Polynuclear Titanocene Complexes with Antimony Ligands: $[(Cp_2Ti)_2(SbR_2)_2]$ (R = Et), $[(Cp_2Ti)_3(SbR)_3Sb]$ [R = 2-$(Me_2NCH_2)C_6H_4$] and $[(Cp_2Ti)_5(SbR)_2Sb_7]$ ($R = Me_3SiCH_2$)

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Experimental details

The R_4Sb_2 used as starting materials were prepared according to previously described methods [R = Et,[1] 2-(Me_2NCH_2)C_6H_4,[2] Me_3SiCH_2,[3]]. Attempts to record EI (70 eV) for **1**-**3** or CI (NH_3) for **1** mass spectra failed.

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Synthesis of [(Cp_2Ti)$_2$(SbR_2)$_2$] (R = Et), 1

[Cp_2Ti(btmsa)] (btmsa = $Me_3SiC_2SiMe_3$) (0.6 g, 1.7 mmol) was added to a solution of Et_4Sb_2 (0.3 g, 0.8 mmol) in 10 mL C_6H_6, under stirring, and the resulting brown mixture was kept for 12 h at 7 °C and for 2 d at r.t. when 0.2 g (25%) red crystals of **1** (mp 180 °C, dec.) were isolated.

Synthesis of [(Cp_2Ti)$_3$(SbR)$_3$Sb] [R = 2-(Me_2NCH_2)C_6H_4], 2

To a solution of [Cp_2Ti(btmsa)] (0.2 g, 0.57 mmol) in 10 mL benzene was added dropwise [2-(Me_2NCH_2)C_6H_4]$_4Sb_2$ (0.45 g, 0.58 mmol) in 5 mL benzene and the resulting green mixture was stirred for 1 h at r.t. The solvent was removed under reduced pressure and the resulting green liquid was dissolved again in benzene and kept at r.t. After 1 d 0.25 g (62%) red crystals of **2** were isolated.

Synthesis of [(Cp_2Ti)$_5$(SbR)$_2$$Sb_7$] (R = Me_3SiCH_2), 3

To a solution of [Cp_2Ti(btmsa)] (0.43 g, 1.2 mmol) in 20 mL benzene was added (Me_3SiCH_2)$_4Sb_2$ (0.73 g, 1.2 mmol) in 10 mL benzene. The resulting mixture was stirred for 0.5 h at r.t., then the solvent was removed at reduced pressure and the remaining oily product was dissolved in benzene. After 2 months at r.t. several black crystals of **3** were obtained.

Crystallography Details

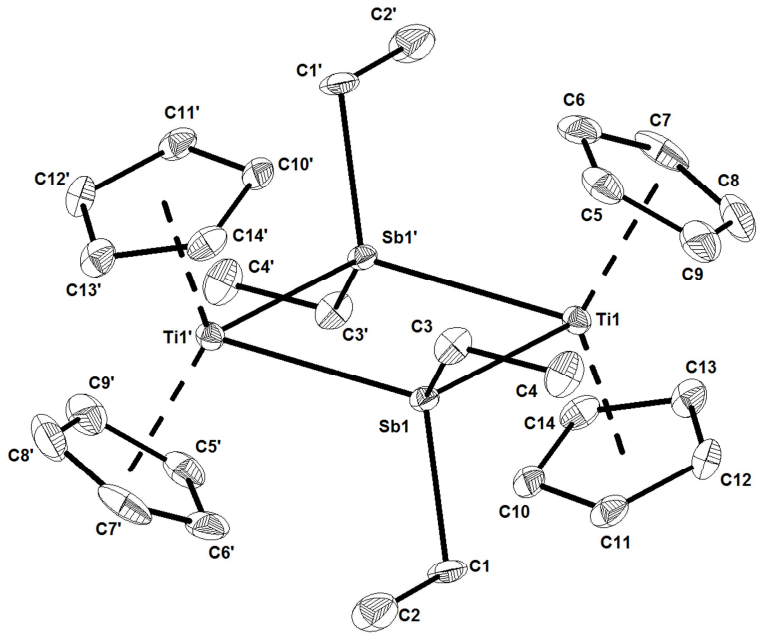

Figure S1. Thermal ellipsoid (30 % probability) representation of the molecule 1 of **1**. The hydrogen atoms were omitted for clarity. Symmetry transformations used to generate equivalent atoms: ' 1-x, 1-y, 1-z

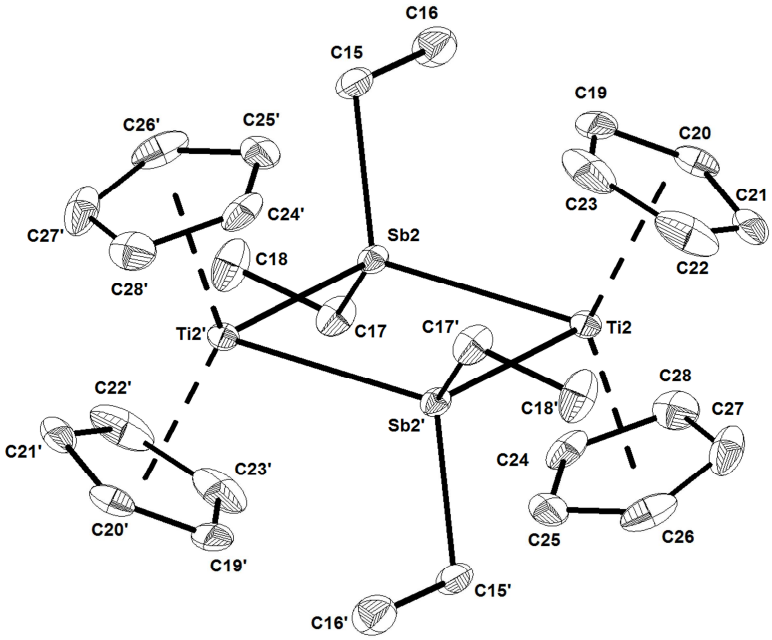

Figure S2. Thermal ellipsoid (30 % probability) representation of the molecule 2 of **1**. The hydrogen atoms were omitted for clarity. Symmetry transformations used to generate equivalent atoms: ' 1-x, 1-y, 1-z

Table S8. Selected bond lengths (Å) and bond angles (°) of **1**.

