis.

each component of the twin can be separated with a blade under the polarized microscope. The photographs of Bzte1 are shown in Fig. 2.3. The other crystal form of Bzte (Bzte2) has not such a twin structure, but gradually decomposes due to the elimination of crystal solvent.

In order to reduce the diffraction from a glass capillary mounting the crystal, the fine glass fiber (strands of glass wool *ca* 20 μm in width) was attached at the top of the normal capillary and the crystal was mounted on the glass fiber (Fig. 2.4(a)). [5)]

The preliminary results have been reported using the platinum complex, $[Pt_2(Hpop)_2(pop)_2]^{2-}$, with the tetrabutylammonium (Bu1) [6)] and tetrapentylammonium (Pn1) cations. [7)]

2.2 Condition of photo irradiation

2.2.1 Spectroscopy of Ptpop compounds

The absorption spectra of the Ptpop complex measured with the uv-vis spectrometer (Shimadzu UV-3100) are shown in Fig. 1.2. The absorption spectra of Ptpop anion are characterized at 367 and 440 nm.

The absorption band at 367 nm was assigned to $5d_z^2 \rightarrow 6p_z$, which is the lowest-energy-allowed transition; i.e. $^1A_{1g} \rightarrow {}^1A_{2u}$ ($1a_{2u} \rightarrow 2a_{1g}$) and the weak emission at 400 nm to the corresponding fluorescence. The weak absorption at 440 nm was assigned to the $^1A_{1g} \rightarrow {}^3A_{2u}$ ($1a_{2u} \rightarrow 2a_{1g}$) transition and the intense emission at 504 nm to the corresponding phosphorescence. [8)]

The lifetime of excited state of Bu and Pn compounds were 6.4 μsec at r.t. and 7.8 μsec at 77 K, respectively. These lifetimes are almost the same as those reported previously. [9,10,11,12)]

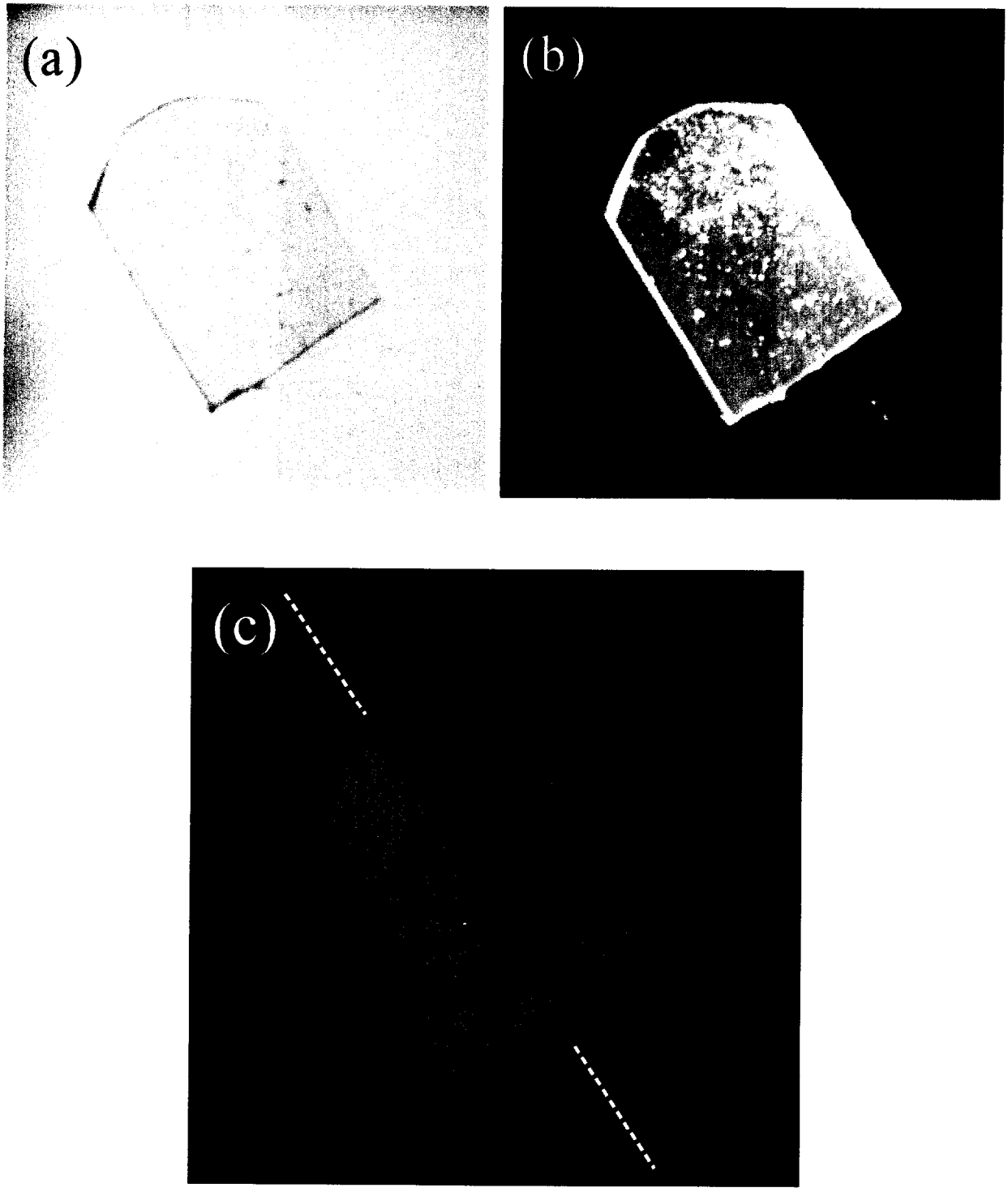

Fig. 2.3 The microscope images of Bzte1 crystal:
(a) The observation without the polarized filter. The crystal seems to be single crystal.
(b) The photo-irradiated crystal image without the polarized filter. The boundary of the twin structure cannot observed and emission was occurred from each components.
(c) The observation with the polarized filters. The boundary of the twin structure can be seen. Crystal was cut before use.

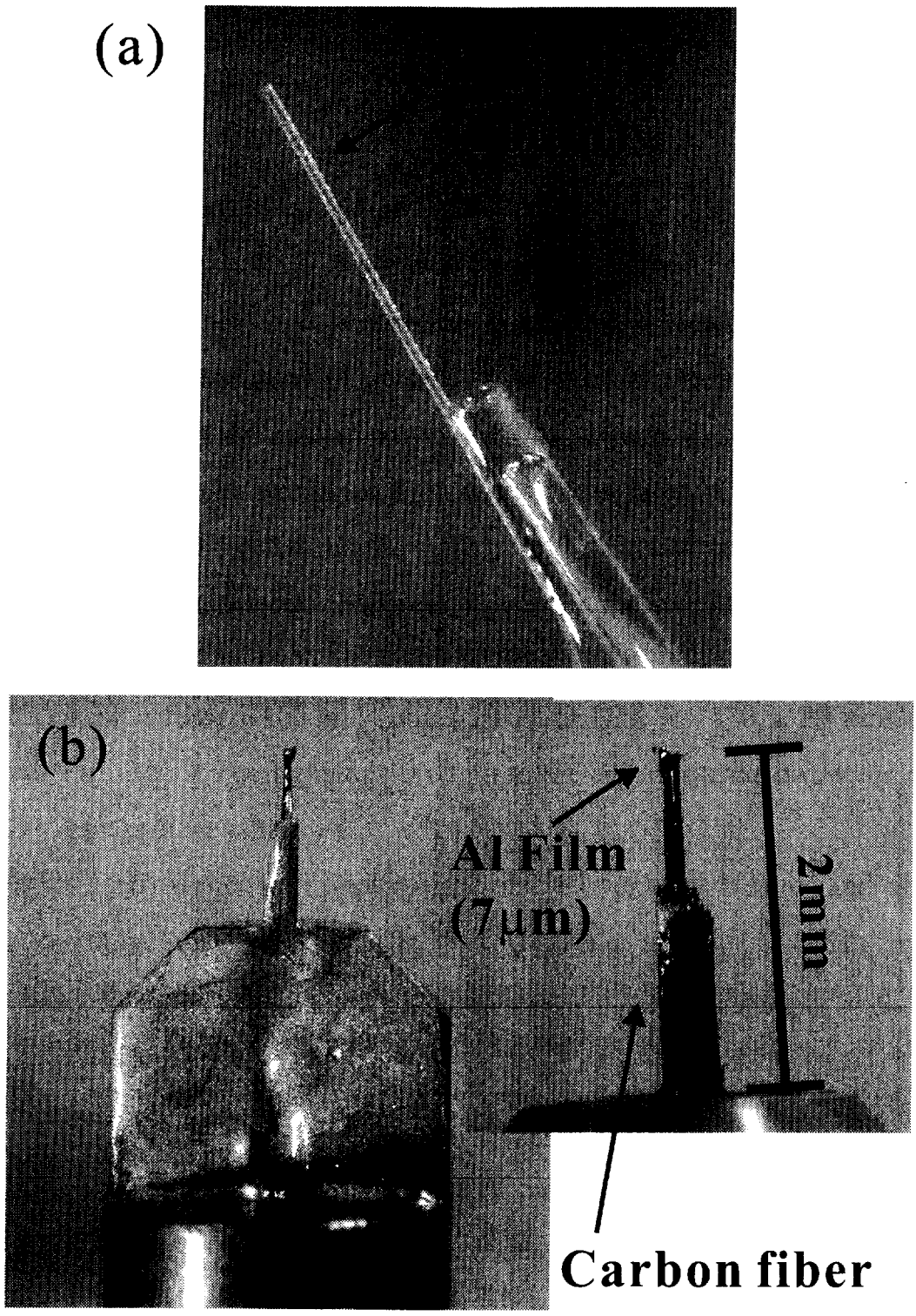

Fig. 2.4 The pictures of mount pins for X-ray measurements:
(a) The mount pin for the measurement at the laboratory system. The glass fiber was attached at the top of normal glass pin.
(b) The mount pin for the measurement at SPring-8 BL02B1 beam line. The carbon fiber, mounting the Al film, was attached on the Cu base.

2.2.2 The condition of excitation light

The excitation light with longer wavelengths can penetrate into the crystal more deeply. The large absorption coefficient generates the heat and increases the temperature of crystal. [13] In order to penetrate the excitation light into the crystal and to avoid the heat generation, the range of the wavelength range of excitation light was selected from 400 to 550 nm. The excitation band from the ground state to triplet-excited state ($^1A_{1g} \rightarrow {}^3A_{2u}$) is included in this range. In order to satisfy the conditions, the 150 W xenon lamp (SAN-EI ELECTRIC SUPER BRIGHT 152S) with filters (HOYA blue filter B460 and long pass filter L39, $\lambda = 470 \pm 80$ nm) was used (Fig. 2.5). The light was brought to the crystal on the diffractometer using a glass-fiber tube.

Figure 2.6 show the photograph of Pn1 crystal before and after photo-irradiation (size 1.70 x 0.16 x 0.05 mm^3). The yellowish green emission was observed when the filtered excitation light was irradiated.

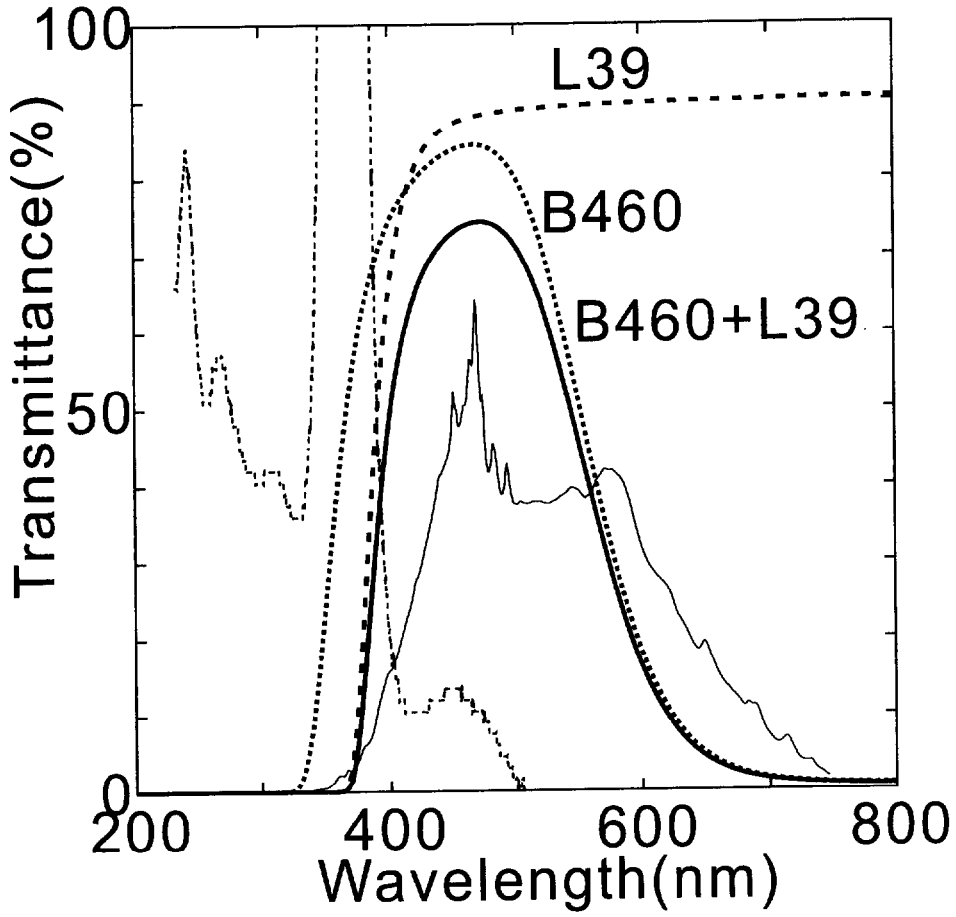

Fig. 2.5 The transmittance of used optical filters:
The thick dotted and broken lines are the transmittance of the optical filters, HOYA blue filter B460 and long pass filter L39, respectively. The thick solid line is the transmittance of a combined B460 and L39 filters.
The thin dotted and solid lines are the absorption spectra of the Ptpop compound and the wavelength distribution of the Xe lamp without optical filter, respectively. Vertical scale of absorption spectra and wavelength distribution are not scaled each other.

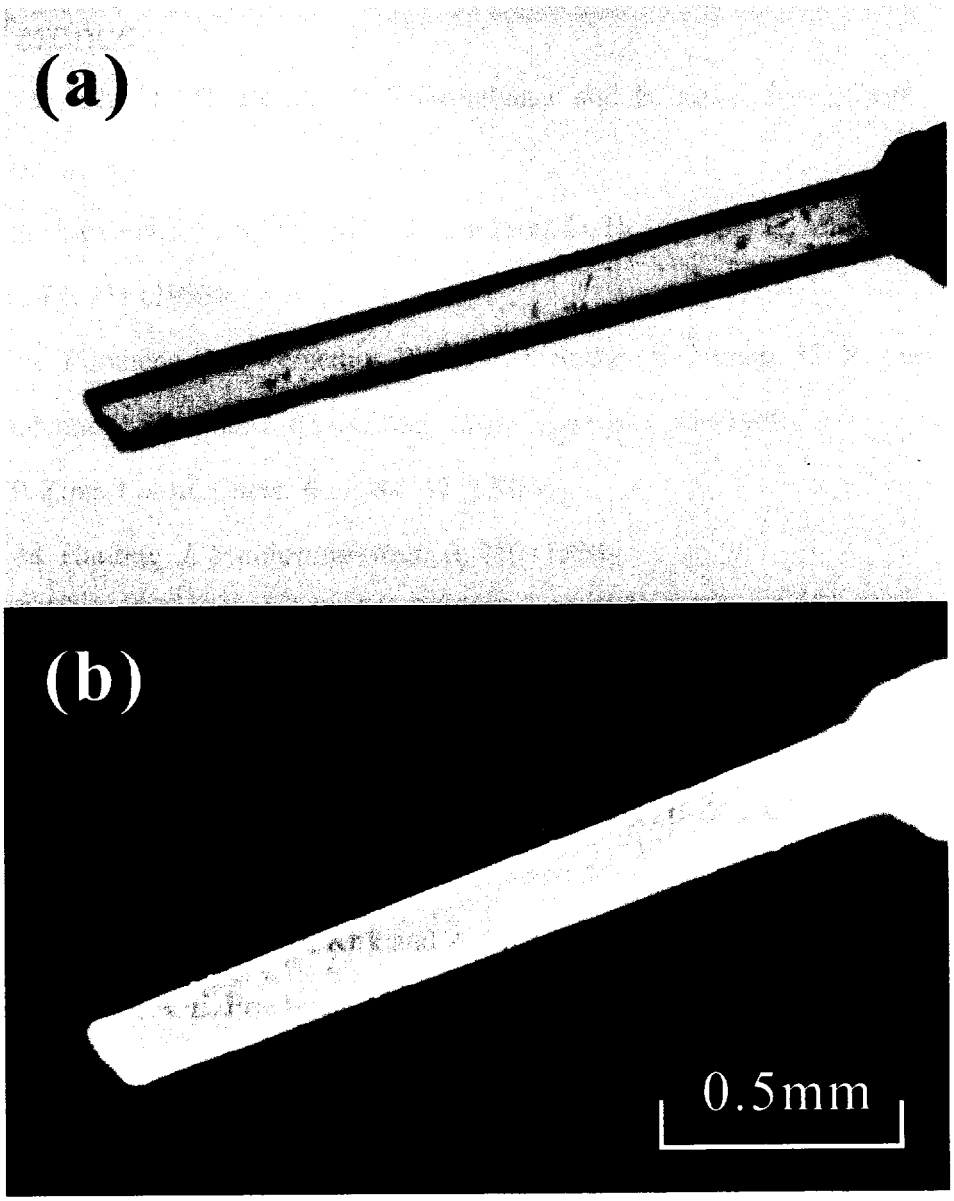

Fig. 2.6 Color change of the Pn1 crystal under the microscope:
(a) at the light-off stage.
(b) at the light-on stage. Intense yellowish green emission was observed. Light condition was described in chapter 2.2.2.

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Chapter 3

Photo-excited structure change of Ptpop compound

3.0 Abstract

The photo-excited structures of $[Pt_2(pop)_4]^{4-}$ and $[Pt_2(Hpop)_2(pop)_2]^{2-}$, (pop = diphosphito; $P_2O_5H_2^{2-}$), in five kinds of complexes were analyzed by single crystal X-ray analysis in laboratory system. Four Ptpop anions, except for Bzdmp compound, are attached by two protons and are represented as $[Pt_2(Hpop)_2(pop)_2]^{2-}$, whereas Ptpop anion of Bzdmp is represented $[Pt_2(pop)_4]^{4-}$.

Since the Bu, Pn and Bzte complexes have two crystal forms, the structures of eight crystals were determined by X-ray analysis before irradiation. The differences between each crystal forms were due to the inclusion of crystal solvent or the orientation of Ptpop anion.

The five crystals of Bu1, Pn1, Bzte1, Bztbu and Bzdmp were irradiated the excitation light with a xenon lamp, and the intensity data were collected at the light-off and light-on stages at low temperatures. Either crystal showed the contraction of the unit-cell volume significantly at light-on stage. The analyzed structures at light-on and light-off stages clearly indicated that the Pt-Pt and Pt-P bond distances became significantly shorter at light-on stage than the corresponding ones at light-off stage. The other bond distances in anions and cations are insignificantly changed. These structural changes are in good agreement with the results observed by spectroscopic methods.

If we assume the equilibrium state between the excited- and ground-state molecules at the light-on stage, the concentration of the excited molecules in the equilibrium structure may be 1 - 6 %.

3.1 Introduction

The (μ-diphosphito)diplatinum complex, $[Pt_2(pop)_4]^{4-}$, is well known as the photo-excited compound. These compounds excite by photo-irradiation and indicate yellowish green fluorescence and phosphorescence. Many spectroscopic studies about the excited state of $[Pt_2(pop)_4]^{4-}$ complex has been reported in 1980's, and the Pt-Pt distance at the excited state was found to become shorter by about 0.21 Å than that at the ground state. [1] This shortening is due to the electron transition from anti-bonding state ($d\sigma^*$) to bonding state ($p\sigma$). [2]

Recently, Coppens et al. have reported the time-resolved stroboscopic diffraction technique to observe the structure of $[N(C_2H_5)_4]_3[Pt_2(Hpop)(pop)_3]$ at the excited state. [3] The frequency and width of the X-ray pulse were 5100 Hz and 33 μs. The laser pulses from a triplet Nd/YAG pump laser (λ = 355 nm) are synchronized with the X-ray pulses. This means that the intensity data were collected within 33 μs just after the photoirradiation. The data collection was repeated in a time interval of 196 μs and the corresponding intensity data of each time-interval were summarized. The intensity data at the light-off and light-on stages were collected at 17 K and the two sets of data were scaled. Analyzing the structural change using the difference intensities, the Pt-Pt bond shortening was obtained to be 0.28(9) Å and the population of the excited state was 2.0 %.

This time-resolved diffraction technique is becoming very effective and powerful method to analyze the transient irreversible structural change. However, it may be not necessary to use this technique for the observation of the unstable structure with reversible change, such as the excited structure. Because the summation of the diffraction by X-ray pulses is

essentially the same as the structure analysis by continuous monochromatic X-ray diffraction if we can assume that the excited structure does not change to the other transient ones and there are only two structures composed of the ground and excited states in the photo-irradiated crystal. The diffraction should be brought about by the periodic structure composed of the equilibrium structure between the ground-state and the excited-state molecules.

If the concentration of the excited molecules exceeds the threshold value in the equilibrium structure, the structure of the excited molecule can be analyzed using the diffraction data at light-on stage (during irradiation). The concentration or occupancy factor of the excited molecules, which is the most important factor, depends mainly on the wavelength of the incident light. The light with the wavelength of absorption maximum may excite only the surface molecules and it would not be able to excite the molecules in the inner part of the crystal. Although the excitation light with longer wavelength can penetrate into the crystal more effectively, the number of the absorbed photons would be small. Because the data collection time is not limited for the reversible photoreactions, the light with longer continuous wavelengths seems to be better than the stronger pulsed-light with the wavelength of absorption maximum.

Ozawa et al. reported the preliminary structure analyses of the excited state of the Bu1 crystal using the continuous laser beam. The crystal was mounted on a new low-temperature vacuum (LTV) X-ray camera installed at the BL02B1 beam line of SPring-8. [4] The crystal was irradiated with a CW He-Cd blue laser (λ = 442 nm). The intensity data at the light-off and light-on stages were recorded on the same imaging plate at 54 K. Analyzing the structural change using the difference intensities, the Pt-Pt

bond shortening was obtained to be 0.23(4) Å and the population of the excited state was 1.4(2) %.

It is valuable to develop the conventional photo-crystallographic method utilizing the irradiation with continuous wavelengths and continuous X-ray with monochromatic wavelength to observe the excited molecule. The crystal would be in the equilibrium state between the ground state and the excited state when it was photo-irradiated and kept at a low temperature. The light with longer wavelengths than the absorption maximum was selected to penetrate the light effectively into the crystal. If the concentration of the excited molecules exceeds the threshold value (≈5%) at the equilibrium condition, the reversible structural change, how quickly it occurs, should be observed by the method.

In laboratory system, Kaizu et al. reported that the powder pattern of the Ptpop complex, $[N(C_4H_9)_4]_4[Pt_2(pop)_4]$, shifted reversibly to its higher diffraction angle when the powdered sample was irradiated with a xenon lamp at a low temperature (Fig. 1.5). [5] This experiment indicated that the structural change of the Ptpop complex in the excited state is significantly large and the concentration of the excited molecules clearly exceeds the threshold value. Such an observation of the reversible lattice change at low temperatures is very important to check the possibility whether the excited structure can be observed by X-ray analysis or not.

The goal in this chapter is the observation of the structural change of the excited Ptpop complex in laboratory system using the conventional photo-crystallographic method. In order to achieve that, the five Ptpop complexes, including three new complexes, were synthesized, measured single crystal X-ray diffraction and compared the structures between the

ground state and the excited state. In addition, single crystal and powder X-ray diffraction measurement were carried out with synchrotron radiation to support the observed structure change. The structural features of each crystal, polymorph structure, hydrogen bond motifs and so on will be also described.

3.2 Experiment

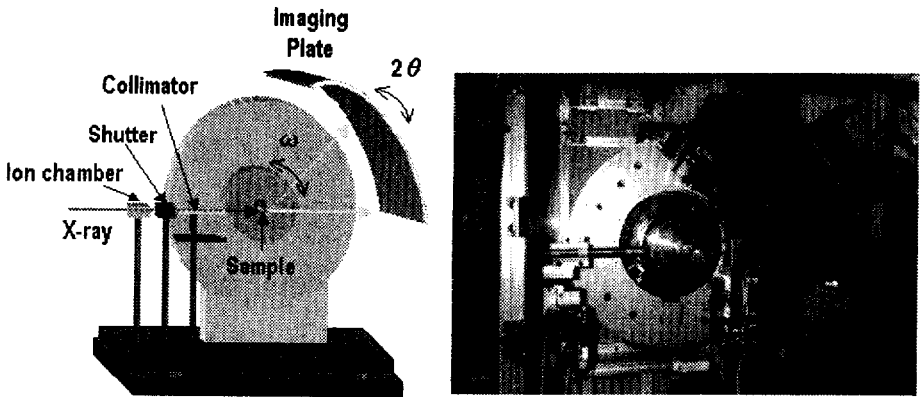
3.2.1 Compounds and condition of photo-irradiation

Eight crystals of five compounds, Bu1, Bu2, Pn1, Pn2, Bzte1, Bzte2, Bztbu and Bzdmp, were synthesized and crystallized by the method described in chapter 2.1.1 and 2.1.2. The reason why such alkylammonium ions are used for the counter cations is to loosen the crystal packing around the Ptpop anion and to make the complex crystal transparent to the excitation light except for the Ptpop anion.

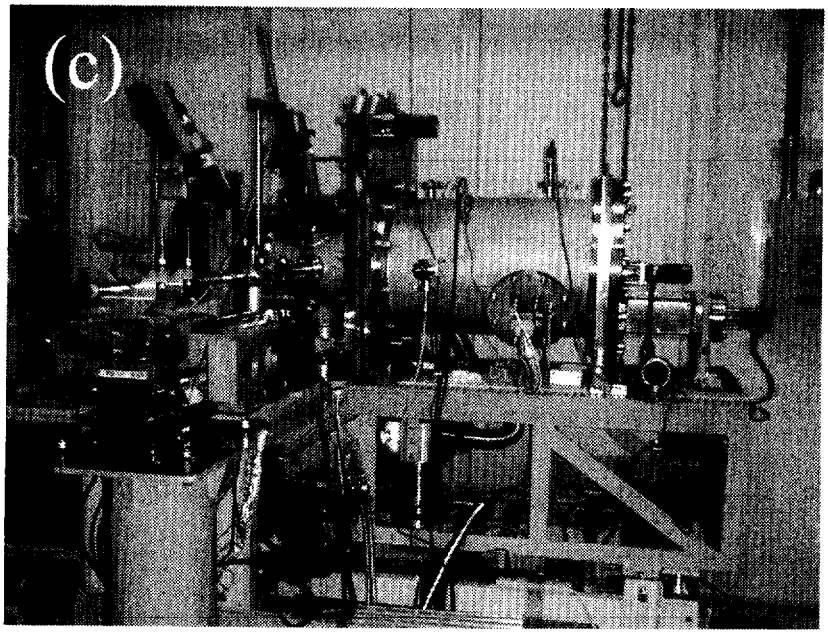
The condition of the excitation light was already described in chapter 2.2.2.

3.2.2 Powder X-ray diffraction measurement at SPring-8

The powder X-ray diffraction of Pn1 was measured at the BL02B2 beam line of SPring-8, in order to investigate the difference of excitation between $[Pt_2(pop)_4]^{4-}$ complex and $[Pt_2(Hpop)_2(pop)_2]^{2-}$ complex. The powdered sample was filled in a glass capillary (0.3 mm diameter) and was mounted on a Debye-Scherrer camera with large diameter shown in Figs. 3.1(a) and (b). This camera has an Imaging Plate (IP) with radius 286.5 mm on the 2θ-arm. The pixel size of IP was selected 50 μm; i.e. the resolution of 2θ angle is 0.01 °. [6,7]



(a) The schematic view (b) The photograph



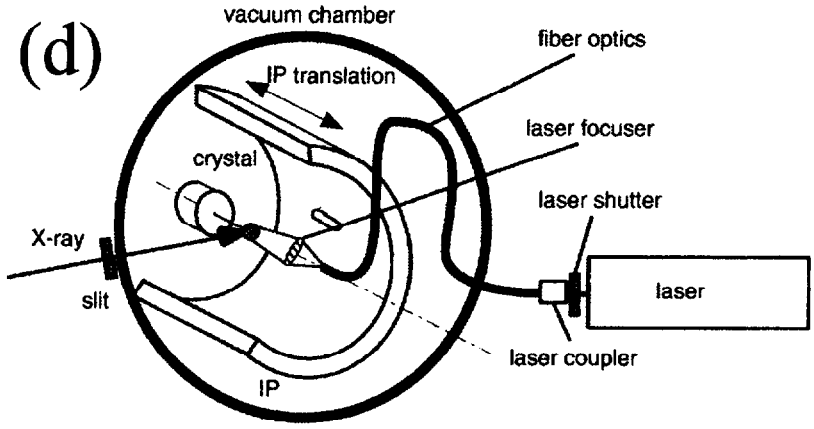


Fig. 3.1 Photograph and schematic images of equipments used at SPring-8:
(a,b) Debye-Scherrer camera with large diameter installed at BL02B2 beam line.
(c,d) Low-temperature vacuum (LTV) X-ray camera installed at BL02B1 beam line. This schematic image was referred from *Chem. Lett.*, **32**, 62 (2003).(Ozawa *et al.*).

The wavelength of X-ray was selected 1.08 Å because the *L* absorption edge of platinum atom is 1.07 Å (Fig. 3.2). [8] $2\theta_{min}$ and $2\theta_{max}$ were 2.5 and 75 °, respectively. The sample was cooled to 173 K with cold-nitrogen-gas stream and was irradiated the excitation light described in chapter 2.2.2.

Although the Pn compound is the mixture of Pn1 and Pn2 crystals, it is almost impossible to separate Pn1 and Pn2 from a large amount of Pn compound. However Pn2 was found to transform to Pn1 form by grinding in mortar. When the grinding time was 2 min, the powder pattern was superimposed those of Pn1 and Pn2. Grinding the sample, the diffraction peak of Pn2 form decreased and that of Pn1 increased as shown in Fig. 3.3. After 8 min grinding, the powder pattern completely transformed to that of Pn1.

3.2.3 Single crystal X-ray diffraction measurement at SPring-8

In order to consider the effect of the degradation of crystallinity, single crystal X-ray diffraction of Bzte1 was measured at the BL02B1 beam line of SPring-8. In laboratory system, the measurement of light-on stage should be the next of the light-off stage because it is impossible to measure the light-on and light-off stages at same time and the degradation of crystallinity due to photo-irradiation is unavoidable. Therefore the degree of the degradation is different between the light-on (degradation by photo-irradiation) and the light-off stages (good crystallinity).

The low-temperature vacuum camera (LTV camera) set at BL02B1 beam line, as shown in Figs. 3.1(c) and (d), enables the special method, called "The multiple-exposure IP method", by which both measured diffraction patterns for the light-on and light-off stages are recorded on the same IP frame with a slight shift (2 mm) of the IP. The diffraction image of Bzte1

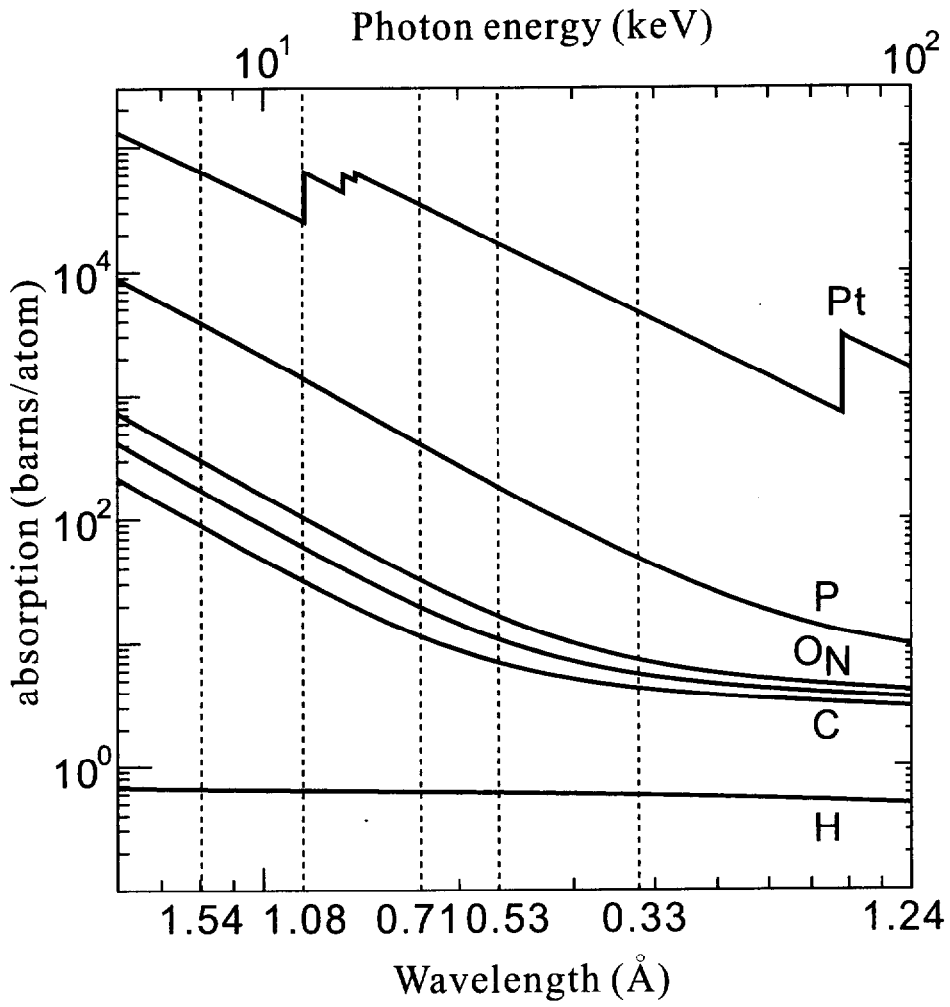


Fig. 3.2 Absorption cross section of Pt, P, O, N, C and H atoms. Dotted lines are the wavelengths for the measurements; 1.54Å (SPring-8 BL44B2) 1.08Å (SPring-8 BL02B2) 0.71Å (Mo$K\alpha$) 0.53Å (SPring-8 BL02B1) and 0.33Å (SPring-8 BL04B2).

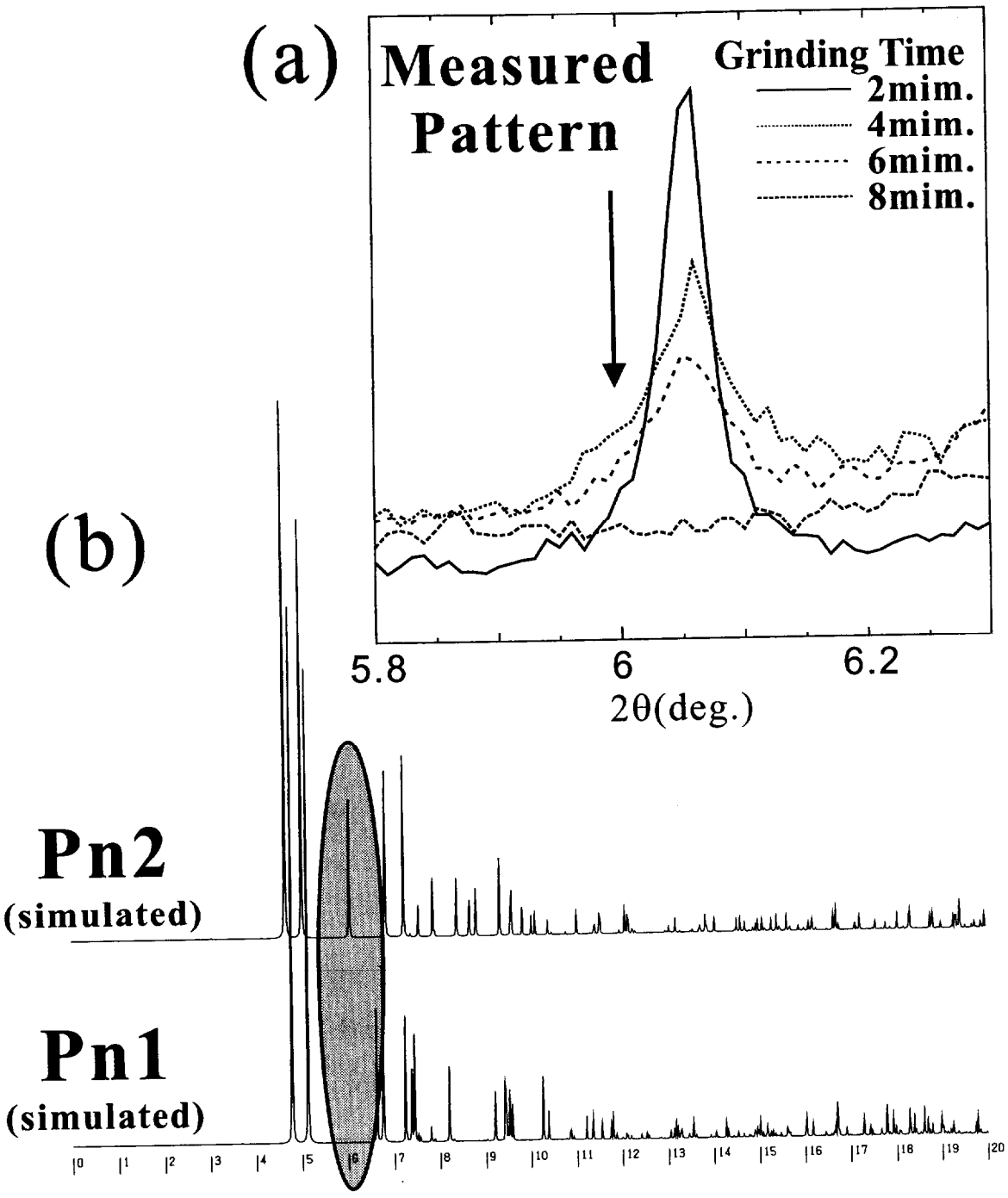


Fig. 3.3 The diffraction pattern change of Pn by grinding:
(a) Measured powder diffraction patterns around $2\theta = 6°$ of Pn at SPring-8 BL02B2 beam line. Pn is the mixture of Pn1 and Pn2 crystal forms. Pn2 form was transform to Pn1 form by grinding. The diffraction peak of Pn2 form gradually decreased with grinding.
(b) Simulated powder diffraction patterns of Pn1 and Pn2 with PLATON. Cell parameters, determined by single crystal X-ray analysis, were used for calculation.

crystal measured by the multiple-exposure IP method is shown in Fig. 3.4(a). These processes minimize the systematic errors in the intensity collection caused by the decay of synchrotron radiation and the fading of diffraction intensity on IP, and the effect of the degradation of crystallinity because crystallinity was almost same between at least the same φ-oscillation ranges. Moreover the measurement in the vacuum chamber and at low temperature (50 K) make possible to obtain accurate intensity with high S/N ratio.

Since the heat conduction was used for cooling the crystal, the pin for crystal mount was made from carbon fiber and cupper pin, and aluminum film (thickness ca. 7μm) was attached on the top of the carbon fiber to reflect the laser beam. The crystal was mounted on the aluminum film with the epoxy glue. The conductive paste, consists of the metal powder, was used to coat the connections between carbon fiber and cupper pin and cupper pin and goniometer to improve the heat conduction. The prepared cupper pin is shown in Fig. 2.4(b).

The intensity data of Bztel crystal (150 x 90 x 30 μm, Fig. 3.4(b)) was collected by the multiple-exposure IP method. The crystal was cooled down to 50 K by the thermal conduction from a cold head of He refrigerator. The 100 mW He-Cd laser (λ=442 nm) was used as the excitation light and brought to the vacuum chamber with an optical fiber. The excitation light was attenuated with 10 % ND filter and didn't focus to the crystal because the crystallinity was significantly degraded by strong and focused laser irradiation. The monochrome image of the crystal during laser-irradiation is shown in Fig. 3.5(c), the reflection of laser beam and probably emission from excited-species were observed.

The wavelength of X-ray was selected 0.538 Å (23 keV) with Si(311)

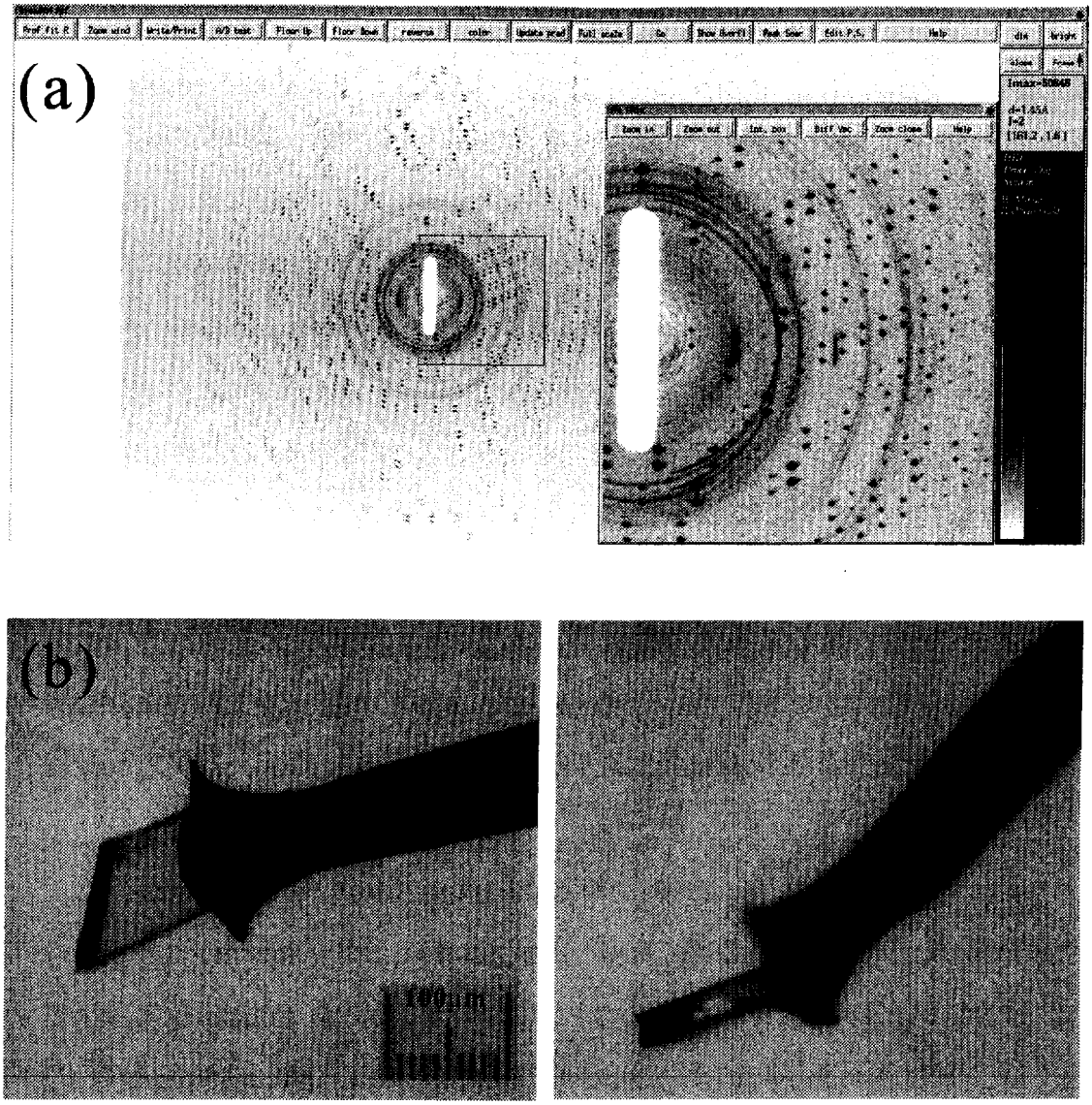


Fig. 3.4 (a) The diffraction image of Bztel crystal measured by the multiple-exposure IP method at SPring-8 BL02B1 beam line. The powder pattern and a few diffraction peaks were diffraction from carbon fiber of the mount pin.
(b) The images of the measured Bztel crystal; the crystal was mounted on the mount pin, consisted of Al film and carbon fiber. (c) The monochrome image of the laser-irradiated crystal during the multiple-exposure IP measurement. The reflection of laser light and probably emission from the crystal were observed.

monochromator. The oscillation range was $\Delta\varphi$ = 3.0 °, and the image overlap was 0.5 °. The 77 images were recorded for each stage and total measurement time was about 16 hours. The intensity decay was about 42 % during the measurement and corrected by the scaling the diffraction image, this decay was due to the degradation of crystal and the intensity decay of synchrotron radiation.

DENZO [9] and MULABS [10] in PLATON [11] were used for the integration of the diffraction intensity and the absorption collection, respectively. The other operations, structure determination, refinement and treatment of hydrogen atoms and so on, were the same as the laboratory systems. Crystal data of each stage are summarized in Table 3.1.

3.2.4 Single crystal X-ray diffraction measurement in laboratory system

All the intensity data of crystals, Bu1, Bu2, Pn1, Pn2, Bzte1, Bzte2, Bztbu and Bzdmp were collected in laboratory system using Bruker Smart CCD diffractometer with the rotating-anode X-ray generator.

The crystals were cooled with cold-nitrogen-gas stream. Bu2, Pn2 and Bzte2 were measured at 103, 223 and 103 K, respectively. Crystal data of each crystal are summarized in Table 3.2. The intensity data of Bu1 at light-on and light-off stages were collected at 173 K, since the cell change was the largest at 173 K as shown in the preliminary work. [12] The intensity data of two crystals, Pn1 and Bzdmp, were collected at light-off and light-on stages under the same conditions as those for Bu1, except the temperature was 103 K for the Bzte1 and Bztbu crystals. Crystal data at light-off and light-on stages are given in Table 3.3.

All structures were solved by the direct method (SHELXS-97) [13] and refined by the full-matrix least-squares method (SHELXL-97). [14] All the

Table 3.1 Crystal data and experimental details of Bzte1 crystal measured by the multiple-exposure IP method at SPring-8 BL02B1 beam line.

	Bzte1-LTV-OFF	Bzte1-LTV-ON
Formula	$C_{26}H_{54}N_2O_{20}P_8Pt_2$	
Formula Weight	1352.65	
Temperature (K)	50(2)	
Wavelength (Å)	0.5379	
Crystal Size (mm^3)	0.15 x 0.09 x 0.03	
Crystal System	Triclinic	
Space Group	$P\bar{1}$	
Z	2	
a (Å)	11.8110(13)	11.8120(12)
b (Å)	12.5010(16)	12.5010(16)
c (Å)	14.6910(18)	14.6890(17)
α (°)	89.315(6)	89.319(6)
β (°)	88.134(9)	88.143(8)
γ (°)	73.426(8)	73.430(8)
V ($Å^3$)	2077.9(4)	2077.8(4)
D_{calc} (Mg/m^3)	2.162	2.162
μ (mm^{-1})	3.856	3.856
θ range (°)	1.66 to 20.44	1.66 to 20.44
Reflections collected/unique	11855 / 7356	11993 / 7412
R int	0.0561	0.0558
Completeness to θ = 20.44 °	0.772	0.778
Data/restraints/parameters	7356 / 0 / 523	7412 / 0 / 523
$R_1[I>2\sigma(I)]$	0.0536	0.0525
No. of $I>2\sigma(I)$ (refs.)	5904	5960
Largest diff. peak ($e.Å^{-3}$)	2.842	3.015
Largest diff. hole ($e.Å^{-3}$)	-2.201	-2.181

Table 3.2 Crystal data and experimental details of Bu2, Pn2 and Bzte2 crystals

	Bu2	Pn2	Bzte2
Formula	$C_{32}H_{82}N_2O_{20}P_8Pt_2/CH_3OH$	$C_{40}H_{98}N_2O_{20}P_8Pt_2$	$C_{26}H_{54}N_2O_{20}P_8Pt_2/CH_3OH$
Formula Weight	1484.98	1565.14	1384.69
Temperature (K)	103(2)	223(2)	103(2)
Wavelength (Å)	0.71069	0.71073	0.71073
Crystal Size (mm^3)	0.40 x 0.06 x 0.06	0.30 x 0.07 x 0.05	0.32 x 0.20 x 0.03
Crystal System	Orthorhombic	Triclinic	Orthorhombic
Space Group	$P2_12_12_1$	$P\bar{1}$	$Pna2_1$
Z	4	2	4
a (Å)	9.4870(3)	9.45410(10)	20.42330(10)
b (Å)	20.3145(7)	16.9411(2)	21.6230(2)
c (Å)	27.7153(13)	20.68590(10)	10.10650(10)
α (°)	90	91.9743(8)	90
β (°)	90	98.3843(3)	90
γ (°)	90	104.2355(9)	90
V ($Å^3$)	5341.4(4)	3168.50(5)	4463.16(6)
D_{calc} (Mg/m^3)	1.847	1.641	2.061
μ (mm^{-1})	5.544	4.677	6.627
θ range (°)	2.27 to 27.48	1.24 to 27.48	1.99 to 27.48
Reflections collected/unique	35286 / 11038	22594 / 14268	30527 / 9974
R int	0.0479	0.0293	0.0557
Completeness to θ = 27.48 °	0.939	0.982	0.998
Data/restraints/parameters	11038 / 0 / 593	14268 / 4 / 669	9974 / 1 / 546
$R_1[I>2\sigma(I)]$	0.0350	0.0343	0.0291
No. of $I>2\sigma(I)$ (refs.)	10525	12040	9538
Largest diff. peak ($e.Å^{-3}$)	1.073	1.631	1.622
Largest diff. hole ($e.Å^{-3}$)	-1.368	-1.468	-1.954

Table 3.3 Crystal data and experimental details of Bu1, Pn1, Bzte1, Bztbu and Bzdmp crystals at light-off and light-on stages.

	Bu1-OFF	Bu1-ON	Pn1-OFF	Pn1-ON	Bzte1-OFF	Bzte1-ON
Formula	$C_{32}H_{82}N_2O_{20}P_8Pt_2$		$C_{40}H_{98}N_2O_{20}P_8Pt_2$		$C_{26}H_{54}N_2O_{20}P_8Pt_2$	
Formula Weight	1452.94		1565.14		1352.65	
Temperature (K)	173(2)		173(2)		103(2)	
Wavelength (Å)	0.71073		0.71073		0.71073	
Crystal Size (mm^3)	0.12 x 0.10 x 0.10		0.40 x 0.05 x 0.02		0.15 x 0.08 x 0.02	
Crystal System	Triclinic		Triclinic		Triclinic	
Space Group	$P\bar{1}$		$P\bar{1}$		$P\bar{1}$	
Z	1		2		2	
a (Å)	12.40780(10)	12.3768(3)	9.69650(10)	9.6758(3)	11.8647(4)	11.8488(3)
b (Å)	12.4747(2)	12.4443(3)	17.2492(3)	17.2106(6)	12.5661(4)	12.5275(4)
c (Å)	9.64630(10)	9.6268(2)	18.7278(2)	18.6822(6)	14.7700(5)	14.7425(5)
α (°)	96.0435(8)	95.9963(6)	93.6649(4)	93.6675(8)	89.3129(9)	89.3304(6)
β (°)	91.3580(8)	91.3709(8)	90.9346(8)	90.9035(4)	88.0813(6)	87.9796(12)
γ (°)	116.8715(3)	116.7862(8)	102.8259(7)	102.8002(8)	73.3677(9)	73.3187(7)
V ($Å^3$)	1320.18(3)	1312.16(5)	3046.45(7)	3026.12(17)	2108.78(12)	2094.92(11)
D_{calc} (Mg/m^3)	1.828	1.839	1.706	1.718	2.130	2.144
μ (mm^{-1})	5.604	5.639	4.864	4.897	7.009	7.055
θ range (°)	1.85 to 27.48	1.85 to 27.48	1.09 to 27.48	1.09 to 27.48	1.38 to 27.48	1.38 to 27.48
Reflections collected/unique	9357 / 5883	9268 / 5821	21788 / 13755	21211 / 13429	15069 / 9552	9429 / 7550
R int	0.0281	0.0257	0.0325	0.0325	0.0346	0.0385
Completeness to θ = 27.48 °	0.971	0.966	0.984	0.967	0.987	0.785
Data/restraints/parameters	5883 / 0 / 289	5821 / 0 / 289	13755 / 0 / 670	13429 / 0 / 673	9552 / 0 / 553	7550 / 0 / 541
$R_1[I>2\sigma(I)]$	0.0284	0.0274	0.0333	0.0335	0.0332	0.0380
No. of $I>2\sigma(I)$ (refs.)	5407	5406	11246	11009	8039	6084
Largest diff. peak ($e.Å^{-3}$)	1.604	1.480	1.372	1.363	2.561	1.603
Largest diff. hole ($e.Å^{-3}$)	-1.652	-1.385	-1.427	-1.453	-2.490	-1.387

	Bztbu-OFF	Bztbu-ON	Bzdmp-OFF	Bzdmp-ON
Formula	$C_{38}H_{78}N_2O_{20}P_8Pt_2$		$C_{31}H_{44}N_2O_{11}P_4Pt$	
Formula Weight	1520.96		939.65	
Temperature (K)	103(2)		173(2)	
Wavelength (Å)	0.71073		0.71073	
Crystal Size (mm^3)	0.18 x 0.08 x 0.05		0.20 x 0.17 x 0.10	
Crystal System	Triclinic		Monoclinic	
Space Group	$P\bar{1}$		$P2_1/n$	
Z	2		4	
a (Å)	9.5229(3)	9.5199(2)	13.74370(10)	13.73350(10)
b (Å)	14.3046(5)	14.2924(4)	12.9901(2)	12.9877(2)
c (Å)	20.8753(7)	20.8590(6)	21.04720(10)	21.03340(10)
α (°)	90.4165(3)	90.4352(7)	90	90
β (°)	97.3252(8)	97.3120(7)	105.9300(10)	105.9380(10)
γ (°)	106.8507(8)	106.8467(5)	90	90
V ($Å^3$)	2696.42(16)	2691.27(12)	3613.30(6)	3607.44(6)
D_{calc} (Mg/m^3)	1.873	1.877	1.727	1.730
μ (mm^{-1})	5.493	5.503	4.120	4.127
θ range (°)	1.49 to 27.48	1.49 to 27.48	2.01 to 27.48	1.86 to 27.48
Reflections collected/unique	13248 / 9927	13212 / 9900	25314 / 8275	25234 / 8264
R int	0.0271	0.0288	0.0340	0.0347
Completeness to θ = 27.48 °	0.802	0.802	0.998	0.998
Data/restraints/parameters	9927 / 0 / 644	9900 / 0 / 655	8275 / 0 / 436	8264 / 0 / 436
$R_1[I>2\sigma(I)]$	0.0336	0.0353	0.0262	0.0274
No. of $I>2\sigma(I)$ (refs.)	8969	8893	7561	7529
Largest diff. peak ($e.Å^{-3}$)	1.831	2.095	1.155	1.417
Largest diff. hole ($e.Å^{-3}$)	-1.515	-1.421	-1.524	-1.482

non-hydrogen atoms were found in the difference Fourier map. All hydrogen atoms of the cations were located geometrically. Some hydrogen atoms of the Ptpop anion were located in difference Fourier map and the other ones were located from the geometrical calculation considering the P-O bond distances and the intermolecular O...O hydrogen bonds. All the non-hydrogen atoms were refined anisotropically and the hydrogen atoms were refined isotropically.

The all crystal data and atomic parameters have been deposited at the CCDC and the deposition numbers are 226198 - 226210.

3.3 Results and discussions

The crystal structures and molecular structures of eight Ptpop complexes were determined by the single crystal X-ray analysis. The detailed crystallographic data, atomic coordination and displacement parameters, bond lengths and bond angles and hydrogen bond tables are summarized in Appendix.

3.3.1 Molecular structure of Ptpop anion

The molecular structures of the Ptpop anion were determined by single crystal X-ray analysis. The bone structures consist of non-hydrogen atoms, were almost the same as that reported before (Fig.1.4). Two Pt atoms were bridged by four diphosphito ligands, and platinum atom formed a square-planer arrangement with four phosphorous atoms. The bone structure of Ptpop anion was seem to have the D_{4h} (4/m) symmetry except for the exocyclic P=O or P-OH groups. Pt-Pt distances at light-off stage were the range from 2.9203(2) Å for Bzdmp to 2.9794(4) Å for Bteal,

these are normal distances by comparison with other d^8-d^8 Ptpop compound, e.g. 2.925(1) Å in $K_4[Pt_2(pop)_4]\cdot 2H_2O$ [15, 16] and 2.949 Å in $Ba_2[Pt_2(pop)_4]$ $8H_2O$. [17,18] If these compounds were not d^8-d^8 ion but d^7-d^7 ion, $[Pt_2(pop)_4X_2]^{4-}$, Pt-Pt distance became shorter, e.g. 2.695(1) Å in $K_4[Pt_2(pop)_4Cl_2]\cdot 2H_2O$.[19]

Considering the Ptpop anion including the hydrogen atom, the Ptpop anions, except for the Bzdmp compounds, are slightly different from those reported previously. There are only two ammonium cations were found per one Ptpop anion. The hydrogen atoms were assigned by the difference Fourier map and the comparison the P-O bond lengths, and extra two hydrogen atoms were found in Ptpop anion. This indicates that Ptpop anion isn't tetravalent but bivalent anion and there are five P-OH bonds and three P=O bonds among the eight independent P-O bonds in a Ptpop anion. For the Bzdmp complex, four ammonium cations are found and extra hydrogen atom isn't found, therefore there are four P-OH and P=O bonds. Thus the Ptpop anions are represented as $[Pt_2(H_3P_2O_5)_2(H_2P_2O_5)_2]^{2-}$ for the crystals of Bu, Pn, Bzte and Bztbu and $[Pt_2(H_2P_2O_5)_4]^{4-}$ for Bzdmp crystal.

For $[Pt_2(H_2P_2O_5)_4]^{4-}$ anion, all hydrogen atom form the intramolecular O-H...O hydrogen bond with neighboring P-O bond. On the other hand, eight of ten hydrogen atoms of most of $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anions form the same intramolecular O-H...O hydrogen bond, whereas the extra two hydrogen atoms are found to direct the external of anion.

The intermolecular O-H...O hydrogen bond are formed using these external hydrogen atoms with neighboring $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anions. The motifs of intermolecular hydrogen bond will be described in chapter 3.3.2. The intermolecular hydrogen bond lengths and angles are summarized in Table 3.4. All hydrogen bond lengths and angles are summarized in

Table 3.4 Inter molecular hydrogen bond lengths (Å) and angles (°) of the Bu, Pn, Bzte, Bztbu and Bzdmp crystals at light-off and light-on stages. All hydrogen bond were summarized in Appendix.

	D-H...A	D-H(Å)	H...A(Å)	D...A(Å)	D-H...A (°)
Bu1-OFF	O8-H8...O7^{i}	0.84	1.72	2.519(4)	157.3
Bu1-ON	O7-H7...O8^{i}	0.84	1.78	2.510(4)	144.8
Bu2	OM-HM0...O17	0.84	2.09	2.93(2)	172.8
	O5-H5...O16^{ii}	0.84	1.69	2.522(7)	169.6
	O15-H15...O6^{iii}	0.84	1.66	2.492(7)	170.8
Pn1-OFF	O8-H8...O7^{iv}	0.86(6)	1.77(6)	2.627(4)	175(6)
	O14-H14...O13^{v}	0.84	1.70	2.537(4)	171.1
Pn1-ON	O8-H8...O7^{iv}	0.79(6)	1.83(6)	2.620(5)	171(6)
	O14-H14...O13^{v}	0.93(6)	1.68(6)	2.526(4)	150(6)
Pn2	O1-H1...O2^{v}	0.83	1.71	2.532(4)	170.3
	O15-H15...O16^{vi}	1.05(6)	1.48(6)	2.506(4)	162(5)
Bzte1-OFF	O2-H2...O17^{vii}	1.20(6)	1.34(7)	2.460(5)	152(6)
	O3-H3...O18^{vii}	0.84(6)	2.06(6)	2.763(5)	141(6)
	O12-H12...O7	0.80(8)	1.74(8)	2.495(6)	158(7)
	O13-H13...O8	0.96(7)	1.59(8)	2.553(6)	173(6)
Bzte1-ON	O3-H3...O18^{vii}	0.77(9)	2.42(9)	2.785(8)	111(8)
	O12-H12...O7	0.86(9)	1.75(9)	2.498(7)	145(9)
	O13-H13...O8	0.84	1.81	2.557(7)	146.9
	O17-H17...O2^{viii}	0.84	1.62	2.459(7)	176.8
Bzte2	O7-H7...O20^{vii}	0.84	1.66	2.468(5)	159.3
	O14-H14...O1^{ix}	0.84	1.74	2.491(6)	147.3
	O50-H50...O6	0.87(11)	2.07(11)	2.926(7)	167(11)
Bztbu-OFF	O7-H7...O8^{i}	0.84	1.72	2.533(4)	163.6
	O17-H17...O18^{x}	1.12(5)	1.38(5)	2.493(4)	171(5)
Bztbu-ON	O7-H7...O8^{i}	1.12(6)	1.40(6)	2.521(5)	175(6)
	O17-H17...O18^{x}	1.14(6)	1.35(6)	2.489(4)	171(6)
Bzdmp-OFF	O50-H50...O1	0.85	1.96	2.813(3)	173.9
Bzdmp-ON	O50-H50...O1	0.85	1.96	2.815(4)	173.9

symmetry operations : i)-x, -y, 1-z; ii)1+x, y, z; iii)-1+x, y, z; iv)-x, 2-y, -z; v)1-x, 1-y, 1-z; vi)1-x, -y, -z; vii)x, y, -1+z; viii)x, y, 1+z; ix)x+0.5, -y+0.5, z; x)-x, 1-y, -z

Appendix.

For Bztel, only six hydrogen atoms of Ptpop form six intramolecular O-H...O hydrogen bonds, and other hydrogen atoms directed to external of Ptpop anion and form the intermolecular hydrogen bond. Therefore two O...O distances without intramolecular hydrogen bond, O2...O3 = 2.903(5) and O12...O13 = 2.984(6) Å, are slightly longer than the others. Although these distances are slightly shorter than the sum of van der Waals radius (1.52 + 1.52 Å), it also close to the threshold of the hydrogen bond with near certainly, < 3.0 Å. [20,21] The other O...O distances, forming the intramolecular hydrogen bond, are 2.4~2.7 Å, these distances are suitable for hydrogen bond.

3.3.2 Crystal structure of Ptpop compounds

The crystal structure of eight Ptpop complexes, Bu1 and Bu2, Pn1 and Pn2, Bztel and Bzte2, Bztbu and Bzdmp crystals, are described in this chapter.

3.3.2.1 Crystal structure of Bu1 and Bu2

Two crystal forms, Bu1 and Bu2, were produced in the same batch. The Bu2 crystal form has one methanol molecule per one Ptpop anion as the crystal solvent, while there is no solvent in the Bu1 crystal. Thus Bu1 and Bu2 are pseudo-polymorph. [22] In order to obtain the precise diffraction data during photo-irradiation, only the Bu1 crystal was used for photo-irradiation, because the elimination of the methanol molecule in Bu2 crystal may complicate to compare the small structure change.

