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Bis[bis(trimethylsilyl)cyclopentadienyl](bromo)uranium(III) bis(t-butylisocyanide)

S.M. Beshouri and A. Zalkin

October 1988

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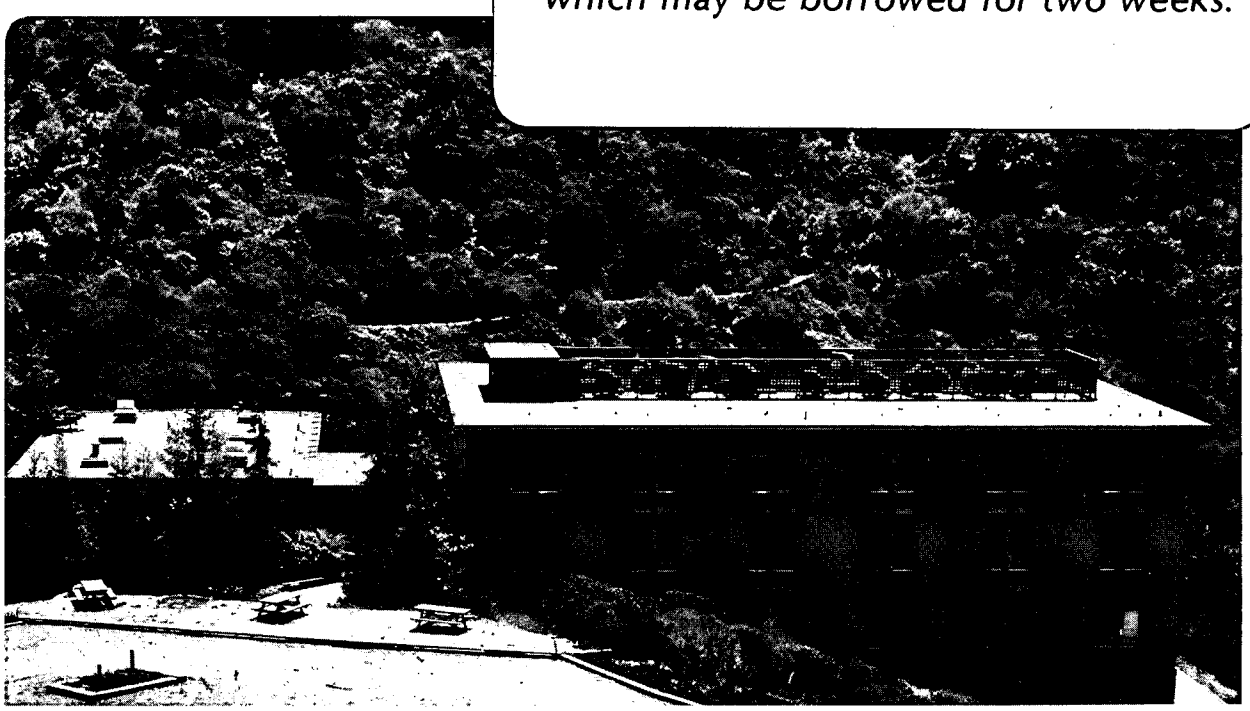

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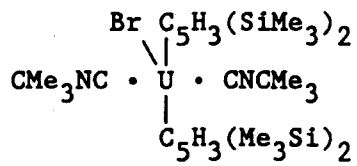
Bis[bis(trimethylsilyl)cyclopentadienyl](bromo)uranium(III) bis(t-butylisocyanide)

By Sharon M. Beshouri and Allan Zalkin

Materials and Chemical Sciences Division, Lawrence Berkeley Laboratory,
1 Cyclotron Rd., Berkeley, CA 94720, USA

Abstract. $[(Me_3Si)_2C_5H_3]_2UBr\cdot 2[CNCMe_3]_2$, M_r = 903.13, monoclinic, $P2_1/n$, a = 11.765(3), b = 12.135(2), c = 30.125(5) Å, β = 92.29(2)°, V = 4297.5, Z = 4, D_x = 1.396 g cm^{-3}, λ(MoKα) = 0.71073 Å, μ = 46.3 cm^{-1}, F(000) = 1796, T = 296 K, R = 0.033 for 4281 $F^2>2\sigma(F^2)$ of 7592 total unique data. The uranium atom is five coordinate with distances: U-Br 2.8761(10); U-Cp 2.514, 2.520; U-C(isocyanide) 2.662(8), 2.697(7); <U-C(cyclopentadiene)> 2.791(18) Å.

