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Bis[bis(trimethylsilyl)cyclopentadienyl](chloro)uranium(III) bis(2,6-dimethylphenylisocyanide)

A. Zalkin and S.M. Beshouri

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Bis[bis(trimethylsilyl)cyclopentadienyl](chloro)uranium(III) bis(2,6-dimethylphenylisocyanide)

By Allan Zalkin and Sharon M. Beshouri

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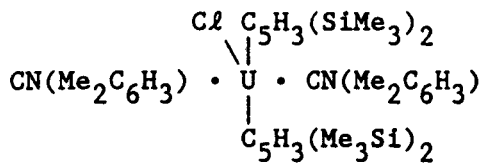
Abstract. $[(Me_3Si)_2C_5H_3]_2C\ell U\cdot 2(CNC_6H_3Me_2)$, M_r = 954.77, monoclinic, $P2_1/n$, a = 16.000(4), b = 22.806(4), c = 13.093(3) Å, β = 92.85(2), V = 4771.7, Z = 4, D_x = 1.33 g cm^{-3}, λ(MoKα) = 0.71073 Å, μ = 34.0 cm^{-1}, F(000) = 1916, T = 296 K, R = 0.031 for 4116 [$F^2>2\sigma(F^2)$] of 8437 total unique data. The uranium atom is five coordinate with distances: U-Cℓ 2.6865(20); U-Cp 2.505, 2.508; U-C(isocyanide) 2.654(9), 2.681(9); <U-C(cyclopentadiene)> 2.781(11).

Experimental. The compound, shown below, was prepared by reaction of one



equivalent of $[<C_5H_3(SiMe_3)_2>_2UC\ell]_2$ with four equivalents of $CN(Me_2C_6H_3)$ in diethyl ether solution. The product was dissolved in hexane solution, and dark crystals were isolated after cooling at -20°C.

A black air-sensitive crystal, 0.18 x 0.36 x 0.72 mm, was sealed inside a quartz capillary in an argon-filled drybox. X-ray diffraction intensities (θ-2θ scans) were obtained using a modified Picker FACS-I automatic diffractometer equipped with a graphite monochromator. Cell dimensions from 28 reflections, $20<2\theta<27°$; analytical absorption correction, range 1.78-3.09; max.$(\sin\theta)/\lambda = 0.60$ Å^{-1}, h -19 to 19, k 0 to 27, ℓ -15 to 15; three standard reflections, 1.1%, 1.6%, 0.8% variation in standards intensities from average, intensities adjusted isotropically; 12995 data, 8441 unique [including 4116, $F^2 < 3\sigma(F^2)$], $R_{int} = 0.075$; structure solved by Patterson and Fourier methods; refined on F, 433 parameters; H atoms included with estimated positional and isotropic thermal parameters; R = 0.12 (all data), R = 0.031 [$F^2>3\sigma(F^2)$ data], wR = 0.031, S = 1.0; $w = 4F^2[\sigma^2(F^2) + (0.035F^2)^2]^{-1}$; max. (shift/$\sigma$) < 0.001; no extinction correction indicated; max.,min. of ΔF synthesis 1.0, -1.8 e Å^{-3}; atomic f from International Tables for X-ray Crystallography (1974); local unpublished programs and ORTEP (Johnson, 1965).

Atomic parameters are listed in Table 1,* and distances and angles are listed in Table 2. Fig. 1 shows the molecule and the numbering scheme.

*Lists of structure factors, anisotropic thermal parameters, calculated hydrogen positions, distances and angles, and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. 00000 (22 pp). Copies may be obtained through The Executive Secretary International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. The U(III) dimer, $[<C_5H_3(SiMe_3)_2>_2UC\ell]_2$, has previously been prepared and structurally characterized (Blake, Lappert, Taylor, Atwood, Hunter & Zhang, 1986). The ability of isocyanides to act as good donor ligands toward uranium metal centers has been previously observed (Kanellakopulos, Fischer, Dornberger & Baumgartner, 1970).

