Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloridobis[1,2-bis(diphenylphosphino)-ethane](ethylimido)molybdenum(IV) tetraphenylborate acetonitrile disolvate

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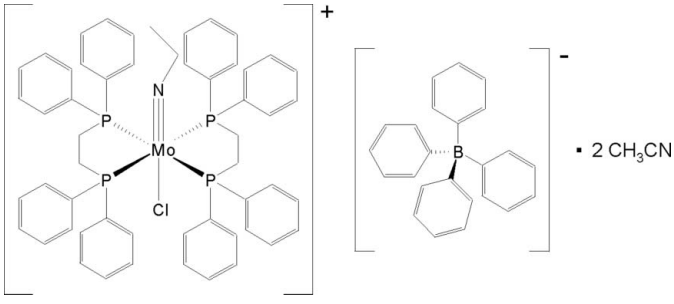
Received 30 March 2007; accepted 18 April 2007

Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 17.8.

In the crystal structure of the title compound, $[Mo(C_2H_5N)Cl(C_{26}H_{24}P_2)_2](C_{24}H_{20}B)\cdot 2C_2H_3N$, $C_{82}H_{79}N_3BClP_4Mo$, the Mo atom is surrounded by four P atoms of two crystallographically independent 1,2-bis(diphenylphosphino)ethane ligands, one Cl atom and one N atom of an ethylimido ligand in a distorted octahedral geomtery.

Related literature

For related literature, see: Alias *et al.* (1997); Bruno *et al.* (2002); Chatt & Dilworth (1977); George & Noble (1978); Mersmann *et al.* (2006).



Experimental

Crystal data

$[Mo(C_2H_5N)Cl(C_{26}H_{24}P_2)_2]\cdot(C_{24}H_{20}B)\cdot 2C_2H_3N$
M_r = 1372.56
Monoclinic, $P2_1/n$
a = 15.3299 (12) Å
b = 21.5840 (11) Å
c = 21.3439 (16) Å
β = 96.387 (9)°
V = 7018.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 170 (2) K
0.2 × 0.15 × 0.1 mm

Data collection

Stoe IPDS-1 diffractometer
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
T_{min} = 0.929, T_{max} = 0.941
48449 measured reflections
15159 independent reflections
12034 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.01
15159 reflections
850 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mo1—N1	1.732 (2)	Mo1—P3	2.5342 (6)
Mo1—Cl1	2.4413 (5)	Mo1—P2	2.5447 (6)
Mo1—P4	2.5308 (6)	Mo1—P1	2.5503 (6)
N1—Mo1—Cl1	178.20 (7)	P4—Mo1—P2	100.388 (19)
N1—Mo1—P4	94.16 (8)	P3—Mo1—P2	175.395 (18)
Cl1—Mo1—P4	84.136 (19)	N1—Mo1—P1	96.28 (8)
N1—Mo1—P3	91.98 (10)	Cl1—Mo1—P1	85.432 (19)
Cl1—Mo1—P3	88.31 (2)	P4—Mo1—P1	169.537 (17)
P4—Mo1—P3	79.981 (19)	P3—Mo1—P1	98.915 (18)
N1—Mo1—P2	92.57 (10)	P2—Mo1—P1	79.879 (18)
Cl1—Mo1—P2	87.16 (2)		

Data collection: *IPDS* Program Package (Stoe & Cie, 1998); cell refinement: *IPDS* Program Package; data reduction: *IPDS* Program Package; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXTL*.

This work is supported by the state of Schleswig-Holstein and the DFG (project No. TU58/12–2).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2011).

References

Alias, Y., Ibrahim, S. K., Queiros, M. A., Fonseca, A., Talarmin, J., Volant, F. & Pickett, C. J. (1997). *J. Chem. Soc. Dalton Trans.* pp. 4807–4815.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P. , Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Chatt, J. & Dilworth, J. R. (1977). *J. Indian Chem. Soc.* **54**, 13–18.
George, T. A. & Noble, M. E. (1978). *Inorg. Chem.* **17**, 1678–1679.
Mersmann, K., Hauser, A., Lehnert, N. & Tuczek, F. (2006). *Inorg. Chem.* **45**, 5044–5056.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (1998). *X-SHAPE* (Version 1.03) and *IPDS* Program Package (Version 2.89). Stoe & Cie, Darmstadt, Germany.

  doi:10.1107/S1600536807019320

supplementary materials

Acta Cryst. (2007). E**63**, m1476 [**doi:10.1107/S1600536807019320**]

Chloridobis[1,2-bis(diphenylphosphino)ethane](ethylimido)molybdenum(IV) tetraphenylborate acetonitrile disolvate

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Comment

The structure determination of this compound was undertaken as part of a project on the asymmetric reduction of dinitrogen via the Chatt cycle (Mersmann *et al.*, 2006). Imido complexes are problematic intermediates in this cycle because of their very negative reduction potentials (Alias *et al.*, 1997). For practical reasons it is instructive to study alkylimido complexes. During these investigations we obtained big crystals of the title compound in order to perform polarised absorption spectroscopy. An absoption band at 510 nm possesses unexpected differences in intensity under polarisation along the a- and b-axis of this molecule. Furthermore a vibrational fine structure of about 530 cm^{-1} was observed on the absorption band, which is attributed to a Mo—N—C bending vibration.

The crystal structure of the title compound consists of discrete $[Mo(Cl)(NC_2H_5)(P_2C_{26}H_{24})_2]^+$ cations and tetraphenylborate anions. The molybdenum atoms are coordinated by four phosphorous atoms of two crystallographically independent 1,2-bis(diphenylphosphino)ethane ligands, one nitrogen atom of an ethylimido ligand and one chlorine atom within distorted octahedra (Fig. 1). All bond lengths and angles are in good agreement with those retrieved from the CSD database (conquest version 1.8, 2007; Bruno *et al.*, 2002) The Mo1—N1 bond lengths of 1.732 (2) Å strongly indicate that this is a Mo—N triple bond. There are two additional acetonitrile ligands per formula unit within the structure, that are located in holes of the crystal. These solvent molecules exhibit slightly enlarged anisotropic displacement parameters indicating some static or dynamic disorder.

Experimental

Under an inert gas atmosphere, 120 mg (0,127 mmol) of the nitrido complex $[Mo(N)(Cl)(dppe)_2]$, prepared following literature procedures (George *et al.*, 1978; Chatt *et al.*, 1977), were dissolved in 15 ml thf. Some drops of ethyliodide were added and the solution was stirred for 3 h. Afterwards the reaction mixture was evaporated to dryness and the residue was redissolved in 30 ml of acetonitrile. After addition of 50 mg (0,15 mmol) sodium tetraphenylborate the product crystallises in rectangular plates.

Refinement

The hydrogen atoms were positioned with idealized geometry (methyl H atoms allowed to rotate but not to tip) and were refined isotropic with $U_{eq} = 1.2\ U_{eq}(C)$ for aromatic and methylene H atoms and $U_{eq} = 1.5\ U_{eq}(C)$ for methyl H atoms using a riding model with C—H = 0.95 Å for aromatic, C—H = 0.99 Å for methylene and C—H = 0.98 Å for methyl H atoms. Both carbon atoms of the ethylimido ligand are disordered in two positions and were refined using a split model.

