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(2,2′-Bipyridyl)dicarbonylbis(triethoxyphosphine-κP)-rhenium(I) hexafluorophosphate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.012 Å
Disorder in main residue
R factor = 0.033
wR factor = 0.073
Data-to-parameter ratio = 15.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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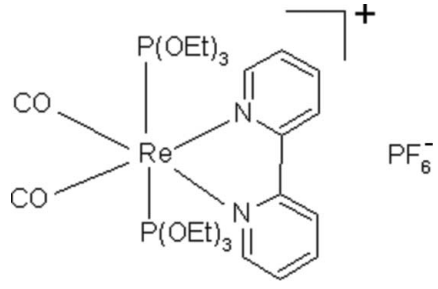
In the title compound, $[Re(C_{10}H_8N_2)(C_6H_{15}O_3P)_2(CO)_2]PF_6$, the carbonyl ligands are mutually *cis* and lie *trans* to the N donors of the 2,2′-bipyridyl ligand, while the triethoxyphosphine ligands are mutually *trans*. The Re^I centres exhibit approximate octahedral coordination, the major distortions from which arise from the narrow bite angle of the 2,2′-bipyridyl ligand which is expressed in the N—Re—N angles of 74.0 (3) and 74.3 (3)°. There are two cations and two anions in the asymmetric unit. The title compound is of interest because it has been shown to be a photocatalyst for CO_2 reduction [Ishitani, George, Ibusuki, Johnson, Koike, Nozaki, Pac, Turner & Westwell (1994). *Inorg. Chem.* **33**, 4712–4717].

Comment

The title compound, (I), is of interest because it has been shown to be a photocatalyst for CO_2 reduction (Ishitani *et al.*, 1994). A structure determination showed that the carbonyl ligands are mutually *cis*, while the triethoxyphosphine ligands are mutually *trans*. The carbonyl groups are *trans* to the N-atom donors of the 2,2′-bipyridyl (2,2′-bipy) ligand. The Re^I centres occupy approximately octahedral coordination environments. The major distortions from ideal octahedral geometry arise from the narrow chelate angle of the 2,2′-bipyridyl ligand; the N—Re—N angles are 74.0 (3) and 74.3 (3)°.



(I)

Rhenium complexes containing similar arrays of ligands are unusual; the only previous example of the (2,2′-bipy)Re-$(CO)_2P_2$ fragment which has been structurally characterized is the less symmetrical *cis*,*trans*-dicarbonyl(4,4′-dimethyl-2,2′-bipyridyl)(triethoxyphosphine)(triphenylphosphine)rhenium(I) hexafluorophosphate (Koike *et al.*, 2000).

Experimental

The title compound was prepared using the method reported previously by Ishitani *et al.* (1994) by photolysis (> 360 nm long-pass

filter) of (2,2′-bipyridyl)tricarbonylrhenium trifluoromethanesulfonate in MeCN in the presence of $P(OEt)_3$. Reaction with NH_4PF_6 in MeOH yielded the title salt which was subjected to column chromatography on silica with $MeCN/CH_2Cl_2$ (1:5 *v*/*v*) as eluant. Crystals were obtained by slow diffusion of diethyl ether into a solution of the product in MeCN.

Crystal data

$[Re(C_{10}H_8N_2)(C_6H_{15}O_3P)_2(CO)_2]PF_6$	D_x = 1.715 Mg m^{-3}
M_r = 875.66	Mo $K\alpha$ radiation
Orthorhombic, $Pca2_1$	Cell parameters from 7686 reflections
a = 30.821 (6) Å	θ = 2.4–28.8°
b = 14.136 (3) Å	μ = 3.80 mm^{-1}
c = 15.571 (3) Å	T = 150 (2) K
V = 6784 (2) Å^3	Cuboid, yellow
Z = 8	0.42 × 0.41 × 0.37 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	12592 independent reflections
ω scans	11418 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)	R_{int} = 0.043
T_{min} = 0.114, T_{max} = 0.245	θ_{max} = 29.0°
42198 measured reflections	$h = -41 \rightarrow 41$
	$k = -19 \rightarrow 19$
	$l = -11 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 11.37P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$(\Delta/\sigma)_{max}$ = 0.003
$wR(F^2)$ = 0.074	$\Delta\rho_{max}$ = 1.26 e Å^{-3}
S = 1.15	$\Delta\rho_{min}$ = −1.28 e Å^{-3}
12592 reflections	Absolute structure: Flack (1983), 3084 Friedel pairs
790 parameters	Flack parameter: 0.265 (7)
H-atom parameters constrained	

The asymmetric unit contains two independent cation–anion pairs. In one of the cations there is disorder in the arms of one of the triethoxyphosphine ligands. A disorder model was developed in which all three O atoms, but only one of the methylene C atoms and none of the methyl C atoms, were refined over split sites. Similarity restraints were applied to all C—O and C—C distances involving disordered atoms. The major and minor disorder components refined to occupancies of 0.53 (1) and 0.47 (1), respectively, and these were fixed at 0.50 in the final cycles of least-squares refinement. The wide range of U_{eq} values for the C atoms is a reflection of the approximate nature of the disorder model. H atoms were placed geometrically and refined using a riding model, with C—H distances of 0.95–0.99 Å and with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for the other H atoms. The Flack parameter refined to 0.265 (7), indicating the presence of some inversion twinning. The highest peak and deepest trough in the final difference Fourier synthesis are located 0.81 Å from atom Re1*A* and 1.48 Å from Re1, respectively.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* and *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004; *PLATON*).

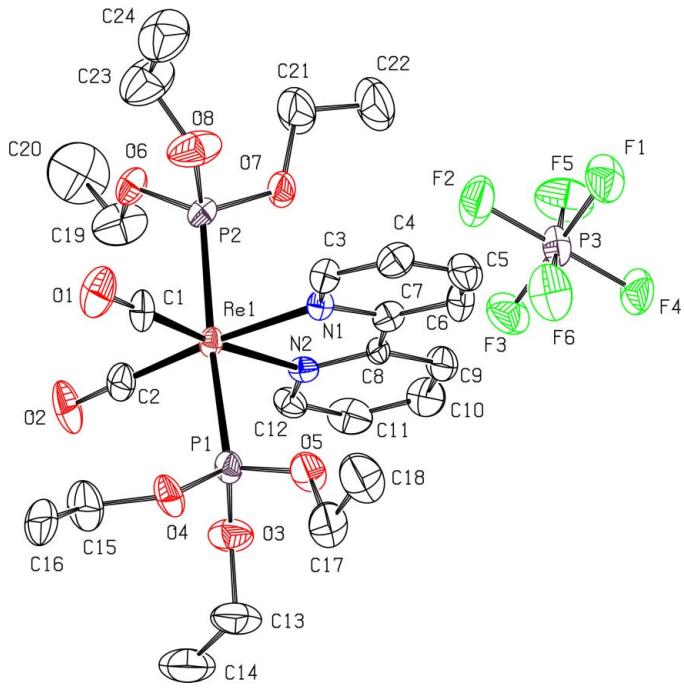


Figure 1
A view of the ordered cation–anion pair with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Except for the orientations of the ethoxy chain, the geometry of the other cation pair is similar.