Experimental. The title compound, as shown below,



was prepared by reaction on one equivalent of $[<C_5H_3(SiMe_3)_2>_2UBr]_2$ with four equivalents of $CN(CMe_3)$ in diethyl ether solution. Product was dissolved in hexane and dark crystals were isolated after cooling to -20°C.

A brown-green air-sensitive crystal, 0.17 x 0.18 x 0.67 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 29 reflections $20< 2\theta <30°$; analytical absorption correction, range 1.96-2.37; max.$(\sin\theta)/\lambda$ = 0.60 $Å^{-1}$, h -14 to 14, k 0 to 14, ℓ -35 to 35; three standard reflections, 1.5%, 1.4%, 2.5% variation in standards intensities from average, intensities adjusted isotropically; 14455 data, 7592 unique [including 3311, $F^2 < 3\sigma(F^2)$], R_{int} = 0.048; structure solved by Patterson and Fourier methods; refined on F, 385 parameters; parameters of the six hydrogen atoms of the cyclopentadienyl rings were included with isotropic thermal parameters; the methyl H atoms included with estimated positional and isotropic thermal parameters and were not refined; R = 0.094 (all data), R = 0.033 [$F^2>2\sigma(F^2)$ data], wR = 0.031, S = 1.0; $w = 4F^2[\sigma^2(F^2) + (0.035F^2)^2]^{-1}$; max. $\Delta/\sigma < 0.02$; max. empirical isotropic correction for extinction 16% of F; max.,min. of ΔF synthesis 1.21,-1.42 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.

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*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 (19 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, $[<C_5H_3(SiMe_3)_2>_2UBr]_2$, has been made and structurally characterized (Blake, Lappert, Taylor, Atwood & Zhang, 1987). The ability of isocyanides to act as good donor ligands toward uranium metal centers has been previously observed (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	0.18863(2)	0.11824(2)	0.35897(1)	3.339(6)
BR	0.20423(9)	0.32988(8)	0.31666(3)	6.40(3)
SI1	-0.04814(17)	-0.12204(21)	0.39988(7)	4.88(6)
SI2	0.02958(18)	0.10755(20)	0.23520(7)	4.59(6)
SI3	0.44003(18)	-0.08801(18)	0.41748(7)	4.79(7)
SI4	0.30450(20)	0.36631(21)	0.44719(8)	5.68(7)
N1	-0.0751(6)	0.2705(6)	0.39312(20)	5.1(2)
N2	0.4408(5)	0.1163(6)	0.28308(21)	5.5(2)
C1	-0.0078(6)	0.0171(6)	0.32377(25)	3.9(2)
C2	0.0352(6)	-0.0609(6)	0.35467(23)	3.9(2)
C3	0.1379(6)	-0.0997(6)	0.33657(25)	4.1(2)
C4	0.1548(6)	-0.0474(6)	0.29623(24)	3.7(2)
C5	0.0640(6)	0.0292(6)	0.28696(22)	3.7(2)
C6	0.3734(6)	0.1462(7)	0.41853(24)	4.2(2)
C7	0.3434(6)	0.0323(6)	0.42288(22)	3.9(2)
C8	0.2362(7)	0.0345(7)	0.44315(24)	4.0(2)
C9	0.2049(6)	0.1444(6)	0.45058(22)	4.2(2)
C10	0.2899(6)	0.2171(6)	0.43543(22)	3.9(2)
C11	0.0051(7)	0.2264(6)	0.38401(25)	4.7(2)
C12	0.3708(6)	0.1122(8)	0.30743(25)	5.4(2)
C13	-0.1774(8)	0.3305(9)	0.4045(3)	6.8(3)
C14	0.5317(7)	0.1299(7)	0.25126(29)	5.7(3)
C15	-0.1787(7)	-0.1862(8)	0.37371(28)	6.8(3)