Helpful discussions with Professor R. A. Andersen are appreciated. This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the US Department of Energy under Contract No. DE-AC03-76SF- 00098.

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International Tables for X-ray Crystallography (1974). Vol. IV; Table 2.2, pp. 71-102. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Johnson, C. K. (1965). ORTEP. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

Kanellakopulos, B., Fischer, E. O., Dornberger, E., & Baumgartner, F., (1970). J. Organomet. Chem., 24, 507-514.

Table 1. Atomic parameters

$$B_{eq} = 1/3 \sum_i \sum_j B_{ij} a_i^* a_j^* \cdot a_i a_j .$$

	x	y	z	B_{eq}(Å^2)
U	0.47976(2)	0.21461(1)	0.13690(2)	3.428(7)
Cℓ	0.56861(15)	0.26416(10)	0.29360(16)	6.13(7)
SI1	0.45200(16)	0.12623(12)	0.40786(17)	5.39(8)
SI2	0.22796(14)	0.18402(11)	0.05526(17)	4.72(7)
SI3	0.59890(17)	0.36651(12)	0.03497(19)	5.77(8)
SI4	0.54570(20)	0.13484(13)	-0.13756(21)	7.1(1)
N1	0.6855(4)	0.1313(3)	0.1778(5)	5.1(2)
N2	0.3692(4)	0.3514(4)	0.2263(5)	5.1(2)
C1	0.3437(5)	0.1708(4)	0.2369(5)	4.2(2)
C2	0.4118(5)	0.1353(4)	0.2728(5)	4.3(2)
C3	0.4351(5)	0.1011(3)	0.1862(6)	4.2(2)
C4	0.3807(5)	0.1154(3)	0.1016(5)	4.0(2)
C5	0.3238(5)	0.1595(3)	0.1306(5)	3.9(2)
C6	0.5818(5)	0.2432(4)	-0.0220(6)	4.8(3)
C7	0.5433(5)	0.2959(3)	0.0019(5)	4.4(3)
C8	0.4573(4)	0.2892(4)	-0.0292(5)	4.1(2)
C9	0.4458(5)	0.2330(4)	-0.0692(5)	4.4(2)
C10	0.5226(5)	0.2030(3)	-0.0652(5)	4.4(2)
C11	0.3966(7)	0.0627(5)	0.4661(7)	7.8(4)
C12	0.4305(7)	0.1937(4)	0.4819(6)	7.6(4)
C13	0.5654(6)	0.1078(4)	0.4167(7)	7.2(3)
C14	0.2267(5)	0.2627(4)	0.0230(7)	6.1(3)
C15	0.2182(6)	0.1388(4)	-0.0644(7)	6.6(3)

C16	0.1346(6)	0.1712(5)	0.1312(8)	8.2(4)
C17	0.6309(9)	0.4001(5)	-0.0858(8)	11.7(5)
C18	0.6949(7)	0.3546(5)	0.1165(8)	9.2(4)
C19	0.5317(8)	0.4178(5)	0.1007(11)	12.1(5)
C20	0.5762(10)	0.0716(5)	-0.0637(9)	13.2(6)
C21	0.6159(11)	0.1524(7)	-0.2363(12)	16.9(8)
C22	0.4474(9)	0.1129(6)	-0.2132(10)	13.6(6)
C23	0.6210(6)	0.1518(4)	0.1612(6)	5.3(3)
C24	0.3936(5)	0.3073(4)	0.1943(6)	4.7(3)
C25	0.7665(6)	0.1083(5)	0.1964(6)	5.4(3)
C26	0.7744(7)	0.0481(5)	0.2037(8)	7.2(4)
C27	0.8552(9)	0.0274(6)	0.2191(9)	9.4(5)
C28	0.9213(8)	0.0640(8)	0.2292(11)	10.8(6)
C29	0.9099(7)	0.1237(7)	0.2265(8)	8.6(5)
C30	0.8311(6)	0.1489(5)	0.2082(6)	6.5(4)
C31	0.3439(6)	0.4049(4)	0.2669(8)	5.6(3)
C32	0.2963(6)	0.4432(4)	0.2056(8)	5.9(3)
C33	0.2707(7)	0.4938(5)	0.2534(10)	7.5(4)
C34	0.2920(9)	0.5064(6)	0.3514(11)	9.8(5)
C35	0.3398(9)	0.4681(6)	0.4114(10)	10.7(6)
C36	0.3667(8)	0.4158(5)	0.3686(8)	8.7(4)
C37	0.6997(7)	0.0078(5)	0.1920(10)	10.3(5)
C38	0.8172(7)	0.2135(6)	0.2006(8)	8.3(4)
C39	0.2749(6)	0.4299(4)	0.0970(7)	7.1(3)
C40	0.4198(10)	0.3723(6)	0.4304(8)	13.5(6)

