

μ_2 -Iodido-bis{dimethyl[methylbis(quinolin-8-yl)silanyl- κ^3 N,Si,N']platinum(IV)} tetrakis(pentafluorophenyl)borate dichloromethane 0.66-solvate

C. A. Marcus Carr, Christopher W. Gribble* and Marcus I. Gibson

Department of Chemistry, University of California, Berkeley, Berkeley,

CA 94720-1460, USA

Correspondence e-mail: cgribble@berkeley.edu

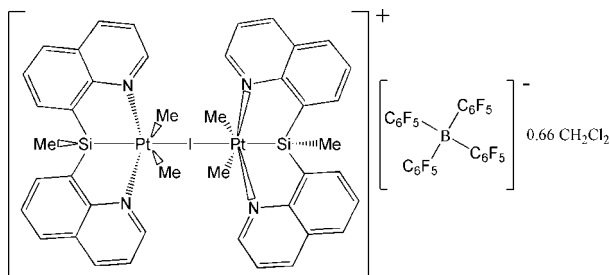
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Key indicators: single-crystal X-ray study; $T = 167$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; disorder in solvent or counterion; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 14.8.

The title complex, $[\text{Pt}_2(\text{CH}_3)_4(\text{C}_{19}\text{H}_{15}\text{N}_2\text{Si})_2\text{I}][\text{B}(\text{C}_6\text{F}_5)_4] \cdot 0.66\text{CH}_2\text{Cl}_2$, resulted from an attempt to synthesize a stable five-coordinate platinum species *via* ligand abstraction of a six-coordinate platinum precursor. However, dimerization occurred after ligand abstraction, thereby yielding the compound described in this study. The cation is a dinuclear Pt^{IV} organometallic complex, in which the metal centers are bridged by an I^- anion. Both metal centers display a coordination geometry close to octahedral, including *cis*-arranged quinoline ligands connected by Si atoms, which form Pt–Si bonds, two *cis*-methyl groups, and the bridging I^- anion. In the crystal structure, voids between cations and anions are partially filled with an average of 0.66 molecules of dichloromethane solvent.

Related literature

Five-coordinate platinum compounds have been speculated to be intermediates in bond-activation processes (Brown *et al.*, 1974). However, ligand abstraction of a six-coordinate platinum precursor carried out in the present study yielded a dinuclear six-coordinate complex.



Experimental

Crystal data

$[\text{Pt}_2(\text{CH}_3)_4(\text{C}_{19}\text{H}_{15}\text{N}_2\text{Si})_2\text{I}] \cdot (\text{C}_{24}\text{F}_{20}\text{B}) \cdot 0.66\text{CH}_2\text{Cl}_2$
 $M_r = 1911.14$
 Triclinic, $P\bar{1}$
 $a = 13.9051$ (10) Å
 $b = 15.3559$ (11) Å
 $c = 17.1261$ (12) Å
 $\alpha = 71.930$ (1)°
 $\beta = 72.045$ (1)°
 $\gamma = 87.621$ (1)°
 $V = 3301.3$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 4.89$ mm⁻¹
 $T = 167$ (2) K
 $0.24 \times 0.11 \times 0.07$ mm

Data collection

Bruker APEX CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
 $T_{\text{min}} = 0.530$, $T_{\text{max}} = 0.710$
 30538 measured reflections
 13293 independent reflections
 11270 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.065$
 $S = 1.08$
 13293 reflections
 898 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.94$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.71$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

I1–Pt2	2.9720 (3)	Pt1–Si1	2.2591 (10)
I1–Pt1	2.9770 (3)	Pt2–Si2	2.2556 (10)
Pt2–I1–Pt1	133.755 (10)		

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *POV-RAY* (Cason, 2002); software used to prepare material for publication: *SHELXL97*.

We thank Dr Fred Hollander and Michael Pluth for assistance throughout the CHEM 208 course, as well as Professor Kenneth Raymond for teaching the course. We thank Preeyanuch Sangtrirutnugul for providing us with a sample.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2154).

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 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

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**2-Iodido-bis{dimethyl[methylbis(quinolin-8-yl)silanyl-³N,Si,N']platinum(IV)}
tetrakis(pentafluorophenyl)borate dichloromethane 0.66-solvate**

C. A. M. Carr, C. W. Gribble and M. I. Gibson

Comment

Five-coordinate platinum compounds have been speculated as intermediates in bond activation processes (Brown *et al.*, 1974). During an attempt to synthesize such a stable five-coordinate platinum species *via* ligand abstraction of six-coordinate platinum precursor, we obtained the title complex (I). We assume that dimerization occurred after ligand abstraction, thereby yielding a dinuclear cationic complex. In the cation, both crystallographically independent Pt^{IV} ions display a coordination geometry close to octahedral, while Si atoms, as expected, are tetrahedrally bonded to two quinoline ligands, one methyl group, and one Pt^{IV} ion (Fig. 1). In the crystal, voids between cations and anions are partially filled with solvent molecules, giving a 0.66 dichloromethane solvate crystal (Fig. 2).

Experimental

Compound (I) was synthesized by addition of lithium tetrakis(perfluorophenyl)borate to a solution of the parent six-coordinate monomer in dichloromethane. X-ray quality single crystals were obtained by vapor diffusion of pentane into dichloromethane.

Refinement

Structure refinement was conducted using least-squares analysis. Thermal parameters for all atoms except H were refined anisotropically. Solvent occupancy was allowed to refine with U_{iso} fixed and subsequently fixed at 0.66 during anisotropic refinement. H atoms were placed in calculated positions, and refined using a riding approximation, with C—H bond lengths constrained to 0.93 (aromatic CH), 0.97 (methylene CH₂) or 0.96 Å (methyl CH₃), and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{carrier C})$ for aromatic CH and methylene CH₂ groups, and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{carrier C})$ for methyl groups. In order to get accurate torsion angles, methyl groups were allowed to rotate about their C—C bonds.

Figures

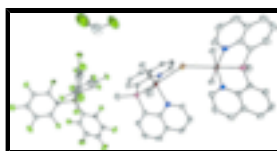


Fig. 1. ORTEP-3 diagram of compound (I). H atoms are omitted for clarity.

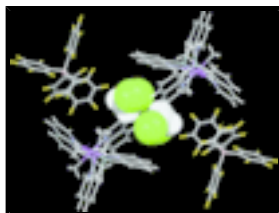


Fig. 2. Packing diagram with co-crystallized dichloromethane shown as the space-filling model.

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Crystal data

$[\text{Pt}_2(\text{CH}_3)_4(\text{C}_{19}\text{H}_{15}\text{N}_2\text{Si})_2\text{I}](\text{C}_{24}\text{F}_{20}\text{B}) \cdot 0.66\text{CH}_2\text{Cl}_2$	$Z = 2$
$M_r = 1911.14$	$F_{000} = 1831.4$
Triclinic, $P\bar{1}$	$D_x = 1.921 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 13.9051 (10) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 15.3559 (11) \text{ \AA}$	Cell parameters from 30538 reflections
$c = 17.1261 (12) \text{ \AA}$	$\theta = 2.1\text{--}26.4^\circ$
$\alpha = 71.930 (1)^\circ$	$\mu = 4.89 \text{ mm}^{-1}$
$\beta = 72.045 (1)^\circ$	$T = 167 (2) \text{ K}$
$\gamma = 87.621 (1)^\circ$	Prism, colourless
$V = 3301.3 (4) \text{ \AA}^3$	$0.24 \times 0.11 \times 0.07 \text{ mm}$

Data collection

Bruker APEX CCD diffractometer	13293 independent reflections
Monochromator: graphite	11270 reflections with $I > 2\sigma(I)$
$T = 167(2) \text{ K}$	$R_{\text{int}} = 0.020$
$P = 101(1) \text{ kPa}$	$\theta_{\text{max}} = 26.4^\circ$
ω scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -11 \rightarrow 17$
$T_{\text{min}} = 0.530$, $T_{\text{max}} = 0.710$	$k = -19 \rightarrow 19$
30538 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained
$wR(F^2) = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
	$(\Delta/\sigma)_{\text{max}} = 0.003$