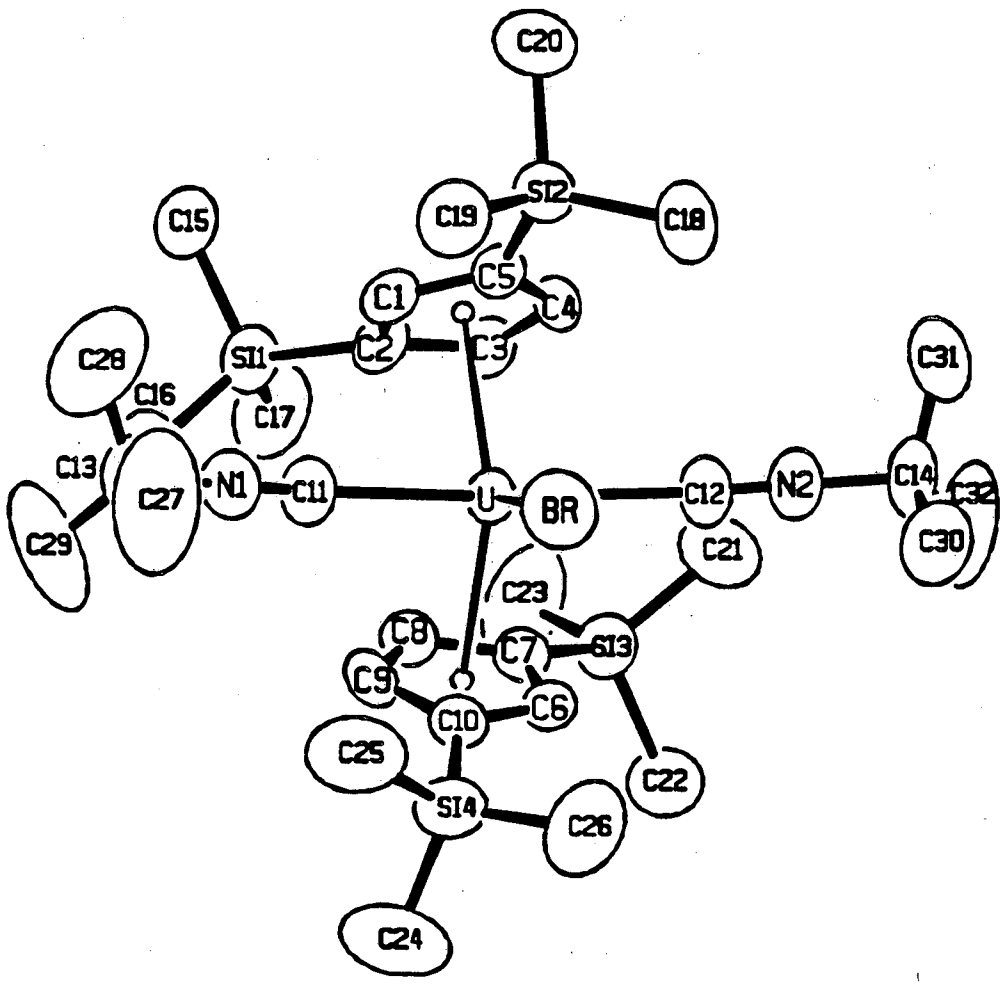
C16	-0.0956(8)	-0.0163(8)	0.44006(28)	7.0(3)
C17	0.0324(8)	-0.2327(8)	0.4300(3)	8.1(3)
C18	0.1632(7)	0.1462(7)	0.20699(26)	6.3(3)
C19	-0.0592(7)	0.2296(7)	0.24854(27)	6.5(3)
C20	-0.0574(8)	0.0197(8)	0.19556(27)	7.3(3)
C21	0.4795(8)	-0.1160(8)	0.35979(28)	7.6(3)
C22	0.5758(7)	-0.0600(9)	0.4497(3)	7.8(3)
C23	0.3701(9)	-0.2108(8)	0.4393(4)	10.1(4)
C24	0.3462(10)	0.3811(9)	0.5074(3)	10.0(4)
C25	0.1702(9)	0.4444(8)	0.4381(4)	8.9(4)
C26	0.4186(9)	0.4271(8)	0.4141(4)	10.1(4)
C27	-0.1685(12)	0.4458(12)	0.3910(5)	14.2(7)
C28	-0.2720(11)	0.2769(14)	0.3779(5)	15.3(7)
C29	-0.1970(12)	0.3198(13)	0.4513(4)	14.2(6)
C30	0.5678(8)	0.2492(8)	0.2525(3)	7.7(4)
C31	0.4829(9)	0.0971(10)	0.2059(3)	10.2(4)
C32	0.6292(9)	0.0546(9)	0.2667(4)	10.4(5)
H1	-0.079(5)	0.055(5)	0.3259(20)	4.2(16)
H2	0.183(5)	-0.157(5)	0.3478(19)	3.9(16)
H3	0.208(5)	-0.059(5)	0.2780(18)	2.5(13)
H4	0.440(5)	0.171(5)	0.4059(19)	3.6(15)
H5	0.202(5)	-0.029(5)	0.4498(19)	2.8(15)
H6	0.134(5)	0.166(5)	0.4625(18)	3.0(13)

