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# Crystal structure of the mixed-valence platinum(II,IV) iodide-bridged chain complex $[Pt(en)_2I](H_2PO_4)_2(H_3PO_4)_2$ within a hydrogen-bonded phosphate framework

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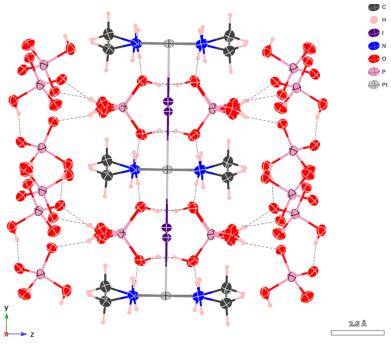
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The crystal structure of the mixed-valence platinum(II,IV) iodide-bridged chain complex *catena*-poly[[[bis(ethylenediamine-$\kappa^2N,N'$)platinum(II,IV)]-$\mu$-iodido] bis(dihydrogen phosphate) bis(phosphoric acid)], $\{[PtI(C_2H_8N_2)_2](H_2PO_4)_2\cdot 2H_3PO_4\}_n$, is reported. The structure consists of one-dimensional Pt–I chains accommodated within an extended hydrogen-bonded framework formed by dihydrogenphosphate anions and neutral phosphoric acid molecules. The $Pt^{II}$ and $Pt^{IV}$ centers are crystallographically indistinguishable, and the bridging iodide ions are positionally disordered over two sites with equal occupancies. The resulting short and long Pt—I distances are consistent with the local coordination environments expected for alternating $Pt^{II}$ and $Pt^{IV}$ centers. Neutral $H_3PO_4$ molecules are located between neighboring *MX* chains along the *a*-axis direction and form N—H···O hydrogen bonds with the ethylenediamine ligands. The crystallographically averaged structure may be associated with weak phase correlations between the charge-ordering patterns of neighboring *MX* chains.

## 1. Chemical context

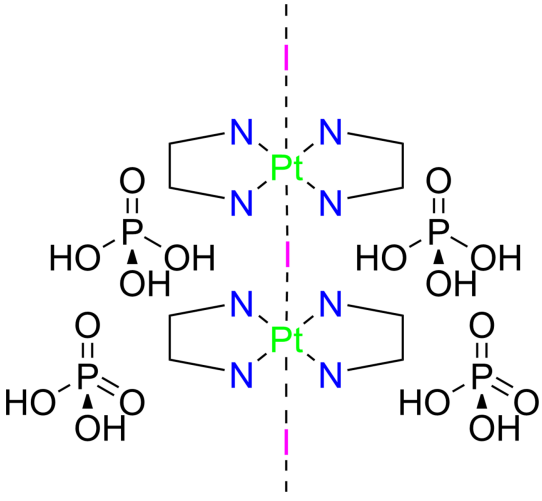
Quasi-one-dimensional halogen-bridged metal complexes (*MX*-chain compounds) have attracted considerable interest as mixed-valence systems characterized by alternating metal oxidation states and unequal metal–halogen distances. In particular, iodide-bridged platinum complexes containing ethylenediamine (en) ligands generally exhibit alternating $Pt^{II}$ and $Pt^{IV}$ centers along the chains. Their crystal structures are strongly influenced by the counter-ions and intermolecular interactions. An iodide-bridged $Pt^{II}/Pt^{IV}$ complex containing perchlorate counter-ions has been structurally characterized (Endres *et al.*, 1979). Hydrogen bonds between diamine ligands and counter-ions can connect neighboring *MX* chains to form higher-dimensional networks (Okamoto *et al.*, 1990). In contrast, neutral *MX*-chain complexes without counter-ions have also been reported, in which the absence of counter-ions allows shorter interchain distances (Otake *et al.*, 2016). These studies illustrate the importance of the surrounding ionic environment in determining the structural organization of *MX* chains.

Among various counter-ions, phosphate species are particularly interesting because of their ability to construct extended hydrogen-bonded frameworks. Dihydrogenphosphate ($H_2PO_4^-$) anions can assemble through O—H···O hydrogen bonds into host lattices that accommodate organic cations (Jagan *et al.*, 2015). The coexistence of $H_2PO_4^-$ anions and neutral phosphoric acid ($H_3PO_4$) molecules can also



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produce hydrogen-bonded phosphate layers, with organic cations located between them (Khemiri *et al.*, 2009). Such hydrogen-bonding interactions are also important in *MX*-chain compounds. Pt–Br chain complexes containing $H_2PO_4^-$ counter-ions have been reported, in which hydrogen bonding contributes to the cohesion of the chain structures (Afrin *et al.*, 2019). Furthermore, a phosphate-containing a Pt–I *MX*-chain complex exhibits three-dimensional valence ordering, with hydrogenphosphate and dihydrogenphosphate anions forming cyclic hydrogen-bonded tetramers (Matsushita, 2006). These examples demonstrate that phosphate-based hydrogen-bonded networks can accommodate cationic species, including mixed-valence metal chains, and contribute to their crystal packing.