The crystal structure of Bu1 is shown in Fig. 3.5. There are two tetrabuthyl ammonium cations per a $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion. Each Ptpop

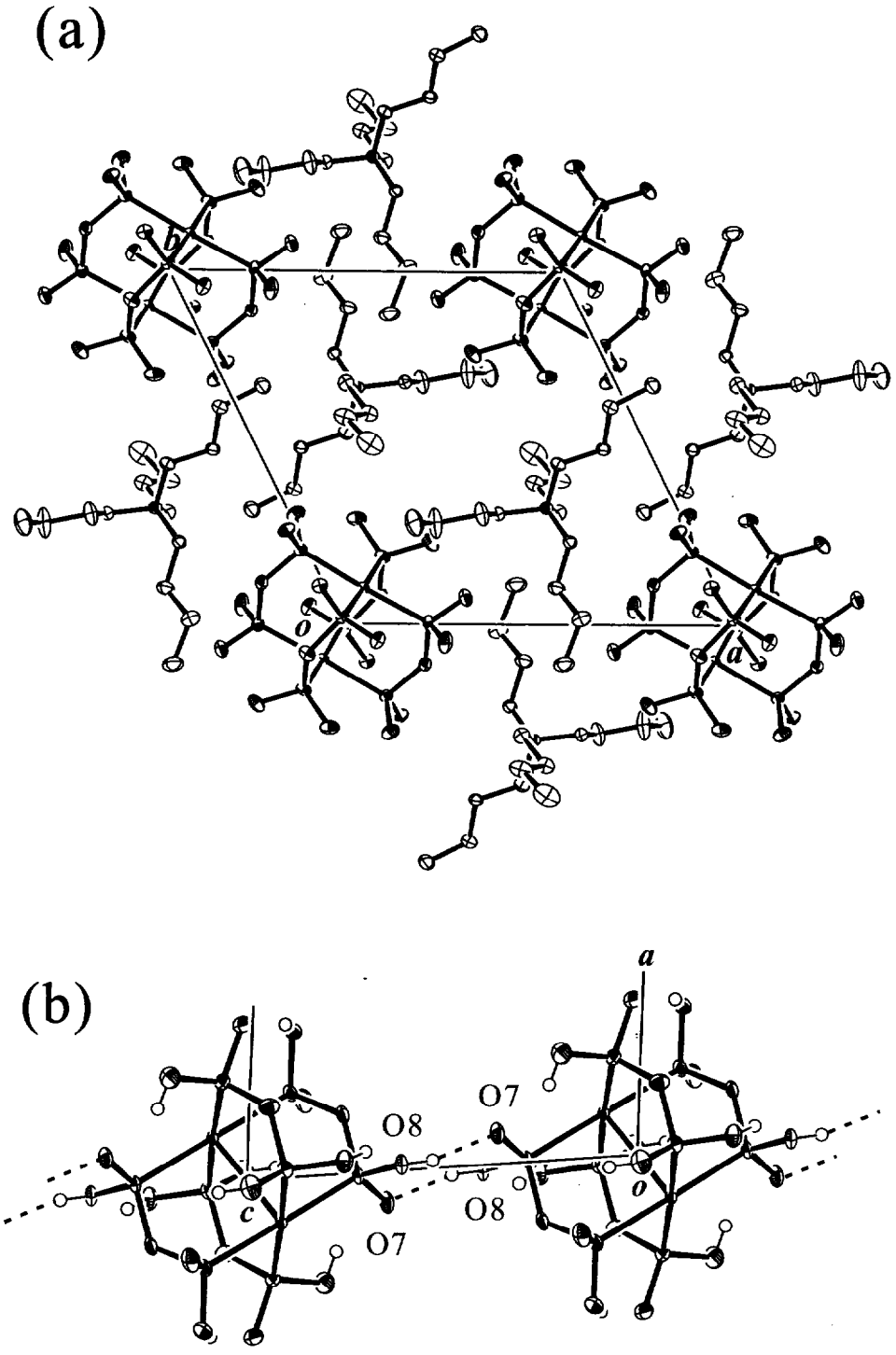


Fig. 3.5
(a) Crystal structure of Bu1 viewed along the c-axis.
(b) O-H...O hydrogen bonding chain along the c-axis.
The ellipsoids are drawn at the 50 % probability level.

anion lie on a center of symmetry. The Ptpop complexes of Bu1 are connected with the neighboring complexes by two O-H...O hydrogen bonds using the two external hydrogen atoms and make a linear chain along the c axis.

The crystal structure of Bu2 is shown in Fig. 3.6. The similar hydrogen bond chain form with the Ptpop complexes along a-axis. The solvent methanol molecule makes O-H...O hydrogen bond with the Ptpop complex.

3.3.2.2 Crystal structure of Pn1 and Pn2

The two crystal structures of Pn1 and Pn2 are shown in Figs. 3.7 and 3.8, respectively. Both of them were obtained in the same batch and have no solvent molecules. In Pn2, one alkyl chain of the cations is disordered (Fig. 3.8(c)), although all the alkyl chains are ordered in Pn1. This is due to the void space that is made by the slight orientation change of the Ptpop anions in Pn2 crystal. Because the Pn1 and Pn2 are different only the orientation of the Ptpop anion, these polymorph are true-polymorph. [22] Because of the disorder structure in the Pn2 crystal, only the Pn1 crystal was used for photo-irradiation, since the thermal energy emitted from the excited molecules may affect the disordered structure.

Either crystal has two crystallographically independent Ptpop anions that occupy the different centers of symmetry and there are two tetrapenthyl ammonium cations per a $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion. The Ptpop complexes are connected with the neighboring complexes by the O-H...O hydrogen bonds to form a linear chain as observed in Bu1 crystal. The chain is extended along a-axis in each crystal.

3.3.2.3 Crystal structure of Bzte1 and Bzte2

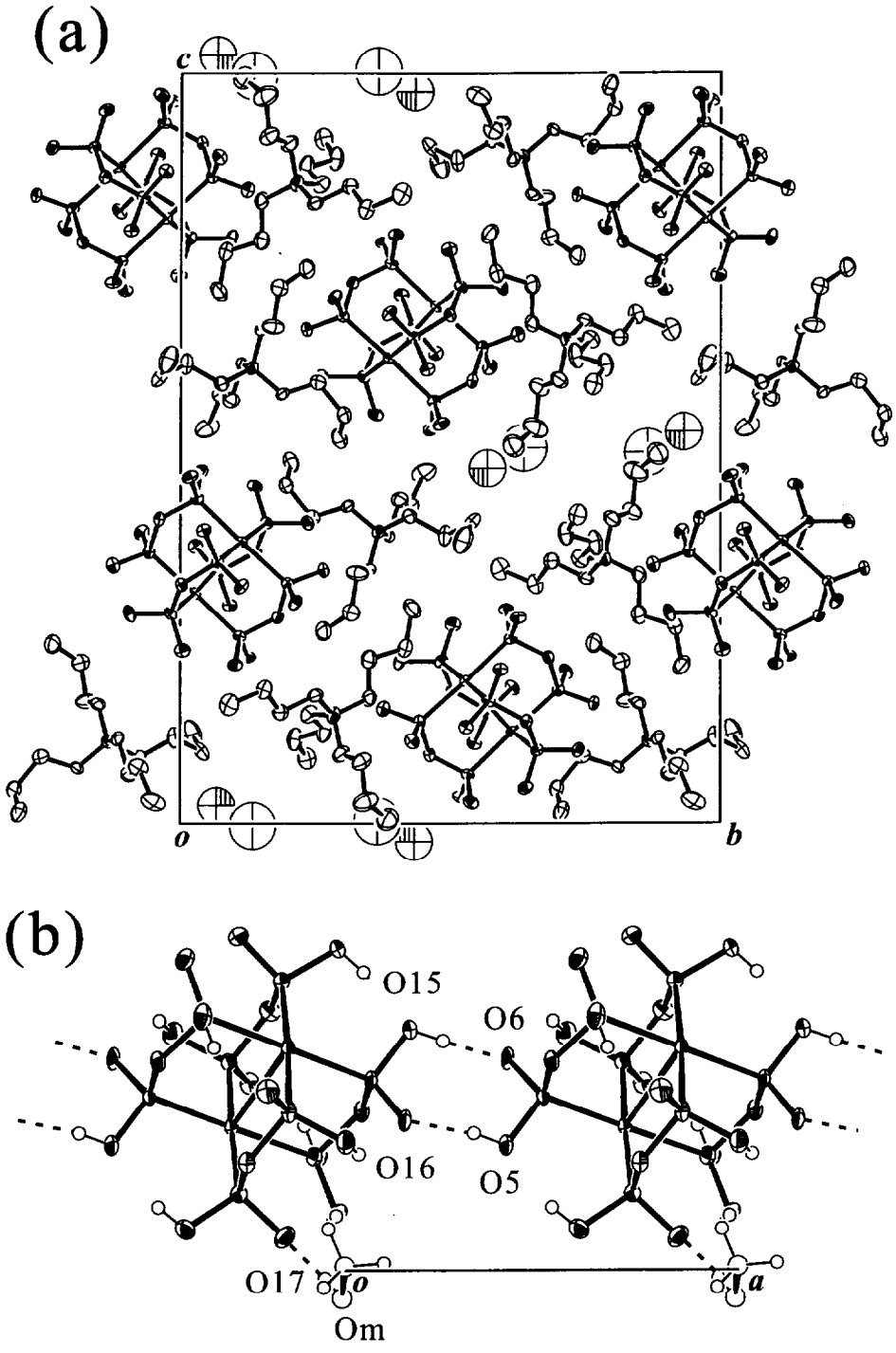


Fig. 3.6
(a)Crystal structure of Bu2 viewed along the a-axis.
(b)The hydrogen bonding chain along the a-axis. Methanol molecule connected to Ptpop anion by O-H...O hydrogen bond. The ellipsoids are drawn at the 50 % probability level.

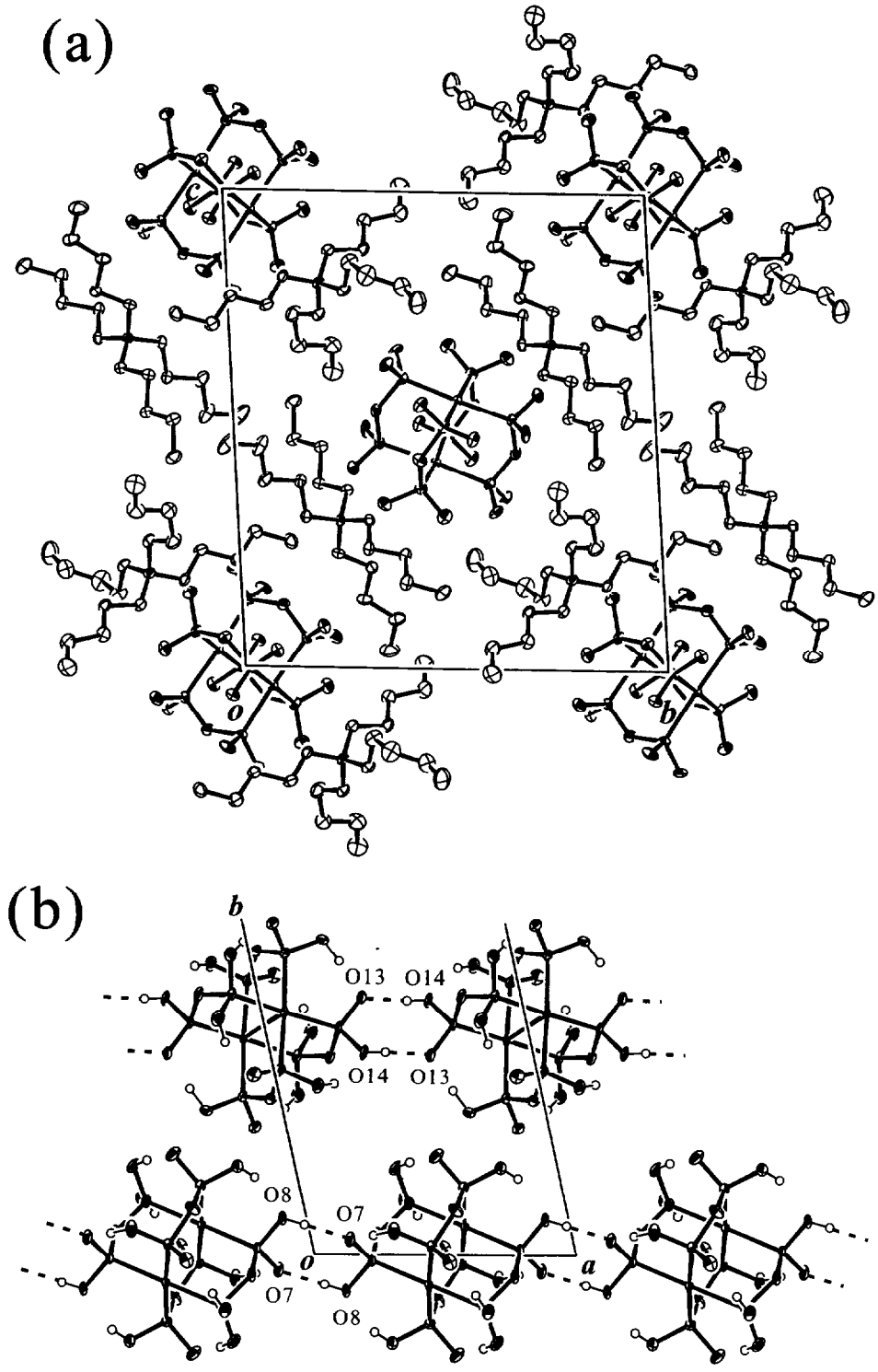


Fig. 3.7·
(a)Crystal structure of Pn1 viewed along the a-axis.
(b)The two crystallographically independent hydrogen bonding chains along the a-axis.
The ellipsoids are drawn at the 50 % probability level.

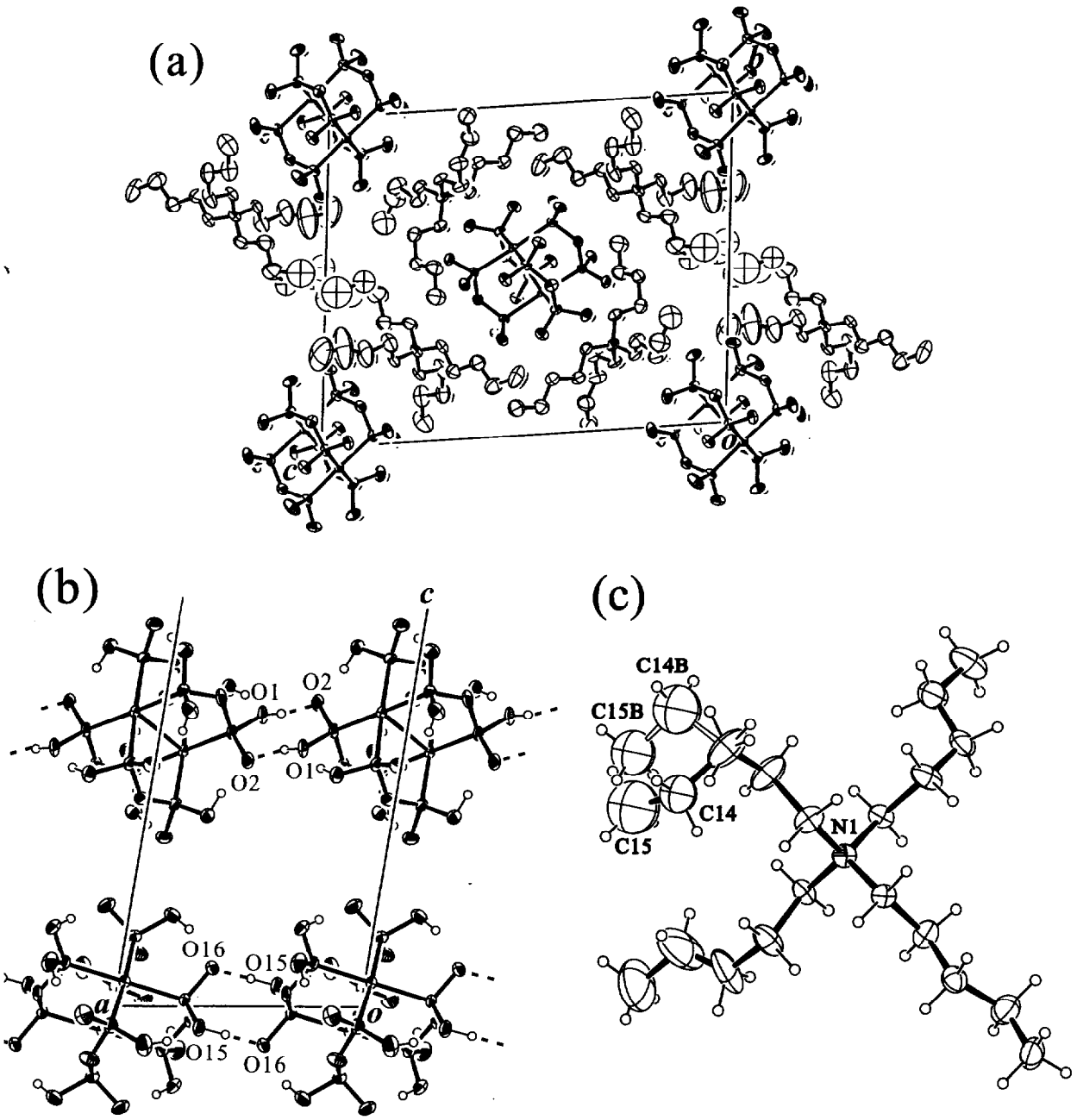


Fig. 3.8
(a)Crystal structure of Pn2 viewed along the a-axis.
(b)The two hydrogen bonding chains along the a-axis.
(c)Disordered alkyl chain of cation (C13-C14 and C13B-C14B) in Pn2 crystal. Occupancy factor of C13-C14 are 0.54(2).
The ellipsoids are drawn at the 50 % probability level for (a) and (b), and 30 % probability level for (c).

There are two crystal forms for the Bzte complexes, Bzte1 and Bzte2. Their crystal structures are shown in Figs. 3.9 and 3.10, respectively. There are two benzyltriethyl ammonium cations per a $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion.

The Bzte1 crystal has no crystal solvent and two Ptpop anions occupy the different centers of symmetry, whereas the Bzte2 crystal has one methanol molecule as a crystal solvent, which is attached to the Ptpop complex with the O-H...O hydrogen bond. Thus Bzte1 and Bzte2 crystals are pseudo-polymorph. [22] In each crystal, the Ptpop complexes are connected with the O-H...O hydrogen bonds to form a two-dimensional sheet. The only Bzte1 crystal was used photo-irradiation because the same reason as the Bu crystal. Indeed the methanol molecule in Bzte2 crystal eliminated within an hour at room temperature.

3.3.2.4 Crystal structure of Bztbu

There is only crystal form for the Bztbu complex, whose crystal structure is shown in Fig. 3.11. The two crystallographically independent Ptpop anions occupy the different inversion centers and there are two benzyltributyl ammonium cations per a $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion. The Ptpop complexes are connected with the neighboring Ptpop complexes by a pair of O-H...O hydrogen bonds to form a chain along the a-axis. This crystal was used for photo-irradiation.

3.3.2.5 Crystal structure of Bzdmp

There is only one crystal form for the Bzdmp complex. The crystal structure is shown in Fig. 3.12. The Ptpop complex has a different structure from those of the above crystals, since no extra protons are attached to the Ptpop moieties. Therefore, the Ptpop complex is written as

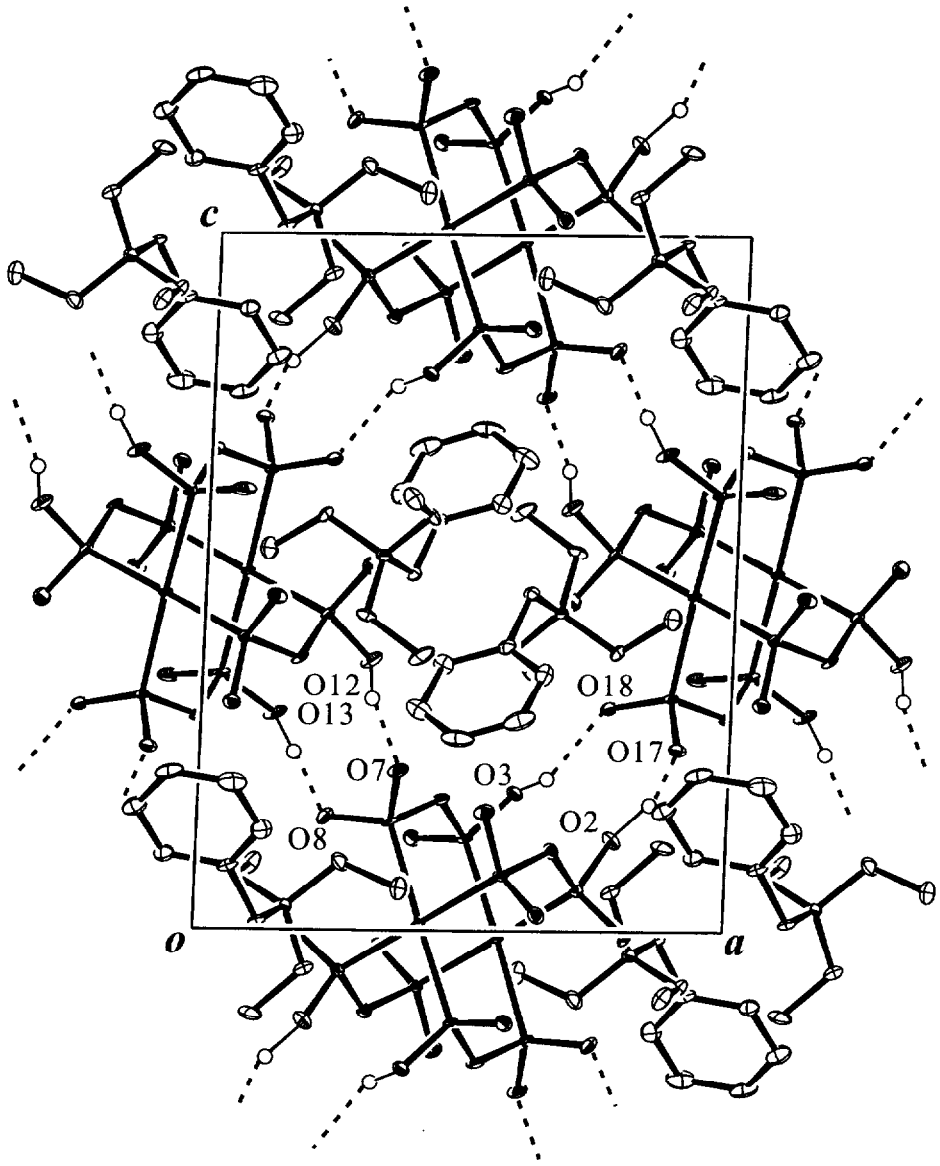


Fig. 3.9 Crystal structure of Bztel viewed along the b-axis and the hydrogen-bonding sheet normal to the b-axis. The ellipsoids are drawn at the 50 % probability level.

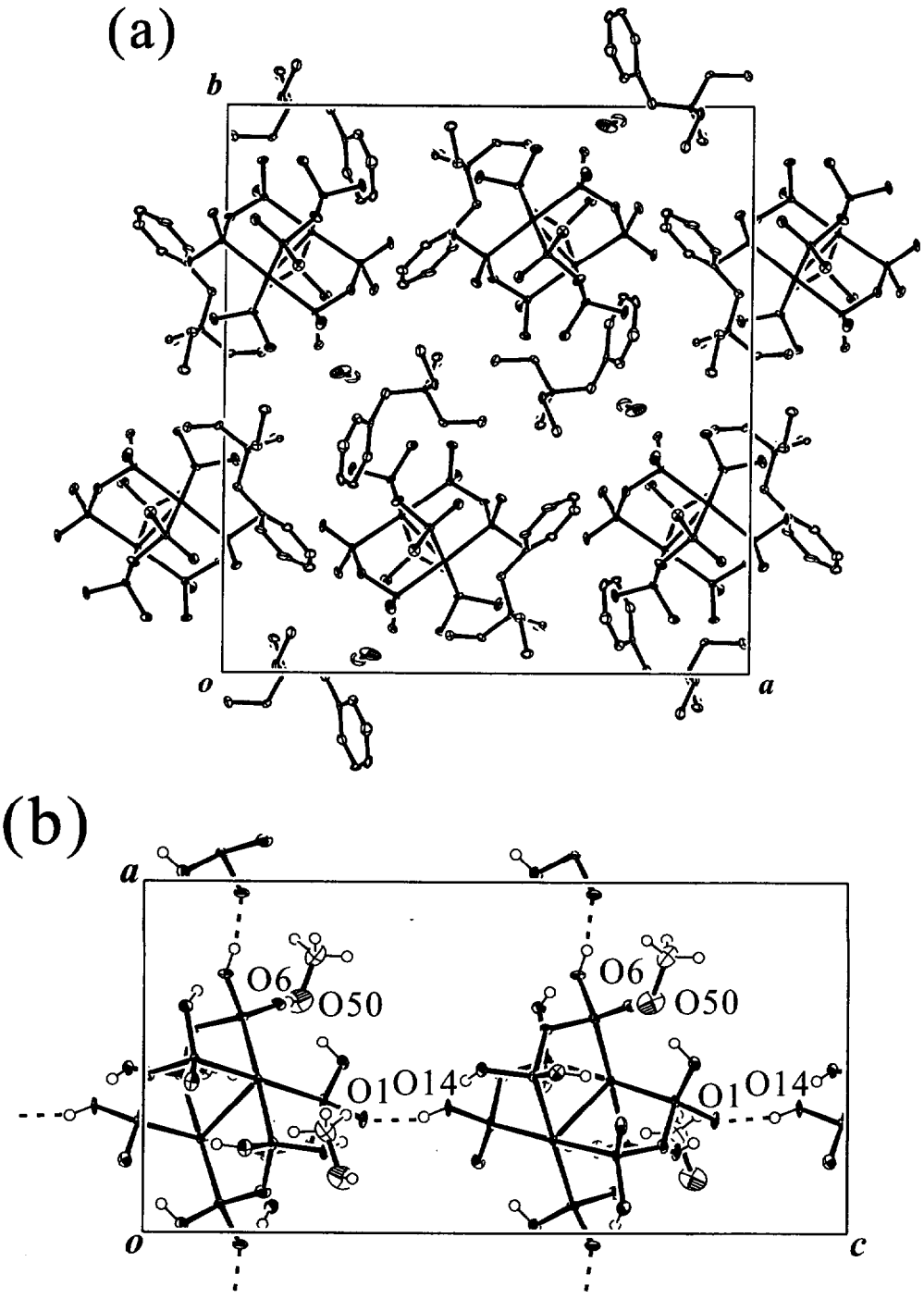


Fig. 3.10
(a)Crystal structure of Bzte2 viewed along the c-axis.
(b)The hydrogen bonding chain along the c-axis.
The ellipsoids are drawn at the 50 % probability level.

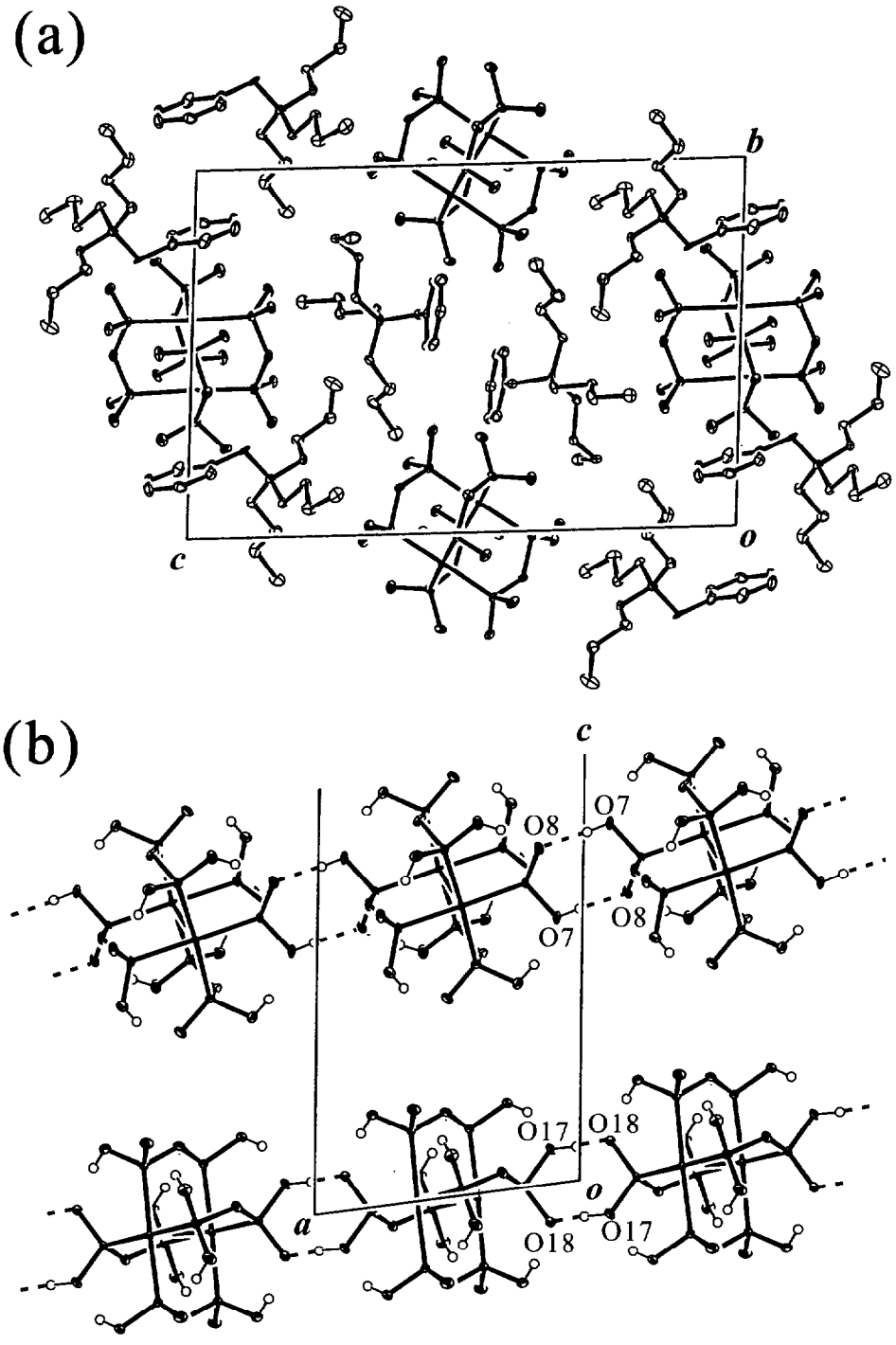


Fig. 3.11
(a) Crystal structure of Bztbu viewed along the a-axis.
(b) The two hydrogen-bonding chains along the a-axis.
The ellipsoids are drawn at the 50 % probability level.

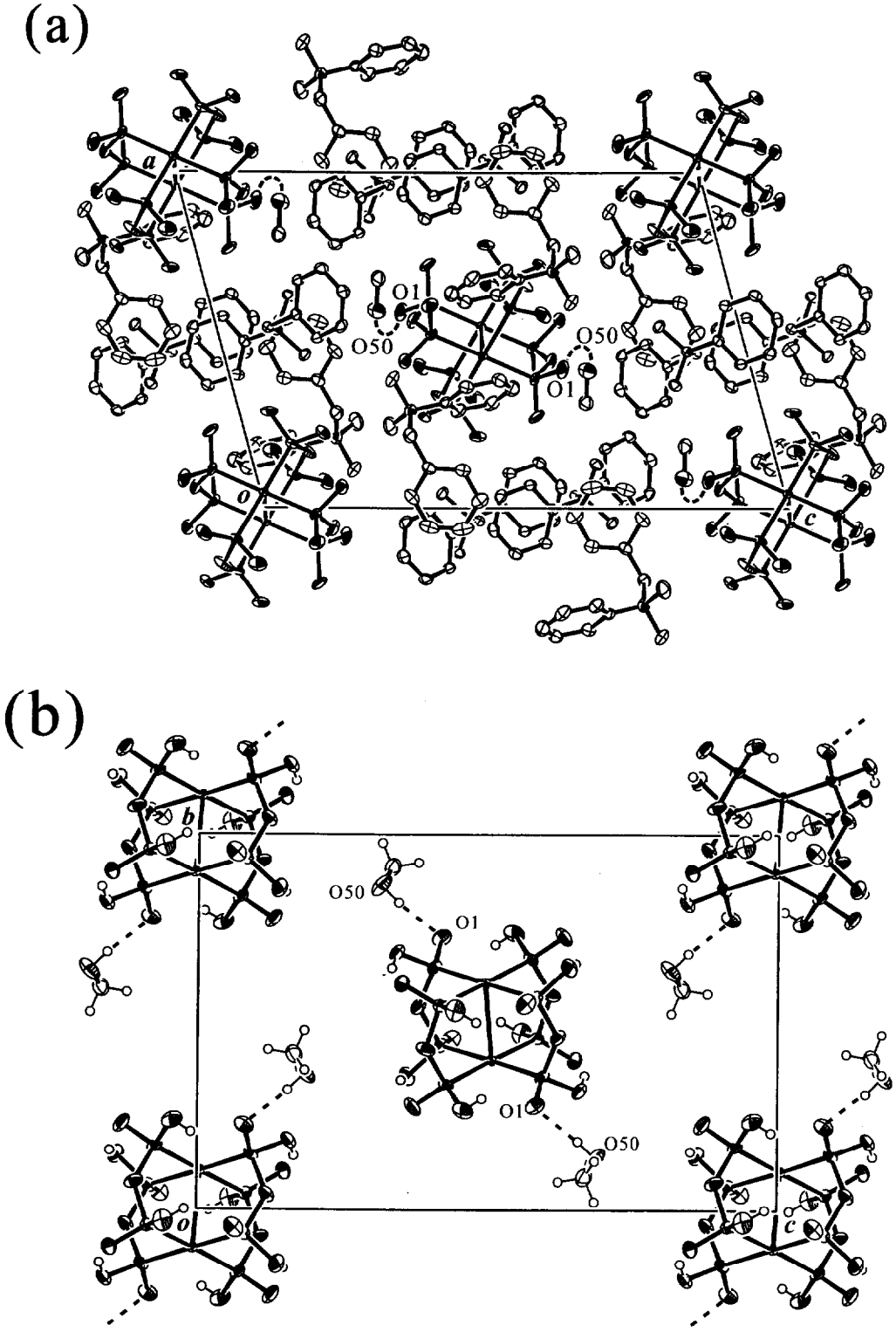


Fig. 3.12
(a)Crystal structure of Bzdmp viewed along the b-axis.
(b)The hydrogen bond between Ptpop anion and two methanol molecules. The hydrogen bond network between Ptpop complex anions don't form.
The ellipsoids are drawn at the 50 % probability level.

$[Pt_2(pop)_4]^{4-}$ and there are four benzyldimethylphenylammonium cations per one Ptpop complex anion.

The Ptpop anion doesn't form hydrogen bonds with the neighboring Ptpop anions and is isolated from the other Ptpop anions. The two solvent methanol molecules are connected with the Ptpop complex by the O-H...O hydrogen bond. The isolated structure is probably closely related to the no-proton attached anion. Although the methanol molecule was included in this crystal, this crystal was used for photo-irradiation because the polymorph crystal without solvent wasn't obtained.

Although the occupancy factor of methanol molecule was refined first, it was almost 1.0. This means the methanol molecule in the crystal didn't eliminate after the measurement at light-off and light-on stages. Therefore occupancy factor was fixed to 1.0 and the structure was refined again.

3.3.3 Powder X-ray analysis of Pn1 at SPring-8

As described in chapter 3.3.1, the Ptpop anions of Bu, Pn, Bzte and Bztbu are represented as $[Pt_2(Hpop)_2(pop)_2]^{2-}$ and $[Pt_2(pop)_4]^{4-}$ for Bzdmp crystal. The compounds represented $[Pt_2(pop)_4]^{4-}$ is suitable for the study of photo-excitation because the photo-excited behavior was confirmed by the powder X-ray measurement. Although the structural difference between $[Pt_2(Hpop)_2(pop)_2]^{2-}$ and $[Pt_2(pop)_4]^{4-}$ is so small, it was worry about the difference of the excited state behaviors of $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion. In order to confirm the behavior of $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion, the powder X-ray analysis was carried out at SPring-8.

For the $[N(C_4H_9)_4]_4[Pt_2(pop)_4]$ compounds, the peak shift to higher 2θ by photo-irradiation was observed previously. [5] The powder X-ray diffraction of Pn1 at the light-off and light-on stages, as the $[Pt_2(Hpop)_2(pop)_2]^{2-}$ anion,

were measured at the BL02B2 beam line of SPring-8. The experimental details are in chapter 3.2.2.

The powder diffraction patterns of light-off and light-on stages are shown in Fig. 3.13(a). The diffraction peak shifted to the higher 2θ angle about 0.02° at the range from 6.5 to 7.5°, when the excitation light was irradiated. The diffraction pattern should shift to the lower diffraction angles if the crystal lattice is expanded thermally due to photo-irradiation. This indicates that the unit cell contracts at the excited state. It is adequate to assume that the excited-state Ptpop complex becomes smaller than that at the ground state, because there are no other substances which contracts on exposure to the Xe lamp.

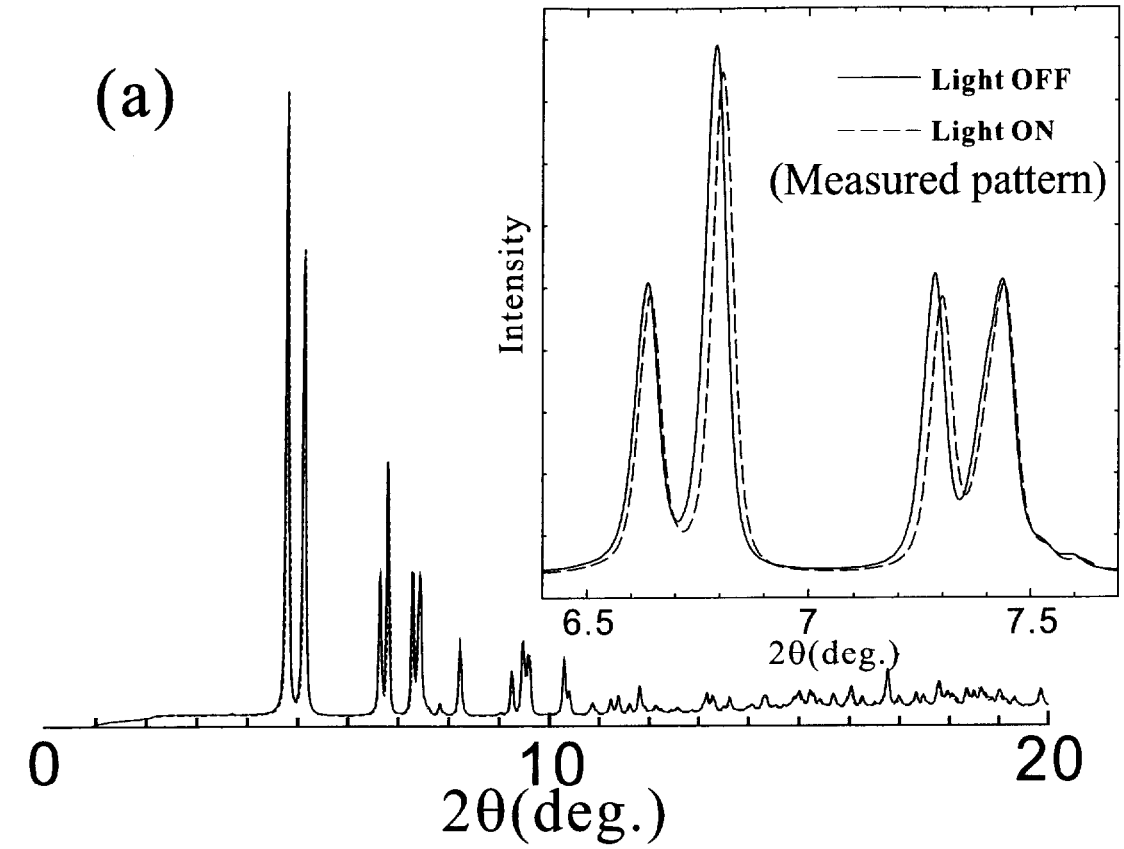
Moreover, it must be emphasized that the diffraction peaks at the light-on stage are sharp and that they indicate no mixing of the original diffraction peaks. This suggests that the structures of the excited state and the ground state reached the equilibrium state after a short period and the new crystalline-lattice corresponding to the equilibrium state was produced.

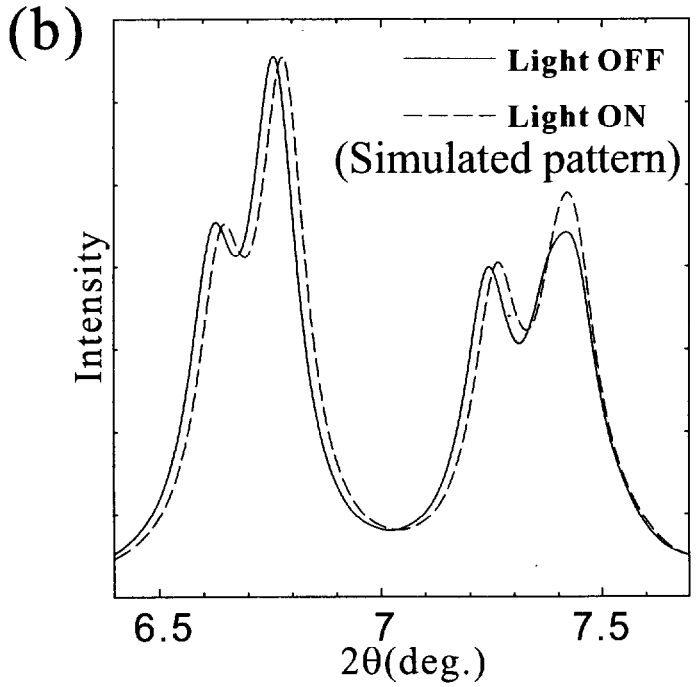
Since this result corresponded with the $[Pt_2(pop)_4]^{4-}$ anion, the four $[Pt_2(Hpop)_2(pop)_2]^{2-}$ crystals, Bu1 Pn1 Bzte1 and Bztbu, were worth to measure the excited-state structure by single crystal X-ray analysis.

3.3.4 Cell-volume change by photo-irradiation

The five crystals of Bu1, Pn1, Bzte1, Bztbu and Bzdmp among the eight crystals were analyzed the photo-excited structure. The measurement condition and details of structure analysis is described in chapter 3.2.4.

After the all refinements were finished, the cell volumes at light-off and light-on stages were compared in order to confirm the decrease of the cell volume by photo-irradiation as observed for the powder diffraction





(c)

	Shift of 2θ (°)
Bu1	0.02
Pn 1	0.02～0.04
Bzte1	0.02～0.04
Bztbu	0～0.02
Bzdmp	0～0.02

Fig. 3.13 The powder diffraction patterns of Pn1 compound at light-off and light-on stages:
(a)Powder diffraction patterns of Pn1 compound measured at SPring-8 BL02B2 beam line. The solid and dotted lines are light-off and light-on stages, respectively.
(b)The simulated powder patterns based on the unit-cell dimensions of the single crystals at the light-off and light-on stages. These patterns calculated with PLATON.
(c)The table of shifted 2θ angles of each crystals calculated by simulated powder diffraction pattern.

measurements of $[N(C_4H_9)_4]_4[Pt_2(pop)_4]$ [5] and Pn1.

The unit-cell dimensions of the five crystals at the light-off and light-on stages are listed in Table 3.3. The cell volume and the changes of the cell volume of five compounds between light-off and light-on stages are summarized in Table 3.5. The cell volumes of all crystals decreased by 5.15(14) ~ 20.33(12) $Å^3$ by photo-irradiation. Although these amounts of decrease have no relation each other, the ratio of the volume change, $\Delta| V_{on} - V_{off} |/V_{off}$, is about 0.6 % for the Bu1 Pn1 and Bzte1 crystals and about 0.2 % for Bztbu and Bzdmp crystals. These correspondences of ratio are very surprisingly and may indicate that there is some threshold for the cell lattice change at the excited state. However the difference between 0.6 % and 0.2 % may be due to the influence of the environment in the crystal.

The simulated pattern of the powder X-ray diffraction can be calculated since the lattice parameters are determined accurately by single crystal analysis. The simulated powder patterns, including the light-off and the light-on stages of each five crystals, were calculated using the program PLATON [11] and overlapped each other. For instance, the simulated powder pattern of Pn1 is shown in Fig. 3.14(b). The cell parameters are a=9.69650(10) b=17.2492(3) c=18.7278(2) Å, α=93.6649(4) β=90.9346(8) and γ=102.8259(7)° for light-off stage and a=9.6758(3) b=17.2106(6) c=18.6822(6) Å, α=93.6675(8) β=90.9035(4) and γ=102.8002(8)° for light-on stage. The diffraction peaks of the light-on stage shift to the higher angle, about 0.02° at the range from 6.5 to 7.5°, than those at the light-off stage.

The amount of the peak shift corresponded with that of powder X-ray analysis measured at SPring-8, described in chapter 3.3.3. The simulated amounts of the peak shift for all complexes are summarized in Fig. 3.13(c).

Table 3.5 Change of the unit-cell volume ($Å^3$) at light-off (V_{off}) and light-on (V_{on}) stages for the Bu1, Pn1, Bzte1, Bztbu and Bzdmp crystals

	V_{off} ($Å^3$)	V_{on} ($Å^3$)	$\Delta(V_{on}-V_{off})$	$\Delta\lvert V_{on}-V_{off}\rvert/V_{off}$ (%)
Bu1	1320.18(3)	1312.16(5)	-8.02(4)	0.61
Pn1	3046.45(7)	3026.12(17)	-20.33(12)	0.67
Bzte1	2108.78(12)	2094.92(11)	-13.86(11)	0.66
Bztbu	2696.42(16)	2691.27(12)	-5.15(14)	0.19
Bzdmp	3613.30(6)	3607.44(6)	-5.86(6)	0.16

This indicates the rate of the excited molecules may be almost the same although the particle size is much different between the single crystal and the powder sample.

3.3.5 Structure change by photo-irradiation

The structures of the five crystals at the light-off and light-on stages are determined by X-ray analysis. The bond lengths of Ptpop anions were summarized in Table 3.6.

The Pt-Pt distance of the Ptpop anion and the averaged N-C bond distances of ammonium cations are summarized in Tables 3.7 and 3.8, respectively. In each crystal, there are no significant structural differences in the cation molecules between the light-off and light-on stages. On the other hand, the bond distances in the Ptpop complex anions are significantly changed from the corresponding ones at light-off stage. The differences of Pt-Pt distance of each crystal were 0.0038(3), 0.0083(3), 0.0135(4), 0.0035(3) and 0.0019(2) Å for Bu1, Pn1, Bzte1, Bztbu and Bzdmp, respectively.

The same result was obtained from the measurement of Bzte1 crystal using LTV camera at SPring-8. The Pt-Pt distance of one Ptpop anion changed shorter from 2.9495(8) to 2.9482(8) Å and Δ(ON-OFF)= -0.0013(8) Å, although the difference was slightly smaller. This result indicates the shortening of Pt-Pt distance didn't occur by the degradation of the crystal, because the effect of crystal degradation was avoided by the multiple-exposure IP method.

Pt-Pt distances of Bu1 crystal at light-off stage were measured at various temperatures, 223, 198, 173 and 148 K. The distances increased with temperature from 2.9415(3) Å for 148 K to 2.9486(3) Å for 223 K. This

Table 3.6 Bond lengths (Å) of the Pt anions with their estimated standard deviations in eight crystals of Bu1, Pn1, Bzte1, Bztbu, Bzdmp, Bu2, Pn2 and Bzte2.

Bu1 OFF						**Bzdmp OFF**					
Pt1-Pt1	2.9419(3)	P2-O3	1.532(3)	P3-O6	1.589(3)	Pt1-Pt1	2.9203(2)	P1-O1	1.518(3)	P3-O6	1.572(3)
		P3-O5	1.509(3)	P4-O8	1.554(3)			P2-O3	1.522(3)	P4-O8	1.584(3)
Pt1-P1	2.3291(10)	P4-O7	1.565(3)	P1-O9	1.623(3)	Pt1-P1	2.3323(8)	P3-O5	1.530(3)	P1-O9	1.640(3)
Pt1-P2	2.3282(10)	P1-O1	1.584(3)	P2-O10	1.639(3)	Pt1-P2	2.3415(8)	P4-O7	1.517(3)	P2-O10	1.634(3)
Pt1-P3	2.3472(10)	P1-O2	1.523(3)	P3-O9	1.644(3)	Pt1-P3	2.3336(8)	P1-O2	1.582(3)	P3-O9	1.640(2)
Pt1-P4	2.3308(10)	P2-O4	1.565(3)	P4-O10	1.621(3)	Pt1-P4	2.3367(8)	P2-O4	1.575(3)	P4-O10	1.636(3)
Pn1 OFF						**Bu2**					
Pt1-Pt1	2.9542(3)	P1-O2	1.514(3)	P6-O14	1.577(3)	Pt1-Pt2	2.9233(4)	P1-O6	1.536(5)	P5-O14	1.536(6)
Pt2-Pt2	2.9387(3)	P3-O5	1.506(4)	P7-O15	1.591(3)			P3-O10	1.519(5)	P6-O15	1.581(5)
		P4-O7	1.533(3)	P8-O17	1.539(4)	Pt1-P1	2.3054(19)	P4-O11	1.506(5)	P7-O20	1.569(6)
Pt1-P1	2.3224(12)	P5-O11	1.520(3)	P8-O18	1.544(3)	Pt1-P3	2.3269(19)	P6-O16	1.523(5)	P8-O18	1.563(6)
Pt1-P2	2.3263(12)	P6-O13	1.524(3)	P1-O9	1.620(3)	Pt1-P5	2.3141(19)	P7-O17	1.512(6)	P1-O1	1.617(5)
Pt1-P3	2.3319(12)	P7-O16	1.512(3)	P2-O10	1.634(3)	Pt1-P7	2.3137(19)	P8-O19	1.517(6)	P2-O1	1.624(5)
Pt1-P4	2.3367(11)	P1-O1	1.579(4)	P3-O9	1.629(3)	Pt2-P2	2.310(2)	P1-O5	1.565(5)	P3-O2	1.624(5)
Pt2-P5	2.3257(11)	P2-O3	1.523(4)	P4-O10	1.621(3)	Pt2-P4	2.3206(19)	P2-O7	1.546(5)	P4-O2	1.628(5)
Pt2-P6	2.3154(11)	P2-O4	1.544(4)	P5-O19	1.628(4)	Pt2-P6	2.3052(19)	P2-O8	1.529(6)	P5-O3	1.619(5)
Pt2-P7	2.3274(11)	P3-O6	1.563(4)	P6-O20	1.621(4)	Pt2-P8	2.3144(19)	P3-O9	1.563(6)	P6-O3	1.625(5)
Pt2-P8	2.3262(11)	P4-O8	1.580(4)	P7-O19	1.625(4)			P4-O12	1.577(5)	P7-O4	1.626(5)
		P5-O12	1.574(4)	P8-O20	1.639(4)			P5-O13	1.554(6)	P8-O4	1.630(5)
Bzte1 OFF						**Pn2**					
Pt1-Pt1	2.9657(3)	P3-O5	1.526(4)	P6-O13	1.559(4)	Pt1-Pt1	2.9468(3)	P1-O2	1.527(3)	P5-O12	1.565(4)
Pt2-Pt2	2.9794(4)	P4-O7	1.542(4)	P6-O14	1.549(4)	Pt2-Pt2	2.9657(3)	P2-O4	1.525(3)	P6-O14	1.573(4)
		P4-O8	1.536(4)	P7-O16	1.579(4)			P4-O7	1.514(3)	P7-O15	1.556(4)
Pt1-P1	2.3304(13)	P5-O11	1.554(4)	P8-O18	1.531(4)	Pt1-P1	2.3206(11)	P6-O13	1.513(4)	P8-O17	1.591(4)
Pt1-P2	2.3369(13)	P7-O15	1.518(4)	P1-O9	1.635(4)	Pt1-P2	2.3382(11)	P7-O16	1.569(3)	P1-O9	1.636(3)
Pt1-P3	2.3327(13)	P8-O17	1.550(4)	P2-O10	1.623(4)	Pt1-P3	2.3271(11)	P8-O18	1.526(4)	P2-O10	1.638(3)
Pt1-P4	2.3412(13)	P1-O1	1.575(4)	P3-O9	1.638(3)	Pt1-P4	2.3299(11)	P1-O1	1.586(3)	P3-O9	1.642(3)
Pt2-P5	2.3389(13)	P1-O2	1.536(4)	P4-O10	1.654(4)	Pt2-P5	2.3267(11)	P2-O3	1.579(3)	P4-O10	1.633(3)
Pt2-P6	2.3458(13)	P2-O3	1.577(4)	P5-O19	1.632(4)	Pt2-P6	2.3325(12)	P3-O5	1.550(4)	P5-O19	1.634(3)
Pt2-P7	2.3359(13)	P2-O4	1.543(4)	P6-O20	1.629(4)	Pt2-P7	2.3244(11)	P3-O6	1.537(4)	P6-O20	1.642(4)
Pt2-P8	2.3370(13)	P3-O6	1.583(4)	P7-O19	1.646(4)	Pt2-P8	2.3174(12)	P4-O8	1.586(3)	P7-O19	1.621(3)
		P5-O12	1.546(4)	P8-O20	1.653(4)			P5-O11	1.532(4)	P8-O20	1.619(4)
Bztbu OFF						**Bzte2**					
Pt1-Pt1	2.9457(3)	P2-O3	1.539(4)	P6-O14	1.532(4)	Pt1-Pt2	2.9425(3)	P1-O1	1.516(4)	P6-O14	1.568(4)
Pt2-Pt2	2.9330(3)	P3-O5	1.514(3)	P6-O13	1.543(4)			P2-O5	1.521(4)	P7-O16	1.530(4)
		P4-O8	1.533(3)	P7-O16	1.579(3)	Pt1-P1	2.3369(15)	P3-O6	1.517(4)	P7-O17	1.576(4)
Pt1-P1	2.3271(12)	P5-O12	1.519(4)	P8-O17	1.576(3)	Pt1-P3	2.3400(14)	P5-O12	1.529(4)	P8-O19	1.560(4)
Pt1-P2	2.3337(11)	P7-O15	1.519(4)	P1-O9	1.626(3)	Pt1-P5	2.3190(15)	P6-O15	1.508(4)	P1-O3	1.655(4)
Pt1-P3	2.3301(12)	P8-O18	1.537(4)	P2-O10	1.630(3)	Pt1-P7	2.3292(15)	P8-O20	1.540(4)	P2-O3	1.609(4)
Pt1-P4	2.3198(11)	P1-O2	1.529(4)	P3-O9	1.632(4)	Pt2-P2	2.3192(15)	P1-O2	1.560(4)	P3-O8	1.670(4)
Pt2-P5	2.3373(13)	P1-O1	1.566(3)	P4-O10	1.626(4)	Pt2-P4	2.3163(15)	P2-O4	1.583(4)	P4-O8	1.618(4)
Pt2-P6	2.3241(11)	P2-O4	1.547(4)	P5-O19	1.624(4)	Pt2-P8	2.3267(14)	P3-O7	1.570(4)	P5-O13	1.623(4)
Pt2-P7	2.3174(13)	P3-O6	1.587(3)	P6-O20	1.632(4)	Pt2-P6	2.3363(14)	P4-O9	1.532(4)	P6-O13	1.652(4)
Pt2-P8	2.3139(11)	P4-O7	1.578(3)	P7-O19	1.635(4)			P4-O10	1.577(4)	P7-O18	1.629(4)
		P5-O11	1.584(3)	P8-O20	1.634(4)			P5-O11	1.578(4)	P8-O18	1.640(5)

Table 3.7 The change of Pt-Pt bond length and the rate of excited molecules. The rate of excited molecules was calculated as the rate with the reported contraction, 0.21 Å.

	Light OFF (Å)	Light ON (Å)	Δ(ON-OFF)	Rate(%)
Bu	2.9419(3)	2.9381(3)	-0.0038(3)	1.80
Pn 1 anionA	2.9622(3)	2.9542(3)	-0.0080(3)	3.80
anionB	2.9470(3)	2.9387(3)	-0.0083(3)	3.95
Bzte1 anionA	2.9657(3)	2.9522(5)	-0.0135(4)	6.43
anionB	2.9794(4)	2.9676(6)	-0.0118(5)	5.62
Bztbu anionA	2.9457(3)	2.9422(3)	-0.0035(3)	1.67
anionB	2.9330(3)	2.9304(4)	-0.0026(3)	1.24
Bzdmp	2.9203(2)	2.9184(2)	-0.0019(2)	0.90

Table 3.8 Averaged N-C bond distances (Å) of ammonium cations at light-off and light-on stages and their differences.

	Light OFF (Å)	Light ON (Å)	Δ(ON-OFF)
Bu1	1.527(5)	1.525(5)	-0.002(5)
Pn1	1.529(6)	1.525(6)	-0.004(6)
Bzte1	1.530(6)	1.524(9)	-0.006(8)
Bztbu	1.527(6)	1.526(6)	-0.001(6)
Bzdmp	1.523(4)	1.522(5)	-0.001(4)

indicates that if the heat was generated in the crystal by photo-irradiation, then Pt-Pt distance should become longer. It may be unavoidable the generation of the some degree of heat by photo-irradiation and Pt-Pt distance may slightly become longer. However actually, Pt-Pt distance became shorter by photo-irradiation rather than the elongation of Pt-Pt distance by heat.

Therefore it was concluded the shortening of the Pt-Pt distance, observed in these experiments, was not due to the degradation of crystal or heat generation, but also occurred by the photo-irradiation, i.e. photo-excitation of Ptpop complex.

For Pn1 and Bzte1 crystals, the differences of the Pt-Pt distance, 0.0083(3) and 0.0135(4) Å respectively, were slightly larger than those of the others. Such differences are probably caused by the different concentration of the excited molecules in each crystal. The differences in transmittance of the incident light and the packing around the Ptpop complex may be responsible to the different concentration of the excited molecules.

In order to see the structural change in more detail, the averaged bond distances of Pn1 and Bzte1 crystals were calculated. It seems adequate that the Ptpop complex has the D_{4h} (4/m) symmetry except for the exocyclic P=O or P-OH groups. Assuming the exocyclic P=O and P-OH bonds were also included the D_{4h} symmetry, the five bond types, Pt-Pt, Pt-P, P-O(-P), P=O and P-O(-H) were averaged and compared them between light-off and light-on stages.

The averaged bond distances of five bond types are summarized in Table 3.9. D_{off} and D_{on} are averaged distance at light-off and light-on stages, respectively, and ΔD is the difference of D_{off} and D_{on}.

Table 3.9 Averaged bond distances (Å) of Pt-Pt, Pt-P, P-O(-P), P=O and P-O(-H) at light-off (D_{off}) and light-on (D_{on}) stages and their differences (ΔD).

	D_{off}	D_{on}	ΔD		D_{off}	D_{on}	ΔD
Bu1				Bztbu			
Pt-Pt	2.9419(3)	2.9381(3)	-0.0038(3)	Pt-Pt	2.9394(3)	2.9363(4)	-0.0031(3)
Pt-P	2.3338(10)	2.3269(10)	-0.0069(10)	Pt-P	2.3254(12)	2.3235(12)	-0.0019(12)
P-O(-P)	1.632(3)	1.629(3)	-0.003(3)	P-O(-P)	1.630(4)	1.628(4)	-0.002(4)
P=O	1.535(3)	1.530(3)	-0.005(3)	P=O	1.527(4)	1.521(4)	-0.006(4)
P-O(-H)	1.563(3)	1.561(3)	-0.002(3)	P-O(-H)	1.562(3)	1.563(4)	0.001(4)
Pn1				Bzdmp			
Pt-Pt	2.9546(3)	2.9465(3)	-0.0081(3)	Pt-Pt	2.9203(2)	2.9184(2)	-0.0019(2)
Pt-P	2.3318(11)	2.3265(11)	-0.0053(11)	Pt-P	2.3360(8)	2.3327(9)	-0.0033(8)
P-O(-P)	1.630(3)	1.627(4)	-0.003(3)	P-O(-P)	1.638(3)	1.636(3)	-0.002(3)
P=O	1.522(3)	1.518(3)	-0.004(3)	P=O	1.522(3)	1.521(3)	-0.001(3)
P-O(-H)	1.565(3)	1.561(4)	-0.004(4)	P-O(-H)	1.578(3)	1.575(3)	-0.003(3)
Bzte1							
Pt-Pt	2.9726(4)	2.9599(6)	-0.0127(5)				
Pt-P	2.3374(13)	2.3289(14)	-0.0085(14)				
P-O(-P)	1.639(4)	1.628(6)	-0.011(5)				
P=O	1.538(4)	1.532(6)	-0.006(5)				
P-O(-H)	1.558(4)	1.553(5)	-0.005(5)				

The Pt-Pt and Pt-P bond distances become significantly shorter at light-on stage than those at light-off stage, and the differences are -0.0081(3) and -0.0053(11) Å for Pn1 and -0.0127(5) and -0.0085(13) Å for Bzte1, respectively. In contrast, the changes of the other bond distances are within the experimental error. The ratios of Δ(Pt-Pt) to Δ(Pt-P) in Pn1 and Bzte1, 1.53 and 1.49, are very close to each other.

The same comparison were adapted for the other compounds, Bu1 Bztbu and Bzdmp, and the shortening of the Pt-Pt and Pt-P bonds are in the range of -0.0019(2) to -0.0038(3) and -0.0019(12) to -0.0069(10) Å, respectively. The differences of P-O(-P) P=O and P-O(-H) bonds are in the range of -0.002(3) to -0.003(3), -0.001(3) to -0.006(4) and 0.001(4) to -0.003(3) Å, respectively.

From the combination of the EXAFS method with rapid-flow laser spectroscopy in an aqueous solution with glycerol, it was estimated that the $^3A_{2u}$ state undergoes a contraction in the Pt-Pt distance of 0.52 ± 0.13 Å and in the Pt-P distance of 0.047 ± 0.011 Å relative to the $^1A_{1g}$ ground state. The Pt-P contraction can be considered as the analogue to the predicted Ni-C contraction of the square-planar complex $Ni(CN)_4^{2-}$. [23,24] These results suggest that the excited Ptpop anion should have the same structure in each crystal although the concentrations of the excited molecules are different among the five crystals. The structural change at the excited stage is schematically drawn in Fig. 3.14.

3.3.6 The concentration of excited molecule in the crystal

It is important to estimate the concentration of the excited molecule in the crystal. However the structural change is too small to separate the ground state molecule and the excited state molecule by X-ray analysis.