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$Z = 8$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7686 reflections
$\theta = 2.4$–$28.8°$
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Cuboid, yellow
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$h = -41 \rightarrow 41$
$k = -19 \rightarrow 19$
$l = -11 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.074$
$S = 1.15$
12592 reflections
790 parameters
17 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 11.37P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 1.26$ e Å^{-3}
$\Delta\rho_{min} = -1.28$ e Å^{-3}
Absolute structure: Flack (1983), 3084 Friedel pairs
Absolute structure parameter: 0.265 (7)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Re1	0.362857 (7)	0.223761 (17)	−0.087268 (12)	0.02148 (6)	
P1	0.43886 (5)	0.25000 (12)	−0.09253 (16)	0.0277 (4)	
P2	0.28643 (5)	0.20979 (12)	−0.07425 (15)	0.0287 (4)	
C1	0.3537 (3)	0.3136 (6)	−0.1759 (6)	0.0344 (18)	
O1	0.3484 (2)	0.3682 (4)	−0.2320 (4)	0.0543 (16)	
C2	0.3685 (3)	0.1268 (7)	−0.1739 (6)	0.033 (2)	
O2	0.3728 (2)	0.0704 (4)	−0.2261 (5)	0.0523 (17)	
N1	0.35976 (16)	0.3203 (5)	0.0202 (5)	0.0220 (14)	
N2	0.37129 (17)	0.1374 (4)	0.0272 (4)	0.0214 (13)	
O3	0.46529 (13)	0.1553 (4)	−0.0823 (5)	0.0466 (14)	
O4	0.45965 (18)	0.3028 (4)	−0.1726 (4)	0.0384 (14)	
O5	0.45462 (16)	0.3191 (5)	−0.0187 (4)	0.0523 (18)	
O6	0.25890 (15)	0.1418 (3)	−0.1351 (3)	0.0342 (11)	
O7	0.27313 (14)	0.1824 (4)	0.0222 (3)	0.0464 (13)	
O8	0.26278 (15)	0.3079 (3)	−0.0920 (5)	0.0620 (17)	
C3	0.3562 (2)	0.4155 (5)	0.0117 (6)	0.0298 (16)	
H3A	0.3518	0.4412	−0.0441	0.036*	
C4	0.3585 (2)	0.4760 (6)	0.0802 (7)	0.039 (2)	
H4A	0.3566	0.5423	0.0715	0.047*	
C5	0.3637 (2)	0.4399 (6)	0.1619 (7)	0.043 (2)	
H5A	0.3652	0.4805	0.2104	0.052*	
C6	0.3668 (2)	0.3437 (6)	0.1711 (6)	0.038 (2)	
H6A	0.3703	0.3168	0.2266	0.046*	
C7	0.36490 (18)	0.2867 (5)	0.1004 (7)	0.0259 (18)	
C8	0.36995 (18)	0.1809 (5)	0.1039 (4)	0.0220 (13)	
C9	0.3736 (2)	0.1318 (5)	0.1817 (5)	0.0366 (16)	
H9A	0.3725	0.1639	0.2352	0.044*	
C10	0.3789 (2)	0.0342 (6)	0.1778 (6)	0.0442 (19)	
H10A	0.3816	−0.0012	0.2293	0.053*	
C11	0.3802 (2)	−0.0115 (5)	0.0997 (6)	0.042 (2)	
H11A	0.3833	−0.0783	0.0966	0.050*	
C12	0.3769 (2)	0.0430 (5)	0.0256 (5)	0.0298 (15)	
H12A	0.3787	0.0122	−0.0285	0.036*	
C13	0.5127 (2)	0.1515 (6)	−0.0887 (9)	0.060 (3)	
H13A	0.5258	0.1545	−0.0308	0.072*	
H13B	0.5235	0.2058	−0.1227	0.072*	
C14	0.5249 (3)	0.0593 (8)	−0.1323 (9)	0.079 (4)	
H14A	0.5565	0.0553	−0.1374	0.119*	

H14B	0.5118	0.0570	−0.1896	0.119*
H14C	0.5143	0.0061	−0.0979	0.119*
C15	0.4557 (3)	0.2603 (6)	−0.2584 (8)	0.054 (2)
H15A	0.4250	0.2452	−0.2705	0.065*
H15B	0.4727	0.2008	−0.2609	0.065*
C16	0.4723 (3)	0.3278 (8)	−0.3227 (6)	0.061 (3)
H16A	0.4694	0.3005	−0.3802	0.091*
H16B	0.5029	0.3413	−0.3111	0.091*
H16C	0.4555	0.3867	−0.3195	0.091*
C17	0.4936 (3)	0.3769 (7)	−0.0161 (7)	0.058 (3)
H17A	0.5076	0.3776	−0.0733	0.069*
H17B	0.5144	0.3502	0.0258	0.069*
C18	0.4816 (3)	0.4753 (7)	0.0095 (8)	0.070 (3)
H18A	0.5078	0.5145	0.0118	0.105*
H18B	0.4679	0.4743	0.0662	0.105*
H18C	0.4614	0.5018	−0.0326	0.105*
C19	0.2668 (3)	0.0429 (5)	−0.1348 (7)	0.062 (3)
H19A	0.2750	0.0226	−0.0762	0.074*
H19B	0.2913	0.0285	−0.1738	0.074*
C20	0.2286 (3)	−0.0098 (7)	−0.1624 (9)	0.099 (4)
H20A	0.2351	−0.0776	−0.1627	0.148*
H20B	0.2203	0.0104	−0.2204	0.148*
H20C	0.2045	0.0026	−0.1227	0.148*
C21	0.2282 (3)	0.1790 (9)	0.0516 (6)	0.082 (3)
H21A	0.2135	0.2390	0.0367	0.098*
H21B	0.2128	0.1268	0.0222	0.098*
C22	0.2262 (3)	0.1649 (9)	0.1417 (6)	0.081 (3)
H22A	0.1958	0.1645	0.1601	0.121*
H22B	0.2417	0.2162	0.1708	0.121*
H22C	0.2397	0.1042	0.1562	0.121*
C23	0.2239 (3)	0.3238 (6)	−0.1366 (8)	0.077 (3)
H23A	0.2006	0.2835	−0.1124	0.093*
H23B	0.2276	0.3067	−0.1978	0.093*
C24	0.2118 (3)	0.4212 (6)	−0.1298 (7)	0.079 (3)
H24A	0.1843	0.4316	−0.1600	0.119*
H24B	0.2345	0.4607	−0.1555	0.119*
H24C	0.2084	0.4380	−0.0691	0.119*
Re1A	0.367270 (7)	0.725429 (16)	0.737972 (12)	0.02039 (6)
P1A	0.44335 (5)	0.75241 (12)	0.74876 (15)	0.0258 (4)
P2A	0.29260 (5)	0.69640 (13)	0.71431 (13)	0.0259 (4)
C1A	0.3700 (2)	0.6348 (6)	0.8267 (7)	0.029 (2)
O1A	0.37199 (19)	0.5784 (4)	0.8817 (5)	0.0526 (18)
C2A	0.3548 (2)	0.8199 (6)	0.8226 (6)	0.0291 (17)
O2A	0.34769 (18)	0.8762 (4)	0.8741 (4)	0.0408 (13)
N1A	0.36712 (14)	0.8149 (5)	0.6244 (5)	0.0224 (14)
N2A	0.38027 (18)	0.6311 (4)	0.6299 (4)	0.0211 (12)
O3A	0.46161 (16)	0.8171 (4)	0.6737 (4)	0.0397 (14)
O4A	0.46906 (13)	0.6550 (3)	0.7461 (5)	0.0422 (14)