C(1)-C(2)	1,523(7)	Ti(1)-Sb(1)	2,9046(10)		
C(1)-Sb(1)	2,190(4)	Ti(1)-Sb(1)#1	2,9105(10)	C(3)-Sb(1)-C(1)	93,5(2)
C(3)-C(4)	1,511(7)	Ti(2)-Sb(2)#2	2,8797(10)	Ti(1)-Sb(1)-Ti(1)#1	104,62(3)
C(3)-Sb(1)	2,186(4)	Ti(2)-Sb(2)	2,8916(11)	Sb(1)-Ti(1)-Sb(1)#1	75,38(2)
C(15)-C(16)	1,526(7)	Sb(1)-Ti(1)#1	2,9105(10)	C(15)-Sb(2)-C(17)	93,4(2)
C(15)-Sb(2)	2,184(5)	Sb(2)-Ti(2)#2	2,8797(10)	Ti(2)#2-Sb(2)-Ti(2)	100,58(3)
C(17)-C(18)	1,528(7)	Ti(1)-Sb(1)	2,9046(10)	Sb(2)#2-Ti(2)-Sb(2)	79,42(3)
C(17)-Sb(2)	2,195(5)	Ti(1)-Sb(1)#1	2,9105(10)		

Symmetry transformations used to generate equivalent atoms: #1 1-x, 1-y, 1-z; #2 -x,-y,-z.

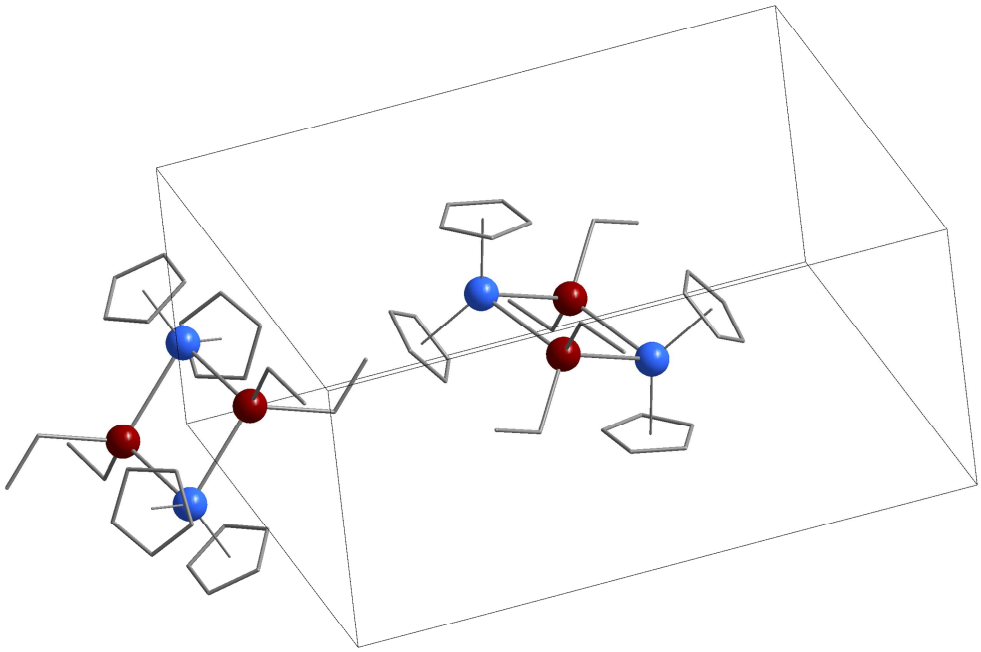

Figure S3. Packing of **1** in the crystal. The inversion centre of the molecule **1** is located on the centre of the unit cell, and the inversion centres of molecules **2** are located on the corners of the unit cell.

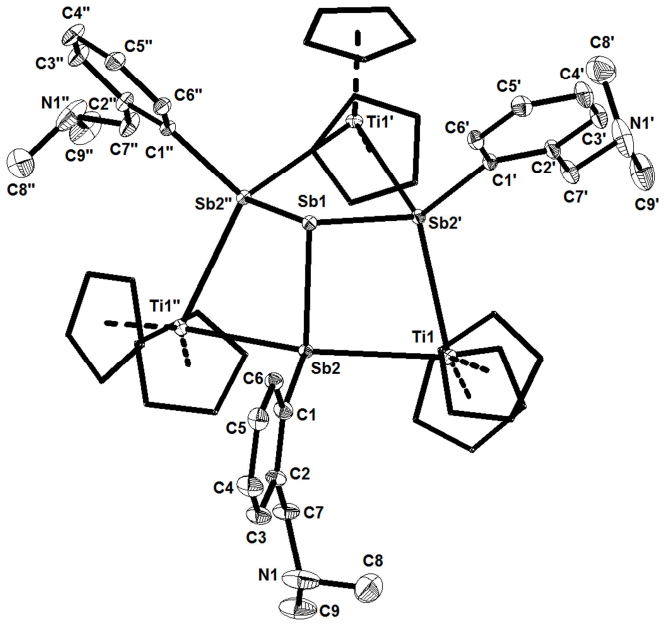

Figure S4. Graphical representation of **2**. The thermal ellipsoids were drawn at 20 % probability. The cyclopentadielnyl groups were drawn as capped sticks and the hydrogen atoms were omitted for clarity. Symmetry transformations used to generate equivalent atoms: ' -x+y, 1-x, z; '' 1-y, 1+x-y, z.

Table S9. Selected bond lengths (Å) and bond angles (°) of **2**.