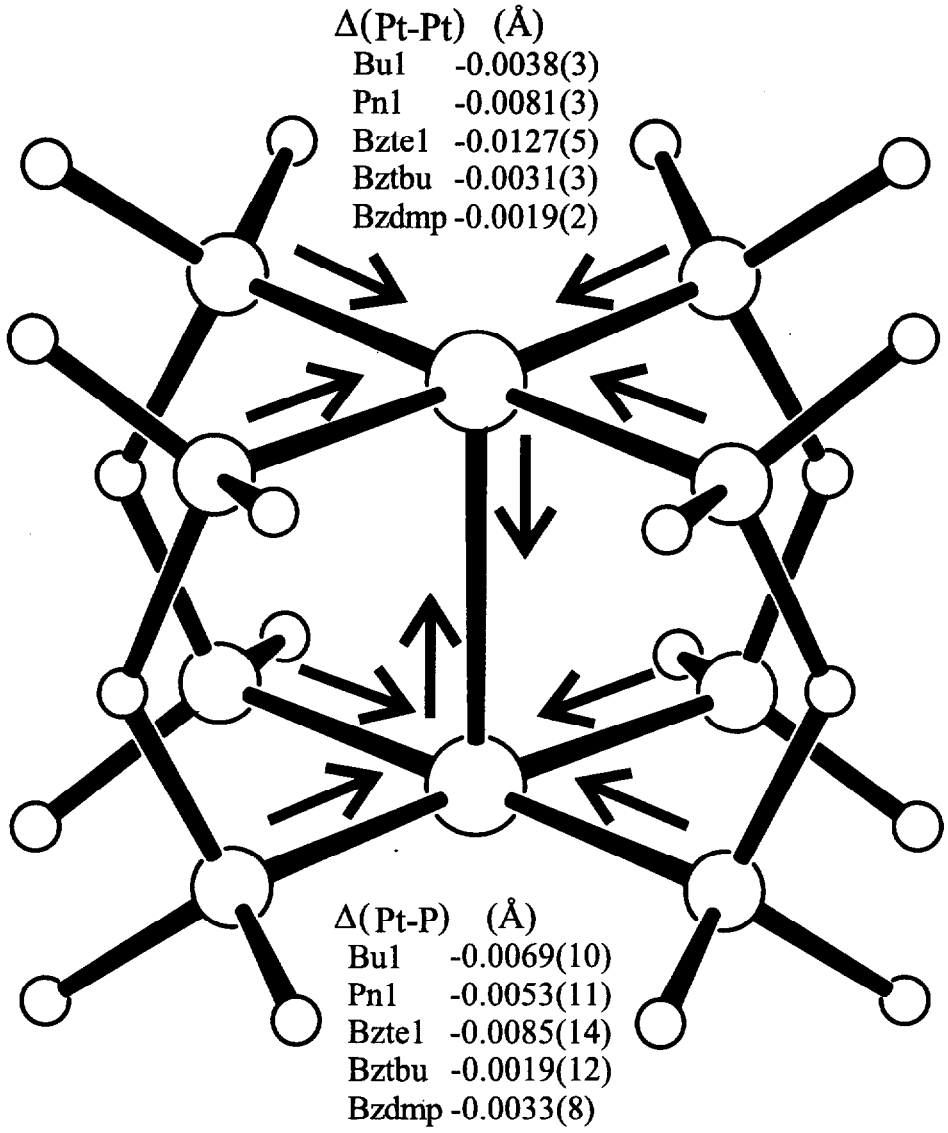


Fig. 3.14 A summary of the structural change of the Ptpop anions at photo-excited state.

Considering more simply, the rate of the Pt-Pt bond shortening to the estimated shortening by spectroscopy, 0.21 Å, [25] are summarized in Table 3.7 and the calculated value are in the range from 0.9 to 6.4 %. Although this estimation is very simple, the estimated value of Bu1 crystal, 1.80 %, corresponds with that derived from structure refinement by Ozawa et al., 1.4 % [4] and Coppens et al., 2.0 %. [3]

Considering the other point of view, if it is assumed that the concentration of the excited molecule in Bu1 is the same as that reported by Ozawa et al., 1.4 %, the shortening for Pt-Pt distance is estimate to be 0.27 Å (0.0038/1.4%). This is in agreement with the corresponding values 0.23 and 0.28 Å.

3.4 Summary

Eight crystals of five compounds containing $[Pt_2(Hpop)_2(pop)_2]^{2-}$ and $[Pt_2(pop)_4]^{4-}$ as an anion and tetrabutyl-, tetrapentyl-, benzyltriethyl-, benzyltributyl- or benzyldimethylphenyl-ammonium as a cation were prepared and their crystal structures were determined at low temperature by single crystal X-ray analysis. The five crystals were investigated the photo-excited structural change.

When each crystal was irradiated the excitation light, the unit-cell dimensions significantly contracted. Moreover the Pt-Pt and Pt-P bond distances were significantly shortened at light-on stage. This is due to the fact that the produced excited-state molecules and the ground-state molecules reach the equilibrium state and the contractions of the bond distances come from the structure of the excited molecule.

The concentration of the excited molecules was estimated 1-6 %. The

agreement of the amount of peak shift from the single crystal and the powder X-ray diffractions may indicate that the concentration of the excited-state molecules in the single crystal and powder sample is almost the same at the equilibrium state.

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Chapter 4

Time-resolved experiment of the photo-excitation process using MSGC

4.0 Abstract

In order to observe the photo-excitation process from the initiation of light irradiation to the equilibrium state, the time-resolved X-ray analysis using micro-strip gas chamber (MSGC) and synchrotron radiation was carried out at 173 K.

The position of a diffraction spot was continuously recorded with several cycles of the light-on and light-off stages. The peak positions at light-on and light-off stages were analyzed at an interval of 100 msec. The direction of the peak shift is consistent alternately with that reported by the powder X-ray measurement, i.e. the shift to higher 2θ angle at light-on stage and to lower 2θ at light-off stage. The peak shift didn't reach the equilibrium state for 20 sec just after the start and stop of the photo-irradiation.

Moreover, for a few seconds just after light-on and -off operations, the discontinuity of the averaged peak position was observed. This discontinuity reflected the early stage of the photo-excited process with many complicated factors.

4.1 Introduction

4.1.1 Time-resolved analysis of Ptpop compound

In chapter 3, the photo-excited structure of the Ptpop complex was discussed. During X-ray measurement, the excitation light was irradiated to the single crystal continuously. This method was intended to keep the molecules at the equilibrium state between excited-state and ground-state in the crystal. As the result, the contraction of cell-volume, Pt-Pt and Pt-P bonds were observed.

However the knowledge of the excitation process to the equilibrium state is also important to understand the mechanism of photo-excitation. In order to observe the photo-excitation process the time-resolved measurement was carried out. Because this process may be observed for very short time and X-ray intensity should be strong to measure the data rapidly and accurately, micro-strip gas chamber (MSGC) was developed and installed at SPring-8 BL44B2 beam line for this time-resolved X-ray measurement.

In this chapter, the time-resolved measurement of Ptpop compound using MSGC was carried out and the photo-excitation process of Ptpop compound was discussed.

4.1.2 Micro-Strip Gas Chamber (MSGC)

The detectors with the gas-amplification process are widely used for detection of γ-ray, X-ray, charged particle and neutrons. The micro-strip gas chamber (MSGC) was proposed as a new type of gas detector by A. Oed in 1988. [1] This detector was anticipated as a new generation of detector with fine position resolution in comparison with wire-type gas chamber. Many groups are developing the various types of MSGC. [2]

Prof. Tanimori group developed MSGC as a X-ray detector. The structure

of MSGC and measured image were shown in Fig. 4.1. [3,4,5,6,7] The detector size was 10 cm x 10 cm. The anode and cathode stripes are printed on the polyimide substrate with 200 μm pitch. The space between the substrate and the drift plane placed at 3~10 mm above the substrate, was filled with noble gas (e.g. argon or xenon) mixed with 20~30 % ethane gas as quencher.

The features of MSGC were; [6]

(i) Real-time-photon-counting type detector.

(ii) Fine position resolution of <100 μm.

(iii) High rate capacity for incident X-ray of 10^7 counts s^{-1} mm^{-2}.

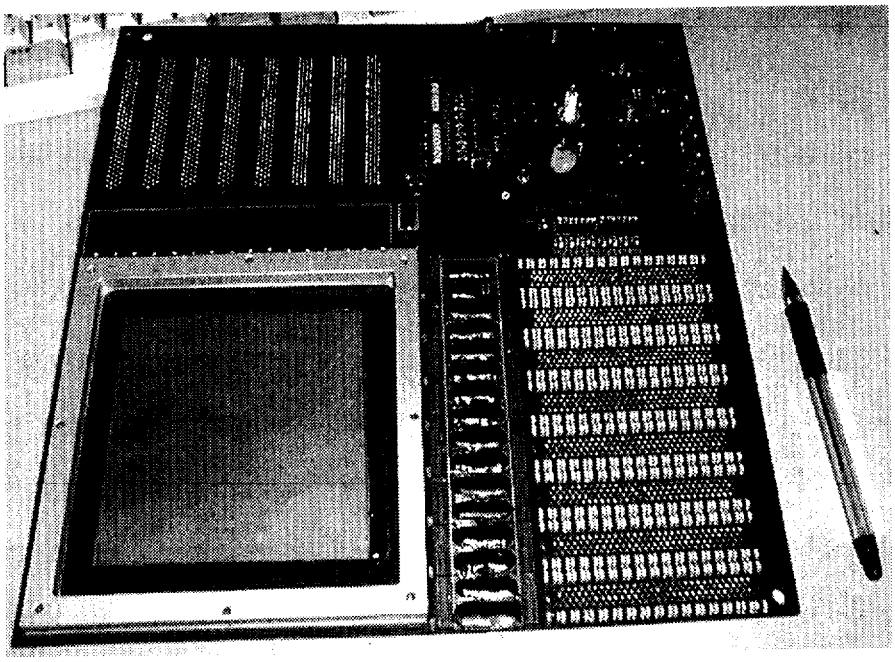
(iv) Fine timing resolution of ~50 ns.

The fine position resolution makes it possible to determine the cell parameters and cell volume correctly, and high rate capacity allows us to use bright X-ray like synchrotron radiation and to collect the weak diffraction intensity accurately. The real-time-photon-counting and the fine resolution are important features for time-resolved measurement, since MSGC enables to obtain the correct ω-angles from the rotation speed and the internal timer and constructs the reciprocal space directly. Moreover MSGC enables watching the measured diffraction data like a movie, because each photon is recorded with the time information.

Furthermore, since the integration time are unnecessary, differing from IP and CCD detectors, MSGC can measure the X-ray diffraction in a short time with continuous rotation of the crystal (continuous rotation method) if the diffraction intensity is significant large.

Generally, more than several tens of thousands of events are necessary to construct two-dimensional images, and a few tens of images are required for a second to obtain the image as a movie. Thus, more than 10^6 counts s^{-1}

(a)



(b)

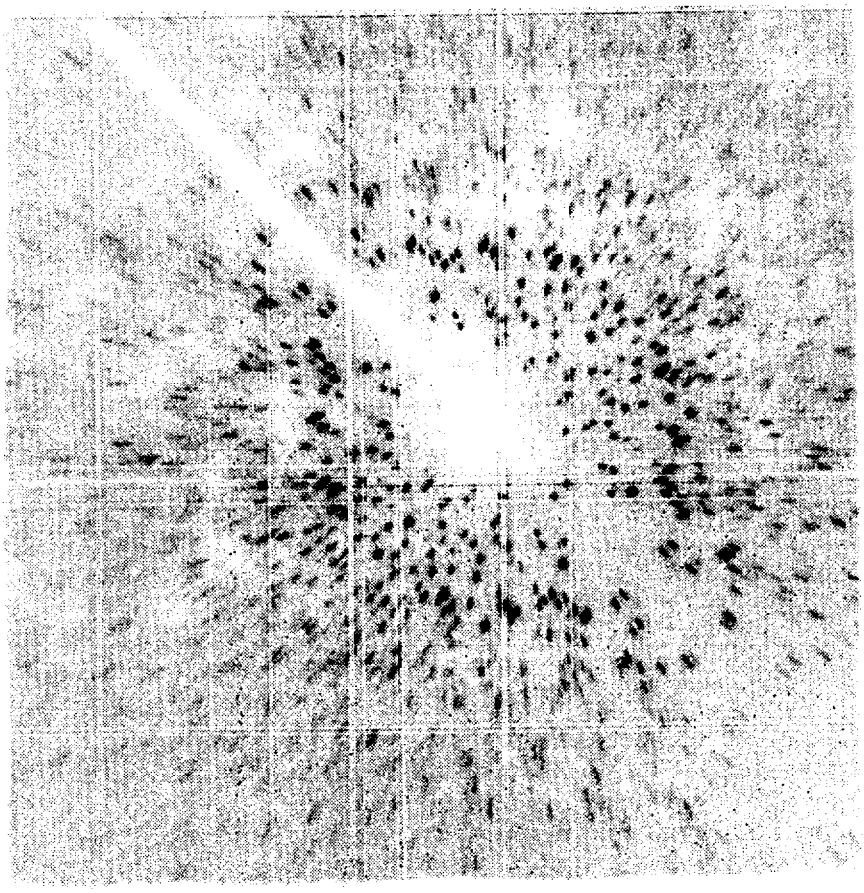


Fig. 4.1
(a)·The main board of MSGC. Detector size was 10 x 10 cm.
(b)Measured diffraction image of ammonium bitartrate crystal ($C_4H_9NO_6$; ABT) by the continuous rotation method. Measurement time for this image took 28 sec and rotation speed was 4 sec/rotation.

capacity is required for real-time X-ray imaging analysis. This detector can obtain the data at up to 10^7 counts s^{-1}. The fine positional and timing resolution and large dynamic range are hopeful characteristics to apply to the time-resolved analysis.

Before the time-resolved analysis, the rapid single crystal X-ray measurements using MSGC were examined for the crystals of cytidine ($C_9H_{13}N_3O_5$) and ammonium bitartrate ($C_4H_9NO_6$; ABT). The both organic compounds were well known as the standard crystals for X-ray measurement. [8] Although the oscillation method was used as the common strategy for the data collection of the detector with imaging plate and CCD, the continuous rotation method was used for the rapid measurement using MSGC.

In laboratory system, the data collection was carried out using the shield-tube (Mo$K\alpha$) at room temperature. Total measurement time was 10 min for cytidine and 17 sec for ABT and R-factor were 6.7 % (4361 reflections) and 9.2 % (1406 reflections), respectively. In SPring-8 BL46XU beam line with inserted undulator, the molecular structure of ABT was obtained by means of 250 msec measurement (one crystal rotation). The R-factor was 14.6 % (2588 reflections).

Therefore MSGC was anticipated to be the best detector to observe the photo-excitation process of Ptpop compound using synchrotron radiation because of the fine positional and time resolution and large dynamic range.

4.2 Experiment

4.2.1 Time-resolved X-ray diffraction measurement using MSGC at SPring-8

Ideally it is the best way for direct observation of photo-excitation process to collect the many sets of all diffraction intensities in a short period at light-on and light-off stages and to analyze the three-dimensional structural change with time. Although the structure analysis of ABT in 250 msec succeeded as described in chapter 4.1.2, the number of photons was insufficient for structure analysis with high structural accuracy. The low accuracy is due to the weak intensity and low redundancy of the measured diffraction peaks even if the synchrotron radiation was used.

It is needless to say that it is very important to determine the molecular structure in a short time with high accuracy in order to discuss the relation of the photo-excitation process and molecular structure, e.g. Pt-Pt and Pt-P distances. To this purpose, many photons should be collected enough to compare the small change of structures, however it is difficult to do the time-resolved structure analysis at present stage.

Fortunately the accuracy of the diffraction-peak position was the same level as the other detector like CCD and imaging plate. Therefore in order to observe the photo-excitation process, the shift of a diffraction peak was measured by neither the oscillation nor continuous-rotation crystal method but by the still-photograph method. It is possible to collect enough photons by still-photograph method. Since the position of diffraction peak reflected the cell lattice and cell volume, the movement of the diffraction peak also reflected the change of the cell lattice and cell volume. Therefore the photo-excitation process in the crystal can be observed indirectly.

Time-resolved measurement was carried out at SPring-8 BL44B2 beam line. This beam line is originally dedicated to macromolecular crystallography in white (Laue) and monochromatic X-ray mode, and XAFS of the diluted biological systems. Synchrotron radiation was

generated by bending magnet and monochromatized with double monochromator for time-resolved measurement. In order to strengthen intensity of the high angle diffraction, wavelength of X-ray was selected 1.54 Å. At this wavelength, although the absorption of X-ray by the diplatinum complex crystal is not so small (Fig. 3.2), it would be enough to observe the shift of the diffraction peak.

MSGC was set at about $2\theta = 30°$ and the distance from crystal to detector was about 60 cm. For detection of the timing of light-on and light-off, the photo-sensor (Akizuki-denshi illuminometer kit) was set and the status whether the light was on or off is recorded in the measurement data.

The Pn1 crystal, whose size is 140 x 80 x 30 μm, was selected and mounted on a glass capillary with epoxy glue. The sample was cooled to 173 K with cold-nitrogen-gas during the measurement. The measurement was not oscillation method but still-photograph method.

The condition of photo-irradiation was the same as the laboratory system described before. The status of light-off and light-on were controlled by the opening and closing a shutter, controlled by the computer every 20 second. The internal timer cycle of MSGC was 256 μsec (st4). Total measurement time was 224 seconds and total events, the number of counted photons, were 6953627 events. The number of events per 1 second was over 30000 events.

4.2.2 Data processing

For data processing, new software programs were made, which includes the converter of the measured binary data into ASCII text data, image viewer, generator of peak profile and powder X-ray pattern, calculator of

average peak center and 2θ angle from MSGC X-Y position, merging from several cycle data to one cycle data and so on.

At the first step of the data processing, the measured binary data, recording the X-Y position, light on/off status and the time information, were converted to ASCII text data. In order to know the 2θ angle of each diffraction peak, the simulated powder pattern of Si sample was generated and fitting to the experimental powder pattern. The 2θ angle of the measured diffraction peak was 31.7°. The measurement images are shown in Figs. 4.2(a) and (b) and intensity distribution map and peak profile of the diffraction peak are shown in Figs. 4.2(c) and (d), respectively.

The measured data were recorded as the data stream with several on-off cycles (OFF1→ON1→OFF2→ON2→OFF3→...). Thus, several cycles of data were merged into one cycle of data in order to increase the number of event and accuracy of diffraction position. Two merged data were made, because the interval time from light-off to light-on stages (or from light-on to light-off stages) was slightly deviated from the preset time although the computer controlled the shutter. Therefore one data set was merged of the point from light-off to light-on stage (OFF→ON), and another data set was merged from light-on to light-off stage (ON→OFF), shown in Fig. 4.3(a).

To determine the area of the diffraction peak, the peak profile was generated (Fig. 4.3(b)). In the determined area, the averaged peak center was calculated in 100 msec and 500 msec time intervals using the merged on-off cycle data (OFF→ON and ON→OFF) and 1000 msec time interval using non-merged data, respectively (Fig. 4.3(c)). For 100 msec averaged data, about 6000 events per one point were used to calculate the peak center and 30000 and 10000 events was used for 500 msec and 1000 msec averaged data, respectively.

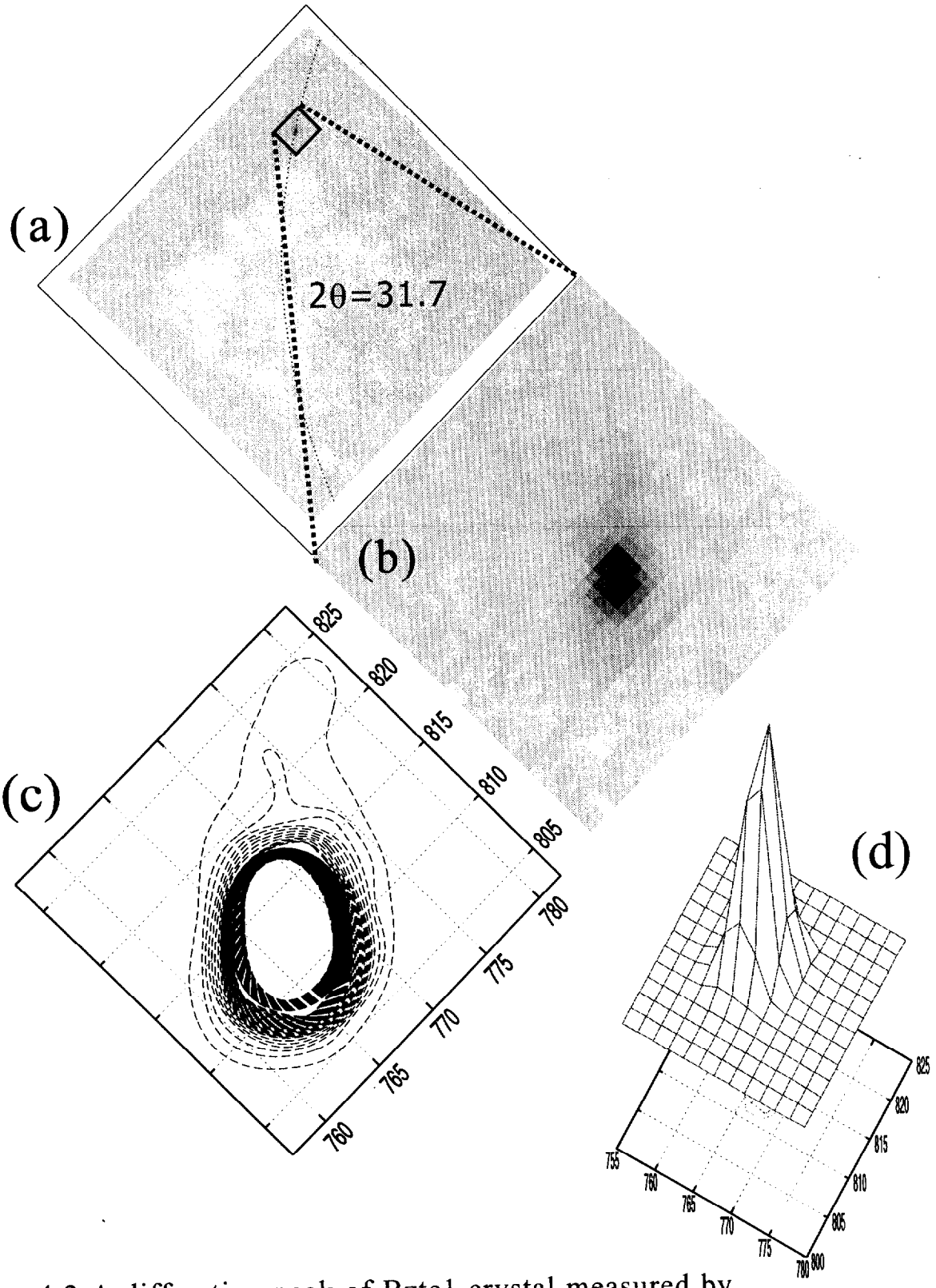


Fig. 4.2 A diffraction peak of Bzte1 crystal measured by MSGC:
(a)Measured image of MSGC, diffraction angle was determined by comparison with the powder pattern of Si.
(b)Measured diffraction peak.
(c)The intensity distribution map of measured diffraction peak.
(d)Peak profile of measured diffraction peak.

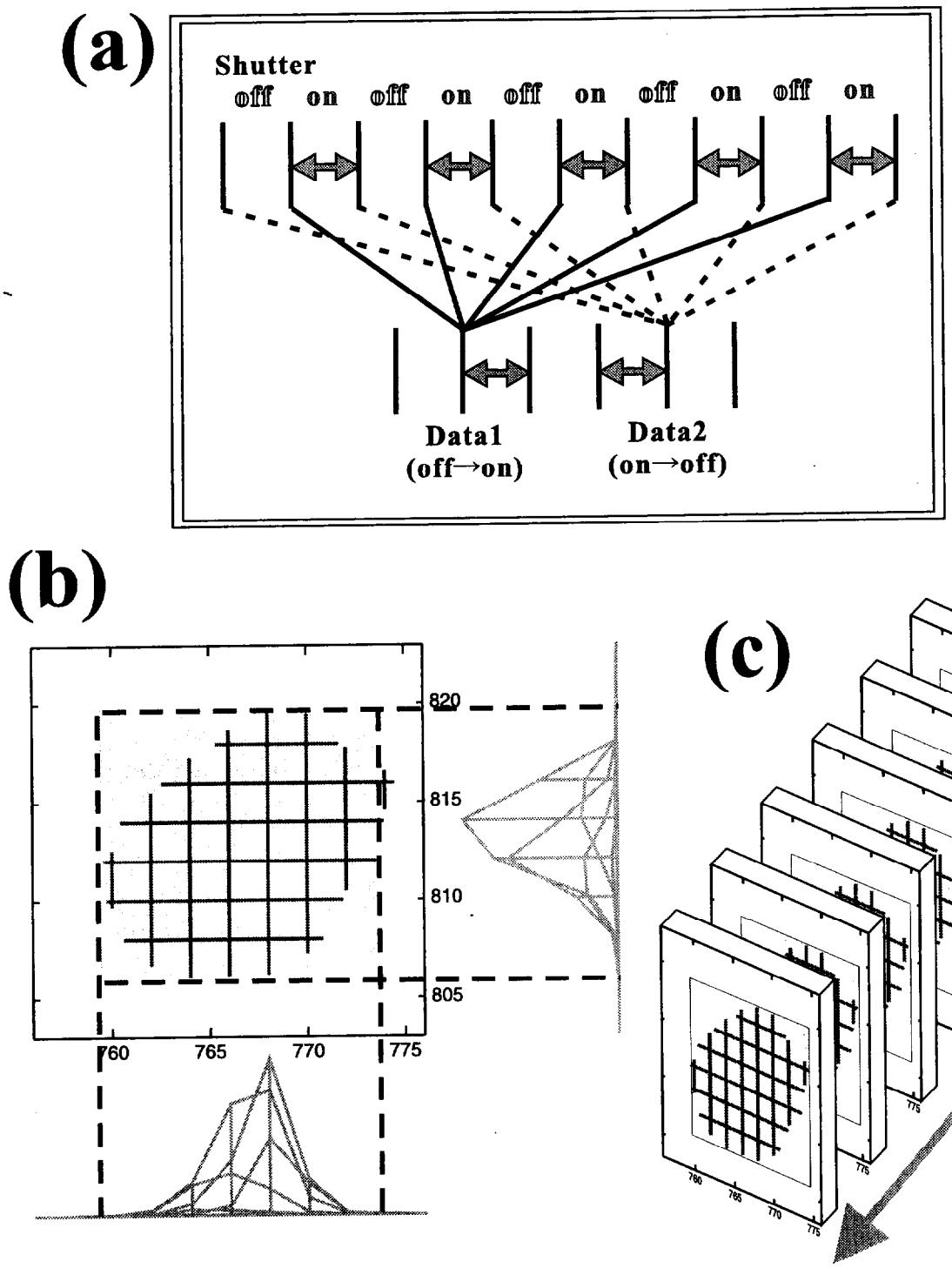


Fig. 4.3 The conceptual scheme of the data processing:
(a)Merge the measured data into the two data; merging at the point from light-off to light-on stage and from light-on to light-off stage.
(b)Determine the area of the diffraction peak.
(c)Calculate the average peak center.

At last each averaged data was three-dimensional data, included X-Y position and time. In order to make the two-dimensional plot, X-Y position was converted into the 2θ angle.

4.3 Results and discussions

The averaged position of the diffraction spot with 1000 msec time-resolution was plotted as shown in Fig. 4.4. From this figure, the point was found to shift with time. The plot of the peak position, averaged in a 100 msec interval using the merged data, shows the tendency clearly in Fig. 4.5. The left side figure is the plot using the merged data from light-off to light-on stage (OFF→ON), and the right side one is the data from light-on to light-off stage (ON→OFF).

It is clearly found that the diffraction peak shifted with time continuously just after the photo-irradiation is started or stopped. Furthermore the direction of shift is the opposite to each other, i.e. shift to the higher 2θ angle at light-on stage and shift to lower 2θ angle at light-off stage, respectively. The direction of the peak shift is consistent with that of the powder X-ray diffraction. Unfortunately both of the peak shifts are not converged after 20 sec. This means that the molecules at the ground state and the excited state didn't reach the equilibrium state within 20 seconds. This also indicates that the excited state molecules remain in the crystal after photo-irradiation was stopped. Although the extra time may be necessary to converge the shift of diffraction peak, these continuous shifts of diffraction peak reflected the photo-excitation process.

In order to see the further details, the averaged position with 500 msec intervals using the merged data is shown in Fig. 4.6. Figure 4.6(a) is the

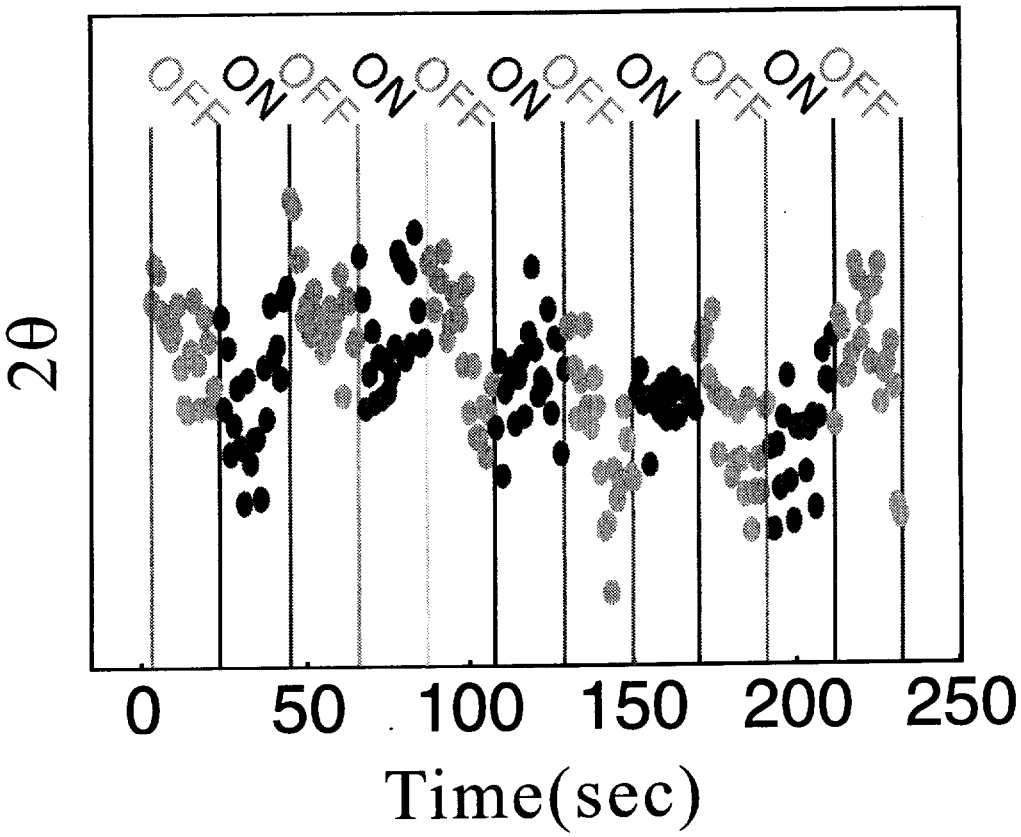


Fig. 4.4 The averaged peak center with 1000 msec time resolutions used no merged data. About 10000 events were used for the calculation of peak center.

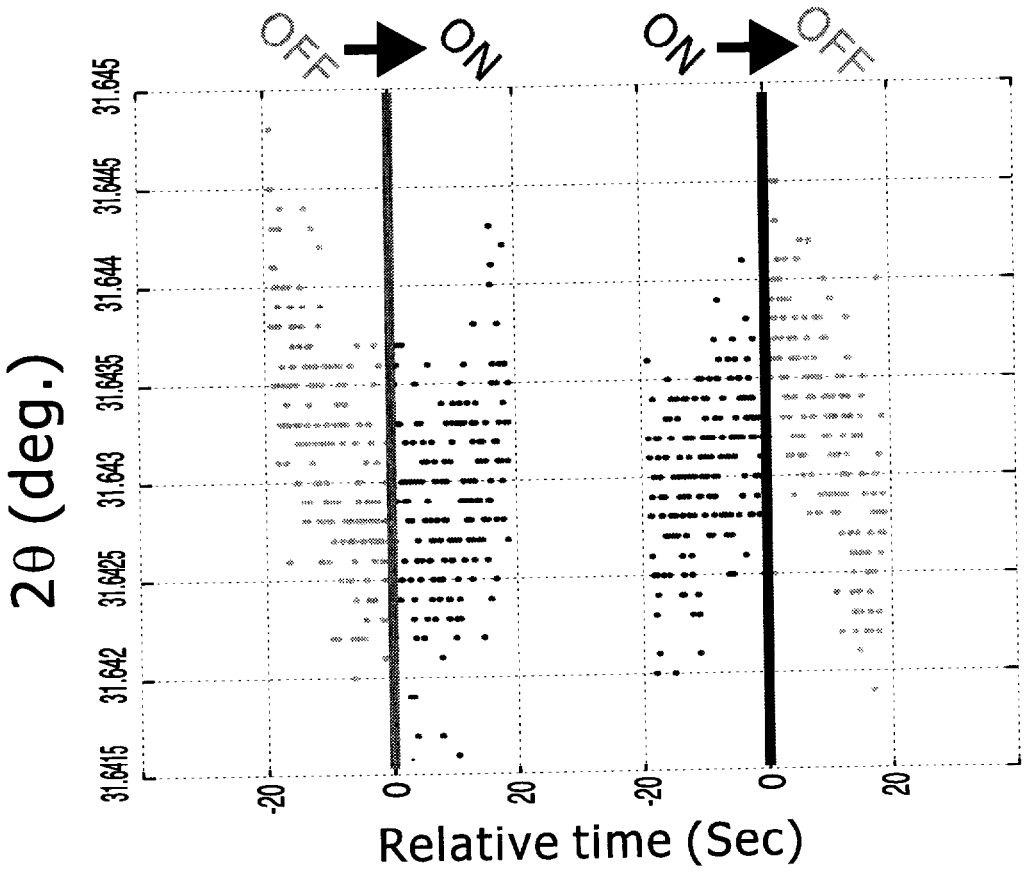


Fig. 4.5 The averaged peak center with 100 msec time resolutions. About 6000 events were used for the calculation of peak center.
(Left side) the positional change from light-off to light-on.
(Right side) the positional change from light-on to light-off.

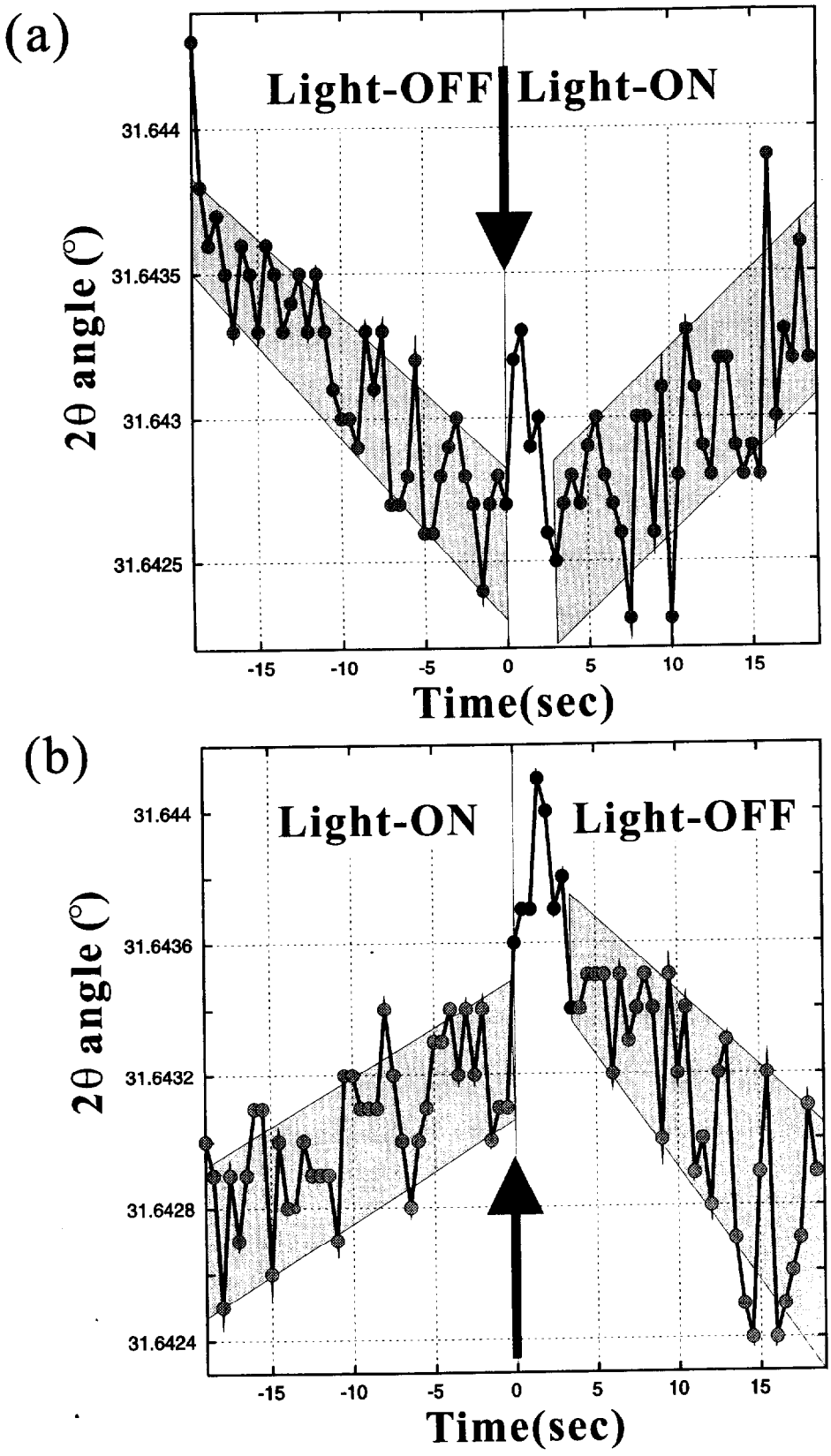


Fig. 4.6 The averaged peak center with 500 msec time resolutions. About 30000 events were used for the calculation of peak center.
(a) The positional change from light-off to light-on stage.
(b) The positional change from light-on to light-off stage.

plots using the merged data from light-off to light-on stage, and Fig. 4.6(b) is for the data from light-on to light-off stage. For each plot, discontinuous peak shift was observed at the boundary between light-on and light-off stages.

When the photo-irradiation began, the diffraction peak shifted to higher 2θ for about 1 second. Then the diffraction peak shifted to lower 2θ for a few seconds, and shifted to higher 2θ again. When the photo-irradiation was stopped, similarly, the diffraction peak shifted to higher 2θ for about 1.5 second, and then shifted to lower 2θ gradually.

One may consider this discontinuous shift was the experimental error for small change of the peak shift. However the additional lines indicate that the tendency of peak shift for a few seconds after the start or stop of irradiation is clearly different from that of the subsequent seconds. Thus, it was concluded this discontinuous shifts of the diffraction peak also reflected the photo-excitation process of the moments when the photo-irradiation was started and stopped.

The explanation of these discontinuous shifts was seemed to be difficult. However this behavior of diffraction peak has complicated relation with the excitation from the ground state to the excited state by photo-absorption, the transition from the excited state to the ground state with luminescence or phosphorescence, the heat generation in crystal by photo-absorption and the cooling by cooled nitrogen gas. Although the factor may be much more, the interaction of each factors make complicate the early stage of the photo-excitation process.

In this experiment, since only one diffraction peak was measured, it is difficult to know the detail of the photo-excitation process in the crystal. However the two possibilities of excitation process in the crystal can be

proposed because the time to form the equilibrium structure isn't so quickly. The first possibility is that the concentration of excited Ptpop molecule reaches the equilibrium state in the short time after the photo-irradiation, while the crystal structure change into the equilibrium structure slowly. The second possibility is that the concentration of excited Ptpop molecule increase with the crystal structure change.

The author support the former excitation process, because the time-resolved experiment using the stroboscopic technique observed the excited-state molecule with the same concentration as that observed at equilibrium state. This quick increase of the concentration may enable us to explain the discontinuous change of the diffraction peak shift.

4.4 Summary

The time-resolved X-ray analysis using the combination of micro-strip gas chamber (MSGC) and synchrotron radiation was carried out to make clear the photo-excitation process of the Ptpop crystal.

The continuous shift of a diffraction spot by photo-irradiation was observed, which reflected the photo-excitation process before reaching the equilibrium state.

For a few seconds just after the light-on and light-off stages, the discontinuous shifts of the diffraction spot were found, which indicates the complicated photo-excitation process at the early stages.

These results indicate that the analysis of the continuous change of cell parameter and cell volume make possible if the positions of all diffraction peaks could be measured.

The two possibilities of the photo-excitation process can be proposed. If

the three dimensional structure change could be analyzed in the short time, we can make clear the photo-excitation process.

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Chapter 5

General discussion and conclusion

In this thesis, the structural change of the photo-excited Ptpop complex in the crystal is investigated by the single crystal X-ray analysis and the time-resolved X-ray analysis.

In chapter 1, the background of this research is described.

In chapter 2, synthetic method of $[Pt_2(pop)_4]^{4-}$ and $[Pt_2(Hpop)_2(pop)_2]^{2-}$ complexes with five kinds of ammonium cations, and the conditions of light-irradiation are described.

In chapter 3, the three-dimensional structural changes of Ptpop complexes are analyzed using the conventional single crystal X-ray analysis. The contractions of the cell volume and Pt-Pt and Pt-P distances are observed at the photo-excited state. The powder diffraction peak shift can be clearly explained by this cell-volume contraction. This suggests that the crystal structure reaches an equilibrium composed of the ground and excited-states. The concentration of the excited state molecule estimated 1-6 % in the crystal.

These results provide the evidence that the conventional single crystal X-ray analysis, using the X-ray generated by the rotating anode and the Xe lamp for excitation, enable us to analyze not only the photo-excited molecules but also the other reversible reactions occurred in the crystal with small change.

In chapter 4, the time-resolved analysis of the photo-excitation process from the initiation of excitation to the equilibrium state is investigated using the combination of MSGC and synchrotron radiation. The averaged position of one diffraction peak shifts to the lower 2θ angle and to the higher 2θ angle at the light-off and light-on stages, respectively. This peak shift shows the change of the unit cell, which reflects indirectly the excitation process in the crystal. The peak shift doesn't finish in the

measurement time. This may indicate the molecules at the ground and excited states don't form the equilibrium state so quickly in the crystal, even if some molecules are already excited. The discontinuous changes, observed at the early stages of light-on and light-off, may indicate more complicate excitation process at the stages.

In this thesis, the structures of the ground and excited states are observed directly but individually, while the excitation process between them is observed continuously but indirectly. If the improvement will achieve enough to collect many diffraction data sets in several seconds, we can watch this structural change directly and continuously. This continuous observation of the reaction process may enable us to discover a lot of new features of the chemical reaction as well as the structures of unstable and metastable species produced in the fast and slow crystalline state reaction.

Through this thesis and the subsequent progress of equipments, the author hopes that the "true" time-resolved structure analysis becomes the conventional method of X-ray analysis in near future.

Appendix

= Crystallographic data =

Bu2, Pn2, Btea2 crystals

Bu1 crystal light-off & on stages
Pn1 crystal light-off & on stages
Bzte1 crystal light-off & on stages
Bztbu1 crystal light-off & on stages
Bzdmp1 crystal light-off & on stages
(Measured at laboratory system)

Bzte1 crystal light-off & on stages
(Measured at SPring-8 BL02B1 beam line)

Crystallographic data of Bu2 crystal measured at laboratory system

Table 1. Crystal data and structure refinement for bu2.

Identification code	ptbu2	
Empirical formula	C33 H86 N2 O21 P8 Pt2	
Formula weight	1484.98	
Temperature	103(2) K	
Wavelength	0.71069 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.4870(3) Å	α= 90°.
	b = 20.3145(7) Å	β= 90°.
	c = 27.7153(13) Å	γ= 90°.
Volume	5341.4(4) Å^3	
Z	4	
Density (calculated)	1.847 Mg/m^3	
Absorption coefficient	5.544 mm^{-1}	
F(000)	2968	
Crystal size	0.40 x 0.06 x 0.06 mm^3	
Theta range for data collection	2.27 to 27.48°.	
Index ranges	-11<=h<=12, -26<=k<=25, -35<=l<=35	
Reflections collected	35286	
Independent reflections	11038 [Rint = 0.0479]	
Completeness to θ = 27.48°	93.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.1928 and 0.5872	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11038 / 0 / 593	
Goodness-of-fit on F^2	1.133	
Final R indices [I>2σ(I)]	R1 = 0.0350, wR2 = 0.0778	
R indices (all data)	R1 = 0.0385, wR2 = 0.0796	
Absolute structure parameter	0.006(6)	
Largest diff. peak and hole	1.073 and -1.368 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bu2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
OM	90(20)	-677(11)	5242(7)	199(9)
CM	20(50)	-1350(20)	4968(16)	320(30)
Pt(1)	2896(1)	1139(1)	3772(1)	15(1)
Pt(2)	1452(1)	275(1)	3088(1)	16(1)
P(1)	4993(2)	697(1)	3505(1)	16(1)
P(2)	3545(2)	-177(1)	2821(1)	20(1)
P(3)	2955(2)	1998(1)	3217(1)	19(1)
P(4)	1614(2)	1106(1)	2516(1)	19(1)
P(5)	792(2)	1602(1)	4024(1)	19(1)
P(6)	-649(2)	704(1)	3364(1)	17(1)
P(7)	2701(2)	316(1)	4345(1)	19(1)
P(8)	1428(2)	-578(1)	3641(1)	20(1)
O(1)	4766(5)	22(2)	3205(2)	19(1)
O(2)	1912(6)	1813(2)	2772(2)	22(1)
O(3)	-409(5)	1404(3)	3635(2)	20(1)
O(4)	2504(5)	-392(2)	4079(2)	20(1)
O(5)	5939(5)	438(3)	3927(2)	22(1)
O(6)	5897(5)	1141(3)	3181(2)	22(1)
O(7)	3627(6)	-937(3)	2820(2)	27(1)
O(8)	4081(6)	41(3)	2326(2)	28(1)
O(9)	4393(6)	2143(3)	2964(2)	26(1)
O(10)	2430(6)	2660(2)	3396(2)	22(1)
O(11)	2718(6)	1025(3)	2130(2)	25(1)
O(12)	199(5)	1253(3)	2238(2)	22(1)
O(13)	733(6)	2367(3)	4025(2)	26(1)
O(14)	221(6)	1384(3)	4517(2)	27(1)
O(15)	-1624(5)	922(3)	2930(2)	21(1)
O(16)	-1499(5)	283(3)	3714(2)	22(1)
O(17)	1534(6)	374(3)	4714(2)	28(1)
O(18)	-6(6)	-714(3)	3901(2)	27(1)
O(19)	1965(6)	-1238(3)	3462(2)	30(1)
O(20)	4070(6)	181(3)	4647(2)	28(1)
N(1)	1493(8)	1328(3)	6091(2)	28(1)
N(2)	3343(8)	2851(4)	1449(3)	33(2)
C(1)	1983(10)	1509(4)	6602(3)	30(2)
C(2)	3509(12)	1717(6)	6641(3)	48(3)
C(3)	3937(10)	1831(5)	7166(3)	38(2)
C(4)	3097(13)	2341(5)	7414(4)	50(3)
C(5)	2328(10)	761(4)	5885(3)	29(2)
C(6)	2140(11)	108(4)	6146(4)	42(2)
C(7)	3219(10)	-393(5)	5966(3)	42(2)
C(8)	4655(12)	-226(6)	6206(6)	70(4)
C(9)	-53(8)	1149(4)	6134(3)	26(2)
C(10)	-747(11)	940(5)	5666(3)	38(2)
C(11)	-2275(11)	769(6)	5754(3)	44(2)
C(12)	-2938(14)	497(7)	5297(4)	64(4)
C(13)	1697(10)	1898(4)	5749(3)	29(2)
C(14)	1086(12)	2552(5)	5899(3)	42(2)
C(15)	1117(11)	3034(5)	5470(3)	42(2)
C(16)	-127(11)	2946(5)	5158(4)	45(2)
C(17)	2039(10)	2400(5)	1464(3)	39(2)
C(18)	731(12)	2678(5)	1249(5)	55(3)
C(19)	-340(11)	2133(5)	1125(5)	50(3)
C(20)	-1599(12)	2357(5)	870(4)	50(3)
C(21)	4523(10)	2513(4)	1717(3)	32(2)
C(22)	5007(10)	1867(5)	1489(3)	35(2)
C(23)	6171(10)	1564(5)	1794(4)	39(2)
C(24)	6652(12)	916(5)	1592(4)	53(3)
C(25)	3705(12)	2989(5)	928(3)	43(2)

C(26)	5024(11)	3366(6)	832(4)	46(3)
C(27)	5314(15)	3439(8)	297(5)	71(4)
C(28)	4048(15)	3841(7)	57(5)	70(4)
C(29)	3004(11)	3501(4)	1680(3)	36(2)
C(30)	2729(12)	3500(5)	2206(4)	42(2)
C(31)	2088(12)	4163(5)	2356(3)	42(2)
C(32)	2025(14)	4290(5)	2886(4)	53(3)

Table 3. Bond lengths [Å] and angles [°] for bu2.

OM-CM	1.57(4)	P(6)-O(15)	1.581(5)	C(14)-C(15)	1.540(13)
Pt(1)-P(1)	2.3054(19)	P(6)-O(3)	1.625(5)	C(15)-C(16)	1.475(15)
Pt(1)-P(7)	2.3137(19)	P(7)-O(17)	1.512(6)	C(17)-C(18)	1.488(14)
Pt(1)-P(5)	2.3141(19)	P(7)-O(20)	1.569(6)	C(18)-C(19)	1.542(14)
Pt(1)-P(3)	2.3269(19)	P(7)-O(4)	1.626(5)	C(19)-C(20)	1.460(15)
Pt(1)-Pt(2)	2.9233(4)	P(8)-O(19)	1.517(6)	C(21)-C(22)	1.527(12)
Pt(2)-P(6)	2.3052(19)	P(8)-O(18)	1.563(6)	C(22)-C(23)	1.521(13)
Pt(2)-P(2)	2.310(2)	P(8)-O(4)	1.630(5)	C(23)-C(24)	1.502(14)
Pt(2)-P(8)	2.3144(19)	N(1)-C(13)	1.508(9)	C(25)-C(26)	1.492(14)
Pt(2)-P(4)	2.3206(19)	N(1)-C(5)	1.510(10)	C(26)-C(27)	1.516(15)
P(1)-O(6)	1.536(5)	N(1)-C(9)	1.516(11)	C(27)-C(28)	1.598(19)
P(1)-O(5)	1.565(5)	N(1)-C(1)	1.535(10)	C(29)-C(30)	1.481(12)
P(1)-O(1)	1.617(5)	N(2)-C(29)	1.503(11)	C(30)-C(31)	1.534(13)
P(2)-O(8)	1.529(6)	N(2)-C(21)	1.509(11)	C(31)-C(32)	1.494(13)
P(2)-O(7)	1.546(5)	N(2)-C(25)	1.509(11)		
P(2)-O(1)	1.624(5)	N(2)-C(17)	1.540(12)	P(1)-Pt(1)-P(7)	90.42(7)
P(3)-O(10)	1.519(5)	C(1)-C(2)	1.512(13)	P(1)-Pt(1)-P(5)	178.51(7)
P(3)-O(9)	1.563(6)	C(2)-C(3)	1.528(12)	P(7)-Pt(1)-P(5)	91.07(7)
P(3)-O(2)	1.624(5)	C(3)-C(4)	1.477(14)	P(1)-Pt(1)-P(3)	93.38(7)
P(4)-O(11)	1.506(5)	C(5)-C(6)	1.521(12)	P(7)-Pt(1)-P(3)	176.19(7)
P(4)-O(12)	1.577(5)	C(6)-C(7)	1.527(13)	P(5)-Pt(1)-P(3)	85.13(7)
P(4)-O(2)	1.628(5)	C(7)-C(8)	1.554(15)	P(1)-Pt(1)-Pt(2)	87.85(5)
P(5)-O(14)	1.536(6)	C(9)-C(10)	1.517(11)	P(7)-Pt(1)-Pt(2)	88.51(5)
P(5)-O(13)	1.554(6)	C(10)-C(11)	1.510(13)	P(5)-Pt(1)-Pt(2)	92.05(5)
P(5)-O(3)	1.619(5)	C(11)-C(12)	1.518(14)	P(3)-Pt(1)-Pt(2)	91.84(5)
P(6)-O(16)	1.523(5)	C(13)-C(14)	1.507(12)	P(6)-Pt(2)-P(2)	178.66(7)

P(6)-Pt(2)-P(8)	93.13(7)	O(14)-P(5)-O(13)	106.0(3)	C(9)-N(1)-C(1)	106.1(6)
P(2)-Pt(2)-P(8)	85.58(7)	O(14)-P(5)-O(3)	105.8(3)	C(29)-N(2)-C(21)	110.3(7)
P(6)-Pt(2)-P(4)	90.53(7)	O(13)-P(5)-O(3)	102.9(3)	C(29)-N(2)-C(25)	107.1(7)
P(2)-Pt(2)-P(4)	90.76(7)	O(14)-P(5)-Pt(1)	117.1(2)	C(21)-N(2)-C(25)	112.7(8)
P(8)-Pt(2)-P(4)	176.34(7)	O(13)-P(5)-Pt(1)	116.0(2)	C(29)-N(2)-C(17)	109.8(8)
P(6)-Pt(2)-Pt(1)	87.90(5)	O(3)-P(5)-Pt(1)	107.8(2)	C(21)-N(2)-C(17)	108.2(7)
P(2)-Pt(2)-Pt(1)	92.51(5)	O(16)-P(6)-O(15)	109.4(3)	C(25)-N(2)-C(17)	108.6(7)
P(8)-Pt(2)-Pt(1)	91.43(5)	O(16)-P(6)-O(3)	105.7(3)	C(2)-C(1)-N(1)	114.9(7)
P(4)-Pt(2)-Pt(1)	88.61(5)	O(15)-P(6)-O(3)	100.8(3)	C(1)-C(2)-C(3)	111.3(8)
O(6)-P(1)-O(5)	108.4(3)	O(16)-P(6)-Pt(2)	117.2(2)	C(4)-C(3)-C(2)	114.0(9)
O(6)-P(1)-O(1)	105.8(3)	O(15)-P(6)-Pt(2)	111.1(2)	N(1)-C(5)-C(6)	115.1(7)
O(5)-P(1)-O(1)	100.2(3)	O(3)-P(6)-Pt(2)	111.3(2)	C(5)-C(6)-C(7)	110.2(7)
O(6)-P(1)-Pt(1)	116.1(2)	O(17)-P(7)-O(20)	105.0(3)	C(6)-C(7)-C(8)	107.6(9)
O(5)-P(1)-Pt(1)	112.7(2)	O(17)-P(7)-O(4)	107.0(3)	N(1)-C(9)-C(10)	114.8(6)
O(1)-P(1)-Pt(1)	112.3(2)	O(20)-P(7)-O(4)	100.6(3)	C(11)-C(10)-C(9)	110.0(7)
O(8)-P(2)-O(7)	105.7(3)	O(17)-P(7)-Pt(1)	117.8(2)	C(10)-C(11)-C(12)	110.3(9)
O(8)-P(2)-O(1)	106.2(3)	O(20)-P(7)-Pt(1)	115.2(2)	C(14)-C(13)-N(1)	117.0(6)
O(7)-P(2)-O(1)	102.4(3)	O(4)-P(7)-Pt(1)	109.66(19)	C(13)-C(14)-C(15)	109.9(7)
O(8)-P(2)-Pt(2)	117.3(2)	O(19)-P(8)-O(18)	106.7(3)	C(16)-C(15)-C(14)	111.2(9)
O(7)-P(2)-Pt(2)	116.1(2)	O(19)-P(8)-O(4)	103.8(3)	C(18)-C(17)-N(2)	115.6(8)
O(1)-P(2)-Pt(2)	107.69(19)	O(18)-P(8)-O(4)	104.1(3)	C(17)-C(18)-C(19)	111.5(8)
O(10)-P(3)-O(9)	105.4(3)	O(19)-P(8)-Pt(2)	116.2(2)	C(20)-C(19)-C(18)	115.0(9)
O(10)-P(3)-O(2)	104.6(3)	O(18)-P(8)-Pt(2)	116.4(2)	N(2)-C(21)-C(22)	114.2(7)
O(9)-P(3)-O(2)	103.6(3)	O(4)-P(8)-Pt(2)	108.2(2)	C(23)-C(22)-C(21)	109.7(8)
O(10)-P(3)-Pt(1)	116.1(2)	P(1)-O(1)-P(2)	130.0(3)	C(24)-C(23)-C(22)	111.5(9)
O(9)-P(3)-Pt(1)	117.4(2)	P(3)-O(2)-P(4)	129.8(3)	C(26)-C(25)-N(2)	117.2(8)
O(2)-P(3)-Pt(1)	108.3(2)	P(5)-O(3)-P(6)	128.6(3)	C(25)-C(26)-C(27)	112.1(9)
O(11)-P(4)-O(12)	105.4(3)	P(7)-O(4)-P(8)	128.0(3)	C(26)-C(27)-C(28)	108.8(11)
O(11)-P(4)-O(2)	106.6(3)	C(13)-N(1)-C(5)	106.4(6)	C(30)-C(29)-N(2)	117.3(7)
O(12)-P(4)-O(2)	101.2(3)	C(13)-N(1)-C(9)	111.0(7)	C(29)-C(30)-C(31)	109.6(8)
O(11)-P(4)-Pt(2)	116.9(2)	C(5)-N(1)-C(9)	110.7(6)	C(32)-C(31)-C(30)	115.6(8)
O(12)-P(4)-Pt(2)	114.6(2)	C(13)-N(1)-C(1)	111.0(6)		
O(2)-P(4)-Pt(2)	110.81(19)	C(5)-N(1)-C(1)	111.8(7)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for bu2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	11(1)	19(1)	16(1)	-1(1)	-1(1)	0(1)
Pt(2)	11(1)	19(1)	18(1)	-2(1)	0(1)	0(1)
P(1)	9(1)	20(1)	20(1)	-1(1)	-1(1)	0(1)
P(2)	14(1)	23(1)	24(1)	-6(1)	3(1)	2(1)
P(3)	15(1)	21(1)	20(1)	-1(1)	-2(1)	0(1)
P(4)	15(1)	23(1)	18(1)	-2(1)	0(1)	-1(1)
P(5)	16(1)	22(1)	20(1)	-2(1)	0(1)	2(1)
P(6)	9(1)	24(1)	19(1)	3(1)	0(1)	2(1)
P(7)	16(1)	25(1)	17(1)	2(1)	0(1)	0(1)
P(8)	12(1)	19(1)	28(1)	1(1)	0(1)	-1(1)
O(1)	13(2)	19(2)	25(3)	-3(2)	-2(2)	4(2)
O(2)	25(3)	19(2)	23(2)	2(2)	-3(2)	-2(2)
O(3)	13(2)	20(3)	26(3)	-1(2)	0(2)	5(2)
O(4)	16(3)	17(3)	28(3)	2(2)	0(2)	0(2)
O(5)	11(2)	30(3)	24(2)	3(2)	0(2)	4(2)
O(6)	9(2)	27(3)	31(3)	10(2)	2(2)	-8(2)
O(7)	19(3)	21(3)	41(3)	-10(2)	2(2)	-4(2)
O(8)	21(3)	37(3)	27(3)	0(2)	6(2)	8(3)
O(9)	23(3)	25(3)	30(3)	10(2)	4(2)	-4(2)
O(10)	22(3)	16(2)	28(3)	-3(2)	-1(2)	1(2)
O(11)	23(3)	32(3)	19(2)	0(2)	3(2)	-3(3)
O(12)	13(2)	37(3)	18(2)	-1(2)	-3(2)	0(2)
O(13)	27(3)	21(3)	28(3)	-5(2)	3(2)	3(3)
O(14)	25(3)	33(3)	24(3)	-6(2)	8(2)	6(2)
O(15)	12(2)	31(3)	21(2)	0(2)	-1(2)	1(2)
O(16)	9(2)	30(3)	28(2)	2(2)	2(2)	1(2)
O(17)	24(3)	34(3)	27(3)	7(2)	9(2)	1(3)
O(18)	19(3)	30(3)	32(3)	5(2)	0(2)	-2(3)
O(19)	31(3)	25(3)	33(3)	-3(2)	0(2)	1(3)
O(20)	24(3)	37(3)	22(3)	9(2)	-4(2)	-4(3)
N(1)	37(4)	23(3)	23(3)	4(2)	8(3)	-1(3)
N(2)	35(4)	24(4)	39(4)	7(3)	-3(3)	-4(3)
C(1)	37(5)	31(4)	21(3)	4(3)	7(3)	-13(4)
C(2)	40(5)	73(7)	31(4)	-5(5)	5(4)	-16(6)
C(3)	32(5)	44(5)	40(5)	-2(4)	3(4)	-14(4)
C(4)	62(7)	35(5)	53(6)	-1(4)	-11(5)	-9(5)
C(5)	30(5)	29(4)	29(4)	-2(3)	4(3)	10(4)
C(6)	40(5)	24(4)	63(6)	4(4)	20(5)	3(4)
C(7)	42(6)	39(5)	46(5)	20(4)	0(4)	5(5)
C(8)	53(7)	55(7)	102(10)	23(8)	-14(7)	8(6)
C(9)	28(4)	22(4)	29(4)	-5(3)	10(3)	5(4)
C(10)	40(5)	41(5)	32(4)	0(4)	4(4)	-10(4)
C(11)	33(5)	55(6)	43(5)	7(4)	-7(4)	-9(5)
C(12)	54(7)	87(10)	51(6)	18(6)	-26(6)	-26(7)
C(13)	43(5)	24(4)	21(3)	6(3)	9(3)	6(4)
C(14)	60(7)	38(5)	30(4)	-3(4)	7(4)	-4(5)
C(15)	58(7)	29(5)	39(5)	-3(4)	8(4)	10(5)
C(16)	44(6)	36(5)	56(6)	-12(5)	14(5)	-3(5)
C(17)	29(5)	43(5)	44(5)	8(4)	1(4)	-6(5)
C(18)	41(6)	34(5)	90(8)	12(6)	-13(6)	-8(5)
C(19)	40(6)	33(5)	76(8)	6(5)	1(5)	-9(5)
C(20)	39(6)	48(6)	64(7)	-2(5)	5(5)	-7(5)
C(21)	36(5)	35(5)	25(4)	5(3)	-4(3)	-4(4)
C(22)	33(5)	36(5)	36(5)	0(4)	0(4)	-6(4)
C(23)	27(5)	37(5)	53(6)	6(4)	2(4)	4(4)
C(24)	35(6)	54(7)	70(7)	4(5)	7(5)	15(5)
C(25)	50(6)	43(5)	36(5)	11(4)	-8(4)	-7(5)
C(26)	39(5)	55(6)	43(5)	14(5)	-7(4)	-16(5)
C(27)	66(9)	89(10)	58(7)	20(7)	1(6)	-25(8)
C(28)	76(9)	65(8)	69(8)	8(7)	-11(7)	-10(8)
C(29)	39(5)	28(4)	40(4)	4(3)	5(4)	12(4)
C(30)	40(6)	35(5)	50(5)	2(4)	2(5)	6(5)
C(31)	47(6)	30(5)	49(5)	6(4)	0(5)	3(5)
C(32)	65(7)	42(6)	51(6)	-16(5)	-16(6)	5(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for bu2.

	x	y	z	U(eq)
HM0	521	-400	5071	299
HM1	549	-1684	5149	485
HM2	431	-1301	4646	485
HM3	-966	-1490	4939	485
H(5)	6758	367	3824	33
H(7)	3337	-1082	3086	41
H(8)	4057	454	2308	42
H(9)	4735	1790	2857	39
H(12)	-459	1303	2437	34
H(13)	1038	2510	3760	38
H(14)	234	971	4534	40
H(15)	-2461	955	3027	32
H(18)	-338	-358	4005	40
H(20)	4762	143	4460	42
H(1A)	1384	1872	6724	35
H(1B)	1831	1124	6815	35
H(2A)	3653	2127	6455	58
H(2B)	4116	1371	6498	58
H(3A)	3841	1411	7344	46
H(3B)	4943	1960	7175	46
H(4A)	3149	2754	7231	75
H(4B)	3473	2410	7739	75
H(4C)	2113	2197	7435	75
H(5A)	3340	879	5891	35
H(5B)	2053	701	5544	35
H(6A)	1176	-62	6089	51
H(6B)	2261	174	6498	51
H(7A)	3303	-367	5610	51
H(7B)	2922	-844	6054	51
H(8A)	4916	229	6129	105
H(8B)	5382	-526	6084	105
H(8C)	4574	-276	6557	105
H(9A)	-569	1533	6265	32
H(9B)	-146	786	6370	32
H(10A)	-685	1302	5428	45
H(10B)	-249	553	5532	45
H(11A)	-2793	1167	5859	52
H(11B)	-2341	437	6015	52
H(12A)	-2972	843	5051	96
H(12B)	-3897	346	5367	96
H(12C)	-2374	127	5178	96
H(13A)	2722	1958	5698	35
H(13B)	1280	1776	5434	35
H(14A)	1639	2735	6170	51
H(14B)	103	2490	6009	51
H(15A)	1140	3491	5593	50
H(15B)	1984	2959	5279	50
H(16A)	-94	2511	5007	68
H(16B)	-129	3286	4907	68
H(16C)	-986	2985	5352	68
H(17A)	2269	1986	1293	46

H(17B)	1844	2286	1805	46
H(18A)	973	2925	952	66
H(18B)	297	2990	1480	66
H(19A)	139	1798	923	60
H(19B)	-636	1915	1428	60
H(20A)	-2185	2618	1089	76
H(20B)	-2136	1975	756	76
H(20C)	-1321	2628	593	76
H(21A)	4209	2424	2051	38
H(21B)	5338	2816	1734	38
H(22A)	4202	1558	1467	42
H(22B)	5360	1950	1158	42
H(23A)	6981	1870	1808	47
H(23B)	5822	1497	2127	47
H(24A)	5867	602	1598	79
H(24B)	7432	745	1787	79
H(24C)	6969	977	1258	79
H(25A)	3774	2562	757	51
H(25B)	2909	3234	783	51
H(26A)	5828	3137	986	55
H(26B)	4945	3808	979	55
H(27A)	5393	3000	145	85
H(27B)	6213	3676	247	85
H(28A)	3211	3559	37	106
H(28B)	4321	3982	-268	106
H(28C)	3834	4229	254	106
H(29A)	3800	3804	1617	43
H(29B)	2165	3685	1517	43
H(30A)	3620	3426	2384	50
H(30B)	2070	3139	2288	50
H(31A)	2644	4519	2203	50
H(31B)	1119	4189	2224	50
H(32A)	1410	3963	3039	79
H(32B)	1649	4732	2944	79
H(32C)	2974	4258	3023	79

Table 6. Hydrogen bonds for bu2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
OM-HM0...O(17)	0.84	2.09	2.93(2)	172.8
O(5)-H(5)...O(16)#1	0.84	1.69	2.522(7)	169.6
O(7)-H(7)...O(19)	0.84	1.70	2.454(8)	148.7
O(8)-H(8)...O(11)	0.84	1.79	2.442(8)	133.1
O(9)-H(9)...O(6)	0.84	1.94	2.557(8)	129.6
O(12)-H(12)...O(15)	0.84	1.92	2.669(7)	148.0
O(13)-H(13)...O(10)	0.84	1.69	2.446(8)	148.5
O(14)-H(14)...O(17)	0.84	1.80	2.461(8)	134.3
O(15)-H(15)...O(6)#2	0.84	1.66	2.492(7)	170.8
O(18)-H(18)...O(16)	0.84	1.89	2.524(8)	131.6
O(20)-H(20)...O(5)	0.84	1.95	2.720(7)	152.6

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x-1,y,z

Crystallographic data of Pn2 crystal measured at laboratory system

Table 1. Crystal data and structure refinement for pn2.