O5A	0.46236 (16)	0.8049 (4)	0.8318 (4)	0.0337 (13)	
O6A	0.2879 (2)	0.5875 (5)	0.6828 (5)	0.0311 (17)*	0.50
O6B	0.2816 (3)	0.6208 (6)	0.6450 (7)	0.033 (2)*	0.50
O7A	0.2614 (3)	0.6643 (8)	0.7862 (5)	0.037 (2)*	0.50
O7B	0.2574 (3)	0.7128 (6)	0.7887 (5)	0.0299 (19)*	0.50
O8A	0.2682 (3)	0.7494 (6)	0.6386 (7)	0.028 (2)*	0.50
O8B	0.2721 (3)	0.7910 (8)	0.6754 (8)	0.061 (3)*	0.50
C3A	0.36113 (19)	0.9097 (5)	0.6266 (6)	0.0268 (16)	
H3AA	0.3554	0.9389	0.6804	0.032*	
C4A	0.36302 (19)	0.9657 (5)	0.5544 (7)	0.0348 (19)	
H4AA	0.3600	1.0324	0.5584	0.042*	
C5A	0.3694 (2)	0.9230 (6)	0.4772 (7)	0.0374 (19)	
H5AA	0.3703	0.9603	0.4264	0.045*	
C6A	0.3744 (2)	0.8261 (5)	0.4715 (5)	0.0281 (14)	
H6AA	0.3783	0.7961	0.4174	0.034*	
C7A	0.3738 (2)	0.7725 (4)	0.5481 (5)	0.0201 (13)	
C8A	0.38072 (17)	0.6702 (4)	0.5504 (4)	0.0220 (13)	
C9A	0.38623 (19)	0.6140 (5)	0.4790 (5)	0.0286 (14)	
H9AA	0.3868	0.6419	0.4235	0.034*	
C10A	0.3910 (2)	0.5181 (5)	0.4872 (6)	0.0361 (18)	
H10B	0.3947	0.4794	0.4380	0.043*	
C11A	0.3902 (2)	0.4791 (5)	0.5677 (6)	0.0349 (17)	
H11B	0.3932	0.4127	0.5749	0.042*	
C12A	0.3851 (2)	0.5365 (4)	0.6374 (5)	0.0285 (15)	
H12B	0.3849	0.5089	0.6931	0.034*	
C13A	0.4999 (2)	0.8780 (6)	0.6731 (7)	0.053 (2)	
H13C	0.5218	0.8526	0.6328	0.063*	
H13D	0.5130	0.8801	0.7312	0.063*	
C14A	0.4869 (4)	0.9744 (8)	0.6464 (10)	0.093 (4)	
H14D	0.5125	1.0158	0.6463	0.140*	
H14E	0.4653	0.9992	0.6866	0.140*	
H14F	0.4745	0.9720	0.5885	0.140*	
C15A	0.5166 (2)	0.6497 (5)	0.7496 (7)	0.048 (2)	
H15C	0.5289	0.6585	0.6914	0.058*	
H15D	0.5281	0.7001	0.7874	0.058*	
C16A	0.5286 (3)	0.5570 (6)	0.7831 (7)	0.059 (3)	
H16D	0.5603	0.5520	0.7855	0.088*	
H16E	0.5171	0.5076	0.7454	0.088*	
H16F	0.5166	0.5493	0.8409	0.088*	
C17A	0.4567 (2)	0.7682 (6)	0.9181 (6)	0.0434 (19)	
H17C	0.4763	0.7137	0.9272	0.052*	
H17D	0.4264	0.7461	0.9257	0.052*	
C18A	0.4664 (3)	0.8432 (6)	0.9813 (7)	0.050 (2)	
H18D	0.4626	0.8182	1.0395	0.075*	
H18E	0.4467	0.8966	0.9725	0.075*	
H18F	0.4965	0.8645	0.9739	0.075*	
C19A	0.2479 (3)	0.5477 (6)	0.6486 (7)	0.077 (3)	
H19C	0.2243	0.5496	0.6918	0.093*	0.50