In the present study, we report a new mixed-valence $Pt^{II}/Pt^{IV}$ iodide-bridged chain complex, $[Pt(en)_2I](H_2PO_4)_2(H_3PO_4)_2$, obtained under phosphoric-acid-rich crystallization conditions. The cationic Pt–I chains are embedded within an extended hydrogen-bonded framework formed by $H_2PO_4^-$ anions and neutral $H_3PO_4$ molecules. Unlike the previously reported phosphate-containing Pt–I *MX*-chain compound (Matsushita, 2006), the present compound incorporates neutral $H_3PO_4$ molecules into the surrounding hydrogen-bonded framework. The crystal structure is characterized by crystallographically averaged Pt sites and positional disorder of the bridging iodide ions.

## 2. Structural commentary

The crystal structure of the title compound consists of one-dimensional iodide-bridged mixed-valence platinum(II,IV) chains extending along the *b*-axis direction, together with dihydrogenphosphate anions and neutral phosphoric acid molecules. A portion of the one-dimensional Pt–I chain is shown in Fig. 1. Each Pt atom is coordinated by four nitrogen atoms from two ethylenediamine ligands in the equatorial plane, while the bridging iodide ions occupy the axial positions, linking the Pt centers into infinite *MX* chains. The local structures of mixed-valence Pt–I chains are generally described in terms of alternating square-planar $Pt^{II}$ and elongated octahedral $Pt^{IV}$ coordination environments. In a fully valence-ordered structure, alternating $Pt^{II}$ and $Pt^{IV}$ centers would give rise to a doubled repeat period along the MX chain. However, in the present structure, the $Pt^{II}$ and $Pt^{IV}$ centers are crystallographically indistinguishable and are represented by a single averaged Pt site located on a crystallographic twofold rotation axis. The bridging iodide ions were modeled as positionally disordered over two sites (I1*A* and I1*B*), each with an occupancy of 0.50, as illustrated in Fig. 1. The resulting short and long Pt-I distances are consistent with the $Pt^{IV}$—I bonds and $Pt^{II}\cdots$I contacts, respectively, expected for a locally charge-ordered mixed-valence *MX* chain. The dihydrogenphosphate anions and neutral phosphoric acid molecules are arranged around the Pt–I chains, forming a hydrogen-bonded framework (Figs. 2 and 3). The P—O bond lengths are consistent with the assigned protonation states of the phosphate species. In contrast, the related phosphate-containing $Pt^{II}/Pt^{IV}$ *MX*-chain complex exhibits crystallographically distinct, alternately arranged square-planar $Pt^{II}$

