

Supplementary Material

Pursuing the excision of carbon-centred hexanuclear scandium clusters {CSc₆} from solid {CSc₆}I₁₂Sc[†]

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Supplementary Material
for
**Pursuing the Excision of Carbon-Centred Hexanuclear Scandium
Clusters {CSc₆} from Solid {CSc₆}I₁₂Sc**

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Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for [Sc(DMA)₆]I₃ **2O**.

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Table S5. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for [Sc(DMA)₆]I₃ **2M**.

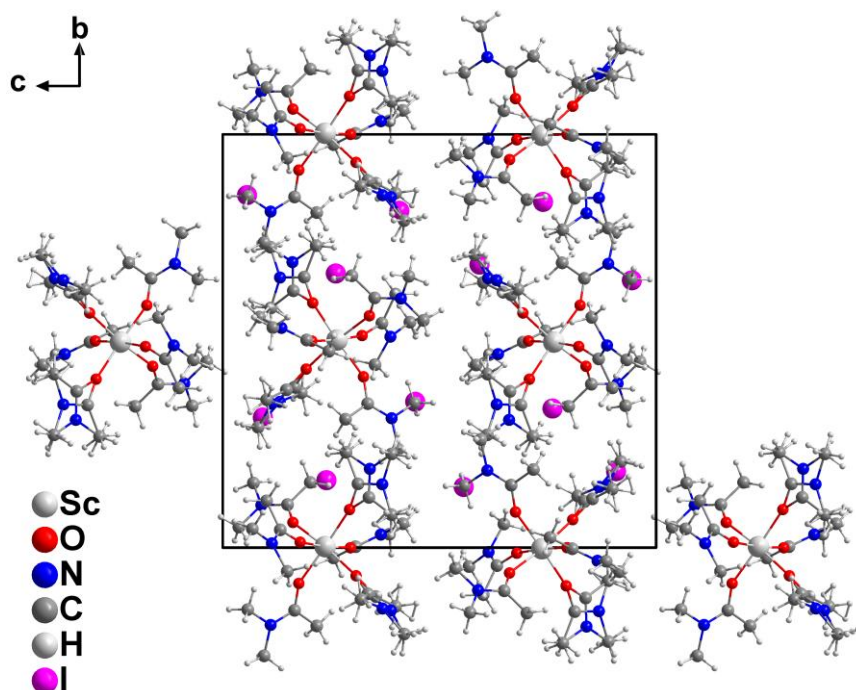


Figure S1. View on the crystal structure of [Sc(DMA)₆]I₃, **2O** along the crystallographic *a* axis.

