- *Supplementary Information* -

A Triamido-Uranium(V) Inverse-Sandwich 10π-Toluene Tetraanion Arene Complex

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Experimental

General

All manipulations were carried out using standard Schlenk techniques, or an MBraun UniLab glovebox, under an atmosphere of dry nitrogen. Solvents were dried by passage through activated alumina towers and degassed before use. All solvents were stored over potassium mirrors except for ethers which were stored over activated 4 Å sieves. Deuterated solvent was distilled from potassium, degassed by three freeze-pump-thaw cycles and stored under nitrogen. [U(Ts^{Tol})(Cl)(THF)] (**2**, Ts^{Tol} = $HC(SiMe_2NAr')_3$; Ar' = 4-MeC_6H_4), and KC_8 were synthesised according to published procedures.[1,2]

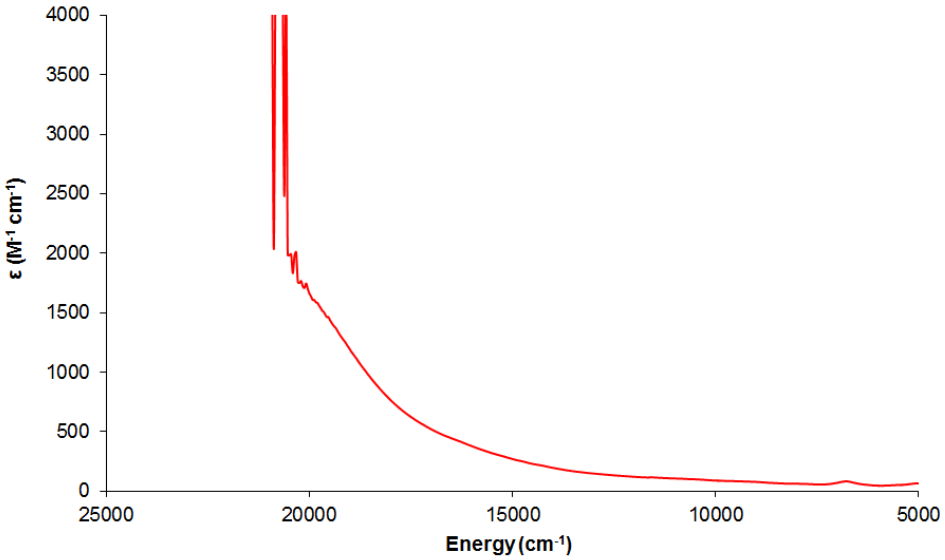
^{1}H NMR spectra were recorded on a Bruker 300 spectrometer operating at 300.13 MHz; chemical shifts are quoted in ppm and are relative to TMS. FTIR spectra were recorded on a Bruker Tensor 27 spectrometer. UV/Vis/NIR spectra were recorded on a Perkin Elmer Lambda 750 spectrometer. Data were collected in 1mm path length cuvettes loaded in an MBraun UniLab glovebox and were run verses the appropriate toluene reference solvent. Variable-temperature magnetic moment data were recorded in an applied dc field of 0.1 T on a Quantum Design MPMS XL5 SQUID magnetometer using doubly recrystallised powdered samples. Samples were checked for purity before and after use and data reproducibility was carefully checked. Care was taken to ensure complete thermalisation of the sample before each data point was measured. A diamagnetic corrections of 831.8×10^{-6} cm^3 mol^{-1} was applied for **3** using tabulated Pascal constants and measurements were corrected for the effect of the blank sample holders (flame sealed Wilmad NMR tube and straw). Solution magnetic moments were recorded at room temperature using the Evans method and the variance of measured solution and solid state magnetic moments is attributed to the different condensed phases and weighing errors. Variable temperature (300-5 K) EPR spectra were measured at S-band (ca. 3.8 GHz) on a Bruker Elexsys E500 spectrometer with a ER4118SMS5 resonator. Polycrystalline samples were sealed under vacuum in 1mm i.d. silica tubing, and double-contained for EPR by insertion into an X-band silica tube or PTFE sleeve. Measurements were made on several independently prepared batches, which were also analysed by SQUID and CHN microanalyses, to ensure reproducibility. Spectra were background corrected against blank sample holders measured under identical conditions. Elemental microanalyses were carried out by Tong Liu at the University of Nottingham.

Preparation of [{U(Ts^{Tol})}$_2$(μ-η^6:η^6-C_6H_5Me)] (3)

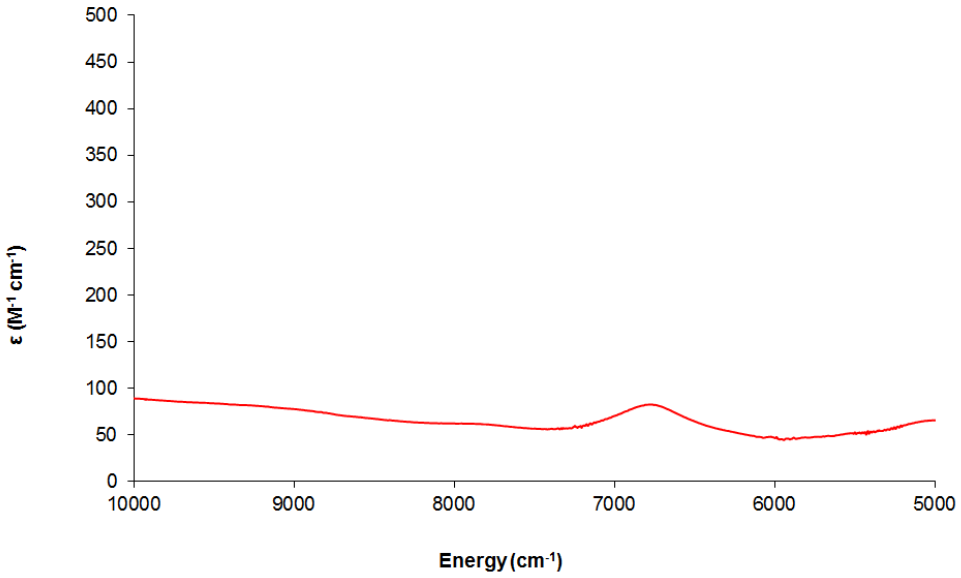
Toluene (15 ml) and THF (15 ml) were added simultaneously to a cold (-78 °C) stirring mixture of **2** (4.24 g, 5.00 mmol) and KC_8 (0.74 g, 5.50 mmol). The mixture was allowed to warm to room temperature over 16 hours with stirring. After this time the mixture was filtered and the black solids washed with toluene (2 × 5 mL). All the volatiles were removed *in vacuo* to afford a dark red solid. The solid was dissolved in hexanes and was stored at -30 °C to yield **3** as dark red crystals. Yield: 3.75 g, 95 %. Dark red blocks of **3**.1.5C_6H_{14} suitable for X-ray diffraction studies were grown from a saturated hexanes solution of **3** stored at -30 °C over 16 hours. Anal. Calcd for $C_{72}H_{109}N_6Si_6U_2$: C, 50.77; H, 6.45; N, 4.93 %. Found: C, 48.97; H, 6.11; N, 4.91 %. Slightly low carbon values for silicon-rich f-block complexes are common.[3] ^{1}H NMR (C_6D_6): δ 32.45 (3H, s, C*H*$_3$-toluene), 11.27 (12H, s, Ar-C*H*), 9.33 (12H, s, Ar-C*H*), 4.01 (18H, s, Ar-C*H*$_3$), -1.97 (36H, s, Si-C*H*$_3$), -18.80 (2H, s, C*H*-toluene), -21.04 (2H, s, C*H*-toluene), -34.95 (1H, s, *p*-C*H*-toluene), -35.11 (2H, s, Si-C*H*). Magnetic moment (Evans method, C_6D_6, 298 K): μ_{eff} = 2.92 μ_B. FTIR ν/cm^{-1} (Nujol): 1602 (m), 1495 (vs), 1464 (vs), 1235 (vs), 1170 (m), 1102 (m), 1043 (m), 974 (s), 930 (m), 907 (vs), 839 (vs), 810 (vs), 748 (m), 727 (m), 707 (m), 699 (m), 637 (w), 542 (w), 502 (m).