H19D	0.2384	0.5820	0.5964	0.093*	0.50
H19E	0.2248	0.5660	0.6096	0.093*	0.50
H19F	0.2357	0.5481	0.7061	0.093*	0.50
C20A	0.2599 (3)	0.4517 (6)	0.6287 (9)	0.087 (4)	
H20D	0.2342	0.4110	0.6321	0.130*	
H20E	0.2817	0.4299	0.6699	0.130*	
H20F	0.2720	0.4490	0.5705	0.130*	
C21A	0.2638 (3)	0.6849 (8)	0.8772 (5)	0.068 (3)	
H21C	0.2775	0.7476	0.8852	0.081*	0.50
H21D	0.2826	0.6372	0.9053	0.081*	0.50
H21E	0.2830	0.7293	0.9057	0.081*	0.50
H21F	0.2768	0.6224	0.8800	0.081*	0.50
C22A	0.2216 (3)	0.6848 (7)	0.9185 (6)	0.067 (2)	
H22D	0.2247	0.6652	0.9785	0.101*	
H22E	0.2023	0.6406	0.8885	0.101*	
H22F	0.2091	0.7486	0.9162	0.101*	
C23A	0.2462 (6)	0.8383 (9)	0.6577 (9)	0.050 (4)*	0.50
H23C	0.2666	0.8840	0.6842	0.060*	0.50
H23D	0.2216	0.8278	0.6975	0.060*	0.50
C23B	0.2280 (4)	0.7971 (9)	0.6403 (9)	0.049 (4)*	0.50
H23E	0.2070	0.8140	0.6858	0.059*	0.50
H23F	0.2192	0.7361	0.6143	0.059*	0.50
C24A	0.2303 (3)	0.8742 (6)	0.5724 (7)	0.076 (3)	
H24D	0.2153	0.9347	0.5806	0.115*	0.50
H24E	0.2102	0.8281	0.5473	0.115*	0.50
H24F	0.2550	0.8833	0.5337	0.115*	0.50
H24G	0.2023	0.8818	0.5463	0.115*	0.50
H24H	0.2511	0.8567	0.5293	0.115*	0.50
H24I	0.2389	0.9328	0.5985	0.115*	0.50
P3	0.39157 (7)	0.72574 (13)	0.21217 (14)	0.0355 (4)	
F1	0.36602 (16)	0.8078 (4)	0.2599 (4)	0.0576 (16)	
F2	0.36496 (19)	0.7472 (6)	0.1267 (5)	0.079 (2)	
F3	0.41680 (15)	0.6437 (4)	0.1636 (4)	0.0556 (14)	
F4	0.41860 (15)	0.7056 (3)	0.2975 (3)	0.0506 (12)	
F5	0.35538 (14)	0.6523 (3)	0.2418 (6)	0.0685 (18)	
F6	0.42756 (18)	0.7991 (3)	0.1839 (4)	0.0609 (15)	
P4	0.60029 (5)	0.78284 (12)	−0.06173 (13)	0.0265 (4)	
F7	0.58061 (16)	0.8604 (4)	0.0002 (4)	0.0638 (17)	
F8	0.57075 (15)	0.8221 (4)	−0.1379 (4)	0.0642 (16)	
F9	0.61997 (18)	0.7056 (4)	−0.1265 (4)	0.0575 (15)	
F10	0.62998 (14)	0.7446 (4)	0.0139 (4)	0.0555 (15)	
F11	0.56293 (13)	0.7092 (3)	−0.0359 (3)	0.0411 (11)	
F12	0.63835 (12)	0.8546 (3)	−0.0910 (5)	0.0432 (11)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Re1	0.02439 (10)	0.02392 (13)	0.01614 (15)	−0.00483 (8)	−0.00090 (10)	0.00229 (14)

P1	0.0277 (7)	0.0359 (8)	0.0196 (10)	−0.0086 (6)	0.0044 (8)	0.0047 (10)
P2	0.0241 (6)	0.0346 (8)	0.0274 (10)	−0.0009 (6)	−0.0057 (7)	−0.0012 (8)
C1	0.049 (4)	0.035 (4)	0.019 (4)	−0.008 (4)	−0.003 (4)	0.000 (3)
O1	0.074 (4)	0.056 (4)	0.033 (4)	−0.008 (3)	−0.011 (3)	0.023 (3)
C2	0.040 (4)	0.038 (4)	0.021 (5)	−0.007 (3)	0.000 (3)	0.008 (4)
O2	0.080 (4)	0.047 (3)	0.030 (4)	−0.019 (3)	0.012 (3)	−0.021 (3)
N1	0.025 (3)	0.019 (3)	0.022 (4)	−0.0056 (19)	−0.001 (2)	0.000 (2)
N2	0.019 (2)	0.021 (3)	0.024 (3)	−0.0012 (19)	0.004 (2)	0.008 (2)
O3	0.030 (2)	0.053 (3)	0.056 (4)	−0.0003 (19)	0.009 (3)	0.012 (4)
O4	0.048 (3)	0.043 (3)	0.024 (3)	−0.015 (2)	0.016 (2)	−0.001 (3)
O5	0.029 (3)	0.084 (5)	0.044 (4)	−0.028 (3)	0.009 (3)	−0.022 (4)
O6	0.037 (2)	0.032 (2)	0.034 (3)	−0.0072 (19)	−0.013 (2)	−0.004 (2)
O7	0.026 (2)	0.091 (4)	0.022 (3)	−0.016 (2)	0.003 (2)	−0.005 (3)
O8	0.043 (3)	0.040 (3)	0.103 (5)	0.010 (2)	−0.017 (4)	−0.017 (3)
C3	0.035 (3)	0.026 (3)	0.028 (4)	−0.002 (3)	−0.004 (3)	0.001 (3)
C4	0.036 (3)	0.037 (4)	0.043 (5)	−0.002 (3)	−0.005 (3)	0.001 (4)
C5	0.045 (4)	0.042 (4)	0.042 (6)	0.002 (3)	0.001 (3)	−0.018 (4)
C6	0.049 (4)	0.045 (4)	0.022 (4)	−0.007 (3)	−0.004 (3)	0.003 (3)
C7	0.026 (3)	0.019 (3)	0.033 (5)	−0.005 (2)	−0.003 (3)	−0.001 (3)
C8	0.020 (3)	0.033 (3)	0.014 (3)	−0.002 (2)	0.002 (2)	0.005 (3)
C9	0.040 (3)	0.045 (4)	0.025 (4)	0.007 (3)	0.003 (3)	0.010 (3)
C10	0.051 (4)	0.048 (4)	0.034 (4)	0.008 (3)	0.006 (4)	0.026 (4)
C11	0.046 (4)	0.027 (3)	0.054 (6)	0.008 (3)	0.009 (4)	0.019 (4)
C12	0.032 (3)	0.028 (3)	0.029 (4)	0.004 (3)	0.008 (3)	0.005 (3)
C13	0.030 (3)	0.071 (6)	0.078 (7)	0.006 (3)	0.008 (5)	−0.005 (7)
C14	0.041 (4)	0.092 (8)	0.105 (11)	0.020 (5)	−0.001 (6)	−0.024 (8)
C15	0.070 (5)	0.059 (5)	0.033 (5)	−0.017 (4)	0.010 (5)	0.009 (5)
C16	0.065 (5)	0.091 (7)	0.027 (5)	0.005 (5)	−0.005 (4)	0.014 (5)
C17	0.039 (4)	0.085 (7)	0.049 (6)	−0.038 (4)	0.004 (4)	−0.014 (5)
C18	0.062 (6)	0.083 (8)	0.065 (8)	−0.027 (5)	0.014 (5)	−0.021 (6)
C19	0.057 (5)	0.032 (4)	0.096 (8)	0.001 (3)	−0.008 (5)	0.003 (4)
C20	0.099 (8)	0.069 (6)	0.129 (12)	−0.035 (6)	0.001 (8)	−0.025 (7)
C21	0.043 (5)	0.157 (10)	0.045 (6)	−0.026 (5)	0.011 (4)	−0.019 (7)
C22	0.072 (6)	0.127 (9)	0.043 (5)	−0.021 (6)	0.018 (5)	−0.009 (6)
C23	0.080 (6)	0.055 (5)	0.097 (9)	0.017 (5)	−0.030 (6)	0.005 (6)
C24	0.095 (7)	0.065 (6)	0.078 (8)	0.021 (5)	−0.019 (6)	0.013 (5)
Re1A	0.02380 (10)	0.02149 (12)	0.01588 (14)	−0.00457 (8)	−0.00004 (10)	0.00149 (14)
P1A	0.0257 (6)	0.0292 (8)	0.0225 (11)	−0.0063 (5)	−0.0015 (8)	−0.0004 (9)
P2A	0.0210 (6)	0.0335 (8)	0.0232 (10)	−0.0037 (6)	0.0031 (6)	0.0020 (7)
C1A	0.026 (3)	0.024 (3)	0.036 (6)	−0.008 (2)	−0.001 (3)	0.011 (4)
O1A	0.074 (4)	0.042 (3)	0.042 (5)	−0.014 (3)	−0.012 (3)	0.020 (3)
C2A	0.027 (3)	0.032 (4)	0.028 (5)	−0.005 (3)	0.009 (3)	0.004 (3)
O2A	0.061 (3)	0.034 (3)	0.027 (3)	−0.001 (2)	0.014 (3)	−0.011 (2)
N1A	0.019 (3)	0.025 (3)	0.023 (4)	−0.0025 (18)	0.002 (2)	0.001 (3)
N2A	0.021 (2)	0.025 (3)	0.017 (3)	−0.004 (2)	−0.001 (2)	−0.002 (2)
O3A	0.042 (3)	0.060 (4)	0.017 (3)	−0.026 (2)	−0.001 (2)	0.002 (3)
O4A	0.029 (2)	0.047 (3)	0.051 (4)	0.0024 (18)	−0.011 (3)	−0.018 (3)
O5A	0.035 (3)	0.048 (3)	0.018 (3)	−0.017 (2)	−0.004 (2)	0.000 (3)