Table 3. Selected Distances (Å) and Angles (°)

Cp1 - U	2.520	C5 - U	2.787(7)
Cp2 - U	2.514	C6 - U	2.784(7)
Br - U	2.8761(10)	C7 - U	2.798(7)
Cl1 - U	2.662(8)	C8 - U	2.769(7)
Cl2 - U	2.697(7)	C9 - U	2.777(7)
C1 - U	2.788(7)	C10 - U	2.819(7)
C2 - U	2.825(7)	C11 - N1	1.128(8)
C3 - U	2.789(7)	C12 - N2	1.126(8)
C4 - U	2.777(7)		

Br - U - Cl1	75.65(17)	C12 - U - Cp1	96.97
Br - U - Cl2	72.73(20)	C12 - U - Cp2	99.22
Cl1- U - Cl2	148.09(25)	Cp1 - U - Cp2	129.08
Br - U - Cp1	118.73	C11 - N1 - C13	178.4(9)
Br - U - Cp2	112.16	C12 - N2 - C14	176.2(10)
Cl1- U - Cp1	94.41	U - C11 - N1	177.1(7)
Cl1- U - Cp2	96.44	U - C12 - N2	173.1(7)

Figure 1. ORTEP drawing showing atomic numbering; 50% probability ellipsoids.



SUPPLEMENTAL MATERIALS

Bis[bis(trimethylsilyl)cyclopentadienyl](bromo)uranium(III) bis(t-butylisocyanide)

By Sharon M. Beshouri and Allan Zalkin

Materials and Chemical Sciences Division, Lawrence Berkeley Laboratory,
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Abstract. $[(Me_3Si)_2C_5H_3]_2UBr\cdot 2[CNCMe_3]_2$, M_r = 903.13, monoclinic, $P2_1/n$, a = 11.765(3), b = 12.135(2), c = 30.125(5) Å, β = 92.29(2)°, V = 4297.5, Z = 4, D_x = 1.396 g cm^{-3}, λ(MoKα) = 0.71073 Å, μ = 46.3 cm^{-1}, F(000) = 1796, T = 296 K, R = 0.033 for 4281 $F^2>2\sigma(F^2)$ of 7592 total unique data. The uranium atom is five coordinate with distances: U-Br 2.8761(10); U-Cp 2.514, 2.520; U-C(isocyanide) 2.662(8), 2.697(7); <U-C(cyclopentadiene)> 2.791(18) Å.