UV/Vis/NIR Electronic Absorption Spectra

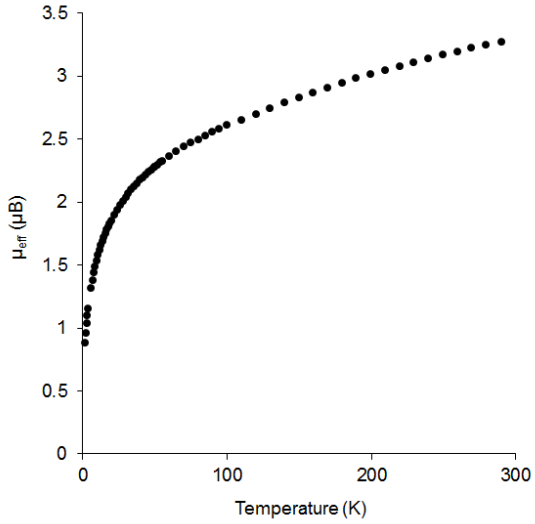
25,000-5,000 cm^{-1} range of 3



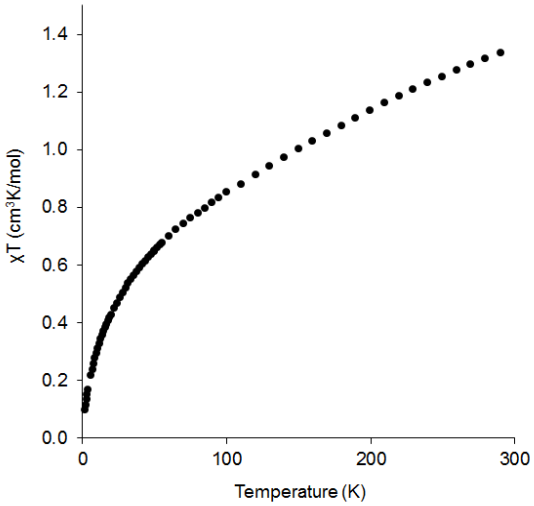
Zoom-in of 10,000-5,000 cm^{-1} region of 3



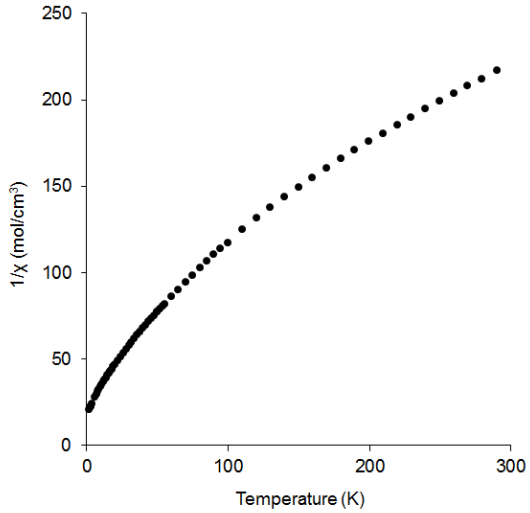
μ_{eff} (μ_B) vs T for 3



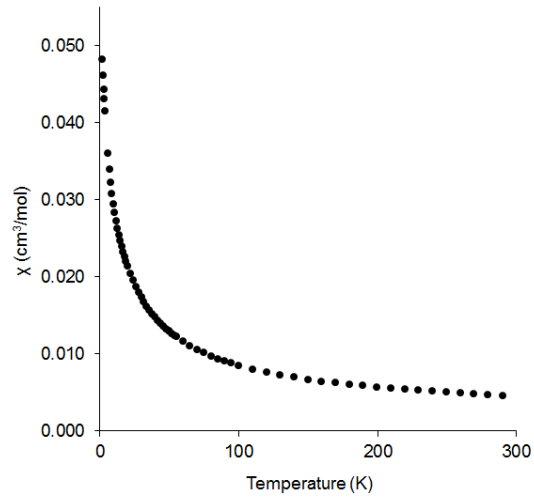
χT vs T for 3



1/χ vs T for 3



χ vs T for 3



X-ray Crystallography

Experimental details for 3 CCDC 904038

Crystal data	
Chemical formula	$C_{63}H_{88}N_6Si_6U_2$1.5(C_6H_{14})
M_r	1703.25
Crystal system, space group	Tetragonal, *P*-42$_1$*m*
Temperature (K)	90
a, *c* (Å)	23.0405 (3), 15.9177 (2)
V (Å^3)	8450.13 (19)
Z	4
Radiation type	Cu *K*a
m (mm^{-1})	11.81
Crystal size (mm)	0.54 × 0.09 × 0.08
Data collection	
Diffractometer	SuperNova, Single source at offset), Atlas diffractometer
Absorption correction	Analytical *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.36 (release 02-08-2010 CrysAlis171 .NET) (compiled Jan 5 2010,16:28:46) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897)
T_{min}, T_{max}	0.102, 0.503
No. of measured, independent and observed [$I > 2s(I)$] reflections	8498, 8498, 7674
R_{int}	0.0000
(sin q/l)$_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2s(F^2)]$, $wR(F^2)$, *S*	0.072, 0.195, 1.10
No. of reflections	8498
No. of parameters	620
No. of restraints	1059
H-atom treatment	H-atom parameters constrained
	$w = 1/[s^2(F_o^2) + (0.1048P)^2 + 79.092P]$ where $P = (F_o^2 + 2F_c^2)/3$
Dρ$_{max}$, Dρ$_{min}$ (e Å^{-3})	3.46, -3.50
Absolute structure	Flack H D (1983), Acta Cryst. A39, 876-881
Flack parameter	0.00 (2)