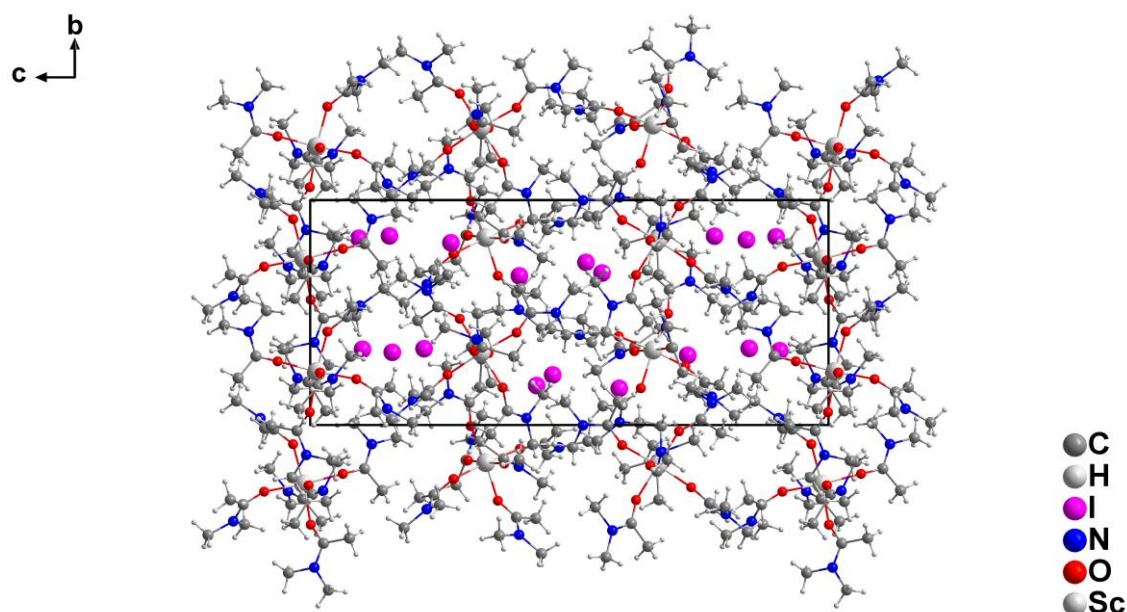


Figure S2. View on the crystal structure of $[\text{Sc}(\text{DMA})_6]\text{I}_3$, **2M** along the crystallographic a axis.

Table S1. Selected crystal structure solution and refinement data for $\{\text{CSc}_6\}\text{I}_{12}\text{Sc}$ (**1**), and $[\text{Sc}(\text{DMA})_6]\text{I}_3$ (**2O** and **2M**).

	1	2O	2M
Formula	$\text{Cl}_{12}\text{Sc}_7$	$\text{C}_{24}\text{H}_{54}\text{I}_3\text{N}_6\text{O}_6\text{Sc}$	$\text{C}_{24}\text{H}_{54}\text{I}_3\text{N}_6\text{O}_6\text{Sc}$
formula weight (g/mol)	1849.50	948.39	2845.17
T (K)	293(2)	170(1)	170(1)
crystal system	trigonal	orthorhombic	monoclinic
space group	$R\bar{3}$ (No. 146)	$P2_12_12_1$ (No. 19)	$P2_1$ (No. 4)
cell a (Å)	14.7206(2)	11.151(5)	19.7554(19)
b (Å)	9.850(1)	18.415(5)	11.4190(7)
c (Å)	-	19.306(5)	26.157(2)
α (°)	-	90	90
β (°)	-	90	91.929(7)
γ (°)	120.00	90	90
Volume (Å ³)	1848.5(3)	3964(2)	5897.3(8)
Z	3	4	6
density calculated (g/cm ³)	5.09	1.589	1.602
absorption coefficient (mm ⁻¹)	16.829	2.560	2.581
$F(000)$	2367	1872.0	2808.0
Theta range for data collection (°)	2.61 to 28.12	3.056 to 54.652	3.116 to 54.744
Index ranges		$-14 \leq h \leq 14$, $-23 \leq k \leq 23$, $-24 \leq l \leq 24$	$-25 \leq h \leq 25$, $-14 \leq k \leq 14$, $-33 \leq l \leq 30$
Reflections collected	3444	45543	74839
Independent reflections	1792 [$R_{\text{int}} = 0.0523$]	8855 [$R_{\text{int}} = 0.0870$, $R_{\text{sigma}} = 0.0581$]	26225 [$R_{\text{int}} = 0.0810$, $R_{\text{sigma}} = 0.1470$]
Completeness to theta	100%	100%	100%
Data / restraints / parameters	1792/0/1595	8855/0/416	26225/1/1083
Goodness-of-fit on F^2	1.012	0.975	0.781
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0295$, $wR_2 = 0.0699$	$R_1 = 0.0412$, $wR_2 = 0.0761$	$R_1 = 0.0753$, $wR_2 = 0.0891$
R indices (all data)	$R_1 = 0.0336$, $wR_2 = 0.0711$	$R_1 = 0.0753$, $wR_2 = 0.0891$	$R_1 = 0.1326$, $wR_2 = 0.0711$
Largest diff. peak and hole (e/Å ⁻³)	0.25/-0.41	0.56/-1.29	0.94/-2.09
CCDC		2114659	2114660

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Sc}(\text{DMA})_6]\text{I}_3 \mathbf{2O}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{II} tensor.