Supplementary Table 1. Anisotropic Thermal Parameters

Atom	B11	B22	B33	B12	B13	B23
U	2.868(10)	3.758(12)	3.407(11)	0.298(14)	0.340(7)	0.026(15)
Br	8.12(6)	4.60(4)	6.49(5)	-0.18(4)	0.54(4)	1.19(4)
Si1	4.19(9)	5.85(12)	4.65(10)	-0.32(11)	0.70(8)	1.03(11)
Si2	4.85(10)	5.03(12)	3.88(9)	-0.22(11)	0.00(8)	0.60(10)
Si3	4.05(10)	5.04(13)	5.25(11)	1.14(9)	-0.14(8)	-0.13(9)
Si4	5.41(11)	5.11(14)	6.42(13)	0.43(11)	-0.75(10)	-1.57(11)
N1	4.5(3)	5.8(4)	5.1(3)	1.2(3)	0.53(28)	-0.12(29)
N2	4.09(29)	6.2(4)	6.2(4)	0.5(4)	1.40(27)	-0.9(4)
C1	3.0(3)	4.1(4)	4.6(4)	-0.3(3)	-0.3(3)	0.0(3)
C2	3.0(3)	3.6(3)	4.9(4)	-0.48(28)	0.15(28)	0.4(3)
C3	3.6(3)	3.7(4)	4.9(4)	0.2(3)	0.37(29)	-0.3(3)
C4	3.7(4)	4.2(4)	3.2(4)	-0.3(3)	0.9(3)	-0.7(3)
C5	3.3(3)	3.9(4)	3.9(4)	-0.34(29)	0.12(28)	-0.21(28)
C6	3.2(3)	5.8(5)	3.6(4)	-0.2(3)	-0.34(27)	-0.9(3)
C7	3.5(4)	4.8(4)	3.2(4)	0.6(3)	-0.45(29)	0.0(3)
C8	4.1(4)	4.6(5)	3.3(4)	-0.2(4)	-0.1(3)	0.4(3)
C9	3.8(4)	5.8(5)	2.9(3)	1.5(3)	0.23(26)	-0.6(3)
C10	3.9(4)	4.2(4)	3.5(4)	0.3(3)	-0.3(3)	-0.36(29)
C11	3.7(4)	4.9(4)	5.5(4)	1.2(3)	0.8(3)	-0.3(3)
C12	3.9(3)	6.8(5)	5.8(4)	0.9(4)	1.3(3)	-0.9(5)
C13	4.6(5)	8.6(6)	7.3(6)	2.6(5)	1.2(4)	0.4(5)
C14	4.7(4)	4.9(5)	7.6(5)	-0.2(4)	3.0(4)	-0.7(4)
C15	5.2(5)	8.5(6)	6.6(5)	-1.4(4)	1.2(4)	-0.7(5)
C16	7.6(5)	8.2(6)	5.4(5)	-1.7(5)	2.5(4)	-0.7(4)
C17	6.8(6)	8.6(6)	9.0(6)	-0.2(5)	0.8(5)	4.5(5)
C18	6.7(5)	7.0(6)	5.4(4)	-0.2(4)	2.1(4)	1.4(4)
C19	5.8(5)	7.0(5)	6.8(5)	1.4(4)	-0.5(4)	1.2(4)
C20	8.5(6)	8.9(6)	4.5(4)	-1.0(5)	-1.4(4)	0.9(4)
C21	7.4(5)	8.7(6)	6.6(5)	3.0(5)	-1.0(4)	-2.0(5)
C22	5.1(5)	10.3(7)	8.0(6)	2.8(5)	-1.2(4)	-3.3(5)
C23	6.7(6)	6.7(6)	16.8(10)	2.5(5)	1.9(6)	4.3(6)
C24	13.2(8)	7.8(6)	8.8(6)	2.9(7)	-3.2(6)	-2.9(6)
C25	9.3(7)	6.1(5)	11.0(7)	2.7(5)	-2.1(6)	-3.3(5)
C26	8.4(7)	6.6(6)	15.6(10)	-2.5(5)	2.9(7)	-3.1(6)
C27	11.5(10)	11.8(10)	19.8(14)	7.6(8)	5.7(9)	5.3(10)
C28	5.6(6)	18.6(14)	21.6(14)	4.3(8)	-0.7(8)	-5.1(12)
C29	14.5(11)	21.1(13)	7.4(7)	10.7(10)	4.8(7)	1.8(8)
C30	7.1(6)	6.9(6)	9.3(6)	-1.5(5)	1.8(5)	-0.3(5)
C31	9.2(7)	13.5(9)	8.3(6)	-4.1(7)	4.7(5)	-3.9(7)
C32	7.1(6)	7.6(7)	17.1(11)	2.2(5)	6.4(7)	2.3(7)

The temperature factor has the form: $\exp[-(B_{11}\ h^2a^{*2} + 2B_{12}hka^*b^* + \ldots)/4]$

Supplemental Table 2. Hydrogen atomic coordinates

Atom	x	y	z	B(Å^2)
H1	-0.079(5)	0.055(5)	0.3259(20)	4.2(16)
H2	0.183(5)	-0.157(5)	0.3478(19)	3.9(16)
H3	0.208(5)	-0.059(5)	0.2780(18)	2.5(13)
H4	0.440(5)	0.171(5)	0.4059(19)	3.6(15)
H5	0.202(5)	-0.029(5)	0.4498(19)	2.8(15)
H6	0.134(5)	0.166(5)	0.4625(18)	3.0(13)