C3A	0.028 (3)	0.022 (3)	0.030 (4)	0.001 (2)	−0.003 (3)	−0.003 (3)
C4A	0.035 (3)	0.029 (3)	0.041 (5)	0.002 (3)	0.000 (3)	0.015 (4)
C5A	0.039 (4)	0.038 (4)	0.035 (4)	0.000 (3)	0.003 (3)	0.019 (4)
C6A	0.036 (3)	0.033 (3)	0.016 (3)	−0.007 (3)	0.003 (3)	0.005 (3)
C7A	0.021 (2)	0.028 (3)	0.011 (3)	−0.002 (2)	−0.002 (2)	−0.002 (3)
C8A	0.017 (3)	0.028 (3)	0.021 (3)	−0.003 (2)	−0.003 (2)	0.000 (3)
C9A	0.030 (3)	0.038 (3)	0.017 (3)	0.003 (3)	−0.001 (3)	0.003 (3)
C10A	0.030 (3)	0.045 (4)	0.034 (4)	0.007 (3)	−0.002 (3)	−0.014 (3)
C11A	0.036 (3)	0.028 (3)	0.041 (5)	−0.003 (3)	0.001 (3)	−0.009 (3)
C12A	0.037 (3)	0.019 (3)	0.030 (4)	−0.002 (2)	−0.002 (3)	0.000 (3)
C13A	0.033 (4)	0.070 (6)	0.054 (7)	−0.026 (4)	−0.002 (4)	0.009 (5)
C14A	0.093 (8)	0.084 (8)	0.102 (11)	−0.045 (6)	−0.034 (8)	0.039 (8)
C15A	0.028 (3)	0.060 (5)	0.057 (6)	0.008 (3)	−0.012 (4)	−0.012 (5)
C16A	0.047 (4)	0.064 (6)	0.066 (8)	0.011 (4)	0.002 (5)	0.005 (5)
C17A	0.050 (4)	0.061 (5)	0.019 (4)	−0.020 (3)	−0.013 (4)	0.027 (4)
C18A	0.052 (5)	0.065 (5)	0.034 (5)	0.003 (4)	0.003 (4)	−0.015 (4)
C19A	0.062 (5)	0.071 (5)	0.099 (9)	−0.027 (5)	0.013 (6)	−0.035 (6)
C20A	0.076 (6)	0.065 (6)	0.119 (11)	−0.006 (5)	−0.019 (7)	−0.021 (6)
C21A	0.047 (4)	0.127 (8)	0.029 (4)	−0.027 (5)	0.009 (4)	−0.007 (5)
C22A	0.062 (5)	0.102 (7)	0.038 (5)	−0.021 (5)	0.022 (5)	−0.006 (5)
C24A	0.082 (6)	0.068 (5)	0.079 (8)	0.025 (5)	−0.019 (6)	0.010 (6)
P3	0.0550 (10)	0.0280 (9)	0.0233 (11)	0.0031 (8)	0.0000 (8)	−0.0006 (8)
F1	0.083 (4)	0.040 (2)	0.049 (4)	0.016 (2)	−0.005 (3)	−0.012 (2)
F2	0.094 (5)	0.102 (5)	0.043 (4)	0.034 (3)	−0.025 (3)	−0.012 (4)
F3	0.058 (3)	0.049 (3)	0.059 (4)	0.006 (2)	0.008 (3)	−0.019 (3)
F4	0.068 (3)	0.056 (3)	0.029 (2)	0.006 (2)	−0.004 (2)	0.011 (2)
F5	0.052 (2)	0.049 (3)	0.104 (6)	−0.013 (2)	0.015 (4)	0.001 (4)
F6	0.092 (4)	0.041 (3)	0.049 (4)	−0.019 (2)	0.011 (3)	0.013 (2)
P4	0.0294 (7)	0.0274 (8)	0.0227 (10)	−0.0061 (6)	−0.0014 (6)	−0.0011 (7)
F7	0.056 (3)	0.053 (3)	0.082 (5)	−0.006 (2)	0.012 (3)	−0.041 (3)
F8	0.056 (3)	0.076 (3)	0.061 (4)	−0.010 (2)	−0.027 (3)	0.030 (3)
F9	0.065 (3)	0.058 (3)	0.049 (3)	−0.007 (3)	0.022 (3)	−0.025 (3)
F10	0.046 (3)	0.075 (3)	0.046 (4)	−0.014 (2)	−0.017 (2)	0.028 (3)
F11	0.036 (2)	0.047 (2)	0.040 (3)	−0.0151 (17)	0.0016 (19)	−0.004 (2)
F12	0.0415 (19)	0.042 (2)	0.046 (3)	−0.0165 (17)	0.002 (2)	−0.002 (3)

Geometric parameters (Å, º)