Atom	x	y	z	U(eq)
Sc01	2265.3(13)	25.1(8)	-2362.6(8)	37.0(3)
O1	1902(6)	-864(3)	-1754(3)	54.5(16)
O2	703(5)	-1(3)	-2945(3)	52.1(14)
O3	3039(6)	-679(3)	-3075(3)	55.1(16)
O4	1326(5)	611(3)	-1618(3)	47.6(13)
O5	3807(5)	133(3)	-1785(3)	55.2(15)
O6	2788(6)	923(3)	-2924(3)	54.6(15)
N1	1957(6)	-1868(4)	-1104(3)	46.8(16)
N2	-790(7)	317(4)	-3647(4)	51.0(18)
N3	-61(6)	1028(3)	-890(4)	44.2(16)
N4	5450(8)	105(5)	-1132(4)	69(3)
N5B	3588(16)	1908(8)	-3393(9)	45(3)
N6A	4110(20)	-1472(10)	-3686(10)	65(5)
C1	1586(8)	-1515(4)	-1656(4)	44.4(18)
C2	818(10)	-1892(5)	-2168(5)	61(3)
C3	1579(11)	-2616(4)	-952(6)	68(3)
C4	2679(11)	-1498(6)	-576(5)	74(3)
C5	-412(7)	25(5)	-3066(4)	43.4(19)
C6	-1282(9)	-247(5)	-2552(5)	58(2)
C7	77(11)	580(6)	-4156(5)	74(3)
C8	-2064(8)	327(5)	-3846(5)	60(3)
C9	93(8)	1580(5)	-2019(4)	47.1(19)
C10	484(7)	1044(4)	-1495(4)	38.4(18)
C11	-976(8)	1566(5)	-706(5)	60(2)
C12	309(10)	498(5)	-371(5)	61(3)
C13	2026(14)	-1420(8)	-3987(9)	115(5)
C14	5088(15)	-1251(10)	-3189(9)	130(6)
C15	4310(10)	800(5)	-3891(6)	68(3)
C16	4426(9)	2269(5)	-3896(5)	60(3)
C17	2925(11)	2307(6)	-2844(6)	72(3)
C18	4442(9)	433(5)	-1327(5)	57(2)
C19	4068(11)	1134(6)	-1010(7)	78(3)
C20	5813(12)	-572(7)	-1487(8)	99(5)
C21	6344(12)	456(7)	-681(6)	101(5)
C22B	3560(20)	1217(11)	-3373(13)	46(4)
C23	4165(15)	-2086(6)	-4186(6)	102(5)
C24A	3110(20)	-1182(11)	-3533(13)	54(5)
N5A	3921(13)	1535(12)	-3680(8)	37(3)
N6B	3330(30)	-1518(14)	-3878(10)	57(6)
C22A	3217(16)	1546(17)	-3120(9)	39(4)
C24B	3740(30)	-1117(15)	-3347(14)	48(7)
I01	-3477.9(6)	1633.7(4)	-2391.1(3)	59.72(17)
I02	1380.2(6)	3530.6(3)	-4440.7(3)	61.04(18)
I03	-3336.6(7)	1849.9(4)	924.6(3)	67.4(2)