Bond lengths (Å) for 3

U1—N1	2.239 (15)	C50—C51	1.3900
U1—N1^{i}	2.239 (15)	C55—C54	1.3900
U1—N2^{i}	2.314 (17)	C54—C53	1.3900
U1—N2	2.314 (17)	C53—C52	1.3900
U1—N3^{i}	2.351 (18)	C53—C56	1.61 (5)
U1—N3	2.351 (18)	C52—C51	1.3900
U1—C59	2.592 (16)	C57—C58	1.55 (3)
U1—C59^{i}	2.592 (16)	C58—C63	1.3900
U1—C58	2.595 (13)	C58—C59	1.3900
U1—C58^{i}	2.595 (13)	C63—C62	1.3900
U1—C60	2.629 (14)	C62—C61	1.3900
U1—C60^{i}	2.629 (15)	C61—C60	1.3900
U1—C63	2.636 (15)	C60—C59	1.3900
U1—C63^{i}	2.636 (16)	C1—H1	1.0000
U1—C61	2.669 (12)	C2—H2C	0.9800
U1—C61^{i}	2.669 (13)	C2—H2B	0.9800
U1—C62	2.673 (16)	C2—H2A	0.9800
U1—C62^{i}	2.673 (18)	C3—H3C	0.9800
U2—N5	2.19 (2)	C3—H3B	0.9800
U2—N5^{i}	2.19 (2)	C3—H3A	0.9800
U2—N4	2.193 (18)	C5—H5	0.9500
U2—N4^{i}	2.193 (18)	C6—H6	0.9500
U2—N6^{i}	2.47 (3)	C8—H8	0.9500
U2—N6	2.47 (3)	C9—H9	0.9500
U2—C60^{i}	2.535 (15)	C10—H10C	0.9800
U2—C60	2.535 (15)	C10—H10B	0.9800
U2—C61^{i}	2.537 (15)	C10—H10A	0.9800
U2—C61	2.537 (14)	C11—H11C	0.9800
U2—C59^{i}	2.581 (15)	C11—H11B	0.9800
U2—C59	2.581 (16)	C11—H11A	0.9800
U2—C62^{i}	2.585 (17)	C12—H12C	0.9800
U2—C62	2.585 (17)	C12—H12B	0.9800
U2—C58^{i}	2.628 (13)	C12—H12A	0.9800
U2—C58	2.628 (13)	C14—H14	0.9500
U2—C63^{i}	2.630 (15)	C15—H15	0.9500
U2—C63	2.630 (15)	C17—H17	0.9500
Si1—N1	1.753 (13)	C18—H18	0.9500
Si1—C1	1.859 (10)	C19—H19C	0.9800
Si1—C3	1.864 (13)	C19—H19B	0.9800
Si1—C2	1.869 (14)	C19—H19A	0.9800
Si2—N2	1.738 (14)	C20—H20C	0.9800
Si2—C1	1.864 (10)	C20—H20B	0.9800
Si2—C12	1.878 (14)	C20—H20A	0.9800
Si2—C11	1.894 (14)	C21—H21C	0.9800
Si3—N3	1.739 (14)	C21—H21B	0.9800
Si3—C21	1.864 (14)	C21—H21A	0.9800

Si3—C1	1.872 (10)	C23—H23	0.9500
Si3—C20	1.881 (14)	C24—H24	0.9500
Si4—N4	1.741 (15)	C26—H26	0.9500
Si4—C29	1.827 (12)	C27—H27	0.9500
Si4—C31	1.868 (16)	C28—H28C	0.9800
Si4—C30	1.880 (15)	C28—H28B	0.9800
Si5—N5	1.767 (15)	C28—H28A	0.9800
Si5—C39	1.868 (16)	C29—H29	1.0000
Si5—C29	1.871 (13)	C30—H30C	0.9800
Si5—C40	1.882 (15)	C30—H30B	0.9800
Si6—N6	1.738 (15)	C30—H30A	0.9800
Si6—C49	1.894 (15)	C31—H31C	0.9800
Si6—C29	1.915 (13)	C31—H31B	0.9800
Si6—C48	1.935 (16)	C31—H31A	0.9800
N1—C4	1.460 (15)	C33—H33	0.9500
N2—C13	1.438 (15)	C34—H34	0.9500
N3—C22	1.455 (16)	C36—H36	0.9500
N4—C32	1.461 (18)	C37—H37	0.9500
N5—C41	1.461 (18)	C38—H38C	0.9800
N6—C50	1.458 (18)	C38—H38B	0.9800
C4—C5	1.3900	C38—H38A	0.9800
C4—C9	1.3900	C39—H39C	0.9800
C5—C6	1.3900	C39—H39B	0.9800
C6—C7	1.3900	C39—H39A	0.9800
C7—C8	1.3900	C40—H40C	0.9800
C7—C10	1.54 (2)	C40—H40B	0.9800
C8—C9	1.3900	C40—H40A	0.9800
C13—C14	1.3900	C42—H42	0.9500
C13—C18	1.3900	C43—H43	0.9500
C14—C15	1.3900	C45—H45	0.9500
C15—C16	1.3900	C46—H46	0.9500
C16—C17	1.3900	C47—H47C	0.9800
C16—C19	1.55 (3)	C47—H47B	0.9800
C17—C18	1.3900	C47—H47A	0.9800
C22—C23	1.3900	C48—H48C	0.9800
C22—C27	1.3900	C48—H48B	0.9800
C23—C24	1.3900	C48—H48A	0.9800
C24—C25	1.3900	C49—H49C	0.9800
C25—C26	1.3900	C49—H49B	0.9800
C25—C28	1.60 (3)	C49—H49A	0.9800
C26—C27	1.3900	C51—H51	0.9500
C33—C32	1.3900	C52—H52	0.9500
C33—C34	1.3900	C54—H54	0.9500
C32—C37	1.3900	C55—H55	0.9500
C37—C36	1.3900	C56—H56C	0.9800
C36—C35	1.3900	C56—H56B	0.9800
C35—C34	1.3900	C56—H56A	0.9800

C35—C38	1.53 (5)	C57—H57C	0.9800
C41—C46	1.3900	C57—H57B	0.9800
C41—C42	1.3900	C57—H57A	0.9800
C46—C45	1.3900	C59—H59	0.9500
C45—C44	1.3900	C60—H60	0.9500
C44—C43	1.3900	C61—H61	0.9500
C44—C47	1.57 (5)	C62—H62	0.9500
C43—C42	1.3900	C63—H63	0.9500
C50—C55	1.3900		