Identification code	pn1of223	
Empirical formula	C40 H98 N2 O20 P8 Pt2	
Formula weight	1565.14	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 9.45410(10) Å	α= 91.9743(8)°.
	b = 16.9411(2) Å	β= 98.3843(3)°.
	c = 20.68590(10) Å	γ = 104.2355(9)°.
Volume	3168.50(5) Å^3	
Z	2	
Density (calculated)	1.641 Mg/m^3	
Absorption coefficient	4.677 mm^{-1}	
F(000)	1576	
Crystal size	0.30 x 0.07 x 0.05 mm^3	
Theta range for data collection	1.24 to 27.48°.	
Index ranges	-12<=h<=12, -13<=k<=22, -26<=l<=26	
Reflections collected	22594	
Independent reflections	14268 [Rint = 0.0293]	
Completeness to θ = 27.48°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.6984	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14268 / 4 / 669	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2σ(I)]	R1 = 0.0343, wR2 = 0.0810	
R indices (all data)	R1 = 0.0444, wR2 = 0.0865	
Largest diff. peak and hole	1.631 and -1.468 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for pn2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	8891(1)	4296(1)	4641(1)	19(1)
P(4)	9022(1)	3583(1)	5582(1)	24(1)
P(1)	7082(1)	4845(1)	4984(1)	23(1)
P(2)	8873(1)	4970(1)	3673(1)	23(1)
P(3)	10705(1)	3762(1)	4277(1)	26(1)
O(1)	5927(3)	4192(2)	5302(2)	31(1)
O(2)	6238(3)	5266(2)	4476(2)	33(1)
O(3)	7486(4)	5320(2)	3464(2)	32(1)
O(4)	9077(4)	4504(2)	3064(2)	34(1)
O(5)	10469(4)	3533(2)	3530(2)	36(1)
O(6)	11074(4)	3024(2)	4610(2)	38(1)
O(7)	9894(4)	2943(2)	5606(2)	34(1)
O(8)	7479(4)	3143(2)	5782(2)	33(1)
O(9)	7743(3)	5517(2)	5610(2)	32(1)
O(10)	10264(3)	5784(2)	3773(2)	28(1)
Pt(2)	9734(1)	629(1)	451(1)	21(1)
P(5)	12268(1)	1131(1)	783(1)	30(1)
P(6)	10000(1)	1568(1)	-349(1)	30(1)
P(7)	7209(1)	98(1)	118(1)	25(1)
P(8)	9635(1)	-264(1)	1277(1)	29(1)
O(11)	12941(4)	883(2)	1440(2)	44(1)
O(12)	12852(4)	2080(2)	800(2)	45(1)
O(13)	11128(4)	2377(2)	-160(2)	45(1)
O(14)	8546(5)	1765(3)	-698(2)	55(1)
O(15)	6444(4)	587(2)	-384(2)	36(1)
O(16)	6302(3)	-75(2)	699(2)	33(1)
O(17)	8251(4)	-378(3)	1651(2)	42(1)
O(18)	10957(4)	-113(3)	1826(2)	49(1)
O(19)	13128(3)	811(2)	237(2)	30(1)
O(20)	10613(4)	1184(2)	-960(2)	42(1)
C(14)	12210(20)	4951(14)	-994(11)	126(9)
C(15)	12790(50)	4680(20)	-319(16)	250(20)
C(14B)	10190(40)	4650(30)	-623(11)	207(19)
C(15B)	11490(40)	4520(20)	-102(17)	178(15)
C(3)	13163(8)	2284(4)	-3831(3)	60(2)
C(4)	13155(10)	1547(5)	-4244(4)	83(2)
N(1)	11452(5)	2764(3)	-2309(2)	41(1)
C(1)	12067(7)	2838(3)	-2950(3)	44(1)
C(2)	12308(8)	2075(4)	-3249(3)	60(2)
C(5)	14015(10)	1775(6)	-4802(4)	99(3)
C(6)	10003(6)	2095(3)	-2376(3)	44(1)
C(7)	8763(7)	2192(5)	-2906(4)	68(2)
C(8)	7424(7)	1447(5)	-2950(3)	69(2)
C(9)	6565(9)	1404(6)	-2419(4)	85(3)
C(10)	5277(9)	644(6)	-2459(5)	102(3)
C(11)	11215(8)	3588(4)	-2131(3)	57(2)
C(12)	10519(12)	3655(5)	-1518(4)	89(3)
C(13)	10614(15)	4537(6)	-1324(5)	119(4)
C(16)	12518(6)	2516(3)	-1772(3)	44(1)
C(17)	14096(8)	3034(5)	-1667(4)	77(2)
C(18)	15030(12)	2746(9)	-1088(5)	134(5)
C(19)	14985(17)	2960(15)	-527(8)	231(11)
C(20)	16130(20)	2819(12)	13(8)	227(9)
C(23)	11195(8)	1626(4)	3219(4)	66(2)
C(24)	11325(9)	847(5)	3485(4)	80(2)
N(2)	15167(5)	2542(3)	2809(2)	40(1)
C(21)	13577(6)	2032(3)	2765(3)	42(1)
C(22)	12713(7)	2275(4)	3273(3)	53(2)

C(25)	9780(10)	225(5)	3414(4)	88(3)
C(26)	16090(6)	2472(3)	3462(3)	40(1)
C(27)	16095(7)	1604(3)	3646(3)	48(1)
C(28)	17165(7)	1622(4)	4272(3)	49(1)
C(29)	17012(8)	784(4)	4537(4)	64(2)
C(30)	18164(13)	788(5)	5139(4)	109(4)
C(31)	15765(6)	2209(3)	2235(3)	45(1)
C(32)	17392(6)	2593(4)	2188(3)	54(2)
C(33)	17876(10)	2125(5)	1650(4)	86(3)
C(34)	19581(12)	2481(6)	1593(5)	104(3)
C(35)	19891(13)	3221(8)	1335(6)	131(4)
C(36)	15236(6)	3449(3)	2761(3)	44(1)
C(37)	14371(7)	3663(4)	2140(3)	56(2)
C(38)	14307(7)	4565(4)	2210(3)	49(1)
C(39)	13285(8)	4727(4)	2666(4)	66(2)
C(40)	13226(10)	5609(5)	2722(4)	82(2)

Table 3. Bond lengths [Å] and angles [°] for pn2.

Pt(1)-P(1)	2.3206(11)	O(10)-P(4)#1	1.633(3)	O(17)-H(17)	0.86(7)
Pt(1)-P(3)	2.3271(11)	Pt(2)-P(8)	2.3174(12)	O(19)-P(7)#2	1.621(3)
Pt(1)-P(4)	2.3299(11)	Pt(2)-P(7)	2.3244(11)	O(20)-P(8)#2	1.619(4)
Pt(1)-P(2)	2.3382(11)	Pt(2)-P(5)	2.3267(11)	C(14)-C(13)	1.543(15)
Pt(1)-Pt(1)#1	2.9468(3)	Pt(2)-P(6)	2.3325(12)	C(14)-C(15)	1.547(18)
P(4)-O(7)	1.514(3)	Pt(2)-Pt(2)#2	2.9657(3)	C(14B)-C(15B)	1.576(19)
P(4)-O(8)	1.586(3)	P(5)-O(11)	1.532(4)	C(14B)-C(13)	1.579(18)
P(4)-O(10)#1	1.633(3)	P(5)-O(12)	1.565(4)	C(3)-C(4)	1.485(10)
P(1)-O(2)	1.527(3)	P(5)-O(19)	1.634(3)	C(3)-C(2)	1.550(9)
P(1)-O(1)	1.586(3)	P(6)-O(13)	1.513(4)	C(4)-C(5)	1.513(11)
P(1)-O(9)	1.636(3)	P(6)-O(14)	1.573(4)	N(1)-C(11)	1.509(7)
P(2)-O(4)	1.525(3)	P(6)-O(20)	1.642(4)	N(1)-C(1)	1.521(7)
P(2)-O(3)	1.579(3)	P(7)-O(15)	1.556(4)	N(1)-C(16)	1.530(7)
P(2)-O(10)	1.638(3)	P(7)-O(16)	1.569(3)	N(1)-C(6)	1.533(7)
P(3)-O(6)	1.537(4)	P(7)-O(19)#2	1.621(3)	C(1)-C(2)	1.495(8)
P(3)-O(5)	1.550(4)	P(8)-O(18)	1.526(4)	C(6)-C(7)	1.529(8)
P(3)-O(9)#1	1.642(3)	P(8)-O(17)	1.591(4)	C(7)-C(8)	1.542(10)
O(3)-H(3)	0.99(6)	P(8)-O(20)#2	1.619(4)	C(8)-C(9)	1.452(10)
O(5)-H(5)	0.97(7)	O(12)-H(12)	0.82(7)	C(9)-C(10)	1.530(11)
O(8)-H(8)	0.86(6)	O(14)-H(14)	0.89(8)	C(11)-C(12)	1.525(9)
O(9)-P(3)#1	1.643(3)	O(15)-H(15)	1.05(6)	C(12)-C(13)	1.510(11)

C(16)-C(17)	1.514(8)	P(4)-Pt(1)-Pt(1)#1	89.15(3)	P(7)-Pt(2)-P(5)	178.73(4)
C(17)-C(18)	1.548(13)	P(2)-Pt(1)-Pt(1)#1	91.18(3)	P(8)-Pt(2)-P(6)	176.10(4)
C(18)-C(19)	1.212(17)	O(7)-P(4)-O(8)	105.34(19)	P(7)-Pt(2)-P(6)	94.95(4)
C(19)-C(20)	1.504(18)	O(7)-P(4)-O(10)#1	106.35(19)	P(5)-Pt(2)-P(6)	85.86(5)
C(23)-C(24)	1.472(10)	O(8)-P(4)-O(10)#1	100.31(18)	P(8)-Pt(2)-Pt(2)#2	89.97(3)
C(23)-C(22)	1.566(8)	O(7)-P(4)-Pt(1)	117.39(14)	P(7)-Pt(2)-Pt(2)#2	88.76(3)
C(24)-C(25)	1.561(10)	O(8)-P(4)-Pt(1)	115.44(14)	P(5)-Pt(2)-Pt(2)#2	90.25(3)
N(2)-C(26)	1.524(7)	O(10)#1-P(4)-Pt(1)	110.32(12)	P(6)-Pt(2)-Pt(2)#2	90.59(3)
N(2)-C(21)	1.526(6)	O(2)-P(1)-O(1)	108.79(18)	O(11)-P(5)-O(12)	105.9(2)
N(2)-C(36)	1.530(7)	O(2)-P(1)-O(9)	105.78(19)	O(11)-P(5)-O(19)	105.6(2)
N(2)-C(31)	1.534(7)	O(1)-P(1)-O(9)	99.81(18)	O(12)-P(5)-O(19)	102.6(2)
C(21)-C(22)	1.525(8)	O(2)-P(1)-Pt(1)	116.87(14)	O(11)-P(5)-Pt(2)	117.51(15)
C(26)-C(27)	1.532(8)	O(1)-P(1)-Pt(1)	111.91(13)	O(12)-P(5)-Pt(2)	115.08(16)
C(27)-C(28)	1.517(8)	O(9)-P(1)-Pt(1)	112.17(12)	O(19)-P(5)-Pt(2)	108.70(11)
C(28)-C(29)	1.522(9)	O(4)-P(2)-O(3)	106.2(2)	O(13)-P(6)-O(14)	107.0(2)
C(29)-C(30)	1.528(10)	O(4)-P(2)-O(10)	104.00(18)	O(13)-P(6)-O(20)	103.1(2)
C(31)-C(32)	1.535(8)	O(3)-P(2)-O(10)	103.53(18)	O(14)-P(6)-O(20)	102.6(2)
C(32)-C(33)	1.531(9)	O(4)-P(2)-Pt(1)	116.79(15)	O(13)-P(6)-Pt(2)	116.88(17)
C(33)-C(34)	1.600(12)	O(3)-P(2)-Pt(1)	115.85(14)	O(14)-P(6)-Pt(2)	116.70(16)
C(34)-C(35)	1.362(13)	O(10)-P(2)-Pt(1)	109.00(12)	O(20)-P(6)-Pt(2)	108.77(14)
C(36)-C(37)	1.524(8)	O(6)-P(3)-O(5)	105.7(2)	O(15)-P(7)-O(16)	109.00(18)
C(37)-C(38)	1.545(8)	O(6)-P(3)-O(9)#1	105.8(2)	O(15)-P(7)-O(19)#2	104.97(19)
C(38)-C(39)	1.509(9)	O(5)-P(3)-O(9)#1	102.44(19)	O(16)-P(7)-O(19)#2	100.98(18)
C(39)-C(40)	1.511(10)	O(6)-P(3)-Pt(1)	117.82(14)	O(15)-P(7)-Pt(2)	115.80(14)
		O(5)-P(3)-Pt(1)	115.41(15)	O(16)-P(7)-Pt(2)	114.05(13)
P(1)-Pt(1)-P(3)	178.72(4)	O(9)#1-P(3)-Pt(1)	108.15(12)	O(19)#2-P(7)-Pt(2)	110.65(12)
P(1)-Pt(1)-P(4)	90.53(4)	P(2)-O(3)-H(3)	106(4)	O(18)-P(8)-O(17)	104.0(2)
P(3)-Pt(1)-P(4)	90.74(4)	P(3)-O(5)-H(5)	110(4)	O(18)-P(8)-O(20)#2	106.9(2)
P(1)-Pt(1)-P(2)	93.21(4)	P(4)-O(8)-H(8)	114(4)	O(17)-P(8)-O(20)#2	100.6(2)
P(3)-Pt(1)-P(2)	85.51(4)	P(1)-O(9)-P(3)#1	127.8(2)	O(18)-P(8)-Pt(2)	117.96(16)
P(4)-Pt(1)-P(2)	176.25(4)	P(4)#1-O(10)-P(2)	130.0(2)	O(17)-P(8)-Pt(2)	116.34(16)
P(1)-Pt(1)-Pt(1)#1	87.84(3)	P(8)-Pt(2)-P(7)	88.92(4)	O(20)#2-P(8)-Pt(2)	109.34(14)
P(3)-Pt(1)-Pt(1)#1	92.09(3)	P(8)-Pt(2)-P(5)	90.28(4)	P(5)-O(12)-H(12)	105(5)

P(6)-O(14)-H(14)	122(5)	C(9)-C(8)-C(7)	116.1(7)	C(22)-C(21)-N(2)	115.7(4)
P(7)-O(15)-H(15)	108(3)	C(8)-C(9)-C(10)	115.2(8)	C(21)-C(22)-C(23)	108.9(5)
P(8)-O(17)-H(17)	112(5)	N(1)-C(11)-C(12)	116.4(5)	N(2)-C(26)-C(27)	116.1(4)
P(7)#2-O(19)-P(5)	128.0(2)	C(13)-C(12)-C(11)	110.7(7)	C(28)-C(27)-C(26)	110.8(5)
P(8)#2-O(20)-P(6)	133.2(2)	C(12)-C(13)-C(14)	108.6(12)	C(27)-C(28)-C(29)	112.5(5)
C(13)-C(14)-C(15)	119(2)	C(12)-C(13)-C(14B)	112.3(17)	C(28)-C(29)-C(30)	112.6(6)
C(15B)-C(14B)-C(13)	108(2)	C(14)-C(13)-C(14B)	85.4(17)	N(2)-C(31)-C(32)	116.2(4)
C(4)-C(3)-C(2)	112.7(6)	C(17)-C(16)-N(1)	115.8(5)	C(33)-C(32)-C(31)	109.9(5)
C(3)-C(4)-C(5)	111.1(7)	C(16)-C(17)-C(18)	110.4(7)	C(32)-C(33)-C(34)	112.2(6)
C(11)-N(1)-C(1)	106.4(4)	C(19)-C(18)-C(17)	120.6(16)	C(35)-C(34)-C(33)	114.3(10)
C(11)-N(1)-C(16)	111.3(5)	C(18)-C(19)-C(20)	119.1(18)	C(37)-C(36)-N(2)	115.5(4)
C(1)-N(1)-C(16)	111.1(4)	C(24)-C(23)-C(22)	113.3(7)	C(36)-C(37)-C(38)	109.9(5)
C(11)-N(1)-C(6)	110.9(5)	C(23)-C(24)-C(25)	110.9(7)	C(39)-C(38)-C(37)	114.3(5)
C(1)-N(1)-C(6)	111.5(4)	C(26)-N(2)-C(21)	111.2(4)	C(38)-C(39)-C(40)	113.5(6)
C(16)-N(1)-C(6)	105.7(4)	C(26)-N(2)-C(36)	106.4(4)		
C(2)-C(1)-N(1)	116.2(5)	C(21)-N(2)-C(36)	111.5(4)	Symmetry transformations used to	
C(1)-C(2)-C(3)	109.5(5)	C(26)-N(2)-C(31)	111.2(4)	generate equivalent atoms:	
C(7)-C(6)-N(1)	115.7(4)	C(21)-N(2)-C(31)	105.7(4)	#1 -x+2,-y+1,-z+1	
C(6)-C(7)-C(8)	109.7(5)	C(36)-N(2)-C(31)	110.9(4)	#2 -x+2,-y,-z	

Table 4. Anisotropic displacement parameters ($Å^3 x\ 10^3$)for pn2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	14(1)	19(1)	22(1)	1(1)	1(1)	4(1)
P(4)	20(1)	22(1)	27(1)	5(1)	1(1)	4(1)
P(1)	14(1)	26(1)	31(1)	5(1)	4(1)	8(1)
P(2)	21(1)	26(1)	22(1)	3(1)	0(1)	4(1)
P(3)	22(1)	26(1)	31(1)	-1(1)	6(1)	9(1)
O(1)	15(1)	34(2)	48(2)	12(1)	9(1)	9(1)
O(2)	21(2)	44(2)	39(2)	13(2)	6(1)	17(1)
O(3)	27(2)	40(2)	30(2)	8(1)	2(1)	11(1)
O(4)	39(2)	36(2)	24(2)	-2(1)	5(1)	7(2)
O(5)	39(2)	40(2)	32(2)	-8(2)	6(2)	17(2)
O(6)	42(2)	36(2)	46(2)	10(2)	17(2)	22(2)
O(7)	41(2)	33(2)	35(2)	11(1)	8(2)	21(2)
O(8)	27(2)	28(2)	41(2)	12(1)	6(2)	3(1)
O(9)	19(2)	37(2)	45(2)	-1(2)	13(1)	9(1)
O(10)	27(2)	31(2)	24(2)	4(1)	4(1)	1(1)
Pt(2)	17(1)	25(1)	21(1)	1(1)	2(1)	4(1)
P(5)	20(1)	34(1)	31(1)	-5(1)	-1(1)	0(1)

P(6)	28(1)	30(1)	34(1)	9(1)	6(1)	8(1)
P(7)	16(1)	35(1)	25(1)	6(1)	3(1)	7(1)
P(8)	25(1)	39(1)	22(1)	7(1)	2(1)	7(1)
O(11)	27(2)	64(3)	30(2)	0(2)	-6(1)	-2(2)
O(12)	34(2)	33(2)	56(3)	-11(2)	-1(2)	-6(2)
O(13)	48(2)	26(2)	58(2)	7(2)	13(2)	1(2)
O(14)	37(2)	66(3)	69(3)	38(2)	12(2)	21(2)
O(15)	20(2)	47(2)	42(2)	16(2)	4(1)	10(2)
O(16)	25(2)	51(2)	28(2)	7(1)	9(1)	14(2)
O(17)	40(2)	64(3)	31(2)	17(2)	15(2)	19(2)
O(18)	37(2)	72(3)	30(2)	16(2)	-8(2)	5(2)
O(19)	12(1)	38(2)	37(2)	-1(1)	5(1)	-1(1)
O(20)	58(2)	36(2)	34(2)	10(2)	16(2)	10(2)
C(3)	60(4)	58(4)	61(4)	6(3)	0(3)	19(3)
C(4)	85(6)	76(5)	87(6)	-10(4)	23(5)	18(5)
N(1)	49(3)	38(2)	38(2)	17(2)	10(2)	12(2)
C(1)	50(3)	47(3)	39(3)	20(2)	12(3)	15(3)
C(2)	74(5)	48(4)	57(4)	4(3)	22(3)	9(3)
C(5)	81(6)	130(8)	67(5)	-36(5)	25(5)	-10(5)
C(6)	42(3)	47(3)	42(3)	23(2)	11(2)	8(2)
C(7)	47(4)	101(6)	59(4)	42(4)	6(3)	18(4)
C(8)	47(4)	105(6)	52(4)	6(4)	-6(3)	20(4)
C(9)	60(5)	125(8)	71(5)	11(5)	10(4)	23(5)
C(10)	58(5)	127(8)	109(8)	45(6)	5(5)	3(5)
C(11)	79(5)	42(3)	61(4)	19(3)	26(4)	24(3)
C(12)	140(8)	62(5)	80(6)	15(4)	62(6)	29(5)
C(13)	193(13)	76(6)	118(9)	11(6)	71(9)	67(7)
C(16)	41(3)	49(3)	36(3)	20(2)	1(2)	0(2)
C(17)	54(4)	92(6)	69(5)	30(4)	-3(4)	-6(4)
C(18)	90(8)	188(12)	79(7)	29(8)	-36(6)	-21(8)
C(19)	116(12)	450(40)	116(13)		60(18)	-11(10)
C(20)	240(20)	270(20)	156(15)		-36(15)	-80(14)
C(23)	58(4)	48(4)	92(6)	-4(4)	33(4)	7(3)
C(24)	80(6)	65(5)	81(6)	13(4)	6(4)	-8(4)
N(2)	36(2)	35(2)	41(3)	-8(2)	-1(2)	2(2)
C(21)	37(3)	30(3)	51(3)	-13(2)	2(2)	-1(2)
C(22)	49(3)	39(3)	66(4)	-12(3)	14(3)	2(3)
C(25)	99(6)	72(5)	77(6)	1(4)	38(5)	-23(5)
C(26)	40(3)	37(3)	38(3)	-5(2)	-2(2)	8(2)
C(27)	50(3)	40(3)	52(4)	-4(3)	4(3)	11(3)
C(28)	48(3)	46(3)	50(4)	-2(3)	4(3)	9(3)
C(29)	70(5)	55(4)	69(5)	10(3)	8(4)	22(3)
C(30)	165(10)	73(6)	77(6)	10(4)	-38(6)	38(6)
C(31)	44(3)	38(3)	44(3)	-9(2)	4(2)	1(2)
C(32)	39(3)	54(4)	65(4)	-10(3)	11(3)	2(3)
C(33)	97(6)	69(5)	92(6)	-15(4)	57(5)	-1(4)
C(34)	133(9)	87(7)	117(8)	17(6)	79(7)	38(6)
C(35)	96(8)	150(11)	141(11)	21(9)	35(8)	9(8)
C(36)	40(3)	35(3)	48(3)	-9(2)	-1(2)	-1(2)
C(37)	58(4)	53(4)	50(4)	0(3)	-4(3)	11(3)
C(38)	52(4)	46(3)	46(3)	8(3)	2(3)	9(3)
C(39)	62(4)	60(4)	80(5)	14(4)	28(4)	12(3)
C(40)	95(6)	70(5)	95(6)	14(4)	50(5)	26(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for pn2.

	x	y	z	U(eq)
H(1)	5186	4364	5328	46
H(3)	7090(60)	5400(30)	3870(30)	48
H(5)	9850(70)	3850(40)	3300(30)	54
H(6)	10917	3039	4994	57
H(8)	6780(70)	3380(40)	5660(30)	49
H(11)	12297	546	1590	66
H(12)	12480(80)	2210(40)	450(30)	67
H(14)	7650(90)	1490(50)	-630(40)	82
H(15)	5330(70)	260(40)	-510(30)	54
H(17)	7500(80)	-280(40)	1410(30)	63
H(14A)	12302	5540	-946	152
H(14B)	12874	4866	-1297	152
H(15A)	13802	4993	-175	378
H(15B)	12742	4106	-355	378
H(15C)	12178	4788	-3	378
H(14C)	10043	5198	-552	249
H(14D)	9266	4248	-584	249
H(15D)	11260	4593	335	267
H(15E)	12396	4925	-145	267
H(15F)	11618	3980	-175	267
H(3A)	12718	2649	-4104	72
H(3B)	14188	2575	-3661	72
H(4A)	12132	1259	-4422	99
H(4B)	13593	1178	-3974	99
H(1A)	11389	3039	-3269	53
H(1B)	13013	3253	-2875	53
H(2A)	11353	1686	-3403	72
H(2B)	12873	1822	-2920	72
H(5A)	13993	1284	-5063	148
H(5B)	15031	2053	-4625	148
H(5C)	13572	2133	-5074	148
H(6A)	10215	1568	-2468	52
H(6B)	9646	2077	-1954	52
H(7A)	9114	2240	-3330	82
H(7B)	8468	2691	-2801	82
H(8A)	6765	1444	-3362	83
H(8B)	7781	951	-2969	83
H(9A)	6173	1887	-2410	102
H(9B)	7229	1425	-2004	102
H(10A)	4774	665	-2084	153
H(10B)	5651	159	-2458	153
H(10C)	4589	625	-2859	153
H(11A)	10586	3737	-2502	69
H(11B)	12174	3991	-2073	69
H(12A)	9481	3345	-1601	107
H(12B)	11032	3420	-1158	107
H(13A)	9923	4567	-1019	142
H(13B)	10349	4817	-1713	142
H(13C)	9949	4739	-1648	142
H(13D)	11624	4864	-1327	142
H(16A)	12132	2533	-1358	53
H(16B)	12526	1949	-1877	53
H(17A)	14108	3607	-1575	93
H(17B)	14526	2992	-2066	93
H(18A)	14750	2148	-1127	161
H(18B)	16065	2918	-1152	161
H(19A)	14010	2684	-428	277
H(19B)	15047	3546	-508	277
H(20A)	15939	3015	431	340
H(20B)	17102	3111	-59	340
H(20C)	16069	2240	16	340

H(23A)	10537	1850	3454	79
H(23B)	10740	1521	2757	79
H(24A)	11767	945	3949	97
H(24B)	11979	617	3251	97
H(21A)	13044	2068	2328	50
H(21B)	13592	1460	2808	50
H(22A)	12548	2815	3196	63
H(22B)	13277	2301	3714	63
H(25A)	9893	-284	3590	132
H(25B)	9346	124	2955	132
H(25C)	9139	448	3653	132
H(26A)	15729	2739	3809	48
H(26B)	17113	2776	3455	48
H(27A)	15097	1310	3706	58
H(27B)	16380	1312	3289	58
H(28A)	16990	1998	4605	58
H(28B)	18178	1832	4187	58
H(29A)	17112	398	4193	76
H(29B)	16022	592	4654	76
H(30A)	18021	242	5289	164
H(30B)	18056	1159	5485	164
H(30C)	19147	966	5025	164
H(31A)	15160	2283	1826	53
H(31B)	15635	1620	2267	53
H(32A)	17520	3165	2089	65
H(32B)	18010	2578	2609	65
H(33A)	17269	2154	1229	103
H(33B)	17707	1549	1744	103
H(34A)	20169	2530	2031	125
H(34B)	19889	2090	1320	125
H(35A)	20945	3405	1331	196
H(35B)	19583	3613	1599	196
H(35C)	19364	3172	891	196
H(36A)	14865	3641	3139	53
H(36B)	16275	3750	2791	53
H(37A)	13366	3307	2064	67
H(37B)	14849	3577	1763	67
H(38A)	15306	4904	2370	59
H(38B)	13987	4733	1776	59
H(39A)	13611	4567	3102	79
H(39B)	12287	4385	2509	79
H(40A)	12557	5674	3022	123
H(40B)	12875	5769	2294	123
H(40C)	14206	5952	2885	123

Table 6. Hydrogen bonds for pn2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#3	0.83	1.71	2.532(4)	170.3
O(3)-H(3)...O(2)	0.99(6)	1.58(6)	2.542(5)	164(5)
O(5)-H(5)...O(4)	0.97(7)	1.53(7)	2.483(5)	166(6)
O(6)-H(6)...O(7)	0.83	1.69	2.473(5)	156.6
O(8)-H(8)...O(1)	0.86(6)	1.88(6)	2.698(5)	156(6)
O(11)-H(11)...O(18)	0.83	1.62	2.444(5)	175.4
O(12)-H(12)...O(13)	0.82(7)	1.74(7)	2.524(6)	159(7)
O(14)-H(14)...O(15)	0.89(8)	1.81(8)	2.621(5)	150(7)
O(15)-H(15)...O(16)#4	1.05(6)	1.48(6)	2.506(4)	162(5)
O(17)-H(17)...O(16)	0.86(7)	1.82(7)	2.650(5)	160(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1 #2 -x+2,-y,-z #3 -x+1,-y+1,-z+1

#4 -x+1,-y,-z

Crystallographic data of Bzte2 crystal measured at laboratory system

Table 1. Crystal data and structure refinement for bzte2.

Identification code	btea10	
Empirical formula	C27 H58 N2 O21 P8 Pt2	
Formula weight	1384.69	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P\,n\,a\,2_1$	
Unit cell dimensions	a = 20.42330(10) Å	α= 90°.
	b = 21.6230(2) Å	β= 90°.
	c = 10.10650(10) Å	γ = 90°.
Volume	4463.16(6) Å^3	
Z	4	
Density (calculated)	2.061 Mg/m^3	
Absorption coefficient	6.627 mm^{-1}	
F(000)	2712	
Crystal size	0.32 x 0.20 x 0.03 mm^3	
Theta range for data collection	1.99 to 27.48°.	
Index ranges	-12<=h<=26, -28<=k<=28, -13<=l<=12	
Reflections collected	30527	
Independent reflections	9974 [Rint = 0.0557]	
Completeness to θ = 27.48°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.400	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9974 / 1 / 546	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2σ(I)]	R1 = 0.0291, wR2 = 0.0639	
R indices (all data)	R1 = 0.0312, wR2 = 0.0646	
Absolute structure parameter	0.177(4)	
Largest diff. peak and hole	1.622 and -1.954 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for bzte2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	8378(1)	2209(1)	5650(1)	6(1)
Pt(2)	9191(1)	3009(1)	7336(1)	6(1)
P(1)	7451(1)	2778(1)	6242(2)	10(1)
P(2)	8287(1)	3629(1)	7753(1)	10(1)
P(3)	8611(1)	2867(1)	3874(1)	9(1)
P(4)	9466(1)	3622(1)	5540(2)	10(1)
P(5)	9279(1)	1608(1)	5100(2)	10(1)
P(6)	10079(1)	2362(1)	6887(1)	10(1)
P(7)	8170(1)	1573(1)	7462(2)	10(1)
P(8)	8901(1)	2429(1)	9184(1)	10(1)
O(1)	6884(2)	2401(2)	6779(4)	17(1)
O(2)	7183(2)	3227(2)	5163(4)	16(1)
O(3)	7628(2)	3238(2)	7500(4)	14(1)
O(4)	8180(2)	3826(2)	9247(4)	21(1)
O(5)	8222(2)	4216(2)	6935(4)	17(1)
O(6)	8096(2)	3345(2)	3512(4)	15(1)
O(7)	8850(2)	2493(2)	2633(4)	15(1)
O(8)	9303(2)	3251(2)	4189(4)	11(1)
O(9)	9141(2)	4258(2)	5430(4)	18(1)
O(10)	10218(2)	3764(2)	5350(4)	17(1)
O(11)	9408(2)	1497(2)	3579(4)	16(1)
O(12)	9319(2)	965(2)	5720(5)	19(1)
O(13)	9943(2)	1975(2)	5505(4)	14(1)
O(14)	10687(2)	2750(2)	6429(4)	16(1)
O(15)	10257(2)	1896(2)	7938(4)	16(1)
O(16)	8560(2)	972(2)	7584(4)	18(1)
O(17)	7429(2)	1390(2)	7659(4)	18(1)
O(18)	8298(2)	1956(2)	8825(4)	18(1)
O(19)	9449(2)	2005(2)	9761(4)	16(1)
O(20)	8618(2)	2811(2)	10335(4)	16(1)
N(1)	9533(2)	6051(2)	5876(4)	9(1)
C(1)	9736(3)	6723(2)	5586(6)	13(1)
C(2)	9247(3)	7211(3)	5994(5)	11(1)
C(3)	9287(3)	7475(2)	7268(7)	16(1)
C(4)	8834(4)	7935(3)	7637(7)	25(2)
C(5)	8363(3)	8138(3)	6731(8)	28(2)
C(6)	8342(3)	7895(3)	5466(8)	24(2)
C(7)	8784(3)	7429(3)	5101(6)	16(1)
C(8)	9376(3)	5996(2)	7346(6)	14(1)
C(9)	9229(3)	5347(3)	7829(6)	18(1)
C(10)	10105(3)	5631(2)	5508(6)	14(1)
C(11)	10698(3)	5668(3)	6429(6)	17(1)
C(12)	8938(3)	5866(3)	5078(6)	13(1)
C(13)	9026(3)	5858(3)	3596(6)	21(1)
N(2)	8802(2)	-20(2)	1536(5)	11(1)
C(14)	8053(3)	57(3)	1375(6)	17(1)
C(15)	7766(3)	589(2)	2151(6)	11(1)
C(16)	7521(3)	501(3)	3438(6)	16(1)
C(17)	7257(3)	991(3)	4150(7)	23(1)
C(18)	7216(3)	1577(3)	3574(7)	23(2)
C(19)	7448(3)	1667(3)	2296(8)	24(1)
C(20)	7724(3)	1176(3)	1579(6)	18(1)
C(21)	8981(3)	-117(3)	2983(6)	16(1)
C(22)	8700(3)	-699(3)	3624(6)	20(1)
C(23)	9015(3)	-593(3)	755(7)	21(1)
C(24)	8957(4)	-518(3)	-741(7)	32(2)
C(25)	9140(3)	560(3)	1033(6)	14(1)
C(26)	9878(3)	539(3)	1008(6)	20(1)

O(50)	7806(4)	4669(3)	3421(6)	46(2)
C(50)	7578(4)	4763(3)	2110(8)	34(2)

Table 3. Bond lengths [Å] and angles [°] for bzte2.

Pt(1)-P(5)	2.3190(15)	P(7)-O(18)	1.629(4)	C(21)-C(22)	1.527(8)
Pt(1)-P(7)	2.3292(15)	P(8)-O(20)	1.540(4)	C(23)-C(24)	1.524(10)
Pt(1)-P(1)	2.3369(15)	P(8)-O(19)	1.560(4)	C(25)-C(26)	1.508(8)
Pt(1)-P(3)	2.3400(14)	P(8)-O(18)	1.640(5)	O(50)-C(50)	1.419(10)
Pt(1)-Pt(2)	2.9425(3)	N(1)-C(12)	1.512(7)	O(50)-H(50)	0.87(11)
Pt(2)-P(4)	2.3163(15)	N(1)-C(8)	1.524(7)		
Pt(2)-P(2)	2.3192(15)	N(1)-C(10)	1.527(7)	P(5)-Pt(1)-P(7)	90.18(5)
Pt(2)-P(8)	2.3267(14)	N(1)-C(1)	1.540(7)	P(5)-Pt(1)-P(1)	177.67(5)
Pt(2)-P(6)	2.3363(14)	C(1)-C(2)	1.510(8)	P(7)-Pt(1)-P(1)	87.77(5)
P(1)-O(1)	1.516(4)	C(2)-C(7)	1.390(8)	P(5)-Pt(1)-P(3)	89.79(5)
P(1)-O(2)	1.560(4)	C(2)-C(3)	1.411(9)	P(7)-Pt(1)-P(3)	178.08(5)
P(1)-O(3)	1.655(4)	C(3)-C(4)	1.408(9)	P(1)-Pt(1)-P(3)	92.30(5)
P(2)-O(5)	1.521(4)	C(4)-C(5)	1.398(11)	P(5)-Pt(1)-Pt(2)	91.19(4)
P(2)-O(4)	1.583(4)	C(5)-C(6)	1.383(11)	P(7)-Pt(1)-Pt(2)	89.72(4)
P(2)-O(3)	1.609(4)	C(6)-C(7)	1.401(9)	P(1)-Pt(1)-Pt(2)	89.91(4)
P(3)-O(6)	1.517(4)	C(8)-C(9)	1.514(8)	P(3)-Pt(1)-Pt(2)	88.37(4)
P(3)-O(7)	1.570(4)	C(10)-C(11)	1.529(8)	P(4)-Pt(2)-P(2)	90.33(5)
P(3)-O(8)	1.670(4)	C(12)-C(13)	1.509(8)	P(4)-Pt(2)-P(8)	177.78(5)
P(4)-O(9)	1.532(4)	N(2)-C(25)	1.519(7)	P(2)-Pt(2)-P(8)	87.91(5)
P(4)-O(10)	1.577(4)	N(2)-C(21)	1.522(7)	P(4)-Pt(2)-P(6)	90.08(5)
P(4)-O(8)	1.618(4)	N(2)-C(23)	1.532(7)	P(2)-Pt(2)-P(6)	178.18(5)
P(5)-O(12)	1.529(4)	N(2)-C(14)	1.546(8)	P(8)-Pt(2)-P(6)	91.72(5)
P(5)-O(11)	1.578(4)	C(14)-C(15)	1.511(8)	P(4)-Pt(2)-Pt(1)	91.12(4)
P(5)-O(13)	1.623(4)	C(15)-C(20)	1.397(8)	P(2)-Pt(2)-Pt(1)	89.79(4)
P(6)-O(15)	1.508(4)	C(15)-C(16)	1.406(8)	P(8)-Pt(2)-Pt(1)	90.22(4)
P(6)-O(14)	1.568(4)	C(16)-C(17)	1.390(9)	P(6)-Pt(2)-Pt(1)	88.43(4)
P(6)-O(13)	1.652(4)	C(17)-C(18)	1.396(10)	O(1)-P(1)-O(2)	108.5(3)
P(7)-O(16)	1.530(4)	C(18)-C(19)	1.390(11)	O(1)-P(1)-O(3)	102.4(2)
P(7)-O(17)	1.576(4)	C(19)-C(20)	1.403(9)	O(2)-P(1)-O(3)	103.8(2)

O(1)-P(1)-Pt(1)	115.32(18)	O(14)-P(6)-O(13)	98.9(2)	C(3)-C(2)-C(1)	119.6(5)
O(2)-P(1)-Pt(1)	115.68(18)	O(15)-P(6)-Pt(2)	116.74(19)	C(4)-C(3)-C(2)	119.3(6)
O(3)-P(1)-Pt(1)	109.67(15)	O(14)-P(6)-Pt(2)	110.61(17)	C(5)-C(4)-C(3)	120.0(7)
O(5)-P(2)-O(4)	106.4(3)	O(13)-P(6)-Pt(2)	109.75(16)	C(6)-C(5)-C(4)	120.5(6)
O(5)-P(2)-O(3)	106.2(2)	O(16)-P(7)-O(17)	106.1(2)	C(5)-C(6)-C(7)	119.8(6)
O(4)-P(2)-O(3)	100.2(2)	O(16)-P(7)-O(18)	106.2(2)	C(2)-C(7)-C(6)	120.7(6)
O(5)-P(2)-Pt(2)	116.91(18)	O(17)-P(7)-O(18)	100.1(2)	C(9)-C(8)-N(1)	115.3(5)
O(4)-P(2)-Pt(2)	115.95(18)	O(16)-P(7)-Pt(1)	118.00(18)	N(1)-C(10)-C(11)	115.3(5)
O(3)-P(2)-Pt(2)	109.49(16)	O(17)-P(7)-Pt(1)	115.02(17)	C(13)-C(12)-N(1)	115.9(5)
O(6)-P(3)-O(7)	111.9(2)	O(18)-P(7)-Pt(1)	109.57(16)	C(25)-N(2)-C(21)	109.1(5)
O(6)-P(3)-O(8)	107.1(2)	O(20)-P(8)-O(19)	107.6(2)	C(25)-N(2)-C(23)	111.4(5)
O(7)-P(3)-O(8)	98.3(2)	O(20)-P(8)-O(18)	102.7(2)	C(21)-N(2)-C(23)	108.3(5)
O(6)-P(3)-Pt(1)	117.30(17)	O(19)-P(8)-O(18)	104.8(2)	C(25)-N(2)-C(14)	109.0(5)
O(7)-P(3)-Pt(1)	111.21(17)	O(20)-P(8)-Pt(2)	114.34(18)	C(21)-N(2)-C(14)	110.7(5)
O(8)-P(3)-Pt(1)	109.14(15)	O(19)-P(8)-Pt(2)	115.77(18)	C(23)-N(2)-C(14)	108.3(5)
O(9)-P(4)-O(10)	103.8(2)	O(18)-P(8)-Pt(2)	110.45(17)	C(15)-C(14)-N(2)	114.4(5)
O(9)-P(4)-O(8)	107.1(2)	P(2)-O(3)-P(1)	128.4(3)	C(20)-C(15)-C(16)	119.0(5)
O(10)-P(4)-O(8)	101.2(2)	P(4)-O(8)-P(3)	125.6(3)	C(20)-C(15)-C(14)	120.0(5)
O(9)-P(4)-Pt(2)	117.69(17)	P(5)-O(13)-P(6)	126.9(3)	C(16)-C(15)-C(14)	121.0(5)
O(10)-P(4)-Pt(2)	116.31(16)	P(7)-O(18)-P(8)	128.7(3)	C(17)-C(16)-C(15)	120.9(6)
O(8)-P(4)-Pt(2)	109.14(16)	C(12)-N(1)-C(8)	109.3(4)	C(16)-C(17)-C(18)	119.9(6)
O(12)-P(5)-O(11)	104.6(3)	C(12)-N(1)-C(10)	109.2(4)	C(19)-C(18)-C(17)	119.6(6)
O(12)-P(5)-O(13)	107.2(2)	C(8)-N(1)-C(10)	110.6(4)	C(18)-C(19)-C(20)	120.7(6)
O(11)-P(5)-O(13)	100.4(2)	C(12)-N(1)-C(1)	111.3(4)	C(15)-C(20)-C(19)	119.9(6)
O(12)-P(5)-Pt(1)	117.01(18)	C(8)-N(1)-C(1)	108.4(4)	N(2)-C(21)-C(22)	115.6(5)
O(11)-P(5)-Pt(1)	116.77(18)	C(10)-N(1)-C(1)	108.0(4)	C(24)-C(23)-N(2)	113.8(5)
O(13)-P(5)-Pt(1)	109.24(16)	C(2)-C(1)-N(1)	115.4(4)	C(26)-C(25)-N(2)	115.8(5)
O(15)-P(6)-O(14)	112.0(2)	C(7)-C(2)-C(3)	119.6(5)	C(50)-O(50)-H(50)	106(7)
O(15)-P(6)-O(13)	107.3(2)	C(7)-C(2)-C(1)	120.6(5)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for bzte2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	5(1)	6(1)	8(1)	0(1)	0(1)	0(1)
Pt(2)	5(1)	6(1)	7(1)	0(1)	0(1)	0(1)
P(1)	5(1)	10(1)	15(1)	-2(1)	-1(1)	1(1)
P(2)	7(1)	9(1)	13(1)	-4(1)	-1(1)	4(1)
P(3)	12(1)	9(1)	7(1)	1(1)	-1(1)	-1(1)
P(4)	13(1)	7(1)	10(1)	2(1)	0(1)	-2(1)
P(5)	7(1)	8(1)	14(1)	-2(1)	-1(1)	1(1)
P(6)	5(1)	10(1)	14(1)	-1(1)	-2(1)	2(1)
P(7)	10(1)	9(1)	13(1)	2(1)	0(1)	-3(1)
P(8)	12(1)	11(1)	6(1)	2(1)	-1(1)	-3(1)
O(1)	5(2)	22(2)	23(2)	1(2)	3(2)	-3(2)
O(2)	11(2)	20(2)	16(2)	-1(2)	-2(2)	5(2)
O(3)	10(2)	16(2)	15(2)	-8(2)	-2(2)	0(2)
O(4)	17(2)	28(3)	17(2)	-7(2)	1(2)	5(2)
O(5)	12(2)	11(2)	27(2)	0(2)	-1(2)	3(2)
O(6)	19(2)	15(2)	11(2)	6(2)	-2(2)	1(2)
O(7)	20(2)	18(2)	6(2)	-2(1)	0(2)	0(2)
O(8)	12(2)	11(2)	9(2)	-4(2)	-2(2)	-4(2)
O(9)	21(2)	10(2)	22(2)	2(2)	3(2)	0(2)
O(10)	10(2)	23(2)	17(2)	4(2)	1(2)	-5(2)
O(11)	17(2)	19(2)	12(2)	-6(2)	-1(2)	3(2)
O(12)	18(2)	8(2)	30(2)	4(2)	2(2)	2(2)
O(13)	15(2)	9(2)	17(2)	-5(2)	-3(2)	0(2)
O(14)	2(2)	18(2)	26(2)	1(2)	-1(2)	0(2)
O(15)	15(2)	12(2)	20(2)	-1(2)	-1(2)	4(2)
O(16)	18(2)	13(2)	24(2)	6(2)	0(2)	-1(2)
O(17)	7(2)	24(2)	23(2)	4(2)	4(2)	-5(2)
O(18)	22(2)	17(2)	14(2)	-2(2)	-1(2)	-8(2)
O(19)	14(2)	19(2)	16(2)	6(2)	-2(2)	0(2)
O(20)	20(2)	20(2)	7(2)	-2(2)	-1(2)	1(2)
N(1)	8(2)	9(2)	8(2)	-2(2)	-2(2)	0(2)
C(1)	12(3)	10(3)	16(2)	1(2)	1(3)	-2(2)
C(2)	14(3)	7(3)	12(3)	0(2)	4(2)	-6(2)
C(3)	19(3)	8(3)	20(3)	-2(3)	4(3)	-4(2)
C(4)	36(4)	8(3)	31(4)	-4(2)	12(3)	-5(3)
C(5)	20(4)	11(3)	54(5)	7(3)	18(3)	1(3)
C(6)	18(3)	14(3)	41(5)	14(3)	3(3)	2(2)
C(7)	19(3)	10(3)	21(3)	5(2)	6(2)	-1(2)
C(8)	17(3)	13(3)	10(2)	1(3)	5(3)	-1(2)
C(9)	22(3)	12(3)	19(3)	4(2)	3(2)	-2(3)
C(10)	11(3)	10(3)	20(3)	-4(2)	1(3)	4(2)
C(11)	11(3)	14(3)	24(3)	-1(2)	-2(2)	1(2)
C(12)	8(3)	9(3)	21(3)	-3(2)	-5(2)	1(2)
C(13)	23(4)	17(3)	23(3)	-7(2)	-10(3)	2(3)
N(2)	5(2)	8(2)	20(2)	-3(2)	-4(2)	-1(2)
C(14)	11(3)	19(3)	20(3)	-3(2)	0(2)	-2(2)
C(15)	6(2)	10(3)	18(3)	-1(2)	-1(2)	-1(2)
C(16)	14(3)	15(3)	20(3)	1(2)	-2(2)	1(3)
C(17)	20(3)	25(3)	23(3)	-2(3)	1(3)	0(3)
C(18)	10(3)	22(3)	37(4)	-11(3)	-10(3)	5(3)
C(19)	18(3)	7(3)	46(4)	1(3)	-16(4)	2(2)
C(20)	13(3)	20(3)	22(3)	6(3)	-3(2)	-3(3)
C(21)	6(3)	21(3)	19(3)	3(2)	1(2)	0(2)
C(22)	14(3)	21(3)	26(3)	7(3)	0(3)	1(3)
C(23)	18(3)	12(3)	31(3)	-8(3)	6(3)	-3(2)
C(24)	38(5)	27(4)	32(4)	-13(3)	6(3)	0(3)
C(25)	12(3)	9(3)	19(3)	-2(2)	3(2)	3(2)
C(26)	11(3)	18(3)	32(4)	-1(2)	4(2)	-4(2)
O(50)	69(5)	23(3)	47(3)	13(3)	8(3)	15(3)

C(50)	36(4)	25(4)	40(5)	7(3)	11(4)	5(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bzte2.

	x	y	z	U(eq)
H(2)	7471	3283	4582	23
H(4)	8302	3537	9746	31
H(7)	8724	2672	1941	22
H(9)	8734	4220	5523	26
H(10)	10440	3471	5660	25
H(11)	9250	1792	3142	24
H(14)	11032	2580	6700	23
H(16)	8961	1047	7486	27
H(17)	7189	1683	7408	27
H(19)	9740	1949	9186	24
H(1A)	10155	6806	6045	15
H(1B)	9816	6764	4624	15
H(3)	9616	7345	7870	19
H(4)	8848	8106	8502	30
H(5)	8056	8446	6986	34
H(6)	8029	8042	4847	29
H(7)	8766	7260	4233	20
H(8A)	9752	6159	7856	16
H(8B)	8994	6262	7544	16
H(9A)	9135	5358	8779	27
H(9B)	9610	5081	7667	27
H(9C)	8849	5184	7353	27
H(10A)	10250	5736	4601	16
H(10B)	9948	5198	5494	16
H(11A)	11039	5383	6117	25
H(11B)	10566	5553	7328	25
H(11C)	10870	6091	6431	25
H(12A)	8799	5449	5365	15
H(12B)	8577	6156	5293	15
H(13A)	8615	5733	3174	31
H(13B)	9372	5563	3363	31
H(13C)	9149	6272	3290	31
H(14A)	7953	119	426	20
H(14B)	7837	-330	1659	20
H(16)	7538	102	3827	20
H(17)	7104	928	5027	27
H(18)	7031	1912	4054	28
H(19)	7419	2066	1903	29
H(20)	7882	1243	707	22
H(21A)	8829	246	3493	19
H(21B)	9464	-133	3055	19
H(22A)	8839	-719	4551	31
H(22B)	8860	-1065	3152	31
H(22C)	8221	-686	3581	31
H(23A)	9476	-689	978	25
H(23B)	8744	-949	1035	25
H(24A)	9100	-900	-1177	48
H(24B)	9233	-174	-1033	48
H(24C)	8500	-433	-974	48
H(25A)	8983	644	124	16
H(25B)	9003	912	1594	16
H(26A)	10048	932	672	31
H(26B)	10022	201	430	31
H(26C)	10043	468	1906	31
H(50)	7960(60)	4290(50)	3450(100)	70
H(50A)	7132	4928	2136	51
H(50B)	7580	4369	1633	51
H(50C)	7866	5058	1656	51

Table 6. Hydrogen bonds for bzte2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(6)	0.84	1.68	2.516(6)	174.0
O(4)-H(4)...O(20)	0.84	1.80	2.612(6)	162.3
O(7)-H(7)...O(20)#1	0.84	1.66	2.468(5)	159.3
O(9)-H(9)...O(5)	0.84	1.77	2.417(6)	132.5
O(10)-H(10)...O(14)	0.84	1.81	2.630(6)	163.5
O(11)-H(11)...O(7)	0.84	1.80	2.617(6)	164.8
O(14)-H(14)...O(1)#2	0.84	1.74	2.491(6)	147.3
O(16)-H(16)...O(12)	0.84	1.94	2.440(6)	117.3
O(17)-H(17)...O(1)	0.84	1.79	2.609(6)	164.7
O(19)-H(19)...O(15)	0.84	1.65	2.483(6)	172.9
O(50)-H(50)...O(6)	0.87(11)	2.07(11)	2.926(7)	167(11)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x+1/2,-y+1/2,z

Crystallographic data of Bu1 crystal light-off stage measured at laboratory system

Table 1. Crystal data and structure refinement for bu1-off.

Identification code	e2off-100	
Empirical formula	C32 H82 N2 O20 P8 Pt2	
Formula weight	1452.94	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 12.40780(10) Å	α= 96.0435(8)°.
	b = 12.4747(2) Å	β= 91.3580(8)°.
	c = 9.64630(10) Å	γ = 116.8715(3)°.
Volume	1320.18(3) Å^3	
Z	1	
Density (calculated)	1.828 Mg/m^3	
Absorption coefficient	5.604 mm^{-1}	
F(000)	724	
Crystal size	0.12 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.85 to 27.48°.	
Index ranges	-16<=h<=16, -13<=k<=16, -12<=l<=12	
Reflections collected	9357	
Independent reflections	5883 [Rint = 0.0281]	
Completeness to θ = 27.48°	97.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8599	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5883 / 0 / 289	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2σ(I)]	R1 = 0.0284, wR2 = 0.0700	
R indices (all data)	R1 = 0.0319, wR2 = 0.0716	
Largest diff. peak and hole	1.604 and -1.652 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bu1-off. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	978(1)	1016(1)	902(1)	11(1)
P(1)	-176(1)	2061(1)	979(1)	16(1)
P(2)	1869(1)	1916(1)	-1043(1)	17(1)
P(3)	2212(1)	42(1)	706(1)	17(1)
P(4)	63(1)	151(1)	2857(1)	14(1)
O(1)	-275(3)	2617(3)	2496(3)	22(1)
O(2)	168(3)	3097(3)	102(3)	28(1)
O(3)	1680(3)	2992(3)	-1396(3)	27(1)
O(4)	3260(3)	2325(3)	-1052(3)	26(1)
O(5)	3463(3)	763(3)	241(3)	24(1)
O(6)	2375(3)	-534(3)	2040(3)	31(1)
O(7)	682(3)	-500(3)	3616(3)	21(1)
O(8)	-128(3)	1033(3)	3966(3)	18(1)
O(9)	-1589(3)	1132(3)	517(3)	21(1)
O(10)	1316(3)	886(3)	-2419(3)	20(1)
N(1)	3356(3)	6711(3)	-2351(3)	16(1)
C(1)	4644(4)	6877(4)	-2454(4)	19(1)
C(2)	5067(4)	6903(5)	-3917(5)	33(1)
C(3)	6359(5)	7166(7)	-3938(6)	50(2)
C(4)	6887(5)	7169(6)	-5273(6)	50(2)
C(5)	3179(4)	7673(4)	-3030(4)	19(1)
C(6)	4120(4)	8983(4)	-2586(6)	31(1)
C(7)	3862(5)	9853(4)	-3337(5)	31(1)
C(8)	4894(5)	11152(4)	-2975(6)	37(1)
C(9)	3110(4)	6825(4)	-808(4)	23(1)
C(10)	3332(4)	5976(4)	47(5)	26(1)
C(11)	2677(5)	5859(5)	1385(5)	36(1)
C(12)	2991(6)	5112(6)	2328(6)	52(2)
C(13)	2486(4)	5454(4)	-3109(4)	20(1)
C(14)	1140(4)	5020(4)	-2955(4)	20(1)
C(15)	435(4)	3844(4)	-3958(5)	22(1)
C(16)	-916(4)	3236(4)	-3779(5)	29(1)

Table 3. Bond lengths [Å] and angles [°] for bu1-off

Pt(1)-P(2)	2.3282(10)	P(2)-O(4)	1.565(3)	O(9)-O(9)#1	5.847(6)
Pt(1)-P(1)	2.3291(10)	P(2)-O(10)	1.639(3)	O(10)-P(4)#1	1.621(3)
Pt(1)-P(4)	2.3308(10)	P(3)-O(5)	1.509(3)	O(10)-O(10)#1	5.805(6)
Pt(1)-P(3)	2.3472(10)	P(3)-O(6)	1.589(3)	N(1)-C(5)	1.521(5)
Pt(1)-Pt(1)#1	2.9419(3)	P(3)-O(9)#1	1.644(3)	N(1)-C(1)	1.524(5)
P(1)-O(2)	1.523(3)	P(4)-O(8)	1.554(3)	N(1)-C(9)	1.531(5)
P(1)-O(1)	1.584(3)	P(4)-O(7)	1.565(3)	N(1)-C(13)	1.533(5)
P(1)-O(9)	1.623(3)	P(4)-O(10)#1	1.621(3)	C(1)-C(2)	1.516(6)
P(2)-O(3)	1.532(3)	O(9)-P(3)#1	1.644(3)	C(2)-C(3)	1.485(7)

C(3)-C(4)	1.458(8)	O(1)-P(1)-Pt(1)	114.90(12)	P(2)-O(10)-O(10)#1	69.05(10)
C(5)-C(6)	1.524(6)	O(9)-P(1)-Pt(1)	110.26(11)	C(5)-N(1)-C(1)	111.1(3)
C(6)-C(7)	1.508(6)	O(3)-P(2)-O(4)	106.41(19)	C(5)-N(1)-C(9)	108.3(3)
C(7)-C(8)	1.539(7)	O(3)-P(2)-O(10)	106.28(17)	C(1)-N(1)-C(9)	109.3(3)
C(9)-C(10)	1.522(6)	O(4)-P(2)-O(10)	102.20(16)	C(5)-N(1)-C(13)	109.4(3)
C(10)-C(11)	1.526(6)	O(3)-P(2)-Pt(1)	117.35(13)	C(1)-N(1)-C(13)	107.9(3)
C(11)-C(12)	1.527(8)	O(4)-P(2)-Pt(1)	115.09(13)	C(9)-N(1)-C(13)	110.9(3)
C(13)-C(14)	1.522(6)	O(10)-P(2)-Pt(1)	108.12(11)	C(2)-C(1)-N(1)	115.6(3)
C(14)-C(15)	1.534(5)	O(5)-P(3)-O(6)	106.73(18)	C(3)-C(2)-C(1)	113.0(4)
C(15)-C(16)	1.519(6)	O(5)-P(3)-O(9)#1	103.28(16)	C(4)-C(3)-C(2)	119.6(5)
		O(6)-P(3)-O(9)#1	103.32(18)	N(1)-C(5)-C(6)	116.5(3)
P(2)-Pt(1)-P(1)	90.01(4)	O(5)-P(3)-Pt(1)	116.50(13)	C(7)-C(6)-C(5)	111.8(4)
P(2)-Pt(1)-P(4)	178.45(4)	O(6)-P(3)-Pt(1)	116.29(13)	C(6)-C(7)-C(8)	110.5(4)
P(1)-Pt(1)-P(4)	88.46(4)	O(9)#1-P(3)-Pt(1)	109.16(11)	C(10)-C(9)-N(1)	114.8(3)
P(2)-Pt(1)-P(3)	86.15(4)	O(8)-P(4)-O(7)	108.49(15)	C(9)-C(10)-C(11)	109.9(4)
P(1)-Pt(1)-P(3)	176.12(4)	O(8)-P(4)-O(10)#1	101.95(16)	C(10)-C(11)-C(12)	110.7(5)
P(4)-Pt(1)-P(3)	95.38(4)	O(7)-P(4)-O(10)#1	104.89(17)	C(14)-C(13)-N(1)	116.8(3)
P(2)-Pt(1)-Pt(1)#1	91.04(3)	O(8)-P(4)-Pt(1)	114.29(12)	C(13)-C(14)-C(15)	108.0(3)
P(1)-Pt(1)-Pt(1)#1	89.72(3)	O(7)-P(4)-Pt(1)	115.55(12)	C(16)-C(15)-C(14)	113.1(4)
P(4)-Pt(1)-Pt(1)#1	89.21(3)	O(10)#1-P(4)-Pt(1)	110.42(11)		
P(3)-Pt(1)-Pt(1)#1	90.87(3)	P(1)-O(9)-P(3)#1	130.79(19)		
O(2)-P(1)-O(1)	104.68(17)	P(1)-O(9)-O(9)#1	67.54(10)		
O(2)-P(1)-O(9)	106.29(18)	P(3)#1-O(9)-O(9)#1	68.82(10)		
O(1)-P(1)-O(9)	100.89(16)	P(4)#1-O(10)-P(2)	129.85(19)		
O(2)-P(1)-Pt(1)	118.14(14)	P(4)#1-O(10)-O(10)#1	67.83(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for bu1-off. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	12(1)	12(1)	8(1)	2(1)	1(1)	4(1)
P(1)	18(1)	15(1)	16(1)	3(1)	2(1)	8(1)
P(2)	18(1)	16(1)	13(1)	5(1)	5(1)	3(1)
P(3)	15(1)	22(1)	14(1)	2(1)	0(1)	9(1)
P(4)	18(1)	16(1)	8(1)	4(1)	3(1)	8(1)
O(1)	33(2)	21(2)	17(1)	-1(1)	2(1)	16(1)
O(2)	38(2)	24(2)	27(2)	10(1)	5(1)	18(2)
O(3)	37(2)	19(2)	22(2)	9(1)	7(1)	9(1)
O(4)	18(2)	31(2)	21(2)	8(1)	6(1)	3(1)
O(5)	16(1)	30(2)	23(2)	-1(1)	0(1)	9(1)
O(6)	29(2)	50(2)	25(2)	16(2)	3(1)	26(2)
O(7)	29(2)	29(2)	12(1)	7(1)	4(1)	19(1)
O(8)	25(2)	20(2)	9(1)	2(1)	2(1)	10(1)
O(9)	17(1)	20(2)	27(2)	-2(1)	1(1)	10(1)
O(10)	21(2)	22(2)	10(1)	4(1)	5(1)	4(1)
N(1)	17(2)	14(2)	16(2)	1(1)	-1(1)	6(1)
C(1)	17(2)	19(2)	21(2)	2(2)	0(2)	8(2)
C(2)	20(2)	57(3)	22(2)	4(2)	3(2)	17(2)
C(3)	28(3)	96(5)	35(3)	6(3)	1(2)	37(3)
C(4)	33(3)	74(4)	42(3)	6(3)	16(3)	24(3)
C(5)	18(2)	17(2)	21(2)	4(2)	-1(2)	7(2)
C(6)	25(2)	18(2)	47(3)	9(2)	-4(2)	5(2)
C(7)	40(3)	26(2)	30(2)	5(2)	5(2)	17(2)
C(8)	44(3)	21(2)	48(3)	11(2)	17(2)	13(2)
C(9)	27(2)	26(2)	15(2)	-2(2)	2(2)	12(2)
C(10)	29(2)	25(2)	19(2)	3(2)	2(2)	8(2)
C(11)	44(3)	28(3)	21(2)	2(2)	8(2)	5(2)
C(12)	59(4)	56(4)	26(3)	20(3)	4(3)	11(3)
C(13)	19(2)	18(2)	18(2)	-1(2)	-1(2)	5(2)
C(14)	19(2)	16(2)	21(2)	0(2)	3(2)	6(2)
C(15)	21(2)	19(2)	22(2)	2(2)	1(2)	5(2)
C(16)	22(2)	26(2)	34(3)	5(2)	-3(2)	8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for bu1-off.

	x	y	z	U(eq)
H(1)	-463	2086	3038	34
H(2)	235	2859	-724	42
H(4)	3404	1757	-862	39
H(6)	1694	-946	2329	46
H(8)	-175	788	4751	27
H(1A)	5205	7645	-1875	23
H(1B)	4707	6209	-2047	23
H(2A)	4558	6109	-4481	40
H(2B)	4951	7528	-4360	40
H(3A)	6849	7972	-3389	60
H(3B)	6464	6566	-3430	60
H(4A)	6371	6416	-5883	74
H(4B)	7697	7230	-5114	74
H(4C)	6948	7863	-5718	74

H(5A)	2372	7600	-2825	23	H(11B)	2916	6675	1892	43
H(5B)	3168	7492	-4056	23	H(12A)	2855	4345	1789	78
H(6A)	4125	9187	-1565	38	H(12B)	2474	4946	3112	78
H(6B)	4933	9073	-2787	38	H(12C)	3843	5567	2688	78
H(7A)	3088	9828	-3061	37	H(13A)	2615	5453	-4118	24
H(7B)	3779	9607	-4359	37	H(13B)	2712	4856	-2767	24
H(8A)	5041	11359	-1957	56	H(14A)	904	5643	-3186	24
H(8B)	4664	11721	-3366	56	H(14B)	957	4870	-1980	24
H(8C)	5633	11204	-3373	56	H(15A)	561	4028	-4933	27
H(9A)	3630	7670	-378	27	H(15B)	764	3273	-3801	27
H(9B)	2256	6667	-754	27	H(16A)	-1050	3026	-2826	43
H(10A)	4212	6297	286	31	H(16B)	-1319	2498	-4451	43
H(10B)	3032	5168	-509	31	H(16C)	-1251	3792	-3945	43
H(11A)	1791	5463	1145	43					

Table 6. Hydrogen bonds for bu1-off [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.84	1.85	2.616(4)	151.2
O(2)-H(2)...O(3)	0.84	1.86	2.436(5)	124.3
O(4)-H(4)...O(5)	0.84	1.74	2.520(5)	153.4
O(6)-H(6)...O(7)	0.84	2.00	2.635(5)	132.2
O(8)-H(8)...O(7)#2	0.84	1.72	2.519(4)	157.3

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,-y,-z+1

Crystallographic data of Bu1 crystal light-on stage measured at laboratory system

Table 1. Crystal data and structure refinement for bu1-on.