Atom	x	y	z	B(Å^2)	Atom	x	y	z	B(Å^2)
H7	-0.1567	-0.2436	0.3528	10.0	H34	0.4186	0.343	0.5137	10.0
H8	-0.2236	-0.1297	0.3578	10.0	H35	0.2873	0.3485	0.5254	10.0
H9	-0.2242	-0.219	0.3968	10.0	H36	0.3547	0.4594	0.5148	10.0
H10	-0.1438	0.0381	0.4244	10.0	H37	0.1126	0.4153	0.4575	10.0
H11	-0.0290	0.0206	0.4538	10.0	H38	0.1434	0.4368	0.407	10.0
H12	-0.1389	-0.0521	0.4631	10.0	H39	0.1837	0.5224	0.4448	10.0
H13	0.1030	-0.2022	0.4433	10.0	H40	0.3997	0.4170	0.3824	10.0
H14	0.0506	-0.2915	0.4091	10.0	H41	0.4910	0.3905	0.4218	10.0
H15	-0.0140	-0.2628	0.4534	10.0	H42	0.4252	0.506	0.4207	10.0
H16	0.2049	0.0793	0.1995	10.0	H43	-0.1597	0.4498	0.3588	10.0
H17	0.2109	0.1921	0.2270	10.0	H44	-0.1023	0.4796	0.4064	10.0
H18	0.1436	0.1875	0.1798	10.0	H45	-0.2376	0.4854	0.3987	10.0
H19	-0.017	0.2770	0.2698	10.0	H46	-0.2766	0.1989	0.3861	10.0
H20	-0.1297	0.2048	0.2616	10.0	H47	-0.2575	0.283	0.3462	10.0
H21	-0.0775	0.271	0.2213	10.0	H48	-0.344	0.3134	0.384	10.0
H22	-0.1282	-0.0018	0.2093	10.0	H49	-0.1318	0.3498	0.4686	10.0
H23	-0.0142	-0.0465	0.1883	10.0	H50	-0.2065	0.2417	0.4587	10.0
H24	-0.0753	0.0614	0.1683	10.0	H51	-0.2659	0.3604	0.4584	10.0
H25	0.5186	-0.0517	0.348	10.0	H52	0.5960	0.2683	0.2826	10.0
H26	0.4107	-0.1313	0.3414	10.0	H53	0.5026	0.296	0.2441	10.0
H27	0.5302	-0.1801	0.3594	10.0	H54	0.6284	0.2608	0.2316	10.0
H28	0.5597	-0.0485	0.481	10.0	H55	0.418	0.1446	0.1978	10.0
H29	0.6117	0.0062	0.4380	10.0	H56	0.4577	0.0201	0.2067	10.0
H30	0.6272	-0.1230	0.447	10.0	H57	0.5414	0.1051	0.1839	10.0
H31	0.2986	-0.2241	0.4223	10.0	H58	0.6025	-0.0219	0.267	10.0
H32	0.3540	-0.1992	0.4706	10.0	H59	0.6561	0.076	0.2967	10.0
H33	0.4202	-0.2748	0.4366	10.0	H60	0.6917	0.0612	0.2463	10.0

Supplemental Table 3. Distances (Å)

Cp1 - U	2.520	C5 - SI2	1.857(7)	C5 - C4	1.435(9
Cp2 - U	2.514	C18 - SI2	1.876(8)	C4 - C5	1.435(9
Br - U	2.8761(10)	C19 - SI2	1.865(9)	C10 - C6	1.415(9
C11 - U	2.662(8)	C20 - SI2	1.874(9)	C7 - C6	1.433(1
C12 - U	2.697(7)	C7 - SI3	1.862(7)	C8 - C7	1.423(1
C1 - U	2.788(7)	C21 - SI3	1.848(9)	C9 - C8	1.403(1
C2 - U	2.825(7)	C22 - SI3	1.867(9)	C10 - C9	1.423(9
C3 - U	2.789(7)	C23 - SI3	1.837(10)	C29 - C13	1.444(1
C4 - U	2.777(7)	C10 - SI4	1.852(8)	C27 - C13	1.462(1
C5 - U	2.787(7)	C24 - SI4	1.870(10)	C28 - C13	1.494(1
C6 - U	2.784(7)	C25 - SI4	1.853(10)	C30 - C14	1.509(1
C7 - U	2.798(7)	C26 - SI4	1.856(11)	C31 - C14	1.515(1
C8 - U	2.769(7)	C11 - N1	1.128(8)	C32 - C14	1.524(1
C9 - U	2.777(7)	C13 - N1	1.459(10)	H1 - C1	0.97(6)
C10 - U	2.819(7)	C12 - N2	1.126(8)	H2 - C3	0.93(6)
C2 - SI1	1.864(7)	C14 - N2	1.473(9)	H3 - C4	0.86(5)
C15 - SI1	1.868(9)	C2 - C1	1.408(9)	H4 - C6	0.94(6)
C16 - SI1	1.864(9)	C5 - C1	1.428(9)	H5 - C8	0.90(6)
C17 - SI1	1.858(9)	C3 - C2	1.425(9)	H6 - C9	0.96(6)
C4 - C3	1.392(9)			Other C-H	0.98