Bond angles (°) for 3

N1—U1—N1^{i}	43.3 (10)	C58—U2—C63^{i}	16.3 (6)
N1—U1—N2^{i}	107.9 (6)	N5—U2—C63	96.2 (6)
N1^{i}—U1—N2^{i}	92.5 (7)	N5^{i}—U2—C63	116.0 (7)
N1—U1—N2	92.5 (7)	N4—U2—C63	136.7 (7)
N1^{i}—U1—N2	107.9 (6)	N4^{i}—U2—C63	144.3 (10)
N2^{i}—U1—N2	41.8 (11)	N6^{i}—U2—C63	88.4 (5)
N1—U1—N3^{i}	50.6 (7)	N6—U2—C63	131.3 (6)
N1^{i}—U1—N3^{i}	89.3 (6)	C60^{i}—U2—C63	45.7 (2)
N2^{i}—U1—N3^{i}	89.5 (6)	C60—U2—C63	65.09 (17)
N2—U1—N3^{i}	52.4 (7)	C61^{i}—U2—C63	64.2 (4)
N1—U1—N3	89.3 (6)	C61—U2—C63	55.5 (2)
N1^{i}—U1—N3	50.6 (7)	C59^{i}—U2—C63	16.1 (3)
N2^{i}—U1—N3	52.4 (7)	C59—U2—C63	55.02 (19)
N2—U1—N3	89.5 (6)	C62^{i}—U2—C63	63.6 (5)
N3^{i}—U1—N3	115.0 (7)	C62—U2—C63	30.90 (18)
N1—U1—C59	102.5 (5)	C58^{i}—U2—C63	16.3 (6)
N1^{i}—U1—C59	126.0 (6)	C58—U2—C63	30.65 (14)
N2^{i}—U1—C59	141.5 (5)	C63^{i}—U2—C63	45.1 (6)
N2—U1—C59	115.0 (6)	N1—Si1—C1	103.9 (8)
N3^{i}—U1—C59	91.9 (5)	N1—Si1—C3	113.5 (9)
N3—U1—C59	151.8 (5)	C1—Si1—C3	113.2 (7)
N1—U1—C59^{i}	126.0 (6)	N1—Si1—C2	108.6 (10)
N1^{i}—U1—C59^{i}	102.5 (5)	C1—Si1—C2	113.3 (7)
N2^{i}—U1—C59^{i}	115.0 (6)	C3—Si1—C2	104.5 (8)
N2—U1—C59^{i}	141.5 (5)	N1—Si1—U1	34.0 (5)
N3^{i}—U1—C59^{i}	151.8 (5)	C1—Si1—U1	73.6 (5)
N3—U1—C59^{i}	91.9 (5)	C3—Si1—U1	141.3 (7)
C59—U1—C59^{i}	60.4 (6)	C2—Si1—U1	107.1 (7)
N1—U1—C58	94.0 (5)	N2—Si2—C1	102.7 (8)
N1^{i}—U1—C58	99.6 (5)	N2—Si2—C12	115.7 (11)
N2^{i}—U1—C58	157.3 (5)	C1—Si2—C12	112.1 (7)
N2—U1—C58	146.0 (6)	N2—Si2—C11	112.2 (10)
N3^{i}—U1—C58	109.7 (5)	C1—Si2—C11	111.2 (8)
N3—U1—C58	123.9 (5)	C12—Si2—C11	103.1 (8)
C59—U1—C58	31.09 (16)	N3—Si3—C21	111.6 (10)

C59^{i}—U1—C58	43.6 (5)	N3—Si3—C1	104.7 (8)
N1—U1—C58^{i}	99.6 (5)	C21—Si3—C1	112.5 (7)
N1^{i}—U1—C58^{i}	94.0 (5)	N3—Si3—C20	112.6 (11)
N2^{i}—U1—C58^{i}	146.0 (6)	C21—Si3—C20	104.9 (8)
N2—U1—C58^{i}	157.3 (5)	C1—Si3—C20	110.8 (7)
N3^{i}—U1—C58^{i}	123.9 (5)	N4—Si4—C29	102.9 (11)
N3—U1—C58^{i}	109.7 (5)	N4—Si4—C31	107.7 (19)
C59—U1—C58^{i}	43.6 (6)	C29—Si4—C31	115.4 (10)
C59^{i}—U1—C58^{i}	31.1 (3)	N4—Si4—C30	112.9 (18)
C58—U1—C58^{i}	15.1 (7)	C29—Si4—C30	114.5 (10)
N1—U1—C60	130.1 (5)	C31—Si4—C30	103.7 (10)
N1^{i}—U1—C60	154.4 (6)	N4—Si4—U2	32.2 (7)
N2^{i}—U1—C60	111.2 (5)	C29—Si4—U2	71.8 (8)
N2—U1—C60	96.5 (5)	C31—Si4—U2	113.6 (11)
N3^{i}—U1—C60	99.9 (5)	C30—Si4—U2	134.7 (12)
N3—U1—C60	139.5 (6)	N5—Si5—C39	118.9 (17)
C59—U1—C60	30.87 (17)	N5—Si5—C29	104.8 (13)
C59^{i}—U1—C60	59.5 (5)	C39—Si5—C29	113.8 (9)
C58—U1—C60	54.9 (2)	N5—Si5—C40	103.1 (16)
C58^{i}—U1—C60	61.1 (4)	C39—Si5—C40	104.0 (10)
N1—U1—C60^{i}	154.4 (5)	C29—Si5—C40	111.8 (9)
N1^{i}—U1—C60^{i}	130.1 (5)	N5—Si5—U2	36.7 (9)
N2^{i}—U1—C60^{i}	96.5 (5)	C39—Si5—U2	113.9 (11)
N2—U1—C60^{i}	111.2 (5)	C29—Si5—U2	75.0 (8)
N3^{i}—U1—C60^{i}	139.5 (5)	C40—Si5—U2	134.7 (11)
N3—U1—C60^{i}	99.9 (5)	N6—Si6—C49	128.4 (17)
C59—U1—C60^{i}	59.5 (6)	N6—Si6—C29	109.0 (13)
C59^{i}—U1—C60^{i}	30.9 (2)	C49—Si6—C29	109.6 (9)
C58—U1—C60^{i}	61.1 (3)	N6—Si6—C48	100.9 (15)
C58^{i}—U1—C60^{i}	54.9 (3)	C49—Si6—C48	100.0 (10)
C60—U1—C60^{i}	40.8 (7)	C29—Si6—C48	105.9 (9)
N1—U1—C63	110.7 (6)	C4—N1—Si1	117.2 (11)
N1^{i}—U1—C63	94.0 (5)	C4—N1—U1	122.7 (10)
N2^{i}—U1—C63	129.8 (6)	Si1—N1—U1	120.0 (8)
N2—U1—C63	155.9 (5)	C13—N2—Si2	119.9 (12)
N3^{i}—U1—C63	140.3 (5)	C13—N2—U1	122.0 (10)
N3—U1—C63	97.1 (5)	Si2—N2—U1	118.0 (8)
C59—U1—C63	54.84 (19)	C22—N3—Si3	122.9 (13)
C59^{i}—U1—C63	16.1 (3)	C22—N3—U1	120.1 (10)
C58—U1—C63	30.81 (14)	Si3—N3—U1	116.4 (8)
C58^{i}—U1—C63	16.4 (6)	C32—N4—Si4	115.1 (14)
C60—U1—C63	63.75 (17)	C32—N4—U2	121.3 (13)
C60^{i}—U1—C63	44.8 (2)	Si4—N4—U2	122.7 (11)
N1—U1—C63^{i}	94.0 (5)	C41—N5—Si5	120.5 (18)
N1^{i}—U1—C63^{i}	110.7 (6)	C41—N5—U2	116.0 (14)
N2^{i}—U1—C63^{i}	155.9 (5)	Si5—N5—U2	114.4 (13)
N2—U1—C63^{i}	129.8 (6)	C50—N6—Si6	110.3 (17)