Table S3. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Sc}(\text{DMA})_6]\text{I}_3$ **2O**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*^2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sc01	34.8(7)	33.0(7)	43.2(7)	-2.2(6)	0.0(7)	1.0(6)
O1	72(5)	38(3)	54(3)	2(3)	2(3)	-5(3)
O2	44(4)	58(3)	54(3)	-4(3)	-10(3)	2(3)
O3	53(4)	55(4)	57(4)	-17(3)	8(3)	6(3)
O4	50(4)	43(3)	50(3)	-4(2)	7(3)	12(3)
O5	41(3)	56(4)	69(4)	-17(3)	-14(3)	1(3)
O6	56(4)	48(3)	59(4)	9(3)	16(3)	-7(3)
N1	52(4)	42(3)	46(4)	6(3)	2(3)	5(3)
N2	49(4)	51(4)	53(4)	-7(3)	-14(4)	7(3)
N3	48(4)	45(4)	39(4)	-5(3)	7(3)	-3(3)
N4	59(5)	92(7)	57(5)	20(5)	-19(4)	-30(5)
N5B	43(8)	52(8)	40(7)	5(8)	2(7)	5(9)
N6A	104(15)	48(9)	45(9)	-10(7)	21(10)	34(11)
C1	47(5)	34(4)	53(4)	1(3)	3(4)	3(4)
C2	73(7)	45(5)	66(6)	-9(5)	-11(5)	-3(5)
C3	88(8)	42(4)	72(6)	12(4)	21(7)	1(5)
C4	80(7)	79(7)	64(6)	-7(6)	-10(6)	1(6)
C5	35(5)	46(4)	49(5)	-12(4)	-8(4)	6(4)
C6	49(6)	65(6)	61(6)	4(4)	5(5)	1(4)
C7	80(8)	90(8)	52(6)	18(6)	1(6)	0(6)
C8	51(6)	67(6)	64(6)	-9(5)	-21(5)	9(4)
C9	43(5)	46(5)	52(5)	2(4)	-5(4)	1(4)
C10	35(4)	37(4)	43(4)	-4(3)	1(4)	-2(3)
C11	49(5)	69(6)	61(5)	-16(5)	14(4)	8(4)
C12	85(8)	52(5)	45(5)	4(4)	6(5)	-5(5)
C13	102(11)	125(11)	119(11)	-31(10)	-18(10)	-45(9)
C14	92(11)	173(17)	125(13)	-18(12)	-41(10)	51(11)
C15	63(7)	61(6)	79(7)	-17(5)	14(6)	4(5)
C16	57(6)	63(6)	59(6)	27(5)	1(5)	-14(5)
C17	73(8)	62(6)	82(7)	-18(5)	23(6)	-1(5)
C18	53(6)	67(6)	51(5)	9(5)	4(5)	-22(5)
C19	81(8)	71(7)	82(7)	-27(6)	15(7)	-23(5)
C20	76(9)	71(8)	149(14)	5(8)	-26(9)	13(6)
C21	102(10)	130(10)	70(7)	37(7)	-57(7)	-64(8)
C22B	33(10)	64(11)	40(9)	6(11)	3(9)	8(10)
C23	196(16)	49(6)	60(7)	-8(5)	34(8)	25(7)
C24A	74(17)	45(10)	43(12)	3(9)	9(11)	-2(11)
N5A	34(8)	42(9)	35(7)	3(9)	18(7)	-3(8)
N6B	90(20)	54(12)	23(10)	2(9)	5(12)	5(15)
C22A	27(9)	52(12)	36(9)	4(11)	17(7)	-4(10)
C24B	58(18)	48(14)	38(14)	-10(11)	-1(14)	12(14)
I01	47.6(3)	83.5(4)	48.1(3)	-0.9(3)	-1.1(3)	6.7(3)
I02	56.3(4)	68.4(4)	58.3(3)	-4.7(3)	-1.4(3)	1.3(3)
I03	77.7(5)	64.8(4)	59.8(4)	-1.7(3)	13.6(4)	18.4(3)

Table S4. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Sc}(\text{DMA})_6]\text{I}_3 \cdot 2\text{M}$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{H} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U(\text{eq})$
C1	12302(6)	1471(11)	8707(5)	43(3)
C2	11621(6)	1682(11)	8459(4)	50(3)
C3	13413(7)	593(13)	8734(5)	66(4)
C4	12570(8)	113(13)	8028(5)	76(5)
C5	12340(6)	-250(10)	10255(5)	40(3)
C6	12028(6)	-25(10)	10757(5)	49(3)
C7	12651(7)	-1569(14)	9581(5)	80(4)
C8	12066(8)	-2329(10)	10351(6)	78(5)
C9	14211(6)	1724(11)	9857(4)	39(3)
C10	14269(6)	723(10)	10213(5)	45(3)
C11	14670(6)	3062(12)	9218(5)	66(4)
C12	15386(6)	1474(13)	9626(6)	71(5)
C13	13405(6)	5269(12)	9184(5)	61(4)
C14	12576(13)	4817(14)	9297(7)	98(8)
C15	11502(7)	4857(14)	9119(7)	98(7)
C16	12359(7)	6072(12)	8577(5)	62(4)
C17	10982(9)	1923(18)	10041(6)	92(7)
C18	10815(7)	633(11)	9699(5)	60(4)
C19	9880(6)	1606(13)	10305(5)	68(4)
C20	10743(7)	3375(12)	10530(5)	72(4)
C21	13062(6)	3062(10)	11048(4)	41(3)
C22	13331(7)	2096(10)	11391(5)	51(4)
C23	12950(7)	5081(10)	10847(5)	52(4)
C24	13559(8)	4442(11)	11658(5)	66(5)
C25	10744(6)	6532(10)	12295(4)	41(3)
C26	9989(6)	6307(12)	12225(5)	62(4)
C27	10940(8)	5253(11)	11567(5)	61(4)
C28	11878(6)	6358(12)	11997(5)	61(4)
C29	10927(8)	5632(13)	13805(6)	66(5)
C30	10627(7)	4602(11)	13484(5)	67(4)
C31	11585(8)	6356(13)	14500(6)	88(5)
C32	11542(9)	4131(12)	14293(6)	90(6)
C33	12458(7)	7939(12)	13307(5)	52(4)
C34	12665(8)	6684(16)	13274(6)	94(6)
C35	12714(9)	9961(16)	13225(8)	98(7)
C36	13601(7)	8470(20)	13113(6)	134(8)
C37	10986(10)	10257(17)	12460(8)	95(7)
C38	11598(7)	9647(12)	12073(5)	57(4)
C39	10267(7)	11683(13)	12652(5)	68(4)
C40	10860(9)	11601(14)	11760(5)	77(5)
C41	9209(8)	8468(15)	13316(8)	101(7)
C42	9086(8)	8053(16)	13931(5)	90(6)
C43	8875(8)	9333(12)	12594(5)	69(4)