13293 reflections $\Delta\rho_{\max} = 0.95 \text{ e } \text{\AA}^{-3}$
 898 parameters $\Delta\rho_{\min} = -0.71 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct methods Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}	Occ. (<1)
C1	0.5927 (3)	0.8330 (2)	0.1569 (2)	0.0282 (8)	
H1A	0.5490	0.8633	0.1916	0.034*	
C2	0.6658 (3)	0.8859 (2)	0.0819 (3)	0.0326 (9)	
H2A	0.6697	0.9495	0.0675	0.039*	
C3	0.7308 (3)	0.8432 (3)	0.0304 (2)	0.0304 (8)	
H3A	0.7804	0.8774	-0.0192	0.036*	
C4	0.7227 (3)	0.7460 (2)	0.0527 (2)	0.0246 (8)	
C5	0.7887 (3)	0.6975 (3)	0.0026 (3)	0.0300 (8)	
H5A	0.8397	0.7291	-0.0473	0.036*	
C6	0.7776 (3)	0.6041 (3)	0.0275 (3)	0.0316 (9)	
H6A	0.8219	0.5721	-0.0050	0.038*	
C7	0.7005 (3)	0.5562 (3)	0.1013 (2)	0.0296 (8)	
H7A	0.6935	0.4926	0.1161	0.035*	
C8	0.6344 (3)	0.6000 (2)	0.1528 (2)	0.0250 (8)	
C9	0.6462 (3)	0.6969 (2)	0.1286 (2)	0.0222 (7)	
C10	0.2819 (3)	0.7299 (3)	0.2598 (3)	0.0356 (9)	
H10A	0.2887	0.7720	0.2871	0.043*	
C11	0.1989 (3)	0.7348 (3)	0.2287 (3)	0.0427 (11)	
H11A	0.1521	0.7790	0.2354	0.051*	
C12	0.1883 (3)	0.6733 (3)	0.1885 (3)	0.0419 (10)	
H12A	0.1342	0.6761	0.1668	0.050*	
C13	0.2582 (3)	0.6064 (3)	0.1796 (3)	0.0331 (9)	
C14	0.2521 (4)	0.5407 (3)	0.1388 (3)	0.0450 (11)	
H14A	0.1992	0.5410	0.1163	0.054*	
C15	0.3226 (4)	0.4770 (3)	0.1321 (3)	0.0472 (12)	
H15A	0.3181	0.4348	0.1043	0.057*	
C16	0.4021 (3)	0.4748 (3)	0.1671 (3)	0.0363 (9)	
H16A	0.4488	0.4300	0.1629	0.044*	
C17	0.4129 (3)	0.5371 (2)	0.2074 (2)	0.0293 (8)	
C18	0.3408 (3)	0.6045 (2)	0.2129 (2)	0.0281 (8)	
C19	0.5971 (3)	0.6374 (3)	0.3545 (3)	0.0363 (9)	
H19A	0.6275	0.5818	0.3480	0.054*	
H19B	0.5726	0.6325	0.4147	0.054*	
H19C	0.6465	0.6881	0.3241	0.054*	
C20	0.3865 (3)	0.5713 (3)	0.4192 (3)	0.0419 (10)	
H20A	0.3339	0.5427	0.4085	0.063*	
H20B	0.3569	0.6055	0.4582	0.063*	
H20C	0.4262	0.5249	0.4445	0.063*	
C21	0.5518 (3)	0.4274 (3)	0.3099 (3)	0.0398 (10)	
H21A	0.5744	0.3907	0.2722	0.060*	

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H21B	0.4919	0.3981	0.3558	0.060*
H21C	0.6040	0.4340	0.3339	0.060*
C22	0.3632 (3)	0.9755 (3)	0.4990 (2)	0.0310 (8)
H22A	0.3746	0.9149	0.5007	0.037*
C23	0.3762 (3)	1.0041 (3)	0.5660 (3)	0.0357 (9)
H23A	0.3941	0.9628	0.6112	0.043*
C24	0.3623 (3)	1.0924 (3)	0.5636 (3)	0.0406 (10)
H24A	0.3728	1.1127	0.6063	0.049*
C25	0.3319 (3)	1.1539 (3)	0.4965 (3)	0.0340 (9)
C26	0.3132 (3)	1.2469 (3)	0.4902 (3)	0.0479 (12)
H26A	0.3221	1.2702	0.5318	0.057*
C27	0.2829 (4)	1.3021 (3)	0.4252 (3)	0.0551 (13)
H27A	0.2730	1.3634	0.4213	0.066*
C28	0.2659 (3)	1.2677 (3)	0.3629 (3)	0.0419 (10)
H28A	0.2439	1.3065	0.3188	0.050*
C29	0.2817 (3)	1.1761 (3)	0.3663 (3)	0.0306 (9)
C30	0.3170 (3)	1.1201 (3)	0.4323 (2)	0.0295 (8)
C31	0.1589 (3)	0.8372 (2)	0.4373 (2)	0.0303 (8)
H31A	0.2132	0.8016	0.4445	0.036*
C32	0.0610 (3)	0.7944 (3)	0.4749 (3)	0.0364 (9)
H32A	0.0514	0.7322	0.5060	0.044*
C33	-0.0188 (3)	0.8446 (3)	0.4653 (3)	0.0353 (9)
H33A	-0.0839	0.8170	0.4886	0.042*
C34	-0.0029 (3)	0.9392 (2)	0.4198 (2)	0.0271 (8)
C35	-0.0832 (3)	0.9962 (3)	0.4075 (3)	0.0328 (9)
H35A	-0.1495	0.9710	0.4304	0.039*
C36	-0.0648 (3)	1.0870 (3)	0.3630 (3)	0.0370 (10)
H36A	-0.1181	1.1238	0.3555	0.044*
C37	0.0360 (3)	1.1255 (3)	0.3280 (3)	0.0341 (9)
H37A	0.0476	1.1879	0.2979	0.041*
C38	0.1173 (3)	1.0737 (2)	0.3371 (2)	0.0250 (8)
C39	0.0981 (3)	0.9787 (2)	0.3836 (2)	0.0228 (7)
C40	0.4696 (3)	1.0604 (3)	0.2528 (3)	0.0361 (9)
H40A	0.4716	1.1166	0.2660	0.054*
H40B	0.4791	1.0741	0.1922	0.054*
H40C	0.5226	1.0233	0.2676	0.054*
C41	0.3279 (3)	0.9685 (3)	0.2114 (2)	0.0318 (9)
H41A	0.3417	1.0258	0.1654	0.048*
H41B	0.2621	0.9430	0.2201	0.048*
H41C	0.3782	0.9266	0.1965	0.048*
C42	0.2777 (4)	1.2036 (3)	0.1814 (3)	0.0450 (11)
H42A	0.2319	1.2520	0.1828	0.068*
H42B	0.2683	1.1723	0.1435	0.068*
H42C	0.3462	1.2291	0.1609	0.068*
C43	0.7438 (3)	0.2082 (2)	0.0728 (2)	0.0231 (7)
C44	0.7338 (3)	0.1558 (2)	0.0219 (2)	0.0270 (8)
C45	0.6554 (3)	0.1602 (3)	-0.0123 (2)	0.0312 (9)
C46	0.5817 (3)	0.2207 (3)	0.0014 (3)	0.0339 (9)
C47	0.5896 (3)	0.2774 (2)	0.0480 (2)	0.0299 (8)