N3^{i}—U1—C63^{i}	97.1 (4)	C50—N6—U2	134.0 (15)
N3—U1—C63^{i}	140.3 (5)	Si6—N6—U2	112.4 (14)
C59—U1—C63^{i}	16.1 (3)	Si1—C1—Si2	114.2 (6)
C59^{i}—U1—C63^{i}	54.8 (2)	Si1—C1—Si3	113.5 (6)
C58—U1—C63^{i}	16.4 (5)	Si2—C1—Si3	114.3 (6)
C58^{i}—U1—C63^{i}	30.81 (19)	C5—C4—C9	120.0
C60—U1—C63^{i}	44.8 (2)	C5—C4—N1	120.8 (12)
C60^{i}—U1—C63^{i}	63.7 (4)	C9—C4—N1	118.7 (12)
C63—U1—C63^{i}	45.0 (6)	C4—C5—C6	120.0
N1—U1—C61	156.4 (5)	C7—C6—C5	120.0
N1^{i}—U1—C61	142.8 (5)	C6—C7—C8	120.0
N2^{i}—U1—C61	95.3 (5)	C6—C7—C10	120.3 (7)
N2—U1—C61	102.0 (5)	C8—C7—C10	119.7 (7)
N3^{i}—U1—C61	127.0 (6)	C9—C8—C7	120.0
N3—U1—C61	109.1 (6)	C8—C9—C4	120.0
C59—U1—C61	54.4 (2)	C14—C13—C18	120.0
C59^{i}—U1—C61	41.9 (3)	C14—C13—N2	116.6 (12)
C58—U1—C61	63.73 (17)	C18—C13—N2	123.3 (12)
C58^{i}—U1—C61	61.0 (2)	C13—C14—C15	120.0
C60—U1—C61	30.40 (13)	C16—C15—C14	120.0
C60^{i}—U1—C61	12.7 (6)	C15—C16—C17	120.0
C63—U1—C61	54.0 (2)	C15—C16—C19	119.2 (7)
C63^{i}—U1—C61	62.4 (3)	C17—C16—C19	120.7 (7)
N1—U1—C61^{i}	142.8 (5)	C16—C17—C18	120.0
N1^{i}—U1—C61^{i}	156.4 (5)	C17—C18—C13	120.0
N2^{i}—U1—C61^{i}	102.0 (5)	C23—C22—C27	120.0
N2—U1—C61^{i}	95.3 (5)	C23—C22—N3	117.7 (11)
N3^{i}—U1—C61^{i}	109.1 (6)	C27—C22—N3	122.2 (11)
N3—U1—C61^{i}	127.0 (6)	C24—C23—C22	120.0
C59—U1—C61^{i}	41.9 (4)	C25—C24—C23	120.0
C59^{i}—U1—C61^{i}	54.4 (4)	C24—C25—C26	120.0
C58—U1—C61^{i}	60.98 (19)	C24—C25—C28	119.8 (7)
C58^{i}—U1—C61^{i}	63.7 (2)	C26—C25—C28	120.2 (7)
C60—U1—C61^{i}	12.7 (6)	C25—C26—C27	120.0
C60^{i}—U1—C61^{i}	30.40 (16)	C26—C27—C22	120.0
C63—U1—C61^{i}	62.4 (4)	Si4—C29—Si5	114.2 (9)
C63^{i}—U1—C61^{i}	54.0 (3)	Si4—C29—Si6	106.8 (9)
C61—U1—C61^{i}	18.7 (8)	Si5—C29—Si6	121.4 (10)
N1—U1—C62	140.5 (6)	C32—C33—C34	120.0
N1^{i}—U1—C62	112.7 (5)	C33—C32—C37	120.0
N2^{i}—U1—C62	103.2 (6)	C33—C32—N4	122 (2)
N2—U1—C62	127.0 (5)	C37—C32—N4	118 (2)
N3^{i}—U1—C62	153.6 (5)	C32—C37—C36	120.0
N3—U1—C62	90.8 (5)	C35—C36—C37	120.0
C59—U1—C62	63.73 (17)	C36—C35—C34	120.0
C59^{i}—U1—C62	14.55 (10)	C36—C35—C38	120.1 (8)
C58—U1—C62	54.4 (2)	C34—C35—C38	119.7 (8)

C58^{i}—U1—C62	44.0 (4)	C35—C34—C33	120.0
C60—U1—C62	54.01 (18)	C46—C41—C42	120.0
C60^{i}—U1—C62	17.9 (4)	C46—C41—N5	121 (2)
C63—U1—C62	30.35 (17)	C42—C41—N5	119 (2)
C63^{i}—U1—C62	62.4 (5)	C45—C46—C41	120.0
C61—U1—C62	30.16 (15)	C46—C45—C44	120.0
C61^{i}—U1—C62	46.0 (7)	C45—C44—C43	120.0
N1—U1—C62^{i}	112.7 (4)	C45—C44—C47	119.9 (8)
N1^{i}—U1—C62^{i}	140.5 (6)	C43—C44—C47	119.9 (8)
N2^{i}—U1—C62^{i}	127.0 (5)	C44—C43—C42	120.0
N2—U1—C62^{i}	103.2 (6)	C43—C42—C41	120.0
N3^{i}—U1—C62^{i}	90.8 (5)	C55—C50—C51	120.0
N3—U1—C62^{i}	153.6 (5)	C55—C50—N6	117 (2)
C59—U1—C62^{i}	14.55 (10)	C51—C50—N6	123 (2)
C59^{i}—U1—C62^{i}	63.7 (2)	C50—C55—C54	120.0
C58—U1—C62^{i}	44.0 (4)	C55—C54—C53	120.0
C58^{i}—U1—C62^{i}	54.4 (4)	C54—C53—C52	120.0
C60—U1—C62^{i}	17.9 (4)	C54—C53—C56	119.7 (8)
C60^{i}—U1—C62^{i}	54.0 (3)	C52—C53—C56	120.3 (8)
C63—U1—C62^{i}	62.4 (5)	C51—C52—C53	120.0
C63^{i}—U1—C62^{i}	30.4 (2)	C52—C51—C50	120.0
C61—U1—C62^{i}	46.0 (5)	C63—C58—C59	120.0
C61^{i}—U1—C62^{i}	30.2 (3)	C63—C58—C57	119.4 (7)
C62—U1—C62^{i}	63.0 (6)	C59—C58—C57	119.8 (7)
N5—U2—N5^{i}	51.0 (18)	C63—C58—U1	76.2 (6)
N5—U2—N4	99.7 (11)	C59—C58—U1	74.3 (6)
N5^{i}—U2—N4	105.2 (8)	C57—C58—U1	129.6 (11)
N5—U2—N4^{i}	105.2 (8)	C63—C58—U2	74.7 (6)
N5^{i}—U2—N4^{i}	99.7 (11)	C59—C58—U2	72.7 (6)
N4—U2—N4^{i}	13 (2)	C57—C58—U2	115.1 (11)
N5—U2—N6^{i}	43.5 (12)	U1—C58—U2	115.3 (5)
N5^{i}—U2—N6^{i}	92.7 (11)	C62—C63—C58	120.0
N4—U2—N6^{i}	76.6 (14)	C62—C63—U2	72.8 (5)
N4^{i}—U2—N6^{i}	87.9 (12)	C58—C63—U2	74.6 (6)
N5—U2—N6	92.7 (11)	C62—C63—U1	76.3 (5)
N5^{i}—U2—N6	43.5 (12)	C58—C63—U1	73.0 (6)
N4—U2—N6	87.9 (12)	U2—C63—U1	113.8 (5)
N4^{i}—U2—N6	76.6 (14)	C63—C62—C61	120.0
N6^{i}—U2—N6	127.5 (10)	C63—C62—U2	76.3 (5)
N5—U2—C60^{i}	128.9 (8)	C61—C62—U2	72.4 (5)
N5^{i}—U2—C60^{i}	159.9 (6)	C63—C62—U1	73.4 (4)
N4—U2—C60^{i}	94.8 (6)	C61—C62—U1	74.8 (5)
N4^{i}—U2—C60^{i}	99.3 (9)	U2—C62—U1	114.1 (5)
N6^{i}—U2—C60^{i}	94.7 (7)	C60—C61—C62	120.0
N6—U2—C60^{i}	136.9 (7)	C60—C61—U2	74.0 (6)
N5—U2—C60	159.9 (6)	C62—C61—U2	76.2 (6)
N5^{i}—U2—C60	128.9 (9)	C60—C61—U1	73.2 (6)