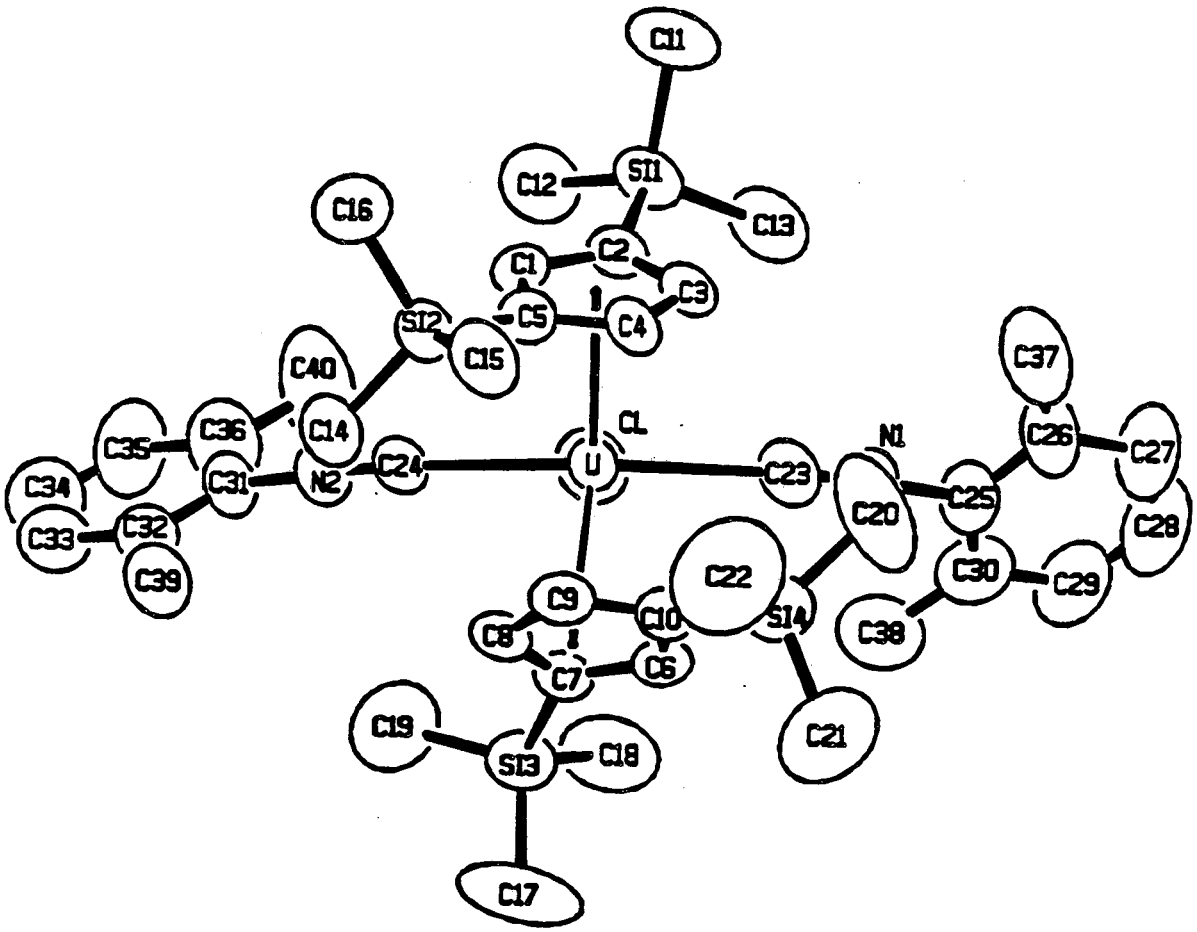
Table 2. Selected distances (Å) and angles(°)