Sb(1)-Sb(2)#1	282.67(4)	Sb(2)#1-Sb(1)-Sb(2)	80.532(14)	C(1)-Sb(2)-Ti(1)#1	107.62(11)
Sb(1)-Sb(2)	282.67(4)	Sb(2)#1-Sb(1)-Sb(2)#2	80.532(14)	Sb(1)-Sb(2)-Ti(1)#1	93.274(16)
Sb(1)-Sb(2)#2	282.67(4)	Sb(2)-Sb(1)-Sb(2)#2	80.532(14)	Ti(1)-Sb(2)-Ti(1)#1	142.79(3)
Sb(2)-C(1)	217.7(4)	C(1)-Sb(2)-Sb(1)	102.86(11)		
Sb(2)-Ti(1)	295.84(8)	C(1)-Sb(2)-Ti(1)	106.41(11)		
Sb(2)-Ti(1)#1	296.76(8)	Sb(1)-Sb(2)-Ti(1)	93.470(16)		

Symmetry transformations used to generate equivalent atoms: #1 1-y, 1+x-y, z; #2 -x+y,-x+1,z.

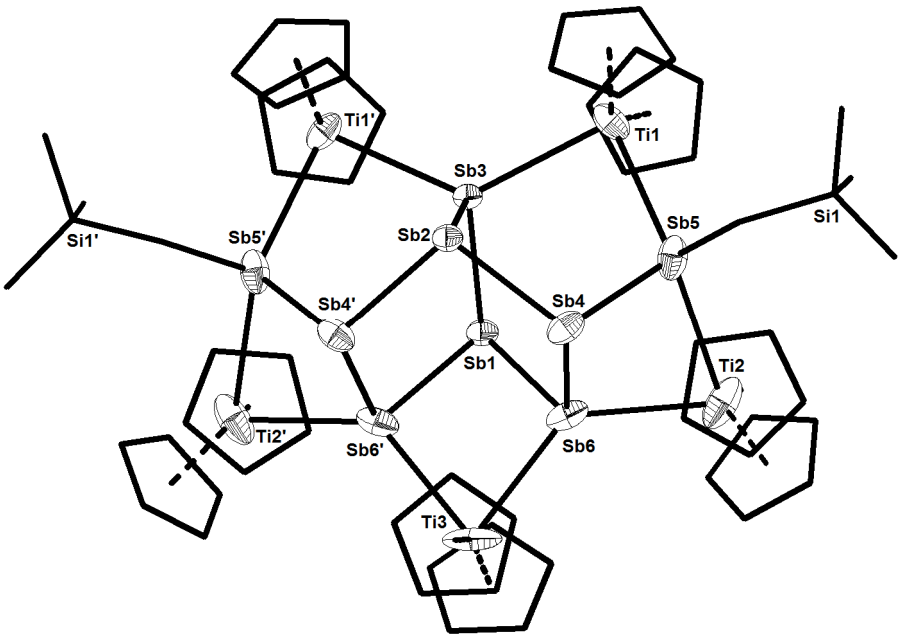

Figure S5. Graphical representation of **3**. The anisotropically refined atoms were drawn at 30 % probability and the isotropically refined atoms as capped sticks. The hydrogen atoms were omitted for clarity. Symmetry transformations used to generate equivalent atoms: ' 1-y, 1-x, z.

Table S10. Selected bond lengths (Å) and bond angles (°) of **3**.

Sb(1)-Sb(3)	2.836(3)	Sb(3)-Sb(1)-Sb(6)#1	104.68(8)	C(31)-Sb(5)-Sb(4)	94.8(9)
Sb(1)-Sb(6)	2.850(3)	Sb(3)-Sb(1)-Sb(6)	104.68(8)	C(31)-Sb(5)-Ti(1)	106.1(9)
Sb(1)-Sb(6)#1	2.850(3)	Sb(6)#1-Sb(1)-Sb(6)	77.14(10)	Sb(4)-Sb(5)-Ti(1)	110.22(11)
Sb(2)-Sb(3)	2.773(4)	Sb(3)-Sb(2)-Sb(4)	98.60(7)	C(31)-Sb(5)-Ti(2)	111.6(8)
Sb(2)-Sb(4)	2.774(2)	Sb(3)-Sb(2)-Sb(4)#1	98.60(7)	Sb(4)-Sb(5)-Ti(2)	89.33(16)
Sb(2)-Sb(4)#1	2.774(2)	Sb(4)-Sb(2)-Sb(4)#1	101.76(10)	Ti(1)-Sb(5)-Ti(2)	135.56(16)
Sb(3)-Ti(1)#1	2.995(4)	Sb(2)-Sb(3)-Sb(1)	100.18(9)	Sb(4)-Sb(6)-Sb(1)	102.26(7)
Sb(3)-Ti(1)	2.995(4)	Sb(2)-Sb(3)-Ti(1)#1	101.80(10)	Sb(4)-Sb(6)-Ti(2)	92.86(14)
Sb(4)-Sb(6)	2.811(3)	Sb(1)-Sb(3)-Ti(1)#1	110.22(11)	Sb(1)-Sb(6)-Ti(2)	115.85(15)
Sb(4)-Sb(5)	2.829(3)	Sb(2)-Sb(3)-Ti(1)	101.80(10)	Sb(4)-Sb(6)-Ti(3)	112.1(2)
Sb(5)-C(31)	2.25(3)	Sb(1)-Sb(3)-Ti(1)	110.22(11)	Sb(1)-Sb(6)-Ti(3)	98.14(16)
Sb(5)-Ti(1)	3.006(6)	Ti(1)#1-Sb(3)-Ti(1)	128.0(2)	Ti(2)-Sb(6)-Ti(3)	132.49(18)
Sb(5)-Ti(2)	3.042(6)	Sb(2)-Sb(4)-Sb(6)	106.14(8)		
Sb(6)-Ti(2)	2.888(7)	Sb(2)-Sb(4)-Sb(5)	102.67(8)		
Sb(6)-Ti(3)	2.892(6)	Sb(6)-Sb(4)-Sb(5)	79.22(8)		

Symmetry transformations used to generate equivalent atoms: #1 1-y, 1-x, z.