N4—U2—C60	99.3 (9)	C62—C61—U1	75.0 (5)
N4^{i}—U2—C60	94.8 (5)	U2—C61—U1	115.8 (5)
N6^{i}—U2—C60	136.9 (7)	C59—C60—C61	120.0
N6—U2—C60	94.7 (7)	C59—C60—U2	76.1 (5)
C60^{i}—U2—C60	42.4 (7)	C61—C60—U2	74.2 (6)
N5—U2—C61^{i}	159.3 (7)	C59—C60—U1	73.1 (5)
N5^{i}—U2—C61^{i}	142.0 (8)	C61—C60—U1	76.4 (6)
N4—U2—C61^{i}	91.5 (7)	U2—C60—U1	117.3 (5)
N4^{i}—U2—C61^{i}	89.4 (6)	C60—C59—C58	120.0
N6^{i}—U2—C61^{i}	124.7 (8)	C60—C59—U2	72.4 (5)
N6—U2—C61^{i}	105.2 (7)	C58—C59—U2	76.4 (5)
C60^{i}—U2—C61^{i}	31.81 (19)	C60—C59—U1	76.1 (4)
C60—U2—C61^{i}	13.3 (7)	C58—C59—U1	74.6 (5)
N5—U2—C61	142.0 (9)	U2—C59—U1	117.0 (5)
N5^{i}—U2—C61	159.3 (7)	Si1—C1—H1	104.4
N4—U2—C61	89.4 (6)	Si2—C1—H1	104.4
N4^{i}—U2—C61	91.5 (7)	Si3—C1—H1	104.4
N6^{i}—U2—C61	105.2 (7)	C4—C5—H5	120.0
N6—U2—C61	124.7 (8)	C6—C5—H5	120.0
C60^{i}—U2—C61	13.3 (6)	C5—C6—H6	120.0
C60—U2—C61	31.81 (16)	C7—C6—H6	120.0
C61^{i}—U2—C61	19.7 (8)	C7—C8—H8	120.0
N5—U2—C59^{i}	103.2 (7)	C9—C8—H8	120.0
N5^{i}—U2—C59^{i}	131.5 (7)	C4—C9—H9	120.0
N4—U2—C59^{i}	120.7 (7)	C8—C9—H9	120.0
N4^{i}—U2—C59^{i}	128.4 (10)	C13—C14—H14	120.0
N6^{i}—U2—C59^{i}	84.1 (5)	C15—C14—H14	120.0
N6—U2—C59^{i}	143.4 (6)	C14—C15—H15	120.0
C60^{i}—U2—C59^{i}	31.5 (2)	C16—C15—H15	120.0
C60—U2—C59^{i}	60.8 (5)	C16—C17—H17	120.0
C61^{i}—U2—C59^{i}	56.1 (4)	C18—C17—H17	120.0
C61—U2—C59^{i}	43.1 (3)	C13—C18—H18	120.0
N5—U2—C59	131.5 (7)	C17—C18—H18	120.0
N5^{i}—U2—C59	103.2 (7)	Si3—C21—H21C	109.5
N4—U2—C59	128.4 (10)	Si3—C21—H21B	109.5
N4^{i}—U2—C59	120.7 (7)	Si3—C21—H21A	109.5
N6^{i}—U2—C59	143.4 (5)	H21B—C21—H21C	109.5
N6—U2—C59	84.1 (5)	H21A—C21—H21C	109.5
C60^{i}—U2—C59	60.8 (6)	H21A—C21—H21B	109.5
C60—U2—C59	31.51 (19)	C22—C23—H23	120.0
C61^{i}—U2—C59	43.1 (4)	C24—C23—H23	120.0
C61—U2—C59	56.1 (2)	C23—C24—H24	120.0
C59^{i}—U2—C59	60.7 (6)	C25—C24—H24	120.0
N5—U2—C62^{i}	146.4 (7)	C25—C26—H26	120.0
N5^{i}—U2—C62^{i}	111.6 (8)	C27—C26—H26	120.0