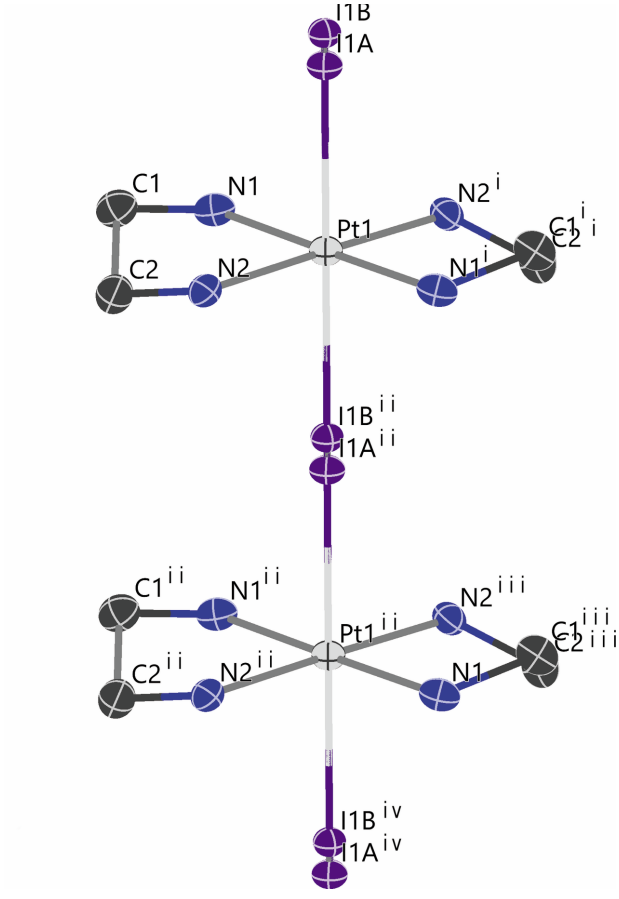



**Figure 1**
A portion of the one-dimensional iodide-bridged Pt chain in the title compound, showing the coordination environment of the Pt atoms and the positional disorder of the bridging iodide ions (I1*A* and I1*B*). The two iodide positions were refined with equal occupancies of 0.50. Displacement ellipsoids are drawn at the 60% probability level. Hydrogen atoms are omitted for clarity. Symmetry codes: (i) $\frac{1}{2}-x, y, 1-z$; (ii) $x, y-1, z$; (iii) $\frac{1}{2}-x, y-1, 1-z$; (iv) $x, y-2, z$.

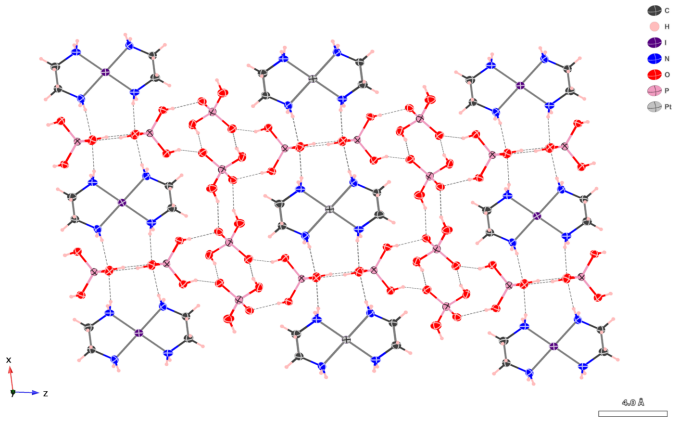


**Figure 2**
Crystal packing viewed along the *b* axis, showing the arrangement of the one-dimensional Pt–I chains within the hydrogen-bonded framework formed by $H_2PO_4^-$ anions and neutral $H_3PO_4$ molecules. The O—H···O and N—H···O hydrogen bonds are indicated by dashed lines.

and elongated-octahedral $Pt^{IV}$ sites, resulting in three-dimensional valence ordering. The oxidation-state assignments are supported by the short $Pt^{IV}$—I bonds of 2.6997 (7) and 2.6921 (7) Å and the substantially longer $Pt^{II}$···I contacts of 3.3239 (8) and 3.2902 (7) Å (Matsushita, 2006). The crystallographically averaged structure observed in the present compound may arise from a lack of long-range phase correlation between the charge-ordering patterns of neighboring *MX* chains, as discussed in Section 3.

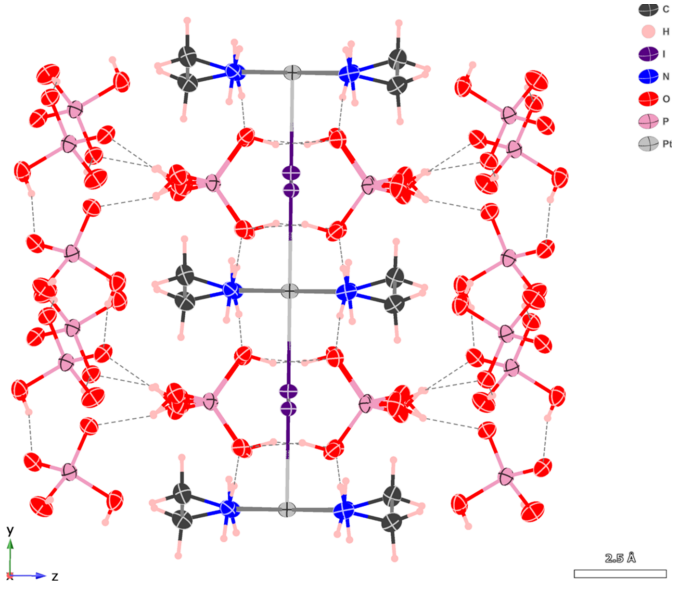


**Figure 3**
Crystal packing viewed along the *c* axis, showing the arrangement of the one-dimensional Pt–I chains and the surrounding hydrogen-bonded phosphate framework. Neutral $H_3PO_4$ molecules are located between neighboring *MX* chains along the *a*-axis direction and form N—H···O hydrogen bonds with the ethylenediamine ligands. The O—H···O and N—H···O hydrogen bonds are indicated by dashed lines.