Due to the poor quality of the measured crystal the collected reflections allowed the anisotropic refinement only of the titanium and antimony atoms. The crystallization solvent (benzene) was found to be disordered over two positions, both refined with a site occupation factor of 0.25. The cyclopentadienyl groups containing the atoms C21 - C23, and C24 - C26 were refined with the 1,2-distances at 1.42 Å, 1,3-distances at 2.30, and restrained to have all the atoms in the same plane. The Si–C distances were restrained at 1.8 Å with an estimated standard deviation of 0.05 Å.

Computational Details

The geometry optimizations and the frequencies calculations were performed using the ADF 2008.01 software package using the BP86 and Slater type orbitals of TZ2P quality.[S1–S3] The relativistic effects were included using the zero order regular approximation (ZORA).

In the frequency calculations carried out there were obtained imaginary frequencies at small wave numbers and with reduced absorption intensity: [$Cp_2TiSbEt$] –24.56 (–0.24); **1** (triplet) –40.04 (–0.04), –23.49 (–0.02), –6.99 (–0.02); **1** (singlet) –46.09 (–0.01), –39.01 (–0.23), –21.45 (–0.13) [wave numbers in cm^{-1} (absorption intensities in km/mole)] corresponding to the rotation of one, or more cyclopentadienyl groups. These frequencies could emerge from the accumulation of errors in the numerical operations.[S4]

An additional set of calculations was performed with GAMESS, 11 April 2008 release, software package[S5,S6] using B3LYP functional and LANL2DZ basis set.[S7–S10] For the antimony atoms the LANL2DZ basis was augmented with two polarization functions.[S11] The calculations for the triplet state of **1** were carried out using RO self consistent field. For the frequencies calculations carried out with GAMESS software package no imaginary frequency was obtained.

The bonds lengths and bond angles obtained for the triplet state of **1** using ADF or GAMESS are in better agreement with the values determined experimentally than the values found for the singlet state of **1**. The Sb–Ti bond lengths found for the triplet state of **1** are slightly (3-4 %) longer than the measured values. The C–Sb–C bond angles were predicted by the DFT methods to be 1 % larger than the determined values. The most important differences were found between the Ti···Ti interatomic distances and Ti···Sb···Ti, and Sb···Ti···Sb bond angles, respectively (Table 1).

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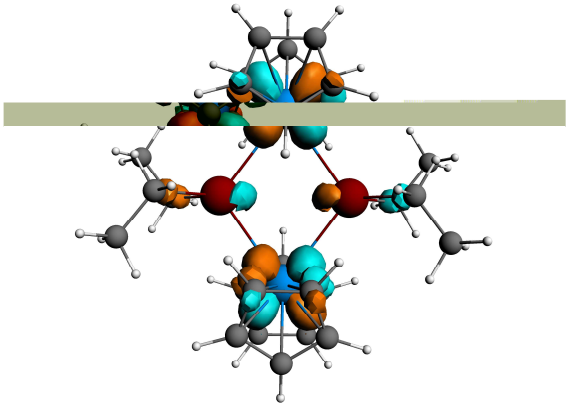
Table S1. Comparison of selected crystallographic and theoretical data of **1**.

Functional		**BP86**		**B3LYP**		**BP86**		**B3LYP**	
Multiplicity	**-**	**triplet**	**Å (%)**	**triplet**	**Å (%)**	**singlet**	**Å (%)**	**singlet**	**Å (%)**
Molecule 1									
Sb–Ti	2.9046(10)	3.016	0.111 (3.8)	3.008	0.103 (3.6)	2.892	-0.013 (0.4)	2.879	-0.026 (0.9)
	2.9105(10)	3.018	0.108 (3.7)	2.995	0.085 (2.9)	2.933	-0.023 (0.8)	2.846	-0.064 (2.2)
Sb···Sb	3.555(1)	3.580	0.025 (0.7)	3.575	0.020 (0.6)	4.027	0.472 (13.3)	4.051	0.496 (14.0)
Ti···Ti	4.602(2)	4.856	0.254 (5.5)	4.823	0.221 (4.8)	4.209	-0.393 (8.5)	4.046	-0.556 (12.1)
C–Sb–C		93,72	0,24 (0.3)	94,41	0,93 (1.0)	95,12	1,64 (1.8)	94,86	1,38 (1.5)
Ti···Sb···Ti		107,19	2,57 (2.5)	106,90	2,28 (2.2)	92,53	-12,09 (11.6)	89,93	-14,69 (14.0)
Sb···Ti···Sb		72,80	-2,58 (3.4)	73,10	-2,28 (3.0)	87,46	14,69 (19.5)	90,07	14,69 (19.5)
Molecule 2									
Sb–Ti	2.8797(10)	3.016	0.136 (4.7)	3.008	0.128 (4.5)	2.892	0.012 (0.4)	2.879	-0.001 (0.0)
	2.8916(11)	3.018	0.126 (4.4)	2.995	0.103 (3.6)	2.933	-0.041 (1.4)	2.846	-0.046 (1.6)
Sb···Sb	3.687(1)	3.580	-0.107 (2.9)	3.575	-0.112 (3.0)	4.027	0.340 (9.2)	4.051	0.364 (9.9)
Ti···Ti	4.440(2)	4.856	0.416 (9.4)	4.823	0.383 (8.6)	4.209	-0.231 (5.2)	4.046	-0.394 (8.9)
C–Sb–C		93,72	0,32 (0.3)	94,40	1,00 (1.1)	95,12	1,72 (1.8)	94,86	1,46 (1.6)
Ti···Sb···Ti		107,19	6,61 (6.6)	106,90	6,32 (6.3)	92,53	-8,05 (8.0)	89,93	-10,65 (10.6)
Sb···Ti···Sb		72,80	-6,62 (8.3)	73,10	-6,32 (8.0)	87,46	8,04 (10.1)	90,07	10,65 (13.4)

Table S2. Frontier alpha molecular orbitals of **1** (triplet) calculated with BP86/TZ2P.