Cp1 - U	2.508	C5 - U	2.792(7)
Cp2 - U	2.505	C6 - U	2.785(8)
C23 - U	2.681(9)	C7 - U	2.788(7)
C24 - U	2.654(9)	C8 - U	2.771(7)
Cℓ - U	2.6865(20)	C9 - U	2.759(7)
C1 - U	2.781(7)	C10 - U	2.779(7)
C2 - U	2.795(7)	C23 - N1	1.144(9)
C3 - U	2.771(7)	C24 - N2	1.164(10)
C4 - U	2.788(7)		

Cℓ -U-Cp1	115.30	Cp1-U -Cp2	129.40
Cℓ -U-Cp2	115.30	Cℓ -U -C23	73.95(19)
C23-U-Cp1	97.96	Cℓ -U -C24	73.22(18)
C23-U-Cp2	95.35	C23-N1-C25	177.4(10)
C24-U-Cp1	98.33	C24-N2-C31	177.1(9)
C24-U-Cp2	96.12		

Cp1 and Cp2 are the centroids of atoms C1-C5 and C6-C10 repectively.

Fig 1. ORTEP drawing; thermal ellipsoids at 50% probability level.



SUPPLEMENTARY MATERIALS

Bis[bis(trimethylsilyl)cyclopentadienyl](chloro)uranium(III) bis(2,6-dimethylphenylisocyanide)

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Abstract. $[(Me_3Si)_2C_5H_3]_2C\ell U\cdot 2(CNC_6H_3Me_2)$, M_r = 954.77, monoclinic, $P2_1/n$, a = 16.000(4), b = 22.806(4), c = 13.093(3) Å, β = 92.85(2), V = 4771.7, Z = 4, D_x = 1.33 g cm^{-3}, λ(MoKα) = 0.71073 Å, μ = 34.0 cm^{-1}, F(000) = 1916, T = 296 K, R = 0.031 for 4116 [$F^2 > 2\sigma(F^2)$] of 8437 total unique data. The Uranium atom is five coordinate with distances: U-Cℓ 2.6865(20); U-Cp 2.505, 2.508; U-C(isocyanide) 2.654(9), 2.681(9); <U-C(cyclopentadiene)> 2.781(11).