Figures

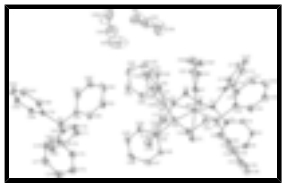


Fig. 1. : Crystal structure of compound I with labelling and displacement ellipsoids drawn at the 50% probability level. The hydrogen atoms are omitted for clarity.

Chloridobis[1,2-bis(diphenylphosphino)ethane](ethylimido)molybdenum(IV) tetraphenylborate acetonitrile disolvate

Crystal data

$[Mo(C_2H_5N)Cl(C_{26}H_{24}P_2)_2](C_{24}H_{20}B)\cdot 2C_2H_3N$	F_{000} = 2864
M_r = 1372.56	D_x = 1.299 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 15.3299 (12) Å	Cell parameters from 8000 reflections
b = 21.5840 (11) Å	θ = 11.3–24.3º
c = 21.3439 (16) Å	μ = 0.36 mm^{-1}
β = 96.387 (9)º	T = 170 (2) K
V = 7018.4 (8) Å^3	Block, red
Z = 4	0.2 × 0.15 × 0.1 mm

Data collection

Stoe IPDS-1 diffractometer	15159 independent reflections
Radiation source: fine-focus sealed tube	12034 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 170(2) K	θ_{max} = 27.0º
φ scans	θ_{min} = 2.1º
Absorption correction: numerical (X-SHAPE; Stoe & Cie, 1998)	h = −19→18
T_{min} = 0.929, T_{max} = 0.941	k = −23→27
48449 measured reflections	l = −27→27

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 1.19P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max}$ = 0.005
$wR(F^2)$ = 0.101	$\Delta\rho_{max}$ = 0.62 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.68 e Å^{-3}

15159 reflections

850 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0024 (2)

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mo1	0.498959 (11)	0.407142 (8)	0.224115 (7)	0.01628 (6)	
Cl1	0.47025 (4)	0.40693 (3)	0.10929 (2)	0.02676 (12)	
N1	0.52061 (19)	0.40494 (9)	0.30548 (9)	0.0443 (6)	
C91	0.5682 (3)	0.40422 (19)	0.37061 (19)	0.0293 (8)	0.60
H91A	0.5967	0.4447	0.3809	0.035*	0.60
H91B	0.6135	0.3714	0.3747	0.035*	0.60
C92	0.4978 (4)	0.3913 (3)	0.4132 (2)	0.0538 (13)	0.60
H92A	0.5243	0.3900	0.4572	0.081*	0.60
H92B	0.4700	0.3513	0.4019	0.081*	0.60
H92C	0.4535	0.4242	0.4083	0.081*	0.60
C91'	0.4942 (4)	0.3962 (3)	0.3708 (3)	0.0281 (12)	0.40
H91C	0.4728	0.3535	0.3768	0.034*	0.40
H91D	0.4483	0.4261	0.3796	0.034*	0.40
C92'	0.5809 (5)	0.4085 (4)	0.4127 (3)	0.050 (2)	0.40
H92D	0.5714	0.4040	0.4572	0.075*	0.40
H92E	0.6011	0.4506	0.4052	0.075*	0.40
H92F	0.6253	0.3786	0.4025	0.075*	0.40
P1	0.39118 (3)	0.49746 (2)	0.21967 (2)	0.01916 (11)	
P2	0.35534 (3)	0.34829 (3)	0.22543 (2)	0.02065 (12)	
C1	0.28036 (15)	0.46342 (11)	0.21360 (12)	0.0289 (5)	
H1A	0.2385	0.4939	0.2277	0.035*	
H1B	0.2610	0.4526	0.1691	0.035*	
C2	0.28130 (15)	0.40533 (10)	0.25447 (11)	0.0270 (5)	
H2A	0.2213	0.3879	0.2527	0.032*	
H2B	0.3014	0.4159	0.2989	0.032*	

C3	0.38091 (14)	0.55426 (10)	0.15561 (9)	0.0219 (4)
C4	0.41413 (16)	0.61398 (11)	0.16549 (10)	0.0267 (5)
H4	0.4416	0.6256	0.2059	0.032*
C5	0.40713 (19)	0.65652 (12)	0.11648 (11)	0.0377 (6)
H5	0.4293	0.6974	0.1235	0.045*
C6	0.3682 (2)	0.63965 (13)	0.05778 (11)	0.0407 (6)
H6	0.3624	0.6691	0.0245	0.049*
C7	0.33749 (19)	0.58018 (13)	0.04703 (11)	0.0388 (6)
H7	0.3122	0.5685	0.0061	0.047*
C8	0.34333 (16)	0.53753 (11)	0.09556 (10)	0.0305 (5)
H8	0.3217	0.4967	0.0880	0.037*
C9	0.39205 (14)	0.54671 (10)	0.28972 (9)	0.0227 (4)
C10	0.46220 (15)	0.54570 (11)	0.33647 (10)	0.0267 (5)
H10	0.5111	0.5196	0.3321	0.032*
C11	0.46172 (18)	0.58257 (11)	0.38987 (11)	0.0336 (5)
H11	0.5096	0.5809	0.4222	0.040*
C12	0.39177 (19)	0.62165 (11)	0.39600 (11)	0.0350 (6)
H12	0.3911	0.6463	0.4328	0.042*
C13	0.32302 (18)	0.62475 (12)	0.34869 (12)	0.0360 (6)
H13	0.2758	0.6525	0.3523	0.043*
C14	0.32282 (16)	0.58740 (11)	0.29599 (11)	0.0296 (5)
H14	0.2750	0.5895	0.2637	0.036*
C15	0.29625 (15)	0.31922 (11)	0.15219 (10)	0.0265 (5)
C16	0.20557 (16)	0.32541 (13)	0.13927 (12)	0.0369 (6)
H16	0.1734	0.3479	0.1673	0.044*
C17	0.1625 (2)	0.29883 (15)	0.08555 (14)	0.0498 (8)
H17	0.1008	0.3037	0.0766	0.060*
C18	0.2080 (2)	0.26536 (15)	0.04495 (13)	0.0497 (8)
H18	0.1775	0.2469	0.0085	0.060*
C19	0.2979 (2)	0.25859 (14)	0.05704 (12)	0.0448 (7)
H19	0.3294	0.2353	0.0293	0.054*
C20	0.34173 (17)	0.28634 (12)	0.11043 (11)	0.0340 (5)
H20	0.4037	0.2827	0.1184	0.041*
C21	0.34541 (14)	0.28166 (10)	0.27740 (10)	0.0248 (4)
C22	0.36671 (16)	0.22305 (11)	0.25682 (12)	0.0330 (5)
H22	0.3863	0.2183	0.2164	0.040*
C23	0.35970 (17)	0.17142 (12)	0.29471 (15)	0.0429 (7)
H23	0.3758	0.1317	0.2807	0.051*
C24	0.3292 (2)	0.17804 (15)	0.35267 (15)	0.0514 (8)
H24	0.3233	0.1427	0.3784	0.062*
C25	0.3075 (2)	0.23580 (15)	0.37329 (13)	0.0479 (7)
H25	0.2861	0.2401	0.4132	0.057*
C26	0.31648 (16)	0.28802 (12)	0.33636 (11)	0.0323 (5)
H26	0.3028	0.3279	0.3515	0.039*
P3	0.63851 (3)	0.46729 (2)	0.21345 (2)	0.01898 (11)
P4	0.60205 (3)	0.31874 (2)	0.20681 (2)	0.02002 (11)
C31	0.72697 (14)	0.41003 (10)	0.22556 (11)	0.0269 (5)
H31A	0.7827	0.4284	0.2150	0.032*
H31B	0.7351	0.3968	0.2702	0.032*