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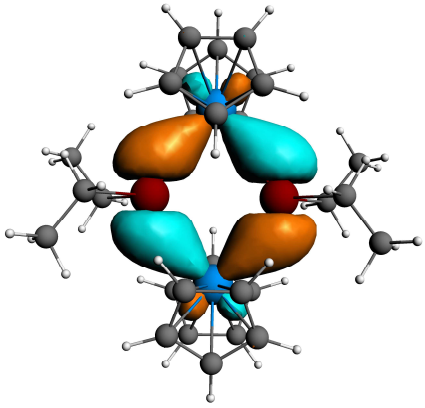

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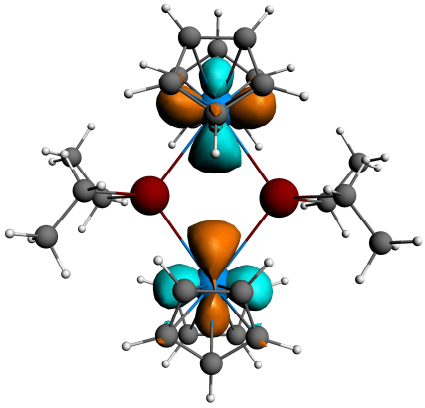

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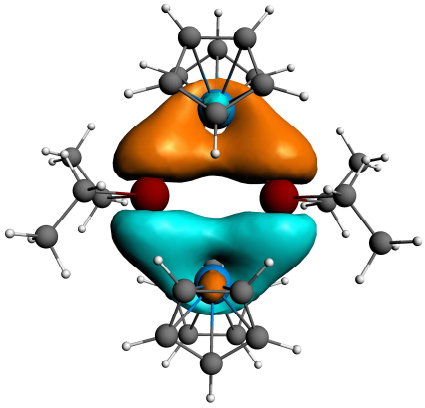

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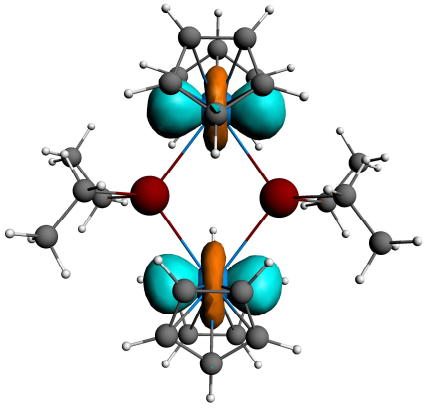

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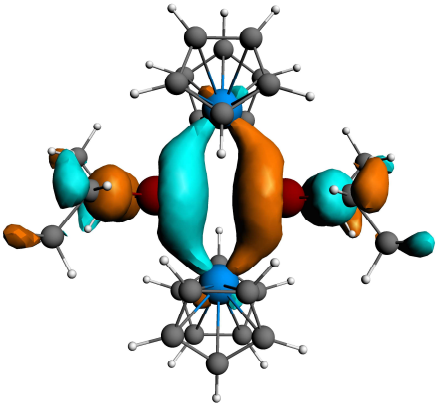
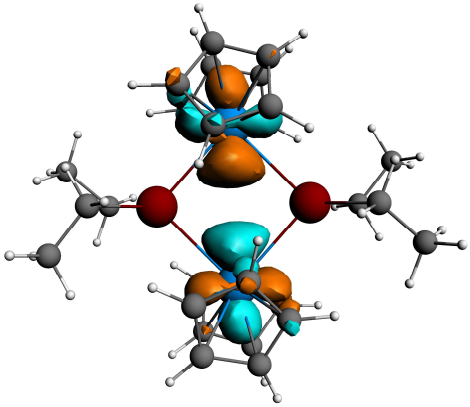


HOMO-4

Table S3. Frontier alpha molecular orbitals of **1** (triplet) calculated with BP86/TZ2P.



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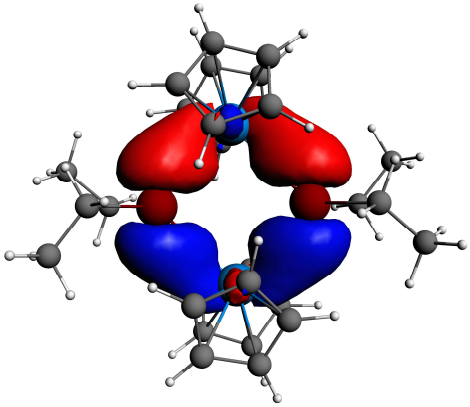

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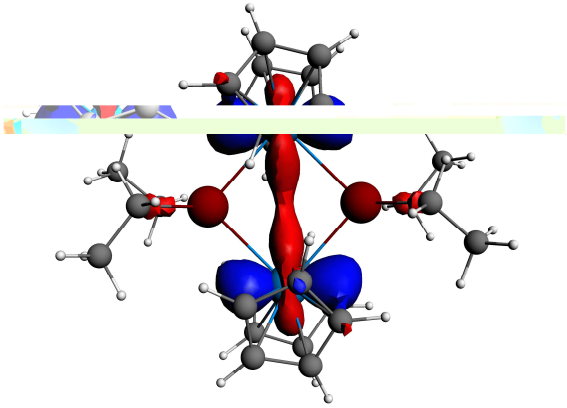

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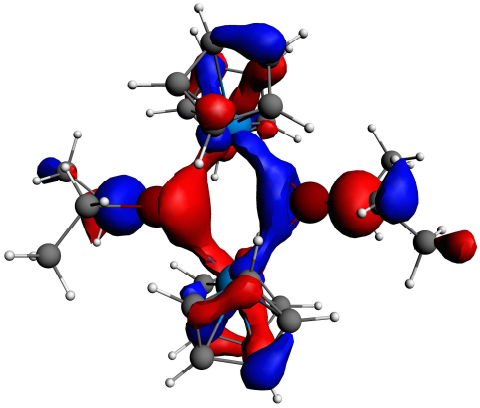