Supplementary Table 1. Anisotropic Thermal Parameters

Atom	B11	B22	B33	B12	B13	B23
U	3.296(12)	3.095(12)	3.863(11)	-0.077(17)	-0.121(7)	-0.097(16)
CL	6.41(13)	5.80(14)	5.94(10)	-0.98(10)	-2.05(9)	-0.77(9)
SI1	6.08(14)	5.29(14)	4.66(11)	-0.60(12)	-1.22(10)	1.21(10)
SI2	3.89(11)	4.72(13)	5.43(11)	0.01(10)	-0.97(9)	0.66(10)
SI3	6.23(15)	4.55(15)	6.57(13)	-1.73(12)	0.62(11)	-0.10(12)
SI4	9.94(23)	5.21(15)	6.33(13)	-0.19(14)	2.96(15)	-1.43(13)
N1	3.8(4)	5.1(4)	6.3(4)	0.7(3)	-0.24(29)	-0.2(3)
N2	5.4(4)	4.4(4)	5.5(4)	0.4(3)	0.44(29)	-0.1(3)
C1	3.3(4)	4.7(5)	4.5(4)	-0.6(3)	0.14(29)	0.8(3)
C2	4.6(4)	4.0(4)	4.4(4)	-0.8(4)	0.2(3)	0.8(3)
C3	4.7(4)	2.9(4)	5.0(4)	-0.3(3)	-0.4(3)	0.6(3)
C4	4.8(4)	3.1(4)	4.0(3)	-0.5(3)	-0.5(3)	0.00(28)
C5	3.5(4)	3.5(4)	4.7(4)	-0.8(3)	-0.32(29)	0.3(3)
C6	4.8(4)	4.8(5)	4.9(4)	-0.2(4)	1.4(3)	0.3(3)
C7	4.6(4)	3.8(5)	4.9(4)	-0.6(3)	0.8(3)	0.8(3)
C8	4.5(4)	4.1(4)	3.77(29)	-0.1(4)	0.13(26)	0.9(4)
C9	5.5(5)	4.0(5)	3.8(3)	-1.5(4)	-0.3(3)	0.36(29)
C10	5.8(5)	3.5(5)	3.9(3)	-0.5(4)	1.4(3)	-0.60(29)
C11	9.3(7)	7.6(6)	6.4(5)	-2.1(6)	-1.3(5)	2.6(5)
C12	10.5(7)	7.8(7)	4.5(4)	0.4(5)	0.5(4)	-0.1(4)
C13	6.2(5)	7.5(6)	7.6(5)	-0.9(5)	-2.8(4)	2.0(5)
C14	5.3(5)	5.5(6)	7.3(5)	0.6(4)	-0.8(4)	0.4(4)
C15	6.9(5)	5.6(6)	7.1(5)	0.2(5)	-2.3(4)	0.1(4)
C16	5.5(5)	9.9(8)	9.2(6)	-0.6(5)	0.0(5)	2.6(6)

C17	17.2(12)	9.5(9)	8.2(7)	-7.3(8)	-1.3(7)	2.8(6)
C18	8.4(7)	8.9(8)	10.0(7)	-4.0(6)	-2.0(5)	0.5(6)
C19	10.7(9)	5.4(7)	20.5(12)	-3.5(6)	5.3(8)	-4.4(8)
C20	24.4(15)	6.7(7)	8.4(7)	6.9(9)	0.7(8)	-1.7(6)
C21	24.3(17)	11.1(11)	16.7(12)	3.6(11)	13.9(12)	-1.4(9)
C22	15.5(12)	13.5(12)	12.0(9)	-2.4(9)	1.1(8)	-7.9(9)
CN23	5.3(5)	4.3(5)	6.1(5)	-0.1(4)	-0.3(4)	0.2(4)
CN24	5.2(5)	3.7(5)	5.3(4)	0.2(4)	0.6(3)	0.0(3)
C25	4.3(5)	6.3(6)	5.5(4)	1.2(5)	-0.7(4)	0.2(4)
C26	5.9(6)	6.6(7)	8.9(6)	2.4(5)	-1.2(5)	-0.1(5)
C27	7.7(8)	10.2(10)	10.0(7)	4.2(7)	-1.6(6)	0.1(7)
C28	4.8(7)	14.9(14)	12.6(9)	4.1(9)	-1.5(6)	0.3(10)
C29	5.5(7)	12.1(11)	8.2(6)	0.2(7)	-0.7(5)	0.1(7)
C30	5.1(5)	9.3(8)	4.8(4)	0.0(6)	-0.2(4)	-0.1(5)
C31	6.3(6)	3.7(5)	7.1(6)	1.3(4)	1.2(4)	-0.6(4)
C32	5.5(5)	3.7(5)	8.5(6)	-0.2(4)	1.5(5)	0.3(4)
C33	7.4(7)	4.2(6)	11.1(8)	0.2(5)	1.1(6)	1.2(5)
C34	12.0(10)	6.1(8)	11.3(9)	0.7(7)	2.2(8)	-3.0(7)
C35	13.5(11)	8.8(9)	9.8(8)	3.4(8)	0.7(7)	-3.8(7)
C36	11.3(9)	7.7(8)	7.0(6)	2.7(7)	0.3(6)	-1.7(6)
C37	8.2(8)	5.1(6)	17.3(10)	0.6(6)	-1.6(7)	-1.1(7)
C38	8.3(6)	7.4(7)	9.1(6)	-2.0(7)	-0.8(5)	0.7(6)
C39	6.9(6)	6.5(6)	7.8(6)	0.7(5)	-0.9(5)	0.3(5)
C40	21.7(14)	11.9(10)	6.5(6)	9.1(10)	-3.4(7)	-3.4(6)