C32	0.70217 (15)	0.35445 (11)	0.18297 (11)	0.0282 (5)
H32A	0.7506	0.3239	0.1867	0.034*
H32B	0.6918	0.3681	0.1385	0.034*
C33	0.65835 (14)	0.50534 (10)	0.13959 (9)	0.0232 (4)
C34	0.74278 (15)	0.51344 (12)	0.12320 (11)	0.0310 (5)
H34	0.7913	0.4959	0.1487	0.037*
C35	0.75663 (17)	0.54724 (13)	0.06962 (12)	0.0363 (6)
H35	0.8146	0.5523	0.0586	0.044*
C36	0.68722 (18)	0.57335 (12)	0.03251 (11)	0.0346 (6)
H36	0.6972	0.5966	−0.0038	0.041*
C37	0.60335 (18)	0.56560 (12)	0.04823 (11)	0.0346 (5)
H37	0.5552	0.5836	0.0227	0.041*
C38	0.58884 (16)	0.53159 (12)	0.10132 (10)	0.0295 (5)
H38	0.5306	0.5262	0.1116	0.035*
C39	0.67054 (13)	0.52817 (10)	0.27102 (9)	0.0211 (4)
C40	0.71922 (15)	0.51613 (11)	0.32870 (10)	0.0276 (5)
H40	0.7373	0.4750	0.3393	0.033*
C41	0.74138 (17)	0.56396 (13)	0.37068 (11)	0.0359 (6)
H41	0.7747	0.5554	0.4099	0.043*
C42	0.71564 (18)	0.62372 (12)	0.35619 (12)	0.0367 (6)
H42	0.7319	0.6564	0.3850	0.044*
C43	0.66570 (18)	0.63605 (11)	0.29926 (12)	0.0348 (5)
H43	0.6466	0.6771	0.2893	0.042*
C44	0.64374 (16)	0.58848 (11)	0.25710 (11)	0.0283 (5)
H44	0.6099	0.5972	0.2181	0.034*
C45	0.57533 (14)	0.25804 (10)	0.14803 (10)	0.0242 (4)
C46	0.57037 (18)	0.27257 (12)	0.08388 (11)	0.0341 (5)
H46	0.5853	0.3130	0.0711	0.041*
C47	0.5437 (2)	0.22822 (13)	0.03898 (12)	0.0428 (7)
H47	0.5408	0.2384	−0.0045	0.051*
C48	0.52136 (19)	0.16919 (13)	0.05671 (12)	0.0405 (6)
H48	0.5031	0.1390	0.0256	0.049*
C49	0.52576 (18)	0.15443 (12)	0.12001 (12)	0.0369 (6)
H49	0.5100	0.1141	0.1324	0.044*
C50	0.55329 (16)	0.19857 (11)	0.16568 (11)	0.0292 (5)
H50	0.5570	0.1879	0.2091	0.035*
C51	0.64005 (15)	0.27452 (10)	0.27751 (10)	0.0253 (5)
C52	0.58005 (17)	0.26072 (11)	0.31972 (10)	0.0310 (5)
H52	0.5224	0.2773	0.3131	0.037*
C53	0.6037 (2)	0.22294 (12)	0.37139 (12)	0.0402 (6)
H53	0.5621	0.2132	0.3997	0.048*
C54	0.6877 (2)	0.19962 (12)	0.38149 (13)	0.0492 (8)
H54	0.7041	0.1739	0.4170	0.059*
C55	0.7475 (2)	0.21340 (15)	0.34061 (15)	0.0555 (9)
H55	0.8053	0.1971	0.3479	0.067*
C56	0.72490 (19)	0.25093 (14)	0.28856 (13)	0.0427 (6)
H56	0.7671	0.2605	0.2606	0.051*
B1	0.48127 (15)	−0.08729 (11)	0.17146 (11)	0.0203 (4)
C61	0.50020 (13)	−0.03005 (10)	0.22225 (10)	0.0215 (4)

C62	0.56562 (15)	0.01470 (10)	0.22030 (11)	0.0272 (5)
H62	0.6006	0.0140	0.1863	0.033*
C63	0.58165 (17)	0.06050 (11)	0.26652 (13)	0.0366 (6)
H63	0.6270	0.0899	0.2634	0.044*
C64	0.53206 (18)	0.06319 (12)	0.31651 (12)	0.0380 (6)
H64	0.5429	0.0942	0.3480	0.046*
C65	0.46630 (17)	0.01994 (12)	0.32005 (12)	0.0366 (6)
H65	0.4311	0.0214	0.3539	0.044*
C66	0.45152 (15)	−0.02579 (11)	0.27405 (11)	0.0289 (5)
H66	0.4065	−0.0554	0.2779	0.035*
C67	0.38780 (14)	−0.07824 (10)	0.12653 (9)	0.0216 (4)
C68	0.36469 (15)	−0.12151 (11)	0.07866 (10)	0.0281 (5)
H68	0.4037	−0.1549	0.0735	0.034*
C69	0.28697 (17)	−0.11773 (13)	0.03827 (10)	0.0345 (6)
H69	0.2736	−0.1483	0.0066	0.041*
C70	0.22974 (16)	−0.06959 (14)	0.04446 (11)	0.0358 (6)
H70	0.1765	−0.0668	0.0172	0.043*
C71	0.25019 (15)	−0.02557 (13)	0.09041 (11)	0.0324 (5)
H71	0.2110	0.0078	0.0949	0.039*
C72	0.32856 (14)	−0.02987 (11)	0.13057 (10)	0.0246 (4)
H72	0.3418	0.0013	0.1616	0.030*
C73	0.55772 (14)	−0.09069 (10)	0.12310 (10)	0.0230 (4)
C74	0.56174 (15)	−0.04456 (11)	0.07683 (10)	0.0273 (5)
H74	0.5204	−0.0117	0.0749	0.033*
C75	0.62368 (16)	−0.04511 (13)	0.03393 (11)	0.0339 (5)
H75	0.6241	−0.0129	0.0036	0.041*
C76	0.68469 (17)	−0.09249 (13)	0.03532 (12)	0.0372 (6)
H76	0.7272	−0.0932	0.0062	0.045*
C77	0.68259 (16)	−0.13894 (13)	0.07998 (12)	0.0356 (5)
H77	0.7242	−0.1717	0.0816	0.043*
C78	0.61981 (15)	−0.13791 (11)	0.12256 (11)	0.0279 (5)
H78	0.6193	−0.1706	0.1523	0.034*
C79	0.47921 (13)	−0.15040 (10)	0.21425 (9)	0.0205 (4)
C80	0.54757 (15)	−0.16243 (11)	0.26222 (10)	0.0275 (5)
H80	0.5954	−0.1342	0.2681	0.033*
C81	0.54804 (16)	−0.21383 (12)	0.30136 (11)	0.0331 (5)
H81	0.5958	−0.2203	0.3330	0.040*
C82	0.47913 (17)	−0.25576 (12)	0.29447 (12)	0.0353 (5)
H82	0.4793	−0.2910	0.3211	0.042*
C83	0.41032 (16)	−0.24545 (11)	0.24836 (11)	0.0309 (5)
H83	0.3622	−0.2734	0.2435	0.037*
C84	0.41126 (14)	−0.19410 (10)	0.20891 (10)	0.0239 (4)
H84	0.3636	−0.1885	0.1769	0.029*
N2	0.2933 (3)	0.2066 (3)	0.54874 (19)	0.1073 (15)
C93	0.3490 (3)	0.2388 (2)	0.53754 (18)	0.0772 (12)
C94	0.4213 (3)	0.2788 (3)	0.5230 (3)	0.1022 (16)
H94A	0.4523	0.2948	0.5623	0.153*
H94B	0.3979	0.3134	0.4966	0.153*
H94C	0.4621	0.2548	0.5003	0.153*