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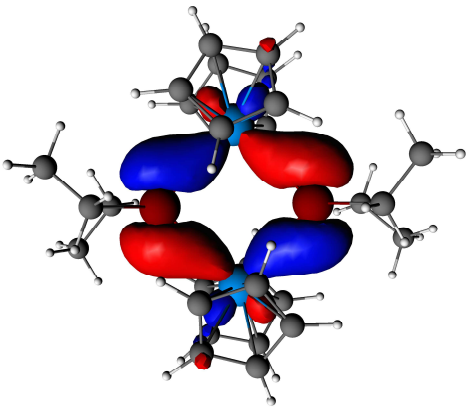

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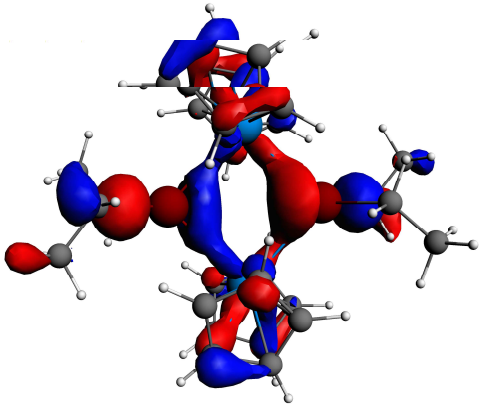
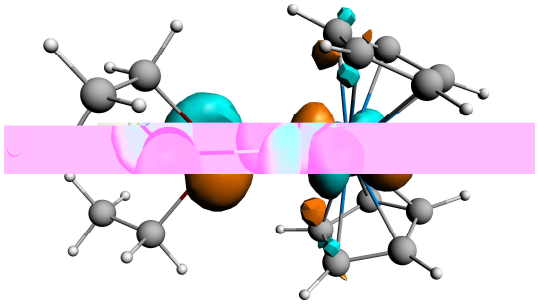
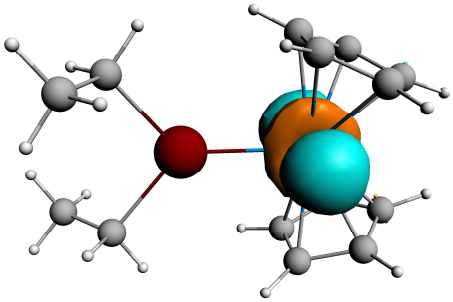


HOMO-4

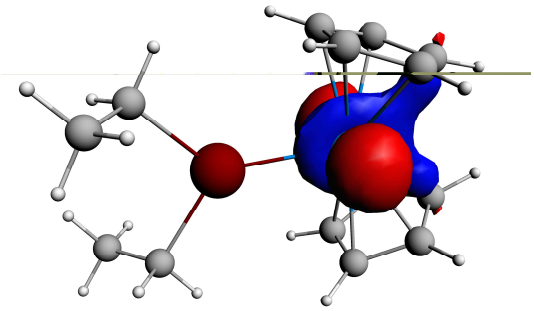
Table S4. Frontier alpha molecular orbitals and localized molecular orbitals* (LMO) of [$Et_2SbTiCp_2$] calculated with BP86/TZ2P.



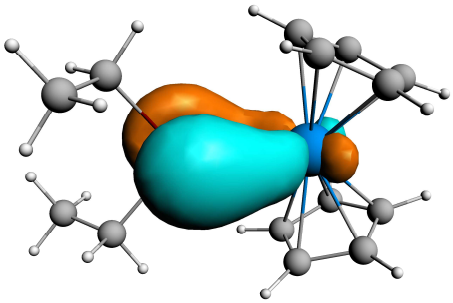
LUMO (44A)



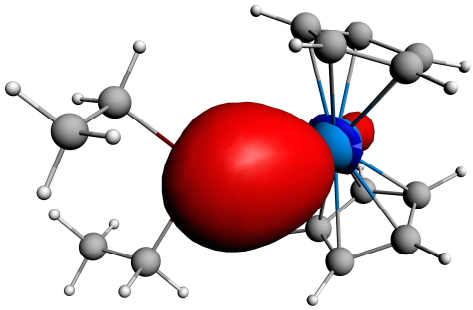
HOMO (43A)



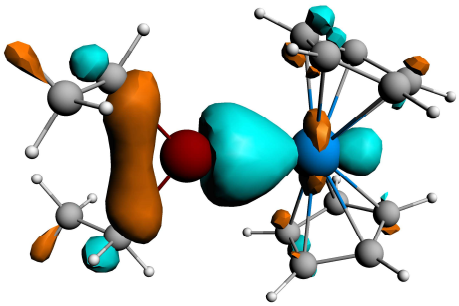
LMO 43



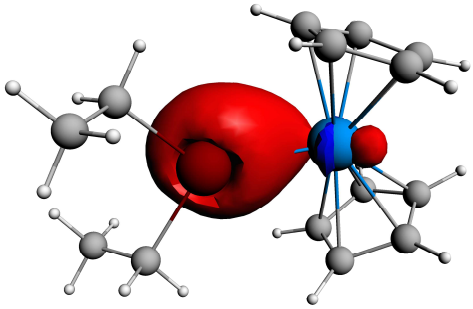
HOMO-1 (42A)



LMO 42



HOMO-3 (40A)



LMO 40

* In the ADF software package the Boys-Foster localisation method is implemented.

Table S5. Cartesian coordinates of the optimized geometry of **1**.