C44	8072(6)	9095(11)	13384(6)	63(4)
C45	10831(6)	10000(9)	14259(5)	39(3)
C46	11176(7)	11063(11)	14054(5)	52(4)
C47	10264(8)	9011(11)	14934(5)	65(4)
C48	10673(7)	11015(11)	15077(5)	59(4)
C49	5593(6)	1897(9)	12387(4)	36(3)
C50	6237(5)	1776(11)	12110(4)	50(3)
C51	4415(6)	1449(13)	12497(5)	64(4)
C52	5082(6)	435(9)	11812(5)	44(3)
C53	6322(7)	903(11)	13980(5)	48(3)
C54	6921(6)	853(11)	14350(5)	56(4)
C55	5277(7)	99(12)	13649(6)	74(5)
C56	5815(7)	-711(10)	14461(5)	56(4)
C57	7651(6)	3438(13)	13007(4)	48(3)
C58	7684(7)	5428(11)	13315(5)	62(4)
C59	8762(6)	4368(12)	13096(6)	66(4)
C60	7993(6)	2344(10)	12812(5)	51(4)
C61	5698(6)	6009(10)	13071(5)	39(3)
C62	5905(6)	6878(11)	13491(5)	57(4)
C63	5180(8)	5633(14)	12234(5)	74(5)
C64	5080(7)	7608(10)	12634(6)	78(5)
C65	4528(8)	3501(13)	13734(6)	72(5)
C66	4213(7)	4277(11)	13267(5)	59(4)
C67	4438(8)	2441(13)	14478(5)	78(5)
C68	3387(6)	3466(15)	14031(5)	71(4)
C69	6569(7)	4185(10)	14534(5)	46(3)
C70	5949(7)	4695(11)	14757(5)	58(4)
C71	7775(6)	3681(11)	14572(5)	59(4)
C72	7182(7)	4280(11)	15358(4)	58(4)
I1	14204.6(5)	6757.1(7)	14369.2(3)	54.9(2)
I2	10229.3(4)	8367.7(9)	11010.1(3)	55.7(2)
I3	7432.3(4)	7230.1(6)	14679.1(3)	50.5(2)
I4	13472.2(4)	8234.4(8)	11583.9(3)	57.4(2)
I5	9198.1(5)	1631.3(8)	14036.4(3)	60.7(3)
I6	6842.8(4)	8394.9(9)	12197.1(3)	63.6(2)
I7	9094.5(4)	3408.9(9)	11528.7(3)	59.3(2)
I8	14781.2(4)	8303.8(9)	9061.5(3)	61.6(2)
I9	12241.8(5)	3101.3(8)	12716.2(4)	68.1(3)
N1	12719(5)	724(9)	8515(4)	44(3)
N2	12345(5)	-1328(7)	10078(4)	47(3)
N3	14712(5)	2055(8)	9570(4)	46(3)
N4	12307(12)	5308(13)	9039(6)	134(9)
N5	10559(7)	2080(20)	10248(7)	146(10)
N6	13171(5)	4151(8)	11186(4)	38(3)
N7	11155(5)	6045(8)	11982(4)	39(3)
N8	11305(8)	5315(11)	14170(5)	79(5)
N9	12880(6)	8797(14)	13234(5)	76(4)