**Table 1**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O2$^{i}$ | 0.91 | 2.10 | 2.989 (7) | 167 |
| N1—H1*B*···O1 | 0.91 | 2.22 | 2.951 (7) | 137 |
| N2—H2*A*···O2$^{ii}$ | 0.91 | 2.13 | 3.018 (7) | 166 |
| N2—H2*B*···O1$^{iii}$ | 0.91 | 2.30 | 3.016 (7) | 135 |
| O1—H1···O2$^{iv}$ | 0.84 | 1.68 | 2.483 (9) | 159 |
| O3—H3···O5 | 0.84 | 1.65 | 2.452 (7) | 158 |
| O4—H4···O7$^{v}$ | 0.84 | 1.78 | 2.501 (7) | 144 |
| O6—H6···O7$^{vi}$ | 0.84 | 1.82 | 2.614 (7) | 158 |
| O8—H8···O5$^{v}$ | 0.84 | 1.78 | 2.603 (6) | 166 |

Symmetry codes: (i) $x, y+1, z$; (ii) $x-\frac{1}{2}, -y, z$; (iii) $x-\frac{1}{2}, -y+1, z$; (iv) $-x+1, -y, -z+1$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (vi) $-x+\frac{3}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$.

## 3. Supramolecular features

The dihydrogenphosphate anions ($H_2PO_4^-$) and neutral phosphoric acid molecules ($H_3PO_4$) are interconnected through O—H···O hydrogen bonds, forming an extended hydrogen-bonded framework that accommodates the one-dimensional iodide-bridged Pt chains (Fig. 2). The O···O distances range from 2.452 (7) to 2.614 (7) Å (Table 1). In particular, the O3—H3···O5 and O4—H4···O7$^{ix}$ hydrogen bonds, with O···O distances of 2.452 (7) and 2.501 (7) Å, respectively, connect the neutral $H_3PO_4$ molecules and $H_2PO_4^-$ anions. Additional O—H···O hydrogen bonds, namely O1—H1···O2$^{viii}$, O6—H6···O7$^{x}$ and O8—H8···O5$^{ix}$, with O···O distances of 2.483 (9), 2.614 (7) and 2.603 (6) Å, respectively, further extend the hydrogen-bonded framework. The $H_2PO_4^-$ anions serve as counter-ions that compensate for the positive charge of the mixed-valence *MX* chains, while also contributing to the hydrogen-bonded framework. In contrast, the neutral $H_3PO_4$ molecules are located between neighboring *MX* chains along the *a*-axis direction, as shown in Fig. 3, and participate in N—H···O hydrogen bonds with the amino groups of the ethylenediamine ligands. Four N—H···O hydrogen bonds are observed, N1—H1*A*···O2$^{v}$, N1—H1*B*···O1, N2—H2*A*···O2$^{vi}$ and N2–H2*B*···O1$^{vii}$, with N···O distances of 2.989 (7), 2.951 (7), 3.018 (7) and 3.016 (7) Å, respectively (Table 1). These interactions connect the MX *chains* to the surrounding phosphate-based hydrogen-bonded framework. Although alternating Pt(II) and Pt(IV) centers are expected within individual *MX* chains, the phases of their charge-ordering patterns may not be correlated between neighboring chains. The presence of neutral $H_3PO_4$ molecules between adjacent chains along the *a*-axis direction (Fig. 3) may weaken the electrostatic coupling between their charge-ordering patterns, thereby reducing the tendency toward coherent interchain charge ordering. Consequently, the lack of long-range interchain phase correlation could account for the crystallographically averaged Pt sites observed in the present structure, rather than crystallographically distinct $Pt^{II}$ and $Pt^{IV}$ sites.