C48	0.6680 (3)	0.2697 (2)	0.0821 (2)	0.0246 (8)	
C49	0.9330 (3)	0.2601 (2)	0.0168 (2)	0.0221 (7)	
C50	1.0032 (3)	0.2259 (2)	-0.0421 (2)	0.0256 (8)	
C51	1.0698 (3)	0.2809 (3)	-0.1188 (2)	0.0266 (8)	
C52	1.0678 (3)	0.3745 (3)	-0.1411 (2)	0.0292 (8)	
C53	0.9984 (3)	0.4116 (2)	-0.0859 (2)	0.0273 (8)	
C54	0.9335 (3)	0.3553 (2)	-0.0105 (2)	0.0245 (8)	
C55	0.8299 (3)	0.2420 (2)	0.1879 (2)	0.0223 (7)	
C56	0.9035 (3)	0.2909 (2)	0.1992 (2)	0.0245 (8)	
C57	0.8893 (3)	0.3211 (2)	0.2696 (2)	0.0284 (8)	
C58	0.7979 (3)	0.3032 (2)	0.3339 (2)	0.0313 (9)	
C59	0.7230 (3)	0.2533 (2)	0.3277 (2)	0.0292 (8)	
C60	0.7413 (3)	0.2234 (2)	0.2565 (2)	0.0254 (8)	
C61	0.8718 (3)	0.0923 (2)	0.1483 (2)	0.0231 (7)	
C62	0.9665 (3)	0.0714 (2)	0.1555 (2)	0.0249 (8)	
C63	0.9933 (3)	-0.0154 (3)	0.1944 (3)	0.0298 (9)	
C64	0.9221 (3)	-0.0866 (2)	0.2319 (2)	0.0305 (9)	
C65	0.8251 (3)	-0.0704 (2)	0.2285 (2)	0.0281 (8)	
C66	0.8022 (3)	0.0170 (2)	0.1872 (2)	0.0248 (8)	
C67	-0.0752 (11)	0.5150 (8)	0.4112 (9)	0.122 (4)	0.66
H67A	-0.1126	0.4909	0.3823	0.147*	0.66
H67B	-0.1082	0.4896	0.4730	0.147*	0.66
N1	0.5823 (2)	0.74187 (18)	0.18139 (18)	0.0220 (6)	
N2	0.3514 (2)	0.66832 (19)	0.25244 (19)	0.0261 (7)	
N3	0.3360 (2)	1.0299 (2)	0.43409 (19)	0.0253 (7)	
N4	0.1783 (2)	0.92465 (19)	0.39265 (18)	0.0232 (6)	
B1	0.8452 (3)	0.2007 (3)	0.1062 (3)	0.0231 (8)	
C11	0.0568 (4)	0.4763 (3)	0.3846 (3)	0.1616 (17)	0.66
C12	-0.0800 (3)	0.6230 (2)	0.3838 (2)	0.1332 (14)	0.66
F1	0.80500 (17)	0.09582 (14)	0.00363 (14)	0.0345 (5)	
F2	0.65082 (19)	0.10489 (16)	-0.05899 (16)	0.0464 (6)	
F3	0.50501 (19)	0.22623 (18)	-0.03129 (17)	0.0510 (7)	
F4	0.51852 (18)	0.33806 (16)	0.06101 (16)	0.0429 (6)	
F5	0.66725 (16)	0.32833 (13)	0.12742 (14)	0.0308 (5)	
F6	1.01229 (16)	0.13451 (13)	-0.02676 (14)	0.0329 (5)	
F7	1.13855 (17)	0.24295 (16)	-0.17102 (14)	0.0390 (6)	
F8	1.13372 (18)	0.42857 (16)	-0.21388 (14)	0.0423 (6)	
F9	0.99416 (18)	0.50378 (14)	-0.10509 (14)	0.0404 (6)	
F10	0.86536 (16)	0.39738 (13)	0.03881 (13)	0.0302 (5)	
F11	0.99707 (16)	0.31049 (14)	0.14062 (13)	0.0294 (5)	
F12	0.96573 (18)	0.36638 (15)	0.27686 (14)	0.0392 (6)	
F13	0.7830 (2)	0.33331 (15)	0.40263 (14)	0.0443 (6)	
F14	0.63277 (17)	0.23398 (15)	0.38999 (13)	0.0387 (6)	
F15	0.66365 (16)	0.17265 (15)	0.25679 (14)	0.0328 (5)	
F16	1.04155 (16)	0.13871 (14)	0.12469 (15)	0.0335 (5)	
F17	1.08923 (18)	-0.02941 (15)	0.19654 (17)	0.0445 (6)	
F18	0.9457 (2)	-0.17045 (14)	0.27213 (16)	0.0462 (6)	
F19	0.75214 (17)	-0.13898 (14)	0.26455 (14)	0.0376 (5)	
F20	0.70486 (16)	0.02546 (13)	0.18756 (14)	0.0331 (5)	

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I1	0.430471 (19)	0.815649 (18)	0.374301 (16)	0.03229 (7)
Pt1	0.478070 (11)	0.658600 (9)	0.304310 (9)	0.02414 (4)
Pt2	0.331383 (10)	0.990179 (9)	0.322963 (8)	0.02269 (4)
Si1	0.52290 (8)	0.54261 (7)	0.24778 (7)	0.0265 (2)
Si2	0.25226 (8)	1.12171 (7)	0.29133 (6)	0.0266 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.030 (2)	0.0266 (19)	0.033 (2)	0.0078 (16)	-0.0137 (17)	-0.0125 (16)
C2	0.038 (2)	0.0187 (18)	0.041 (2)	-0.0007 (16)	-0.0136 (19)	-0.0070 (16)
C3	0.025 (2)	0.032 (2)	0.031 (2)	-0.0043 (16)	-0.0069 (17)	-0.0069 (16)
C4	0.0215 (19)	0.0306 (19)	0.0257 (19)	0.0018 (15)	-0.0117 (16)	-0.0103 (15)
C5	0.021 (2)	0.039 (2)	0.034 (2)	0.0022 (16)	-0.0084 (17)	-0.0172 (17)
C6	0.025 (2)	0.041 (2)	0.038 (2)	0.0112 (17)	-0.0107 (18)	-0.0243 (19)
C7	0.026 (2)	0.0279 (19)	0.037 (2)	0.0045 (16)	-0.0079 (17)	-0.0150 (17)
C8	0.023 (2)	0.0248 (18)	0.030 (2)	0.0029 (15)	-0.0096 (16)	-0.0106 (15)
C9	0.0219 (19)	0.0233 (17)	0.0265 (18)	0.0042 (14)	-0.0135 (15)	-0.0091 (14)
C10	0.028 (2)	0.038 (2)	0.049 (3)	0.0072 (18)	-0.0157 (19)	-0.0207 (19)
C11	0.029 (2)	0.042 (2)	0.062 (3)	0.0119 (19)	-0.020 (2)	-0.017 (2)
C12	0.030 (2)	0.046 (3)	0.057 (3)	0.0048 (19)	-0.024 (2)	-0.016 (2)
C13	0.027 (2)	0.033 (2)	0.041 (2)	-0.0037 (17)	-0.0148 (19)	-0.0089 (18)
C14	0.046 (3)	0.044 (3)	0.056 (3)	-0.006 (2)	-0.030 (2)	-0.017 (2)
C15	0.056 (3)	0.039 (2)	0.063 (3)	0.000 (2)	-0.032 (3)	-0.025 (2)
C16	0.037 (2)	0.028 (2)	0.047 (3)	0.0009 (18)	-0.015 (2)	-0.0143 (18)
C17	0.025 (2)	0.0246 (18)	0.035 (2)	-0.0016 (15)	-0.0071 (17)	-0.0070 (16)
C18	0.024 (2)	0.0255 (18)	0.032 (2)	-0.0060 (15)	-0.0071 (17)	-0.0061 (16)
C19	0.036 (2)	0.039 (2)	0.041 (2)	0.0079 (19)	-0.023 (2)	-0.0129 (19)
C20	0.041 (3)	0.045 (2)	0.033 (2)	0.001 (2)	-0.006 (2)	-0.0075 (19)
C21	0.043 (3)	0.027 (2)	0.044 (2)	0.0059 (18)	-0.014 (2)	-0.0039 (18)
C22	0.025 (2)	0.041 (2)	0.028 (2)	0.0012 (17)	-0.0071 (17)	-0.0132 (17)
C23	0.025 (2)	0.057 (3)	0.026 (2)	-0.0005 (19)	-0.0082 (17)	-0.0142 (19)
C24	0.023 (2)	0.071 (3)	0.037 (2)	-0.005 (2)	-0.0051 (18)	-0.032 (2)
C25	0.023 (2)	0.046 (2)	0.035 (2)	-0.0100 (18)	-0.0017 (17)	-0.0210 (19)
C26	0.045 (3)	0.051 (3)	0.055 (3)	-0.011 (2)	-0.009 (2)	-0.032 (2)
C27	0.061 (3)	0.037 (2)	0.070 (4)	-0.006 (2)	-0.012 (3)	-0.029 (2)
C28	0.044 (3)	0.028 (2)	0.047 (3)	-0.0074 (19)	-0.007 (2)	-0.0069 (19)
C29	0.019 (2)	0.034 (2)	0.035 (2)	-0.0111 (16)	0.0020 (17)	-0.0158 (17)
C30	0.0191 (19)	0.037 (2)	0.030 (2)	-0.0086 (16)	0.0017 (16)	-0.0160 (17)
C31	0.028 (2)	0.0264 (19)	0.034 (2)	0.0035 (16)	-0.0057 (17)	-0.0099 (16)
C32	0.028 (2)	0.027 (2)	0.041 (2)	-0.0037 (17)	0.0011 (19)	-0.0039 (17)
C33	0.024 (2)	0.036 (2)	0.037 (2)	-0.0094 (17)	0.0018 (18)	-0.0098 (18)
C34	0.023 (2)	0.033 (2)	0.0257 (19)	0.0006 (16)	-0.0065 (16)	-0.0115 (16)
C35	0.0159 (19)	0.047 (2)	0.036 (2)	0.0026 (17)	-0.0062 (17)	-0.0152 (19)
C36	0.026 (2)	0.042 (2)	0.042 (2)	0.0094 (18)	-0.0118 (19)	-0.0117 (19)
C37	0.035 (2)	0.032 (2)	0.035 (2)	0.0048 (18)	-0.0134 (19)	-0.0078 (17)
C38	0.023 (2)	0.0305 (19)	0.0222 (18)	0.0027 (15)	-0.0082 (15)	-0.0082 (15)
C39	0.0232 (19)	0.0260 (18)	0.0190 (17)	0.0010 (15)	-0.0055 (15)	-0.0076 (14)