N10	10777(12)	10972(16)	12248(6)	147(10)
N11	8732(7)	8803(11)	13205(8)	114(7)
N12	10640(5)	9989(8)	14738(4)	40(2)
N13	5056(5)	1259(8)	12248(4)	37(3)
N14	5838(5)	125(8)	14030(4)	48(3)
N15	8001(6)	4346(10)	13134(4)	53(3)
N16	5327(5)	6386(8)	12673(4)	46(3)
N17	4131(6)	3158(14)	14023(6)	92(5)
N18	7128(5)	4009(8)	14803(4)	46(3)
O1	12486(4)	2041(7)	9111(3)	47(2)
O2	12616(4)	573(6)	10009(3)	43(2)
O3	13656(4)	2335(7)	9812(3)	45(2)
O4	12557(4)	4152(6)	9669(3)	39(2)
O5	11582(4)	2324(7)	9969(3)	41.1(19)
O6	12730(4)	2833(6)	10629(3)	41(2)
O7	10959(4)	7234(7)	12649(3)	41.2(19)
O8	10727(4)	6669(7)	13713(3)	44.5(19)
O9	11867(4)	8199(8)	13439(3)	50(2)
O10	10941(4)	9723(7)	12885(3)	44(2)
O11	9796(4)	8296(8)	13163(3)	43.5(17)
O12	10752(4)	9111(6)	13982(3)	44(2)
O13	5558(4)	2606(6)	12764(3)	43(2)
O14	6298(4)	1638(7)	13620(3)	51(2)
O15	7013(3)	3434(8)	13044(3)	44.8(18)
O16	5894(4)	4955(7)	13096(3)	46(2)
O17	5170(3)	3286(8)	13745(2)	43.0(17)
O18	6558(4)	3947(6)	14046(3)	43(2)
Sc1	12609.1(12)	2384.5(18)	9872.9(8)	32.8(5)
Sc2	10823.7(9)	8225(2)	13292.7(7)	33.4(5)
Sc3	6087.6(9)	3333(2)	13387.5(7)	34.8(4)

Table S5. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Sc}(\text{DMA})_6]\text{I}_3$ **2M**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U_{11}+2hka*b*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	30(7)	52(8)	46(8)	6(7)	1(6)	14(6)
C2	34(7)	61(8)	54(8)	6(8)	-8(6)	5(7)
C3	33(8)	102(11)	62(10)	-15(9)	-8(7)	20(8)
C4	84(12)	93(11)	50(10)	-31(9)	3(9)	8(9)
C5	26(7)	29(6)	63(9)	4(6)	-3(6)	-2(5)
C6	51(9)	56(8)	42(8)	-3(7)	2(7)	-7(6)
C7	96(11)	53(8)	94(11)	-6(10)	30(9)	-8(10)
C8	95(13)	32(7)	107(13)	14(8)	10(10)	-17(7)
C9	28(7)	54(7)	35(7)	-13(7)	-1(6)	1(6)
C10	43(8)	48(7)	45(8)	8(7)	-10(7)	1(6)
C11	36(7)	68(10)	95(10)	22(9)	12(7)	-12(7)
C12	28(8)	89(11)	97(12)	-16(10)	3(8)	24(8)
C13	29(8)	84(10)	71(10)	11(8)	7(7)	-6(7)