Re1—C1	1.896 (9)	P4—F7	1.581 (5)
Re1—C2	1.931 (10)	P4—F8	1.595 (5)
Re1—N1	2.162 (8)	P4—F9	1.605 (5)
Re1—N2	2.176 (6)	P4—F10	1.587 (6)
Re1—P1	2.3730 (15)	P4—F11	1.603 (4)
Re1—P2	2.3724 (16)	P4—F12	1.616 (4)
P1—O3	1.575 (5)	C3—H3A	0.95
P1—O4	1.588 (6)	C4—H4A	0.95
P1—O5	1.585 (7)	C5—H5A	0.95
P2—O6	1.594 (5)	C6—H6A	0.95

P2—O7	1.604 (5)	C9—H9A	0.95
P2—O8	1.591 (5)	C10—H10A	0.95
C1—O1	1.178 (10)	C11—H11A	0.95
C2—O2	1.147 (11)	C12—H12A	0.95
N1—C7	1.346 (13)	C13—H13A	0.99
N1—C3	1.357 (10)	C13—H13B	0.99
N2—C8	1.344 (9)	C14—H14A	0.98
N2—C12	1.346 (9)	C14—H14B	0.98
O3—C13	1.466 (7)	C14—H14C	0.98
O4—C15	1.470 (13)	C15—H15A	0.99
O5—C17	1.454 (8)	C15—H15B	0.99
O6—C19	1.419 (8)	C16—H16A	0.98
O7—C21	1.458 (9)	C16—H16B	0.98
O8—C23	1.405 (10)	C16—H16C	0.98
C3—C4	1.368 (12)	C17—H17A	0.99
C4—C5	1.381 (14)	C17—H17B	0.99
C5—C6	1.370 (12)	C18—H18A	0.98
C6—C7	1.366 (13)	C18—H18B	0.98
C7—C8	1.504 (10)	C18—H18C	0.98
C8—C9	1.400 (10)	C19—H19A	0.99
C9—C10	1.390 (11)	C19—H19B	0.99
C10—C11	1.377 (13)	C20—H20A	0.98
C11—C12	1.392 (11)	C20—H20B	0.98
C13—C14	1.516 (13)	C20—H20C	0.98
C15—C16	1.474 (13)	C21—H21A	0.99
C17—C18	1.493 (13)	C21—H21B	0.99
C19—C20	1.459 (11)	C22—H22A	0.98
C21—C22	1.417 (13)	C22—H22B	0.98
C23—C24	1.431 (11)	C22—H22C	0.98
Re1A—C1A	1.886 (9)	C23—H23A	0.99
Re1A—C2A	1.915 (9)	C23—H23B	0.99
Re1A—N1A	2.174 (8)	C24—H24A	0.98
Re1A—N2A	2.184 (6)	C24—H24B	0.98
Re1A—P1A	2.3817 (15)	C24—H24C	0.98
Re1A—P2A	2.3664 (16)	C3A—H3AA	0.95
P1A—O3A	1.587 (6)	C4A—H4AA	0.95
P1A—O4A	1.589 (5)	C5A—H5AA	0.95
P1A—O5A	1.602 (6)	C6A—H6AA	0.95
P2A—O6B	1.557 (9)	C9A—H9AA	0.95
P2A—O7A	1.545 (10)	C10A—H10B	0.95
P2A—O8A	1.586 (10)	C11A—H11B	0.95
P2A—O8B	1.598 (11)	C12A—H12B	0.95
P2A—O7B	1.604 (8)	C13A—H13C	0.99
P2A—O6A	1.623 (7)	C13A—H13D	0.99
C1A—O1A	1.172 (11)	C14A—H14D	0.98
C2A—O2A	1.151 (10)	C14A—H14E	0.98
N1A—C7A	1.346 (11)	C14A—H14F	0.98
N1A—C3A	1.354 (10)	C15A—H15C	0.99

N2A—C12A	1.351 (8)	C15A—H15D	0.99
N2A—C8A	1.356 (9)	C16A—H16D	0.98
O3A—C13A	1.462 (8)	C16A—H16E	0.98
O4A—C15A	1.468 (7)	C16A—H16F	0.98
O5A—C17A	1.450 (10)	C17A—H17C	0.99
O6A—C19A	1.457 (8)	C17A—H17D	0.99
O6B—C19A	1.467 (8)	C18A—H18D	0.98
O7A—C21A	1.448 (8)	C18A—H18E	0.98
O7B—C21A	1.447 (8)	C18A—H18F	0.98
O8A—C23A	1.458 (9)	C19A—H19C	0.99
O8B—C23B	1.467 (8)	C19A—H19D	0.99
C3A—C4A	1.376 (12)	C19A—H19E	0.97
C4A—C5A	1.360 (14)	C19A—H19F	0.97
C5A—C6A	1.382 (11)	C20A—H20D	0.98
C6A—C7A	1.413 (10)	C20A—H20E	0.98
C7A—C8A	1.461 (9)	C20A—H20F	0.98
C8A—C9A	1.378 (9)	C21A—H21C	0.99
C9A—C10A	1.368 (9)	C21A—H21D	0.99
C10A—C11A	1.369 (12)	C21A—H21E	0.97
C11A—C12A	1.364 (11)	C21A—H21F	0.97
C13A—C14A	1.479 (13)	C22A—H22D	0.98
C15A—C16A	1.458 (11)	C22A—H22E	0.98
C17A—C18A	1.478 (13)	C22A—H22F	0.98
C19A—C20A	1.440 (11)	C23A—H23C	0.99
C21A—C22A	1.453 (10)	C23A—H23D	0.99
C23A—C24A	1.506 (15)	C23B—H23E	0.99
C23B—C24A	1.521 (14)	C23B—H23F	0.99
P3—F1	1.586 (5)	C24A—H24D	0.98
P3—F2	1.592 (7)	C24A—H24E	0.98
P3—F3	1.588 (5)	C24A—H24F	0.98
P3—F4	1.594 (5)	C24A—H24G	0.96
P3—F5	1.592 (5)	C24A—H24H	0.96
P3—F6	1.581 (5)	C24A—H24I	0.96

C1—Re1—C2	88.9 (4)	C17—C18—H18B	109.5
C1—Re1—N1	97.7 (3)	H18A—C18—H18B	109.5
C2—Re1—N1	173.2 (3)	C17—C18—H18C	109.5
C1—Re1—N2	171.7 (3)	H18A—C18—H18C	109.5
C2—Re1—N2	99.4 (3)	H18B—C18—H18C	109.5
N1—Re1—N2	74.0 (3)	O6—C19—H19A	109.1
C1—Re1—P2	88.3 (3)	C20—C19—H19A	109.1
C2—Re1—P2	95.2 (2)	O6—C19—H19B	109.1
N1—Re1—P2	86.71 (14)	C20—C19—H19B	109.1
N2—Re1—P2	90.11 (15)	H19A—C19—H19B	107.8
C1—Re1—P1	90.9 (3)	C19—C20—H20A	109.5
C2—Re1—P1	89.9 (2)	C19—C20—H20B	109.5
N1—Re1—P1	88.37 (14)	H20A—C20—H20B	109.5
N2—Re1—P1	89.89 (15)	C19—C20—H20C	109.5