C40	0.023 (2)	0.050 (2)	0.033 (2)	-0.0066 (18)	-0.0069 (18)	-0.0100 (19)
C41	0.033 (2)	0.040 (2)	0.030 (2)	0.0048 (18)	-0.0141 (18)	-0.0167 (17)
C42	0.051 (3)	0.041 (2)	0.034 (2)	-0.003 (2)	-0.011 (2)	-0.0003 (19)
C43	0.0203 (19)	0.0215 (17)	0.0249 (18)	-0.0007 (14)	-0.0063 (15)	-0.0041 (14)
C44	0.028 (2)	0.0244 (18)	0.029 (2)	0.0018 (15)	-0.0063 (17)	-0.0106 (15)
C45	0.039 (2)	0.031 (2)	0.029 (2)	-0.0019 (17)	-0.0135 (18)	-0.0128 (16)
C46	0.032 (2)	0.041 (2)	0.032 (2)	-0.0040 (18)	-0.0189 (18)	-0.0066 (17)
C47	0.027 (2)	0.031 (2)	0.031 (2)	0.0049 (16)	-0.0101 (17)	-0.0070 (16)
C48	0.027 (2)	0.0216 (17)	0.0259 (19)	-0.0005 (15)	-0.0079 (16)	-0.0087 (14)
C49	0.0234 (19)	0.0218 (17)	0.0244 (18)	-0.0006 (14)	-0.0113 (15)	-0.0079 (14)
C50	0.027 (2)	0.0264 (18)	0.030 (2)	0.0014 (15)	-0.0126 (17)	-0.0142 (15)
C51	0.023 (2)	0.036 (2)	0.0249 (19)	0.0027 (16)	-0.0082 (16)	-0.0150 (16)
C52	0.027 (2)	0.038 (2)	0.0196 (18)	-0.0052 (17)	-0.0067 (16)	-0.0050 (16)
C53	0.030 (2)	0.0235 (18)	0.030 (2)	0.0014 (16)	-0.0147 (17)	-0.0064 (15)
C54	0.024 (2)	0.0263 (18)	0.0263 (19)	0.0054 (15)	-0.0099 (16)	-0.0111 (15)
C55	0.0236 (19)	0.0178 (16)	0.0267 (19)	0.0062 (14)	-0.0102 (16)	-0.0069 (14)
C56	0.026 (2)	0.0209 (17)	0.0268 (19)	0.0061 (15)	-0.0090 (16)	-0.0068 (14)
C57	0.034 (2)	0.0236 (18)	0.035 (2)	0.0036 (16)	-0.0185 (18)	-0.0124 (16)
C58	0.050 (3)	0.0279 (19)	0.0225 (19)	0.0107 (18)	-0.0155 (19)	-0.0140 (16)
C59	0.037 (2)	0.0258 (18)	0.0197 (18)	0.0090 (17)	-0.0048 (17)	-0.0047 (15)
C60	0.026 (2)	0.0230 (18)	0.0276 (19)	0.0065 (15)	-0.0106 (16)	-0.0066 (15)
C61	0.027 (2)	0.0216 (17)	0.0232 (18)	0.0035 (15)	-0.0068 (15)	-0.0109 (14)
C62	0.024 (2)	0.0241 (18)	0.0297 (19)	0.0009 (15)	-0.0084 (16)	-0.0131 (15)
C63	0.029 (2)	0.033 (2)	0.040 (2)	0.0115 (17)	-0.0191 (18)	-0.0206 (17)
C64	0.041 (2)	0.0207 (18)	0.033 (2)	0.0080 (17)	-0.0154 (19)	-0.0089 (15)
C65	0.031 (2)	0.0205 (18)	0.029 (2)	-0.0015 (15)	-0.0021 (17)	-0.0092 (15)
C66	0.022 (2)	0.0254 (18)	0.0288 (19)	0.0053 (15)	-0.0064 (16)	-0.0134 (15)
C67	0.143 (13)	0.089 (8)	0.153 (12)	-0.002 (8)	-0.070 (10)	-0.036 (8)
N1	0.0207 (16)	0.0228 (15)	0.0270 (16)	0.0059 (12)	-0.0123 (13)	-0.0095 (12)
N2	0.0222 (17)	0.0270 (16)	0.0294 (17)	0.0026 (13)	-0.0087 (14)	-0.0089 (13)
N3	0.0203 (16)	0.0320 (16)	0.0239 (16)	-0.0031 (13)	-0.0038 (13)	-0.0114 (13)
N4	0.0196 (16)	0.0273 (15)	0.0239 (15)	0.0021 (12)	-0.0068 (13)	-0.0098 (12)
B1	0.022 (2)	0.0231 (19)	0.026 (2)	0.0051 (16)	-0.0076 (18)	-0.0109 (16)
Cl1	0.230 (5)	0.125 (3)	0.132 (3)	-0.012 (3)	-0.052 (3)	-0.046 (3)
Cl2	0.227 (4)	0.0683 (17)	0.109 (2)	0.004 (2)	-0.059 (3)	-0.0270 (17)
F1	0.0365 (13)	0.0351 (12)	0.0415 (13)	0.0090 (10)	-0.0138 (11)	-0.0243 (10)
F2	0.0575 (17)	0.0516 (15)	0.0496 (15)	0.0035 (13)	-0.0287 (13)	-0.0308 (12)
F3	0.0483 (16)	0.0623 (17)	0.0609 (17)	0.0088 (13)	-0.0394 (14)	-0.0230 (14)
F4	0.0345 (14)	0.0459 (14)	0.0552 (15)	0.0181 (11)	-0.0223 (12)	-0.0193 (12)
F5	0.0315 (12)	0.0289 (11)	0.0412 (13)	0.0090 (9)	-0.0164 (10)	-0.0197 (10)
F6	0.0344 (13)	0.0274 (11)	0.0356 (12)	0.0053 (10)	-0.0037 (10)	-0.0156 (9)
F7	0.0351 (14)	0.0508 (14)	0.0324 (12)	0.0082 (11)	-0.0041 (10)	-0.0218 (11)
F8	0.0413 (15)	0.0462 (14)	0.0259 (12)	-0.0078 (11)	-0.0004 (11)	-0.0015 (10)
F9	0.0503 (16)	0.0245 (11)	0.0375 (13)	-0.0016 (10)	-0.0089 (11)	-0.0014 (10)
F10	0.0314 (12)	0.0259 (11)	0.0321 (12)	0.0082 (9)	-0.0054 (10)	-0.0125 (9)
F11	0.0254 (12)	0.0312 (11)	0.0338 (12)	-0.0026 (9)	-0.0078 (10)	-0.0141 (9)
F12	0.0512 (16)	0.0380 (13)	0.0384 (13)	-0.0025 (11)	-0.0218 (12)	-0.0174 (11)
F13	0.0676 (18)	0.0432 (14)	0.0308 (13)	0.0115 (12)	-0.0183 (12)	-0.0215 (11)
F14	0.0389 (14)	0.0422 (13)	0.0259 (12)	0.0090 (11)	0.0002 (10)	-0.0092 (10)

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F15	0.0253 (12)	0.0407 (13)	0.0308 (12)	-0.0036 (10)	-0.0047 (10)	-0.0122 (10)
F16	0.0258 (12)	0.0298 (11)	0.0483 (14)	0.0018 (9)	-0.0151 (11)	-0.0133 (10)
F17	0.0377 (14)	0.0392 (13)	0.0698 (17)	0.0144 (11)	-0.0332 (13)	-0.0204 (12)
F18	0.0625 (17)	0.0247 (12)	0.0569 (16)	0.0114 (11)	-0.0330 (14)	-0.0071 (11)
F19	0.0394 (14)	0.0227 (11)	0.0410 (13)	-0.0037 (10)	-0.0002 (11)	-0.0082 (10)
F20	0.0224 (12)	0.0244 (11)	0.0470 (14)	0.0016 (9)	-0.0054 (10)	-0.0091 (10)
I1	0.02772 (14)	0.04357 (15)	0.03540 (14)	0.01162 (11)	-0.01362 (11)	-0.02336 (12)
Pt1	0.02348 (8)	0.02635 (8)	0.02421 (8)	0.00427 (6)	-0.00920 (6)	-0.00873 (6)
Pt2	0.01752 (8)	0.03071 (8)	0.02077 (7)	-0.00020 (6)	-0.00455 (6)	-0.01054 (6)
Si1	0.0257 (6)	0.0216 (5)	0.0317 (6)	0.0034 (4)	-0.0097 (5)	-0.0072 (4)
Si2	0.0246 (6)	0.0280 (5)	0.0243 (5)	-0.0037 (4)	-0.0058 (4)	-0.0054 (4)