	ADF				GAMESS		
Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
H	-1,35197060	3,31463729	-4,38111273	H	-0,155749964	4,620683322	-3,390538748
H	0,32725020	1,90717493	-3,07292714	H	0,178228656	2,111855341	-3,073491040
H	-1,31145658	1,26489277	-2,88845910	H	-1,515203205	2,552102720	-2,896395411
C	-0,67208291	2,13206238	-2,67828995	C	-0,522568604	2,673730971	-2,438186233
C	-1,24150548	3,41187277	-3,28861376	C	-0,139321430	4,170358209	-2,385345723
H	2,63156905	2,91531545	-1,70744470	H	2,125772622	1,932254151	-2,114402714
H	-0,59249411	4,27654529	-3,09364101	H	0,865914534	4,313450840	-1,967199138
H	-2,23469357	3,64907346	-2,88291990	H	-0,839759532	4,738858124	-1,758605519
H	-3,51722463	1,24326830	-1,31704928	H	-3,389083504	3,283824241	-1,434213760
C	2,98370701	2,17442114	-0,99752567	C	2,712003218	1,790233934	-1,219947791
H	2,04798104	0,27556337	-1,73856438	H	2,787271045	-0,451056142	-1,009227313
C	2,67337374	0,78317293	-1,01258217	C	3,094809016	0,523778540	-0,653702365
H	-3,18705282	0,44271827	0,22697803	H	-3,904611964	1,848082137	-0,530201819
Sb	-0,40667536	2,20518568	-0,45850423	Sb	-0,627768107	1,632581536	-0,503958769
C	-3,48575018	1,39626556	-0,22942236	C	-3,521279820	2,872328380	-0,424079355
H	4,26903770	3,38750899	0,37681592	H	3,300560623	3,891603178	-0,662978413
C	3,84090435	2,42772576	0,10675591	C	3,359176269	2,829410449	-0,465025930
H	-4,51528688	1,61687816	0,09744639	H	-4,297847524	3,472765367	0,074557770
C	-2,53338032	2,52770787	0,15514222	C	-2,197532098	2,901326433	0,375435816
C	3,33726283	0,16996338	0,08348307	C	3,957653738	0,782364571	0,452608683
H	-2,84169795	3,48319042	-0,28830611	H	-1,823875722	3,932396514	0,453449066
C	4,07065209	1,18473925	0,76499762	C	4,127526047	2,204574448	0,564858101
H	3,31813105	-0,88579215	0,33277062	H	4,414050696	0,035276666	1,089071255
Ti	1,77784197	1,69161897	1,04710456	Ti	1,779861285	1,738468696	0,979611399
H	-2,49267187	2,66996139	1,24287906	H	-2,367357457	2,535964430	1,398880566
H	4,71558336	1,03214147	1,62232419	H	4,735297456	2,713993136	1,301406862
H	-0,25473772	3,44486880	2,66050007	H	-0,206602924	3,567333178	2,606590092
C	0,45612428	2,64475335	2,83725368	C	0,486088847	2,757364540	2,788975103
H	2,34861295	3,76024566	3,27081982	H	2,422000545	3,813174817	3,199980293
H	-0,79146187	0,79596699	2,60265104	H	-0,813454262	0,931414642	2,589151258
C	1,83154531	2,81397115	3,15074694	C	1,875580462	2,885023234	3,093249619
C	0,17320137	1,24802693	2,80569834	C	0,164474283	1,357954360	2,767193935
C	2,39385473	1,51674333	3,32584786	C	2,413635986	1,561576527	3,264354361
C	1,37369988	0,54703127	3,09767215	C	1,353671768	0,616699565	3,065324220
H	3,41752227	1,30413041	3,61083415	H	3,434593186	1,323426355	3,529510744
H	1,48368790	-0,53009837	3,16807895	H	1,429164558	-0,458891104	3,156819979

Table S6. Cartesian coordinates of the optimized geometry of **1** (triplet).