N3	0.5099 (5)	0.1161 (4)	0.4785 (2)	0.178 (3)
C95	0.4699 (4)	0.0975 (3)	0.5157 (2)	0.0936 (16)
C96	0.4198 (4)	0.0808 (3)	0.5645 (3)	0.121 (2)
H96A	0.4565	0.0831	0.6050	0.182*
H96B	0.3980	0.0384	0.5576	0.182*
H96C	0.3700	0.1093	0.5648	0.182*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.01982 (9)	0.01424 (9)	0.01485 (9)	0.00141 (7)	0.00219 (6)	−0.00022 (6)
Cl1	0.0357 (3)	0.0260 (3)	0.0177 (2)	−0.0009 (2)	−0.00102 (19)	−0.00043 (19)
N1	0.0904 (19)	0.0166 (10)	0.0249 (10)	0.0166 (11)	0.0015 (11)	−0.0020 (8)
C91	0.031 (2)	0.031 (2)	0.026 (2)	0.0033 (17)	0.0032 (16)	0.0022 (16)
C92	0.060 (3)	0.071 (4)	0.033 (3)	−0.011 (3)	0.014 (2)	0.005 (2)
C91'	0.040 (4)	0.028 (3)	0.016 (3)	−0.001 (3)	0.003 (2)	0.005 (2)
C92'	0.051 (4)	0.076 (6)	0.022 (3)	−0.009 (4)	−0.008 (3)	0.004 (3)
P1	0.0214 (3)	0.0154 (3)	0.0211 (2)	0.0021 (2)	0.00404 (19)	0.00153 (19)
P2	0.0205 (3)	0.0159 (3)	0.0263 (3)	0.0004 (2)	0.0058 (2)	0.0011 (2)
C1	0.0241 (11)	0.0187 (11)	0.0441 (13)	0.0015 (9)	0.0046 (9)	0.0048 (9)
C2	0.0247 (11)	0.0187 (11)	0.0398 (12)	0.0025 (9)	0.0130 (9)	0.0026 (9)
C3	0.0230 (10)	0.0192 (10)	0.0238 (10)	0.0026 (8)	0.0044 (8)	0.0013 (8)
C4	0.0360 (12)	0.0213 (11)	0.0238 (10)	−0.0013 (10)	0.0071 (9)	0.0007 (8)
C5	0.0609 (17)	0.0218 (12)	0.0325 (12)	−0.0044 (12)	0.0150 (11)	0.0029 (9)
C6	0.0618 (18)	0.0324 (14)	0.0295 (12)	0.0070 (13)	0.0117 (12)	0.0122 (10)
C7	0.0539 (16)	0.0381 (15)	0.0228 (11)	0.0070 (12)	−0.0026 (10)	0.0033 (10)
C8	0.0377 (13)	0.0250 (12)	0.0276 (11)	0.0023 (10)	−0.0019 (9)	0.0000 (9)
C9	0.0297 (11)	0.0174 (10)	0.0224 (9)	0.0020 (9)	0.0093 (8)	0.0022 (8)
C10	0.0318 (12)	0.0212 (11)	0.0280 (10)	0.0019 (9)	0.0071 (9)	−0.0018 (8)
C11	0.0438 (14)	0.0272 (13)	0.0297 (11)	−0.0033 (11)	0.0034 (10)	−0.0026 (9)
C12	0.0565 (16)	0.0229 (12)	0.0284 (11)	−0.0003 (11)	0.0169 (11)	−0.0036 (9)
C13	0.0465 (15)	0.0273 (13)	0.0376 (13)	0.0116 (11)	0.0191 (11)	0.0003 (10)
C14	0.0344 (12)	0.0269 (12)	0.0287 (11)	0.0089 (10)	0.0083 (9)	0.0033 (9)
C15	0.0263 (11)	0.0213 (11)	0.0314 (11)	−0.0042 (9)	0.0010 (9)	0.0036 (9)
C16	0.0279 (12)	0.0377 (15)	0.0439 (14)	−0.0041 (11)	−0.0009 (10)	0.0093 (11)
C17	0.0376 (15)	0.060 (2)	0.0479 (16)	−0.0145 (14)	−0.0142 (12)	0.0151 (14)
C18	0.0580 (18)	0.0558 (19)	0.0316 (13)	−0.0279 (15)	−0.0111 (13)	0.0091 (12)
C19	0.0565 (18)	0.0440 (16)	0.0337 (13)	−0.0173 (14)	0.0035 (12)	−0.0068 (11)
C20	0.0329 (12)	0.0339 (14)	0.0345 (12)	−0.0068 (11)	0.0008 (10)	−0.0054 (10)
C21	0.0183 (10)	0.0223 (11)	0.0338 (11)	−0.0011 (9)	0.0022 (8)	0.0056 (9)
C22	0.0280 (12)	0.0222 (12)	0.0490 (14)	0.0004 (10)	0.0058 (10)	0.0047 (10)
C23	0.0314 (13)	0.0207 (13)	0.0739 (19)	−0.0018 (11)	−0.0050 (12)	0.0114 (12)
C24	0.0483 (17)	0.0387 (17)	0.0651 (19)	−0.0092 (14)	−0.0028 (14)	0.0293 (14)
C25	0.0494 (17)	0.0516 (19)	0.0428 (14)	−0.0097 (14)	0.0055 (12)	0.0212 (13)
C26	0.0311 (12)	0.0338 (13)	0.0322 (11)	−0.0037 (10)	0.0052 (9)	0.0076 (10)
P3	0.0181 (2)	0.0159 (3)	0.0224 (2)	0.0006 (2)	0.00004 (19)	−0.00067 (19)
P4	0.0214 (3)	0.0157 (3)	0.0230 (2)	0.0019 (2)	0.00261 (19)	−0.00274 (19)
C31	0.0201 (10)	0.0193 (11)	0.0403 (12)	0.0006 (9)	−0.0004 (9)	−0.0030 (9)