N4—U2—C62^{i}	113.5 (10)	C22—C27—H27	120.0
N4^{i}—U2—C62^{i}	106.3 (7)	C26—C27—H27	120.0
N6^{i}—U2—C62^{i}	148.7 (6)	Si4—C29—H29	104.2
N6—U2—C62^{i}	83.4 (6)	Si5—C29—H29	104.2
C60^{i}—U2—C62^{i}	56.1 (3)	Si6—C29—H29	104.2
C60—U2—C62^{i}	18.5 (4)	C32—C33—H33	120.0
C61^{i}—U2—C62^{i}	31.5 (3)	C34—C33—H33	120.0
C61—U2—C62^{i}	48.0 (6)	C33—C34—H34	120.0
C59^{i}—U2—C62^{i}	65.1 (2)	C35—C34—H34	120.0
C59—U2—C62^{i}	14.93 (12)	C35—C36—H36	120.0
N5—U2—C62	111.6 (8)	C37—C36—H36	120.0
N5^{i}—U2—C62	146.4 (8)	C32—C37—H37	120.0
N4—U2—C62	106.3 (7)	C36—C37—H37	120.0
N4^{i}—U2—C62	113.5 (10)	Si5—C39—H39C	109.5
N6^{i}—U2—C62	83.4 (6)	Si5—C39—H39B	109.5
N6—U2—C62	148.7 (6)	Si5—C39—H39A	109.5
C60^{i}—U2—C62	18.5 (4)	H39B—C39—H39C	109.5
C60—U2—C62	56.1 (2)	H39A—C39—H39C	109.5
C61^{i}—U2—C62	48.0 (7)	H39A—C39—H39B	109.5
C61—U2—C62	31.47 (18)	C41—C42—H42	120.0
C59^{i}—U2—C62	14.93 (11)	C43—C42—H42	120.0
C59—U2—C62	65.11 (17)	C42—C43—H43	120.0
C62^{i}—U2—C62	65.4 (6)	C44—C43—H43	120.0
N5—U2—C58^{i}	98.1 (6)	C44—C45—H45	120.0
N5^{i}—U2—C58^{i}	104.6 (6)	C46—C45—H45	120.0
N4—U2—C58^{i}	150.2 (6)	C41—C46—H46	120.0
N4^{i}—U2—C58^{i}	153.6 (7)	C45—C46—H46	120.0
N6^{i}—U2—C58^{i}	100.9 (6)	H47B—C47—H47C	109.5
N6—U2—C58^{i}	115.0 (6)	H47A—C47—H47C	109.5
C60^{i}—U2—C58^{i}	55.5 (3)	H47A—C47—H47B	109.5
C60—U2—C58^{i}	61.8 (3)	C44—C47—H47C	109.5
C61^{i}—U2—C58^{i}	65.1 (2)	C44—C47—H47B	109.5
C61—U2—C58^{i}	62.3 (2)	C44—C47—H47A	109.5
C59^{i}—U2—C58^{i}	30.9 (3)	Si6—C49—H49C	109.5
C59—U2—C58^{i}	43.4 (5)	Si6—C49—H49B	109.5
C62^{i}—U2—C58^{i}	55.0 (4)	Si6—C49—H49A	109.5
C62—U2—C58^{i}	44.5 (4)	H49B—C49—H49C	109.5
N5—U2—C58	104.6 (6)	H49A—C49—H49C	109.5
N5^{i}—U2—C58	98.1 (5)	H49A—C49—H49B	109.5

N4—U2—C58	153.6 (7)	C50—C51—H51	120.0
N4^{i}—U2—C58	150.2 (6)	C52—C51—H51	120.0
N6^{i}—U2—C58	115.0 (6)	C51—C52—H52	120.0
N6—U2—C58	100.9 (6)	C53—C52—H52	120.0
C60^{i}—U2—C58	61.8 (3)	C53—C54—H54	120.0
C60—U2—C58	55.5 (2)	C55—C54—H54	120.0
C61^{i}—U2—C58	62.3 (2)	C50—C55—H55	120.0
C61—U2—C58	65.09 (17)	C54—C55—H55	120.0
C59^{i}—U2—C58	43.4 (5)	U1—C59—H59	120.4
C59—U2—C58	30.93 (16)	U2—C59—H59	122.5
C62^{i}—U2—C58	44.5 (4)	C58—C59—H59	120.0
C62—U2—C58	55.0 (2)	C60—C59—H59	120.0
C58^{i}—U2—C58	14.9 (6)	U1—C60—H60	121.8
N5—U2—C63^{i}	116.0 (7)	U2—C60—H60	120.9
N5^{i}—U2—C63^{i}	96.2 (6)	C59—C60—H60	120.0
N4—U2—C63^{i}	144.3 (10)	C61—C60—H60	120.0
N4^{i}—U2—C63^{i}	136.7 (7)	U1—C61—H61	123.2
N6^{i}—U2—C63^{i}	131.3 (6)	U2—C61—H61	121.0
N6—U2—C63^{i}	88.4 (6)	C60—C61—H61	120.0
C60^{i}—U2—C63^{i}	65.1 (4)	C62—C61—H61	120.0
C60—U2—C63^{i}	45.7 (2)	U1—C62—H62	123.3
C61^{i}—U2—C63^{i}	55.5 (3)	U2—C62—H62	122.6
C61—U2—C63^{i}	64.2 (3)	C61—C62—H62	120.0
C59^{i}—U2—C63^{i}	55.0 (2)	C63—C62—H62	120.0
C59—U2—C63^{i}	16.1 (3)	U1—C63—H63	122.0
C62^{i}—U2—C63^{i}	30.9 (2)	U2—C63—H63	124.2
C62—U2—C63^{i}	63.6 (5)	C58—C63—H63	120.0
C58^{i}—U2—C63^{i}	30.65 (18)	C62—C63—H63	120.0

DFT Calculations

General

Unrestricted geometry optimisations were performed for the full model of **3** using coordinates derived from the X-ray crystal structure. No constraints were imposed on the structure during the geometry optimisations. The calculations were performed using the Amsterdam Density Functional (ADF) suite version 2010.01.[4,5] The DFT geometry optimisations employed Slater type orbital (STO) triple-ζ-plus polarisation all-electron basis sets (from the ZORA/TZP database of the ADF suite). Scalar relativistic approaches were used within the ZORA Hamiltonian for the inclusion of relativistic effects and the local density

approximation (LDA) with the correlation potential due to Vosko et al[6] was used in all of the calculations. Gradient corrections were performed using the functionals of Becke[7] and Perdew.[8] MOLEKEL[9] was used to prepare the three-dimensional plot of the electron density. Nalewajski-Mrozek bond indices are reported as they account for covalent as well as ionic contributions to the bonding.

Final coordinates and single point energy for geometry optimised 3

1.C	1.579147	3.710291	-6.131773
2.C	0.381891	1.565485	-5.456997
3.C	-4.186913	0.873699	-5.494938
4.C	0.567009	2.948043	-5.306436
5.C	-0.572564	0.868343	-4.709116
6.C	-3.511186	-2.421002	-4.518788
7.C	-0.232895	3.606056	-4.356938
8.C	-1.387010	1.530249	-3.770104
9.C	-4.620650	2.833104	-3.266772
10.C	-1.184003	2.916876	-3.605448
11.C	2.916028	-5.943277	-3.145498
12.C	-5.070141	-0.276958	-2.717793
13.C	3.702892	-3.551583	-2.768502
14.C	-5.602892	-3.367390	-2.591571
15.C	2.456342	6.562313	-1.983191
16.C	3.069887	-4.709704	-2.285768
17.C	3.049037	4.097219	-1.779967
18.C	-1.842430	-4.174361	-1.779708
19.C	3.888538	-2.428525	-1.958863
20.C	-1.441350	-5.394542	-1.230400
21.C	2.681968	5.306821	-1.169466
22.C	-6.809523	1.594404	-0.888148
23.C	-2.624795	-3.264577	-1.039997
24.C	3.298348	2.947365	-1.029625
25.C	0.522304	-0.639490	-1.213724
26.C	2.615598	-4.688834	-0.958384
27.C	0.478657	0.804042	-1.113819
28.C	6.153204	0.194128	-0.614870
29.C	3.458679	-2.416512	-0.615007
30.C	-1.787457	-5.762517	0.079468
31.C	-6.277609	-1.200738	0.092192
32.C	2.808096	-3.574619	-0.140275
33.C	-2.971628	-3.636189	0.276721
34.C	2.560030	5.311046	0.230694
35.C	0.076757	-1.451858	-0.102941
36.C	-0.388255	2.940314	0.036227