Identification code	e2on-100-3	
Empirical formula	C32 H82 N2 O20 P8 Pt2	
Formula weight	1452.94	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 12.3768(3) Å	α= 95.9963(6)°.
	b = 12.4443(3) Å	β= 91.3709(8)°.
	c = 9.6268(2) Å	γ = 116.7862(8)°.
Volume	1312.16(5) Å^3	
Z	1	
Density (calculated)	1.839 Mg/m^3	
Absorption coefficient	5.639 mm^{-1}	
F(000)	724	
Crystal size	0.12 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.85 to 27.48°.	
Index ranges	-15<=h<=16, -13<=k<=16, -12<=l<=12	
Reflections collected	9268	
Independent reflections	5821 [Rint = 0.0257]	
Completeness to θ = 27.48°	96.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.0000 and 0.8193	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5821 / 0 / 289	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2σ(I)]	R1 = 0.0274, wR2 = 0.0669	
R indices (all data)	R1 = 0.0305, wR2 = 0.0684	
Largest diff. peak and hole	1.480 and -1.385 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for bu1-on. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	978(1)	1016(1)	902(1)	11(1)
P(1)	-176(1)	2060(1)	979(1)	16(1)
P(2)	1869(1)	1914(1)	-1043(1)	17(1)
P(3)	2210(1)	40(1)	707(1)	17(1)
P(4)	63(1)	152(1)	2856(1)	14(1)
O(1)	-279(3)	2616(3)	2495(3)	23(1)
O(2)	175(3)	3101(3)	105(3)	27(1)
O(3)	1676(3)	2988(3)	-1396(3)	26(1)
O(4)	3260(3)	2324(3)	-1048(3)	27(1)
O(5)	3464(3)	759(3)	244(3)	24(1)
O(6)	2375(3)	-532(3)	2037(3)	31(1)
O(7)	688(3)	-493(3)	3615(3)	21(1)
O(8)	-132(3)	1032(2)	3973(3)	18(1)
O(9)	-1584(3)	1135(3)	514(3)	21(1)
O(10)	1319(3)	889(3)	-2420(3)	20(1)
N(1)	3360(3)	6710(3)	-2352(3)	17(1)
C(1)	4649(4)	6878(4)	-2452(4)	19(1)
C(2)	5068(4)	6902(5)	-3910(5)	35(1)
C(3)	6352(5)	7161(7)	-3942(6)	49(2)
C(4)	6893(5)	7174(6)	-5273(6)	52(2)
C(5)	3178(4)	7676(4)	-3035(4)	20(1)
C(6)	4122(4)	8988(4)	-2575(6)	32(1)
C(7)	3863(5)	9861(4)	-3333(5)	31(1)
C(8)	4889(5)	11146(4)	-2979(6)	39(1)
C(9)	3111(4)	6827(4)	-811(4)	23(1)
C(10)	3333(4)	5973(4)	48(4)	25(1)
C(11)	2678(5)	5863(5)	1389(5)	36(1)
C(12)	2981(6)	5112(6)	2338(6)	54(2)
C(13)	2493(4)	5456(3)	-3105(4)	19(1)
C(14)	1139(4)	5017(3)	-2946(4)	20(1)
C(15)	439(4)	3842(4)	-3963(4)	23(1)
C(16)	-916(4)	3245(4)	-3769(5)	29(1)

Table 3. Bond lengths [Å] and angles [°] for bu1-on.

Pt(1)-P(1)	2.3213(10)	P(2)-O(10)	1.634(3)	O(10)-O(10)#1	5.800(5)
Pt(1)-P(2)	2.3223(10)	P(3)-O(5)	1.507(3)	N(1)-C(1)	1.520(5)
Pt(1)-P(4)	2.3248(9)	P(3)-O(6)	1.580(3)	N(1)-C(13)	1.526(5)
Pt(1)-P(3)	2.3393(10)	P(3)-O(9)#1	1.642(3)	N(1)-C(5)	1.527(5)
Pt(1)-Pt(1)#1	2.9381(3)	P(4)-O(8)	1.555(3)	N(1)-C(9)	1.527(5)
P(1)-O(2)	1.521(3)	P(4)-O(7)	1.560(3)	C(1)-C(2)	1.507(6)
P(1)-O(1)	1.582(3)	P(4)-O(10)#1	1.623(3)	C(2)-C(3)	1.474(7)
P(1)-O(9)	1.616(3)	O(9)-P(3)#1	1.642(3)	C(3)-C(4)	1.459(8)
P(2)-O(3)	1.529(3)	O(9)-O(9)#1	5.824(5)	C(5)-C(6)	1.526(6)
P(2)-O(4)	1.561(3)	O(10)-P(4)#1	1.623(3)	C(6)-C(7)	1.511(6)

C(7)-C(8)	1.524(7)	O(3)-P(2)-O(4)	106.46(18)	P(2)-O(10)-O(10)#1	68.94(10)
C(9)-C(10)	1.525(6)	O(3)-P(2)-O(10)	106.09(17)	C(1)-N(1)-C(13)	108.1(3)
C(10)-C(11)	1.526(6)	O(4)-P(2)-O(10)	102.34(16)	C(1)-N(1)-C(5)	111.1(3)
C(11)-C(12)	1.526(8)	O(3)-P(2)-Pt(1)	117.17(13)	C(13)-N(1)-C(5)	109.3(3)
C(13)-C(14)	1.528(5)	O(4)-P(2)-Pt(1)	115.09(13)	C(1)-N(1)-C(9)	109.3(3)
C(14)-C(15)	1.538(5)	O(10)-P(2)-Pt(1)	108.34(11)	C(13)-N(1)-C(9)	110.9(3)
C(15)-C(16)	1.524(6)	O(5)-P(3)-O(6)	106.42(18)	C(5)-N(1)-C(9)	108.0(3)
P(1)-Pt(1)-P(2)	90.12(4)	O(5)-P(3)-O(9)#1	103.42(16)	C(2)-C(1)-N(1)	115.4(3)
P(1)-Pt(1)-P(4)	88.40(4)	O(6)-P(3)-O(9)#1	103.36(18)	C(3)-C(2)-C(1)	113.3(4)
P(2)-Pt(1)-P(4)	178.50(3)	O(5)-P(3)-Pt(1)	116.64(13)	C(4)-C(3)-C(2)	120.5(5)
P(1)-Pt(1)-P(3)	176.18(4)	O(6)-P(3)-Pt(1)	116.33(13)	C(6)-C(5)-N(1)	115.9(3)
P(2)-Pt(1)-P(3)	86.09(4)	O(9)#1-P(3)-Pt(1)	109.12(11)	C(7)-C(6)-C(5)	111.3(4)
P(4)-Pt(1)-P(3)	95.38(4)	O(8)-P(4)-O(7)	108.19(15)	C(6)-C(7)-C(8)	110.3(4)
P(1)-Pt(1)-Pt(1)#1	89.74(3)	O(8)-P(4)-O(10)#1	101.84(15)	C(10)-C(9)-N(1)	114.6(3)
P(2)-Pt(1)-Pt(1)#1	91.03(3)	O(7)-P(4)-O(10)#1	105.04(16)	C(9)-C(10)-C(11)	109.6(4)
P(4)-Pt(1)-Pt(1)#1	89.21(2)	O(8)-P(4)-Pt(1)	114.62(11)	C(10)-C(11)-C(12)	110.9(5)
P(3)-Pt(1)-Pt(1)#1	90.81(3)	O(7)-P(4)-Pt(1)	115.35(12)	N(1)-C(13)-C(14)	116.9(3)
O(2)-P(1)-O(1)	104.51(17)	O(10)#1-P(4)-Pt(1)	110.54(11)	C(13)-C(14)-C(15)	107.7(3)
O(2)-P(1)-O(9)	106.55(17)	P(1)-O(9)-P(3)#1	131.06(19)	C(16)-C(15)-C(14)	112.0(4)
O(1)-P(1)-O(9)	100.92(16)	P(1)-O(9)-O(9)#1	67.67(10)		
O(2)-P(1)-Pt(1)	117.92(13)	P(3)#1-O(9)-O(9)#1	68.87(10)		
O(1)-P(1)-Pt(1)	115.06(12)	P(4)#1-O(10)-P(2)	129.72(18)		
O(9)-P(1)-Pt(1)	110.24(11)	P(4)#1-O(10)-O(10)#1	67.68(10)		

Symmetry transformations:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for bu1-on. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	12(1)	12(1)	8(1)	2(1)	1(1)	4(1)
P(1)	19(1)	15(1)	16(1)	2(1)	2(1)	8(1)
P(2)	19(1)	17(1)	12(1)	4(1)	4(1)	3(1)
P(3)	15(1)	22(1)	14(1)	2(1)	1(1)	9(1)
P(4)	19(1)	15(1)	7(1)	3(1)	3(1)	8(1)
O(1)	31(2)	21(2)	18(1)	0(1)	2(1)	14(1)
O(2)	36(2)	22(2)	28(2)	12(1)	6(1)	16(1)
O(3)	38(2)	17(1)	21(2)	10(1)	8(1)	9(1)
O(4)	20(2)	31(2)	24(2)	9(1)	6(1)	4(1)

O(5)	17(1)	29(2)	23(2)	-1(1)	0(1)	9(1)
O(6)	29(2)	49(2)	25(2)	15(1)	4(1)	26(2)
O(7)	29(2)	27(2)	13(1)	10(1)	8(1)	17(1)
O(8)	26(2)	19(1)	10(1)	2(1)	5(1)	12(1)
O(9)	18(1)	20(1)	25(2)	-3(1)	-1(1)	9(1)
O(10)	21(1)	24(2)	10(1)	4(1)	6(1)	5(1)
N(1)	18(2)	16(2)	17(2)	2(1)	1(1)	7(1)
C(1)	17(2)	19(2)	19(2)	2(2)	1(2)	8(2)
C(2)	22(2)	62(3)	21(2)	2(2)	3(2)	20(2)
C(3)	27(3)	92(5)	31(3)	0(3)	1(2)	33(3)
C(4)	35(3)	80(5)	43(3)	6(3)	13(3)	29(3)
C(5)	20(2)	19(2)	23(2)	5(2)	1(2)	10(2)
C(6)	25(2)	24(2)	43(3)	8(2)	-4(2)	9(2)
C(7)	40(3)	30(2)	28(2)	7(2)	6(2)	19(2)
C(8)	47(3)	27(2)	49(3)	10(2)	19(3)	19(2)
C(9)	26(2)	24(2)	15(2)	1(2)	2(2)	9(2)
C(10)	31(2)	21(2)	17(2)	4(2)	3(2)	6(2)
C(11)	43(3)	31(3)	20(2)	6(2)	8(2)	5(2)
C(12)	63(4)	60(4)	24(3)	19(3)	4(3)	11(3)
C(13)	19(2)	17(2)	17(2)	-1(1)	1(2)	6(2)
C(14)	19(2)	16(2)	22(2)	1(2)	4(2)	6(2)
C(15)	23(2)	21(2)	20(2)	-2(2)	-1(2)	6(2)
C(16)	21(2)	26(2)	36(3)	5(2)	-2(2)	7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bu1-on.

	x	y	z	U(eq)
H(1)	-471	2082	3038	34
H(2)	246	2865	-722	40
H(4)	3405	1755	-859	41
H(6)	1693	-943	2330	46
H(7)	241	-884	4214	31
H(1A)	5209	7649	-1874	22
H(1B)	4715	6212	-2040	22
H(2A)	4556	6106	-4472	42
H(2B)	4949	7527	-4354	42
H(3A)	6842	7965	-3386	58
H(3B)	6457	6557	-3437	58
H(4A)	6494	6361	-5805	78
H(4B)	7761	7419	-5096	78
H(4C)	6789	7751	-5813	78
H(5A)	3173	7501	-4063	24
H(5B)	2368	7601	-2833	24
H(6A)	4119	9187	-1553	38
H(6B)	4938	9079	-2770	38
H(7A)	3089	9840	-3055	38
H(7B)	3777	9612	-4356	38
H(8A)	5026	11361	-1959	59
H(8B)	4669	11715	-3391	59
H(8C)	5633	11188	-3359	59
H(9A)	3633	7673	-382	27
H(9B)	2256	6670	-758	27
H(10A)	4215	6291	287	30
H(10B)	3030	5162	-507	30
H(11A)	1790	5474	1147	43
H(11B)	2922	6683	1893	43
H(12A)	2879	4358	1791	81
H(12B)	2436	4918	3097	81

H(12C)	3824	5577	2737	81
H(13A)	2722	4857	-2763	23
H(13B)	2620	5454	-4116	23
H(14A)	899	5642	-3171	24
H(14B)	956	4860	-1970	24
H(15A)	565	4030	-4938	28
H(15B)	767	3267	-3808	28
H(16A)	-1045	3055	-2806	43
H(16B)	-1326	2495	-4424	43
H(16C)	-1250	3801	-3954	43

Table 6. Hydrogen bonds for bu1-on [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.84	1.85	2.615(4)	150.8
O(2)-H(2)...O(3)	0.84	1.85	2.425(5)	124.7
O(4)-H(4)...O(5)	0.84	1.74	2.517(5)	153.3
O(6)-H(6)...O(7)	0.84	1.99	2.626(4)	132.1
O(7)-H(7)...O(8)#2	0.84	1.78	2.510(4)	144.8

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,-y,-z+1

Crystallographic data of Pn1 crystal light-off stage measured at laboratory system

Table 1. Crystal data and structure refinement for pn1-off.

Identification code	off173K-1	
Empirical formula	C40 H98 N2 O20 P8 Pt2	
Formula weight	1565.14	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 9.69650(10) Å	α= 93.6649(4)°.
	b = 17.2492(3) Å	β= 90.9346(8)°.
	c = 18.7278(2) Å	γ = 102.8259(7)°.
Volume	3046.45(7) Å^3	
Z	2	
Density (calculated)	1.706 Mg/m^3	
Absorption coefficient	4.864 mm^{-1}	
F(000)	1576	
Crystal size	0.40 x 0.05 x 0.02 mm^3	
Theta range for data collection	1.09 to 27.48°.	
Index ranges	-12<=h<=12, -21<=k<=22, -24<=l<=16	
Reflections collected	21788	
Independent reflections	13755 [Rint = 0.0325]	
Completeness to θ = 27.48°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.907 and 0.741	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13755 / 0 / 670	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2σ(I)]	R1 = 0.0333, wR2 = 0.0712	
R indices (all data)	R1 = 0.0469, wR2 = 0.0765	
Largest diff. peak and hole	1.372 and -1.427 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for pn1-off. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4069(1)	9368(1)	380(1)	12(1)
P(1)	3783(1)	8509(1)	-649(1)	16(1)
P(2)	5997(1)	8872(1)	742(1)	18(1)
P(3)	4497(1)	10186(1)	1440(1)	17(1)
P(4)	2132(1)	9877(1)	33(1)	15(1)
O(1)	2204(4)	8090(2)	-883(2)	24(1)
O(2)	4577(4)	7839(2)	-686(2)	28(1)
O(3)	6200(4)	8097(2)	361(2)	29(1)
O(4)	6123(4)	8767(2)	1554(2)	26(1)
O(5)	5052(4)	9846(2)	2082(2)	25(1)
O(6)	3201(4)	10529(2)	1698(2)	28(1)
O(7)	1473(3)	10342(2)	607(2)	22(1)
O(8)	900(3)	9214(2)	-351(2)	22(1)
O(9)	4273(3)	9019(2)	-1335(2)	24(1)
O(10)	2557(3)	10458(2)	-617(2)	20(1)
Pt(2)	9107(1)	4709(1)	4351(1)	13(1)
P(5)	8596(1)	3428(1)	4753(1)	17(1)
P(6)	7194(1)	5048(1)	4923(1)	16(1)
P(7)	9734(1)	5967(1)	3906(1)	17(1)
P(8)	11005(1)	4334(1)	3784(1)	19(1)
O(11)	8821(3)	2776(2)	4212(2)	24(1)
O(12)	7068(4)	3118(2)	5044(2)	27(1)
O(13)	6055(3)	4370(2)	5180(2)	23(1)
O(14)	6435(3)	5576(2)	4461(2)	23(1)
O(15)	8459(3)	6323(2)	3630(2)	25(1)
O(16)	10795(4)	6087(2)	3316(2)	28(1)
O(17)	11729(4)	4859(2)	3200(2)	31(1)
O(18)	10714(4)	3470(2)	3454(2)	26(1)
O(19)	9648(3)	3382(2)	5428(2)	22(1)
O(20)	12263(3)	4341(2)	4382(2)	23(1)
N(1)	371(4)	7825(2)	1923(2)	20(1)
C(1)	140(5)	8655(3)	1804(3)	24(1)
C(2)	-469(6)	9072(3)	2417(3)	29(1)
C(3)	-481(5)	9927(3)	2241(3)	26(1)
C(4)	-1030(6)	10397(3)	2830(3)	35(1)
C(5)	-1126(6)	11234(3)	2640(3)	34(1)
C(6)	1341(5)	7853(3)	2583(3)	25(1)
C(7)	2745(6)	8437(4)	2577(3)	41(1)
C(8)	3719(6)	8360(3)	3221(3)	38(1)
C(9)	4145(6)	7578(4)	3216(3)	44(2)
C(10)	5369(7)	7588(4)	3739(4)	53(2)
C(11)	1033(5)	7564(3)	1244(3)	24(1)
C(12)	1366(6)	6737(3)	1208(3)	28(1)
C(13)	2370(6)	6674(3)	604(3)	30(1)
C(14)	2564(7)	5832(3)	428(3)	41(2)
C(15)	3699(7)	5795(4)	-114(4)	52(2)
C(16)	-1010(5)	7236(3)	2083(3)	24(1)
C(17)	-2149(6)	7072(4)	1496(3)	36(1)
C(18)	-3597(6)	6685(4)	1776(4)	47(2)
C(19)	-3739(6)	5865(4)	2006(4)	46(2)
C(20)	-5172(8)	5527(4)	2340(4)	62(2)
N(2)	4446(4)	2411(2)	3132(2)	16(1)
C(21)	3575(5)	2609(3)	3768(2)	19(1)
C(22)	2263(5)	1965(3)	3903(2)	22(1)
C(23)	1830(5)	2048(3)	4684(3)	23(1)
C(24)	508(5)	1428(3)	4840(3)	27(1)
C(25)	171(6)	1457(3)	5634(3)	35(1)
C(26)	3583(5)	2326(3)	2438(2)	21(1)
C(27)	3309(5)	3095(3)	2165(3)	22(1)

C(28)	2338(5)	2888(3)	1494(3)	28(1)
C(29)	2261(6)	3618(3)	1091(3)	35(1)
C(30)	1258(7)	3406(4)	438(3)	49(2)
C(31)	5752(5)	3095(2)	3134(3)	19(1)
C(32)	6769(5)	3047(3)	2531(3)	22(1)
C(33)	7595(5)	3892(3)	2396(3)	23(1)
C(34)	8716(5)	3887(3)	1831(3)	30(1)
C(35)	9376(6)	4730(3)	1617(3)	38(1)
C(36)	4878(5)	1615(3)	3201(3)	19(1)
C(37)	5501(5)	1525(3)	3931(3)	22(1)
C(38)	5847(6)	700(3)	3953(3)	34(1)
C(39)	6587(6)	619(3)	4662(4)	42(2)
C(40)	7103(7)	-153(4)	4695(4)	61(2)

Table 3. Bond lengths [Å] and angles [°] for pn1-off.

Pt(1)-P(1)	2.3281(12)	Pt(2)-P(6)	2.3226(11)	N(1)-C(1)	1.527(5)
Pt(1)-P(2)	2.3302(11)	Pt(2)-P(5)	2.3305(11)	N(1)-C(6)	1.533(6)
Pt(1)-P(3)	2.3368(12)	Pt(2)-P(7)	2.3318(11)	N(1)-C(16)	1.538(6)
Pt(1)-P(4)	2.3425(11)	Pt(2)-P(8)	2.3319(11)	C(1)-C(2)	1.512(6)
Pt(1)-Pt(1)#1	2.9622(3)	Pt(2)-Pt(2)#2	2.9470(3)	C(2)-C(3)	1.535(6)
P(1)-O(2)	1.523(3)	P(5)-O(11)	1.521(3)	C(3)-C(4)	1.501(7)
P(1)-O(1)	1.582(4)	P(5)-O(12)	1.578(3)	C(4)-C(5)	1.530(7)
P(1)-O(9)	1.621(3)	P(5)-O(19)	1.629(3)	C(6)-C(7)	1.503(7)
P(2)-O(3)	1.529(3)	P(6)-O(13)	1.529(3)	C(7)-C(8)	1.550(8)
P(2)-O(4)	1.548(4)	P(6)-O(14)	1.580(3)	C(8)-C(9)	1.495(8)
P(2)-O(10)#1	1.637(3)	P(6)-O(20)#2	1.625(4)	C(9)-C(10)	1.522(8)
P(3)-O(5)	1.511(3)	P(7)-O(16)	1.516(3)	C(11)-C(12)	1.528(6)
P(3)-O(6)	1.574(3)	P(7)-O(15)	1.590(3)	C(12)-C(13)	1.518(6)
P(3)-O(9)#1	1.630(3)	P(7)-O(19)#2	1.634(3)	C(13)-C(14)	1.522(7)
P(4)-O(7)	1.531(3)	P(8)-O(18)	1.540(4)	C(14)-C(15)	1.518(8)
P(4)-O(8)	1.585(3)	P(8)-O(17)	1.542(4)	C(16)-C(17)	1.513(7)
P(4)-O(10)	1.627(3)	P(8)-O(20)	1.640(4)	C(17)-C(18)	1.532(7)
O(1)-H(1)	0.80(6)	O(12)-H(12)	1.02(6)	C(18)-C(19)	1.481(8)
O(4)-H(4)	0.85(6)	O(17)-H(17)	0.93(6)	C(19)-C(20)	1.542(8)
O(6)-H(6)	1.05(6)	O(18)-H(18)	0.80(6)	N(2)-C(26)	1.515(6)
O(8)-H(8)	0.86(6)	O(19)-P(7)#2	1.634(3)	N(2)-C(31)	1.527(5)
O(9)-P(3)#1	1.630(3)	O(20)-P(6)#2	1.625(4)	N(2)-C(36)	1.534(5)
O(10)-P(2)#1	1.637(3)	N(1)-C(11)	1.520(6)	N(2)-C(21)	1.537(5)

C(21)-C(22)	1.528(6)	O(3)-P(2)-O(4)	106.1(2)	P(8)-Pt(2)-Pt(2)#2	90.69(3)
C(22)-C(23)	1.535(6)	O(3)-P(2)-O(10)#1	105.93(18)	O(11)-P(5)-O(12)	105.48(19)
C(23)-C(24)	1.522(7)	O(4)-P(2)-O(10)#1	101.80(18)	O(11)-P(5)-O(19)	104.30(18)
C(24)-C(25)	1.528(7)	O(3)-P(2)-Pt(1)	117.73(15)	O(12)-P(5)-O(19)	103.91(19)
C(26)-C(27)	1.526(6)	O(4)-P(2)-Pt(1)	115.57(14)	O(11)-P(5)-Pt(2)	115.01(13)
C(27)-C(28)	1.533(7)	O(10)#1-P(2)-Pt(1)	108.17(12)	O(12)-P(5)-Pt(2)	116.93(13)
C(28)-C(29)	1.522(7)	O(5)-P(3)-O(6)	106.6(2)	O(19)-P(5)-Pt(2)	109.94(12)
C(29)-C(30)	1.525(8)	O(5)-P(3)-O(9)#1	102.67(19)	O(13)-P(6)-O(14)	107.85(18)
C(31)-C(32)	1.522(6)	O(6)-P(3)-O(9)#1	103.63(19)	O(13)-P(6)-O(20)#2	106.51(19)
C(32)-C(33)	1.537(6)	O(5)-P(3)-Pt(1)	117.10(14)	O(14)-P(6)-O(20)#2	100.85(18)
C(33)-C(34)	1.530(6)	O(6)-P(3)-Pt(1)	114.61(14)	O(13)-P(6)-Pt(2)	117.44(13)
C(34)-C(35)	1.536(7)	O(9)#1-P(3)-Pt(1)	110.73(13)	O(14)-P(6)-Pt(2)	112.44(13)
C(36)-C(37)	1.517(7)	O(7)-P(4)-O(8)	107.92(18)	O(20)#2-P(6)-Pt(2)	110.31(12)
C(37)-C(38)	1.534(6)	O(7)-P(4)-O(10)	106.98(17)	O(16)-P(7)-O(15)	104.90(18)
C(38)-C(39)	1.528(8)	O(8)-P(4)-O(10)	100.12(17)	O(16)-P(7)-O(19)#2	107.88(19)
C(39)-C(40)	1.527(8)	O(7)-P(4)-Pt(1)	117.65(14)	O(15)-P(7)-O(19)#2	100.02(17)
		O(8)-P(4)-Pt(1)	112.49(13)	O(16)-P(7)-Pt(2)	118.04(14)
P(1)-Pt(1)-P(2)	89.76(4)	O(10)-P(4)-Pt(1)	110.13(11)	O(15)-P(7)-Pt(2)	115.87(13)
P(1)-Pt(1)-P(3)	175.62(4)	P(1)-O(1)-H(1)	114(4)	O(19)#2-P(7)-Pt(2)	108.43(12)
P(2)-Pt(1)-P(3)	85.87(4)	P(2)-O(4)-H(4)	105(4)	O(18)-P(8)-O(17)	105.9(2)
P(1)-Pt(1)-P(4)	91.14(4)	P(3)-O(6)-H(6)	112(3)	O(18)-P(8)-O(20)	101.97(19)
P(2)-Pt(1)-P(4)	179.09(4)	P(4)-O(8)-H(8)	118(4)	O(17)-P(8)-O(20)	105.1(2)
P(3)-Pt(1)-P(4)	93.23(4)	P(1)-O(9)-P(3)#1	132.8(2)	O(18)-P(8)-Pt(2)	115.68(14)
P(1)-Pt(1)-Pt(1)#1	90.65(3)	P(4)-O(10)-P(2)#1	130.7(2)	O(17)-P(8)-Pt(2)	117.49(14)
P(2)-Pt(1)-Pt(1)#1	91.38(3)	P(6)-Pt(2)-P(5)	92.75(4)	O(20)-P(8)-Pt(2)	109.12(12)
P(3)-Pt(1)-Pt(1)#1	89.67(3)	P(6)-Pt(2)-P(7)	90.90(4)	P(5)-O(12)-H(12)	108(3)
P(4)-Pt(1)-Pt(1)#1	88.74(3)	P(5)-Pt(2)-P(7)	176.33(4)	P(8)-O(17)-H(17)	108(4)
O(2)-P(1)-O(1)	104.75(19)	P(6)-Pt(2)-P(8)	178.52(4)	P(8)-O(18)-H(18)	113(4)
O(2)-P(1)-O(9)	105.66(19)	P(5)-Pt(2)-P(8)	85.80(4)	P(5)-O(19)-P(7)#2	130.70(19)
O(1)-P(1)-O(9)	101.01(18)	P(7)-Pt(2)-P(8)	90.55(4)	P(6)#2-O(20)-P(8)	130.0(2)
O(2)-P(1)-Pt(1)	118.40(15)	P(6)-Pt(2)-Pt(2)#2	89.61(3)	C(11)-N(1)-C(1)	105.6(3)
O(1)-P(1)-Pt(1)	115.91(14)	P(5)-Pt(2)-Pt(2)#2	89.96(3)	C(11)-N(1)-C(6)	111.6(4)
O(9)-P(1)-Pt(1)	109.30(13)	P(7)-Pt(2)-Pt(2)#2	90.40(3)	C(1)-N(1)-C(6)	110.4(4)

C(11)-N(1)-C(16)	112.0(4)	C(16)-C(17)-C(18)	111.7(5)	C(28)-C(29)-C(30)	111.9(5)
C(1)-N(1)-C(16)	112.3(4)	C(19)-C(18)-C(17)	115.6(5)	C(32)-C(31)-N(2)	116.0(4)
C(6)-N(1)-C(16)	105.0(3)	C(18)-C(19)-C(20)	113.6(5)	C(31)-C(32)-C(33)	109.3(4)
C(2)-C(1)-N(1)	116.7(4)	C(26)-N(2)-C(31)	111.7(3)	C(34)-C(33)-C(32)	112.3(4)
C(1)-C(2)-C(3)	109.8(4)	C(26)-N(2)-C(36)	106.5(3)	C(33)-C(34)-C(35)	111.8(4)
C(4)-C(3)-C(2)	113.7(4)	C(31)-N(2)-C(36)	110.6(3)	C(37)-C(36)-N(2)	114.2(4)
C(3)-C(4)-C(5)	113.9(4)	C(26)-N(2)-C(21)	110.5(3)	C(36)-C(37)-C(38)	110.1(4)
C(7)-C(6)-N(1)	115.3(4)	C(31)-N(2)-C(21)	106.1(3)	C(39)-C(38)-C(37)	111.1(5)
C(6)-C(7)-C(8)	111.7(4)	C(36)-N(2)-C(21)	111.4(3)	C(40)-C(39)-C(38)	114.2(6)
C(9)-C(8)-C(7)	114.2(5)	C(22)-C(21)-N(2)	114.9(4)		
C(8)-C(9)-C(10)	113.0(5)	C(21)-C(22)-C(23)	110.3(4)		
N(1)-C(11)-C(12)	117.2(4)	C(24)-C(23)-C(22)	112.3(4)		
C(13)-C(12)-C(11)	109.3(4)	C(23)-C(24)-C(25)	112.0(5)		
C(12)-C(13)-C(14)	113.8(4)	N(2)-C(26)-C(27)	116.3(4)		
C(15)-C(14)-C(13)	113.0(5)	C(26)-C(27)-C(28)	108.9(4)		
C(17)-C(16)-N(1)	116.0(4)	C(29)-C(28)-C(27)	112.6(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z

#2 -x+2,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pn1-off. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	8(1)	14(1)	14(1)	2(1)	0(1)	3(1)
P(1)	14(1)	16(1)	19(1)	0(1)	0(1)	4(1)
P(2)	12(1)	21(1)	23(1)	6(1)	-1(1)	7(1)
P(3)	13(1)	21(1)	15(1)	0(1)	2(1)	2(1)
P(4)	7(1)	19(1)	18(1)	0(1)	0(1)	4(1)
O(1)	17(2)	22(2)	33(2)	-4(2)	1(2)	5(1)
O(2)	33(2)	26(2)	30(2)	-7(2)	-5(2)	18(2)
O(3)	28(2)	26(2)	38(2)	-1(2)	-10(2)	17(2)
O(4)	22(2)	34(2)	26(2)	8(2)	-4(1)	11(2)
O(5)	26(2)	33(2)	15(2)	2(1)	-3(1)	4(2)
O(6)	18(2)	41(2)	24(2)	-12(2)	-3(1)	9(2)
O(7)	14(2)	30(2)	22(2)	-4(1)	1(1)	9(1)
O(8)	8(2)	25(2)	31(2)	-4(2)	-6(1)	5(1)
O(9)	23(2)	24(2)	21(2)	4(1)	2(1)	-5(1)
O(10)	9(2)	28(2)	23(2)	6(1)	-2(1)	6(1)
Pt(2)	7(1)	16(1)	16(1)	1(1)	0(1)	5(1)
P(5)	14(1)	15(1)	23(1)	1(1)	-1(1)	5(1)
P(6)	7(1)	21(1)	23(1)	5(1)	2(1)	7(1)
P(7)	14(1)	19(1)	21(1)	5(1)	0(1)	6(1)
P(8)	13(1)	23(1)	22(1)	1(1)	3(1)	9(1)
O(11)	22(2)	19(2)	31(2)	-2(1)	-1(1)	8(1)
O(12)	20(2)	13(2)	48(2)	3(2)	9(2)	1(1)
O(13)	12(2)	23(2)	37(2)	10(2)	5(1)	7(1)

O(14)	12(2)	29(2)	35(2)	13(2)	4(1)	13(1)
O(15)	19(2)	30(2)	30(2)	13(2)	1(1)	10(1)
O(16)	32(2)	31(2)	23(2)	16(2)	8(2)	9(2)
O(17)	26(2)	36(2)	35(2)	8(2)	14(2)	14(2)
O(18)	21(2)	29(2)	29(2)	-5(2)	5(2)	7(1)
O(19)	20(2)	17(2)	29(2)	5(1)	-8(1)	6(1)
O(20)	15(2)	30(2)	26(2)	-5(2)	0(1)	13(1)
N(1)	21(2)	22(2)	19(2)	5(2)	3(2)	8(2)
C(1)	30(3)	19(2)	25(3)	8(2)	2(2)	9(2)
C(2)	38(3)	34(3)	21(3)	8(2)	8(2)	21(2)
C(3)	28(3)	28(3)	24(3)	4(2)	2(2)	9(2)
C(4)	41(3)	37(3)	32(3)	3(2)	7(3)	19(3)
C(5)	41(3)	29(3)	35(3)	-4(2)	-5(3)	16(2)
C(6)	26(3)	25(2)	27(3)	9(2)	2(2)	11(2)
C(7)	38(3)	41(3)	40(3)	13(3)	-10(3)	-1(3)
C(8)	28(3)	41(3)	41(3)	3(3)	-8(3)	-2(2)
C(9)	35(3)	55(4)	44(4)	-2(3)	-16(3)	14(3)
C(10)	31(3)	66(4)	61(4)	4(4)	-17(3)	11(3)
C(11)	25(3)	26(2)	24(3)	6(2)	7(2)	12(2)
C(12)	34(3)	25(2)	29(3)	9(2)	9(2)	15(2)
C(13)	26(3)	31(3)	36(3)	3(2)	7(2)	13(2)
C(14)	48(4)	37(3)	46(4)	7(3)	14(3)	23(3)
C(15)	57(4)	56(4)	52(4)	-4(3)	16(3)	34(4)
C(16)	21(2)	28(2)	24(3)	9(2)	8(2)	9(2)
C(17)	25(3)	47(3)	39(3)	10(3)	0(2)	11(2)
C(18)	19(3)	58(4)	66(5)	11(4)	-3(3)	7(3)
C(19)	34(3)	46(3)	57(4)	0(3)	0(3)	6(3)
C(20)	52(4)	46(4)	85(6)	9(4)	17(4)	-3(3)
N(2)	15(2)	15(2)	19(2)	2(2)	2(2)	6(1)
C(21)	18(2)	23(2)	19(2)	2(2)	3(2)	13(2)
C(22)	17(2)	29(2)	19(2)	-1(2)	1(2)	6(2)
C(23)	19(2)	30(3)	22(2)	4(2)	1(2)	11(2)
C(24)	25(3)	37(3)	25(3)	8(2)	5(2)	14(2)
C(25)	39(3)	43(3)	29(3)	13(3)	17(2)	15(3)
C(26)	21(2)	27(2)	15(2)	-2(2)	0(2)	6(2)
C(27)	24(2)	22(2)	22(2)	1(2)	-2(2)	7(2)
C(28)	26(3)	39(3)	20(2)	1(2)	-4(2)	12(2)
C(29)	35(3)	46(3)	27(3)	8(3)	-4(2)	16(3)
C(30)	60(4)	63(4)	30(3)	5(3)	-10(3)	29(4)
C(31)	17(2)	16(2)	24(2)	0(2)	-3(2)	1(2)
C(32)	20(2)	18(2)	30(3)	4(2)	4(2)	5(2)
C(33)	16(2)	23(2)	30(3)	5(2)	4(2)	2(2)
C(34)	26(3)	27(3)	39(3)	8(2)	12(2)	8(2)
C(35)	34(3)	40(3)	40(3)	16(3)	11(3)	7(3)
C(36)	17(2)	17(2)	26(3)	2(2)	4(2)	8(2)
C(37)	17(2)	21(2)	27(3)	4(2)	-2(2)	6(2)
C(38)	41(3)	34(3)	38(3)	15(3)	14(3)	25(3)
C(39)	20(3)	42(3)	67(4)	29(3)	-3(3)	9(2)
C(40)	53(4)	73(5)	78(5)	49(4)	28(4)	43(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for pn1-off.

	x	y	z	U(eq)
H(1)	1630(60)	8320(30)	-730(30)	36
H(3)	5639	7975	4	44
H(4)	5780(60)	9130(30)	1760(30)	39
H(6)	2390(60)	10430(30)	1300(30)	42
H(8)	130(60)	9350(30)	-460(30)	33
H(12)	6620(60)	3590(30)	5130(30)	41
H(14)	5621	5563	4614	35

H(15)	7829	6274	3937	38
H(17)	11650(70)	5380(40)	3320(30)	46
H(18)	10110(70)	3180(30)	3650(30)	39
H(1A)	1061	8998	1690	28
H(1B)	-499	8613	1379	28
H(2A)	109	9082	2860	34
H(2B)	-1445	8777	2500	34
H(3A)	495	10207	2139	31
H(3B)	-1074	9908	1802	31
H(4A)	-403	10444	3260	42
H(4B)	-1983	10100	2952	42
H(5A)	-1489	11506	3046	51
H(5B)	-1766	11194	2222	51
H(5C)	-183	11538	2529	51
H(6A)	836	7988	3013	30
H(6B)	1515	7314	2629	30
H(7A)	2588	8986	2593	49
H(7B)	3218	8343	2126	49
H(8A)	4584	8791	3222	46
H(8B)	3225	8438	3669	46
H(9A)	4420	7434	2727	53
H(9B)	3320	7162	3340	53
H(10A)	5605	7063	3711	79
H(10B)	5094	7713	4227	79
H(10C)	6194	7993	3616	79
H(11A)	1924	7959	1178	29
H(11B)	387	7584	835	29
H(12A)	1806	6650	1668	33
H(12B)	481	6324	1122	33
H(13A)	3304	7026	737	36
H(13B)	2006	6870	169	36
H(14A)	2819	5610	874	49
H(14B)	1655	5493	238	49
H(15A)	3772	5241	-209	78
H(15B)	4609	6116	77	78
H(15C)	3448	6006	-560	78
H(16A)	-779	6723	2189	28
H(16B)	-1403	7444	2521	28
H(17A)	-1893	6715	1110	43
H(17B)	-2205	7579	1290	43
H(18A)	-3804	7026	2187	57
H(18B)	-4324	6672	1396	57
H(19A)	-2970	5865	2360	56
H(19B)	-3620	5510	1586	56
H(20A)	-5201	4985	2477	94
H(20B)	-5941	5517	1991	94
H(20C)	-5287	5866	2766	94
H(21A)	4193	2709	4206	22
H(21B)	3273	3109	3686	22
H(22A)	2467	1432	3799	26
H(22B)	1474	2013	3579	26
H(23A)	2619	1992	5004	28
H(23B)	1654	2587	4787	28
H(24A)	646	890	4689	33
H(24B)	-305	1520	4558	33
H(25A)	-686	1052	5712	53
H(25B)	19	1986	5785	53
H(25C)	964	1353	5915	53
H(26A)	2657	1960	2504	25
H(26B)	4074	2070	2063	25
H(27A)	4215	3451	2049	27
H(27B)	2856	3376	2539	27
H(28A)	2688	2503	1170	33
H(28B)	1374	2629	1634	33
H(29A)	3219	3869	937	42
H(29B)	1936	4011	1417	42

H(30A)	1239	3889	193	73
H(30B)	304	3168	590	73
H(30C)	1586	3023	110	73
H(31A)	5431	3600	3113	23
H(31B)	6279	3121	3595	23
H(32A)	6233	2796	2090	27
H(32B)	7435	2716	2662	27
H(33A)	6925	4208	2237	28
H(33B)	8062	4154	2851	28
H(34A)	8277	3553	1402	36
H(34B)	9470	3646	2022	36
H(35A)	10083	4703	1254	56
H(35B)	9831	5058	2039	56
H(35C)	8634	4968	1422	56
H(36A)	4035	1176	3098	23
H(36B)	5581	1560	2835	23
H(37A)	4817	1589	4304	26
H(37B)	6374	1944	4031	26
H(38A)	4962	283	3890	41
H(38B)	6467	620	3553	41
H(39A)	7408	1076	4746	50
H(39B)	5924	650	5053	50
H(40A)	7566	-161	5162	92
H(40B)	7778	-184	4316	92
H(40C)	6295	-610	4627	92

Table 6. Hydrogen bonds for pn1-off [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.80(6)	1.94(6)	2.690(5)	158(6)
O(3)-H(3)...O(2)	0.84	1.61	2.448(5)	174.1
O(4)-H(4)...O(5)	0.85(6)	1.64(6)	2.487(5)	175(6)
O(6)-H(6)...O(7)	1.05(6)	1.55(6)	2.579(5)	167(5)
O(8)-H(8)...O(7)#3	0.86(6)	1.77(6)	2.627(4)	175(6)
O(12)-H(12)...O(13)	1.02(6)	1.55(6)	2.563(4)	172(5)
O(14)-H(14)...O(13)#4	0.84	1.70	2.537(4)	171.1
O(15)-H(15)...O(14)	0.84	1.93	2.676(4)	148.2
O(17)-H(17)...O(16)	0.93(6)	1.62(6)	2.481(5)	152(6)
O(18)-H(18)...O(11)	0.80(6)	1.70(6)	2.478(5)	165(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z #2 -x+2,-y+1,-z+1 #3 -x,-y+2,-z

#4 -x+1,-y+1,-z+1

Crystallographic data of Pn1 crystal light-on stage measured at laboratory system

Table 1. Crystal data and structure refinement for pn1-on.

Identification code	on173K-1	
Empirical formula	C40 H98 N2 O20 P8 Pt2	
Formula weight	1565.14	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.6758(3) Å	α= 93.6675(8)°.
	b = 17.2106(6) Å	β= 90.9035(4)°.
	c = 18.6822(6) Å	γ= 102.8002(8)°.
Volume	3026.12(17) Å^3	
Z	2	
Density (calculated)	1.718 Mg/m^3	
Absorption coefficient	4.897 mm^{-1}	
F(000)	1576	
Crystal size	0.40 x 0.05 x 0.02 mm^3	
Theta range for data collection	1.09 to 27.48°.	
Index ranges	-12<=h<=12, -21<=k<=22, -24<=l<=16	
Reflections collected	21211	
Independent reflections	13429 [Rint = 0.0325]	
Completeness to θ = 27.48°	96.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.907 and 0.695	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13429 / 0 / 673	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2σ(I)]	R1 = 0.0335, wR2 = 0.0720	
R indices (all data)	R1 = 0.0475, wR2 = 0.0778	
Largest diff. peak and hole	1.363 and -1.453 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for pn1-on. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4069(1)	9368(1)	380(1)	13(1)
P(1)	3784(1)	8509(1)	-649(1)	17(1)
P(2)	5997(1)	8870(1)	742(1)	19(1)
P(3)	4494(1)	10187(1)	1440(1)	18(1)
P(4)	2132(1)	9876(1)	33(1)	16(1)
O(1)	2205(4)	8093(2)	-883(2)	25(1)
O(2)	4569(4)	7839(2)	-684(2)	29(1)
O(3)	6197(4)	8096(2)	361(2)	32(1)
O(4)	6123(4)	8768(2)	1554(2)	27(1)
O(5)	5046(4)	9845(2)	2080(2)	28(1)
O(6)	3206(4)	10529(2)	1699(2)	30(1)
O(7)	1468(3)	10341(2)	609(2)	23(1)
O(8)	903(3)	9215(2)	-352(2)	22(1)
O(9)	4271(4)	9018(2)	-1337(2)	25(1)
O(10)	2562(3)	10458(2)	-615(2)	21(1)
Pt(2)	9108(1)	4710(1)	4352(1)	13(1)
P(5)	8596(1)	3429(1)	4754(1)	18(1)
P(6)	7194(1)	5048(1)	4921(1)	17(1)
P(7)	9735(1)	5968(1)	3907(1)	18(1)
P(8)	11005(1)	4335(1)	3784(1)	19(1)
O(11)	8821(4)	2777(2)	4208(2)	23(1)
O(12)	7065(4)	3120(2)	5042(2)	28(1)
O(13)	6059(3)	4372(2)	5181(2)	24(1)
O(14)	6431(3)	5580(2)	4465(2)	24(1)
O(15)	8458(4)	6325(2)	3628(2)	26(1)
O(16)	10793(4)	6086(2)	3315(2)	28(1)
O(17)	11737(4)	4864(2)	3204(2)	33(1)
O(18)	10709(4)	3465(2)	3455(2)	26(1)
O(19)	9647(4)	3382(2)	5431(2)	23(1)
O(20)	12264(3)	4341(2)	4383(2)	24(1)
N(1)	371(4)	7825(2)	1928(2)	21(1)
C(1)	138(6)	8653(3)	1800(3)	26(1)
C(2)	-467(6)	9073(3)	2422(3)	31(1)
C(3)	-476(6)	9927(3)	2241(3)	25(1)
C(4)	-1025(7)	10399(3)	2829(3)	37(1)
C(5)	-1128(6)	11232(3)	2638(3)	35(1)
C(6)	1342(5)	7851(3)	2582(3)	26(1)
C(7)	2750(6)	8432(4)	2576(3)	39(1)
C(8)	3717(6)	8363(4)	3219(3)	38(1)
C(9)	4149(7)	7579(4)	3213(4)	45(2)
C(10)	5369(7)	7598(4)	3743(4)	53(2)
C(11)	1032(5)	7566(3)	1244(3)	25(1)
C(12)	1360(6)	6738(3)	1207(3)	31(1)
C(13)	2374(6)	6669(3)	602(3)	30(1)
C(14)	2571(7)	5829(3)	434(4)	43(2)
C(15)	3716(8)	5795(4)	-116(4)	58(2)
C(16)	-1010(5)	7234(3)	2084(3)	25(1)
C(17)	-2147(6)	7073(4)	1498(3)	36(1)
C(18)	-3601(6)	6676(4)	1777(4)	49(2)
C(19)	-3743(7)	5864(4)	2008(4)	47(2)
C(20)	-5172(8)	5534(4)	2340(5)	63(2)
N(2)	4450(4)	2414(2)	3133(2)	17(1)
C(21)	3579(5)	2607(3)	3768(3)	21(1)
C(22)	2262(5)	1968(3)	3905(2)	22(1)
C(23)	1839(5)	2051(3)	4688(3)	25(1)
C(24)	519(5)	1434(3)	4848(3)	25(1)
C(25)	173(6)	1458(3)	5634(3)	34(1)
C(26)	3579(5)	2325(3)	2438(2)	20(1)
C(27)	3311(5)	3095(3)	2168(3)	25(1)

C(28)	2341(6)	2891(3)	1493(3)	27(1)	C(35)	9375(6)	4729(3)	1614(3)	37(1)
C(29)	2258(6)	3619(4)	1099(3)	36(1)	C(36)	4879(5)	1618(3)	3201(3)	20(1)
C(30)	1263(8)	3400(4)	439(3)	51(2)	C(37)	5508(5)	1522(3)	3934(3)	24(1)
C(31)	5752(5)	3097(3)	3138(2)	20(1)	C(38)	5832(6)	693(3)	3948(3)	33(1)
C(32)	6768(5)	3050(3)	2534(3)	24(1)	C(39)	6597(6)	617(4)	4657(4)	42(2)
C(33)	7580(5)	3886(3)	2391(3)	26(1)	C(40)	7100(8)	-155(4)	4691(4)	67(3)
C(34)	8719(6)	3882(3)	1831(3)	31(1)					

Table 3. Bond lengths [Å] and angles [°] for pn1-on.

Pt(1)-P(1)	2.3224(12)	O(9)-P(3)#1	1.629(3)	O(20)-P(6)#2	1.621(4)
Pt(1)-P(2)	2.3263(12)	O(10)-P(2)#1	1.634(3)	N(1)-C(6)	1.521(6)
Pt(1)-P(3)	2.3319(12)	Pt(2)-P(6)	2.3154(11)	N(1)-C(11)	1.523(6)
Pt(1)-P(4)	2.3367(11)	Pt(2)-P(5)	2.3257(11)	N(1)-C(1)	1.523(6)
Pt(1)-Pt(1)#1	2.9542(3)	Pt(2)-P(8)	2.3262(11)	N(1)-C(16)	1.535(6)
P(1)-O(2)	1.514(3)	Pt(2)-P(7)	2.3274(11)	C(1)-C(2)	1.523(7)
P(1)-O(1)	1.579(4)	Pt(2)-Pt(2)#2	2.9387(3)	C(2)-C(3)	1.532(7)
P(1)-O(9)	1.620(3)	P(5)-O(11)	1.520(3)	C(3)-C(4)	1.497(7)
P(2)-O(3)	1.523(4)	P(5)-O(12)	1.574(4)	C(4)-C(5)	1.523(7)
P(2)-O(4)	1.544(4)	P(5)-O(19)	1.628(4)	C(6)-C(7)	1.502(7)
P(2)-O(10)#1	1.634(3)	P(6)-O(13)	1.524(3)	C(7)-C(8)	1.538(8)
P(3)-O(5)	1.506(4)	P(6)-O(14)	1.577(3)	C(8)-C(9)	1.500(8)
P(3)-O(6)	1.563(4)	P(6)-O(20)#2	1.621(4)	C(9)-C(10)	1.523(8)
P(3)-O(9)#1	1.629(3)	P(7)-O(16)	1.512(3)	C(11)-C(12)	1.525(6)
P(4)-O(7)	1.533(3)	P(7)-O(15)	1.591(3)	C(12)-C(13)	1.525(7)
P(4)-O(8)	1.580(4)	P(7)-O(19)#2	1.625(4)	C(13)-C(14)	1.513(7)
P(4)-O(10)	1.621(3)	P(8)-O(17)	1.539(4)	C(14)-C(15)	1.532(8)
O(1)-H(1)	0.83(6)	P(8)-O(18)	1.544(3)	C(16)-C(17)	1.508(8)
O(2)-H(3)	1.47(7)	P(8)-O(20)	1.639(4)	C(17)-C(18)	1.536(8)
O(3)-H(3)	0.98(7)	O(12)-H(12)	1.02(6)	C(18)-C(19)	1.466(8)
O(4)-H(4)	0.94(6)	O(14)-H(14)	0.93(6)	C(19)-C(20)	1.531(9)
O(6)-H(6)	0.84(7)	O(17)-H(17)	0.88(6)	N(2)-C(26)	1.518(6)
O(8)-H(8)	0.79(6)	O(19)-P(7)#2	1.625(4)	N(2)-C(31)	1.520(6)

N(2)-C(21)	1.528(5)	O(1)-P(1)-Pt(1)	115.87(14)	P(8)-Pt(2)-P(7)	90.51(4)
N(2)-C(36)	1.531(5)	O(9)-P(1)-Pt(1)	109.36(13)	P(6)-Pt(2)-Pt(2)#2	89.72(3)
C(21)-C(22)	1.525(6)	O(3)-P(2)-O(4)	106.3(2)	P(5)-Pt(2)-Pt(2)#2	89.97(3)
C(22)-C(23)	1.531(6)	O(3)-P(2)-O(10)#1	106.1(2)	P(8)-Pt(2)-Pt(2)#2	90.67(3)
C(23)-C(24)	1.517(7)	O(4)-P(2)-O(10)#1	101.88(19)	P(7)-Pt(2)-Pt(2)#2	90.39(3)
C(24)-C(25)	1.511(7)	O(3)-P(2)-Pt(1)	117.65(16)	O(11)-P(5)-O(12)	105.50(19)
C(26)-C(27)	1.520(6)	O(4)-P(2)-Pt(1)	115.53(14)	O(11)-P(5)-O(19)	104.61(18)
C(27)-C(28)	1.534(7)	O(10)#1-P(2)-Pt(1)	107.87(12)	O(12)-P(5)-O(19)	104.03(19)
C(28)-C(29)	1.509(7)	O(5)-P(3)-O(6)	106.6(2)	O(11)-P(5)-Pt(2)	114.78(13)
C(29)-C(30)	1.527(8)	O(5)-P(3)-O(9)#1	102.6(2)	O(12)-P(5)-Pt(2)	116.77(13)
C(31)-C(32)	1.518(6)	O(6)-P(3)-O(9)#1	103.7(2)	O(19)-P(5)-Pt(2)	109.96(13)
C(32)-C(33)	1.521(6)	O(5)-P(3)-Pt(1)	116.86(15)	O(13)-P(6)-O(14)	107.85(18)
C(33)-C(34)	1.532(6)	O(6)-P(3)-Pt(1)	114.81(15)	O(13)-P(6)-O(20)#2	106.3(2)
C(34)-C(35)	1.538(7)	O(9)#1-P(3)-Pt(1)	110.83(13)	O(14)-P(6)-O(20)#2	100.50(19)
C(36)-C(37)	1.522(7)	O(7)-P(4)-O(8)	107.87(19)	O(13)-P(6)-Pt(2)	117.50(13)
C(37)-C(38)	1.528(6)	O(7)-P(4)-O(10)	107.02(18)	O(14)-P(6)-Pt(2)	112.91(13)
C(38)-C(39)	1.535(8)	O(8)-P(4)-O(10)	100.25(18)	O(20)#2-P(6)-Pt(2)	110.23(12)
C(39)-C(40)	1.517(8)	O(7)-P(4)-Pt(1)	117.61(14)	O(16)-P(7)-O(15)	104.72(19)
		O(8)-P(4)-Pt(1)	112.58(13)	O(16)-P(7)-O(19)#2	107.9(2)
P(1)-Pt(1)-P(2)	89.72(4)	O(10)-P(4)-Pt(1)	109.98(12)	O(15)-P(7)-O(19)#2	100.09(18)
P(1)-Pt(1)-P(3)	175.67(4)	P(1)-O(1)-H(1)	123(4)	O(16)-P(7)-Pt(2)	117.97(14)
P(2)-Pt(1)-P(3)	85.96(4)	P(1)-O(2)-H(3)	108(2)	O(15)-P(7)-Pt(2)	115.91(13)
P(1)-Pt(1)-P(4)	91.10(4)	P(2)-O(3)-H(3)	110(4)	O(19)#2-P(7)-Pt(2)	108.58(12)
P(2)-Pt(1)-P(4)	179.15(4)	P(2)-O(4)-H(4)	103(4)	O(17)-P(8)-O(18)	106.4(2)
P(3)-Pt(1)-P(4)	93.22(4)	P(3)-O(6)-H(6)	120(4)	O(17)-P(8)-O(20)	104.8(2)
P(1)-Pt(1)-Pt(1)#1	90.71(3)	P(4)-O(8)-H(8)	118(4)	O(18)-P(8)-O(20)	101.96(18)
P(2)-Pt(1)-Pt(1)#1	91.44(3)	P(1)-O(9)-P(3)#1	132.5(2)	O(17)-P(8)-Pt(2)	117.54(15)
P(3)-Pt(1)-Pt(1)#1	89.65(3)	P(4)-O(10)-P(2)#1	131.1(2)	O(18)-P(8)-Pt(2)	115.46(14)
P(4)-Pt(1)-Pt(1)#1	88.78(3)	P(6)-Pt(2)-P(5)	92.75(4)	O(20)-P(8)-Pt(2)	109.06(13)
O(2)-P(1)-O(1)	104.7(2)	P(6)-Pt(2)-P(8)	178.54(4)	P(5)-O(12)-H(12)	113(3)
O(2)-P(1)-O(9)	105.86(19)	P(5)-Pt(2)-P(8)	85.84(4)	P(5)-O(14)-H(14)	119(3)
O(1)-P(1)-O(9)	100.71(19)	P(6)-Pt(2)-P(7)	90.90(4)	P(8)-O(17)-H(17)	109(4)
O(2)-P(1)-Pt(1)	118.44(15)	P(5)-Pt(2)-P(7)	176.33(4)	P(7)#2-O(19)-P(5)	130.7(2)

P(6)#2-O(20)-P(8)	130.1(2)	C(14)-C(13)-C(12)	113.8(4)	C(26)-C(27)-C(28)	108.9(4)
C(6)-N(1)-C(11)	111.4(4)	C(13)-C(14)-C(15)	112.5(5)	C(29)-C(28)-C(27)	112.7(4)
C(6)-N(1)-C(1)	111.3(4)	C(17)-C(16)-N(1)	116.1(4)	C(28)-C(29)-C(30)	111.5(5)
C(11)-N(1)-C(1)	104.7(3)	C(16)-C(17)-C(18)	111.8(5)	C(32)-C(31)-N(2)	115.9(4)
C(6)-N(1)-C(16)	105.4(3)	C(19)-C(18)-C(17)	116.1(5)	C(31)-C(32)-C(33)	109.7(4)
C(11)-N(1)-C(16)	111.7(4)	C(18)-C(19)-C(20)	113.3(5)	C(32)-C(33)-C(34)	112.7(4)
C(1)-N(1)-C(16)	112.5(4)	C(26)-N(2)-C(31)	112.1(3)	C(33)-C(34)-C(35)	111.7(4)
N(1)-C(1)-C(2)	115.8(4)	C(26)-N(2)-C(21)	110.5(4)	C(37)-C(36)-N(2)	114.5(4)
C(1)-C(2)-C(3)	109.3(4)	C(31)-N(2)-C(21)	106.2(3)	C(36)-C(37)-C(38)	109.7(4)
C(4)-C(3)-C(2)	113.5(4)	C(26)-N(2)-C(36)	106.2(3)	C(37)-C(38)-C(39)	110.2(5)
C(3)-C(4)-C(5)	114.0(5)	C(31)-N(2)-C(36)	110.8(3)	C(40)-C(39)-C(38)	114.1(6)
C(7)-C(6)-N(1)	115.5(4)	C(21)-N(2)-C(36)	111.2(3)		
C(6)-C(7)-C(8)	112.1(4)	C(22)-C(21)-N(2)	115.6(4)	Symmetry transformations used to	
C(9)-C(8)-C(7)	113.6(5)	C(21)-C(22)-C(23)	110.3(4)	generate equivalent atoms:	
C(8)-C(9)-C(10)	112.3(6)	C(24)-C(23)-C(22)	112.3(4)	#1 -x+1,-y+2,-z	
N(1)-C(11)-C(12)	116.9(4)	C(25)-C(24)-C(23)	112.7(5)	#2 -x+2,-y+1,-z+1	
C(13)-C(12)-C(11)	109.6(4)	N(2)-C(26)-C(27)	115.7(4)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for pn1-on. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	10(1)	15(1)	15(1)	2(1)	1(1)	3(1)
P(1)	14(1)	16(1)	18(1)	-1(1)	0(1)	3(1)
P(2)	14(1)	22(1)	23(1)	7(1)	0(1)	7(1)
P(3)	14(1)	22(1)	16(1)	0(1)	1(1)	2(1)
P(4)	9(1)	20(1)	19(1)	0(1)	0(1)	4(1)
O(1)	16(2)	23(2)	34(2)	-5(2)	-1(2)	2(1)
O(2)	32(2)	28(2)	32(2)	-4(2)	-4(2)	17(2)
O(3)	28(2)	28(2)	42(2)	-2(2)	-7(2)	16(2)
O(4)	20(2)	36(2)	29(2)	15(2)	1(2)	12(2)
O(5)	31(2)	33(2)	18(2)	2(2)	-4(2)	5(2)
O(6)	16(2)	43(2)	29(2)	-13(2)	-4(2)	7(2)
O(7)	16(2)	31(2)	24(2)	-5(2)	1(1)	9(1)
O(8)	7(2)	27(2)	33(2)	-3(2)	-5(1)	6(1)
O(9)	26(2)	24(2)	20(2)	0(1)	2(1)	-6(1)
O(10)	10(2)	27(2)	26(2)	6(2)	-2(1)	7(1)
Pt(2)	8(1)	16(1)	17(1)	1(1)	0(1)	5(1)
P(5)	15(1)	15(1)	24(1)	2(1)	-1(1)	4(1)
P(6)	8(1)	21(1)	24(1)	5(1)	2(1)	7(1)
P(7)	16(1)	19(1)	21(1)	5(1)	0(1)	6(1)
P(8)	15(1)	24(1)	21(1)	0(1)	5(1)	9(1)
O(11)	22(2)	16(2)	31(2)	-2(1)	-1(2)	5(1)

O(12)	24(2)	12(2)	45(2)	1(2)	5(2)	0(1)
O(13)	11(2)	25(2)	38(2)	11(2)	5(1)	9(1)
O(14)	12(2)	31(2)	34(2)	15(2)	2(1)	12(1)
O(15)	21(2)	30(2)	31(2)	13(2)	2(2)	10(2)
O(16)	30(2)	31(2)	25(2)	15(2)	9(2)	7(2)
O(17)	30(2)	40(2)	35(2)	12(2)	18(2)	19(2)
O(18)	19(2)	29(2)	31(2)	-6(2)	5(2)	7(2)
O(19)	23(2)	21(2)	26(2)	4(1)	-5(1)	6(1)
O(20)	16(2)	30(2)	28(2)	-8(2)	0(1)	12(1)
N(1)	25(2)	22(2)	18(2)	7(2)	4(2)	6(2)
C(1)	36(3)	24(2)	20(2)	6(2)	5(2)	12(2)
C(2)	32(3)	39(3)	27(3)	10(2)	8(2)	18(2)
C(3)	29(3)	28(3)	21(2)	5(2)	1(2)	11(2)
C(4)	47(4)	33(3)	35(3)	4(3)	8(3)	16(3)
C(5)	40(3)	31(3)	37(3)	-5(2)	-6(3)	16(3)
C(6)	29(3)	27(3)	23(3)	8(2)	2(2)	8(2)
C(7)	35(3)	39(3)	38(3)	12(3)	-8(3)	-2(3)
C(8)	27(3)	46(3)	37(3)	1(3)	-11(3)	0(3)
C(9)	33(3)	55(4)	45(4)	0(3)	-13(3)	11(3)
C(10)	28(3)	77(5)	55(4)	5(4)	-13(3)	11(3)
C(11)	27(3)	29(3)	21(2)	8(2)	8(2)	10(2)
C(12)	35(3)	29(3)	32(3)	7(2)	9(2)	14(2)
C(13)	28(3)	34(3)	30(3)	2(2)	8(2)	11(2)
C(14)	54(4)	35(3)	46(4)	1(3)	17(3)	20(3)
C(15)	62(5)	63(4)	60(5)	-2(4)	17(4)	38(4)
C(16)	20(2)	29(2)	26(3)	5(2)	10(2)	7(2)
C(17)	24(3)	49(3)	36(3)	9(3)	-3(2)	8(3)
C(18)	25(3)	55(4)	66(5)	11(4)	-4(3)	6(3)
C(19)	42(4)	49(4)	49(4)	5(3)	0(3)	10(3)
C(20)	51(5)	43(4)	90(6)	10(4)	20(4)	-2(3)
N(2)	16(2)	18(2)	17(2)	0(2)	1(2)	4(2)
C(21)	20(2)	23(2)	20(2)	1(2)	3(2)	8(2)
C(22)	18(2)	26(2)	20(2)	-2(2)	1(2)	5(2)
C(23)	20(2)	32(3)	26(3)	5(2)	4(2)	9(2)
C(24)	19(2)	34(3)	26(3)	9(2)	5(2)	11(2)
C(25)	36(3)	41(3)	29(3)	11(3)	14(2)	11(3)
C(26)	20(2)	26(2)	15(2)	-3(2)	-2(2)	6(2)
C(27)	23(3)	28(3)	24(3)	2(2)	-4(2)	10(2)
C(28)	26(3)	38(3)	21(2)	2(2)	-3(2)	16(2)
C(29)	35(3)	51(3)	25(3)	9(3)	0(2)	15(3)
C(30)	62(5)	65(4)	33(3)	7(3)	-9(3)	29(4)
C(31)	18(2)	19(2)	20(2)	1(2)	2(2)	-1(2)
C(32)	20(2)	22(2)	32(3)	4(2)	5(2)	8(2)
C(33)	22(3)	28(3)	29(3)	5(2)	4(2)	5(2)
C(34)	29(3)	29(3)	37(3)	10(2)	12(2)	9(2)
C(35)	32(3)	38(3)	45(4)	10(3)	13(3)	9(3)
C(36)	22(2)	15(2)	25(3)	1(2)	3(2)	10(2)
C(37)	16(2)	23(2)	32(3)	4(2)	-3(2)	6(2)
C(38)	36(3)	33(3)	36(3)	11(2)	16(3)	19(2)
C(39)	22(3)	44(3)	64(4)	28(3)	-5(3)	7(2)
C(40)	59(5)	81(5)	87(6)	56(5)	33(4)	53(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for pn1-on.

	x	y	z	U(eq)
H(1)	1520(70)	8290(30)	-790(30)	37
H(3)	5600(70)	7970(40)	-80(30)	47
H(4)	5770(70)	9190(30)	1760(30)	41
H(6)	2480(70)	10480(40)	1430(30)	44
H(8)	150(60)	9320(30)	-400(30)	34

H(12)	6580(60)	3570(30)	5180(30)	41
H(14)	5450(60)	5490(30)	4460(30)	36
H(15)	7760	6193	3891	39
H(17)	11540(70)	5340(40)	3260(30)	49
H(18)	10057	3182	3677	39
H(1A)	-511	8605	1376	31
H(1B)	1057	8995	1679	31
H(2A)	118	9084	2864	37
H(2B)	-1445	8779	2509	37
H(3A)	501	10207	2138	30
H(3B)	-1071	9906	1801	30
H(4A)	-393	10449	3259	44
H(4B)	-1977	10101	2955	44
H(5A)	-1493	11505	3046	53
H(5B)	-1773	11189	2220	53
H(5C)	-186	11538	2525	53
H(6A)	841	7985	3015	31
H(6B)	1515	7309	2625	31
H(7A)	2594	8982	2586	46
H(7B)	3228	8332	2125	46
H(8A)	4580	8798	3222	46
H(8B)	3216	8439	3668	46
H(9A)	4436	7438	2723	54
H(9B)	3325	7158	3332	54
H(10A)	5616	7075	3720	80
H(10B)	5082	7725	4230	80
H(10C)	6194	8006	3621	80
H(11A)	1926	7961	1178	30
H(11B)	383	7588	835	30
H(12A)	1795	6649	1669	37
H(12B)	471	6325	1120	37
H(13A)	2012	6861	164	36
H(13B)	3310	7023	735	36
H(14A)	1660	5486	247	52
H(14B)	2832	5612	883	52
H(15A)	3793	5240	-213	87
H(15B)	4628	6117	75	87
H(15C)	3461	6007	-562	87
H(16A)	-777	6720	2188	30
H(16B)	-1406	7440	2524	30
H(17A)	-1885	6720	1108	44
H(17B)	-2208	7582	1296	44
H(18A)	-3817	7018	2188	59
H(18B)	-4326	6662	1394	59
H(19A)	-2974	5864	2363	56
H(19B)	-3625	5506	1588	56
H(20A)	-5206	4990	2478	94
H(20B)	-5940	5525	1990	94
H(20C)	-5283	5875	2766	94
H(21A)	4199	2703	4206	25
H(21B)	3282	3110	3689	25
H(22A)	2455	1432	3798	26
H(22B)	1470	2023	3584	26
H(23A)	2633	1993	5006	30
H(23B)	1668	2592	4794	30
H(24A)	-294	1527	4564	30
H(24B)	657	895	4696	30
H(25A)	-686	1051	5708	52
H(25B)	18	1987	5786	52
H(25C)	965	1352	5917	52
H(26A)	2652	1960	2505	24
H(26B)	4069	2068	2061	24
H(27A)	4221	3451	2054	30
H(27B)	2855	3375	2544	30
H(28A)	2699	2510	1167	33
H(28B)	1377	2626	1632	33

H(29A)	3217	3878	949	43
H(29B)	1915	4006	1427	43
H(30A)	1241	3883	193	77
H(30B)	306	3158	588	77
H(30C)	1603	3019	113	77
H(31A)	5430	3603	3118	24
H(31B)	6279	3121	3600	24
H(32A)	6232	2792	2094	29
H(32B)	7442	2723	2668	29
H(33A)	8036	4158	2846	32
H(33B)	6905	4196	2222	32
H(34A)	8292	3544	1400	37
H(34B)	9475	3645	2029	37
H(35A)	10084	4702	1250	56
H(35B)	9830	5059	2036	56
H(35C)	8629	4964	1418	56
H(36A)	4033	1179	3098	24
H(36B)	5582	1562	2833	24
H(37A)	4829	1590	4311	28
H(37B)	6391	1936	4033	28
H(38A)	6437	606	3541	39
H(38B)	4938	281	3894	39
H(39A)	7426	1072	4732	51
H(39B)	5947	656	5055	51
H(40A)	7565	-163	5159	101
H(40B)	7774	-190	4311	101
H(40C)	6285	-609	4625	101

Table 6. Hydrogen bonds for pn1-on [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.83(6)	1.95(6)	2.678(5)	146(6)
O(3)-H(3)...O(2)	0.98(7)	1.47(7)	2.443(5)	173(6)
O(4)-H(4)...O(5)	0.94(6)	1.54(6)	2.479(5)	174(6)
O(6)-H(6)...O(7)	0.84(7)	1.79(7)	2.578(5)	157(6)
O(8)-H(8)...O(7)#3	0.79(6)	1.83(6)	2.620(5)	171(6)
O(12)-H(12)...O(13)	1.02(6)	1.56(6)	2.554(4)	162(5)
O(14)-H(14)...O(13)#4	0.93(6)	1.68(6)	2.526(4)	150(6)
O(15)-H(15)...O(14)	0.84	1.87	2.678(5)	160.5
O(17)-H(17)...O(16)	0.88(6)	1.61(6)	2.471(5)	166(7)
O(18)-H(18)...O(11)	0.84	1.63	2.461(5)	169.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z #2 -x+2,-y+1,-z+1 #3 -x,-y+2,-z

#4 -x+1,-y+1,-z+1

Crystallographic data of Bztel crystal light-off stage measured at laboratory system

Table 1. Crystal data and structure refinement for bztel-off.