Geometric parameters (Å, °)

C1—N1	1.331 (4)	C36—H36A	0.9300
C1—C2	1.399 (5)	C37—C38	1.375 (5)
C1—H1A	0.9300	C37—H37A	0.9300
C2—C3	1.357 (5)	C38—C39	1.419 (5)
C2—H2A	0.9300	C38—Si2	1.879 (4)
C3—C4	1.421 (5)	C39—N4	1.380 (4)
C3—H3A	0.9300	C40—Pt2	2.060 (4)
C4—C5	1.409 (5)	C40—H40A	0.9600
C4—C9	1.413 (5)	C40—H40B	0.9600
C5—C6	1.364 (5)	C40—H40C	0.9600
C5—H5A	0.9300	C41—Pt2	2.054 (3)
C6—C7	1.393 (5)	C41—H41A	0.9600
C6—H6A	0.9300	C41—H41B	0.9600
C7—C8	1.376 (5)	C41—H41C	0.9600
C7—H7A	0.9300	C42—Si2	1.846 (4)
C8—C9	1.418 (5)	C42—H42A	0.9600
C8—Si1	1.870 (4)	C42—H42B	0.9600
C9—N1	1.387 (4)	C42—H42C	0.9600
C10—N2	1.328 (5)	C43—C48	1.391 (5)
C10—C11	1.403 (6)	C43—C44	1.395 (5)
C10—H10A	0.9300	C43—B1	1.664 (5)
C11—C12	1.366 (6)	C44—F1	1.355 (4)
C11—H11A	0.9300	C44—C45	1.379 (5)
C12—C13	1.395 (6)	C45—F2	1.349 (4)
C12—H12A	0.9300	C45—C46	1.371 (5)
C13—C14	1.412 (6)	C46—F3	1.337 (4)
C13—C18	1.427 (5)	C46—C47	1.378 (5)
C14—C15	1.360 (6)	C47—F4	1.346 (4)
C14—H14A	0.9300	C47—C48	1.373 (5)
C15—C16	1.406 (6)	C48—F5	1.357 (4)
C15—H15A	0.9300	C49—C50	1.387 (5)
C16—C17	1.380 (5)	C49—C54	1.388 (5)
C16—H16A	0.9300	C49—B1	1.656 (5)
C17—C18	1.414 (5)	C50—F6	1.354 (4)
C17—Si1	1.877 (4)	C50—C51	1.387 (5)

C18—N2	1.387 (4)	C51—F7	1.342 (4)
C19—Pt1	2.059 (4)	C51—C52	1.370 (5)
C19—H19A	0.9600	C52—F8	1.342 (4)
C19—H19B	0.9600	C52—C53	1.369 (5)
C19—H19C	0.9600	C53—F9	1.354 (4)
C20—Pt1	2.062 (4)	C53—C54	1.372 (5)
C20—H20A	0.9600	C54—F10	1.351 (4)
C20—H20B	0.9600	C55—C60	1.381 (5)
C20—H20C	0.9600	C55—C56	1.387 (5)
C21—Si1	1.860 (4)	C55—B1	1.663 (5)
C21—H21A	0.9600	C56—F11	1.353 (4)
C21—H21B	0.9600	C56—C57	1.378 (5)
C21—H21C	0.9600	C57—F12	1.350 (4)
C22—N3	1.316 (5)	C57—C58	1.372 (5)
C22—C23	1.411 (5)	C58—F13	1.350 (4)
C22—H22A	0.9300	C58—C59	1.367 (6)
C23—C24	1.352 (6)	C59—F14	1.345 (4)
C23—H23A	0.9300	C59—C60	1.381 (5)
C24—C25	1.408 (6)	C60—F15	1.355 (4)
C24—H24A	0.9300	C61—C62	1.376 (5)
C25—C26	1.418 (6)	C61—C66	1.391 (5)
C25—C30	1.422 (5)	C61—B1	1.673 (5)
C26—C27	1.346 (7)	C62—F16	1.359 (4)
C26—H26A	0.9300	C62—C63	1.385 (5)
C27—C28	1.410 (6)	C63—F17	1.353 (4)
C27—H27A	0.9300	C63—C64	1.361 (5)
C28—C29	1.400 (5)	C64—F18	1.339 (4)
C28—H28A	0.9300	C64—C65	1.376 (5)
C29—C30	1.402 (6)	C65—F19	1.349 (4)
C29—Si2	1.879 (4)	C65—C66	1.385 (5)
C30—N3	1.393 (5)	C66—F20	1.352 (4)
C31—N4	1.314 (4)	C67—Cl2	1.582 (11)
C31—C32	1.404 (5)	C67—Cl1	1.869 (14)
C31—H31A	0.9300	C67—H67A	0.9700
C32—C33	1.347 (5)	C67—H67B	0.9700
C32—H32A	0.9300	N1—Pt1	2.184 (3)
C33—C34	1.409 (5)	N2—Pt1	2.186 (3)
C33—H33A	0.9300	N3—Pt2	2.190 (3)
C34—C35	1.416 (5)	N4—Pt2	2.199 (3)
C34—C39	1.424 (5)	I1—Pt2	2.9720 (3)
C35—C36	1.357 (6)	I1—Pt1	2.9770 (3)
C35—H35A	0.9300	Pt1—Si1	2.2591 (10)
C36—C37	1.415 (6)	Pt2—Si2	2.2556 (10)
N1—C1—C2	123.7 (3)	H42A—C42—H42C	109.5
N1—C1—H1A	118.1	H42B—C42—H42C	109.5
C2—C1—H1A	118.1	C48—C43—C44	112.5 (3)
C3—C2—C1	119.2 (3)	C48—C43—B1	127.1 (3)
C3—C2—H2A	120.4	C44—C43—B1	120.1 (3)
C1—C2—H2A	120.4	F1—C44—C45	116.2 (3)

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C2—C3—C4	119.6 (4)	F1—C44—C43	119.2 (3)
C2—C3—H3A	120.2	C45—C44—C43	124.6 (3)
C4—C3—H3A	120.2	F2—C45—C46	119.9 (3)
C5—C4—C9	119.4 (3)	F2—C45—C44	120.3 (3)
C5—C4—C3	122.4 (3)	C46—C45—C44	119.8 (3)
C9—C4—C3	118.2 (3)	F3—C46—C45	120.9 (3)
C6—C5—C4	119.7 (4)	F3—C46—C47	120.6 (4)
C6—C5—H5A	120.1	C45—C46—C47	118.5 (3)
C4—C5—H5A	120.1	F4—C47—C48	121.0 (3)
C5—C6—C7	120.7 (3)	F4—C47—C46	119.2 (3)
C5—C6—H6A	119.7	C48—C47—C46	119.7 (3)
C7—C6—H6A	119.7	F5—C48—C47	114.4 (3)
C8—C7—C6	122.0 (3)	F5—C48—C43	120.7 (3)
C8—C7—H7A	119.0	C47—C48—C43	124.9 (3)
C6—C7—H7A	119.0	C50—C49—C54	113.0 (3)
C7—C8—C9	118.0 (3)	C50—C49—B1	127.2 (3)
C7—C8—Si1	125.0 (3)	C54—C49—B1	119.4 (3)
C9—C8—Si1	116.8 (3)	F6—C50—C49	121.2 (3)
N1—C9—C4	121.1 (3)	F6—C50—C51	115.1 (3)
N1—C9—C8	118.7 (3)	C49—C50—C51	123.7 (3)
C4—C9—C8	120.2 (3)	F7—C51—C52	119.3 (3)
N2—C10—C11	123.6 (4)	F7—C51—C50	120.4 (3)
N2—C10—H10A	118.2	C52—C51—C50	120.3 (3)
C11—C10—H10A	118.2	F8—C52—C53	120.8 (3)
C12—C11—C10	118.7 (4)	F8—C52—C51	121.0 (3)
C12—C11—H11A	120.7	C53—C52—C51	118.2 (3)
C10—C11—H11A	120.7	F9—C53—C52	120.2 (3)
C11—C12—C13	120.4 (4)	F9—C53—C54	119.8 (3)
C11—C12—H12A	119.8	C52—C53—C54	120.0 (3)
C13—C12—H12A	119.8	F10—C54—C53	116.1 (3)
C12—C13—C14	123.5 (4)	F10—C54—C49	119.1 (3)
C12—C13—C18	118.4 (4)	C53—C54—C49	124.7 (3)
C14—C13—C18	118.1 (4)	C60—C55—C56	112.9 (3)
C15—C14—C13	120.9 (4)	C60—C55—B1	121.3 (3)
C15—C14—H14A	119.5	C56—C55—B1	125.6 (3)
C13—C14—H14A	119.5	F11—C56—C57	115.1 (3)
C14—C15—C16	120.2 (4)	F11—C56—C55	120.8 (3)
C14—C15—H15A	119.9	C57—C56—C55	124.0 (3)
C16—C15—H15A	119.9	F12—C57—C58	119.6 (3)
C17—C16—C15	121.9 (4)	F12—C57—C56	120.5 (3)
C17—C16—H16A	119.1	C58—C57—C56	119.9 (3)
C15—C16—H16A	119.1	F13—C58—C59	120.7 (4)
C16—C17—C18	117.9 (4)	F13—C58—C57	120.3 (4)
C16—C17—Si1	123.5 (3)	C59—C58—C57	118.9 (3)
C18—C17—Si1	118.4 (3)	F14—C59—C58	120.3 (3)
N2—C18—C17	118.5 (3)	F14—C59—C60	120.7 (4)
N2—C18—C13	120.5 (3)	C58—C59—C60	119.0 (4)
C17—C18—C13	120.9 (3)	F15—C60—C59	115.0 (3)
Pt1—C19—H19A	109.5	F15—C60—C55	119.9 (3)