The temperature factor has the form: $T = \exp[-1/4(B11\ h^2 a^{*2} + 2B12\ hk\ a^* b^*)]$

Supplementary Table 2. Estimated Hydrogen Atom Parameters

	x	y	z	B(Å^2)		x	y	z	B(Å^2)
H1	0.3144	0.1990	0.2788	10.0	H31	0.5141	0.3999	0.1642	15.0
H2	0.4810	0.0727	0.186	10.0	H32	0.4823	0.4269	0.0564	15.0
H3	0.3820	0.0977	0.0335	10.0	H33	0.5628	0.4539	0.1166	15.0
H4	0.6417	0.2351	-0.0105	10.0	H34	0.5316	0.0611	-0.0186	15.0
H5	0.4137	0.319	-0.0234	10.0	H35	0.6275	0.0804	-0.0222	15.0
H6	0.3923	0.2169	-0.0961	10.0	H36	0.5868	0.0388	-0.1096	15.0
H7	0.4073	0.0270	0.4273	10.0	H37	0.668	0.1684	-0.2052	15.0
H8	0.3363	0.0705	0.4641	10.0	H38	0.5898	0.1814	-0.2828	15.0
H9	0.4174	0.0576	0.5372	10.0	H39	0.6284	0.1167	-0.2746	15.0
H10	0.370	0.2008	0.4805	10.0	H40	0.4304	0.1445	-0.2604	15.0
H11	0.4584	0.2273	0.4514	10.0	H41	0.4026	0.1056	-0.1661	15.0
H12	0.4518	0.1888	0.5529	10.0	H42	0.4578	0.0771	-0.2518	15.0
H13	0.5972	0.1393	0.3857	10.0	H43	0.6723	0.0132	0.1240	15.0
H14	0.5745	0.0709	0.3803	10.0	H44	0.6602	0.017	0.2444	15.0
H15	0.584	0.1034	0.4887	10.0	H45	0.7183	-0.033	0.1996	15.0
H16	0.2747	0.2719	-0.0179	10.0	H46	0.779	0.2258	0.2528	15.0
H17	0.230	0.2859	0.086	10.0	H47	0.7925	0.223	0.1326	15.0
H18	0.1747	0.2721	-0.0163	10.0	H48	0.8707	0.2340	0.2113	15.0
H19	0.2135	0.0972	-0.0463	10.0	H49	0.2428	0.3932	0.0922	15.0
H20	0.2679	0.1446	-0.1042	10.0	H50	0.3264	0.4256	0.0601	15.0
H21	0.1682	0.1509	-0.1054	10.0	H51	0.2412	0.4618	0.0665	15.0
H22	0.1402	0.1936	0.1952	10.0	H52	0.4737	0.3673	0.3987	15.0
H23	0.1300	0.1294	0.1468	10.0	H53	0.391	0.3346	0.4324	15.0
H24	0.0842	0.1841	0.0918	10.0	H54	0.4299	0.3872	0.5003	15.0
H25	0.5812	0.4077	-0.1306	15.0	H55	0.8647	-0.0151	0.2229	10.0
H26	0.6684	0.3733	-0.1199	15.0	H56	0.978	0.0479	0.2384	10.0
H27	0.6601	0.437	-0.0707	15.0	H57	0.9586	0.1495	0.2378	10.0
H28	0.7334	0.3294	0.0805	15.0	H58	0.2353	0.5217	0.2139	10.0
H29	0.6804	0.3356	0.1804	15.0	H59	0.2734	0.5436	0.3807	10.0
H30	0.7218	0.3924	0.1319	15.0	H60	0.3546	0.4775	0.4832	10.0