Identification code	off103k	
Empirical formula	C26 H54 N2 O20 P8 Pt2	
Formula weight	1352.65	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 11.8647(4) Å	α= 89.3129(9)°.
	b = 12.5661(4) Å	β= 88.0813(6)°.
	c = 14.7700(5) Å	γ = 73.3677(9)°.
Volume	2108.78(12) Å^3	
Z	2	
Density (calculated)	2.130 Mg/m^3	
Absorption coefficient	7.009 mm^{-1}	
F(000)	1320	
Crystal size	0.15 x 0.08 x 0.02 mm^3	
Theta range for data collection	1.38 to 27.48°.	
Index ranges	-15<=h<=15, -16<=k<=14, -11<=l<=19	
Reflections collected	15069	
Independent reflections	9552 [Rint = 0.0346]	
Completeness to θ = 27.48°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.571	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9552 / 0 / 553	
Goodness-of-fit on F^2	0.975	
Final R indices [I>2σ(I)]	R1 = 0.0332, wR2 = 0.0752	
R indices (all data)	R1 = 0.0424, wR2 = 0.0786	
Largest diff. peak and hole	2.561 and -2.490 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bztel-off. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4259(1)	4233(1)	109(1)	6(1)
P(1)	2784(1)	5606(1)	-583(1)	9(1)
P(2)	4941(1)	3509(1)	-1323(1)	9(1)
P(3)	5759(1)	2882(1)	799(1)	9(1)
P(4)	3638(1)	4930(1)	1561(1)	10(1)
O(1)	1833(3)	6369(3)	80(3)	15(1)
O(2)	2163(3)	5138(3)	-1311(3)	15(1)
O(3)	4038(3)	3258(3)	-1989(3)	12(1)
O(4)	5936(3)	2406(3)	-1328(3)	14(1)
O(5)	6463(3)	1893(3)	231(3)	13(1)
O(6)	5401(4)	2374(3)	1713(3)	17(1)
O(7)	3747(3)	4035(3)	2303(3)	15(1)
O(8)	2421(3)	5786(3)	1637(3)	16(1)
O(9)	3306(3)	6490(3)	-1157(3)	11(1)
O(10)	5433(3)	4402(3)	-1895(2)	12(1)
Pt(2)	776(1)	5720(1)	5163(1)	6(1)
P(5)	2312(1)	4274(1)	4552(1)	9(1)
P(6)	346(1)	6433(1)	3700(1)	10(1)
P(7)	-788(1)	7122(1)	5790(1)	9(1)
P(8)	1144(1)	5013(1)	6629(1)	9(1)
O(11)	3089(3)	3484(3)	5251(3)	16(1)
O(12)	3167(3)	4648(3)	3894(3)	18(1)
O(13)	1402(4)	6612(3)	3124(3)	18(1)
O(14)	-633(4)	7552(3)	3654(3)	19(1)
O(15)	-1349(3)	8119(3)	5202(3)	14(1)
O(16)	-573(3)	7613(3)	6727(3)	14(1)
O(17)	978(3)	5909(3)	7373(3)	13(1)
O(18)	2306(3)	4117(3)	6779(3)	14(1)
O(19)	1822(3)	3463(3)	3915(2)	10(1)
O(20)	-94(3)	5567(3)	3089(2)	10(1)
N(1)	1722(4)	1958(3)	336(3)	10(1)
C(1)	1224(4)	993(4)	124(3)	9(1)
C(2)	630(5)	559(4)	917(4)	13(1)
C(3)	1243(5)	-345(5)	1436(4)	20(1)
C(4)	649(6)	-785(5)	2112(4)	25(1)
C(5)	-553(6)	-341(5)	2259(4)	22(1)
C(6)	-1181(5)	546(5)	1751(4)	20(1)
C(7)	-589(5)	1001(5)	1074(4)	16(1)
C(8)	2741(5)	1600(4)	978(4)	16(1)
C(9)	3846(5)	761(5)	600(4)	20(1)
C(10)	2139(5)	2362(4)	-562(4)	13(1)
C(11)	1176(5)	2903(5)	-1214(4)	19(1)
C(12)	753(4)	2878(4)	799(4)	12(1)
C(13)	1069(5)	3961(4)	951(4)	18(1)
N(2)	6688(4)	2028(3)	4594(3)	10(1)
C(14)	6127(4)	1114(4)	4863(4)	11(1)
C(15)	5696(5)	549(4)	4093(4)	12(1)
C(16)	4518(5)	953(4)	3842(4)	16(1)
C(17)	4091(6)	388(5)	3186(4)	24(1)
C(18)	4837(6)	-580(5)	2780(4)	27(2)
C(19)	5992(6)	-978(5)	3045(4)	28(2)
C(20)	6429(5)	-417(5)	3702(4)	19(1)
C(21)	5818(5)	2892(4)	4022(4)	15(1)
C(22)	6181(5)	3928(4)	3777(4)	19(1)
C(23)	6970(5)	2538(4)	5467(4)	14(1)
C(24)	5906(5)	3152(5)	6045(4)	23(1)
C(25)	7812(4)	1575(4)	4018(4)	14(1)
C(26)	8835(5)	782(5)	4505(4)	21(1)

Table 3. Bond lengths [Å] and angles [°] for bztel-off.

Pt(1)-P(1)	2.3304(13)	P(5)-O(12)	1.546(4)	C(8)-C(9)	1.522(7)
Pt(1)-P(3)	2.3327(13)	P(5)-O(11)	1.554(4)	C(10)-C(11)	1.519(7)
Pt(1)-P(2)	2.3369(13)	P(5)-O(19)	1.632(4)	C(12)-C(13)	1.532(7)
Pt(1)-P(4)	2.3412(13)	P(6)-O(14)	1.549(4)	N(2)-C(25)	1.526(7)
Pt(1)-Pt(1)#1	2.9657(3)	P(6)-O(13)	1.559(4)	N(2)-C(14)	1.526(6)
P(1)-O(2)	1.536(4)	P(6)-O(20)	1.629(4)	N(2)-C(21)	1.533(6)
P(1)-O(1)	1.575(4)	P(7)-O(15)	1.518(4)	N(2)-C(23)	1.535(6)
P(1)-O(9)	1.635(4)	P(7)-O(16)	1.579(4)	C(14)-C(15)	1.525(7)
P(2)-O(4)	1.543(4)	P(7)-O(19)#2	1.646(4)	C(15)-C(20)	1.394(8)
P(2)-O(3)	1.577(4)	P(8)-O(18)	1.531(4)	C(15)-C(16)	1.405(7)
P(2)-O(10)	1.623(4)	P(8)-O(17)	1.550(4)	C(16)-C(17)	1.398(8)
P(3)-O(5)	1.526(4)	P(8)-O(20)#2	1.653(4)	C(17)-C(18)	1.410(9)
P(3)-O(6)	1.583(4)	O(11)-H(18)	1.39(7)	C(18)-C(19)	1.386(9)
P(3)-O(9)#1	1.638(3)	O(12)-O(13)	2.984(6)	C(19)-C(20)	1.402(8)
P(3)-H(6)	1.91(8)	O(12)-H(12)	0.80(8)	C(21)-C(22)	1.520(7)
P(4)-O(8)	1.536(4)	O(13)-H(13)	0.96(7)	C(23)-C(24)	1.518(8)
P(4)-O(7)	1.542(4)	O(14)-H(14)	0.84(8)	C(25)-C(26)	1.527(7)
P(4)-O(10)#1	1.654(4)	O(16)-H(16)	0.86(6)		
O(1)-H(1)	1.01(7)	O(18)-H(18)	1.10(7)	P(1)-Pt(1)-P(3)	178.90(4)
O(2)-H(2)	1.20(6)	O(19)-P(7)#2	1.646(4)	P(1)-Pt(1)-P(2)	89.01(5)
O(3)-H(3)	0.84(6)	O(20)-P(8)#2	1.653(4)	P(3)-Pt(1)-P(2)	91.00(5)
O(4)-H(4)	1.00(7)	N(1)-C(8)	1.523(6)	P(1)-Pt(1)-P(4)	92.76(5)
O(5)-H(4)	1.44(7)	N(1)-C(12)	1.527(7)	P(3)-Pt(1)-P(4)	87.22(5)
O(6)-H(6)	0.76(7)	N(1)-C(10)	1.532(7)	P(2)-Pt(1)-P(4)	178.08(5)
O(8)-H(1)	1.47(7)	N(1)-C(1)	1.534(6)	P(1)-Pt(1)-Pt(1)#1	86.64(3)
O(9)-P(3)#1	1.638(3)	C(1)-C(2)	1.522(7)	P(3)-Pt(1)-Pt(1)#1	92.26(3)
O(10)-P(4)#1	1.654(4)	C(2)-C(3)	1.396(8)	P(2)-Pt(1)-Pt(1)#1	88.69(3)
Pt(2)-P(7)	2.3359(13)	C(2)-C(7)	1.406(8)	P(4)-Pt(1)-Pt(1)#1	90.66(3)
Pt(2)-P(8)	2.3370(13)	C(3)-C(4)	1.401(9)	O(2)-P(1)-O(1)	109.3(2)
Pt(2)-P(5)	2.3389(13)	C(4)-C(5)	1.385(9)	O(2)-P(1)-O(9)	102.6(2)
Pt(2)-P(6)	2.3458(13)	C(5)-C(6)	1.379(8)	O(1)-P(1)-O(9)	103.4(2)
Pt(2)-Pt(2)#2	2.9794(4)	C(6)-C(7)	1.410(8)	O(2)-P(1)-Pt(1)	112.61(15)

O(1)-P(1)-Pt(1)	115.50(16)	P(7)-Pt(2)-P(8)	87.53(5)	O(20)#2-P(8)-Pt(2)	106.91(14)
O(9)-P(1)-Pt(1)	112.29(14)	P(7)-Pt(2)-P(5)	178.20(4)	P(5)-O(11)-H(18)	114(2)
O(4)-P(2)-O(3)	102.4(2)	P(8)-Pt(2)-P(5)	91.59(5)	P(5)-O(12)-H(12)	128(5)
O(4)-P(2)-O(10)	107.0(2)	P(7)-Pt(2)-P(6)	91.32(5)	P(6)-O(13)-H(13)	130(4)
O(3)-P(2)-O(10)	102.2(2)	P(8)-Pt(2)-P(6)	178.29(4)	P(6)-O(14)-H(14)	111(5)
O(4)-P(2)-Pt(1)	115.59(16)	P(5)-Pt(2)-P(6)	89.52(5)	P(7)-O(16)-H(16)	112(4)
O(3)-P(2)-Pt(1)	118.79(15)	P(7)-Pt(2)-Pt(2)#2	92.03(3)	P(8)-O(18)-H(18)	114(3)
O(10)-P(2)-Pt(1)	109.47(14)	P(8)-Pt(2)-Pt(2)#2	91.50(3)	P(5)-O(19)-P(7)#2	125.7(2)
O(5)-P(3)-O(6)	105.9(2)	P(5)-Pt(2)-Pt(2)#2	86.42(3)	P(6)-O(20)-P(8)#2	126.4(2)
O(5)-P(3)-O(9)#1	107.1(2)	P(6)-Pt(2)-Pt(2)#2	87.27(3)	C(8)-N(1)-C(12)	107.9(4)
O(6)-P(3)-O(9)#1	101.3(2)	O(12)-P(5)-O(11)	106.4(2)	C(8)-N(1)-C(10)	110.1(4)
O(5)-P(3)-Pt(1)	118.19(15)	O(12)-P(5)-O(19)	102.2(2)	C(12)-N(1)-C(10)	111.2(4)
O(6)-P(3)-Pt(1)	115.98(16)	O(11)-P(5)-O(19)	104.8(2)	C(8)-N(1)-C(1)	111.4(4)
O(9)#1-P(3)-Pt(1)	106.79(14)	O(12)-P(5)-Pt(2)	114.79(17)	C(12)-N(1)-C(1)	108.7(4)
O(5)-P(3)-H(6)	127(2)	O(11)-P(5)-Pt(2)	115.75(16)	C(10)-N(1)-C(1)	107.6(4)
O(6)-P(3)-H(6)	23(2)	O(19)-P(5)-Pt(2)	111.56(14)	C(2)-C(1)-N(1)	115.8(4)
O(9)#1-P(3)-H(6)	101(2)	O(14)-P(6)-O(13)	105.3(2)	C(3)-C(2)-C(7)	118.9(5)
Pt(1)-P(3)-H(6)	95(2)	O(14)-P(6)-O(20)	105.8(2)	C(3)-C(2)-C(1)	121.6(5)
O(8)-P(4)-O(7)	110.0(2)	O(13)-P(6)-O(20)	103.0(2)	C(7)-C(2)-C(1)	119.3(5)
O(8)-P(4)-O(10)#1	104.9(2)	O(14)-P(6)-Pt(2)	115.12(17)	C(2)-C(3)-C(4)	120.2(5)
O(7)-P(4)-O(10)#1	102.16(19)	O(13)-P(6)-Pt(2)	115.95(16)	C(5)-C(4)-C(3)	120.2(5)
O(8)-P(4)-Pt(1)	116.07(16)	O(20)-P(6)-Pt(2)	110.48(14)	C(6)-C(5)-C(4)	120.8(6)
O(7)-P(4)-Pt(1)	114.62(16)	O(15)-P(7)-O(16)	105.7(2)	C(5)-C(6)-C(7)	119.4(6)
O(10)#1-P(4)-Pt(1)	107.67(14)	O(15)-P(7)-O(19)#2	107.3(2)	C(2)-C(7)-C(6)	120.5(5)
P(1)-O(1)-H(1)	111(4)	O(16)-P(7)-O(19)#2	101.0(2)	C(9)-C(8)-N(1)	115.8(5)
P(1)-O(2)-H(2)	125(3)	O(15)-P(7)-Pt(2)	118.05(16)	C(11)-C(10)-N(1)	115.6(4)
P(2)-O(3)-H(3)	122(4)	O(16)-P(7)-Pt(2)	116.66(15)	N(1)-C(12)-C(13)	114.9(4)
P(2)-O(4)-H(4)	111(4)	O(19)#2-P(7)-Pt(2)	106.47(13)	C(25)-N(2)-C(14)	111.6(4)
P(3)-O(5)-H(4)	106(3)	O(18)-P(8)-O(17)	108.4(2)	C(25)-N(2)-C(21)	107.6(4)
P(3)-O(6)-H(6)	104(6)	O(18)-P(8)-O(20)#2	105.8(2)	C(14)-N(2)-C(21)	108.5(4)
P(4)-O(8)-H(1)	110(3)	O(17)-P(8)-O(20)#2	101.9(2)	C(25)-N(2)-C(23)	109.8(4)
P(1)-O(9)-P(3)#1	126.4(2)	O(18)-P(8)-Pt(2)	117.68(16)	C(14)-N(2)-C(23)	107.8(4)
P(2)-O(10)-P(4)#1	127.6(2)	O(17)-P(8)-Pt(2)	114.55(15)	C(21)-N(2)-C(23)	111.7(4)

C(15)-C(14)-N(2)	116.5(4)	C(19)-C(18)-C(17)	119.6(5)
C(20)-C(15)-C(16)	120.3(5)	C(18)-C(19)-C(20)	120.6(6)
C(20)-C(15)-C(14)	120.4(5)	C(15)-C(20)-C(19)	119.8(5)
C(16)-C(15)-C(14)	119.1(5)	C(22)-C(21)-N(2)	115.5(4)
C(17)-C(16)-C(15)	119.4(5)	C(24)-C(23)-N(2)	115.1(4)
C(16)-C(17)-C(18)	120.3(6)	N(2)-C(25)-C(26)	115.4(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1.-y+1.-z

#2 -x.-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for bzte1-off. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	7(1)	8(1)	2(1)	0(1)	1(1)	-3(1)
P(1)	8(1)	11(1)	8(1)	1(1)	0(1)	-3(1)
P(2)	11(1)	11(1)	3(1)	-2(1)	2(1)	-3(1)
P(3)	10(1)	10(1)	6(1)	2(1)	-1(1)	-4(1)
P(4)	11(1)	15(1)	3(1)	-2(1)	4(1)	-6(1)
O(1)	8(2)	20(2)	14(2)	-1(2)	5(1)	1(2)
O(2)	15(2)	16(2)	15(2)	2(2)	-7(2)	-6(2)
O(3)	12(2)	14(2)	9(2)	-1(2)	-3(2)	-2(2)
O(4)	14(2)	14(2)	12(2)	-3(2)	-2(2)	1(2)
O(5)	13(2)	12(2)	13(2)	-2(2)	-3(2)	-1(1)
O(6)	20(2)	18(2)	12(2)	5(2)	2(2)	-7(2)
O(7)	19(2)	20(2)	9(2)	1(2)	4(2)	-11(2)
O(8)	12(2)	23(2)	13(2)	-4(2)	6(2)	-5(2)
O(9)	11(2)	13(2)	12(2)	2(2)	-2(1)	-6(1)
O(10)	15(2)	19(2)	6(2)	-1(2)	2(1)	-10(2)
Pt(2)	8(1)	8(1)	3(1)	0(1)	2(1)	-2(1)
P(5)	9(1)	10(1)	7(1)	-1(1)	4(1)	-2(1)
P(6)	16(1)	11(1)	3(1)	1(1)	2(1)	-4(1)
P(7)	10(1)	7(1)	7(1)	0(1)	1(1)	-1(1)
P(8)	10(1)	13(1)	4(1)	3(1)	1(1)	-2(1)
O(11)	14(2)	17(2)	15(2)	-4(2)	0(2)	0(2)
O(12)	21(2)	23(2)	12(2)	-6(2)	9(2)	-13(2)
O(13)	25(2)	24(2)	9(2)	-2(2)	8(2)	-17(2)
O(14)	29(2)	15(2)	8(2)	3(2)	-1(2)	0(2)
O(15)	18(2)	10(2)	11(2)	1(2)	-2(2)	-2(2)
O(16)	15(2)	15(2)	10(2)	-2(2)	-1(2)	-3(2)
O(17)	15(2)	16(2)	7(2)	0(2)	-2(1)	-5(2)
O(18)	13(2)	16(2)	8(2)	1(2)	1(2)	2(2)
O(19)	12(2)	11(2)	7(2)	-4(1)	6(1)	-3(1)
O(20)	11(2)	13(2)	7(2)	3(1)	1(1)	-5(1)
N(1)	11(2)	11(2)	8(2)	1(2)	-1(2)	-4(2)
C(1)	15(2)	8(2)	5(2)	-2(2)	3(2)	-5(2)
C(2)	21(3)	12(2)	8(3)	-3(2)	5(2)	-10(2)
C(3)	21(3)	18(3)	19(3)	0(2)	0(2)	-4(2)
C(4)	42(4)	15(3)	17(3)	7(2)	-2(3)	-6(3)
C(5)	38(4)	20(3)	11(3)	1(2)	6(2)	-16(3)
C(6)	28(3)	20(3)	17(3)	-5(2)	6(2)	-13(2)
C(7)	19(3)	17(3)	13(3)	2(2)	1(2)	-7(2)
C(8)	14(3)	16(3)	16(3)	3(2)	-5(2)	-1(2)
C(9)	12(3)	20(3)	25(3)	-1(2)	1(2)	0(2)
C(10)	17(3)	12(3)	9(3)	-2(2)	4(2)	-4(2)
C(11)	27(3)	25(3)	9(3)	7(2)	-5(2)	-14(3)
C(12)	12(2)	11(2)	13(3)	-2(2)	5(2)	-3(2)
C(13)	18(3)	13(3)	24(3)	-4(2)	8(2)	-7(2)
N(2)	11(2)	11(2)	7(2)	1(2)	0(2)	-2(2)
C(14)	12(2)	12(2)	9(3)	2(2)	0(2)	-6(2)
C(15)	15(3)	15(3)	10(3)	1(2)	2(2)	-9(2)
C(16)	19(3)	12(3)	18(3)	-1(2)	-2(2)	-8(2)
C(17)	33(3)	25(3)	21(3)	9(3)	-10(3)	-19(3)
C(18)	52(4)	25(3)	13(3)	-2(3)	-4(3)	-24(3)
C(19)	49(4)	19(3)	19(3)	-7(3)	11(3)	-14(3)
C(20)	16(3)	19(3)	22(3)	1(2)	2(2)	-5(2)
C(21)	13(3)	16(3)	16(3)	1(2)	-8(2)	-6(2)
C(22)	21(3)	13(3)	25(3)	6(2)	-8(2)	-6(2)
C(23)	19(3)	17(3)	8(3)	-3(2)	-4(2)	-6(2)
C(24)	31(3)	28(3)	16(3)	-14(3)	12(3)	-17(3)
C(25)	10(2)	17(3)	11(3)	-5(2)	4(2)	0(2)
C(26)	15(3)	20(3)	23(3)	-1(2)	0(2)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for bzte1-off.

	x	y	z	U(eq)
H(1)	1980(50)	6110(50)	730(50)	22
H(2)	1460(50)	5690(50)	-1820(50)	22
H(3)	3450(50)	3760(50)	-2170(50)	18
H(4)	6200(50)	2190(50)	-700(50)	22
H(6)	4870(60)	2820(60)	1890(50)	25
H(12)	3220(60)	4590(60)	3360(50)	26
H(13)	1790(60)	6240(50)	2580(50)	27
H(14)	-900(60)	7770(60)	4180(50)	28
H(16)	20(60)	7180(50)	7000(50)	21
H(18)	2770(50)	3760(50)	6150(50)	20
H(1A)	645	1235	-359	11
H(1B)	1874	371	-122	11
H(3)	2064	-662	1331	23
H(4)	1073	-1390	2472	30
H(5)	-949	-651	2714	26
H(6)	-2005	848	1857	25
H(7)	-1018	1611	722	19
H(8A)	2953	2269	1166	19
H(8B)	2467	1278	1529	19
H(9A)	3646	105	385	30
H(9B)	4424	541	1077	30
H(9C)	4181	1097	95	30
H(10A)	2576	2901	-428	16
H(10B)	2698	1719	-870	16
H(11A)	692	2403	-1316	28
H(11B)	1533	3054	-1792	28
H(11C)	681	3602	-955	28
H(12A)	546	2600	1393	14
H(12B)	44	3044	427	14
H(13A)	1755	3814	1335	27
H(13B)	401	4503	1249	27
H(13C)	1253	4259	366	27
H(14A)	6709	538	5202	13
H(14B)	5451	1437	5284	13
H(16)	4015	1605	4115	19
H(17)	3295	657	3014	29
H(18)	4549	-957	2328	33
H(19)	6492	-1636	2779	34
H(20)	7222	-695	3879	23
H(21A)	5699	2532	3455	18
H(21B)	5050	3121	4358	18

H(22A)	6331	4279	4331	29	H(24C)	5470	2633	6247	35
H(22B)	5549	4449	3450	29	H(25A)	8072	2209	3782	16
H(22C)	6898	3722	3391	29	H(25B)	7626	1183	3491	16
H(23A)	7475	1936	5836	17	H(26A)	9118	1191	4965	31
H(23B)	7430	3060	5302	17	H(26B)	9475	457	4066	31
H(24A)	5395	3748	5688	35	H(26C)	8568	189	4798	31
H(24B)	6167	3470	6574	35					

Table 6. Hydrogen bonds for bzte1-off [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	1.01(7)	1.47(7)	2.468(5)	169(6)
O(2)-H(2)...O(17)#3	1.20(6)	1.34(7)	2.460(5)	152(6)
O(3)-H(3)...O(18)#3	0.84(6)	2.06(6)	2.763(5)	141(6)
O(3)-H(3)...O(2)	0.84(6)	2.31(6)	2.903(5)	128(6)
O(4)-H(4)...O(5)	1.00(7)	1.44(7)	2.437(5)	175(6)
O(6)-H(6)...O(7)	0.76(7)	1.81(7)	2.559(6)	171(7)
O(18)-H(18)...O(11)	1.10(7)	1.39(7)	2.463(5)	165(6)
O(12)-H(12)...O(7)	0.80(8)	1.74(8)	2.495(6)	158(7)
O(13)-H(13)...O(8)	0.96(7)	1.59(8)	2.553(6)	173(6)
O(14)-H(14)...O(15)	0.84(8)	1.61(8)	2.453(6)	176(7)
O(16)-H(16)...O(17)	0.86(6)	1.77(7)	2.588(5)	158(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+1,-z+1 #3 x,y,z-1

Crystallographic data of Bzte1 crystal light-on stage measured at laboratory system

Table 1. Crystal data and structure refinement for bzte1-on.

Identification code	on103k	
Empirical formula	C26 H54 N2 O20 P8 Pt2	
Formula weight	1352.65	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.8488(3) Å	α= 89.3304(6)°.
	b = 12.5275(4) Å	β= 87.9796(12)°.
	c = 14.7425(5) Å	γ = 73.3187(7)°.
Volume	2094.92(11) Å^3	
Z	2	
Density (calculated)	2.144 Mg/m^3	
Absorption coefficient	7.055 mm^{-1}	
F(000)	1320	
Crystal size	0.15 x 0.08 x 0.02 mm^3	
Theta range for data collection	1.38 to 27.48°.	
Index ranges	-15<=h<=6, -15<=k<=13, -10<=l<=19	
Reflections collected	9429	
Independent reflections	7550 [Rint = 0.0385]	
Completeness to θ = 27.48°	78.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.572	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7550 / 0 / 541	
Goodness-of-fit on F^2	0.963	
Final R indices [I>2σ(I)]	R1 = 0.0380, wR2 = 0.0884	
R indices (all data)	R1 = 0.0486, wR2 = 0.0917	
Largest diff. peak and hole	1.603 and -1.387 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for bzte1-on. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4259(1)	4237(1)	107(1)	10(1)
P(1)	2790(2)	5598(2)	-599(1)	14(1)
P(2)	4947(2)	3503(2)	-1318(1)	14(1)
P(3)	5749(2)	2892(2)	804(1)	14(1)
P(4)	3629(2)	4943(2)	1553(1)	14(1)
O(1)	1831(4)	6352(5)	57(3)	21(1)
O(2)	2172(4)	5140(5)	-1322(4)	21(1)
O(3)	4046(5)	3266(5)	-1987(3)	17(1)
O(4)	5938(4)	2390(5)	-1331(3)	19(1)
O(5)	6454(4)	1891(5)	232(3)	19(1)
O(6)	5387(5)	2382(5)	1709(4)	23(1)
O(7)	3743(5)	4041(5)	2295(3)	20(1)
O(8)	2406(4)	5803(5)	1624(3)	19(1)
O(9)	3313(4)	6494(4)	-1156(3)	16(1)
O(10)	5442(4)	4386(4)	-1887(3)	16(1)
Pt(2)	778(1)	5714(1)	5164(1)	11(1)
P(5)	2312(2)	4264(2)	4553(1)	14(1)
P(6)	359(2)	6431(2)	3703(1)	15(1)
P(7)	-783(2)	7120(2)	5789(1)	13(1)
P(8)	1135(2)	5000(2)	6624(1)	14(1)
O(11)	3085(4)	3475(5)	5244(3)	20(1)
O(12)	3173(5)	4635(5)	3899(4)	22(1)
O(13)	1428(5)	6610(5)	3137(3)	23(1)
O(14)	-615(5)	7551(5)	3655(4)	24(1)
O(15)	-1342(4)	8114(4)	5197(3)	16(1)
O(16)	-573(5)	7602(5)	6725(3)	18(1)
O(17)	967(4)	5896(4)	7367(3)	15(1)
O(18)	2292(4)	4102(5)	6769(3)	18(1)
O(19)	1821(4)	3454(4)	3918(3)	14(1)
O(20)	-81(4)	5575(4)	3098(3)	14(1)
N(1)	1718(5)	1952(5)	339(4)	16(1)
C(1)	1236(6)	988(6)	121(5)	16(2)
C(2)	617(7)	561(6)	915(5)	15(2)
C(3)	1245(7)	-344(8)	1438(6)	28(2)
C(4)	633(9)	-783(8)	2101(6)	32(2)
C(5)	-564(8)	-339(8)	2258(6)	30(2)
C(6)	-1188(7)	549(7)	1736(5)	24(2)
C(7)	-593(6)	991(7)	1067(5)	20(2)
C(8)	2740(6)	1598(7)	979(5)	20(2)
C(9)	3848(6)	756(8)	596(6)	26(2)
C(10)	2141(6)	2344(7)	-551(5)	17(2)
C(11)	1183(7)	2897(8)	-1209(5)	24(2)
C(12)	748(6)	2882(7)	801(5)	21(2)
C(13)	1065(7)	3957(7)	951(5)	24(2)
N(2)	6684(5)	2033(5)	4592(4)	15(1)
C(14)	6118(6)	1117(7)	4848(5)	18(2)
C(15)	5689(7)	553(7)	4105(5)	19(2)
C(16)	4521(7)	959(7)	3829(5)	21(2)
C(17)	4101(8)	386(8)	3181(6)	32(2)
C(18)	4852(9)	-580(8)	2794(6)	33(2)
C(19)	5999(9)	-985(8)	3066(6)	32(2)
C(20)	6414(7)	-424(7)	3711(5)	22(2)
C(21)	5819(6)	2892(7)	4015(5)	16(2)
C(22)	6191(7)	3924(7)	3746(6)	27(2)
C(23)	6959(7)	2553(8)	5456(5)	23(2)
C(24)	5892(8)	3166(8)	6027(6)	34(2)
C(25)	7813(6)	1560(7)	4011(5)	18(2)
C(26)	8827(7)	774(8)	4507(6)	31(2)

Table 3. Bond lengths [Å] and angles [°] for bzte1-on.

Pt(1)-P(3)	2.321(2)	P(6)-O(20)	1.611(6)	C(14)-C(15)	1.490(11)
Pt(1)-P(1)	2.324(2)	P(7)-O(15)	1.513(5)	C(15)-C(20)	1.397(11)
Pt(1)-P(2)	2.3264(17)	P(7)-O(16)	1.568(6)	C(15)-C(16)	1.404(11)
Pt(1)-P(4)	2.3325(17)	P(7)-O(19)#2	1.637(5)	C(16)-C(17)	1.388(12)
Pt(1)-Pt(1)#1	2.9522(5)	P(8)-O(18)	1.524(5)	C(17)-C(18)	1.394(13)
P(1)-O(2)	1.521(6)	P(8)-O(17)	1.544(5)	C(18)-C(19)	1.380(13)
P(1)-O(1)	1.564(5)	P(8)-O(20)#2	1.648(5)	C(19)-C(20)	1.373(12)
P(1)-O(9)	1.631(5)	O(11)-H(18)	1.26(8)	C(21)-C(22)	1.526(11)
P(2)-O(4)	1.544(5)	O(12)-H(12)	0.86(9)	C(23)-C(24)	1.509(10)
P(2)-O(3)	1.570(6)	O(14)-H(14)	0.83(9)	C(25)-C(26)	1.521(11)
P(2)-O(10)	1.608(5)	O(16)-H(16)	0.84(9)		
P(2)-H(3)	1.91(9)	O(18)-H(18)	1.21(8)	P(3)-Pt(1)-P(1)	179.05(6)
P(3)-O(5)	1.535(5)	O(19)-P(7)#2	1.637(5)	P(3)-Pt(1)-P(2)	91.07(7)
P(3)-O(6)	1.572(5)	O(20)-P(8)#2	1.648(5)	P(1)-Pt(1)-P(2)	88.69(7)
P(3)-O(9)#1	1.624(6)	N(1)-C(10)	1.515(8)	P(3)-Pt(1)-P(4)	87.18(7)
P(4)-O(8)	1.538(5)	N(1)-C(1)	1.518(10)	P(1)-Pt(1)-P(4)	93.05(7)
P(4)-O(7)	1.545(6)	N(1)-C(8)	1.522(10)	P(2)-Pt(1)-P(4)	178.14(7)
P(4)-O(10)#1	1.656(6)	N(1)-C(12)	1.528(9)	P(3)-Pt(1)-Pt(1)#1	92.09(5)
O(3)-H(3)	0.77(9)	C(1)-C(2)	1.531(9)	P(1)-Pt(1)-Pt(1)#1	86.99(5)
O(6)-H(6)	1.02(9)	C(2)-C(7)	1.391(10)	P(2)-Pt(1)-Pt(1)#1	88.85(5)
O(9)-P(3)#1	1.624(6)	C(2)-C(3)	1.403(12)	P(4)-Pt(1)-Pt(1)#1	90.56(5)
O(10)-P(4)#1	1.656(6)	C(3)-C(4)	1.396(11)	O(2)-P(1)-O(1)	108.5(3)
Pt(2)-P(8)	2.3271(19)	C(4)-C(5)	1.379(12)	O(2)-P(1)-O(9)	103.2(3)
Pt(2)-P(7)	2.3291(18)	C(5)-C(6)	1.386(12)	O(1)-P(1)-O(9)	103.1(3)
Pt(2)-P(5)	2.3329(18)	C(6)-C(7)	1.393(10)	O(2)-P(1)-Pt(1)	113.6(2)
Pt(2)-P(6)	2.3381(19)	C(8)-C(9)	1.524(10)	O(1)-P(1)-Pt(1)	115.2(2)
Pt(2)-Pt(2)#2	2.9676(6)	C(10)-C(11)	1.523(11)	O(9)-P(1)-Pt(1)	112.15(19)
P(5)-O(11)	1.541(6)	C(12)-C(13)	1.518(12)	O(4)-P(2)-O(3)	102.3(3)
P(5)-O(12)	1.542(5)	N(2)-C(14)	1.524(10)	O(4)-P(2)-O(10)	106.9(3)
P(5)-O(19)	1.626(6)	N(2)-C(23)	1.524(10)	O(3)-P(2)-O(10)	101.7(3)
P(6)-O(14)	1.542(6)	N(2)-C(21)	1.529(9)	O(4)-P(2)-Pt(1)	116.3(2)
P(6)-O(13)	1.560(5)	N(2)-C(25)	1.534(8)	O(3)-P(2)-Pt(1)	118.7(2)

O(10)-P(2)-Pt(1)	109.4(2)	O(12)-P(5)-O(19)	102.6(3)	C(1)-N(1)-C(12)	109.6(5)
O(4)-P(2)-H(3)	124(3)	O(11)-P(5)-Pt(2)	115.9(2)	C(8)-N(1)-C(12)	107.9(6)
O(3)-P(2)-H(3)	23(3)	O(12)-P(5)-Pt(2)	114.8(2)	N(1)-C(1)-C(2)	115.5(6)
O(10)-P(2)-H(3)	99(3)	O(19)-P(5)-Pt(2)	111.51(19)	C(7)-C(2)-C(3)	119.3(7)
Pt(1)-P(2)-H(3)	100(3)	O(14)-P(6)-O(13)	105.3(3)	C(7)-C(2)-C(1)	120.3(7)
O(5)-P(3)-O(6)	105.4(3)	O(14)-P(6)-O(20)	105.7(3)	C(3)-C(2)-C(1)	120.2(7)
O(5)-P(3)-O(9)#1	106.9(3)	O(13)-P(6)-O(20)	103.7(3)	C(4)-C(3)-C(2)	118.8(8)
O(6)-P(3)-O(9)#1	101.8(3)	O(14)-P(6)-Pt(2)	115.3(2)	C(5)-C(4)-C(3)	121.5(8)
O(5)-P(3)-Pt(1)	117.8(2)	O(13)-P(6)-Pt(2)	115.5(2)	C(4)-C(5)-C(6)	119.7(7)
O(6)-P(3)-Pt(1)	116.1(2)	O(20)-P(6)-Pt(2)	110.27(19)	C(5)-C(6)-C(7)	119.5(7)
O(9)#1-P(3)-Pt(1)	107.4(2)	O(15)-P(7)-O(16)	106.4(3)	C(2)-C(7)-C(6)	121.1(8)
O(8)-P(4)-O(7)	110.5(3)	O(15)-P(7)-O(19)#2	106.9(3)	N(1)-C(8)-C(9)	115.6(6)
O(8)-P(4)-O(10)#1	105.0(3)	O(16)-P(7)-O(19)#2	100.7(3)	N(1)-C(10)-C(11)	115.7(6)
O(7)-P(4)-O(10)#1	102.2(3)	O(15)-P(7)-Pt(2)	117.86(19)	C(13)-C(12)-N(1)	115.1(6)
O(8)-P(4)-Pt(1)	116.0(2)	O(16)-P(7)-Pt(2)	116.6(2)	C(14)-N(2)-C(23)	109.0(5)
O(7)-P(4)-Pt(1)	114.1(2)	O(19)#2-P(7)-Pt(2)	106.73(19)	C(14)-N(2)-C(21)	107.8(5)
O(10)#1-P(4)-Pt(1)	107.59(16)	O(18)-P(8)-O(17)	108.8(3)	C(23)-N(2)-C(21)	111.5(6)
P(2)-O(3)-H(3)	104(7)	O(18)-P(8)-O(20)#2	106.0(3)	C(14)-N(2)-C(25)	110.5(6)
P(3)-O(6)-H(6)	107(5)	O(17)-P(8)-O(20)#2	101.9(3)	C(23)-N(2)-C(25)	110.3(6)
P(3)#1-O(9)-P(1)	127.1(3)	O(18)-P(8)-Pt(2)	117.46(19)	C(21)-N(2)-C(25)	107.6(5)
P(2)-O(10)-P(4)#1	127.7(3)	O(17)-P(8)-Pt(2)	114.3(2)	C(15)-C(14)-N(2)	118.2(6)
P(8)-Pt(2)-P(7)	87.63(7)	O(20)#2-P(8)-Pt(2)	106.95(19)	C(20)-C(15)-C(16)	118.8(8)
P(8)-Pt(2)-P(5)	91.54(7)	P(5)-O(11)-H(18)	115(4)	C(20)-C(15)-C(14)	120.8(7)
P(7)-Pt(2)-P(5)	178.19(7)	P(5)-O(12)-H(12)	119(6)	C(16)-C(15)-C(14)	120.3(7)
P(8)-Pt(2)-P(6)	178.25(6)	P(6)-O(14)-H(14)	114(7)	C(17)-C(16)-C(15)	120.1(8)
P(7)-Pt(2)-P(6)	91.29(7)	P(7)-O(16)-H(16)	104(6)	C(16)-C(17)-C(18)	119.7(9)
P(5)-Pt(2)-P(6)	89.51(7)	P(8)-O(18)-H(18)	113(4)	C(19)-C(18)-C(17)	120.5(9)
P(8)-Pt(2)-Pt(2)#2	91.27(5)	P(5)-O(19)-P(7)#2	125.7(3)	C(20)-C(19)-C(18)	119.9(8)
P(7)-Pt(2)-Pt(2)#2	91.87(5)	P(6)-O(20)-P(8)#2	126.7(3)	C(19)-C(20)-C(15)	121.0(8)
P(5)-Pt(2)-Pt(2)#2	86.54(5)	C(10)-N(1)-C(1)	107.0(6)	C(22)-C(21)-N(2)	115.8(6)
P(6)-Pt(2)-Pt(2)#2	87.40(5)	C(10)-N(1)-C(8)	109.5(5)	C(24)-C(23)-N(2)	114.8(7)
O(11)-P(5)-O(12)	105.9(3)	C(1)-N(1)-C(8)	111.6(6)	C(26)-C(25)-N(2)	115.0(6)
O(11)-P(5)-O(19)	104.8(3)	C(10)-N(1)-C(12)	111.3(6)		

Symmetry transformations used to generate equivalent atoms:	#2 -x,-y+1,-z+1
#1 -x+1,-y+1,-z	

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for bzte1-on. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	13(1)	10(1)	7(1)	-1(1)	1(1)	-4(1)
P(1)	14(1)	13(1)	14(1)	-1(1)	-1(1)	-5(1)
P(2)	17(1)	12(1)	11(1)	-4(1)	2(1)	-3(1)
P(3)	18(1)	13(1)	12(1)	2(1)	-2(1)	-6(1)
P(4)	16(1)	18(1)	9(1)	-3(1)	4(1)	-7(1)
O(1)	13(2)	25(4)	23(3)	-2(2)	1(2)	-1(2)
O(2)	22(3)	20(3)	25(3)	2(2)	-7(2)	-9(2)
O(3)	22(3)	11(3)	18(3)	-5(2)	-1(2)	-5(2)
O(4)	20(2)	21(3)	14(3)	-5(2)	-1(2)	-4(2)
O(5)	21(3)	12(3)	22(3)	0(2)	-2(2)	-1(2)
O(6)	27(3)	24(4)	20(3)	11(3)	-5(2)	-9(3)
O(7)	29(3)	23(3)	10(2)	-2(2)	3(2)	-12(3)
O(8)	14(2)	23(3)	18(3)	-7(2)	8(2)	-4(2)
O(9)	20(2)	8(3)	19(3)	1(2)	-8(2)	-4(2)
O(10)	20(2)	20(3)	8(2)	-2(2)	3(2)	-4(2)
Pt(2)	15(1)	9(1)	8(1)	0(1)	2(1)	-3(1)
P(5)	15(1)	13(1)	13(1)	-2(1)	4(1)	-3(1)
P(6)	24(1)	13(1)	9(1)	2(1)	3(1)	-5(1)
P(7)	16(1)	7(1)	13(1)	0(1)	0(1)	-1(1)
P(8)	17(1)	14(1)	10(1)	2(1)	1(1)	-2(1)
O(11)	19(2)	17(3)	19(3)	-1(2)	2(2)	1(2)
O(12)	29(3)	28(4)	14(3)	-6(3)	7(2)	-15(3)
O(13)	39(3)	19(3)	15(3)	-4(2)	7(2)	-18(3)
O(14)	32(3)	15(4)	19(3)	2(2)	2(2)	0(3)
O(15)	21(2)	11(3)	16(3)	-1(2)	-2(2)	-1(2)
O(16)	22(3)	14(3)	16(3)	-4(2)	0(2)	-2(2)
O(17)	16(2)	19(3)	8(2)	3(2)	-6(2)	-2(2)
O(18)	18(2)	19(3)	13(3)	4(2)	1(2)	0(2)
O(19)	20(2)	9(3)	12(2)	-2(2)	6(2)	-6(2)
O(20)	19(2)	12(3)	10(2)	2(2)	-2(2)	-4(2)
N(1)	19(3)	12(4)	17(3)	-1(3)	3(3)	-6(3)
C(1)	21(3)	12(5)	15(4)	-2(3)	4(3)	-6(3)
C(2)	26(4)	6(4)	16(4)	0(3)	-1(3)	-8(3)
C(3)	25(4)	27(6)	35(5)	-4(4)	0(4)	-10(4)
C(4)	51(6)	10(5)	30(5)	12(4)	-1(4)	-3(4)
C(5)	46(5)	25(6)	22(4)	3(4)	7(4)	-16(4)
C(6)	33(4)	18(5)	22(4)	3(4)	4(3)	-12(4)
C(7)	20(4)	16(5)	24(4)	7(3)	2(3)	-5(3)
C(8)	22(4)	21(5)	18(4)	-1(3)	-9(3)	-9(3)
C(9)	18(4)	25(5)	33(5)	-5(4)	-4(3)	-4(4)
C(10)	22(4)	12(4)	22(4)	-1(3)	6(3)	-12(3)
C(11)	28(4)	31(6)	17(4)	7(4)	-1(3)	-14(4)
C(12)	16(3)	23(5)	21(4)	-3(4)	3(3)	0(3)
C(13)	24(4)	18(5)	27(4)	-3(4)	8(3)	-3(3)
N(2)	16(3)	15(4)	13(3)	0(3)	-3(2)	-2(3)
C(14)	21(4)	20(5)	13(4)	-1(3)	5(3)	-6(3)
C(15)	25(4)	13(5)	21(4)	-2(3)	3(3)	-11(3)
C(16)	31(4)	13(5)	20(4)	-3(3)	-9(3)	-10(4)
C(17)	40(5)	30(6)	34(5)	9(4)	-18(4)	-19(5)

C(18)	61(6)	29(6)	19(4)	3(4)	-5(4)	-27(5)
C(19)	52(6)	16(5)	30(5)	-8(4)	9(4)	-14(4)
C(20)	27(4)	16(5)	22(4)	-3(4)	0(3)	-6(4)
C(21)	23(4)	14(5)	12(4)	4(3)	-14(3)	-6(3)
C(22)	26(4)	21(5)	33(5)	3(4)	-6(4)	-5(4)
C(23)	25(4)	33(6)	11(4)	-2(4)	-3(3)	-7(4)
C(24)	40(5)	42(7)	27(5)	-20(4)	11(4)	-24(5)
C(25)	16(3)	18(5)	19(4)	-3(3)	-3(3)	-2(3)
C(26)	18(4)	42(6)	32(5)	-9(4)	2(3)	-7(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bzte1-on.

	x	y	z	U(eq)
H(1)	2160	6614	459	32
H(3)	3480(80)	3740(80)	-1900(60)	25
H(4)	6472	2435	-987	28
H(6)	4610(80)	2910(80)	1940(60)	35
H(12)	3080(80)	4620(80)	3330(60)	33
H(13)	1543	6215	2667	34
H(14)	-810(80)	7860(80)	4150(60)	36
H(16)	-10(80)	7100(80)	6940(60)	27
H(17)	1401	5631	7802	23
H(18)	2800(70)	3720(70)	6070(60)	27
H(1A)	1896	362	-112	19
H(1B)	671	1223	-372	19
H(3)	2071	-653	1343	34
H(4)	1051	-1401	2453	38
H(5)	-960	-640	2722	36
H(6)	-2015	853	1834	28
H(7)	-1021	1598	709	24
H(8A)	2468	1275	1532	24
H(8B)	2950	2271	1165	24
H(9A)	3647	98	380	39
H(9B)	4428	534	1071	39
H(9C)	4181	1094	89	39
H(10A)	2697	1695	-858	21
H(10B)	2586	2879	-415	21
H(11A)	694	2401	-1314	36
H(11B)	1548	3045	-1785	36
H(11C)	690	3601	-950	36
H(12A)	41	3050	427	25
H(12B)	537	2606	1396	25
H(13A)	1752	3807	1336	36
H(13B)	397	4502	1250	36
H(13C)	1252	4254	365	36
H(14A)	6699	538	5188	22
H(14B)	5442	1442	5271	22
H(16)	4017	1626	4085	25
H(17)	3306	651	3003	39
H(18)	4571	-962	2340	40
H(19)	6501	-1651	2808	38
H(20)	7207	-705	3892	26
H(21A)	5692	2520	3454	19
H(21B)	5052	3136	4355	19
H(22A)	6346	4289	4293	41
H(22B)	5559	4441	3414	41
H(22C)	6908	3704	3357	41
H(23A)	7467	1956	5830	28
H(23B)	7416	3079	5287	28
H(24A)	5383	3763	5665	51
H(24B)	6146	3488	6558	51
H(24C)	5454	2645	6227	51
H(25A)	7624	1157	3490	22
H(25B)	8078	2189	3764	22
H(26A)	9105	1190	4966	47
H(26B)	9474	442	4072	47
H(26C)	8557	183	4803	47

Table 6. Hydrogen bonds for bzte1-on [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.84	1.97	2.465(7)	116.6
O(3)-H(3)...O(2)	0.77(9)	2.14(9)	2.883(8)	163(9)
O(3)-H(3)...O(18)#3	0.77(9)	2.42(9)	2.785(8)	111(8)
O(4)-H(4)...O(5)	0.84	1.92	2.433(7)	118.7
O(6)-H(6)...O(7)	1.02(9)	1.58(9)	2.541(8)	157(8)
O(18)-H(18)...O(11)	1.21(8)	1.26(8)	2.455(7)	165(8)
O(12)-H(12)...O(7)	0.86(9)	1.75(9)	2.498(7)	145(9)
O(13)-H(13)...O(8)	0.84	1.81	2.557(7)	146.9
O(14)-H(14)...O(15)	0.83(9)	1.64(9)	2.442(7)	161(10)
O(16)-H(16)...O(17)	0.84(9)	1.75(9)	2.575(7)	168(9)
O(17)-H(17)...O(2)#4	0.84	1.62	2.459(7)	176.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+1,-z+1 #3 x,y,z-1

#4 x,y,z+1

Crystallographic data of Bztbu crystal light-off stage measured at laboratory system

Table 1. Crystal data and structure refinement for bztbu-off.

Identification code	off2103k	
Empirical formula	C38 H78 N2 O20 P8 Pt2	
Formula weight	1520.96	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 9.5229(3) Å	α= 90.4165(3)°.
	b = 14.3046(5) Å	β= 97.3252(8)°.
	c = 20.8753(7) Å	γ = 106.8507(8)°.
Volume	2696.42(16) Å^3	
Z	2	
Density (calculated)	1.873 Mg/m^3	
Absorption coefficient	5.493 mm^{-1}	
F(000)	1512	
Crystal size	0.180 x 0.075 x 0.050 mm^3	
Theta range for data collection	1.49 to 27.48°.	
Index ranges	-12<=h<=3, -15<=k<=18, -23<=l<=25	
Reflections collected	13248	
Independent reflections	9927 [Rint = 0.0271]	
Completeness to θ = 27.48°	80.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.827	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9927 / 0 / 644	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2σ(I)]	R1 = 0.0336, wR2 = 0.0827	
R indices (all data)	R1 = 0.0381, wR2 = 0.0859	
Largest diff. peak and hole	1.831 and -1.515 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bztbu-off. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4551(1)	796(1)	4671(1)	6(1)
P(1)	5252(1)	1773(1)	5621(1)	9(1)
P(2)	6965(1)	1516(1)	4455(1)	10(1)
P(3)	3988(1)	-137(1)	3702(1)	9(1)
P(4)	2164(1)	109(1)	4909(1)	9(1)
O(1)	3981(4)	1927(3)	5979(2)	17(1)
O(2)	6295(4)	2800(3)	5571(2)	16(1)
O(3)	7612(3)	2603(3)	4674(2)	14(1)
O(4)	7253(4)	1428(3)	3748(2)	18(1)
O(5)	5066(4)	145(3)	3212(2)	16(1)
O(6)	2401(3)	-242(3)	3313(2)	15(1)
O(7)	967(3)	-34(3)	4292(2)	14(1)
O(8)	1666(3)	618(3)	5450(2)	15(1)
O(9)	6197(3)	1281(2)	6149(2)	13(1)
O(10)	8077(3)	1017(3)	4890(2)	13(1)
Pt(2)	3852(1)	4054(1)	-34(1)	8(1)
P(5)	3591(1)	4056(1)	-1162(1)	10(1)
P(6)	5576(1)	3210(1)	-116(1)	11(1)
P(7)	4206(1)	3981(1)	1082(1)	10(1)
P(8)	2123(1)	4887(1)	42(1)	10(1)
O(11)	2126(3)	4247(3)	-1508(2)	15(1)
O(12)	3703(4)	3143(3)	-1503(2)	16(1)
O(13)	5146(4)	2431(3)	-678(2)	16(1)
O(14)	6088(4)	2721(3)	483(2)	19(1)
O(15)	5038(4)	3288(3)	1367(2)	18(1)
O(16)	2769(3)	3751(3)	1426(2)	13(1)
O(17)	1124(3)	4497(3)	586(2)	13(1)
O(18)	1116(3)	4935(3)	-586(2)	15(1)
O(19)	4901(4)	4930(3)	-1404(2)	15(1)
O(20)	7083(3)	3981(3)	-306(2)	14(1)
N(1)	5733(4)	4178(3)	3426(2)	11(1)
C(1)	5439(5)	4027(4)	4131(2)	13(1)
C(2)	3895(5)	4026(4)	4265(2)	12(1)
C(3)	3479(5)	4888(4)	4291(2)	15(1)
C(4)	2063(5)	4858(4)	4406(3)	18(1)
C(5)	1050(5)	3974(4)	4514(3)	18(1)
C(6)	1463(6)	3120(4)	4512(3)	21(1)
C(7)	2889(6)	3154(4)	4391(3)	18(1)
C(8)	4439(5)	3549(4)	2962(2)	12(1)
C(9)	4150(5)	2442(4)	2996(3)	16(1)
C(10)	2699(6)	1910(4)	2569(3)	21(1)
C(11)	1320(6)	1915(4)	2867(3)	27(1)
C(12)	7131(5)	3888(4)	3377(2)	13(1)
C(13)	7592(5)	3953(4)	2697(3)	16(1)
C(14)	8940(6)	3585(4)	2685(3)	21(1)
C(15)	9393(6)	3617(4)	2012(3)	22(1)
C(16)	5917(5)	5236(4)	3248(3)	13(1)
C(17)	7175(5)	6030(4)	3641(3)	20(1)
C(18)	8636(6)	6377(4)	3358(3)	27(1)
C(19)	9762(6)	7229(5)	3763(3)	32(2)
N(2)	8350(4)	1581(3)	8509(2)	12(1)
C(20)	9344(5)	2368(4)	9008(2)	14(1)
C(21)	10035(5)	1977(4)	9604(3)	17(1)
C(22)	11363(5)	1752(4)	9596(3)	16(1)
C(23)	12036(5)	1421(4)	10151(3)	20(1)
C(24)	11407(6)	1360(4)	10717(3)	24(1)
C(25)	10094(6)	1591(5)	10728(3)	26(1)
C(26)	9413(6)	1904(4)	10181(3)	23(1)
C(27)	7081(5)	956(4)	8834(3)	14(1)

C(28)	5914(5)	176(4)	8388(3)	17(1)	C(34)	7703(6)	4144(5)	7411(4)	36(2)
C(29)	4611(5)	-328(4)	8745(3)	22(1)	C(35)	9202(5)	921(4)	8272(2)	13(1)
C(30)	3474(5)	-1151(4)	8333(3)	26(1)	C(36)	10437(5)	1422(4)	7878(3)	14(1)
C(31)	7817(5)	2093(4)	7926(2)	13(1)	C(37)	11401(6)	742(4)	7802(3)	24(1)
C(32)	6694(5)	2627(4)	8039(3)	17(1)	C(38)	12484(6)	1111(5)	7317(3)	27(1)
C(33)	6432(5)	3220(4)	7448(3)	19(1)					

Table 3. Bond lengths [Å] and angles [°] for bztbu-off.