37.C	-0.149496	1.447953	0.019883
38.C	-1.349486	-7.082975	0.672393
39.C	3.174543	2.946997	0.376264
40.C	-2.558389	-4.851846	0.822034
41.C	6.447401	-2.448170	0.763990
42.C	2.793039	4.162914	0.986686
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45.C	-0.540405	-0.818543	1.040523
46.C	-0.601675	0.624386	1.120781
47.C	6.205962	2.790212	1.768264
48.C	-3.996620	0.646458	2.266587
49.C	5.206532	-0.108811	2.416904
50.C	-3.882035	3.422122	2.371342
51.C	4.200131	-2.961147	3.429844
52.C	-3.936048	1.302387	3.496520
53.C	-3.876397	2.703009	3.577685
54.C	4.181208	2.492721	3.956953
55.C	0.747283	0.699083	4.376281
56.C	1.363162	-0.516880	4.014045
57.C	-3.839180	3.410600	4.912119
58.C	-0.287617	0.739747	5.312855
59.C	0.877599	-1.691221	4.631191
60.C	4.392982	-0.711660	5.386316
61.C	-0.749566	-0.424063	5.944269
62.C	-0.147066	-1.640699	5.576964
63.C	-1.821410	-0.367246	7.007949
64.H	2.023576	3.075313	-6.908828
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69.H	-3.942024	-0.131111	-5.861903
70.H	2.400664	4.099079	-5.510664
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72.H	-4.238748	-2.353495	-5.341335
73.H	-2.664141	-1.762554	-4.748888
74.H	-3.142317	-3.457661	-4.496530
75.H	-5.688567	2.967171	-3.498789
76.H	2.857816	-5.689459	-4.212670
77.H	-0.115632	4.681280	-4.203001
78.H	-4.054695	3.525988	-3.907893
79.H	-6.227495	-3.433985	-3.497803
80.H	4.058388	-3.526023	-3.802577
81.H	-6.033478	-0.331447	-3.268276
82.H	3.772474	-6.625407	-3.018834
83.H	2.108740	6.325569	-2.996752
84.H	2.011581	-6.507808	-2.880367
85.H	3.148329	4.051178	-2.865989
86.H	-1.542134	-3.909434	-2.792878

87.H	-1.788754	3.452082	-2.874481
88.H	-4.457303	3.124106	-2.220949
89.H	3.386275	7.142943	-2.084330
90.H	-6.266985	-3.191468	-1.735867
91.H	4.370168	-1.539634	-2.366187
92.H	-7.672186	1.326279	-1.520361
93.H	-5.120340	-4.347572	-2.451232
94.H	-0.843366	-6.077525	-1.837414
95.H	1.712620	7.217942	-1.512008
96.H	0.975754	-1.113539	-2.083273
97.H	0.842255	1.414919	-1.938937
98.H	3.602353	2.027455	-1.529130
99.H	6.215631	-0.355945	-1.566302
100.H	-6.422032	2.558101	-1.242840
101.H	5.598057	1.123375	-0.792084
102.H	-7.251530	-1.515045	-0.313644
103.H	0.332920	3.462379	-0.605315
104.H	2.105536	-5.563073	-0.550415
105.H	-7.181862	1.737889	0.138217
106.H	-0.885556	-7.727004	-0.085737
107.H	6.559427	-2.894040	-0.236960
108.H	7.183069	0.458939	-0.328196
109.H	0.135127	-2.536544	-0.167623
110.H	-5.626397	-2.081423	0.143994
111.H	-1.399838	3.196777	-0.319551
112.H	-3.941378	3.350930	0.213265
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115.H	-3.589510	-2.955772	0.864023
116.H	-6.451714	-0.841314	1.118146
117.H	2.454481	-3.590259	0.891863
118.H	7.452596	-2.149503	1.108071
119.H	-0.303280	3.341490	1.055462
120.H	6.653205	2.472729	0.817555
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122.H	5.907155	3.844860	1.665049
123.H	6.077660	-3.230392	1.440420
124.H	-2.853823	-5.104258	1.843651
125.H	2.665567	4.191270	2.068578
126.H	-0.901962	-1.421084	1.872137
127.H	-1.053215	1.091665	1.994880
128.H	-4.030016	-0.443074	2.230706
129.H	6.987149	2.742412	2.544773
130.H	3.974481	-3.341769	2.426964
131.H	-3.833560	4.513431	2.396650
132.H	6.217787	-0.157864	2.870537
133.H	5.217545	-3.286068	3.696898
134.H	1.104370	1.624321	3.920404
135.H	3.942974	3.556602	3.808232
136.H	3.511507	-3.440470	4.142303

137.H	3.297954	1.999866	4.380500
138.H	-3.924373	0.709568	4.413596
139.H	4.988720	2.446685	4.703238
140.H	-3.294392	4.362372	4.849254
141.H	-0.736494	1.703080	5.564706
142.H	1.313941	-2.651092	4.354033
143.H	-4.855442	3.639354	5.270730
144.H	4.372392	0.355647	5.641136
145.H	5.393875	-1.102207	5.635979
146.H	-3.356308	2.792678	5.681019
147.H	3.667345	-1.227586	6.034473
148.H	-0.487860	-2.570192	6.040742
149.H	-2.462082	0.516361	6.885445
150.H	-2.463679	-1.258435	6.986795
151.H	-1.379219	-0.309192	8.015624
152.N	-2.389649	0.832284	-3.036846
153.N	-3.061012	-2.023950	-1.578003
154.N	-3.992087	0.706417	-0.205120
155.N	3.670959	-1.301625	0.241582
156.N	3.419392	1.764316	1.120119
157.N	2.419484	-0.534539	3.070142
158.Si	-4.050620	1.055502	-3.615479
159.Si	-4.299438	-2.016283	-2.838449
160.Si	-5.519446	0.207092	-0.928390
161.Si	5.343229	-0.912525	0.695902
162.Si	4.732547	1.730392	2.307958
163.Si	4.033435	-1.075489	3.562770
164.U	-2.034925	-0.093317	-0.998872
165.U	1.971390	0.029051	0.920241

Energy: -983.35980820 eV

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