Supplementary Table 3. Interatomic Distances (Å)

Cp1-U	2.508	C11-SI1	1.881(10)	C25-N1	1.408(10)	C27-C26	1.381(14)
Cp2-U	2.505	C12-SI1	1.861(10)	C24-N2	1.164(10)	C37-C26	1.508(14)
C23-U	2.681(9)	C13-SI1	1.860(10)	C31-N2	1.400(10)	C28-C27	1.349(18)
C24-U	2.654(9)	C5 -SI2	1.867(7)	C2 -C1	1.417(10)	C29-C28	1.376(18)
Cℓ -U	2.6865(20)	C14-SI2	1.843(9)	C5 -C1	1.437(10)	C30-C29	1.394(14)
C1 -U	2.781(7)	C15-SI2	1.876(9)	C3 -C2	1.441(10)	C38-C30	1.493(14)
C2 -U	2.795(7)	C16-SI2	1.859(10)	C4 -C3	1.413(9)	C36-C31	1.385(12)
C3 -U	2.771(7)	C7 -SI3	1.880(8)	C5 -C4	1.420(10)	C32-C31	1.388(12)
C4 -U	2.788(7)	C17-SI3	1.851(11)	C7 -C6	1.392(11)	C33-C32	1.384(13)
C5 -U	2.792(7)	C18-SI3	1.846(10)	C10-C6	1.416(10)	C39-C32	1.478(12)
C6 -U	2.785(8)	C19-SI3	1.832(12)	C8 -C7	1.424(9)	C34-C33	1.342(14)
C7 -U	2.788(7)	C10-SI4	1.867(8)	C9 -C8	1.395(10)	C35-C34	1.381(16)
C8 -U	2.771(7)	C20-SI4	1.791(12)	C10-C9	1.406(11)	C36-C35	1.395(14)
C9 -U	2.759(7)	C21-SI4	1.800(13)	C26-C25	1.383(12)	C40-C36	1.514(14)
C10-U	2.779(7)	C22-SI4	1.884(14)	C30-C25	1.390(12)	C -H	0.98
C2 -SI1	1.863(7)	C23-N1	1.144(9)				

Supplementary Table 4. Angles (°)