C32	0.0239 (11)	0.0211 (11)	0.0406 (12)	0.0015 (9)	0.0074 (9)	−0.0041 (9)
C33	0.0254 (11)	0.0202 (11)	0.0245 (10)	−0.0051 (9)	0.0048 (8)	−0.0046 (8)
C34	0.0260 (11)	0.0339 (13)	0.0335 (12)	−0.0064 (10)	0.0046 (9)	−0.0047 (10)
C35	0.0352 (13)	0.0388 (15)	0.0374 (13)	−0.0126 (11)	0.0158 (10)	−0.0047 (11)
C36	0.0504 (15)	0.0298 (13)	0.0248 (11)	−0.0124 (11)	0.0103 (10)	−0.0032 (9)
C37	0.0418 (14)	0.0341 (14)	0.0275 (11)	−0.0033 (11)	0.0025 (10)	0.0045 (10)
C38	0.0295 (12)	0.0321 (13)	0.0275 (11)	−0.0013 (10)	0.0054 (9)	0.0044 (9)
C39	0.0176 (9)	0.0203 (10)	0.0253 (10)	−0.0012 (8)	0.0026 (8)	−0.0017 (8)
C40	0.0299 (11)	0.0275 (12)	0.0249 (10)	0.0067 (10)	0.0005 (9)	−0.0023 (9)
C41	0.0369 (13)	0.0421 (15)	0.0269 (11)	0.0070 (12)	−0.0044 (10)	−0.0099 (10)
C42	0.0406 (14)	0.0338 (14)	0.0353 (12)	−0.0036 (11)	0.0025 (10)	−0.0162 (10)
C43	0.0459 (14)	0.0197 (11)	0.0390 (13)	0.0011 (11)	0.0055 (11)	−0.0042 (9)
C44	0.0325 (12)	0.0219 (11)	0.0294 (11)	0.0012 (9)	−0.0014 (9)	−0.0010 (9)
C45	0.0251 (10)	0.0201 (11)	0.0280 (10)	0.0025 (9)	0.0058 (8)	−0.0062 (8)
C46	0.0494 (15)	0.0270 (12)	0.0287 (11)	−0.0083 (11)	0.0171 (10)	−0.0072 (9)
C47	0.0626 (18)	0.0392 (15)	0.0291 (12)	−0.0108 (14)	0.0165 (12)	−0.0130 (11)
C48	0.0524 (16)	0.0319 (14)	0.0386 (13)	−0.0087 (12)	0.0111 (12)	−0.0176 (11)
C49	0.0449 (15)	0.0214 (12)	0.0440 (14)	−0.0041 (11)	0.0034 (11)	−0.0065 (10)
C50	0.0350 (12)	0.0204 (11)	0.0318 (11)	−0.0002 (10)	0.0020 (9)	−0.0031 (9)
C51	0.0296 (11)	0.0168 (10)	0.0276 (10)	0.0031 (9)	−0.0049 (8)	−0.0041 (8)
C52	0.0369 (13)	0.0241 (12)	0.0301 (11)	−0.0002 (10)	−0.0048 (9)	0.0043 (9)
C53	0.0628 (18)	0.0246 (13)	0.0309 (12)	−0.0033 (12)	−0.0057 (11)	0.0051 (10)
C54	0.080 (2)	0.0257 (13)	0.0349 (13)	0.0163 (14)	−0.0223 (14)	0.0003 (10)
C55	0.0589 (19)	0.0484 (19)	0.0532 (17)	0.0296 (16)	−0.0195 (15)	−0.0048 (14)
C56	0.0395 (14)	0.0445 (16)	0.0420 (14)	0.0175 (13)	−0.0045 (11)	−0.0025 (12)
B1	0.0185 (11)	0.0177 (11)	0.0252 (11)	−0.0002 (9)	0.0043 (8)	0.0006 (8)
C61	0.0185 (9)	0.0161 (10)	0.0293 (10)	0.0013 (8)	0.0005 (8)	0.0000 (8)
C62	0.0242 (11)	0.0195 (11)	0.0368 (12)	−0.0025 (9)	−0.0012 (9)	0.0029 (9)
C63	0.0338 (13)	0.0196 (12)	0.0530 (15)	−0.0059 (10)	−0.0107 (11)	−0.0011 (10)
C64	0.0413 (14)	0.0243 (13)	0.0445 (14)	0.0063 (11)	−0.0120 (11)	−0.0127 (10)
C65	0.0403 (14)	0.0330 (14)	0.0366 (13)	0.0053 (11)	0.0050 (10)	−0.0103 (10)
C66	0.0272 (11)	0.0238 (12)	0.0362 (12)	−0.0026 (9)	0.0065 (9)	−0.0066 (9)
C67	0.0210 (10)	0.0234 (11)	0.0212 (9)	−0.0035 (8)	0.0064 (8)	0.0012 (8)
C68	0.0286 (11)	0.0288 (12)	0.0271 (11)	−0.0002 (10)	0.0036 (9)	−0.0035 (9)
C69	0.0370 (13)	0.0426 (15)	0.0229 (10)	−0.0090 (12)	−0.0012 (9)	−0.0042 (10)
C70	0.0233 (11)	0.0559 (17)	0.0276 (11)	−0.0025 (11)	−0.0003 (9)	0.0059 (11)
C71	0.0257 (11)	0.0433 (15)	0.0293 (11)	0.0079 (11)	0.0074 (9)	0.0055 (10)
C72	0.0229 (10)	0.0271 (12)	0.0250 (10)	0.0019 (9)	0.0073 (8)	−0.0003 (8)
C73	0.0213 (10)	0.0208 (11)	0.0272 (10)	−0.0028 (8)	0.0045 (8)	−0.0019 (8)
C74	0.0242 (11)	0.0272 (12)	0.0309 (11)	−0.0033 (9)	0.0054 (9)	0.0012 (9)
C75	0.0339 (13)	0.0396 (14)	0.0291 (11)	−0.0113 (11)	0.0077 (10)	0.0013 (10)
C76	0.0315 (12)	0.0476 (16)	0.0355 (12)	−0.0091 (12)	0.0169 (10)	−0.0090 (11)
C77	0.0289 (12)	0.0366 (14)	0.0431 (13)	0.0029 (11)	0.0122 (10)	−0.0082 (11)
C78	0.0261 (11)	0.0247 (12)	0.0342 (11)	0.0000 (9)	0.0085 (9)	−0.0016 (9)
C79	0.0203 (10)	0.0173 (10)	0.0250 (10)	−0.0009 (8)	0.0077 (8)	−0.0037 (8)
C80	0.0256 (11)	0.0230 (12)	0.0331 (11)	−0.0064 (9)	−0.0001 (9)	0.0030 (9)
C81	0.0321 (12)	0.0304 (13)	0.0356 (12)	0.0024 (10)	−0.0010 (10)	0.0058 (10)
C82	0.0430 (14)	0.0219 (12)	0.0427 (13)	−0.0012 (11)	0.0127 (11)	0.0098 (10)
C83	0.0318 (12)	0.0180 (11)	0.0441 (13)	−0.0054 (9)	0.0096 (10)	0.0011 (9)