## 4. Database survey

A search of the Cambridge Structural Database (CSD, version 6.0; Groom *et al.*, 2016), carried out on 24 October 2026, using

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[PtI(C_2H_8N_2)_2](H_2PO_4)_2{\cdot}2H_3PO_4$ |
| $M_r$ | 832.16 |
| Crystal system, space group | Monoclinic, *I*2/*a* |
| Temperature (K) | 100 |
| *a*, *b*, *c* (Å) | 15.2100 (6), 5.9034 (3), 24.0418 (11) |
| $\beta$ (°) | 99.156 (4) |
| $V$ (Å$^3$) | 2131.20 (16) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 8.41 |
| Crystal size (mm) | 0.36 × 0.07 × 0.03 × 0.05 (radius) |
| Data collection | |
| Diffractometer | XtaLAB Synergy R, DW system, HyPix |
| Absorption correction | Gaussian (*CrysAlis PRO*; Rigaku OD, 2024) |
| $T_{min}$, $T_{max}$ | 0.422, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 7459, 2170, 1798 |
| $R_{int}$ | 0.072 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.625 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.040, 0.102, 1.08 |
| No. of reflections | 2170 |
| No. of parameters | 151 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.15, −1.57 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*b*), *SHELXL2018/3* (Sheldrick, 2015*a*) and *OLEX2* (Dolomanov *et al.*, 2009).

the molecular structure and unit-cell parameters of the title compound returned no matches. A search for related iodide-bridged $Pt^{II}/Pt^{IV}$ mixed-valence chain complexes containing ethylenediamine ligands and phosphate-based counter-ions identified one previously reported structure, HEFYIB, $\{[Pt(II)Pt(IV)I_2(en)_4](HPO_4)(H_2PO_4)I{\cdot}3H_2O\}_n$ (Matsushita, 2006). In this compound, the $Pt^{II}$ and $Pt^{IV}$ centers are crystallographically distinct, exhibiting three-dimensional valence ordering. The hydrogenphosphate and dihydrogenphosphate anions form cyclic hydrogen-bonded tetramers. In contrast, the title compound, $[Pt(en)_2I](H_2PO_4)_2(H_3PO_4)_2$, crystallized under phosphoric-acid-rich conditions and exhibits a substantially different chemical composition and crystal structure. Unlike the previously reported compound, the present structure contains neutral phosphoric acid molecules in addition to dihydrogenphosphate anions, but no hydrogenphosphate anions, additional iodide counter-ions or water molecules of crystallization. The dihydrogenphosphate anions and phosphoric acid molecules form an extended hydrogen-bonded framework accommodating the one-dimensional *MX* chains, rather than the cyclic phosphate tetramers observed in the previously reported structure. Furthermore, the $Pt^{II}$ and $Pt^{IV}$ sites are crystallographically averaged, and the bridging iodide ions exhibit positional disorder, in contrast to the three-dimensionally valence-ordered structure reported by Matsushita (2006).

## 5. Synthesis and crystallization

A small fragment of the $Pt^{II}$ ethylenediamine complex was dissolved in two drops of water, followed by the addition of one drop of 85% phosphoric acid ($H_3PO_4$). The resulting solution was left undisturbed overnight, yielding crystals of the mixed-valence $Pt^{II}/Pt^{IV}$ *MX*-chain complex.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The bridging iodide atom was modeled as positionally disordered over two sites (I1*A* and I1*B*), each with an occupancy of 0.50. The Pt and bridging I atoms occupy crystallographic twofold rotation axes. Hydrogen atoms bonded to carbon and nitrogen atoms were placed in geometrically calculated positions and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C,N)$. The hydrogen atoms of the hydroxyl groups were treated using a rotating-group model (AFIX 147). The isotropic displacement parameter of H1 was fixed at $1.5U_{eq}(O1)$, whereas those of H3, H4, H6 and H8 were refined independently. No geometric restraints were applied.

## Acknowledgements

The authors thank Professor Shinya Takaishi (Tohoku University) for conducting the Cambridge Structural Database (CSD) search.

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# supporting information

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# Crystal structure of the mixed-valence platinum(II,IV) iodide-bridged chain complex $[Pt(en)_2I](H_2PO_4)_2(H_3PO_4)_2$ within a hydrogen-bonded phosphate framework

**Yuki Matsumoto and Takefumi Yoshida**

## Computing details

***catena*-Poly[[[bis(ethylenediamine-$\kappa^2N,N'$)platinum(II,IV)]-$\mu$-iodido] bis(dihydrogen phosphate) bis(phosphoric acid)]**

*Crystal data*

$[PtI(C_2H_8N_2)_2](H_2PO_4)_2\cdot 2H_3PO_4$
$M_r = 832.16$
Monoclinic, $I2/a$
$a = 15.2100$ (6) Å
$b = 5.9034$ (3) Å
$c = 24.0418$ (11) Å
$\beta = 99.156$ (4)°
$V = 2131.20$ (16) Å$^3$
$Z = 4$
$F(000) = 1588$
$D_x = 2.594$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3086 reflections
$\theta = 2.7$–$28.3°$
$\mu = 8.41$ mm$^{-1}$
$T = 100$ K
Sphere, dark yellow
0.36 × 0.07 × 0.03 × 0.05 (radius) mm