P2—Re1—P1	174.88 (7)	H20A—C20—H20C	109.5
O3—P1—O5	107.0 (4)	H20B—C20—H20C	109.5
O3—P1—O4	105.7 (3)	C22—C21—H21A	109.4
O5—P1—O4	99.0 (3)	O7—C21—H21A	109.5
O3—P1—Re1	111.99 (18)	C22—C21—H21B	109.5
O5—P1—Re1	112.0 (2)	O7—C21—H21B	109.5
O4—P1—Re1	119.9 (2)	H21A—C21—H21B	108.0
O8—P2—O6	100.3 (3)	C21—C22—H22A	109.5
O8—P2—O7	104.8 (4)	C21—C22—H22B	109.5
O6—P2—O7	105.9 (3)	H22A—C22—H22B	109.5
O8—P2—Re1	111.6 (2)	C21—C22—H22C	109.5
O6—P2—Re1	121.9 (2)	H22A—C22—H22C	109.5
O7—P2—Re1	110.72 (18)	H22B—C22—H22C	109.5
O1—C1—Re1	178.8 (9)	O8—C23—H23A	109.9
O2—C2—Re1	178.2 (8)	C24—C23—H23A	110.0
C7—N1—C3	116.8 (8)	O8—C23—H23B	110.0
C7—N1—Re1	119.3 (5)	C24—C23—H23B	110.0
C3—N1—Re1	123.6 (6)	H23A—C23—H23B	108.4
C8—N2—C12	118.3 (7)	C23—C24—H24A	109.5
C8—N2—Re1	117.9 (4)	C23—C24—H24B	109.4
C12—N2—Re1	123.8 (6)	H24A—C24—H24B	109.5
C13—O3—P1	122.7 (5)	C23—C24—H24C	109.5
C15—O4—P1	119.2 (5)	H24A—C24—H24C	109.5
C17—O5—P1	128.3 (6)	H24B—C24—H24C	109.5
C19—O6—P2	120.1 (5)	N1A—C3A—H3AA	118.7
C21—O7—P2	123.0 (5)	C4A—C3A—H3AA	118.7
C23—O8—P2	128.0 (5)	C5A—C4A—H4AA	120.8
N1—C3—C4	122.5 (9)	C3A—C4A—H4AA	120.9
C3—C4—C5	119.6 (8)	C4A—C5A—H5AA	119.6
C6—C5—C4	118.1 (9)	C6A—C5A—H5AA	119.6
C7—C6—C5	119.9 (9)	C5A—C6A—H6AA	120.8
N1—C7—C6	123.0 (7)	C7A—C6A—H6AA	120.8
N1—C7—C8	113.4 (7)	C10A—C9A—H9AA	119.6
C6—C7—C8	123.6 (8)	C8A—C9A—H9AA	119.6
N2—C8—C9	122.6 (6)	C9A—C10A—H10B	120.5
N2—C8—C7	115.2 (6)	C11A—C10A—H10B	120.4
C9—C8—C7	122.2 (7)	C12A—C11A—H11B	120.6
C10—C9—C8	117.7 (7)	C10A—C11A—H11B	120.6
C11—C10—C9	120.5 (7)	N2A—C12A—H12B	119.0
C10—C11—C12	118.1 (7)	C11A—C12A—H12B	119.0
N2—C12—C11	122.9 (8)	O3A—C13A—H13C	110.0
O3—C13—C14	108.0 (7)	C14A—C13A—H13C	110.0
O4—C15—C16	108.9 (7)	O3A—C13A—H13D	110.0
O5—C17—C18	109.1 (7)	C14A—C13A—H13D	110.0
O6—C19—C20	111.3 (7)	H13C—C13A—H13D	108.4
C22—C21—O7	110.9 (8)	C13A—C14A—H14D	109.5
O8—C23—C24	109.8 (8)	C13A—C14A—H14E	109.5
C1A—Re1A—C2A	88.8 (4)	H14D—C14A—H14E	109.5

C1A—Re1A—N1A	172.4 (4)	C13A—C14A—H14F	109.5
C2A—Re1A—N1A	98.8 (3)	H14D—C14A—H14F	109.5
C1A—Re1A—N2A	98.1 (3)	H14E—C14A—H14F	109.5
C2A—Re1A—N2A	173.1 (3)	C16A—C15A—H15C	110.1
N1A—Re1A—N2A	74.3 (3)	O4A—C15A—H15C	110.1
C1A—Re1A—P2A	92.3 (2)	C16A—C15A—H15D	110.1
C2A—Re1A—P2A	91.9 (2)	O4A—C15A—H15D	110.1
N1A—Re1A—P2A	88.41 (13)	H15C—C15A—H15D	108.4
N2A—Re1A—P2A	87.28 (15)	C15A—C16A—H16D	109.5
C1A—Re1A—P1A	90.8 (2)	C15A—C16A—H16E	109.5
C2A—Re1A—P1A	92.2 (2)	H16D—C16A—H16E	109.5
N1A—Re1A—P1A	88.07 (13)	C15A—C16A—H16F	109.5
N2A—Re1A—P1A	88.36 (15)	H16D—C16A—H16F	109.5
P2A—Re1A—P1A	175.01 (8)	H16E—C16A—H16F	109.5
O3A—P1A—O4A	107.6 (4)	O5A—C17A—H17C	109.8
O3A—P1A—O5A	101.4 (3)	C18A—C17A—H17C	109.9
O4A—P1A—O5A	103.9 (3)	O5A—C17A—H17D	109.9
O3A—P1A—Re1A	112.9 (2)	C18A—C17A—H17D	109.8
O4A—P1A—Re1A	110.51 (17)	H17C—C17A—H17D	108.3
O5A—P1A—Re1A	119.4 (2)	C17A—C18A—H18D	109.5
O7A—P2A—O8A	112.4 (5)	C17A—C18A—H18E	109.5
O6B—P2A—O8B	103.0 (6)	H18D—C18A—H18E	109.5
O6B—P2A—O7B	116.9 (4)	C17A—C18A—H18F	109.4
O8B—P2A—O7B	83.4 (5)	H18D—C18A—H18F	109.5
O7A—P2A—O6A	83.3 (5)	H18E—C18A—H18F	109.5
O8A—P2A—O6A	100.4 (5)	C20A—C19A—H19C	111.0
O7A—P2A—Re1A	123.0 (3)	O6A—C19A—H19C	111.0
O6B—P2A—Re1A	116.1 (3)	O6B—C19A—H19C	121.3
O8A—P2A—Re1A	119.7 (3)	C20A—C19A—H19D	111.0
O8B—P2A—Re1A	107.4 (4)	O6A—C19A—H19D	111.0
O7B—P2A—Re1A	121.4 (3)	H19C—C19A—H19D	109.0
O6A—P2A—Re1A	107.4 (2)	C20A—C19A—H19E	107.3
O1A—C1A—Re1A	179.5 (8)	O6B—C19A—H19E	107.8
O2A—C2A—Re1A	179.1 (8)	C20A—C19A—H19F	107.4
C7A—N1A—C3A	119.0 (8)	O6B—C19A—H19F	107.5
C7A—N1A—Re1A	117.3 (5)	H19E—C19A—H19F	107.1
C3A—N1A—Re1A	123.8 (6)	C19A—C20A—H20D	109.5
C12A—N2A—C8A	118.8 (6)	C19A—C20A—H20E	109.5
C12A—N2A—Re1A	124.0 (5)	H20D—C20A—H20E	109.5
C8A—N2A—Re1A	117.2 (4)	C19A—C20A—H20F	109.5
C13A—O3A—P1A	129.1 (6)	H20D—C20A—H20F	109.5
C15A—O4A—P1A	122.8 (4)	H20E—C20A—H20F	109.5
C17A—O5A—P1A	122.5 (5)	O7A—C21A—H21C	109.0
C19A—O6A—P2A	123.6 (6)	C22A—C21A—H21C	109.0
C19A—O6B—P2A	127.8 (8)	O7A—C21A—H21D	108.9
C21A—O7A—P2A	128.1 (7)	C22A—C21A—H21D	108.9
C21A—O7B—P2A	123.8 (6)	H21C—C21A—H21D	107.8
C23A—O8A—P2A	118.4 (8)	O7B—C21A—H21E	110.1