Pt(1)-P(4)	2.3198(11)	Pt(2)-P(6)	2.3241(11)	N(1)-C(1)	1.538(6)
Pt(1)-P(1)	2.3271(12)	Pt(2)-P(5)	2.3373(13)	C(1)-C(2)	1.532(6)
Pt(1)-P(3)	2.3301(12)	Pt(2)-Pt(2)#2	2.9330(3)	C(2)-C(7)	1.386(7)
Pt(1)-P(2)	2.3337(11)	P(5)-O(12)	1.519(4)	C(2)-C(3)	1.402(7)
Pt(1)-Pt(1)#1	2.9457(3)	P(5)-O(11)	1.584(3)	C(3)-C(4)	1.388(6)
P(1)-O(2)	1.529(4)	P(5)-O(19)	1.624(4)	C(4)-C(5)	1.390(8)
P(1)-O(1)	1.566(3)	P(6)-O(14)	1.532(4)	C(5)-C(6)	1.387(7)
P(1)-O(9)	1.626(3)	P(6)-O(13)	1.543(4)	C(6)-C(7)	1.400(7)
P(2)-O(3)	1.539(4)	P(6)-O(20)	1.632(4)	C(8)-C(9)	1.530(7)
P(2)-O(4)	1.547(4)	P(6)-H(13)	1.85(7)	C(9)-C(10)	1.533(7)
P(2)-O(10)	1.630(3)	P(7)-O(15)	1.519(4)	C(10)-C(11)	1.525(8)
P(3)-O(5)	1.514(3)	P(7)-O(16)	1.579(3)	C(12)-C(13)	1.534(7)
P(3)-O(6)	1.587(3)	P(7)-O(19)#2	1.635(4)	C(13)-C(14)	1.525(6)
P(3)-O(9)#1	1.632(4)	P(8)-O(18)	1.537(4)	C(14)-C(15)	1.519(7)
P(4)-O(8)	1.533(3)	P(8)-O(17)	1.576(3)	C(16)-C(17)	1.532(7)
P(4)-O(7)	1.578(3)	P(8)-O(20)#2	1.634(4)	C(17)-C(18)	1.531(7)
P(4)-O(10)#1	1.626(4)	O(13)-H(13)	0.75(7)	C(18)-C(19)	1.532(8)
O(1)-H(1)	0.87(6)	O(16)-H(16)	0.87(6)	N(2)-C(27)	1.520(6)
O(2)-H(2)	0.94(6)	O(17)-H(17)	1.12(5)	N(2)-C(35)	1.527(5)
O(4)-H(4)	0.77(7)	O(19)-P(7)#2	1.635(4)	N(2)-C(31)	1.531(6)
O(9)-P(3)#1	1.632(4)	O(20)-P(8)#2	1.634(4)	N(2)-C(20)	1.537(6)
O(10)-P(4)#1	1.626(4)	N(1)-C(8)	1.519(6)	C(20)-C(21)	1.519(7)
Pt(2)-P(8)	2.3139(11)	N(1)-C(12)	1.519(5)	C(21)-C(22)	1.395(6)
Pt(2)-P(7)	2.3174(13)	N(1)-C(16)	1.527(7)	C(21)-C(26)	1.400(7)

C(22)-C(23)	1.403(7)	O(3)-P(2)-Pt(1)	114.63(13)	O(12)-P(5)-Pt(2)	115.63(16)
C(23)-C(24)	1.383(8)	O(4)-P(2)-Pt(1)	116.76(15)	O(11)-P(5)-Pt(2)	116.16(14)
C(24)-C(25)	1.386(8)	O(10)-P(2)-Pt(1)	108.94(13)	O(19)-P(5)-Pt(2)	110.83(13)
C(25)-C(26)	1.382(8)	O(5)-P(3)-O(6)	105.7(2)	O(14)-P(6)-O(13)	106.5(2)
C(27)-C(28)	1.532(7)	O(5)-P(3)-O(9)#1	107.14(19)	O(14)-P(6)-O(20)	105.02(19)
C(28)-C(29)	1.529(7)	O(6)-P(3)-O(9)#1	99.60(18)	O(13)-P(6)-O(20)	102.82(19)
C(29)-C(30)	1.519(7)	O(5)-P(3)-Pt(1)	117.50(15)	O(14)-P(6)-Pt(2)	118.35(14)
C(31)-C(32)	1.522(6)	O(6)-P(3)-Pt(1)	115.45(13)	O(13)-P(6)-Pt(2)	114.53(14)
C(32)-C(33)	1.537(8)	O(9)#1-P(3)-Pt(1)	109.67(13)	O(20)-P(6)-Pt(2)	108.16(13)
C(33)-C(34)	1.522(8)	O(8)-P(4)-O(7)	108.20(18)	O(14)-P(6)-H(13)	130(2)
C(35)-C(36)	1.530(6)	O(8)-P(4)-O(10)#1	106.2(2)	O(13)-P(6)-H(13)	23(2)
C(36)-C(37)	1.538(6)	O(7)-P(4)-O(10)#1	100.90(18)	O(20)-P(6)-H(13)	97(2)
C(37)-C(38)	1.525(7)	O(8)-P(4)-Pt(1)	117.29(14)	Pt(2)-P(6)-H(13)	96(2)
		O(7)-P(4)-Pt(1)	112.17(14)	O(15)-P(7)-O(16)	104.7(2)
P(4)-Pt(1)-P(1)	92.66(4)	O(10)#1-P(4)-Pt(1)	110.67(11)	O(15)-P(7)-O(19)#2	106.9(2)
P(4)-Pt(1)-P(3)	90.76(4)	P(1)-O(1)-H(1)	113(4)	O(16)-P(7)-O(19)#2	100.22(18)
P(1)-Pt(1)-P(3)	176.57(4)	P(1)-O(2)-H(2)	100(4)	O(15)-P(7)-Pt(2)	117.66(15)
P(4)-Pt(1)-P(2)	178.44(4)	P(2)-O(4)-H(4)	126(5)	O(16)-P(7)-Pt(2)	116.29(14)
P(1)-Pt(1)-P(2)	85.78(4)	P(1)-O(9)-P(3)#1	130.7(2)	O(19)#2-P(7)-Pt(2)	109.34(14)
P(3)-Pt(1)-P(2)	90.79(4)	P(4)#1-O(10)-P(2)	130.4(2)	O(18)-P(8)-O(17)	108.70(18)
P(4)-Pt(1)-Pt(1)#1	89.30(3)	P(8)-Pt(2)-P(7)	90.18(4)	O(18)-P(8)-O(20)#2	106.0(2)
P(1)-Pt(1)-Pt(1)#1	90.90(3)	P(8)-Pt(2)-P(6)	179.54(5)	O(17)-P(8)-O(20)#2	100.77(18)
P(3)-Pt(1)-Pt(1)#1	89.41(3)	P(7)-Pt(2)-P(6)	90.14(4)	O(18)-P(8)-Pt(2)	116.28(13)
P(2)-Pt(1)-Pt(1)#1	90.92(3)	P(8)-Pt(2)-P(5)	93.62(4)	O(17)-P(8)-Pt(2)	112.46(13)
O(2)-P(1)-O(1)	105.1(2)	P(7)-Pt(2)-P(5)	176.15(4)	O(20)#2-P(8)-Pt(2)	111.36(12)
O(2)-P(1)-O(9)	103.43(19)	P(6)-Pt(2)-P(5)	86.06(4)	P(6)-O(13)-H(13)	102(5)
O(1)-P(1)-O(9)	104.5(2)	P(8)-Pt(2)-Pt(2)#2	88.63(3)	P(7)-O(16)-H(16)	117(4)
O(2)-P(1)-Pt(1)	116.01(15)	P(7)-Pt(2)-Pt(2)#2	91.00(3)	P(8)-O(17)-H(17)	112(3)
O(1)-P(1)-Pt(1)	117.07(14)	P(6)-Pt(2)-Pt(2)#2	91.69(3)	P(5)-O(19)-P(7)#2	131.0(2)
O(9)-P(1)-Pt(1)	109.30(12)	P(5)-Pt(2)-Pt(2)#2	89.74(3)	P(6)-O(20)-P(8)#2	128.9(2)
O(3)-P(2)-O(4)	106.7(2)	O(12)-P(5)-O(11)	105.7(2)	C(8)-N(1)-C(12)	110.9(3)
O(3)-P(2)-O(10)	102.31(18)	O(12)-P(5)-O(19)	103.71(19)	C(8)-N(1)-C(16)	106.6(4)
O(4)-P(2)-O(10)	106.19(19)	O(11)-P(5)-O(19)	103.42(19)	C(12)-N(1)-C(16)	111.6(4)

C(8)-N(1)-C(1)	110.9(4)	C(15)-C(14)-C(13)	111.3(4)	C(26)-C(25)-C(24)	120.8(5)
C(12)-N(1)-C(1)	105.7(3)	N(1)-C(16)-C(17)	117.3(4)	C(25)-C(26)-C(21)	120.2(5)
C(16)-N(1)-C(1)	111.2(4)	C(18)-C(17)-C(16)	116.9(4)	N(2)-C(27)-C(28)	115.0(4)
C(2)-C(1)-N(1)	115.6(4)	C(17)-C(18)-C(19)	112.1(5)	C(29)-C(28)-C(27)	110.4(4)
C(7)-C(2)-C(3)	118.5(4)	C(27)-N(2)-C(35)	108.5(4)	C(30)-C(29)-C(28)	112.0(4)
C(7)-C(2)-C(1)	119.3(4)	C(27)-N(2)-C(31)	112.6(3)	C(32)-C(31)-N(2)	115.7(4)
C(3)-C(2)-C(1)	122.1(4)	C(35)-N(2)-C(31)	108.0(4)	C(31)-C(32)-C(33)	109.7(4)
C(4)-C(3)-C(2)	120.6(5)	C(27)-N(2)-C(20)	108.1(4)	C(34)-C(33)-C(32)	113.0(4)
C(3)-C(4)-C(5)	120.3(5)	C(35)-N(2)-C(20)	111.3(3)	N(2)-C(35)-C(36)	115.2(4)
C(6)-C(5)-C(4)	119.7(4)	C(31)-N(2)-C(20)	108.3(4)	C(35)-C(36)-C(37)	109.1(4)
C(5)-C(6)-C(7)	119.7(5)	C(21)-C(20)-N(2)	115.0(4)	C(38)-C(37)-C(36)	112.0(5)
C(2)-C(7)-C(6)	121.1(5)	C(22)-C(21)-C(26)	118.9(5)		
N(1)-C(8)-C(9)	116.1(4)	C(22)-C(21)-C(20)	120.1(5)	Symmetry transformations used to	
C(8)-C(9)-C(10)	109.9(4)	C(26)-C(21)-C(20)	120.9(4)	generate equivalent atoms:	
C(11)-C(10)-C(9)	113.5(4)	C(21)-C(22)-C(23)	120.5(5)	#1 -x+1,-y,-z+1	
N(1)-C(12)-C(13)	114.0(4)	C(24)-C(23)-C(22)	119.6(5)	#2 -x+1,-y+1,-z	
C(14)-C(13)-C(12)	110.3(4)	C(23)-C(24)-C(25)	120.0(5)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for bztbu-off. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	5(1)	7(1)	7(1)	0(1)	1(1)	2(1)
P(1)	9(1)	10(1)	10(1)	-2(1)	0(1)	3(1)
P(2)	7(1)	11(1)	12(1)	4(1)	4(1)	2(1)
P(3)	10(1)	11(1)	8(1)	0(1)	1(1)	4(1)
P(4)	4(1)	12(1)	10(1)	-1(1)	1(1)	3(1)
O(1)	11(2)	18(2)	21(2)	-8(2)	4(1)	2(1)
O(2)	19(2)	14(2)	13(2)	-4(2)	1(1)	2(1)
O(3)	9(1)	12(2)	21(2)	3(2)	3(1)	0(1)
O(4)	14(2)	23(2)	13(2)	-1(2)	4(1)	1(1)
O(5)	15(2)	20(2)	14(2)	1(2)	8(1)	3(1)
O(6)	10(1)	19(2)	14(2)	-1(2)	-1(1)	5(1)
O(7)	5(1)	19(2)	18(2)	1(2)	-1(1)	2(1)
O(8)	9(1)	19(2)	17(2)	-6(2)	5(1)	3(1)
O(9)	17(2)	7(2)	13(2)	-3(1)	-5(1)	6(1)
O(10)	5(1)	17(2)	18(2)	2(2)	1(1)	3(1)
Pt(2)	6(1)	11(1)	7(1)	0(1)	2(1)	4(1)
P(5)	8(1)	15(1)	7(1)	-1(1)	2(1)	3(1)
P(6)	10(1)	14(1)	12(1)	0(1)	3(1)	7(1)
P(7)	9(1)	15(1)	8(1)	1(1)	2(1)	5(1)
P(8)	7(1)	17(1)	9(1)	2(1)	2(1)	6(1)
O(11)	14(2)	23(2)	9(2)	0(2)	1(1)	7(1)

O(12)	20(2)	17(2)	12(2)	-3(2)	4(1)	7(1)
O(13)	22(2)	12(2)	17(2)	-3(2)	2(1)	10(1)
O(14)	21(2)	26(2)	16(2)	3(2)	7(1)	16(2)
O(15)	21(2)	24(2)	13(2)	6(2)	2(1)	16(2)
O(16)	12(2)	18(2)	10(2)	3(2)	4(1)	4(1)
O(17)	11(1)	19(2)	12(2)	7(2)	6(1)	9(1)
O(18)	10(1)	29(2)	11(2)	3(2)	3(1)	13(1)
O(19)	15(2)	19(2)	8(2)	-2(2)	4(1)	-1(1)
O(20)	11(1)	17(2)	14(2)	-3(2)	5(1)	6(1)
N(1)	10(2)	18(2)	6(2)	-1(2)	0(1)	8(2)
C(2)	14(2)	17(3)	4(3)	0(2)	-1(2)	5(2)
C(3)	12(2)	16(3)	14(3)	-1(2)	2(2)	1(2)
C(4)	17(2)	21(3)	16(3)	-6(2)	2(2)	8(2)
C(5)	13(2)	26(3)	15(3)	-2(2)	1(2)	6(2)
C(6)	20(2)	18(3)	21(3)	-1(2)	7(2)	0(2)
C(7)	26(3)	19(3)	14(3)	-1(2)	5(2)	11(2)
C(8)	12(2)	14(3)	12(3)	3(2)	1(2)	4(2)
C(9)	25(2)	14(3)	11(3)	2(2)	5(2)	9(2)
C(10)	35(3)	9(3)	16(3)	0(2)	2(2)	4(2)
C(11)	19(2)	20(3)	38(4)	-2(3)	-4(2)	2(2)
C(12)	14(2)	21(3)	10(3)	5(2)	7(2)	10(2)
C(13)	17(2)	18(3)	15(3)	1(2)	5(2)	9(2)
C(14)	20(2)	30(3)	19(3)	10(2)	11(2)	13(2)
C(15)	19(2)	26(3)	25(3)	2(2)	12(2)	7(2)
C(16)	17(2)	11(3)	13(3)	4(2)	4(2)	5(2)
C(17)	19(2)	23(3)	18(3)	-2(2)	2(2)	5(2)
C(18)	23(3)	25(3)	28(4)	8(3)	5(2)	0(2)
C(19)	25(3)	31(4)	30(4)	2(3)	0(2)	-5(2)
N(2)	11(2)	12(2)	13(2)	-1(2)	1(1)	4(2)
C(20)	12(2)	9(3)	18(3)	-10(2)	1(2)	0(2)
C(21)	15(2)	17(3)	14(3)	-4(2)	-1(2)	0(2)
C(22)	16(2)	18(3)	16(3)	-1(2)	2(2)	4(2)
C(23)	16(2)	15(3)	25(3)	3(2)	-3(2)	2(2)
C(24)	32(3)	24(3)	12(3)	5(2)	-2(2)	2(2)
C(25)	30(3)	31(4)	12(3)	-4(3)	3(2)	5(2)
C(26)	18(2)	32(3)	22(3)	-7(3)	4(2)	10(2)
C(27)	12(2)	18(3)	15(3)	2(2)	6(2)	4(2)
C(28)	12(2)	15(3)	21(3)	0(2)	1(2)	0(2)
C(29)	13(2)	31(3)	19(3)	-1(2)	5(2)	2(2)
C(30)	14(2)	25(3)	35(4)	5(3)	4(2)	-2(2)
C(31)	18(2)	14(3)	7(3)	0(2)	0(2)	4(2)
C(32)	16(2)	18(3)	21(3)	3(2)	3(2)	10(2)
C(33)	17(2)	20(3)	20(3)	1(2)	-2(2)	7(2)
C(34)	25(3)	32(4)	51(5)	20(3)	5(3)	8(3)
C(35)	11(2)	15(3)	15(3)	-3(2)	6(2)	6(2)
C(36)	10(2)	15(3)	16(3)	0(2)	5(2)	3(2)
C(37)	18(2)	22(3)	35(4)	0(3)	12(2)	7(2)
C(38)	21(2)	32(4)	31(4)	-4(3)	11(2)	12(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bztbu-off.

	x	y	z	U(eq)
H(1)	3110(70)	1560(50)	5820(30)	25
H(2)	6690(70)	2710(40)	5190(30)	24
H(4)	6710(70)	1110(50)	3470(30)	27
H(6)	1797	-250	3575	22
H(7)	128	-331	4389	21
H(11)	1699	4449	-1232	22
H(13)	4790(70)	2680(50)	-940(30)	24
H(14)	5613	2788	784	28
H(16)	2020(70)	3920(40)	1240(30)	20
H(17)	170(60)	4810(40)	570(30)	19
H(1A)	5595	3397	4261	16
H(1B)	6182	4551	4408	16
H(3)	4173	5497	4230	18
H(4)	1785	5444	4411	21
H(5)	78	3954	4588	22
H(6)	782	2516	4593	25
H(7)	3172	2569	4395	22
H(8A)	4612	3731	2516	15
H(8B)	3532	3709	3044	15
H(9A)	4086	2252	3449	19
H(9B)	4980	2251	2848	19
H(10A)	2674	2223	2148	25
H(10B)	2679	1224	2486	25
H(11A)	434	1569	2571	41
H(11B)	1320	2592	2944	41
H(11C)	1319	1589	3278	41
H(12A)	6975	3208	3514	16
H(12B)	7951	4317	3681	16
H(13A)	6760	3555	2384	19
H(13B)	7830	4640	2568	19
H(14A)	9776	3995	2991	25
H(14B)	8708	2905	2827	25
H(15A)	10264	3381	2019	34
H(15B)	9633	4291	1872	34
H(15C)	8575	3199	1710	34
H(16A)	4976	5382	3287	16
H(16B)	6068	5288	2787	16
H(17A)	6819	6605	3704	25
H(17B)	7383	5783	4074	25
H(18A)	8438	6585	2912	32
H(18B)	9062	5825	3334	32
H(19A)	10664	7443	3557	48
H(19B)	10003	7015	4197	48
H(19C)	9339	7773	3793	48
H(20A)	10148	2796	8794	16
H(20B)	8748	2776	9148	16
H(22)	11816	1823	9213	20
H(23)	12917	1241	10138	24
H(24)	11875	1159	11098	29
H(25)	9656	1535	11116	31
H(26)	8520	2069	10196	28
H(27A)	6586	1391	9023	17
H(27B)	7497	627	9194	17
H(28A)	5555	485	8003	21
H(28B)	6364	-316	8240	21
H(29A)	4984	-595	9146	26
H(29B)	4128	160	8870	26
H(30A)	2672	-1466	8582	39
H(30B)	3949	-1634	8206	39
H(30C)	3068	-885	7945	39

H(31A)	8690	2569	7785	16
H(31B)	7373	1598	7567	16
H(32A)	7067	3070	8429	20
H(32B)	5749	2148	8111	20
H(33A)	6290	2803	7050	23
H(33B)	5510	3402	7466	23
H(34A)	7478	4490	7026	54
H(34B)	8616	3968	7384	54
H(34C)	7833	4568	7798	54
H(35A)	8491	371	8004	15
H(35B)	9640	642	8652	15
H(36A)	11052	2047	8101	16
H(36B)	10003	1566	7447	16
H(37A)	11961	692	8227	29
H(37B)	10752	80	7656	29
H(38A)	13073	659	7281	40
H(38B)	13143	1761	7465	40
H(38C)	11932	1152	6894	40

Table 6. Hydrogen bonds for bztbu-off [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.87(6)	1.71(6)	2.557(5)	163(6)
O(2)-H(2)...O(3)	0.94(6)	1.51(6)	2.441(5)	168(6)
O(4)-H(4)...O(5)	0.77(7)	1.78(7)	2.473(5)	149(7)
O(6)-H(6)...O(7)	0.84	1.84	2.658(5)	163.0
O(7)-H(7)...O(8)#3	0.84	1.72	2.533(4)	163.6
O(11)-H(11)...O(18)	0.84	1.74	2.568(5)	170.3
O(13)-H(13)...O(12)	0.75(7)	1.73(7)	2.475(5)	170(7)
O(14)-H(14)...O(15)	0.84	1.64	2.445(5)	161.1
O(16)-H(16)...O(17)	0.87(6)	1.84(6)	2.639(5)	153(6)
O(17)-H(17)...O(18)#4	1.12(5)	1.38(5)	2.493(4)	171(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,-y+1,-z #3 -x,-y,-z+1

#4 -x,-y+1,-z

Crystallographic data of Bztbu crystal light-on stage measured at laboratory system

Table 1. Crystal data and structure refinement for bztbu-on.

Identification code	on1103k	
Empirical formula	C38 H78 N2 O20 P8 Pt2	
Formula weight	1520.96	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 9.5199(2) Å	α= 90.4352(7)°.
	b = 14.2924(4) Å	β= 97.3120(7)°.
	c = 20.8590(6) Å	γ = 106.8467(5)°.
Volume	2691.27(12) Å^3	
Z	2	
Density (calculated)	1.877 Mg/m^3	
Absorption coefficient	5.503 mm^{-1}	
F(000)	1512	
Crystal size	0.180 x 0.075 x 0.050 mm^3	
Theta range for data collection	1.49 to 27.48°.	
Index ranges	-12<=h<=3, -15<=k<=18, -23<=l<=25	
Reflections collected	13212	
Independent reflections	9900 [Rint = 0.0288]	
Completeness to θ = 27.48°	80.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.821	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9900 / 0 / 655	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2σ(I)]	R1 = 0.0353, wR2 = 0.0878	
R indices (all data)	R1 = 0.0401, wR2 = 0.0913	
Largest diff. peak and hole	2.095 and -1.421 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bztbu-on. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4551(1)	795(1)	4671(1)	7(1)
P(1)	5252(1)	1773(1)	5621(1)	10(1)
P(2)	6964(1)	1517(1)	4455(1)	12(1)
P(3)	3988(1)	-139(1)	3703(1)	11(1)
P(4)	2166(1)	111(1)	4910(1)	10(1)
O(1)	3981(4)	1928(3)	5978(2)	20(1)
O(2)	6300(4)	2804(3)	5572(2)	16(1)
O(3)	7610(4)	2600(3)	4671(2)	16(1)
O(4)	7246(4)	1423(3)	3749(2)	20(1)
O(5)	5064(4)	141(3)	3215(2)	18(1)
O(6)	2392(4)	-248(3)	3314(2)	17(1)
O(7)	956(3)	-40(3)	4294(2)	16(1)
O(8)	1666(4)	617(3)	5448(2)	16(1)
O(9)	6200(4)	1287(3)	6144(2)	16(1)
O(10)	8070(3)	1011(3)	4888(2)	14(1)
Pt(2)	3852(1)	4055(1)	-34(1)	9(1)
P(5)	3591(1)	4058(1)	-1162(1)	11(1)
P(6)	5575(1)	3212(1)	-118(1)	13(1)
P(7)	4206(1)	3980(1)	1081(1)	11(1)
P(8)	2123(1)	4888(1)	42(1)	11(1)
O(11)	2128(4)	4247(3)	-1509(2)	16(1)
O(12)	3700(4)	3146(3)	-1502(2)	17(1)
O(13)	5155(4)	2431(3)	-682(2)	18(1)
O(14)	6080(4)	2718(3)	485(2)	19(1)
O(15)	5036(4)	3290(3)	1365(2)	20(1)
O(16)	2774(4)	3753(3)	1426(2)	18(1)
O(17)	1124(4)	4495(3)	584(2)	16(1)
O(18)	1114(3)	4937(3)	-583(2)	15(1)
O(19)	4903(4)	4928(3)	-1406(2)	16(1)
O(20)	7080(4)	3983(3)	-309(2)	15(1)
N(1)	5725(4)	4171(3)	3427(2)	13(1)
C(1)	5433(5)	4018(4)	4131(2)	14(1)
C(2)	3888(5)	4023(4)	4266(2)	15(1)
C(3)	3487(5)	4885(4)	4293(3)	15(1)
C(4)	2060(5)	4858(4)	4402(3)	19(1)
C(5)	1048(5)	3974(4)	4512(3)	21(1)
C(6)	1459(6)	3118(4)	4514(3)	22(1)
C(7)	2886(6)	3151(4)	4390(3)	18(1)
C(8)	4430(5)	3543(4)	2959(3)	15(1)
C(9)	4153(6)	2448(4)	2994(3)	18(1)
C(10)	2693(7)	1910(4)	2571(3)	25(1)
C(11)	1319(6)	1916(5)	2867(3)	30(2)
C(12)	7130(5)	3887(4)	3375(3)	16(1)
C(13)	7588(5)	3950(4)	2694(3)	16(1)
C(14)	8944(6)	3585(5)	2693(3)	24(1)
C(15)	9393(6)	3615(5)	2011(3)	25(1)
C(16)	5906(5)	5221(4)	3249(3)	17(1)
C(17)	7183(6)	6020(5)	3644(3)	23(1)
C(18)	8622(7)	6374(5)	3358(3)	32(2)
C(19)	9748(7)	7230(5)	3768(3)	32(2)
N(2)	8349(4)	1583(3)	8506(2)	14(1)
C(20)	9338(5)	2369(4)	9007(3)	17(1)
C(21)	10031(5)	1985(4)	9603(3)	16(1)
C(22)	11364(5)	1753(4)	9603(3)	19(1)
C(23)	12037(6)	1425(4)	10150(3)	21(1)
C(24)	11408(6)	1354(5)	10718(3)	26(1)
C(25)	10079(7)	1584(5)	10727(3)	27(1)
C(26)	9410(6)	1905(5)	10182(3)	23(1)

C(27)	7071(5)	956(4)	8832(3)	15(1)
C(28)	5917(5)	179(4)	8385(3)	17(1)
C(29)	4609(6)	-331(5)	8745(3)	24(1)
C(30)	3474(6)	-1146(5)	8336(3)	30(1)
C(31)	7818(5)	2088(4)	7928(3)	15(1)
C(32)	6686(6)	2627(4)	8031(3)	19(1)
C(33)	6437(6)	3229(4)	7446(3)	21(1)
C(34)	7702(7)	4140(5)	7408(4)	38(2)
C(35)	9211(5)	924(4)	8270(3)	14(1)
C(36)	10437(5)	1421(4)	7877(3)	16(1)
C(37)	11396(6)	748(5)	7798(3)	26(1)
C(38)	12475(6)	1103(5)	7314(3)	29(2)

Table 3. Bond lengths [Å] and angles [°] for bztbu-on.

Pt(1)-P(4)	2.3175(11)	O(10)-P(4)#1	1.621(4)	O(17)-H(17)	1.14(6)
Pt(1)-P(1)	2.3253(13)	Pt(2)-P(8)	2.3140(11)	O(19)-P(7)#2	1.638(4)
Pt(1)-P(3)	2.3269(13)	Pt(2)-P(7)	2.3165(13)	O(20)-P(8)#2	1.630(4)
Pt(1)-P(2)	2.3324(12)	Pt(2)-P(6)	2.3212(11)	N(1)-C(16)	1.515(7)
Pt(1)-Pt(1)#1	2.9422(3)	Pt(2)-P(5)	2.3343(13)	N(1)-C(8)	1.522(6)
P(1)-O(2)	1.534(4)	Pt(2)-Pt(2)#2	2.9304(4)	N(1)-C(12)	1.523(5)
P(1)-O(1)	1.565(4)	P(5)-O(12)	1.514(4)	N(1)-C(1)	1.534(7)
P(1)-O(9)	1.617(4)	P(5)-O(11)	1.582(3)	C(1)-C(2)	1.534(6)
P(2)-O(3)	1.531(4)	P(5)-O(19)	1.623(4)	C(2)-C(7)	1.381(8)
P(2)-O(4)	1.542(4)	P(6)-O(14)	1.538(4)	C(2)-C(3)	1.395(7)
P(2)-O(10)	1.630(4)	P(6)-O(13)	1.548(4)	C(3)-C(4)	1.394(6)
P(3)-O(5)	1.510(4)	P(6)-O(20)	1.631(4)	C(4)-C(5)	1.390(8)
P(3)-O(6)	1.593(3)	P(6)-H(13)	1.89(7)	C(5)-C(6)	1.388(8)
P(3)-O(9)#1	1.637(4)	P(7)-O(15)	1.512(4)	C(6)-C(7)	1.402(7)
P(4)-O(8)	1.528(4)	P(7)-O(16)	1.574(4)	C(8)-C(9)	1.513(8)
P(4)-O(7)	1.581(4)	P(7)-O(19)#2	1.638(4)	C(9)-C(10)	1.537(8)
P(4)-O(10)#1	1.621(4)	P(8)-O(18)	1.533(4)	C(10)-C(11)	1.519(9)
O(1)-H(1)	0.88(7)	P(8)-O(17)	1.573(4)	C(12)-C(13)	1.533(7)
O(2)-H(2)	1.05(7)	P(8)-O(20)#2	1.630(4)	C(13)-C(14)	1.526(6)
O(3)-H(2)	1.40(7)	O(13)-H(13)	0.77(7)	C(14)-C(15)	1.536(8)
O(4)-H(4)	0.75(7)	O(14)-H(15)	1.09(7)	C(16)-C(17)	1.545(8)
O(7)-H(7)	1.12(6)	O(15)-H(15)	1.36(7)	C(17)-C(18)	1.515(8)
O(9)-P(3)#1	1.637(4)	O(16)-H(16)	0.78(7)	C(18)-C(19)	1.538(9)

N(2)-C(31)	1.518(7)	O(1)-P(1)-O(9)	104.9(2)	P(7)-Pt(2)-P(5)	176.15(4)
N(2)-C(27)	1.527(6)	O(2)-P(1)-Pt(1)	116.13(16)	P(6)-Pt(2)-P(5)	86.07(5)
N(2)-C(35)	1.532(6)	O(1)-P(1)-Pt(1)	117.05(15)	P(8)-Pt(2)-Pt(2)#2	88.64(3)
N(2)-C(20)	1.536(7)	O(9)-P(1)-Pt(1)	109.28(14)	P(7)-Pt(2)-Pt(2)#2	90.98(3)
C(20)-C(21)	1.515(8)	O(3)-P(2)-O(4)	106.9(2)	P(6)-Pt(2)-Pt(2)#2	91.64(3)
C(21)-C(22)	1.401(7)	O(3)-P(2)-O(10)	102.58(19)	P(5)-Pt(2)-Pt(2)#2	89.74(3)
C(21)-C(26)	1.402(8)	O(4)-P(2)-O(10)	106.0(2)	O(12)-P(5)-O(11)	105.5(2)
C(22)-C(23)	1.389(8)	O(3)-P(2)-Pt(1)	114.79(14)	O(12)-P(5)-O(19)	103.6(2)
C(23)-C(24)	1.387(8)	O(4)-P(2)-Pt(1)	116.59(16)	O(11)-P(5)-O(19)	103.5(2)
C(24)-C(25)	1.398(8)	O(10)-P(2)-Pt(1)	108.72(14)	O(12)-P(5)-Pt(2)	115.58(17)
C(25)-C(26)	1.380(9)	O(5)-P(3)-O(6)	106.0(2)	O(11)-P(5)-Pt(2)	116.32(14)
C(27)-C(28)	1.525(7)	O(5)-P(3)-O(9)#1	107.3(2)	O(19)-P(5)-Pt(2)	111.00(14)
C(28)-C(29)	1.539(7)	O(6)-P(3)-O(9)#1	99.46(19)	O(14)-P(6)-O(13)	106.4(2)
C(29)-C(30)	1.508(8)	O(5)-P(3)-Pt(1)	117.48(16)	O(14)-P(6)-O(20)	105.5(2)
C(31)-C(32)	1.529(7)	O(6)-P(3)-Pt(1)	115.41(14)	O(13)-P(6)-O(20)	102.4(2)
C(32)-C(33)	1.531(8)	O(9)#1-P(3)-Pt(1)	109.48(14)	O(14)-P(6)-Pt(2)	118.08(15)
C(33)-C(34)	1.507(9)	O(8)-P(4)-O(7)	107.94(19)	O(13)-P(6)-Pt(2)	114.83(15)
C(35)-C(36)	1.520(7)	O(8)-P(4)-O(10)#1	106.1(2)	O(20)-P(6)-Pt(2)	108.16(13)
C(36)-C(37)	1.526(7)	O(7)-P(4)-O(10)#1	100.75(19)	O(14)-P(6)-H(13)	129(2)
C(37)-C(38)	1.517(8)	O(8)-P(4)-Pt(1)	117.49(15)	O(13)-P(6)-H(13)	23(2)
		O(7)-P(4)-Pt(1)	112.61(14)	O(20)-P(6)-H(13)	98(2)
P(4)-Pt(1)-P(1)	92.61(4)	O(10)#1-P(4)-Pt(1)	110.50(12)	Pt(2)-P(6)-H(13)	96(2)
P(4)-Pt(1)-P(3)	90.80(4)	P(1)-O(1)-H(1)	116(4)	O(15)-P(7)-O(16)	104.8(2)
P(1)-Pt(1)-P(3)	176.58(4)	P(1)-O(2)-H(2)	103(3)	O(15)-P(7)-O(19)#2	106.8(2)
P(4)-Pt(1)-P(2)	178.35(5)	P(2)-O(3)-H(2)	105(3)	O(16)-P(7)-O(19)#2	100.0(2)
P(1)-Pt(1)-P(2)	85.77(4)	P(2)-O(4)-H(4)	125(6)	O(15)-P(7)-Pt(2)	117.68(16)
P(3)-Pt(1)-P(2)	90.82(5)	P(4)-O(7)-H(7)	115(3)	O(16)-P(7)-Pt(2)	116.31(15)
P(4)-Pt(1)-Pt(1)#1	89.38(3)	P(1)-O(9)-P(3)#1	130.7(2)	O(19)#2-P(7)-Pt(2)	109.40(15)
P(1)-Pt(1)-Pt(1)#1	90.87(3)	P(4)#1-O(10)-P(2)	130.9(2)	O(18)-P(8)-O(17)	108.41(19)
P(3)-Pt(1)-Pt(1)#1	89.41(3)	P(8)-Pt(2)-P(7)	90.20(4)	O(18)-P(8)-O(20)#2	106.2(2)
P(2)-Pt(1)-Pt(1)#1	90.95(3)	P(8)-Pt(2)-P(6)	179.57(5)	O(17)-P(8)-O(20)#2	100.9(2)
O(2)-P(1)-O(1)	105.0(2)	P(7)-Pt(2)-P(6)	90.12(5)	O(18)-P(8)-Pt(2)	116.43(14)
O(2)-P(1)-O(9)	103.0(2)	P(8)-Pt(2)-P(5)	93.60(4)	O(17)-P(8)-Pt(2)	112.37(14)

O(20)#2-P(8)-Pt(2)	111.21(12)	C(5)-C(6)-C(7)	119.5(5)	C(23)-C(22)-C(21)	121.6(5)
P(6)-O(13)-H(13)	105(5)	C(2)-C(7)-C(6)	120.9(5)	C(24)-C(23)-C(22)	119.5(5)
P(6)-O(14)-H(15)	111(4)	C(9)-C(8)-N(1)	115.7(4)	C(23)-C(24)-C(25)	119.5(6)
P(7)-O(15)-H(15)	111(3)	C(8)-C(9)-C(10)	109.8(4)	C(26)-C(25)-C(24)	120.7(6)
P(7)-O(16)-H(16)	114(5)	C(11)-C(10)-C(9)	113.8(5)	C(25)-C(26)-C(21)	120.6(5)
P(8)-O(17)-H(17)	113(3)	N(1)-C(12)-C(13)	114.3(4)	C(28)-C(27)-N(2)	114.7(4)
P(5)-O(19)-P(7)#2	130.7(2)	C(14)-C(13)-C(12)	109.4(4)	C(27)-C(28)-C(29)	110.0(4)
P(8)#2-O(20)-P(6)	128.8(2)	C(13)-C(14)-C(15)	110.2(5)	C(30)-C(29)-C(28)	112.2(5)
C(16)-N(1)-C(8)	106.3(4)	N(1)-C(16)-C(17)	117.1(4)	N(2)-C(31)-C(32)	116.5(4)
C(16)-N(1)-C(12)	111.2(4)	C(18)-C(17)-C(16)	117.2(5)	C(31)-C(32)-C(33)	110.6(5)
C(8)-N(1)-C(12)	111.0(4)	C(17)-C(18)-C(19)	112.0(5)	C(34)-C(33)-C(32)	113.4(5)
C(16)-N(1)-C(1)	111.5(4)	C(31)-N(2)-C(27)	112.3(4)	C(36)-C(35)-N(2)	115.4(4)
C(8)-N(1)-C(1)	111.1(4)	C(31)-N(2)-C(35)	108.1(4)	C(35)-C(36)-C(37)	109.4(4)
C(12)-N(1)-C(1)	105.9(4)	C(27)-N(2)-C(35)	108.8(4)	C(38)-C(37)-C(36)	112.8(5)
N(1)-C(1)-C(2)	115.5(4)	C(31)-N(2)-C(20)	108.6(4)		
C(7)-C(2)-C(3)	119.1(5)	C(27)-N(2)-C(20)	107.9(4)		
C(7)-C(2)-C(1)	118.9(5)	C(35)-N(2)-C(20)	111.2(3)		
C(3)-C(2)-C(1)	122.0(5)	C(21)-C(20)-N(2)	115.3(4)		
C(4)-C(3)-C(2)	120.4(5)	C(22)-C(21)-C(26)	117.9(5)		
C(5)-C(4)-C(3)	120.1(5)	C(22)-C(21)-C(20)	120.8(5)		
C(6)-C(5)-C(4)	119.9(5)	C(26)-C(21)-C(20)	121.1(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

#2 -x+1,-y+1,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for bztbu-on. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	6(1)	7(1)	9(1)	1(1)	2(1)	3(1)
P(1)	9(1)	10(1)	12(1)	-2(1)	1(1)	2(1)
P(2)	9(1)	12(1)	15(1)	5(1)	5(1)	2(1)
P(3)	12(1)	12(1)	9(1)	-1(1)	1(1)	4(1)
P(4)	5(1)	13(1)	12(1)	0(1)	2(1)	3(1)
O(1)	14(2)	21(2)	24(2)	-8(2)	3(1)	5(2)
O(2)	18(2)	7(2)	19(2)	-3(2)	3(1)	-1(1)
O(3)	11(2)	11(2)	26(2)	5(2)	4(1)	2(1)
O(4)	17(2)	25(2)	17(2)	0(2)	8(1)	1(2)
O(5)	17(2)	27(2)	12(2)	1(2)	8(1)	6(2)
O(6)	15(2)	23(2)	13(2)	-2(2)	-1(1)	9(1)
O(7)	8(1)	20(2)	19(2)	1(2)	2(1)	5(1)

O(8)	11(2)	20(2)	18(2)	-7(2)	5(1)	2(1)
O(9)	22(2)	10(2)	17(2)	-1(2)	-2(1)	7(1)
O(10)	5(1)	13(2)	25(2)	6(2)	2(1)	3(1)
Pt(2)	7(1)	12(1)	8(1)	0(1)	3(1)	4(1)
P(5)	9(1)	16(1)	8(1)	-1(1)	2(1)	3(1)
P(6)	13(1)	14(1)	15(1)	0(1)	4(1)	8(1)
P(7)	10(1)	16(1)	9(1)	2(1)	3(1)	5(1)
P(8)	8(1)	16(1)	11(1)	2(1)	4(1)	6(1)
O(11)	16(2)	22(2)	12(2)	1(2)	1(1)	9(2)
O(12)	17(2)	21(2)	14(2)	-4(2)	3(1)	6(1)
O(13)	23(2)	17(2)	18(2)	-2(2)	3(2)	12(2)
O(14)	24(2)	23(2)	17(2)	4(2)	6(2)	17(2)
O(15)	23(2)	27(2)	15(2)	6(2)	3(1)	17(2)
O(16)	12(2)	26(2)	17(2)	4(2)	5(1)	7(2)
O(17)	14(2)	25(2)	14(2)	9(2)	7(1)	12(2)
O(18)	10(2)	27(2)	13(2)	0(2)	2(1)	11(1)
O(19)	16(2)	17(2)	12(2)	-2(2)	5(1)	-3(1)
O(20)	16(2)	16(2)	17(2)	-3(2)	7(1)	9(1)
N(1)	14(2)	17(2)	11(2)	1(2)	3(2)	8(2)
C(1)	19(2)	21(3)	4(3)	-1(2)	-2(2)	10(2)
C(2)	18(2)	22(3)	5(3)	1(2)	0(2)	7(2)
C(3)	15(2)	17(3)	13(3)	-1(2)	2(2)	2(2)
C(4)	18(2)	23(3)	17(3)	-3(2)	4(2)	9(2)
C(5)	15(2)	30(4)	17(3)	-3(2)	2(2)	7(2)
C(6)	21(2)	21(3)	23(3)	3(3)	6(2)	2(2)
C(7)	25(3)	16(3)	17(3)	0(2)	6(2)	9(2)
C(8)	14(2)	16(3)	16(3)	1(2)	-1(2)	6(2)
C(9)	27(3)	17(3)	12(3)	0(2)	3(2)	9(2)
C(10)	40(3)	15(3)	15(3)	0(2)	0(2)	4(2)
C(11)	25(3)	21(4)	40(4)	-8(3)	-7(2)	4(2)
C(12)	13(2)	28(3)	13(3)	5(2)	6(2)	11(2)
C(13)	17(2)	19(3)	14(3)	3(2)	5(2)	7(2)
C(14)	21(3)	29(4)	28(4)	12(3)	12(2)	15(2)
C(15)	23(3)	26(4)	28(4)	0(3)	12(2)	6(2)
C(16)	18(2)	19(3)	15(3)	3(2)	3(2)	7(2)
C(17)	23(3)	25(3)	21(3)	-2(3)	7(2)	6(2)
C(18)	28(3)	35(4)	30(4)	5(3)	6(2)	2(3)
C(19)	32(3)	28(4)	28(4)	7(3)	-2(2)	-1(3)
N(2)	13(2)	17(3)	14(2)	-2(2)	2(2)	6(2)
C(20)	13(2)	15(3)	23(3)	-4(2)	1(2)	2(2)
C(21)	17(2)	13(3)	15(3)	-2(2)	-1(2)	2(2)
C(22)	15(2)	18(3)	21(3)	-2(2)	4(2)	-1(2)
C(23)	18(2)	20(3)	24(3)	5(2)	1(2)	5(2)
C(24)	29(3)	22(4)	22(4)	8(3)	-6(2)	2(2)
C(25)	31(3)	30(4)	20(4)	2(3)	3(2)	7(3)
C(26)	22(2)	32(4)	17(3)	-3(3)	5(2)	12(2)
C(27)	13(2)	20(3)	13(3)	2(2)	5(2)	7(2)
C(28)	15(2)	21(3)	13(3)	0(2)	0(2)	1(2)
C(29)	17(2)	29(4)	26(4)	2(3)	8(2)	2(2)
C(30)	22(3)	26(4)	40(4)	9(3)	7(2)	2(2)
C(31)	17(2)	19(3)	10(3)	3(2)	1(2)	7(2)
C(32)	19(2)	19(3)	22(3)	4(2)	6(2)	7(2)
C(33)	20(2)	25(3)	20(3)	2(2)	0(2)	11(2)
C(34)	27(3)	35(4)	53(5)	15(3)	4(3)	10(3)
C(35)	13(2)	13(3)	17(3)	-1(2)	4(2)	5(2)
C(36)	14(2)	19(3)	15(3)	0(2)	2(2)	4(2)
C(37)	21(2)	20(3)	40(4)	2(3)	12(2)	7(2)
C(38)	22(3)	35(4)	36(4)	-5(3)	12(2)	13(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bztbu-on.

	x	y	z	U(eq)
H(1)	3070(80)	1570(50)	5820(30)	30
H(2)	6810(70)	2730(50)	5160(30)	23
H(4)	6730(80)	1080(50)	3490(30)	30
H(6)	1884	-41	3550	25
H(7)	-220(70)	-260(50)	4400(30)	23
H(11)	1822	4584	-1259	24
H(13)	4760(80)	2650(50)	-960(30)	28
H(15)	5580(70)	2880(50)	900(30)	30
H(16)	2130(80)	3920(50)	1240(30)	26
H(17)	160(60)	4820(40)	570(30)	23
H(1A)	6180	4539	4410	17
H(1B)	5583	3385	4259	17
H(3)	4188	5494	4237	19
H(4)	1780	5444	4402	22
H(5)	77	3956	4586	25
H(6)	778	2514	4598	27
H(7)	3167	2565	4391	22
H(8A)	3521	3701	3042	18
H(8B)	4603	3727	2513	18
H(9A)	4100	2259	3448	22
H(9B)	4981	2260	2842	22
H(10A)	2663	2218	2148	29
H(10B)	2674	1223	2490	29
H(11A)	433	1570	2570	45
H(11B)	1319	2594	2944	45
H(11C)	1317	1590	3279	45
H(12A)	6983	3208	3514	20
H(12B)	7951	4320	3678	20
H(13A)	6761	3545	2381	19
H(13B)	7823	4635	2562	19
H(14A)	8716	2906	2839	28
H(14B)	9776	4001	2998	28
H(15A)	10265	3379	2016	38
H(15B)	9630	4289	1870	38
H(15C)	8572	3195	1710	38
H(16A)	4968	5369	3291	20
H(16B)	6050	5271	2787	20
H(17A)	6825	6593	3714	27
H(17B)	7402	5768	4074	27
H(18A)	8415	6586	2915	39
H(18B)	9055	5826	3329	39
H(19A)	10653	7446	3563	48
H(19B)	9987	7015	4203	48
H(19C)	9323	7773	3799	48
H(20A)	10141	2801	8794	21
H(20B)	8738	2775	9147	21
H(22)	11818	1821	9219	23
H(23)	12923	1251	10135	25
H(24)	11876	1150	11099	32
H(25)	9632	1518	11113	33
H(26)	8521	2075	10199	28
H(27A)	7483	629	9194	18
H(27B)	6571	1392	9018	18
H(28A)	6372	-311	8236	21
H(28B)	5557	488	8000	21
H(29A)	4986	-600	9144	29
H(29B)	4129	158	8873	29
H(30A)	2673	-1459	8586	45
H(30B)	3944	-1631	8207	45
H(30C)	3067	-878	7949	45

H(31A)	7377	1590	7569	18
H(31B)	8692	2563	7786	18
H(32A)	7047	3066	8424	23
H(32B)	5736	2148	8096	23
H(33A)	6287	2815	7046	25
H(33B)	5521	3417	7466	25
H(34A)	7480	4489	7024	57
H(34B)	8612	3960	7381	57
H(34C)	7838	4565	7796	57
H(35A)	9652	648	8651	17
H(35B)	8502	370	8003	17
H(36A)	11053	2046	8100	19
H(36B)	10001	1565	7446	19
H(37A)	11959	699	8223	31
H(37B)	10745	84	7655	31
H(38A)	13059	646	7282	44
H(38B)	13139	1753	7459	44
H(38C)	11924	1140	6890	44

Table 6. Hydrogen bonds for bztbu-on [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.88(7)	1.71(7)	2.558(5)	160(6)
O(2)-H(2)...O(3)	1.05(7)	1.40(7)	2.443(5)	173(6)
O(4)-H(4)...O(5)	0.75(7)	1.78(7)	2.467(5)	152(8)
O(6)-H(6)...O(7)	0.84	1.88	2.659(5)	153.7
O(7)-H(7)...O(8)#3	1.12(6)	1.40(6)	2.521(5)	175(6)
O(11)-H(11)...O(18)	0.84	1.77	2.576(5)	160.8
O(13)-H(13)...O(12)	0.77(7)	1.71(7)	2.476(5)	173(8)
O(14)-H(15)...O(15)	1.09(7)	1.36(7)	2.436(5)	167(6)
O(16)-H(16)...O(17)	0.78(7)	1.89(7)	2.640(5)	159(7)
O(17)-H(17)...O(18)#4	1.14(6)	1.35(6)	2.489(4)	171(6)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1 #2 -x+1,-y+1,-z #3 -x,-y,-z+1

#4 -x,-y+1,-z

Crystallographic data of Bzdmp crystal light-off stage measured at laboratory system

Table 1. Crystal data and structure refinement for bzdmp-off.

Identification code	off3173k	
Empirical formula	C31 H44 N2 O11 P4 Pt	
Formula weight	939.65	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 13.74370(10) Å	α= 90°.
	b = 12.9901(2) Å	β= 105.9300(10)°.
	c = 21.04720(10) Å	γ = 90°.
Volume	3613.30(6) Å^3	
Z	4	
Density (calculated)	1.727 Mg/m^3	
Absorption coefficient	4.120 mm^{-1}	
F(000)	1880	
Crystal size	0.20 x 0.17 x 0.10 mm^3	
Theta range for data collection	2.01 to 27.48°.	
Index ranges	-17<=h<=17, -16<=k<=16, -24<=l<=27	
Reflections collected	25314	
Independent reflections	8275 [Rint = 0.0340]	
Completeness to θ = 27.48°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.798	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8275 / 0 / 436	
Goodness-of-fit on F^2	1.065	
Final R indices [I>2σ(I)]	R1 = 0.0262, wR2 = 0.0633	
R indices (all data)	R1 = 0.0299, wR2 = 0.0648	
Largest diff. peak and hole	1.155 and -1.524 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bzdmp-off. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	451(1)	1025(1)	56(1)	12(1)
P(1)	-201(1)	1460(1)	932(1)	22(1)
P(2)	1901(1)	434(1)	841(1)	20(1)
P(3)	1130(1)	630(1)	-817(1)	22(1)
P(4)	-973(1)	1671(1)	-723(1)	23(1)
O(1)	-1058(2)	2237(2)	812(1)	36(1)
O(2)	616(2)	1838(2)	1576(1)	31(1)
O(3)	2240(2)	1017(2)	1492(1)	32(1)
O(4)	2857(2)	309(2)	572(2)	41(1)
O(5)	2276(2)	477(2)	-645(1)	38(1)
O(6)	855(2)	1443(2)	-1392(1)	40(1)
O(7)	-781(2)	2263(2)	-1298(1)	40(1)
O(8)	-1699(2)	2359(2)	-431(2)	41(1)
O(9)	-611(2)	411(2)	1207(1)	31(1)
O(10)	1712(2)	-728(2)	1079(2)	41(1)
N(1)	5310(2)	-1275(2)	1137(1)	19(1)
C(1)	5381(2)	-116(2)	982(2)	18(1)
C(2)	5764(2)	565(2)	1584(2)	20(1)
C(3)	5086(3)	1034(2)	1882(2)	25(1)
C(4)	5430(3)	1743(3)	2394(2)	27(1)
C(5)	6457(3)	1986(3)	2605(2)	29(1)
C(6)	7137(3)	1525(3)	2306(2)	27(1)
C(7)	6795(2)	811(3)	1800(2)	22(1)
C(8)	4560(3)	-1444(3)	1542(2)	26(1)
C(9)	6325(2)	-1668(3)	1541(2)	25(1)
C(10)	4970(2)	-1807(2)	474(2)	20(1)
C(11)	5697(2)	-2162(3)	171(2)	26(1)
C(12)	5370(3)	-2641(3)	-443(2)	29(1)
C(13)	4351(3)	-2748(3)	-756(2)	28(1)
C(14)	3636(3)	-2366(3)	-464(2)	27(1)
C(15)	3946(2)	-1889(3)	157(2)	24(1)
N(2)	2099(2)	4771(2)	1722(2)	28(1)
C(16)	2827(3)	5702(3)	1857(2)	30(1)
C(17)	3798(3)	5520(3)	1666(2)	26(1)
C(18)	3857(3)	5752(3)	1031(2)	28(1)
C(19)	4768(3)	5621(3)	862(2)	37(1)
C(20)	5622(3)	5264(3)	1335(3)	46(1)
C(21)	5565(3)	5035(4)	1968(2)	47(1)
C(22)	4664(3)	5159(3)	2140(2)	38(1)
C(23)	1149(3)	5117(4)	1905(2)	45(1)
C(24)	2564(4)	3901(3)	2184(2)	43(1)
C(25)	1842(2)	4471(3)	1005(2)	25(1)
C(26)	2088(3)	3512(3)	808(2)	31(1)
C(27)	1868(3)	3294(3)	135(2)	38(1)
C(28)	1418(3)	4016(3)	-332(2)	43(1)
C(29)	1174(3)	4981(3)	-131(2)	38(1)
C(30)	1377(2)	5230(2)	537(1)	31(1)
O(50)	-894(2)	3641(2)	1854(1)	49(1)
C(50)	-1857(2)	4126(2)	1661(1)	37(1)

Table 3. Bond lengths [Å] and angles [°] for bzdmp-off.

Pt(1)-P(1)	2.3323(8)	C(11)-C(12)	1.393(5)	O(1)-P(1)-O(2)	105.88(15)
Pt(1)-P(3)	2.3336(8)	C(12)-C(13)	1.382(5)	O(1)-P(1)-O(9)	106.63(15)
Pt(1)-P(4)	2.3367(8)	C(13)-C(14)	1.388(5)	O(2)-P(1)-O(9)	100.83(14)
Pt(1)-P(2)	2.3415(8)	C(14)-C(15)	1.402(5)	O(1)-P(1)-Pt(1)	118.53(12)
Pt(1)-Pt(1)#1	2.9203(2)	N(2)-C(25)	1.505(4)	O(2)-P(1)-Pt(1)	114.54(10)
P(1)-O(1)	1.518(3)	N(2)-C(24)	1.513(5)	O(9)-P(1)-Pt(1)	108.75(9)
P(1)-O(2)	1.582(3)	N(2)-C(23)	1.527(5)	O(3)-P(2)-O(4)	107.18(16)
P(1)-O(9)	1.640(3)	N(2)-C(16)	1.545(5)	O(3)-P(2)-O(10)	102.65(15)
P(2)-O(3)	1.522(3)	C(16)-C(17)	1.514(5)	O(4)-P(2)-O(10)	103.45(17)
P(2)-O(4)	1.575(3)	C(17)-C(18)	1.393(5)	O(3)-P(2)-Pt(1)	117.62(11)
P(2)-O(10)	1.634(3)	C(17)-C(22)	1.408(5)	O(4)-P(2)-Pt(1)	114.32(11)
P(3)-O(5)	1.530(3)	C(18)-C(19)	1.403(5)	O(10)-P(2)-Pt(1)	110.09(10)
P(3)-O(6)	1.572(3)	C(19)-C(20)	1.394(6)	O(5)-P(3)-O(6)	106.48(16)
P(3)-O(9)#1	1.640(2)	C(20)-C(21)	1.387(7)	O(5)-P(3)-O(9)#1	106.81(15)
P(4)-O(7)	1.517(3)	C(21)-C(22)	1.392(6)	O(6)-P(3)-O(9)#1	100.88(15)
P(4)-O(8)	1.584(3)	C(25)-C(26)	1.385(5)	O(5)-P(3)-Pt(1)	116.75(11)
P(4)-O(10)#1	1.636(3)	C(25)-C(30)	1.416(4)	O(6)-P(3)-Pt(1)	113.26(11)
O(9)-P(3)#1	1.640(2)	C(26)-C(27)	1.394(6)	O(9)#1-P(3)-Pt(1)	111.27(9)
O(10)-P(4)#1	1.636(3)	C(27)-C(28)	1.375(6)	O(7)-P(4)-O(8)	106.82(16)
N(1)-C(9)	1.510(4)	C(28)-C(29)	1.393(6)	O(7)-P(4)-O(10)#1	103.72(16)
N(1)-C(10)	1.512(4)	C(29)-C(30)	1.393(4)	O(8)-P(4)-O(10)#1	102.82(16)
N(1)-C(8)	1.523(4)			O(7)-P(4)-Pt(1)	116.49(11)
N(1)-C(1)	1.549(4)	P(1)-Pt(1)-P(3)	178.47(3)	O(8)-P(4)-Pt(1)	115.19(11)
C(1)-C(2)	1.516(4)	P(1)-Pt(1)-P(4)	92.19(3)	O(10)#1-P(4)-Pt(1)	110.35(10)
C(2)-C(3)	1.399(4)	P(3)-Pt(1)-P(4)	88.02(3)	P(3)#1-O(9)-P(1)	130.76(16)
C(2)-C(7)	1.400(4)	P(1)-Pt(1)-P(2)	87.59(3)	P(2)-O(10)-P(4)#1	133.04(17)
C(3)-C(4)	1.397(5)	P(3)-Pt(1)-P(2)	92.15(3)	C(9)-N(1)-C(10)	111.7(2)
C(4)-C(5)	1.395(5)	P(4)-Pt(1)-P(2)	178.07(3)	C(9)-N(1)-C(8)	107.3(3)
C(5)-C(6)	1.396(5)	P(1)-Pt(1)-Pt(1)#1	92.13(2)	C(10)-N(1)-C(8)	111.4(2)
C(6)-C(7)	1.392(5)	P(3)-Pt(1)-Pt(1)#1	89.38(2)	C(9)-N(1)-C(1)	110.2(2)
C(10)-C(15)	1.386(4)	P(4)-Pt(1)-Pt(1)#1	90.89(2)	C(10)-N(1)-C(1)	105.8(2)
C(10)-C(11)	1.403(4)	P(2)-Pt(1)-Pt(1)#1	91.03(2)	C(8)-N(1)-C(1)	110.5(2)

C(2)-C(1)-N(1)	114.8(2)	C(13)-C(14)-C(15)	120.0(3)	C(20)-C(21)-C(22)	120.9(4)
C(3)-C(2)-C(7)	119.6(3)	C(10)-C(15)-C(14)	119.4(3)	C(21)-C(22)-C(17)	119.6(4)
C(3)-C(2)-C(1)	120.5(3)	C(25)-N(2)-C(24)	113.1(3)	C(26)-C(25)-C(30)	121.2(3)
C(7)-C(2)-C(1)	119.5(3)	C(25)-N(2)-C(23)	110.3(3)	C(26)-C(25)-N(2)	121.7(3)
C(4)-C(3)-C(2)	120.4(3)	C(24)-N(2)-C(23)	107.4(3)	C(30)-C(25)-N(2)	117.0(3)
C(5)-C(4)-C(3)	119.7(3)	C(25)-N(2)-C(16)	110.4(3)	C(25)-C(26)-C(27)	119.0(4)
C(4)-C(5)-C(6)	120.1(3)	C(24)-N(2)-C(16)	109.2(3)	C(28)-C(27)-C(26)	121.1(4)
C(7)-C(6)-C(5)	120.2(3)	C(23)-N(2)-C(16)	106.2(3)	C(27)-C(28)-C(29)	119.7(4)
C(6)-C(7)-C(2)	120.0(3)	C(17)-C(16)-N(2)	113.7(3)	C(30)-C(29)-C(28)	121.1(4)
C(15)-C(10)-C(11)	120.9(3)	C(18)-C(17)-C(22)	119.4(3)	C(29)-C(30)-C(25)	117.9(3)
C(15)-C(10)-N(1)	119.7(3)	C(18)-C(17)-C(16)	120.6(3)		
C(11)-C(10)-N(1)	119.4(3)	C(22)-C(17)-C(16)	119.9(3)		
C(12)-C(11)-C(10)	118.6(3)	C(17)-C(18)-C(19)	120.6(4)		
C(13)-C(12)-C(11)	121.0(3)	C(20)-C(19)-C(18)	119.6(4)		
C(12)-C(13)-C(14)	120.1(3)	C(21)-C(20)-C(19)	119.9(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for bzdmp-off. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	10(1)	12(1)	14(1)	1(1)	3(1)	0(1)
P(1)	22(1)	21(1)	25(1)	-7(1)	12(1)	-3(1)
P(2)	14(1)	19(1)	22(1)	2(1)	-2(1)	-1(1)
P(3)	25(1)	24(1)	22(1)	-4(1)	14(1)	-8(1)
P(4)	19(1)	18(1)	27(1)	7(1)	-3(1)	0(1)
O(1)	31(1)	34(1)	46(2)	-10(1)	16(1)	10(1)
O(2)	37(1)	32(1)	26(1)	-12(1)	11(1)	-9(1)
O(3)	29(1)	35(1)	26(1)	-4(1)	-4(1)	-5(1)
O(4)	15(1)	58(2)	46(2)	-1(1)	3(1)	8(1)
O(5)	25(1)	50(2)	47(2)	-11(1)	24(1)	-8(1)
O(6)	52(2)	42(2)	30(2)	7(1)	21(1)	-13(1)
O(7)	42(2)	39(2)	32(2)	19(1)	-3(1)	-3(1)
O(8)	32(1)	34(2)	52(2)	10(1)	4(1)	16(1)
O(9)	41(1)	31(1)	28(1)	-10(1)	21(1)	-16(1)
O(10)	36(2)	23(1)	46(2)	10(1)	-20(1)	-6(1)
N(1)	18(1)	19(1)	19(1)	0(1)	4(1)	-1(1)
C(1)	18(1)	18(1)	19(2)	0(1)	3(1)	0(1)
C(2)	21(2)	19(2)	20(2)	-1(1)	5(1)	0(1)
C(3)	19(2)	26(2)	31(2)	-6(1)	9(1)	-3(1)
C(4)	28(2)	29(2)	30(2)	-9(1)	14(1)	0(1)
C(5)	31(2)	28(2)	27(2)	-12(1)	5(1)	-5(1)
C(6)	22(2)	29(2)	30(2)	-7(1)	4(1)	-5(1)
C(7)	19(2)	24(2)	26(2)	-3(1)	8(1)	0(1)
C(8)	25(2)	31(2)	25(2)	-1(1)	13(1)	-5(1)
C(9)	22(2)	24(2)	24(2)	2(1)	1(1)	6(1)

C(10)	21(2)	17(1)	21(2)	-2(1)	4(1)	-2(1)
C(11)	18(2)	32(2)	27(2)	-5(1)	6(1)	-1(1)
C(12)	28(2)	34(2)	27(2)	-7(1)	12(1)	1(2)
C(13)	35(2)	28(2)	21(2)	-6(1)	5(1)	-3(2)
C(14)	23(2)	29(2)	26(2)	-3(1)	2(1)	-3(1)
C(15)	18(2)	24(2)	29(2)	-6(1)	3(1)	1(1)
N(2)	29(2)	32(2)	25(2)	1(1)	9(1)	-2(1)
C(16)	35(2)	28(2)	28(2)	-9(1)	8(2)	-4(2)
C(17)	26(2)	22(2)	27(2)	-7(1)	1(1)	-4(1)
C(18)	26(2)	21(2)	36(2)	4(1)	5(2)	-2(1)
C(19)	38(2)	27(2)	50(2)	-1(2)	19(2)	-6(2)
C(20)	28(2)	33(2)	78(3)	-4(2)	16(2)	0(2)
C(21)	28(2)	46(3)	57(3)	0(2)	-6(2)	0(2)
C(22)	37(2)	40(2)	29(2)	-2(2)	-3(2)	-3(2)
C(23)	40(2)	66(3)	38(2)	-3(2)	25(2)	1(2)
C(24)	53(3)	43(2)	31(2)	10(2)	7(2)	-5(2)
C(25)	19(2)	29(2)	27(2)	-5(1)	8(1)	-7(1)
C(26)	32(2)	24(2)	40(2)	-1(2)	17(2)	-8(2)
C(27)	38(2)	34(2)	49(2)	-18(2)	24(2)	-18(2)
C(28)	40(2)	55(3)	35(2)	-14(2)	12(2)	-21(2)
C(29)	30(2)	49(2)	33(2)	4(2)	4(2)	-4(2)
C(30)	26(2)	32(2)	33(2)	2(2)	5(1)	1(2)
O(50)	40(2)	54(2)	49(2)	-30(2)	4(1)	9(1)
C(50)	41(2)	39(2)	32(2)	-6(2)	11(2)	3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bzdmp-off.

	x	y	z	U(eq)
H(2)	1109	1429	1664	47
H(4)	2693	-12	212	61
H(6)	228	1549	-1502	59
H(8)	-1822	2053	-110	61
H(1A)	5837	-36	693	22
H(1B)	4702	128	731	22
H(3)	4386	869	1736	30
H(4)	4968	2058	2596	33
H(5)	6695	2466	2954	35
H(6)	7834	1698	2448	33
H(7)	7260	492	1602	27
H(8A)	4800	-1089	1967	39
H(8B)	4500	-2183	1618	39
H(8C)	3898	-1169	1301	39
H(9A)	6520	-1309	1967	37
H(9B)	6834	-1540	1303	37
H(9C)	6280	-2409	1616	37
H(11)	6399	-2077	381	31
H(12)	5855	-2898	-649	34
H(13)	4140	-3083	-1173	34
H(14)	2935	-2427	-684	32
H(15)	3459	-1626	359	29
H(16A)	2475	6304	1609	36
H(16B)	2998	5872	2333	36
H(18)	3276	6001	710	34
H(19)	4803	5775	427	44
H(20)	6243	5178	1225	55
H(21)	6149	4789	2288	57
H(22)	4635	5003	2575	45
H(23A)	1326	5311	2373	68
H(23B)	658	4552	1825	68
H(23C)	852	5711	1633	68
H(24A)	2717	4141	2643	65
H(24B)	3190	3674	2089	65
H(24C)	2087	3325	2120	65
H(26)	2401	3009	1126	37
H(27)	2032	2637	-5	46
H(28)	1273	3857	-789	51
H(29)	864	5478	-454	46
H(30)	1209	5888	674	37
H(50)	-960	3182	1554	73
H(50A)	-2359	3709	1842	56
H(50B)	-1827	4774	1838	56
H(50C)	-2021	4248	1216	56

Table 6. Hydrogen bonds for bzdmp-off [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(3)	0.84	1.77	2.522(4)	147.5
O(4)-H(4)...O(5)	0.84	1.85	2.474(4)	130.2
O(6)-H(6)...O(7)	0.84	1.82	2.545(4)	144.2
O(8)-H(8)...O(1)	0.84	1.95	2.526(4)	124.7
O(50)-H(50)...O(1)	0.85	1.96	2.813(3)	173.9

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Crystallographic data of Bzdmp crystal light-on stage measured at laboratory system

Table 1. Crystal data and structure refinement for bzdmp-on.