C14	210(30)	39(10)	39(11)	-7(8)	-13(13)	39(12)
C15	13(8)	99(12)	180(20)	44(13)	16(10)	-1(8)
C16	68(11)	73(9)	44(9)	26(7)	19(8)	30(8)
C17	51(11)	158(19)	67(11)	71(12)	9(9)	29(13)
C18	73(11)	49(8)	56(9)	-14(7)	4(8)	12(7)
C19	37(8)	83(10)	84(11)	13(9)	22(7)	-4(8)
C20	84(10)	32(6)	99(11)	-23(9)	-5(8)	8(9)
C21	42(7)	43(8)	38(7)	-6(6)	4(6)	-7(6)
C22	79(11)	33(7)	41(8)	6(6)	-3(7)	8(6)
C23	60(9)	40(7)	55(9)	10(7)	-4(7)	-6(6)
C24	91(12)	55(8)	49(9)	-29(7)	-42(8)	-2(8)
C25	51(8)	37(7)	34(7)	3(6)	6(6)	3(6)
C26	36(8)	78(10)	74(10)	-29(8)	19(7)	-15(7)
C27	75(11)	49(8)	58(10)	-38(7)	-11(8)	-4(7)
C28	25(7)	80(10)	80(11)	-12(8)	11(7)	-14(7)
C29	62(11)	64(10)	73(12)	29(9)	17(9)	18(8)
C30	51(9)	59(9)	90(12)	-37(8)	-12(8)	-16(7)
C31	96(13)	94(12)	73(11)	-41(10)	-13(10)	-15(10)
C32	123(16)	66(10)	83(13)	25(9)	12(11)	65(10)
C33	30(8)	78(10)	46(8)	-7(7)	-7(7)	3(7)
C34	70(12)	130(15)	79(12)	-56(12)	-32(10)	62(12)
C35	56(12)	86(13)	150(20)	13(13)	-11(12)	-29(11)
C36	37(9)	250(20)	116(14)	94(19)	7(9)	18(16)
C37	106(16)	91(14)	85(15)	37(12)	-62(13)	-71(12)
C38	48(9)	69(9)	56(9)	-18(8)	21(8)	-3(7)
C39	69(10)	83(10)	55(9)	-20(9)	24(8)	15(9)
C40	121(14)	72(10)	38(8)	34(9)	-8(9)	10(10)
C41	36(9)	55(10)	210(20)	-58(13)	-22(12)	9(9)
C42	94(12)	123(15)	54(9)	49(10)	9(8)	22(11)
C43	81(12)	82(11)	43(9)	22(8)	-4(8)	1(8)
C44	30(8)	71(9)	87(12)	-9(8)	4(8)	6(7)
C45	51(8)	28(6)	39(8)	-10(6)	-4(7)	3(6)
C46	54(10)	55(8)	48(9)	-11(7)	11(8)	-12(7)
C47	82(12)	65(9)	47(9)	-2(7)	5(8)	7(8)
C48	74(10)	59(8)	41(8)	-32(7)	-15(7)	19(7)
C49	42(7)	35(7)	31(6)	1(6)	0(6)	-8(5)
C50	31(7)	63(8)	56(8)	-8(7)	11(6)	-2(6)
C51	31(8)	108(12)	52(9)	-4(9)	3(7)	-14(8)
C52	50(8)	33(6)	48(8)	-19(6)	-5(7)	-9(6)
C53	39(8)	45(8)	62(10)	-8(7)	3(7)	5(7)
C54	40(8)	59(8)	69(10)	10(7)	-13(8)	-14(7)
C55	68(11)	64(9)	86(12)	4(8)	-46(10)	4(8)
C56	64(10)	40(7)	65(10)	21(7)	-3(8)	-10(6)
C57	54(8)	64(8)	25(6)	4(8)	-3(6)	-4(9)
C58	74(11)	44(8)	70(10)	-21(7)	12(9)	-1(7)
C59	27(8)	87(10)	82(11)	7(9)	-6(8)	-11(7)
C60	53(9)	42(7)	56(9)	-11(7)	-2(7)	20(6)