N1A—C3A—C4A	122.9 (8)	C22A—C21A—H21E	109.9
C5A—C4A—C3A	118.3 (7)	O7B—C21A—H21F	110.6
C4A—C5A—C6A	120.8 (8)	C22A—C21A—H21F	110.4
C5A—C6A—C7A	118.5 (8)	H21E—C21A—H21F	108.5
N1A—C7A—C6A	120.5 (6)	C21A—C22A—H22D	109.5
N1A—C7A—C8A	116.2 (7)	C21A—C22A—H22E	109.5
C6A—C7A—C8A	123.2 (7)	H22D—C22A—H22E	109.5
N2A—C8A—C9A	120.2 (6)	C21A—C22A—H22F	109.4
N2A—C8A—C7A	115.1 (6)	H22D—C22A—H22F	109.5
C9A—C8A—C7A	124.7 (6)	H22E—C22A—H22F	109.5
C10A—C9A—C8A	120.6 (7)	O8A—C23A—H23C	110.6
C9A—C10A—C11A	118.9 (7)	C24A—C23A—H23C	110.6
C12A—C11A—C10A	119.4 (7)	O8A—C23A—H23D	110.6
N2A—C12A—C11A	122.2 (7)	C24A—C23A—H23D	110.6
O3A—C13A—C14A	109.0 (7)	H23C—C23A—H23D	108.7
C16A—C15A—O4A	108.3 (7)	O8B—C23B—H23E	110.7
O5A—C17A—C18A	109.6 (7)	C24A—C23B—H23E	110.7
C20A—C19A—O6A	102.9 (8)	O8B—C23B—H23F	110.7
O7B—C21A—C22A	107.4 (8)	C24A—C23B—H23F	110.7
O7A—C21A—C22A	112.6 (8)	H23E—C23B—H23F	108.8
O8A—C23A—C24A	105.2 (9)	C23A—C24A—H24D	109.5
N1—C3—H3A	118.5	C23A—C24A—H24E	109.5
C4—C3—H3A	118.5	H24D—C24A—H24E	109.5
C3—C4—H4A	120.3	C23A—C24A—H24F	109.4
C5—C4—H4A	120.3	H24D—C24A—H24F	109.5
C6—C5—H5A	121.0	H24E—C24A—H24F	109.5
C4—C5—H5A	121.0	C23B—C24A—H24G	109.6
C7—C6—H6A	119.6	C23B—C24A—H24H	109.1
C5—C6—H6A	119.6	H24D—C24A—H24H	129.4
C10—C9—H9A	120.9	H24G—C24A—H24H	109.5
C8—C9—H9A	120.9	C23B—C24A—H24I	109.7
C9—C10—H10A	119.8	H24G—C24A—H24I	109.5
C10—C11—H11A	120.9	H24H—C24A—H24I	109.5
C12—C11—H11A	120.9	F6—P3—F1	90.0 (3)
N2—C12—H12A	118.6	F6—P3—F3	90.1 (3)
C11—C12—H12A	118.6	F1—P3—F3	179.4 (3)
O3—C13—H13A	110.0	F6—P3—F2	90.2 (4)
C14—C13—H13A	110.0	F1—P3—F2	89.8 (4)
O3—C13—H13B	110.0	F3—P3—F2	89.6 (3)
C14—C13—H13B	110.0	F6—P3—F5	179.3 (4)
H13A—C13—H13B	108.4	F1—P3—F5	89.6 (3)
C13—C14—H14A	109.5	F3—P3—F5	90.3 (3)
C13—C14—H14B	109.5	F2—P3—F5	90.3 (4)
H14A—C14—H14B	109.5	F6—P3—F4	89.0 (3)
C13—C14—H14C	109.5	F1—P3—F4	90.0 (3)
H14A—C14—H14C	109.5	F3—P3—F4	90.6 (3)
H14B—C14—H14C	109.5	F2—P3—F4	179.2 (4)
O4—C15—H15A	110.1	F5—P3—F4	90.5 (4)

C16—C15—H15A	110.2	F7—P4—F10	90.3 (4)
O4—C15—H15B	110.1	F7—P4—F8	89.6 (3)
C16—C15—H15B	110.1	F10—P4—F8	179.5 (3)
H15A—C15—H15B	108.4	F7—P4—F11	91.2 (3)
C15—C16—H16A	109.5	F10—P4—F11	90.4 (3)
C15—C16—H16B	109.5	F8—P4—F11	90.1 (3)
H16A—C16—H16B	109.5	F7—P4—F9	178.6 (4)
C15—C16—H16C	109.4	F10—P4—F9	91.0 (4)
H16A—C16—H16C	109.5	F8—P4—F9	89.1 (3)
H16B—C16—H16C	109.5	F11—P4—F9	89.3 (3)
O5—C17—H17A	109.9	F7—P4—F12	90.9 (3)
C18—C17—H17A	109.9	F10—P4—F12	90.3 (3)
O5—C17—H17B	109.8	F8—P4—F12	89.2 (3)
C18—C17—H17B	109.9	F11—P4—F12	177.8 (3)
H17A—C17—H17B	108.3	F9—P4—F12	88.6 (3)
C17—C18—H18A	109.5		