*Data collection*

XtaLAB Synergy R, DW system, HyPix diffractometer
Detector resolution: 10.0000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2024)
$T_{min} = 0.422$, $T_{max} = 1.000$
7459 measured reflections
2170 independent reflections
1798 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.7°$
$h = -17\rightarrow19$
$k = -7\rightarrow6$
$l = -30\rightarrow30$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.102$
$S = 1.08$
2170 reflections
151 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.15$ e Å$^{-3}$
$\Delta\rho_{min} = -1.57$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Pt1 | 0.250000 | 0.48970 (5) | 0.500000 | 0.02350 (15) | |
| I1A | 0.250000 | 0.9486 (3) | 0.500000 | 0.0257 (5) | 0.5 |
| I1B | 0.250000 | 1.0282 (3) | 0.500000 | 0.0245 (5) | 0.5 |
| N1 | 0.3237 (3) | 0.4920 (8) | 0.4353 (3) | 0.0294 (13) | |
| H1A | 0.367127 | 0.599025 | 0.442115 | 0.035* | |
| H1B | 0.350244 | 0.354829 | 0.433213 | 0.035* | |
| C1 | 0.2649 (4) | 0.5421 (12) | 0.3808 (3) | 0.0370 (17) | |
| H1C | 0.254352 | 0.707178 | 0.376884 | 0.044* | |
| H1D | 0.293514 | 0.489993 | 0.348861 | 0.044* | |
| N2 | 0.1446 (4) | 0.4858 (8) | 0.4331 (2) | 0.0288 (13) | |
| H2A | 0.102850 | 0.383485 | 0.439864 | 0.035* | |
| H2B | 0.118638 | 0.624927 | 0.428921 | 0.035* | |
| C2 | 0.1803 (4) | 0.4226 (13) | 0.3808 (3) | 0.0355 (16) | |
| H2C | 0.189892 | 0.256879 | 0.379775 | 0.043* | |
| H2D | 0.137268 | 0.465809 | 0.347123 | 0.043* | |
| P1 | 0.47906 (10) | 0.0040 (2) | 0.41114 (7) | 0.0231 (4) | |
| O1 | 0.4884 (3) | 0.2196 (7) | 0.4487 (2) | 0.0318 (11) | |
| H1 | 0.500271 | 0.181683 | 0.482713 | 0.048* | |
| O2 | 0.4833 (3) | −0.2061 (8) | 0.4468 (2) | 0.0289 (10) | |
| O3 | 0.5563 (3) | 0.0011 (9) | 0.3773 (2) | 0.0398 (13) | |
| H3 | 0.539869 | 0.061472 | 0.345670 | 0.15 (6)* | |
| O4 | 0.3891 (3) | 0.0390 (9) | 0.3724 (2) | 0.0336 (11) | |
| H4 | 0.381574 | −0.064298 | 0.348079 | 0.34 (14)* | |
| P2 | 0.61015 (10) | 0.1716 (3) | 0.24717 (7) | 0.0285 (4) | |
| O5 | 0.5478 (3) | 0.2152 (8) | 0.28916 (18) | 0.0345 (11) | |
| O6 | 0.6844 (4) | 0.0122 (7) | 0.2780 (3) | 0.0434 (14) | |
| H6 | 0.733269 | 0.044168 | 0.267895 | 0.04 (2)* | |
| O7 | 0.6496 (3) | 0.3823 (8) | 0.22506 (18) | 0.0320 (10) | |
| O8 | 0.5599 (3) | 0.0432 (9) | 0.1949 (2) | 0.0373 (11) | |
| H8 | 0.527319 | −0.057401 | 0.205617 | 0.11 (4)* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pt1 | 0.0208 (2) | 0.0224 (2) | 0.0274 (2) | 0.000 | 0.00428 (14) | 0.000 |
| I1A | 0.0247 (8) | 0.0210 (12) | 0.0314 (9) | 0.000 | 0.0046 (5) | 0.000 |
| I1B | 0.0258 (8) | 0.0212 (12) | 0.0267 (8) | 0.000 | 0.0048 (5) | 0.000 |
| N1 | 0.020 (3) | 0.028 (3) | 0.041 (4) | 0.0003 (18) | 0.004 (2) | 0.003 (2) |