C61	35(7)	37(7)	44(8)	5(6)	4(6)	5(5)
C62	55(9)	68(9)	48(8)	-16(7)	-5(7)	-2(7)
C63	71(12)	118(13)	32(9)	-10(9)	-11(8)	-20(10)
C64	49(9)	57(9)	130(15)	37(9)	5(9)	21(7)
C65	77(11)	51(9)	91(11)	-41(9)	43(10)	-27(9)
C66	70(10)	56(8)	50(9)	14(7)	-12(8)	5(7)
C67	96(13)	93(11)	45(9)	42(9)	-8(9)	-6(9)
C68	31(7)	89(10)	93(10)	-16(11)	18(7)	6(9)
C69	53(9)	33(7)	51(9)	6(6)	-17(8)	-5(6)
C70	56(10)	52(8)	67(10)	-3(7)	27(8)	3(7)
C71	37(8)	62(10)	76(10)	-9(7)	-5(7)	5(6)
C72	72(10)	75(9)	25(7)	1(7)	-16(7)	-26(8)
I1	56.4(6)	55.7(5)	52.5(5)	-5.6(5)	-0.6(4)	-1.0(5)
I2	43.1(5)	56.5(5)	67.3(6)	1.7(6)	-1.4(4)	-7.0(5)
I3	49.0(6)	45.0(4)	57.4(6)	-3.6(4)	0.4(4)	-2.4(4)
I4	41.2(5)	49.4(5)	81.1(6)	-6.4(6)	-4.2(4)	-4.4(5)
I5	53.9(6)	75.3(6)	52.4(6)	-12.3(5)	-6.3(5)	14.0(5)
I6	53.9(5)	62.4(5)	74.4(6)	-1.5(6)	3.2(5)	0.3(6)
I7	51.9(5)	49.4(5)	77.1(6)	-4.7(6)	7.3(4)	-8.1(5)
I8	59.1(5)	53.9(5)	71.6(6)	1.3(6)	-0.4(4)	13.6(6)
I9	67.9(6)	68.9(7)	67.4(6)	-5.3(6)	-0.1(5)	-11.9(5)
N1	38(7)	49(6)	44(7)	-6(5)	6(5)	6(5)
N2	45(7)	33(6)	62(7)	0(5)	-3(6)	2(4)
N3	33(6)	46(6)	60(7)	1(5)	0(5)	3(5)
N4	280(30)	82(12)	43(10)	11(8)	25(13)	88(14)
N5	27(8)	260(20)	150(16)	156(18)	6(9)	0(12)
N6	43(7)	37(6)	34(6)	-9(5)	-3(5)	0(5)
N7	43(7)	37(6)	39(6)	0(5)	4(5)	-6(5)
N8	95(12)	77(9)	67(9)	35(8)	30(9)	36(8)
N9	39(8)	126(13)	64(9)	9(8)	7(7)	0(8)
N10	240(20)	120(15)	78(12)	61(11)	-84(14)	-120(16)
N11	26(8)	67(9)	250(20)	-74(11)	18(11)	-6(6)
N12	35(6)	48(6)	36(6)	-9(5)	3(5)	-1(5)
N13	46(7)	37(5)	26(6)	5(4)	1(5)	-1(5)
N14	52(7)	39(6)	54(7)	6(5)	-8(6)	5(5)
N15	39(7)	68(8)	52(8)	9(6)	-6(6)	-11(6)
N16	41(6)	46(6)	52(7)	8(5)	7(5)	3(5)
N17	59(8)	95(11)	125(12)	-49(11)	36(8)	-29(9)
N18	47(7)	41(6)	49(7)	7(5)	-13(6)	-8(5)
O1	45(5)	63(6)	33(5)	-7(4)	-2(4)	1(4)
O2	32(5)	44(4)	52(5)	0(4)	1(4)	1(4)
O3	23(4)	54(5)	59(5)	2(4)	0(4)	2(4)
O4	33(5)	42(4)	42(5)	4(4)	6(4)	-3(4)
O5	24(4)	53(5)	46(5)	-5(4)	3(4)	-10(4)
O6	42(5)	45(5)	36(5)	-5(4)	-4(4)	-6(3)
O7	35(5)	51(5)	37(5)	-17(4)	0(4)	-1(4)
O8	53(5)	30(4)	51(5)	6(4)	7(4)	0(4)

O9	33(4)	58(5)	58(5)	-7(5)	-2(4)	1(5)
O10	56(6)	37(5)	41(5)	4(4)	7(5)	2(4)
O11	35(4)	49(4)	47(4)	2(5)	1(3)	1(5)
O12	59(6)	37(4)	35(5)	-2(4)	-2(4)	-1(4)
O13	35(5)	51(5)	43(5)	-16(4)	-4(4)	-2(4)
O14	57(6)	40(4)	57(6)	4(5)	2(4)	5(4)
O15	28(4)	61(5)	45(4)	-6(5)	2(3)	-3(5)
O16	48(5)	41(5)	50(6)	0(4)	0(4)	5(4)
O17	28(4)	64(5)	37(4)	-6(5)	0(3)	-1(5)
O18	41(5)	49(5)	39(5)	-11(4)	-5(4)	5(4)
Sc1	32.2(14)	35.2(11)	31.0(13)	-0.4(10)	0.9(10)	-1.3(10)
Sc2	36.0(11)	31.8(11)	32.4(11)	-0.8(12)	1.6(9)	1.6(12)
Sc3	32.6(11)	36.9(10)	34.9(11)	-1.9(13)	-1.0(9)	0.4(13)