Pt1—C19—H19B	109.5	C59—C60—C55	125.1 (4)
H19A—C19—H19B	109.5	C62—C61—C66	113.1 (3)
Pt1—C19—H19C	109.5	C62—C61—B1	121.0 (3)
H19A—C19—H19C	109.5	C66—C61—B1	125.6 (3)
H19B—C19—H19C	109.5	F16—C62—C61	120.1 (3)
Pt1—C20—H20A	109.5	F16—C62—C63	115.1 (3)
Pt1—C20—H20B	109.5	C61—C62—C63	124.8 (3)
H20A—C20—H20B	109.5	F17—C63—C64	119.8 (3)
Pt1—C20—H20C	109.5	F17—C63—C62	120.4 (3)
H20A—C20—H20C	109.5	C64—C63—C62	119.7 (3)
H20B—C20—H20C	109.5	F18—C64—C63	120.6 (4)
Si1—C21—H21A	109.5	F18—C64—C65	120.8 (4)
Si1—C21—H21B	109.5	C63—C64—C65	118.5 (3)
H21A—C21—H21B	109.5	F19—C65—C64	120.6 (3)
Si1—C21—H21C	109.5	F19—C65—C66	119.5 (3)
H21A—C21—H21C	109.5	C64—C65—C66	119.9 (3)
H21B—C21—H21C	109.5	F20—C66—C65	115.1 (3)
N3—C22—C23	123.6 (4)	F20—C66—C61	121.0 (3)
N3—C22—H22A	118.2	C65—C66—C61	123.9 (3)
C23—C22—H22A	118.2	Cl2—C67—Cl1	113.3 (8)
C24—C23—C22	119.1 (4)	Cl2—C67—H67A	108.9
C24—C23—H23A	120.5	Cl1—C67—H67A	108.9
C22—C23—H23A	120.5	Cl2—C67—H67B	108.9
C23—C24—C25	120.2 (4)	Cl1—C67—H67B	108.9
C23—C24—H24A	119.9	H67A—C67—H67B	107.7
C25—C24—H24A	119.9	C1—N1—C9	118.1 (3)
C24—C25—C26	123.8 (4)	C1—N1—Pt1	123.7 (2)
C24—C25—C30	118.0 (4)	C9—N1—Pt1	118.1 (2)
C26—C25—C30	118.1 (4)	C10—N2—C18	118.4 (3)
C27—C26—C25	121.2 (4)	C10—N2—Pt1	123.4 (3)
C27—C26—H26A	119.4	C18—N2—Pt1	118.2 (2)
C25—C26—H26A	119.4	C22—N3—C30	118.3 (3)
C26—C27—C28	120.5 (4)	C22—N3—Pt2	123.7 (2)
C26—C27—H27A	119.8	C30—N3—Pt2	117.8 (2)
C28—C27—H27A	119.8	C31—N4—C39	118.7 (3)
C29—C28—C27	121.0 (4)	C31—N4—Pt2	124.3 (2)
C29—C28—H28A	119.5	C39—N4—Pt2	116.9 (2)
C27—C28—H28A	119.5	C49—B1—C55	113.0 (3)
C28—C29—C30	118.1 (4)	C49—B1—C43	101.6 (3)
C28—C29—Si2	124.2 (3)	C55—B1—C43	113.4 (3)
C30—C29—Si2	117.7 (3)	C49—B1—C61	114.6 (3)
N3—C30—C29	118.1 (3)	C55—B1—C61	101.8 (3)
N3—C30—C25	120.8 (4)	C43—B1—C61	113.0 (3)
C29—C30—C25	121.1 (4)	Pt2—I1—Pt1	133.755 (10)
N4—C31—C32	123.8 (4)	C19—Pt1—C20	89.23 (18)
N4—C31—H31A	118.1	C19—Pt1—N1	88.67 (14)
C32—C31—H31A	118.1	C20—Pt1—N1	175.45 (14)
C33—C32—C31	119.2 (4)	C19—Pt1—N2	175.02 (13)
C33—C32—H32A	120.4	C20—Pt1—N2	88.42 (15)

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C31—C32—H32A	120.4	N1—Pt1—N2	93.36 (11)
C32—C33—C34	119.6 (4)	C19—Pt1—Si1	90.71 (11)
C32—C33—H33A	120.2	C20—Pt1—Si1	92.18 (12)
C34—C33—H33A	120.2	N1—Pt1—Si1	83.81 (7)
C33—C34—C35	122.7 (4)	N2—Pt1—Si1	84.99 (8)
C33—C34—C39	118.6 (3)	C19—Pt1—I1	87.36 (11)
C35—C34—C39	118.7 (3)	C20—Pt1—I1	90.20 (12)
C36—C35—C34	120.9 (4)	N1—Pt1—I1	93.73 (7)
C36—C35—H35A	119.5	N2—Pt1—I1	97.04 (7)
C34—C35—H35A	119.5	Si1—Pt1—I1	176.91 (3)
C35—C36—C37	119.7 (4)	C41—Pt2—C40	87.51 (16)
C35—C36—H36A	120.1	C41—Pt2—N3	173.53 (13)
C37—C36—H36A	120.1	C40—Pt2—N3	89.24 (14)
C38—C37—C36	122.2 (4)	C41—Pt2—N4	91.29 (14)
C38—C37—H37A	118.9	C40—Pt2—N4	175.47 (14)
C36—C37—H37A	118.9	N3—Pt2—N4	91.53 (10)
C37—C38—C39	118.2 (3)	C41—Pt2—Si2	90.71 (11)
C37—C38—Si2	123.6 (3)	C40—Pt2—Si2	90.25 (12)
C39—C38—Si2	118.2 (3)	N3—Pt2—Si2	83.72 (8)
N4—C39—C38	119.5 (3)	N4—Pt2—Si2	85.39 (8)
N4—C39—C34	120.2 (3)	C41—Pt2—I1	91.84 (11)
C38—C39—C34	120.3 (3)	C40—Pt2—I1	91.38 (12)
Pt2—C40—H40A	109.5	N3—Pt2—I1	93.82 (8)
Pt2—C40—H40B	109.5	N4—Pt2—I1	93.03 (7)
H40A—C40—H40B	109.5	Si2—Pt2—I1	177.03 (3)
Pt2—C40—H40C	109.5	C21—Si1—C8	111.53 (18)
H40A—C40—H40C	109.5	C21—Si1—C17	112.32 (18)
H40B—C40—H40C	109.5	C8—Si1—C17	108.13 (16)
Pt2—C41—H41A	109.5	C21—Si1—Pt1	123.55 (14)
Pt2—C41—H41B	109.5	C8—Si1—Pt1	100.08 (11)
H41A—C41—H41B	109.5	C17—Si1—Pt1	99.61 (12)
Pt2—C41—H41C	109.5	C42—Si2—C38	111.40 (19)
H41A—C41—H41C	109.5	C42—Si2—C29	111.50 (19)
H41B—C41—H41C	109.5	C38—Si2—C29	109.66 (16)
Si2—C42—H42A	109.5	C42—Si2—Pt2	124.05 (15)
Si2—C42—H42B	109.5	C38—Si2—Pt2	99.38 (11)
H42A—C42—H42B	109.5	C29—Si2—Pt2	99.48 (13)
Si2—C42—H42C	109.5		
N1—C1—C2—C3	-0.3 (6)	F17—C63—C64—F18	1.0 (5)
C1—C2—C3—C4	1.0 (6)	C62—C63—C64—F18	-178.0 (3)
C2—C3—C4—C5	-179.1 (4)	F17—C63—C64—C65	-179.8 (3)
C2—C3—C4—C9	0.0 (5)	C62—C63—C64—C65	1.2 (5)
C9—C4—C5—C6	0.5 (5)	F18—C64—C65—F19	-1.1 (5)
C3—C4—C5—C6	179.6 (3)	C63—C64—C65—F19	179.8 (3)
C4—C5—C6—C7	1.1 (6)	F18—C64—C65—C66	179.5 (3)
C5—C6—C7—C8	-1.5 (6)	C63—C64—C65—C66	0.4 (5)
C6—C7—C8—C9	0.3 (6)	F19—C65—C66—F20	0.6 (5)
C6—C7—C8—Si1	175.0 (3)	C64—C65—C66—F20	180.0 (3)
C5—C4—C9—N1	177.5 (3)	F19—C65—C66—C61	179.8 (3)