C84	0.0219 (10)	0.0191 (11)	0.0310 (10)	−0.0031 (8)	0.0050 (8)	−0.0026 (8)
N2	0.090 (3)	0.153 (5)	0.077 (2)	−0.033 (3)	−0.001 (2)	0.018 (3)
C93	0.075 (3)	0.094 (3)	0.059 (2)	0.000 (3)	−0.007 (2)	0.002 (2)
C94	0.086 (3)	0.096 (4)	0.119 (4)	−0.018 (3)	−0.015 (3)	0.004 (3)
N3	0.176 (6)	0.278 (9)	0.083 (3)	−0.106 (6)	0.030 (3)	−0.022 (4)
C95	0.095 (3)	0.107 (4)	0.078 (3)	−0.044 (3)	0.002 (3)	0.004 (3)
C96	0.107 (4)	0.115 (5)	0.145 (5)	0.001 (4)	0.035 (4)	0.051 (4)

Geometric parameters (Å, °)

Mo1—N1	1.732 (2)	C37—C38	1.389 (3)
Mo1—Cl1	2.4413 (5)	C37—H37	0.9500
Mo1—P4	2.5308 (6)	C38—H38	0.9500
Mo1—P3	2.5342 (6)	C39—C44	1.387 (3)
Mo1—P2	2.5447 (6)	C39—C40	1.391 (3)
Mo1—P1	2.5503 (6)	C40—C41	1.384 (3)
N1—C91	1.496 (4)	C40—H40	0.9500
N1—C91'	1.507 (6)	C41—C42	1.374 (4)
C91—C92	1.513 (6)	C41—H41	0.9500
C91—H91A	0.9900	C42—C43	1.388 (4)
C91—H91B	0.9900	C42—H42	0.9500
C92—H92A	0.9800	C43—C44	1.382 (3)
C92—H92B	0.9800	C43—H43	0.9500
C92—H92C	0.9800	C44—H44	0.9500
C91'—C92'	1.540 (9)	C45—C50	1.390 (3)
C91'—H91C	0.9900	C45—C46	1.399 (3)
C91'—H91D	0.9900	C46—C47	1.384 (3)
C92'—H92D	0.9800	C46—H46	0.9500
C92'—H92E	0.9800	C47—C48	1.383 (4)
C92'—H92F	0.9800	C47—H47	0.9500
P1—C3	1.830 (2)	C48—C49	1.382 (4)
P1—C9	1.833 (2)	C48—H48	0.9500
P1—C1	1.842 (2)	C49—C50	1.394 (3)
P2—C15	1.828 (2)	C49—H49	0.9500
P2—C2	1.829 (2)	C50—H50	0.9500
P2—C21	1.833 (2)	C51—C52	1.389 (3)
C1—C2	1.527 (3)	C51—C56	1.392 (3)
C1—H1A	0.9900	C52—C53	1.387 (3)
C1—H1B	0.9900	C52—H52	0.9500
C2—H2A	0.9900	C53—C54	1.376 (4)
C2—H2B	0.9900	C53—H53	0.9500
C3—C8	1.393 (3)	C54—C55	1.367 (5)
C3—C4	1.393 (3)	C54—H54	0.9500
C4—C5	1.387 (3)	C55—C56	1.388 (4)
C4—H4	0.9500	C55—H55	0.9500
C5—C6	1.376 (4)	C56—H56	0.9500
C5—H5	0.9500	B1—C79	1.642 (3)
C6—C7	1.378 (4)	B1—C67	1.645 (3)
C6—H6	0.9500	B1—C73	1.647 (3)

C7—C8	1.381 (3)	B1—C61	1.648 (3)
C7—H7	0.9500	C61—C62	1.396 (3)
C8—H8	0.9500	C61—C66	1.404 (3)
C9—C10	1.383 (3)	C62—C63	1.399 (3)
C9—C14	1.395 (3)	C62—H62	0.9500
C10—C11	1.391 (3)	C63—C64	1.378 (4)
C10—H10	0.9500	C63—H63	0.9500
C11—C12	1.382 (4)	C64—C65	1.382 (4)
C11—H11	0.9500	C64—H64	0.9500
C12—C13	1.378 (4)	C65—C66	1.393 (3)
C12—H12	0.9500	C65—H65	0.9500
C13—C14	1.384 (3)	C66—H66	0.9500
C13—H13	0.9500	C67—C72	1.393 (3)
C14—H14	0.9500	C67—C68	1.400 (3)
C15—C20	1.386 (3)	C68—C69	1.393 (3)
C15—C16	1.393 (3)	C68—H68	0.9500
C16—C17	1.382 (4)	C69—C70	1.376 (4)
C16—H16	0.9500	C69—H69	0.9500
C17—C18	1.376 (5)	C70—C71	1.376 (4)
C17—H17	0.9500	C70—H70	0.9500
C18—C19	1.381 (4)	C71—C72	1.399 (3)
C18—H18	0.9500	C71—H71	0.9500
C19—C20	1.392 (3)	C72—H72	0.9500
C19—H19	0.9500	C73—C78	1.395 (3)
C20—H20	0.9500	C73—C74	1.409 (3)
C21—C26	1.387 (3)	C74—C75	1.391 (3)
C21—C22	1.390 (3)	C74—H74	0.9500
C22—C23	1.388 (4)	C75—C76	1.384 (4)
C22—H22	0.9500	C75—H75	0.9500
C23—C24	1.378 (5)	C76—C77	1.386 (4)
C23—H23	0.9500	C76—H76	0.9500
C24—C25	1.375 (5)	C77—C78	1.395 (3)
C24—H24	0.9500	C77—H77	0.9500
C25—C26	1.391 (4)	C78—H78	0.9500
C25—H25	0.9500	C79—C84	1.401 (3)
C26—H26	0.9500	C79—C80	1.405 (3)
P3—C39	1.829 (2)	C80—C81	1.388 (3)
P3—C31	1.832 (2)	C80—H80	0.9500
P3—C33	1.833 (2)	C81—C82	1.386 (4)
P4—C51	1.825 (2)	C81—H81	0.9500
P4—C45	1.828 (2)	C82—C83	1.378 (4)
P4—C32	1.839 (2)	C82—H82	0.9500
C31—C32	1.528 (3)	C83—C84	1.393 (3)
C31—H31A	0.9900	C83—H83	0.9500
C31—H31B	0.9900	C84—H84	0.9500
C32—H32A	0.9900	N2—C93	1.147 (6)
C32—H32B	0.9900	C93—C94	1.465 (7)
C33—C38	1.389 (3)	C94—H94A	0.9800
C33—C34	1.389 (3)	C94—H94B	0.9800