| C1 | 0.031 (4) | 0.037 (4) | 0.042 (4) | −0.001 (3) | 0.006 (3) | 0.005 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.032 (3) | 0.026 (3) | 0.028 (3) | 0.0007 (19) | 0.002 (2) | 0.004 (2) |
| C2 | 0.028 (4) | 0.044 (4) | 0.034 (4) | −0.004 (3) | 0.003 (3) | 0.004 (3) |
| P1 | 0.0215 (8) | 0.0266 (9) | 0.0213 (9) | 0.0013 (6) | 0.0037 (6) | −0.0003 (6) |
| O1 | 0.035 (3) | 0.029 (3) | 0.031 (3) | −0.0012 (19) | 0.004 (2) | 0.008 (2) |
| O2 | 0.028 (2) | 0.030 (2) | 0.031 (3) | 0.0005 (19) | 0.0095 (19) | 0.000 (2) |
| O3 | 0.032 (3) | 0.059 (4) | 0.031 (3) | 0.0105 (19) | 0.009 (2) | 0.006 (2) |
| O4 | 0.026 (2) | 0.041 (3) | 0.032 (3) | 0.0041 (19) | 0.0009 (19) | −0.005 (2) |
| P2 | 0.0278 (8) | 0.0309 (9) | 0.0271 (8) | 0.0006 (7) | 0.0056 (6) | 0.0013 (8) |
| O5 | 0.034 (2) | 0.036 (3) | 0.035 (3) | 0.0075 (18) | 0.011 (2) | 0.009 (2) |
| O6 | 0.034 (3) | 0.043 (3) | 0.054 (4) | 0.004 (2) | 0.009 (2) | 0.014 (2) |
| O7 | 0.029 (2) | 0.032 (3) | 0.034 (3) | 0.0026 (19) | 0.0022 (18) | 0.004 (2) |
| O8 | 0.042 (3) | 0.044 (3) | 0.028 (3) | −0.013 (2) | 0.011 (2) | −0.003 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pt1—I1A | 2.7088 (17) | N2—C2 | 1.494 (9) |
| Pt1—I1A$^{i}$ | 3.1946 (17) | C2—H2C | 0.9900 |
| Pt1—I1B$^{i}$ | 2.7246 (18) | C2—H2D | 0.9900 |
| Pt1—I1B | 3.1788 (18) | P1—O1 | 1.554 (5) |
| Pt1—N1 | 2.056 (6) | P1—O2 | 1.503 (5) |
| Pt1—N1$^{ii}$ | 2.056 (6) | P1—O3 | 1.532 (5) |
| Pt1—N2 | 2.083 (6) | P1—O4 | 1.541 (5) |
| Pt1—N2$^{ii}$ | 2.082 (6) | O1—H1 | 0.8400 |
| N1—H1A | 0.9100 | O3—H3 | 0.8400 |
| N1—H1B | 0.9100 | O4—H4 | 0.8400 |
| N1—C1 | 1.493 (9) | P2—O5 | 1.514 (4) |
| C1—H1C | 0.9900 | P2—O6 | 1.563 (5) |
| C1—H1D | 0.9900 | P2—O7 | 1.514 (5) |
| C1—C2 | 1.468 (9) | P2—O8 | 1.560 (5) |
| N2—H2A | 0.9100 | O6—H6 | 0.8400 |
| N2—H2B | 0.9100 | O8—H8 | 0.8400 |
| | | | |
| I1A—Pt1—I1A$^{i}$ | 180.0 | N1—C1—H1C | 110.1 |
| I1A—Pt1—I1B$^{i}$ | 180.0 | N1—C1—H1D | 110.1 |
| I1A—Pt1—I1B | 0.0 | H1C—C1—H1D | 108.4 |
| I1B—Pt1—I1A$^{i}$ | 180.0 | C2—C1—N1 | 107.9 (6) |
| I1B$^{i}$—Pt1—I1A$^{i}$ | 0.0 | C2—C1—H1C | 110.1 |
| I1B$^{i}$—Pt1—I1B | 180.0 | C2—C1—H1D | 110.1 |
| N1—Pt1—I1A$^{i}$ | 90.38 (13) | Pt1—N2—H2A | 110.0 |
| N1—Pt1—I1A | 89.62 (13) | Pt1—N2—H2B | 110.0 |
| N1$^{ii}$—Pt1—I1A | 89.62 (13) | H2A—N2—H2B | 108.4 |
| N1$^{ii}$—Pt1—I1A$^{i}$ | 90.38 (13) | C2—N2—Pt1 | 108.4 (4) |
| N1—Pt1—I1B$^{i}$ | 90.38 (13) | C2—N2—H2A | 110.0 |
| N1$^{ii}$—Pt1—I1B | 89.62 (13) | C2—N2—H2B | 110.0 |
| N1$^{ii}$—Pt1—I1B$^{i}$ | 90.38 (13) | C1—C2—N2 | 108.4 (6) |
| N1—Pt1—I1B | 89.62 (13) | C1—C2—H2C | 110.0 |
| N1—Pt1—N1$^{ii}$ | 179.2 (3) | C1—C2—H2D | 110.0 |
| N1$^{ii}$—Pt1—N2$^{ii}$ | 82.0 (2) | N2—C2—H2C | 110.0 |