Identification code	on1173k	
Empirical formula	C31 H44 N2 O11 P4 Pt	
Formula weight	939.65	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/n$	
Unit cell dimensions	a = 13.73350(10) Å	α= 90°.
	b = 12.9877(2) Å	β= 105.9380(10)°.
	c = 21.03340(10) Å	γ = 90°.
Volume	3607.44(6) Å^3	
Z	4	
Density (calculated)	1.730 Mg/m^3	
Absorption coefficient	4.127 mm^{-1}	
F(000)	1880	
Crystal size	0.20 x 0.17 x 0.10 mm^3	
Theta range for data collection	1.86 to 27.48°.	
Index ranges	-17<=h<=17, -16<=k<=16, -24<=l<=27	
Reflections collected	25234	
Independent reflections	8264 [Rint = 0.0347]	
Completeness to θ = 27.48°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.808	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8264 / 0 / 436	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2σ(I)]	R1 = 0.0274, wR2 = 0.0658	
R indices (all data)	R1 = 0.0313, wR2 = 0.0676	
Largest diff. peak and hole	1.417 and -1.482 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bzdmp-on. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	452(1)	1024(1)	54(1)	13(1)
P(1)	-204(1)	1462(1)	929(1)	24(1)
P(2)	1897(1)	436(1)	841(1)	22(1)
P(3)	1134(1)	627(1)	-815(1)	24(1)
P(4)	-970(1)	1668(1)	-726(1)	26(1)
O(1)	-1059(2)	2239(2)	808(2)	40(1)
O(2)	610(2)	1841(2)	1572(1)	34(1)
O(3)	2238(2)	1019(2)	1493(1)	35(1)
O(4)	2855(2)	312(3)	576(2)	44(1)
O(5)	2281(2)	475(2)	-640(2)	41(1)
O(6)	860(3)	1436(2)	-1391(1)	44(1)
O(7)	-776(2)	2258(2)	-1300(2)	46(1)
O(8)	-1695(2)	2355(2)	-434(2)	44(1)
O(9)	-615(2)	413(2)	1204(1)	35(1)
O(10)	1708(2)	-726(2)	1080(2)	46(1)
N(1)	5307(2)	-1273(2)	1135(1)	21(1)
C(1)	5384(2)	-116(2)	985(2)	20(1)
C(2)	5763(2)	564(3)	1585(2)	21(1)
C(3)	5082(3)	1033(3)	1880(2)	26(1)
C(4)	5429(3)	1738(3)	2393(2)	29(1)
C(5)	6456(3)	1985(3)	2604(2)	32(1)
C(6)	7134(3)	1527(3)	2307(2)	28(1)
C(7)	6791(3)	813(3)	1801(2)	24(1)
C(8)	4558(3)	-1444(3)	1543(2)	27(1)
C(9)	6323(3)	-1668(3)	1542(2)	25(1)
C(10)	4969(2)	-1806(2)	472(2)	21(1)
C(11)	5697(3)	-2164(3)	174(2)	27(1)
C(12)	5369(3)	-2642(3)	-441(2)	31(1)
C(13)	4349(3)	-2743(3)	-757(2)	30(1)
C(14)	3638(3)	-2365(3)	-461(2)	29(1)
C(15)	3947(3)	-1886(3)	158(2)	25(1)
N(2)	2099(2)	4776(3)	1724(2)	31(1)
C(16)	2828(3)	5705(3)	1857(2)	32(1)
C(17)	3797(3)	5520(3)	1666(2)	28(1)
C(18)	3860(3)	5747(3)	1033(2)	31(1)
C(19)	4773(3)	5616(3)	863(2)	39(1)
C(20)	5622(3)	5260(3)	1337(3)	49(1)
C(21)	5569(3)	5037(4)	1968(3)	51(1)
C(22)	4663(3)	5163(3)	2143(2)	41(1)
C(23)	1149(3)	5122(4)	1905(2)	49(1)
C(24)	2562(4)	3907(4)	2183(2)	47(1)
C(25)	1844(3)	4478(3)	1004(2)	26(1)
C(26)	2089(3)	3511(3)	808(2)	33(1)
C(27)	1867(3)	3297(3)	133(2)	41(1)
C(28)	1414(4)	4019(4)	-334(2)	46(1)
C(29)	1174(3)	4983(4)	-129(2)	39(1)
C(30)	1382(2)	5230(2)	537(1)	32(1)
O(50)	-890(2)	3640(2)	1854(1)	52(1)
C(50)	-1853(2)	4126(2)	1661(1)	41(1)

Table 3. Bond lengths [Å] and angles [°] for bzdmp-on.

Pt(1)-P(1)	2.3297(9)	C(11)-C(12)	1.392(5)	O(1)-P(1)-O(2)	105.66(16)
Pt(1)-P(3)	2.3309(8)	C(12)-C(13)	1.382(5)	O(1)-P(1)-O(9)	106.69(16)
Pt(1)-P(4)	2.3338(9)	C(13)-C(14)	1.384(5)	O(2)-P(1)-O(9)	100.89(15)
Pt(1)-P(2)	2.3365(8)	C(14)-C(15)	1.399(5)	O(1)-P(1)-Pt(1)	118.68(13)
Pt(1)-Pt(1)#1	2.9184(2)	N(2)-C(24)	1.507(5)	O(2)-P(1)-Pt(1)	114.54(11)
P(1)-O(1)	1.516(3)	N(2)-C(25)	1.508(5)	O(9)-P(1)-Pt(1)	108.69(10)
P(1)-O(2)	1.579(3)	N(2)-C(23)	1.525(5)	O(3)-P(2)-O(4)	106.83(17)
P(1)-O(9)	1.639(3)	N(2)-C(16)	1.545(5)	O(3)-P(2)-O(10)	102.61(16)
P(2)-O(3)	1.523(3)	C(16)-C(17)	1.511(5)	O(4)-P(2)-O(10)	103.51(18)
P(2)-O(4)	1.571(3)	C(17)-C(18)	1.388(5)	O(3)-P(2)-Pt(1)	117.77(12)
P(2)-O(10)	1.634(3)	C(17)-C(22)	1.407(5)	O(4)-P(2)-Pt(1)	114.43(12)
P(3)-O(5)	1.529(3)	C(18)-C(19)	1.405(6)	O(10)-P(2)-Pt(1)	110.14(10)
P(3)-O(6)	1.570(3)	C(19)-C(20)	1.389(7)	O(5)-P(3)-O(6)	106.53(17)
P(3)-O(9)#1	1.638(3)	C(20)-C(21)	1.380(7)	O(5)-P(3)-O(9)#1	107.02(16)
P(4)-O(7)	1.514(3)	C(21)-C(22)	1.400(7)	O(6)-P(3)-O(9)#1	100.84(16)
P(4)-O(8)	1.581(3)	C(25)-C(26)	1.393(5)	O(5)-P(3)-Pt(1)	116.74(12)
P(4)-O(10)#1	1.632(3)	C(25)-C(30)	1.406(4)	O(6)-P(3)-Pt(1)	113.25(13)
O(9)-P(3)#1	1.637(3)	C(26)-C(27)	1.394(6)	O(9)#1-P(3)-Pt(1)	111.10(10)
O(10)-P(4)#1	1.632(3)	C(27)-C(28)	1.378(7)	O(7)-P(4)-O(8)	106.97(18)
N(1)-C(10)	1.510(4)	C(28)-C(29)	1.394(7)	O(7)-P(4)-O(10)#1	103.81(18)
N(1)-C(9)	1.512(4)	C(29)-C(30)	1.388(5)	O(8)-P(4)-O(10)#1	102.84(18)
N(1)-C(8)	1.527(4)			O(7)-P(4)-Pt(1)	116.45(13)
N(1)-C(1)	1.545(4)	P(1)-Pt(1)-P(3)	178.46(3)	O(8)-P(4)-Pt(1)	115.04(13)
C(1)-C(2)	1.511(4)	P(1)-Pt(1)-P(4)	92.15(4)	O(10)#1-P(4)-Pt(1)	110.32(10)
C(2)-C(3)	1.396(5)	P(3)-Pt(1)-P(4)	88.09(4)	P(3)#1-O(9)-P(1)	130.91(17)
C(2)-C(7)	1.398(5)	P(1)-Pt(1)-P(2)	87.62(3)	P(4)#1-O(10)-P(2)	133.09(19)
C(3)-C(4)	1.395(5)	P(3)-Pt(1)-P(2)	92.09(3)	C(10)-N(1)-C(9)	111.7(3)
C(4)-C(5)	1.394(5)	P(4)-Pt(1)-P(2)	178.09(3)	C(10)-N(1)-C(8)	111.5(3)
C(5)-C(6)	1.390(5)	P(1)-Pt(1)-Pt(1)#1	92.07(2)	C(9)-N(1)-C(8)	106.9(3)
C(6)-C(7)	1.393(5)	P(3)-Pt(1)-Pt(1)#1	89.45(2)	C(10)-N(1)-C(1)	106.2(2)
C(10)-C(15)	1.382(5)	P(4)-Pt(1)-Pt(1)#1	90.90(2)	C(9)-N(1)-C(1)	110.0(2)
C(10)-C(11)	1.398(5)	P(2)-Pt(1)-Pt(1)#1	91.00(2)	C(8)-N(1)-C(1)	110.5(3)

C(2)-C(1)-N(1)	115.1(3)	C(13)-C(14)-C(15)	120.3(3)	C(20)-C(21)-C(22)	120.9(4)
C(3)-C(2)-C(7)	119.7(3)	C(10)-C(15)-C(14)	119.2(3)	C(21)-C(22)-C(17)	119.3(4)
C(3)-C(2)-C(1)	120.5(3)	C(24)-N(2)-C(25)	113.1(3)	C(26)-C(25)-C(30)	121.3(3)
C(7)-C(2)-C(1)	119.5(3)	C(24)-N(2)-C(23)	107.4(3)	C(26)-C(25)-N(2)	121.3(3)
C(4)-C(3)-C(2)	120.1(3)	C(25)-N(2)-C(23)	110.4(3)	C(30)-C(25)-N(2)	117.3(3)
C(5)-C(4)-C(3)	119.9(3)	C(24)-N(2)-C(16)	109.3(3)	C(25)-C(26)-C(27)	118.5(4)
C(6)-C(5)-C(4)	120.1(3)	C(25)-N(2)-C(16)	110.1(3)	C(28)-C(27)-C(26)	121.4(4)
C(5)-C(6)-C(7)	120.1(3)	C(23)-N(2)-C(16)	106.3(3)	C(27)-C(28)-C(29)	119.3(4)
C(6)-C(7)-C(2)	120.1(3)	C(17)-C(16)-N(2)	113.7(3)	C(30)-C(29)-C(28)	121.3(4)
C(15)-C(10)-C(11)	121.1(3)	C(18)-C(17)-C(22)	119.4(4)	C(29)-C(30)-C(25)	118.2(3)
C(15)-C(10)-N(1)	119.5(3)	C(18)-C(17)-C(16)	120.8(3)		
C(11)-C(10)-N(1)	119.3(3)	C(22)-C(17)-C(16)	119.7(4)	Symmetry transformations used to	
C(12)-C(11)-C(10)	118.5(3)	C(17)-C(18)-C(19)	120.9(4)	generate equivalent atoms:	
C(13)-C(12)-C(11)	121.0(3)	C(20)-C(19)-C(18)	119.3(4)	#1 -x,-y,-z	
C(12)-C(13)-C(14)	119.8(3)	C(21)-C(20)-C(19)	120.3(4)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for bzdmp-on. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	11(1)	13(1)	14(1)	1(1)	3(1)	0(1)
P(1)	25(1)	23(1)	29(1)	-9(1)	14(1)	-4(1)
P(2)	15(1)	21(1)	24(1)	2(1)	-3(1)	-2(1)
P(3)	28(1)	26(1)	23(1)	-5(1)	16(1)	-10(1)
P(4)	21(1)	20(1)	30(1)	9(1)	-4(1)	-1(1)
O(1)	35(2)	36(2)	51(2)	-12(1)	18(1)	11(1)
O(2)	41(2)	34(1)	29(1)	-13(1)	14(1)	-11(1)
O(3)	32(2)	39(2)	26(1)	-2(1)	-6(1)	-7(1)
O(4)	17(1)	59(2)	52(2)	-1(2)	1(1)	7(1)
O(5)	28(1)	51(2)	54(2)	-13(2)	28(1)	-8(1)
O(6)	59(2)	50(2)	29(2)	7(1)	21(1)	-17(2)
O(7)	47(2)	42(2)	38(2)	22(1)	-4(1)	-4(1)
O(8)	34(2)	36(2)	58(2)	9(1)	3(1)	16(1)
O(9)	46(2)	37(2)	30(1)	-13(1)	23(1)	-20(1)
O(10)	38(2)	26(1)	51(2)	12(1)	-24(1)	-8(1)
N(1)	20(1)	21(1)	20(1)	0(1)	4(1)	-1(1)
C(1)	21(2)	19(2)	19(2)	1(1)	5(1)	0(1)
C(2)	21(2)	21(2)	21(2)	-2(1)	4(1)	-1(1)
C(3)	21(2)	27(2)	31(2)	-6(1)	9(1)	-4(1)
C(4)	30(2)	30(2)	30(2)	-8(2)	15(2)	1(2)
C(5)	33(2)	32(2)	29(2)	-14(2)	6(2)	-7(2)
C(6)	22(2)	30(2)	32(2)	-7(2)	4(1)	-6(1)
C(7)	21(2)	25(2)	26(2)	-5(1)	7(1)	0(1)
C(8)	26(2)	32(2)	27(2)	0(2)	13(1)	-6(2)
C(9)	22(2)	25(2)	25(2)	2(1)	0(1)	7(1)

C(10)	22(2)	17(2)	22(2)	-3(1)	5(1)	-1(1)
C(11)	18(2)	35(2)	29(2)	-2(2)	7(1)	0(1)
C(12)	29(2)	38(2)	27(2)	-7(2)	12(2)	3(2)
C(13)	37(2)	28(2)	24(2)	-6(1)	6(2)	-2(2)
C(14)	24(2)	29(2)	30(2)	-4(2)	1(1)	-4(1)
C(15)	20(2)	26(2)	27(2)	-4(1)	3(1)	2(1)
N(2)	32(2)	36(2)	25(2)	-1(1)	10(1)	-2(1)
C(16)	36(2)	31(2)	27(2)	-8(2)	7(2)	-4(2)
C(17)	30(2)	21(2)	28(2)	-5(1)	2(1)	-4(1)
C(18)	31(2)	22(2)	38(2)	3(2)	6(2)	-4(2)
C(19)	42(2)	29(2)	51(3)	1(2)	19(2)	-7(2)
C(20)	34(2)	33(2)	82(4)	-6(2)	20(2)	-2(2)
C(21)	32(2)	47(3)	64(3)	0(2)	-6(2)	0(2)
C(22)	39(2)	42(2)	33(2)	-3(2)	-4(2)	-5(2)
C(23)	43(2)	72(3)	40(3)	-4(2)	25(2)	1(2)
C(24)	59(3)	48(3)	33(2)	13(2)	9(2)	-7(2)
C(25)	20(2)	30(2)	30(2)	-3(2)	9(1)	-5(1)
C(26)	36(2)	25(2)	42(2)	-1(2)	17(2)	-9(2)
C(27)	41(2)	34(2)	55(3)	-18(2)	26(2)	-19(2)
C(28)	45(3)	60(3)	34(2)	-12(2)	13(2)	-23(2)
C(29)	30(2)	51(3)	34(2)	3(2)	4(2)	-6(2)
C(30)	28(2)	35(2)	33(2)	1(2)	7(2)	0(2)
O(50)	44(2)	57(2)	51(2)	-31(2)	6(2)	10(2)
C(50)	46(3)	42(2)	34(2)	-8(2)	11(2)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bzdmp-on.

	x	y	z	U(eq)
H(2)	1104	1433	1661	51
H(4)	2694	-9	215	66
H(6)	233	1542	-1502	66
H(8)	-1819	2050	-113	67
H(1A)	5842	-35	697	24
H(1B)	4705	130	732	24
H(3)	4381	872	1731	32
H(4)	4967	2049	2598	34
H(5)	6692	2467	2952	38
H(6)	7832	1701	2450	34
H(7)	7258	495	1602	29
H(8A)	4799	-1088	1968	41
H(8B)	4499	-2183	1620	41
H(8C)	3893	-1170	1303	41
H(9A)	6517	-1309	1968	38
H(9B)	6834	-1543	1305	38
H(9C)	6275	-2409	1618	38
H(11)	6398	-2082	385	33
H(12)	5855	-2903	-646	37
H(13)	4137	-3070	-1176	36
H(14)	2937	-2432	-679	35
H(15)	3460	-1619	359	30
H(16A)	2476	6307	1608	38
H(16B)	3000	5877	2334	38
H(18)	3279	5994	712	37
H(19)	4808	5769	428	47
H(20)	6243	5170	1227	59
H(21)	6155	4795	2288	62
H(22)	4633	5009	2579	49
H(23A)	1327	5316	2373	73
H(23B)	657	4558	1826	73
H(23C)	853	5717	1633	73
H(24A)	2715	4146	2642	71
H(24B)	3187	3680	2087	71
H(24C)	2083	3331	2118	71
H(26)	2400	3007	1126	39
H(27)	2031	2640	-6	49
H(28)	1267	3861	-792	55
H(29)	862	5482	-451	47
H(30)	1216	5889	674	39
H(50)	-956	3181	1554	78
H(50A)	-2355	3708	1842	61
H(50B)	-1823	4774	1838	61
H(50C)	-2017	4248	1216	61

Table 6. Hydrogen bonds for bzdmp-on [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(3)	0.84	1.77	2.524(4)	147.7
O(4)-H(4)...O(5)	0.84	1.84	2.471(5)	130.3
O(6)-H(6)...O(7)	0.84	1.81	2.543(5)	144.1
O(8)-H(8)...O(1)	0.84	1.95	2.521(5)	124.7
O(50)-H(50)...O(1)	0.85	1.96	2.815(4)	173.9

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Crystallographic data of Bzte1 crystal light-off stage measured at SPring-8 BL02B1 beam line

Table 1. Crystal data and structure refinement for bzte50k-off.

Identification code	bteaoff	
Empirical formula	C26 H54 N2 O20 P8 Pt2	
Formula weight	1352.65	
Temperature	50(2) K	
Wavelength	0.5379 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 11.8110(13) Å	α= 89.315(6)°.
	b = 12.5010(16) Å	β= 88.134(9)°.
	c = 14.6910(18) Å	γ = 73.426(8)°.
Volume	2077.9(4) Å^3	
Z	2	
Density (calculated)	2.162 Mg/m^3	
Absorption coefficient	3.856 mm^{-1}	
F(000)	1320	
Crystal size	0.15 x 0.09 x 0.03 mm^3	
Theta range for data collection	1.66 to 20.44°.	
Index ranges	-14<=h<=14, -16<=k<=16, -19<=l<=19	
Reflections collected	11855	
Independent reflections	7356 [Rint = 0.0561]	
Completeness to θ = 20.44°	77.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.86040 and 0.82724	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7356 / 0 / 523	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2σ(I)]	R1 = 0.0536, wR2 = 0.1171	
R indices (all data)	R1 = 0.0712, wR2 = 0.1242	
Largest diff. peak and hole	2.842 and -2.201 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for bzte50k-off. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4256(1)	4236(1)	109(1)	11(1)
P(1)	2781(3)	5607(2)	-586(2)	12(1)
P(2)	4930(3)	3514(2)	-1322(2)	13(1)
P(3)	5748(3)	2881(2)	800(2)	14(1)
P(4)	3641(3)	4929(2)	1560(2)	14(1)
O(1)	1830(8)	6367(6)	65(5)	19(2)
O(2)	2164(8)	5140(6)	-1311(5)	20(2)
O(3)	4029(7)	3279(6)	-1992(4)	14(2)
O(4)	5920(8)	2422(6)	-1345(5)	16(2)
O(5)	6458(8)	1885(6)	226(5)	18(2)
O(6)	5391(8)	2383(6)	1708(5)	20(2)
O(7)	3746(8)	4036(7)	2302(5)	19(2)
O(8)	2419(8)	5796(7)	1641(5)	18(2)
O(9)	3312(7)	6491(6)	-1156(5)	14(2)
O(10)	5427(7)	4413(6)	-1892(4)	16(2)
Pt(2)	778(1)	5718(1)	5161(1)	12(1)
P(5)	2310(3)	4274(2)	4551(2)	14(1)
P(6)	353(3)	6435(2)	3699(2)	14(1)
P(7)	-775(3)	7126(2)	5786(2)	12(1)
P(8)	1141(3)	5013(2)	6624(2)	14(1)
O(11)	3072(8)	3495(6)	5246(5)	20(2)
O(12)	3154(8)	4646(7)	3881(5)	24(2)
O(13)	1413(8)	6615(7)	3122(5)	21(2)
O(14)	-624(9)	7556(6)	3654(5)	26(2)
O(15)	-1339(8)	8131(6)	5197(5)	17(2)
O(16)	-542(8)	7609(6)	6727(5)	18(2)
O(17)	983(8)	5910(6)	7370(5)	18(2)
O(18)	2292(8)	4110(7)	6772(5)	24(2)
O(19)	1808(7)	3456(6)	3913(4)	14(2)
O(20)	-89(8)	5569(6)	3086(4)	18(2)
N(1)	1722(9)	1962(8)	335(6)	17(2)
C(1)	1236(11)	988(9)	129(6)	15(2)
C(2)	613(12)	567(9)	926(7)	22(3)
C(3)	1242(13)	-350(10)	1445(8)	26(3)
C(4)	625(13)	-800(10)	2117(8)	28(3)
C(5)	-564(13)	-358(11)	2268(8)	28(3)
C(6)	-1174(14)	559(11)	1742(8)	28(3)
C(7)	-609(11)	997(9)	1075(7)	20(2)
C(8)	2745(11)	1593(9)	977(7)	20(3)
C(9)	3819(11)	762(9)	595(7)	19(2)
C(10)	2154(11)	2331(9)	-571(7)	20(2)
C(11)	1156(13)	2905(10)	-1209(8)	27(3)
C(12)	756(11)	2883(9)	796(7)	17(2)
C(13)	1064(12)	3953(9)	948(7)	20(2)
N(2)	6695(10)	2045(8)	4596(6)	22(2)
C(14)	6113(11)	1120(9)	4859(7)	17(2)
C(15)	5681(12)	566(9)	4099(7)	21(3)
C(16)	4498(12)	950(9)	3832(7)	22(3)
C(17)	4078(14)	395(10)	3192(8)	28(3)
C(18)	4820(13)	-574(11)	2783(7)	26(3)
C(19)	6000(14)	-961(10)	3048(8)	29(3)
C(20)	6408(13)	-420(10)	3718(8)	26(3)
C(21)	5802(12)	2890(9)	4025(7)	20(2)
C(22)	6215(13)	3922(9)	3762(9)	26(3)
C(23)	6959(12)	2543(10)	5458(7)	21(3)
C(24)	5883(13)	3193(11)	6027(8)	28(3)
C(25)	7802(11)	1572(9)	4029(7)	19(2)
C(26)	8824(12)	786(10)	4506(7)	24(3)

Table 3. Bond lengths [Å] and angles [°] for bzte50k-off.

Pt(1)-P(3)	2.319(3)	P(7)-O(19)#2	1.635(8)	C(23)-C(24)	1.528(17)
Pt(1)-P(1)	2.321(3)	P(8)-O(18)	1.519(9)	C(25)-C(26)	1.508(17)
Pt(1)-P(2)	2.322(3)	P(8)-O(17)	1.547(8)		
Pt(1)-P(4)	2.325(3)	P(8)-O(20)#2	1.652(8)	P(3)-Pt(1)-P(1)	179.20(10)
Pt(1)-Pt(1)#1	2.9495(8)	O(19)-P(7)#2	1.635(8)	P(3)-Pt(1)-P(2)	91.09(10)
P(1)-O(2)	1.523(7)	O(20)-P(8)#2	1.652(8)	P(1)-Pt(1)-P(2)	88.82(10)
P(1)-O(1)	1.556(8)	N(1)-C(12)	1.518(14)	P(3)-Pt(1)-P(4)	87.18(10)
P(1)-O(9)	1.629(7)	N(1)-C(8)	1.520(14)	P(1)-Pt(1)-P(4)	92.91(10)
P(2)-O(4)	1.523(8)	N(1)-C(10)	1.523(13)	P(2)-Pt(1)-P(4)	178.17(11)
P(2)-O(3)	1.562(7)	N(1)-C(1)	1.524(14)	P(3)-Pt(1)-Pt(1)#1	92.38(7)
P(2)-O(10)	1.623(7)	C(1)-C(2)	1.529(15)	P(1)-Pt(1)-Pt(1)#1	86.82(7)
P(3)-O(5)	1.532(8)	C(2)-C(7)	1.401(19)	P(2)-Pt(1)-Pt(1)#1	88.70(7)
P(3)-O(6)	1.562(7)	C(2)-C(3)	1.406(16)	P(4)-Pt(1)-Pt(1)#1	90.78(7)
P(3)-O(9)#1	1.633(8)	C(3)-C(4)	1.413(16)	O(2)-P(1)-O(1)	108.9(5)
P(4)-O(7)	1.533(7)	C(4)-C(5)	1.37(2)	O(2)-P(1)-O(9)	102.9(4)
P(4)-O(8)	1.539(9)	C(5)-C(6)	1.405(18)	O(1)-P(1)-O(9)	103.3(4)
P(4)-O(10)#1	1.640(8)	C(6)-C(7)	1.363(17)	O(2)-P(1)-Pt(1)	112.7(3)
O(9)-P(3)#1	1.633(8)	C(8)-C(9)	1.490(17)	O(1)-P(1)-Pt(1)	115.9(3)
O(10)-P(4)#1	1.640(8)	C(10)-C(11)	1.535(17)	O(9)-P(1)-Pt(1)	111.9(3)
Pt(2)-P(8)	2.319(2)	C(12)-C(13)	1.503(15)	O(4)-P(2)-O(3)	102.4(4)
Pt(2)-P(7)	2.322(3)	N(2)-C(23)	1.498(13)	O(4)-P(2)-O(10)	106.2(4)
Pt(2)-P(5)	2.325(3)	N(2)-C(25)	1.500(16)	O(3)-P(2)-O(10)	101.8(4)
Pt(2)-P(6)	2.331(2)	N(2)-C(21)	1.528(14)	O(4)-P(2)-Pt(1)	116.5(3)
Pt(2)-Pt(2)#2	2.9637(8)	N(2)-C(14)	1.544(14)	O(3)-P(2)-Pt(1)	119.1(3)
P(5)-O(11)	1.528(8)	C(14)-C(15)	1.499(15)	O(10)-P(2)-Pt(1)	109.2(3)
P(5)-O(12)	1.539(8)	C(15)-C(20)	1.396(17)	O(5)-P(3)-O(6)	106.2(4)
P(5)-O(19)	1.638(8)	C(15)-C(16)	1.409(18)	O(5)-P(3)-O(9)#1	106.9(5)
P(6)-O(14)	1.543(9)	C(16)-C(17)	1.361(16)	O(6)-P(3)-O(9)#1	101.3(4)
P(6)-O(13)	1.556(8)	C(17)-C(18)	1.405(19)	O(5)-P(3)-Pt(1)	118.3(3)
P(6)-O(20)	1.623(8)	C(18)-C(19)	1.41(2)	O(6)-P(3)-Pt(1)	115.9(4)
P(7)-O(15)	1.518(7)	C(19)-C(20)	1.376(17)	O(9)#1-P(3)-Pt(1)	106.6(3)
P(7)-O(16)	1.579(7)	C(21)-C(22)	1.545(15)	O(7)-P(4)-O(8)	109.9(4)

O(7)-P(4)-O(10)#1	102.1(4)	O(20)-P(6)-Pt(2)	110.3(3)	C(7)-C(6)-C(5)	121.4(14)
O(8)-P(4)-O(10)#1	104.9(4)	O(15)-P(7)-O(16)	106.0(4)	C(6)-C(7)-C(2)	120.3(11)
O(7)-P(4)-Pt(1)	114.7(3)	O(15)-P(7)-O(19)#2	107.5(4)	C(9)-C(8)-N(1)	115.2(9)
O(8)-P(4)-Pt(1)	116.3(3)	O(16)-P(7)-O(19)#2	100.9(4)	N(1)-C(10)-C(11)	113.8(10)
O(10)#1-P(4)-Pt(1)	107.5(3)	O(15)-P(7)-Pt(2)	118.3(3)	C(13)-C(12)-N(1)	115.3(10)
P(1)-O(9)-P(3)#1	126.8(4)	O(16)-P(7)-Pt(2)	116.1(3)	C(23)-N(2)-C(25)	111.0(10)
P(2)-O(10)-P(4)#1	127.8(4)	O(19)#2-P(7)-Pt(2)	106.4(3)	C(23)-N(2)-C(21)	112.3(9)
P(8)-Pt(2)-P(7)	87.53(10)	O(18)-P(8)-O(17)	108.6(4)	C(25)-N(2)-C(21)	109.0(8)
P(8)-Pt(2)-P(5)	91.65(10)	O(18)-P(8)-O(20)#2	105.1(5)	C(23)-N(2)-C(14)	107.8(8)
P(7)-Pt(2)-P(5)	178.48(9)	O(17)-P(8)-O(20)#2	101.9(4)	C(25)-N(2)-C(14)	110.5(9)
P(8)-Pt(2)-P(6)	178.31(11)	O(18)-P(8)-Pt(2)	117.6(3)	C(21)-N(2)-C(14)	106.2(10)
P(7)-Pt(2)-P(6)	91.25(10)	O(17)-P(8)-Pt(2)	114.5(3)	C(15)-C(14)-N(2)	117.1(8)
P(5)-Pt(2)-P(6)	89.54(10)	O(20)#2-P(8)-Pt(2)	107.4(3)	C(20)-C(15)-C(16)	118.7(11)
P(8)-Pt(2)-Pt(2)#2	91.28(7)	P(7)#2-O(19)-P(5)	125.7(4)	C(20)-C(15)-C(14)	120.1(12)
P(7)-Pt(2)-Pt(2)#2	92.19(7)	P(6)-O(20)-P(8)#2	126.0(5)	C(16)-C(15)-C(14)	120.7(10)
P(5)-Pt(2)-Pt(2)#2	86.55(7)	C(12)-N(1)-C(8)	108.2(8)	C(17)-C(16)-C(15)	120.9(12)
P(6)-Pt(2)-Pt(2)#2	87.60(7)	C(12)-N(1)-C(10)	112.6(8)	C(16)-C(17)-C(18)	120.5(13)
O(11)-P(5)-O(12)	107.3(5)	C(8)-N(1)-C(10)	109.8(10)	C(17)-C(18)-C(19)	118.9(11)
O(11)-P(5)-O(19)	104.9(4)	C(12)-N(1)-C(1)	109.2(9)	C(20)-C(19)-C(18)	120.3(12)
O(12)-P(5)-O(19)	101.8(4)	C(8)-N(1)-C(1)	110.3(8)	C(19)-C(20)-C(15)	120.5(13)
O(11)-P(5)-Pt(2)	115.5(3)	C(10)-N(1)-C(1)	106.7(8)	N(2)-C(21)-C(22)	112.8(10)
O(12)-P(5)-Pt(2)	114.8(3)	N(1)-C(1)-C(2)	115.9(8)	N(2)-C(23)-C(24)	115.6(10)
O(19)-P(5)-Pt(2)	111.3(3)	C(7)-C(2)-C(3)	119.3(10)	N(2)-C(25)-C(26)	116.5(9)
O(14)-P(6)-O(13)	105.3(5)	C(7)-C(2)-C(1)	120.5(10)		
O(14)-P(6)-O(20)	105.9(5)	C(3)-C(2)-C(1)	119.8(12)		
O(13)-P(6)-O(20)	103.0(4)	C(2)-C(3)-C(4)	119.0(13)		
O(14)-P(6)-Pt(2)	115.1(3)	C(5)-C(4)-C(3)	121.1(11)		
O(13)-P(6)-Pt(2)	116.1(3)	C(4)-C(5)-C(6)	118.9(11)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z

#2 -x,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for bzte50k-off. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	16(1)	10(1)	7(1)	-1(1)	0(1)	-6(1)
P(1)	12(2)	13(1)	14(1)	0(1)	-2(1)	-6(1)
P(2)	18(2)	12(1)	9(1)	-3(1)	1(1)	-6(1)
P(3)	21(2)	12(1)	10(1)	1(1)	0(1)	-8(1)
P(4)	16(2)	17(1)	10(1)	-3(1)	3(1)	-8(1)
O(1)	18(5)	19(4)	17(4)	4(3)	3(3)	-2(3)
O(2)	25(6)	15(4)	22(4)	3(3)	-12(3)	-10(3)
O(3)	17(5)	11(3)	17(3)	-5(3)	-3(3)	-8(3)
O(4)	20(5)	13(4)	15(3)	-2(3)	-2(3)	-3(3)
O(5)	29(6)	11(3)	12(3)	3(3)	-3(3)	-3(3)
O(6)	30(6)	20(4)	14(3)	5(3)	-1(3)	-14(4)
O(7)	22(6)	25(4)	13(3)	-2(3)	3(3)	-11(4)
O(8)	16(6)	25(4)	14(3)	-7(3)	5(3)	-7(3)
O(9)	13(5)	16(4)	15(3)	2(3)	-5(3)	-6(3)
O(10)	18(5)	20(4)	12(3)	-2(3)	0(3)	-8(3)
Pt(2)	19(1)	9(1)	8(1)	-1(1)	2(1)	-4(1)
P(5)	16(2)	13(1)	14(1)	-3(1)	4(1)	-6(1)
P(6)	24(2)	11(1)	11(1)	1(1)	2(1)	-8(1)
P(7)	15(2)	9(1)	12(1)	-1(1)	2(1)	-3(1)
P(8)	15(2)	15(1)	12(1)	1(1)	1(1)	-4(1)
O(11)	14(6)	18(4)	25(4)	-6(3)	7(3)	-1(3)
O(12)	26(6)	24(4)	23(4)	-13(3)	12(3)	-11(4)
O(13)	34(6)	23(4)	11(3)	-1(3)	7(3)	-17(4)
O(14)	48(7)	17(4)	11(4)	5(3)	2(3)	-2(4)
O(15)	23(6)	11(3)	16(3)	-1(3)	2(3)	-4(3)
O(16)	26(6)	14(4)	14(3)	-2(3)	-4(3)	-5(3)
O(17)	24(6)	15(4)	12(3)	2(3)	-4(3)	-1(3)
O(18)	30(6)	25(4)	14(4)	0(3)	3(3)	-5(4)
O(19)	11(5)	14(3)	14(3)	-3(3)	3(3)	1(3)
O(20)	26(6)	16(4)	11(3)	0(3)	4(3)	-5(3)
N(1)	21(7)	15(4)	15(4)	-3(3)	3(3)	-5(4)
C(1)	17(7)	14(5)	11(5)	-4(4)	-1(4)	5(4)
C(2)	41(9)	10(5)	17(5)	4(4)	1(5)	-10(5)
C(3)	33(9)	19(6)	23(6)	0(4)	4(5)	-5(5)
C(4)	43(10)	20(6)	22(6)	10(4)	2(5)	-9(6)
C(5)	38(10)	29(7)	22(6)	2(5)	10(5)	-20(6)
C(6)	39(10)	26(6)	21(6)	-4(5)	0(5)	-12(6)
C(7)	17(8)	18(5)	25(6)	4(4)	-4(4)	-4(5)
C(8)	19(8)	16(5)	24(5)	7(4)	-6(5)	-1(5)
C(9)	14(7)	18(5)	22(5)	-1(4)	0(4)	0(4)
C(10)	25(8)	19(5)	16(5)	0(4)	5(4)	-9(5)
C(11)	39(10)	22(6)	25(6)	14(5)	-11(5)	-17(6)
C(12)	12(7)	17(5)	20(5)	2(4)	4(4)	-1(4)
C(13)	21(8)	20(6)	21(5)	-4(4)	7(4)	-8(5)
N(2)	36(8)	20(5)	8(4)	-1(3)	-2(4)	-5(5)
C(14)	18(8)	23(6)	16(5)	0(4)	2(4)	-16(5)
C(15)	26(8)	16(5)	19(5)	0(4)	2(4)	-6(5)
C(16)	25(8)	16(5)	23(6)	-1(4)	-3(5)	-5(5)
C(17)	37(10)	21(6)	32(6)	6(5)	-9(5)	-16(6)
C(18)	40(10)	30(7)	18(5)	-8(4)	4(5)	-25(6)
C(19)	45(11)	21(6)	22(6)	-5(4)	10(5)	-13(6)
C(20)	30(9)	15(5)	32(6)	-4(4)	-3(5)	-5(5)
C(21)	19(8)	20(5)	19(5)	-1(4)	-1(4)	0(5)
C(22)	29(9)	8(5)	42(7)	3(5)	-7(5)	-6(5)
C(23)	28(9)	28(6)	11(5)	-8(4)	-1(4)	-13(6)
C(24)	31(9)	34(7)	20(6)	-19(5)	8(5)	-13(6)
C(25)	23(8)	11(5)	21(5)	-1(4)	4(4)	-3(5)
C(26)	27(9)	23(6)	21(5)	2(4)	1(5)	-5(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bzte50k-off.

	x	y	z	U(eq)
H(1)	2005	6197	608	28
H(3)	3370	3754	-1913	21
H(5)	6313	2017	-327	27
H(6)	4839	2865	1974	30
H(11)	2811	3696	5775	30
H(12)	3194	4307	3385	36
H(13)	1535	6202	2661	32
H(14)	-878	7759	4184	40
H(16)	-41	7116	7010	27
H(17)	1392	5633	7818	27
H(1A)	1898	358	-99	19
H(1B)	671	1215	-370	19
H(3)	2069	-662	1345	31
H(4)	1044	-1420	2470	34
H(5)	-972	-666	2722	33
H(6)	-1997	880	1854	34
H(7)	-1047	1595	711	24
H(8A)	2968	2261	1166	25
H(8B)	2469	1270	1531	25
H(9A)	3605	107	382	28
H(9B)	4406	534	1069	28
H(9C)	4150	1097	84	28
H(10A)	2683	1670	-883	24
H(10B)	2625	2852	-450	24
H(11A)	666	2407	-1314	41
H(11B)	1496	3076	-1790	41
H(11C)	668	3598	-928	41
H(12A)	45	3049	421	20
H(12B)	548	2603	1393	20
H(13A)	1754	3807	1334	31
H(13B)	393	4494	1249	31
H(13C)	1247	4255	361	31
H(14A)	6691	536	5201	20
H(14B)	5434	1447	5281	20
H(16)	3986	1604	4103	26
H(17)	3278	666	3020	34
H(18)	4528	-961	2336	32
H(19)	6520	-1600	2762	34
H(20)	7190	-719	3924	31
H(21A)	5041	3138	4374	24
H(21B)	5664	2522	3464	24
H(22A)	6368	4283	4315	39
H(22B)	5597	4451	3420	39
H(22C)	6941	3688	3383	39
H(23A)	7446	3049	5301	26
H(23B)	7441	1934	5839	26
H(24A)	5383	3787	5655	41
H(24B)	6145	3523	6554	41
H(24C)	5430	2687	6238	41
H(25A)	8068	2202	3778	23
H(25B)	7603	1173	3508	23
H(26A)	9111	1195	4968	36
H(26B)	9463	466	4060	36
H(26C)	8563	185	4798	36

Table 6. Hydrogen bonds for bzte50k-off [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.84	1.64	2.477(10)	176.2
O(3)-H(3)...O(2)	0.84	2.09	2.873(12)	155.6
O(3)-H(3)...O(18)#3	0.84	2.32	2.751(11)	112.6
O(5)-H(5)...O(4)	0.84	1.61	2.449(9)	172.6
O(6)-H(6)...O(7)	0.84	1.71	2.539(12)	166.6
O(11)-H(11)...O(18)	0.84	1.60	2.443(11)	178.4
O(12)-H(12)...O(7)	0.84	1.70	2.467(10)	150.6
O(13)-H(13)...O(8)	0.84	1.79	2.527(10)	145.2
O(14)-H(14)...O(15)	0.84	1.60	2.436(10)	178.9
O(16)-H(16)...O(17)	0.84	1.73	2.554(11)	166.4
O(17)-H(17)...O(2)#4	0.84	1.61	2.448(10)	178.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+1,-z+1 #3 x,y,z-1

#4 x,y,z+1

Crystallographic data of Bzte1 crystal light-on stage measured at SPring-8 BL02B1 beam line

Table 1. Crystal data and structure refinement for bzte50k-on.

Identification code	bteaon	
Empirical formula	C26 H54 N2 O20 P8 Pt2	
Formula weight	1352.65	
Temperature	50(2) K	
Wavelength	0.5379 Å	
Crystal system	Triclinic	
Space group	*P* 1	
Unit cell dimensions	a = 11.8120(12) Å	α= 89.319(6)°.
	b = 12.5010(16) Å	β= 88.143(8)°.
	c = 14.6890(17) Å	γ = 73.430(8)°.
Volume	2077.8(4) Å^3	
Z	2	
Density (calculated)	2.162 Mg/m^3	
Absorption coefficient	3.856 mm^{-1}	
F(000)	1320	
Crystal size	0.15 x 0.09 x 0.03 mm^3	
Theta range for data collection	1.66 to 20.44°.	
Index ranges	-14<=h<=14, -16<=k<=16, -19<=l<=19	
Reflections collected	11993	
Independent reflections	7412 [Rint = 0.0558]	
Completeness to θ = 20.44°	77.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.86025 and 0.83171	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7412 / 0 / 523	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2σ(I)]	R1 = 0.0525, wR2 = 0.1164	
R indices (all data)	R1 = 0.0701, wR2 = 0.1239	
Largest diff. peak and hole	3.015 and -2.181 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for bzte50k-on. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	4256(1)	4237(1)	109(1)	11(1)
P(1)	2779(3)	5607(2)	-586(2)	13(1)
P(2)	4930(3)	3517(2)	-1321(2)	14(1)
P(3)	5750(3)	2881(2)	797(2)	14(1)
P(4)	3639(3)	4935(2)	1562(2)	15(1)
O(1)	1825(8)	6377(6)	68(5)	21(2)
O(2)	2154(8)	5140(6)	-1312(5)	21(2)
O(3)	4036(7)	3278(6)	-1987(4)	16(2)
O(4)	5920(8)	2415(6)	-1339(4)	18(2)
O(5)	6448(7)	1894(6)	227(5)	18(2)
O(6)	5395(8)	2382(6)	1706(5)	22(2)
O(7)	3753(7)	4032(6)	2299(4)	19(2)
O(8)	2431(8)	5792(7)	1645(5)	21(2)
O(9)	3310(7)	6484(6)	-1154(4)	15(2)
O(10)	5423(7)	4412(6)	-1896(4)	16(2)
Pt(2)	778(1)	5718(1)	5161(1)	12(1)
P(5)	2304(3)	4274(2)	4549(2)	14(1)
P(6)	358(3)	6432(2)	3698(2)	15(1)
P(7)	-776(3)	7124(2)	5786(2)	13(1)
P(8)	1138(3)	5013(2)	6625(2)	15(1)
O(11)	3084(7)	3491(6)	5243(5)	19(2)
O(12)	3170(8)	4645(7)	3891(5)	26(2)
O(13)	1412(8)	6625(7)	3116(5)	23(2)
O(14)	-632(8)	7548(6)	3648(4)	24(2)
O(15)	-1337(8)	8130(6)	5197(5)	19(2)
O(16)	-556(7)	7614(6)	6719(4)	19(2)
O(17)	974(7)	5919(6)	7367(4)	19(2)
O(18)	2293(8)	4109(6)	6772(5)	24(2)
O(19)	1813(7)	3459(6)	3916(4)	14(2)
O(20)	-88(7)	5567(6)	3092(4)	16(2)
N(1)	1712(9)	1966(8)	333(6)	20(2)
C(1)	1241(11)	995(9)	127(7)	17(2)
C(2)	609(11)	558(9)	916(7)	19(2)
C(3)	1250(13)	-355(9)	1439(7)	24(3)
C(4)	629(14)	-794(10)	2115(7)	31(3)
C(5)	-580(13)	-342(10)	2263(7)	28(3)
C(6)	-1179(13)	553(10)	1747(7)	25(3)
C(7)	-594(12)	996(9)	1077(7)	23(3)
C(8)	2741(12)	1600(10)	981(7)	25(3)
C(9)	3828(11)	774(9)	583(8)	22(2)
C(10)	2138(11)	2346(9)	-573(7)	20(2)
C(11)	1174(12)	2915(10)	-1205(7)	24(3)
C(12)	740(10)	2885(8)	801(7)	16(2)
C(13)	1056(11)	3960(10)	948(7)	22(2)
N(2)	6684(9)	2028(8)	4602(5)	20(2)
C(14)	6116(10)	1107(9)	4856(7)	17(2)
C(15)	5678(12)	547(9)	4095(7)	22(3)
C(16)	4507(11)	963(9)	3833(8)	21(2)
C(17)	4070(13)	391(10)	3187(8)	29(3)
C(18)	4823(13)	-570(10)	2791(7)	28(3)
C(19)	5977(13)	-947(10)	3055(8)	28(3)
C(20)	6415(12)	-415(8)	3716(7)	22(3)
C(21)	5800(10)	2890(8)	4028(7)	17(2)
C(22)	6210(12)	3919(9)	3770(8)	25(3)
C(23)	6950(12)	2549(9)	5465(7)	25(3)
C(24)	5883(14)	3169(12)	6036(8)	36(4)
C(25)	7817(10)	1559(8)	4027(7)	16(2)
C(26)	8835(12)	784(10)	4510(8)	28(3)

Table 3. Bond lengths [Å] and angles [°] for bzte50k-on.

Pt(1)-P(3)	2.319(3)	P(7)-O(19)#2	1.640(8)	C(23)-C(24)	1.511(18)
Pt(1)-P(2)	2.320(3)	P(8)-O(18)	1.523(9)	C(25)-C(26)	1.505(16)
Pt(1)-P(1)	2.323(3)	P(8)-O(17)	1.549(7)		
Pt(1)-P(4)	2.329(2)	P(8)-O(20)#2	1.646(8)	P(3)-Pt(1)-P(2)	90.99(10)
Pt(1)-Pt(1)#1	2.9482(8)	O(19)-P(7)#2	1.640(8)	P(3)-Pt(1)-P(1)	179.21(9)
P(1)-O(2)	1.528(7)	O(20)-P(8)#2	1.646(8)	P(2)-Pt(1)-P(1)	88.81(10)
P(1)-O(1)	1.566(8)	N(1)-C(1)	1.510(14)	P(3)-Pt(1)-P(4)	87.37(10)
P(1)-O(9)	1.621(7)	N(1)-C(12)	1.525(14)	P(2)-Pt(1)-P(4)	178.21(11)
P(2)-O(4)	1.532(8)	N(1)-C(10)	1.526(13)	P(1)-Pt(1)-P(4)	92.82(10)
P(2)-O(3)	1.554(8)	N(1)-C(8)	1.530(15)	P(3)-Pt(1)-Pt(1)#1	92.32(7)
P(2)-O(10)	1.620(7)	C(1)-C(2)	1.536(13)	P(2)-Pt(1)-Pt(1)#1	88.62(7)
P(3)-O(5)	1.518(8)	C(2)-C(7)	1.383(18)	P(1)-Pt(1)-Pt(1)#1	86.91(7)
P(3)-O(6)	1.562(7)	C(2)-C(3)	1.411(15)	P(4)-Pt(1)-Pt(1)#1	90.72(7)
P(3)-O(9)#1	1.639(8)	C(3)-C(4)	1.412(16)	O(2)-P(1)-O(1)	108.9(5)
P(4)-O(8)	1.522(9)	C(4)-C(5)	1.39(2)	O(2)-P(1)-O(9)	103.1(4)
P(4)-O(7)	1.536(7)	C(5)-C(6)	1.375(17)	O(1)-P(1)-O(9)	103.2(4)
P(4)-O(10)#1	1.641(8)	C(6)-C(7)	1.383(16)	O(2)-P(1)-Pt(1)	112.8(3)
O(9)-P(3)#1	1.639(8)	C(8)-C(9)	1.505(17)	O(1)-P(1)-Pt(1)	116.0(3)
O(10)-P(4)#1	1.641(8)	C(10)-C(11)	1.503(16)	O(9)-P(1)-Pt(1)	111.7(3)
Pt(2)-P(8)	2.321(2)	C(12)-C(13)	1.514(14)	O(4)-P(2)-O(3)	102.2(4)
Pt(2)-P(7)	2.322(3)	N(2)-C(23)	1.514(13)	O(4)-P(2)-O(10)	106.7(4)
Pt(2)-P(5)	2.323(3)	N(2)-C(14)	1.527(14)	O(3)-P(2)-O(10)	101.7(4)
Pt(2)-P(6)	2.331(2)	N(2)-C(25)	1.529(15)	O(4)-P(2)-Pt(1)	116.2(3)
Pt(2)-Pt(2)#2	2.9633(8)	N(2)-C(21)	1.535(13)	O(3)-P(2)-Pt(1)	119.1(3)
P(5)-O(11)	1.539(8)	C(14)-C(15)	1.507(14)	O(10)-P(2)-Pt(1)	109.5(3)
P(5)-O(12)	1.547(8)	C(15)-C(20)	1.379(16)	O(5)-P(3)-O(6)	106.1(4)
P(5)-O(19)	1.623(8)	C(15)-C(16)	1.397(17)	O(5)-P(3)-O(9)#1	107.3(5)
P(6)-O(14)	1.547(9)	C(16)-C(17)	1.391(16)	O(6)-P(3)-O(9)#1	101.4(4)
P(6)-O(13)	1.560(8)	C(17)-C(18)	1.396(19)	O(5)-P(3)-Pt(1)	118.2(3)
P(6)-O(20)	1.618(7)	C(18)-C(19)	1.38(2)	O(6)-P(3)-Pt(1)	115.9(4)
P(7)-O(15)	1.519(7)	C(19)-C(20)	1.376(16)	O(9)#1-P(3)-Pt(1)	106.4(3)
P(7)-O(16)	1.567(7)	C(21)-C(22)	1.538(15)	O(8)-P(4)-O(7)	110.1(4)

O(8)-P(4)-O(10)#1	105.1(4)	O(20)-P(6)-Pt(2)	110.1(3)	C(5)-C(6)-C(7)	120.8(13)
O(7)-P(4)-O(10)#1	101.9(4)	O(15)-P(7)-O(16)	105.4(4)	C(2)-C(7)-C(6)	120.9(11)
O(8)-P(4)-Pt(1)	116.6(3)	O(15)-P(7)-O(19)#2	107.5(4)	C(9)-C(8)-N(1)	114.6(9)
O(7)-P(4)-Pt(1)	114.1(3)	O(16)-P(7)-O(19)#2	101.1(4)	C(11)-C(10)-N(1)	114.9(10)
O(10)#1-P(4)-Pt(1)	107.5(3)	O(15)-P(7)-Pt(2)	118.2(3)	C(13)-C(12)-N(1)	114.5(9)
P(1)-O(9)-P(3)#1	127.0(4)	O(16)-P(7)-Pt(2)	116.6(3)	C(23)-N(2)-C(14)	109.0(8)
P(2)-O(10)-P(4)#1	127.3(4)	O(19)#2-P(7)-Pt(2)	106.4(3)	C(23)-N(2)-C(25)	110.4(9)
P(8)-Pt(2)-P(7)	87.44(9)	O(18)-P(8)-O(17)	109.1(4)	C(14)-N(2)-C(25)	110.7(8)
P(8)-Pt(2)-P(5)	91.80(10)	O(18)-P(8)-O(20)#2	105.4(4)	C(23)-N(2)-C(21)	111.0(8)
P(7)-Pt(2)-P(5)	178.32(9)	O(17)-P(8)-O(20)#2	102.2(4)	C(14)-N(2)-C(21)	107.3(9)
P(8)-Pt(2)-P(6)	178.35(11)	O(18)-P(8)-Pt(2)	117.4(3)	C(25)-N(2)-C(21)	108.5(8)
P(7)-Pt(2)-P(6)	91.43(9)	O(17)-P(8)-Pt(2)	114.1(3)	C(15)-C(14)-N(2)	117.7(8)
P(5)-Pt(2)-P(6)	89.30(10)	O(20)#2-P(8)-Pt(2)	107.2(3)	C(20)-C(15)-C(16)	121.1(11)
P(8)-Pt(2)-Pt(2)#2	91.20(7)	P(5)-O(19)-P(7)#2	125.7(4)	C(20)-C(15)-C(14)	119.3(11)
P(7)-Pt(2)-Pt(2)#2	92.11(7)	P(6)-O(20)-P(8)#2	126.7(4)	C(16)-C(15)-C(14)	119.4(10)
P(5)-Pt(2)-Pt(2)#2	86.40(7)	C(1)-N(1)-C(12)	109.3(9)	C(17)-C(16)-C(15)	119.6(11)
P(6)-Pt(2)-Pt(2)#2	87.63(7)	C(1)-N(1)-C(10)	106.8(8)	C(16)-C(17)-C(18)	119.2(13)
O(11)-P(5)-O(12)	105.6(5)	C(12)-N(1)-C(10)	112.5(8)	C(19)-C(18)-C(17)	119.6(11)
O(11)-P(5)-O(19)	104.8(4)	C(1)-N(1)-C(8)	110.3(8)	C(18)-C(19)-C(20)	122.1(12)
O(12)-P(5)-O(19)	102.6(4)	C(12)-N(1)-C(8)	107.9(8)	C(19)-C(20)-C(15)	118.4(12)
O(11)-P(5)-Pt(2)	115.8(3)	C(10)-N(1)-C(8)	110.0(9)	N(2)-C(21)-C(22)	113.7(9)
O(12)-P(5)-Pt(2)	115.0(3)	N(1)-C(1)-C(2)	116.7(8)	C(24)-C(23)-N(2)	115.5(10)
O(19)-P(5)-Pt(2)	111.8(3)	C(7)-C(2)-C(3)	119.7(10)	C(26)-C(25)-N(2)	116.0(9)
O(14)-P(6)-O(13)	105.1(5)	C(7)-C(2)-C(1)	120.8(10)		
O(14)-P(6)-O(20)	105.2(4)	C(3)-C(2)-C(1)	119.4(11)	Symmetry transformations used to	
O(13)-P(6)-O(20)	103.5(4)	C(2)-C(3)-C(4)	118.2(13)	generate equivalent atoms:	
O(14)-P(6)-Pt(2)	115.2(3)	C(5)-C(4)-C(3)	121.1(11)	#1 -x+1,-y+1,-z	
O(13)-P(6)-Pt(2)	116.6(3)	C(6)-C(5)-C(4)	119.3(11)	#2 -x,-y+1,-z+1	

Table 4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for bzte50k-on. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	16(1)	11(1)	7(1)	-1(1)	1(1)	-6(1)
P(1)	13(2)	13(1)	15(1)	0(1)	-3(1)	-7(1)
P(2)	20(2)	13(1)	10(1)	-2(1)	1(1)	-7(1)
P(3)	20(2)	13(1)	11(1)	2(1)	-1(1)	-9(1)
P(4)	18(2)	18(1)	10(1)	-3(1)	3(1)	-10(1)
O(1)	13(5)	23(4)	22(4)	5(3)	3(3)	2(3)
O(2)	27(6)	14(4)	26(4)	7(3)	-18(3)	-10(3)
O(3)	21(5)	12(3)	16(3)	-2(3)	0(3)	-6(3)
O(4)	28(5)	16(4)	12(3)	-1(3)	-1(3)	-7(3)
O(5)	25(5)	7(3)	20(4)	-1(3)	-3(3)	0(3)
O(6)	30(6)	20(4)	17(4)	4(3)	0(3)	-11(4)
O(7)	22(5)	27(4)	11(3)	2(3)	1(3)	-10(4)
O(8)	25(6)	26(4)	14(3)	-2(3)	8(3)	-9(4)
O(9)	13(5)	18(4)	14(3)	3(3)	-2(3)	-4(3)
O(10)	16(5)	18(4)	13(3)	0(3)	-1(3)	-3(3)
Pt(2)	19(1)	10(1)	8(1)	-1(1)	2(1)	-4(1)
P(5)	15(2)	15(1)	14(1)	-3(1)	5(1)	-6(1)
P(6)	26(2)	11(1)	12(1)	0(1)	2(1)	-9(1)
P(7)	16(2)	10(1)	12(1)	-1(1)	1(1)	-3(1)
P(8)	19(2)	16(1)	10(1)	-1(1)	1(1)	-5(1)
O(11)	14(5)	24(4)	18(4)	-5(3)	2(3)	-4(3)
O(12)	27(6)	26(4)	28(4)	-13(3)	12(3)	-15(4)
O(13)	39(6)	22(4)	14(4)	0(3)	8(3)	-18(4)
O(14)	46(6)	17(4)	7(3)	5(3)	-3(3)	-7(4)
O(15)	26(5)	12(4)	19(4)	2(3)	0(3)	-5(3)
O(16)	23(5)	20(4)	14(3)	-3(3)	2(3)	-5(3)
O(17)	23(5)	20(4)	11(3)	-2(3)	-1(3)	-2(3)
O(18)	36(6)	22(4)	12(3)	0(3)	-2(3)	-5(4)
O(19)	8(5)	18(4)	13(3)	-5(3)	6(3)	-1(3)
O(20)	25(5)	14(3)	10(3)	1(2)	3(3)	-8(3)
N(1)	29(7)	19(5)	12(4)	2(3)	-2(4)	-6(4)
C(1)	22(7)	17(5)	15(5)	0(4)	5(4)	-9(5)
C(2)	33(8)	14(5)	15(5)	4(4)	1(4)	-12(5)
C(3)	33(9)	17(5)	21(5)	-2(4)	6(5)	-8(5)
C(4)	56(11)	22(6)	14(5)	1(4)	-1(5)	-7(6)
C(5)	41(10)	27(6)	18(5)	-2(4)	10(5)	-14(6)
C(6)	39(9)	24(6)	18(5)	-4(4)	0(5)	-16(6)
C(7)	31(9)	14(5)	17(5)	1(4)	1(4)	3(5)
C(8)	26(9)	24(6)	21(5)	1(4)	6(4)	0(5)
C(9)	23(8)	10(5)	33(6)	5(4)	-6(5)	-4(5)
C(10)	21(8)	22(6)	18(5)	-2(4)	3(4)	-9(5)
C(11)	35(9)	23(6)	18(5)	10(4)	-6(5)	-16(5)
C(12)	11(7)	15(5)	22(5)	-2(4)	3(4)	-3(4)
C(13)	20(8)	29(6)	18(5)	-6(4)	11(4)	-12(5)
N(2)	30(7)	21(5)	9(4)	-3(3)	-2(3)	-5(4)
C(14)	14(7)	18(5)	16(5)	-2(4)	0(4)	-3(4)
C(15)	35(9)	15(5)	15(5)	-1(4)	2(4)	-7(5)
C(16)	20(8)	9(5)	35(6)	-3(4)	1(5)	-7(4)
C(17)	37(9)	27(6)	28(6)	4(5)	-8(5)	-18(6)
C(18)	55(10)	27(6)	12(5)	-3(4)	-5(5)	-24(6)
C(19)	31(9)	22(6)	34(6)	-10(5)	7(5)	-16(6)
C(20)	27(8)	8(5)	32(6)	-2(4)	-4(5)	-5(5)
C(21)	10(7)	11(5)	29(5)	-3(4)	-5(4)	-1(4)
C(22)	23(8)	9(5)	41(7)	1(4)	-7(5)	0(5)
C(23)	45(9)	21(6)	12(5)	-1(4)	-8(5)	-12(6)
C(24)	50(11)	42(8)	26(6)	-27(5)	14(5)	-31(7)
C(25)	14(7)	13(5)	20(5)	-4(4)	3(4)	0(4)
C(26)	26(9)	26(6)	28(6)	3(5)	-3(5)	-4(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for bzte50k-on.

	x	y	z	U(eq)
H(1)	2000	6207	611	31
H(3)	3376	3752	-1908	24
H(4)	6117	2221	-804	27
H(6)	4843	2864	1972	32
H(11)	2827	3687	5773	29
H(12)	3212	4317	3390	39
H(13)	1545	6203	2660	35
H(14)	-885	7756	4176	35
H(16)	-55	7125	7007	29
H(17)	1382	5648	7816	28
H(1A)	1909	371	-98	20
H(1B)	683	1220	-376	20
H(3)	2078	-666	1339	28
H(4)	1045	-1409	2474	37
H(5)	-989	-648	2717	34
H(6)	-2004	871	1851	31
H(7)	-1025	1609	722	27
H(8A)	2957	2269	1176	30
H(8B)	2472	1265	1532	30
H(9A)	3621	116	368	33
H(9B)	4424	547	1051	33
H(9C)	4146	1119	71	33
H(10A)	2610	2865	-446	24
H(10B)	2669	1687	-887	24
H(11A)	678	2424	-1316	36
H(11B)	1526	3081	-1784	36
H(11C)	689	3612	-929	36
H(12A)	26	3049	430	20
H(12B)	539	2603	1400	20
H(13A)	1746	3813	1334	32
H(13B)	387	4506	1247	32
H(13C)	1241	4256	359	32
H(14A)	6699	523	5194	20
H(14B)	5439	1428	5281	20
H(16)	4012	1632	4094	25
H(17)	3268	652	3018	34
H(18)	4542	-962	2341	34
H(19)	6487	-1594	2773	33
H(20)	7206	-704	3905	27
H(21A)	5037	3138	4373	20
H(21B)	5663	2527	3463	20
H(22A)	6362	4277	4324	38
H(22B)	5592	4448	3429	38
H(22C)	6936	3687	3391	38
H(23A)	7455	1952	5843	30
H(23B)	7412	3073	5297	30
H(24A)	5375	3766	5672	53
H(24B)	6142	3492	6568	53
H(24C)	5441	2650	6239	53
H(25A)	7628	1156	3503	20
H(25B)	8076	2194	3779	20
H(26A)	9115	1201	4971	42
H(26B)	9479	462	4068	42
H(26C)	8575	184	4805	42

Table 6. Hydrogen bonds for bzte50k-on [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(8)	0.84	1.65	2.487(10)	175.4
O(3)-H(3)...O(2)	0.84	2.09	2.882(12)	156.0
O(3)-H(3)...O(18)#3	0.84	2.33	2.761(11)	112.7
O(4)-H(4)...O(5)	0.84	1.60	2.436(9)	177.7
O(6)-H(6)...O(7)	0.84	1.71	2.535(12)	166.6
O(11)-H(11)...O(18)	0.84	1.61	2.451(10)	177.5
O(12)-H(12)...O(7)	0.84	1.71	2.482(10)	152.2
O(13)-H(13)...O(8)	0.84	1.79	2.524(11)	145.5
O(14)-H(14)...O(15)	0.84	1.60	2.444(10)	178.5
O(16)-H(16)...O(17)	0.84	1.73	2.557(11)	165.9
O(17)-H(17)...O(2)#4	0.84	1.61	2.452(10)	179.2

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x,-y+1,-z+1 #3 x,y,z-1

#4 x,y,z+1