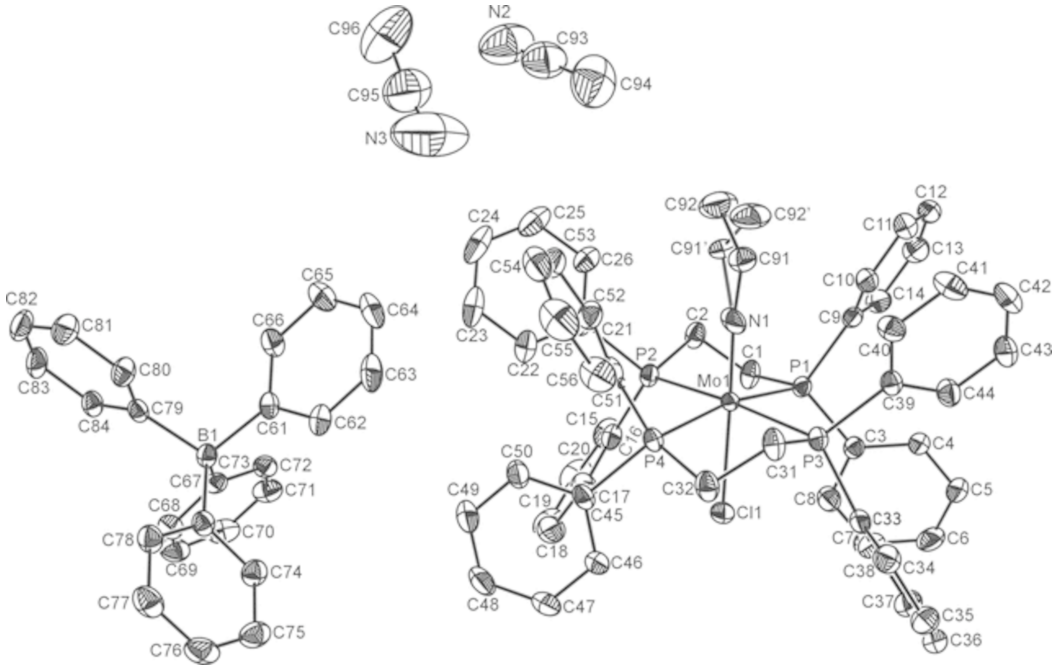
C34—C35	1.392 (3)	C94—H94C	0.9800
C34—H34	0.9500	N3—C95	1.129 (6)
C35—C36	1.375 (4)	C95—C96	1.408 (7)
C35—H35	0.9500	C96—H96A	0.9800
C36—C37	1.375 (4)	C96—H96B	0.9800
C36—H36	0.9500	C96—H96C	0.9800
N1—Mo1—Cl1	178.20 (7)	C38—C33—P3	119.92 (17)
N1—Mo1—P4	94.16 (8)	C34—C33—P3	121.44 (17)
Cl1—Mo1—P4	84.136 (19)	C33—C34—C35	120.3 (2)
N1—Mo1—P3	91.98 (10)	C33—C34—H34	119.9
Cl1—Mo1—P3	88.31 (2)	C35—C34—H34	119.9
P4—Mo1—P3	79.981 (19)	C36—C35—C34	120.6 (2)
N1—Mo1—P2	92.57 (10)	C36—C35—H35	119.7
Cl1—Mo1—P2	87.16 (2)	C34—C35—H35	119.7
P4—Mo1—P2	100.388 (19)	C35—C36—C37	119.6 (2)
P3—Mo1—P2	175.395 (18)	C35—C36—H36	120.2
N1—Mo1—P1	96.28 (8)	C37—C36—H36	120.2
Cl1—Mo1—P1	85.432 (19)	C36—C37—C38	120.2 (2)
P4—Mo1—P1	169.537 (17)	C36—C37—H37	119.9
P3—Mo1—P1	98.915 (18)	C38—C37—H37	119.9
P2—Mo1—P1	79.879 (18)	C37—C38—C33	120.9 (2)
C91—N1—C91'	44.9 (3)	C37—C38—H38	119.6
C91—N1—Mo1	162.0 (3)	C33—C38—H38	119.6
C91'—N1—Mo1	152.9 (3)	C44—C39—C40	118.8 (2)
N1—C91—C92	104.7 (3)	C44—C39—P3	118.66 (16)
N1—C91—H91A	110.8	C40—C39—P3	122.54 (17)
C92—C91—H91A	110.8	C41—C40—C39	120.1 (2)
N1—C91—H91B	110.8	C41—C40—H40	119.9
C92—C91—H91B	110.8	C39—C40—H40	119.9
H91A—C91—H91B	108.9	C42—C41—C40	120.7 (2)
C91—C92—H92A	109.5	C42—C41—H41	119.6
C91—C92—H92B	109.5	C40—C41—H41	119.6
H92A—C92—H92B	109.5	C41—C42—C43	119.6 (2)
C91—C92—H92C	109.5	C41—C42—H42	120.2
H92A—C92—H92C	109.5	C43—C42—H42	120.2
H92B—C92—H92C	109.5	C44—C43—C42	119.9 (2)
N1—C91'—C92'	102.3 (5)	C44—C43—H43	120.1
N1—C91'—H91C	111.3	C42—C43—H43	120.1
C92'—C91'—H91C	111.3	C43—C44—C39	120.9 (2)
N1—C91'—H91D	111.3	C43—C44—H44	119.6
C92'—C91'—H91D	111.3	C39—C44—H44	119.6
H91C—C91'—H91D	109.2	C50—C45—C46	118.9 (2)
C91'—C92'—H92D	109.5	C50—C45—P4	121.23 (17)
C91'—C92'—H92E	109.5	C46—C45—P4	119.65 (17)
H92D—C92'—H92E	109.5	C47—C46—C45	120.2 (2)
C91'—C92'—H92F	109.5	C47—C46—H46	119.9
H92D—C92'—H92F	109.5	C45—C46—H46	119.9
H92E—C92'—H92F	109.5	C46—C47—C48	120.7 (2)
C3—P1—C9	102.30 (10)	C46—C47—H47	119.6