| | | | |
|---|---|---|---|
| N1$^{ii}$—Pt1—N2 | 98.0 (2) | N2—C2—H2D | 110.0 |
| N1—Pt1—N2$^{ii}$ | 98.0 (2) | H2C—C2—H2D | 108.4 |
| N1—Pt1—N2 | 82.0 (2) | O2—P1—O1 | 110.7 (3) |
| N2—Pt1—I1A$^{i}$ | 89.37 (13) | O2—P1—O3 | 109.1 (3) |
| N2$^{ii}$—Pt1—I1A$^{i}$ | 89.37 (13) | O2—P1—O4 | 114.1 (3) |
| N2$^{ii}$—Pt1—I1A | 90.63 (13) | O3—P1—O1 | 108.1 (3) |
| N2—Pt1—I1A | 90.63 (13) | O3—P1—O4 | 111.2 (3) |
| N2—Pt1—I1B | 90.63 (13) | O4—P1—O1 | 103.4 (3) |
| N2—Pt1—I1B$^{i}$ | 89.37 (13) | P1—O1—H1 | 109.5 |
| N2$^{ii}$—Pt1—I1B | 90.63 (13) | P1—O3—H3 | 109.5 |
| N2$^{ii}$—Pt1—I1B$^{i}$ | 89.37 (13) | P1—O4—H4 | 109.5 |
| N2$^{ii}$—Pt1—N2 | 178.7 (3) | O5—P2—O6 | 105.6 (3) |
| Pt1—I1A—Pt1$^{iii}$ | 180.0 | O5—P2—O7 | 114.8 (3) |
| Pt1$^{iii}$—I1B—Pt1 | 180.0 | O5—P2—O8 | 110.0 (3) |
| Pt1—N1—H1A | 109.7 | O7—P2—O6 | 111.4 (3) |
| Pt1—N1—H1B | 109.7 | O7—P2—O8 | 106.7 (3) |
| H1A—N1—H1B | 108.2 | O8—P2—O6 | 108.3 (3) |
| C1—N1—Pt1 | 110.0 (4) | P2—O6—H6 | 109.5 |
| C1—N1—H1A | 109.7 | P2—O8—H8 | 109.5 |
| C1—N1—H1B | 109.7 | | |
| | | | |
| Pt1—N1—C1—C2 | −39.3 (6) | N1—C1—C2—N2 | 53.3 (7) |
| Pt1—N2—C2—C1 | −41.7 (6) | | |

Symmetry codes: (i) $x$, $y-1$, $z$; (ii) $-x+1/2$, $y$, $-z+1$; (iii) $x$, $y+1$, $z$.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O2$^{iii}$ | 0.91 | 2.10 | 2.989 (7) | 167 |
| N1—H1*B*···O1 | 0.91 | 2.22 | 2.951 (7) | 137 |
| N2—H2*A*···O2$^{iv}$ | 0.91 | 2.13 | 3.018 (7) | 166 |
| N2—H2*B*···O1$^{v}$ | 0.91 | 2.30 | 3.016 (7) | 135 |
| O1—H1···O2$^{vi}$ | 0.84 | 1.68 | 2.483 (9) | 159 |
| O3—H3···O5 | 0.84 | 1.65 | 2.452 (7) | 158 |
| O4—H4···O7$^{vii}$ | 0.84 | 1.78 | 2.501 (7) | 144 |
| O6—H6···O7$^{viii}$ | 0.84 | 1.82 | 2.614 (7) | 158 |
| O8—H8···O5$^{vii}$ | 0.84 | 1.78 | 2.603 (6) | 166 |

Symmetry codes: (iii) $x$, $y+1$, $z$; (iv) $x-1/2$, $-y$, $z$; (v) $x-1/2$, $-y+1$, $z$; (vi) $-x+1$, $-y$, $-z+1$; (vii) $-x+1$, $y-1/2$, $-z+1/2$; (viii) $-x+3/2$, $-y+1/2$, $-z+1/2$.