Cℓ -U -Cp1	115.30	C18-SI3-C19	108.3(6)	C6 -C10-C9	105.4(7)
Cℓ -U -Cp2	115.30	C10-SI4-C20	116.9(4)	N1 -C25-C26	117.5(9)
C23-U -Cp1	97.96	C10-SI4-C21	109.0(6)	N1 -C25-C30	116.4(9)
C23-U -Cp2	95.35	C10-SI4-C22	107.8(5)	C26-C25-C30	126.0(9)
C24-U -Cp1	98.33	C20-SI4-C21	113.8(7)	C25-C26-C27	115.5(11)
C24-U -Cp2	96.12	C20-SI4-C22	105.6(7)	C25-C26-C37	121.9(9)
Cp1-U -Cp2	129.40	C21-SI4-C22	102.5(8)	C27-C26-C37	122.6(12)
Cℓ -U -C23	74.0(2)	C23-N1 -C25	177.4(10	C26-C27-C28	121.8(13)
Cℓ -U -C24	73.2(2)	C24-N2 -C31	177.1(9)	C27-C28-C29	120.5(12)
C2 -SI1-C11	108.9(4)	C2 -C1 -C5	110.5(7)	C28-C29-C30	122.0(12)
C2 -SI1-C12	109.8(4)	SI1-C2 -C1	127.0(6)	C25-C30-C29	114.0(11)
C2 -SI1-C13	112.0(4)	SI1-C2 -C3	126.6(6)	C25-C30-C38	122.8(10)
C11-SI1-C12	108.9(5)	C1 -C2 -C3	105.8(6)	C29-C30-C38	123.3(11)
C11-SI1-C13	106.2(5)	C2 -C3 -C4	108.6(7)	N2 -C31-C32	119.3(9)
C12-SI1-C13	111.1(5)	C3 -C4 -C5	109.4(6)	N2 -C31-C36	117.0(9)
C5 -SI2-C14	114.3(4)	SI2-C5 -C1	126.6(6)	C32-C31-C36	123.6(10)
C5 -SI2-C15	108.0(4)	SI2-C5 -C4	126.3(6)	C31-C32-C33	115.4(10)
C5 -SI2-C16	109.4(4)	C1 -C5 -C4	105.7(6)	C31-C32-C39	121.4(9)
C14-SI2-C15	110.1(4)	C7 -C6 -C10	110.8(7)	C33-C32-C39	123.2(10)
C14-SI2-C16	106.0(5)	SI3-C7 -C6	125.6(6)	C32-C33-C34	123.0(11)
C15-SI2-C16	109.0(5)	SI3-C7 -C8	126.6(7)	C33-C34-C35	121.0(12)
C7 -SI3-C17	107.8(4)	C6 -C7 -C8	106.0(7)	C34-C35-C36	119.1(12)
C7 -SI3-C18	112.1(5)	C7 -C8 -C9	108.3(7)	C31-C36-C35	117.9(11)
C7 -SI3-C19	111.9(4)	C8 -C9 -C10	109.5(7)	C31-C36-C40	120.7(10)
C17-SI3-C18	107.3(6)	SI4-C10-C6	126.6(7)	C35-C36-C40	121.4(11)
C17-SI3-C19	109.3(7)	SI4-C10-C9	125.5(6)		

Supplementary Table 5. Least-Squares Planes

Plane 1
Equation of plane: 10.43476 x + 16.28043 y - 3.76022 z = 5.47779
Distance to the Plane from atoms

Forming the Plane:		Not Forming the Plane:	
C1	-0.002(10)	U	2.508(03)
C2	-0.004(10)	SI1	-0.240(13)
C3	0.008(10)	SI2	-0.311(13)
C4	-0.009(10)		
C5	0.007(10)		

Plane 2
Equation of plane: 3.642264x + 7.88068 y - 12.05286 z = 4.29363
Distance to the Plane from atoms

Forming the Plane:		Not Forming the Plane:	
C6	0.008(11)	U	2.505(4)
C7	-0.005(10)	SI3	-0.355(14)
C8	0.003(11)	SI4	-0.415(15)
C9	-0.001(11)		
C10	0.005(11)		

Plane 3
Equation of plane: 13.53475 x + 10.43139 y - 4.13679 z = 7.77678
Distance to the Plane from atoms

Forming the Plane:		Not Forming the Plane:	
C31	-0.003(12)	N2	-0.051(16)
C32	0.006(13)	C24	-0.048(21)
C33	-0.010(16)	C39	0.027(18)
C34	0.005(12)	C40	0.009(22)
C35	0.003(18)		
C36	-0.001(15)		

Plane 4
Equation of plane: -2.59541 x + 0.74020 y + 13.00223 z = 0.65743
Distance to the Plane from atoms

Forming the Plane:		Not Forming the Plane:	
C25	-0.013(13)	N1	-0.027(17)
C26	0.017(14)	C23	-0.061(24)
C27	-0.008(17)	C37	0.028(21)
C28	-0.021(22)	C38	-0.013(21)
C29	0.018(19)		
C30	0.003(16)		

Angle Between Planes:

1	2	51.1(4)
3	4	-66.9(5)

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