C3—C4—C9—N1	-1.6 (5)	C64—C65—C66—C61	-0.8 (5)
C5—C4—C9—C8	-1.8 (5)	C62—C61—C66—F20	178.8 (3)
C3—C4—C9—C8	179.1 (3)	B1—C61—C66—F20	5.5 (5)
C7—C8—C9—N1	-177.9 (3)	C62—C61—C66—C65	-0.3 (5)
Si1—C8—C9—N1	6.9 (4)	B1—C61—C66—C65	-173.7 (3)
C7—C8—C9—C4	1.3 (5)	C2—C1—N1—C9	-1.3 (5)
Si1—C8—C9—C4	-173.8 (3)	C2—C1—N1—Pt1	174.0 (3)
N2—C10—C11—C12	-0.1 (7)	C4—C9—N1—C1	2.3 (5)
C10—C11—C12—C13	0.8 (7)	C8—C9—N1—C1	-178.5 (3)
C11—C12—C13—C14	180.0 (4)	C4—C9—N1—Pt1	-173.3 (2)
C11—C12—C13—C18	-0.5 (7)	C8—C9—N1—Pt1	6.0 (4)
C12—C13—C14—C15	-180.0 (4)	C11—C10—N2—C18	-0.9 (6)
C18—C13—C14—C15	0.5 (7)	C11—C10—N2—Pt1	-178.2 (3)
C13—C14—C15—C16	1.0 (7)	C17—C18—N2—C10	-178.0 (3)
C14—C15—C16—C17	-1.3 (7)	C13—C18—N2—C10	1.2 (5)
C15—C16—C17—C18	0.0 (6)	C17—C18—N2—Pt1	-0.6 (4)
C15—C16—C17—Si1	-175.3 (3)	C13—C18—N2—Pt1	178.6 (3)
C16—C17—C18—N2	-179.3 (3)	C23—C22—N3—C30	-1.3 (5)
Si1—C17—C18—N2	-3.8 (5)	C23—C22—N3—Pt2	173.2 (3)
C16—C17—C18—C13	1.5 (6)	C29—C30—N3—C22	-175.9 (3)
Si1—C17—C18—C13	177.1 (3)	C25—C30—N3—C22	3.2 (5)
C12—C13—C18—N2	-0.5 (6)	C29—C30—N3—Pt2	9.2 (4)
C14—C13—C18—N2	179.0 (4)	C25—C30—N3—Pt2	-171.6 (3)
C12—C13—C18—C17	178.7 (4)	C32—C31—N4—C39	1.8 (5)
C14—C13—C18—C17	-1.8 (6)	C32—C31—N4—Pt2	-173.9 (3)
N3—C22—C23—C24	-1.5 (6)	C38—C39—N4—C31	178.7 (3)
C22—C23—C24—C25	2.1 (6)	C34—C39—N4—C31	-2.1 (5)
C23—C24—C25—C26	178.4 (4)	C38—C39—N4—Pt2	-5.3 (4)
C23—C24—C25—C30	-0.2 (6)	C34—C39—N4—Pt2	173.9 (2)
C24—C25—C26—C27	-179.0 (4)	C50—C49—B1—C55	141.1 (3)
C30—C25—C26—C27	-0.4 (7)	C54—C49—B1—C55	-46.3 (4)
C25—C26—C27—C28	1.9 (7)	C50—C49—B1—C43	-97.1 (4)
C26—C27—C28—C29	-1.0 (7)	C54—C49—B1—C43	75.6 (4)
C27—C28—C29—C30	-1.4 (6)	C50—C49—B1—C61	25.0 (5)
C27—C28—C29—Si2	175.3 (3)	C54—C49—B1—C61	-162.4 (3)
C28—C29—C30—N3	-177.9 (3)	C60—C55—B1—C49	158.0 (3)
Si2—C29—C30—N3	5.1 (5)	C56—C55—B1—C49	-27.3 (5)
C28—C29—C30—C25	3.0 (6)	C60—C55—B1—C43	43.1 (4)
Si2—C29—C30—C25	-174.0 (3)	C56—C55—B1—C43	-142.3 (3)
C24—C25—C30—N3	-2.5 (6)	C60—C55—B1—C61	-78.6 (4)
C26—C25—C30—N3	178.8 (4)	C56—C55—B1—C61	96.1 (4)
C24—C25—C30—C29	176.6 (4)	C48—C43—B1—C49	-97.3 (4)
C26—C25—C30—C29	-2.1 (6)	C44—C43—B1—C49	75.6 (4)
N4—C31—C32—C33	0.0 (6)	C48—C43—B1—C55	24.3 (5)
C31—C32—C33—C34	-1.5 (6)	C44—C43—B1—C55	-162.8 (3)
C32—C33—C34—C35	-179.7 (4)	C48—C43—B1—C61	139.5 (3)
C32—C33—C34—C39	1.1 (6)	C44—C43—B1—C61	-47.6 (4)
C33—C34—C35—C36	-179.8 (4)	C62—C61—B1—C49	44.8 (4)
C39—C34—C35—C36	-0.6 (6)	C66—C61—B1—C49	-142.4 (3)

supplementary materials

C34—C35—C36—C37	0.1 (6)	C62—C61—B1—C55	-77.6 (4)
C35—C36—C37—C38	0.3 (6)	C66—C61—B1—C55	95.3 (4)
C36—C37—C38—C39	-0.3 (6)	C62—C61—B1—C43	160.4 (3)
C36—C37—C38—Si2	179.6 (3)	C66—C61—B1—C43	-26.7 (5)
C37—C38—C39—N4	178.9 (3)	C1—N1—Pt1—C19	-97.0 (3)
Si2—C38—C39—N4	-1.0 (4)	C9—N1—Pt1—C19	78.3 (3)
C37—C38—C39—C34	-0.2 (5)	C1—N1—Pt1—N2	87.6 (3)
Si2—C38—C39—C34	179.9 (3)	C9—N1—Pt1—N2	-97.1 (2)
C33—C34—C39—N4	0.7 (5)	C1—N1—Pt1—Si1	172.2 (3)
C35—C34—C39—N4	-178.5 (3)	C9—N1—Pt1—Si1	-12.5 (2)
C33—C34—C39—C38	179.9 (3)	C1—N1—Pt1—I1	-9.7 (3)
C35—C34—C39—C38	0.7 (5)	C9—N1—Pt1—I1	165.6 (2)
C48—C43—C44—F1	176.9 (3)	C10—N2—Pt1—C20	88.5 (3)
B1—C43—C44—F1	3.1 (5)	C18—N2—Pt1—C20	-88.9 (3)
C48—C43—C44—C45	-3.0 (5)	C10—N2—Pt1—N1	-95.7 (3)
B1—C43—C44—C45	-176.8 (3)	C18—N2—Pt1—N1	87.0 (3)
F1—C44—C45—F2	1.9 (5)	C10—N2—Pt1—Si1	-179.2 (3)
C43—C44—C45—F2	-178.3 (3)	C18—N2—Pt1—Si1	3.5 (3)
F1—C44—C45—C46	-178.4 (3)	C10—N2—Pt1—I1	-1.5 (3)
C43—C44—C45—C46	1.5 (6)	C18—N2—Pt1—I1	-178.9 (2)
F2—C45—C46—F3	-0.3 (6)	Pt2—I1—Pt1—C19	152.31 (12)
C44—C45—C46—F3	179.9 (4)	Pt2—I1—Pt1—C20	-118.47 (13)
F2—C45—C46—C47	-178.8 (3)	Pt2—I1—Pt1—N1	63.82 (7)
C44—C45—C46—C47	1.4 (6)	Pt2—I1—Pt1—N2	-30.04 (8)
F3—C46—C47—F4	0.6 (6)	C22—N3—Pt2—C40	-99.6 (3)
C45—C46—C47—F4	179.1 (3)	C30—N3—Pt2—C40	75.0 (3)
F3—C46—C47—C48	179.0 (3)	C22—N3—Pt2—N4	84.9 (3)
C45—C46—C47—C48	-2.5 (6)	C30—N3—Pt2—N4	-100.6 (3)
F4—C47—C48—F5	-1.0 (5)	C22—N3—Pt2—Si2	170.1 (3)
C46—C47—C48—F5	-179.3 (3)	C30—N3—Pt2—Si2	-15.4 (2)
F4—C47—C48—C43	179.1 (3)	C22—N3—Pt2—I1	-8.2 (3)
C46—C47—C48—C43	0.8 (6)	C30—N3—Pt2—I1	166.3 (2)
C44—C43—C48—F5	-178.0 (3)	C31—N4—Pt2—C41	92.5 (3)
B1—C43—C48—F5	-4.7 (6)	C39—N4—Pt2—C41	-83.2 (2)
C44—C43—C48—C47	1.8 (5)	C39—N4—Pt2—N3	91.0 (2)
B1—C43—C48—C47	175.1 (3)	C31—N4—Pt2—Si2	-176.9 (3)
C54—C49—C50—F6	-179.1 (3)	C39—N4—Pt2—Si2	7.4 (2)
B1—C49—C50—F6	-6.0 (5)	C31—N4—Pt2—I1	0.6 (3)
C54—C49—C50—C51	2.2 (5)	C39—N4—Pt2—I1	-175.1 (2)
B1—C49—C50—C51	175.2 (3)	Pt1—I1—Pt2—C41	-7.74 (12)
F6—C50—C51—F7	-1.5 (5)	Pt1—I1—Pt2—C40	-95.29 (11)
C49—C50—C51—F7	177.3 (3)	Pt1—I1—Pt2—N3	175.38 (8)
F6—C50—C51—C52	-179.9 (3)	Pt1—I1—Pt2—N4	83.64 (7)
C49—C50—C51—C52	-1.0 (6)	C7—C8—Si1—C21	38.2 (4)
F7—C51—C52—F8	-0.4 (5)	C9—C8—Si1—C21	-147.0 (3)
C50—C51—C52—F8	178.0 (3)	C7—C8—Si1—C17	-85.8 (3)
F7—C51—C52—C53	-178.6 (3)	C9—C8—Si1—C17	89.0 (3)
C50—C51—C52—C53	-0.3 (6)	C7—C8—Si1—Pt1	170.5 (3)
F8—C52—C53—F9	1.3 (5)	C9—C8—Si1—Pt1	-14.7 (3)