Supplemental Table 4. Angles (°)

BR -U-C11	75.65(17)	C7 -S-C21	113.8(4)	SI3-C-C6	126.5(6)
BR -U-C12	72.73(20)	C7 -S-C22	108.9(4)	SI3-C-C8	127.3(6)
C11-U-C12	148.09(25)	C7 -S-C23	108.7(4)	C6 -C-C8	104.3(7)
BR -U-Cp1	118.73	C21-S-C22	106.3(4)	C7 -C-C9	109.2(7)
BR -U-Cp2	112.16	C21-S-C23	108.7(5)	C8 -C-C10	110.2(7)
C11-U-Cp1	94.41	C22-S-C23	110.4(5)	SI4-C-C6	127.1(6)
C11-U-Cp2	96.44	C10-S-C24	107.4(4)	SI4-C-C9	127.3(6)
C12-U-Cp1	96.97	C10-S-C25	113.6(4)	C6 -C-C9	104.2(7)
C12-U-Cp2	99.22	C10-S-C26	110.5(4)	U -C-N1	177.1(7)
Cp1-U-Cp2	129.08	C24-S-C25	106.5(5)	U -C-N2	173.1(7)
C2 -S-C15	107.8(4)	C25-S-C26	110.3(6)	N1 -C-C27	110.1(9)
C2 -S-C16	112.4(4)	C11-N-C13	178.4(9)	N1 -C-C28	105.1(8)
C2 -S-C17	111.8(4)	C12-N-C14	176.2(10)	N1 -C-C29	110.4(8)
C15-S-C16	107.4(4)	C2 -C-C5	112.0(7)	C27-C-C28	109.2(11)
C15-S-C17	107.4(5)	SI1-C-C1	124.4(5)	C27-C-C29	111.9(11)
C16-S-C17	109.9(5)	SI1-C-C3	128.8(6)	C28-C-C29	109.9(12)
C5 -S-C18	110.5(4)	C1 -C-C3	104.9(7)	N2 -C-C30	107.6(7)
C5 -S-C19	109.3(3)	C3 -C-C5	109.5(6)	N2 -C-C31	107.4(7)
C5 -S-C20	109.8(4)	SI2-C-C1	126.1(5)	N2 -C-C32	106.9(7)
C18-S-C19	112.7(4)	SI2-C-C4	129.1(5)	C30-C-C31	111.7(8)
C18-S-C20	107.4(4)	C1 -C-C4	103.9(6)	C30-C-C32	111.1(8)
C19-S-C20	107.0(4)	C7 -C-C10	112.1(7)	C31-C-C32	111.8(9)

Supplementary Table 5. Least-Squares Planes

Plane No. 1

Equation of the Plane: 5.82930 x + 8.73758 y + 14.02834 z = 4.64921

Distance (Å) to the Plane From the Atoms

Forming the Plane		Not Forming the Plane	
C1	-0.003(9)	U	2.519(3)
C2	-0.001(9)	SI1	-0.387(12)
C3	0.005(10)	SI2	-0.238(12)
C4	-0.006(9)	H1	-0.05(6)
C5	0.005(9)	H2	-0.08(6)
		H3	-0.05(6)

Plane No. 2

Equation of the Plane: 5.06086 x - 0.34940 y + 26.64205 z = 12.99119

Distance (Å) to the Plane From the Atoms

Forming the Plane		Not Forming the Plane	
C6	-0.000(14)	U	-2.514(4)
C7	0.003(12)	SI3	0.389(13)
C8	-0.006(13)	SI4	0.356(13)
C9	-0.007(14)	H4	-0.01(6)
C10	0.004(13)	H5	0.02(6)
		H6	-0.05(6)

Angle Between the Planes: -50.9(3)°

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720