C3—P1—C1	102.27 (10)	C48—C47—H47	119.6
C9—P1—C1	102.22 (11)	C49—C48—C47	119.5 (2)
C3—P1—Mo1	122.78 (7)	C49—C48—H48	120.2
C9—P1—Mo1	117.84 (7)	C47—C48—H48	120.2
C1—P1—Mo1	106.64 (7)	C48—C49—C50	120.3 (2)
C15—P2—C2	104.69 (11)	C48—C49—H49	119.9
C15—P2—C21	100.46 (10)	C50—C49—H49	119.9
C2—P2—C21	103.10 (10)	C45—C50—C49	120.4 (2)
C15—P2—Mo1	120.59 (8)	C45—C50—H50	119.8
C2—P2—Mo1	103.77 (8)	C49—C50—H50	119.8
C21—P2—Mo1	121.91 (7)	C52—C51—C56	119.0 (2)
C2—C1—P1	109.72 (15)	C52—C51—P4	118.34 (17)
C2—C1—H1A	109.7	C56—C51—P4	122.5 (2)
P1—C1—H1A	109.7	C53—C52—C51	120.5 (2)
C2—C1—H1B	109.7	C53—C52—H52	119.7
P1—C1—H1B	109.7	C51—C52—H52	119.7
H1A—C1—H1B	108.2	C54—C53—C52	119.8 (3)
C1—C2—P2	109.03 (15)	C54—C53—H53	120.1
C1—C2—H2A	109.9	C52—C53—H53	120.1
P2—C2—H2A	109.9	C55—C54—C53	120.2 (2)
C1—C2—H2B	109.9	C55—C54—H54	119.9
P2—C2—H2B	109.9	C53—C54—H54	119.9
H2A—C2—H2B	108.3	C54—C55—C56	120.8 (3)
C8—C3—C4	119.1 (2)	C54—C55—H55	119.6
C8—C3—P1	120.41 (17)	C56—C55—H55	119.6
C4—C3—P1	120.47 (16)	C55—C56—C51	119.6 (3)
C5—C4—C3	120.1 (2)	C55—C56—H56	120.2
C5—C4—H4	119.9	C51—C56—H56	120.2
C3—C4—H4	119.9	C79—B1—C67	110.70 (17)
C6—C5—C4	120.1 (2)	C79—B1—C73	111.75 (17)
C6—C5—H5	120.0	C67—B1—C73	105.93 (16)
C4—C5—H5	120.0	C79—B1—C61	105.59 (16)
C5—C6—C7	120.3 (2)	C67—B1—C61	111.88 (17)
C5—C6—H6	119.9	C73—B1—C61	111.11 (17)
C7—C6—H6	119.9	C62—C61—C66	115.1 (2)
C6—C7—C8	120.2 (2)	C62—C61—B1	124.99 (19)
C6—C7—H7	119.9	C66—C61—B1	119.80 (19)
C8—C7—H7	119.9	C61—C62—C63	122.6 (2)
C7—C8—C3	120.2 (2)	C61—C62—H62	118.7
C7—C8—H8	119.9	C63—C62—H62	118.7
C3—C8—H8	119.9	C64—C63—C62	120.5 (2)
C10—C9—C14	118.6 (2)	C64—C63—H63	119.8
C10—C9—P1	120.90 (16)	C62—C63—H63	119.8
C14—C9—P1	120.43 (17)	C63—C64—C65	118.8 (2)
C9—C10—C11	120.5 (2)	C63—C64—H64	120.6
C9—C10—H10	119.8	C65—C64—H64	120.6
C11—C10—H10	119.8	C64—C65—C66	120.2 (2)
C12—C11—C10	120.1 (2)	C64—C65—H65	119.9
C12—C11—H11	119.9	C66—C65—H65	119.9

C10—C11—H11	119.9	C65—C66—C61	122.8 (2)
C13—C12—C11	119.9 (2)	C65—C66—H66	118.6
C13—C12—H12	120.0	C61—C66—H66	118.6
C11—C12—H12	120.0	C72—C67—C68	115.5 (2)
C12—C13—C14	120.0 (2)	C72—C67—B1	125.79 (19)
C12—C13—H13	120.0	C68—C67—B1	118.65 (19)
C14—C13—H13	120.0	C69—C68—C67	122.8 (2)
C13—C14—C9	120.8 (2)	C69—C68—H68	118.6
C13—C14—H14	119.6	C67—C68—H68	118.6
C9—C14—H14	119.6	C70—C69—C68	119.7 (2)
C20—C15—C16	118.9 (2)	C70—C69—H69	120.2
C20—C15—P2	119.25 (17)	C68—C69—H69	120.2
C16—C15—P2	121.66 (19)	C69—C70—C71	119.5 (2)
C17—C16—C15	119.9 (3)	C69—C70—H70	120.2
C17—C16—H16	120.1	C71—C70—H70	120.2
C15—C16—H16	120.1	C70—C71—C72	120.2 (2)
C18—C17—C16	120.7 (3)	C70—C71—H71	119.9
C18—C17—H17	119.6	C72—C71—H71	119.9
C16—C17—H17	119.6	C67—C72—C71	122.2 (2)
C17—C18—C19	120.2 (3)	C67—C72—H72	118.9
C17—C18—H18	119.9	C71—C72—H72	118.9
C19—C18—H18	119.9	C78—C73—C74	115.3 (2)
C18—C19—C20	119.2 (3)	C78—C73—B1	124.84 (19)
C18—C19—H19	120.4	C74—C73—B1	119.84 (19)
C20—C19—H19	120.4	C75—C74—C73	122.8 (2)
C15—C20—C19	121.0 (2)	C75—C74—H74	118.6
C15—C20—H20	119.5	C73—C74—H74	118.6
C19—C20—H20	119.5	C76—C75—C74	120.1 (2)
C26—C21—C22	119.1 (2)	C76—C75—H75	119.9
C26—C21—P2	121.87 (18)	C74—C75—H75	120.0
C22—C21—P2	118.99 (18)	C75—C76—C77	118.8 (2)
C23—C22—C21	120.7 (3)	C75—C76—H76	120.6
C23—C22—H22	119.7	C77—C76—H76	120.6
C21—C22—H22	119.7	C76—C77—C78	120.4 (2)
C24—C23—C22	119.7 (3)	C76—C77—H77	119.8
C24—C23—H23	120.1	C78—C77—H77	119.8
C22—C23—H23	120.1	C73—C78—C77	122.5 (2)
C25—C24—C23	120.0 (3)	C73—C78—H78	118.7
C25—C24—H24	120.0	C77—C78—H78	118.7
C23—C24—H24	120.0	C84—C79—C80	115.0 (2)
C24—C25—C26	120.7 (3)	C84—C79—B1	125.00 (18)
C24—C25—H25	119.7	C80—C79—B1	119.97 (18)
C26—C25—H25	119.7	C81—C80—C79	122.7 (2)
C21—C26—C25	119.7 (3)	C81—C80—H80	118.7
C21—C26—H26	120.1	C79—C80—H80	118.7
C25—C26—H26	120.1	C82—C81—C80	120.3 (2)
C39—P3—C31	104.53 (10)	C82—C81—H81	119.8
C39—P3—C33	101.42 (10)	C80—C81—H81	119.8
C31—P3—C33	103.45 (11)	C83—C82—C81	118.9 (2)

C39—P3—Mo1	118.30 (7)	C83—C82—H82	120.5
C31—P3—Mo1	105.12 (8)	C81—C82—H82	120.5
C33—P3—Mo1	121.96 (7)	C82—C83—C84	120.1 (2)
C51—P4—C45	102.66 (10)	C82—C83—H83	120.0
C51—P4—C32	104.39 (11)	C84—C83—H83	120.0
C45—P4—C32	103.92 (10)	C83—C84—C79	123.0 (2)
C51—P4—Mo1	114.87 (7)	C83—C84—H84	118.5
C45—P4—Mo1	122.99 (7)	C79—C84—H84	118.5
C32—P4—Mo1	106.16 (8)	N2—C93—C94	178.7 (6)
C32—C31—P3	108.33 (15)	C93—C94—H94A	109.5
C32—C31—H31A	110.0	C93—C94—H94B	109.5
P3—C31—H31A	110.0	H94A—C94—H94B	109.5
C32—C31—H31B	110.0	C93—C94—H94C	109.5
P3—C31—H31B	110.0	H94A—C94—H94C	109.5
H31A—C31—H31B	108.4	H94B—C94—H94C	109.5
C31—C32—P4	108.95 (16)	N3—C95—C96	173.9 (7)
C31—C32—H32A	109.9	C95—C96—H96A	109.5
P4—C32—H32A	109.9	C95—C96—H96B	109.5
C31—C32—H32B	109.9	H96A—C96—H96B	109.5
P4—C32—H32B	109.9	C95—C96—H96C	109.5
H32A—C32—H32B	108.3	H96A—C96—H96C	109.5
C38—C33—C34	118.4 (2)	H96B—C96—H96C	109.5

Fig. 1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