C51—C52—C53—F9	179.6 (3)	C16—C17—Si1—C21	-46.6 (4)
F8—C52—C53—C54	-178.0 (3)	C18—C17—Si1—C21	138.1 (3)
C51—C52—C53—C54	0.3 (6)	C16—C17—Si1—C8	76.9 (4)
F9—C53—C54—F10	2.8 (5)	C18—C17—Si1—C8	-98.4 (3)
C52—C53—C54—F10	-177.9 (3)	C16—C17—Si1—Pt1	-179.1 (3)
F9—C53—C54—C49	-178.2 (3)	C18—C17—Si1—Pt1	5.6 (3)
C52—C53—C54—C49	1.1 (6)	C19—Pt1—Si1—C21	48.3 (2)
C50—C49—C54—F10	176.8 (3)	C20—Pt1—Si1—C21	-41.0 (2)
B1—C49—C54—F10	3.2 (5)	N1—Pt1—Si1—C21	136.86 (19)
C50—C49—C54—C53	-2.3 (5)	N2—Pt1—Si1—C21	-129.2 (2)
B1—C49—C54—C53	-175.9 (3)	C19—Pt1—Si1—C8	-76.13 (17)
C60—C55—C56—F11	176.2 (3)	C20—Pt1—Si1—C8	-165.39 (17)
B1—C55—C56—F11	1.2 (5)	N1—Pt1—Si1—C8	12.45 (14)
C60—C55—C56—C57	-2.3 (5)	N2—Pt1—Si1—C8	106.39 (14)
B1—C55—C56—C57	-177.4 (3)	C19—Pt1—Si1—C17	173.35 (17)
F11—C56—C57—F12	-0.3 (5)	C20—Pt1—Si1—C17	84.08 (17)
C55—C56—C57—F12	178.3 (3)	N1—Pt1—Si1—C17	-98.07 (14)
F11—C56—C57—C58	-178.6 (3)	N2—Pt1—Si1—C17	-4.13 (14)
C55—C56—C57—C58	0.0 (5)	C37—C38—Si2—C42	-41.5 (4)
F12—C57—C58—F13	2.3 (5)	C39—C38—Si2—C42	138.4 (3)
C56—C57—C58—F13	-179.3 (3)	C37—C38—Si2—C29	82.4 (3)
F12—C57—C58—C59	-176.7 (3)	C39—C38—Si2—C29	-97.7 (3)
C56—C57—C58—C59	1.6 (5)	C37—C38—Si2—Pt2	-173.9 (3)
F13—C58—C59—F14	0.5 (5)	C39—C38—Si2—Pt2	6.0 (3)
C57—C58—C59—F14	179.5 (3)	C28—C29—Si2—C42	35.5 (4)
F13—C58—C59—C60	-179.8 (3)	C30—C29—Si2—C42	-147.7 (3)
C57—C58—C59—C60	-0.7 (5)	C28—C29—Si2—C38	-88.3 (4)
F14—C59—C60—F15	-1.8 (5)	C30—C29—Si2—C38	88.5 (3)
C58—C59—C60—F15	178.5 (3)	C28—C29—Si2—Pt2	168.1 (3)
F14—C59—C60—C55	177.8 (3)	C30—C29—Si2—Pt2	-15.2 (3)
C58—C59—C60—C55	-1.9 (5)	C41—Pt2—Si2—C42	-38.8 (2)
C56—C55—C60—F15	-177.1 (3)	C40—Pt2—Si2—C42	48.7 (2)
B1—C55—C60—F15	-1.9 (5)	N3—Pt2—Si2—C42	137.9 (2)
C56—C55—C60—C59	3.3 (5)	N4—Pt2—Si2—C42	-130.0 (2)
B1—C55—C60—C59	178.6 (3)	C41—Pt2—Si2—C38	85.15 (16)
C66—C61—C62—F16	-176.6 (3)	C40—Pt2—Si2—C38	172.66 (16)
B1—C61—C62—F16	-2.9 (5)	N3—Pt2—Si2—C38	-98.14 (13)
C66—C61—C62—C63	2.0 (5)	N4—Pt2—Si2—C38	-6.08 (13)
B1—C61—C62—C63	175.7 (3)	C41—Pt2—Si2—C29	-162.93 (16)
F16—C62—C63—F17	-2.9 (5)	C40—Pt2—Si2—C29	-75.42 (16)
C61—C62—C63—F17	178.5 (3)	N3—Pt2—Si2—C29	13.79 (14)
F16—C62—C63—C64	176.1 (3)	N4—Pt2—Si2—C29	105.84 (14)
C61—C62—C63—C64	-2.5 (6)		

Fig. 1

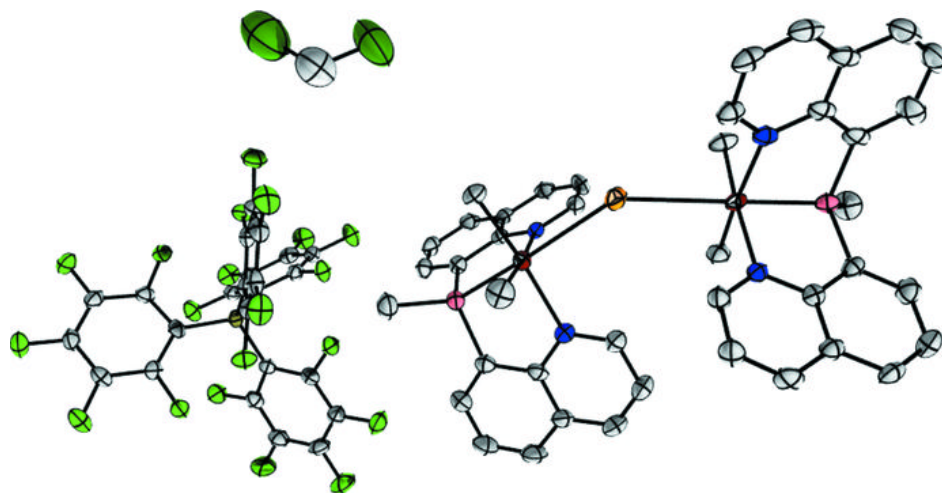


Fig. 2