	ADF				GAMESS		
Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
H	-1,63597996	0,37241330	-3,67295600	Sb	-0,768429652	1,506561630	-0,578670290
H	-3,49750009	-1,55775853	-3,61196275	Ti	-1,773347159	-1,281156330	-1,014196472
C	-1,47953890	-0,64977399	-3,35006189	Sb	0,768432463	-1,506557773	0,578669775
C	-2,45707092	-1,67017466	-3,32575707	Ti	1,773345305	1,281158671	1,014201558
H	-0,05253133	4,62710218	-3,32449623	H	-1,623494842	0,391546241	-3,696839175
H	0,03829238	2,09042514	-3,16746507	H	-3,495402235	-1,532904649	-3,630569059
H	-1,61940779	2,65997574	-2,94251686	C	-1,472422758	-0,623010492	-3,360766498
C	-0,25216952	-1,21190393	-2,88843152	C	-2,461837783	-1,645434207	-3,331405725
C	-1,83886527	-2,86932956	-2,86637776	H	-0,032148025	4,549991384	-3,341618086
H	0,69716833	-0,69282365	-2,81169908	H	0,060483569	2,040896786	-3,140302409
H	-2,32571648	-3,83083319	-2,74053881	H	-1,607962929	2,584017631	-2,949240380
C	-0,47777693	-2,59224870	-2,60630950	C	-0,238049105	-1,192149776	-2,891787042
C	-0,61152595	2,67880246	-2,50517585	C	-1,839402996	-2,860238738	-2,874749787
C	-0,10191192	4,11034014	-2,35202586	H	0,715905566	-0,684701663	-2,833787104
H	0,26215516	-3,30636861	-2,26528699	H	-2,325235508	-3,820326001	-2,762966125
H	2,05319514	1,83989372	-2,07643089	C	-0,466686681	-2,585932760	-2,617672804
H	0,90413818	4,13745526	-1,91335930	C	-0,612309393	2,610705700	-2,481884326
H	-0,75717508	4,70640716	-1,70195332	C	-0,129022203	4,072710210	-2,354343443
H	-3,37186292	3,49777335	-1,42980122	H	0,272071891	-3,306743173	-2,299841743
H	-4,43376035	-2,77530546	-1,43321681	H	2,072239611	1,979844740	-2,076404772
C	2,67907959	1,73321569	-1,19839193	H	0,848542983	4,129892040	-1,858569024
H	2,39662840	-2,59176896	-1,39129717	H	-0,832063428	4,676881183	-1,765207592
H	3,19297971	-0,44029503	-1,21551644	H	-3,336071266	3,498643900	-1,461219158
Ti	-1,77956158	-1,28894613	-1,03203245	H	-4,499600256	-2,700094400	-1,480162342
H	-4,65152013	-0,12980458	-0,96671090	C	2,689132246	1,818028119	-1,206361654
C	3,28038878	0,53212239	-0,74565916	H	2,391831465	-2,583798145	-1,351823401
H	-4,07832743	2,16758765	-0,50177699	H	3,182647818	-0,363136758	-1,343112849
C	-3,93643532	-2,22719131	-0,64094886	H	-4,662284484	-0,073950184	-0,887920356
Sb	-0,76216084	1,51320460	-0,57693138	C	3,277359902	0,574442792	-0,814355208
C	-3,54044747	3,12059223	-0,41167056	H	-4,057786851	2,170118583	-0,535569864
H	1,69447699	-3,91034379	-0,44716617	C	-3,987638404	-2,202247546	-0,668491652
H	2,79272310	3,82909777	-0,41098367	C	-3,512625720	3,117925647	-0,446177423
C	3,07275498	2,78477981	-0,32445298	H	1,661938227	-3,892314747	-0,417363689
C	-4,05224473	-0,83158804	-0,39652104	H	2,865565534	3,878976910	-0,323147390
C	2,22891317	-2,95337232	-0,36749794	C	3,115866888	2,827234411	-0,280964950
H	-4,21365626	3,83418103	0,09129912	C	-4,069112629	-0,807593027	-0,359006717
H	4,21593940	-3,83035780	-0,12078943	C	2,188896876	-2,930736169	-0,327836175
C	-2,22854726	2,95718117	0,35304373	H	-4,173562133	3,836075529	0,063317547
C	4,05268816	0,83106771	0,41182332	H	4,173533162	-3,836115281	-0,063314123
C	-3,06816741	-2,78432341	0,33715459	C	-2,188902994	2,930737234	0,327824731
H	-2,78777732	-3,82855142	0,42310616	C	4,069113542	0,807601721	0,359017677
H	-1,69323164	3,91351216	0,43493430	C	-3,115870796	-2,827228482	0,280974144
C	3,54653930	-3,11659577	0,38707127	H	-2,865572280	-3,878971451	0,323157251
Sb	0,76532999	-1,51338610	0,57291159	H	-1,661949385	3,892321285	0,417344026
C	3,93679715	2,22641156	0,65676662	C	3,512633123	-3,117907524	0,446147477
H	4,08488447	-2,16358117	0,47224253	C	3,987633167	2,202255551	0,668503494
C	-3,27518962	-0,53127046	0,75731957	H	4,057791284	-2,170109487	0,535568417
H	4,64969066	0,12893346	0,98414099	C	-3,277353284	-0,574437062	0,814362720
Ti	1,77754039	1,28890094	1,03758151	H	4,662285308	0,073960980	0,887934518
H	-3,18653716	0,44138115	1,22642960	H	-3,182637268	0,363141844	1,343120948
H	-2,40330651	2,59671523	1,37606182	H	-2,391832953	2,583809625	1,351814808
C	-2,67149855	-1,73182575	1,20870438	C	-2,689126592	-1,818023462	1,206367640
H	4,43064876	2,77384654	1,45169932	H	4,499589641	2,700103114	1,480177160

H	3,38585229	-3,49317193	1,40666572	H	3,336069815	-3,498659842	1,461181451
H	0,75563778	-4,70866737	1,68783014	H	0,832068410	-4,676880060	1,765198929
H	-0,90354470	-4,13483960	1,90339676	H	-0,848536943	-4,129895907	1,858549131
H	-2,04326755	-1,83808718	2,08489020	H	-2,072234255	-1,979841972	2,076410550
H	-0,25992628	3,31559221	2,25943315	H	-0,272083759	3,306734271	2,299849396
C	0,10314749	-4,11278376	2,34084117	C	0,129019890	-4,072710995	2,354334009
C	0,61715916	-2,68346558	2,49830326	C	0,612322311	-2,610711833	2,481878608
C	0,47346731	2,59701740	2,60494403	C	0,466676972	2,585925774	2,617680897
H	2,32700839	3,82568708	2,75371706	H	2,325219525	3,820329643	2,762982484
H	-0,71299361	0,70371171	2,80178973	H	-0,715903981	0,684686919	2,833789234
C	1,83429547	2,86653446	2,87452255	C	1,839391652	2,860239153	2,874758847
C	0,23881974	1,21755081	2,88448921	C	0,238047674	1,192140809	2,891791395
H	1,62586152	-2,66879221	2,93381050	H	1,607977002	-2,584024555	2,949231001
H	-0,02986085	-2,09557972	3,16403629	H	-0,060472235	-2,040907191	3,140300124
H	0,05323366	-4,63256818	3,31173107	H	0,032179151	-4,550008531	3,341603354
C	2,44367221	1,66359774	3,33603038	C	2,461833136	1,645436672	3,331411439
C	1,46039131	0,64844810	3,35295603	C	1,472424727	0,623006309	3,360767686
H	3,48188179	1,54561938	3,62851266	H	3,495398354	1,532911221	3,630574462
H	1,60870487	-0,37464139	3,67547164	H	1,623500976	-0,391550055	3,696839919

Table S7. Cartesian coordinates of the optimized geometry of **1** (singlet).

	ADF				GAMESS		
Atom	X (Å)	Y (Å)	Z (Å)	Atom	X (Å)	Y (Å)	Z (Å)
H	1,74811881	-0,87173225	-3,72322368	Ti	0,778114011	-1,664872844	-0,845392951
H	2,04970574	4,06428315	-3,74097141	Sb	1,493319487	1,089485046	-0,828007691
H	1,76347783	-3,52003745	-3,23120945	Ti	-0,778101732	1,664871849	0,845393890
C	0,94933136	-1,44281741	-3,26625302	Sb	-1,493314601	-1,089483547	0,828004654
H	0,78381992	1,89633316	-3,38272926	H	1,735296225	-0,853233663	-3,710927025
H	2,52091851	1,58945214	-3,33520352	H	2,102572350	4,030312410	-3,702754978
C	0,95234211	-2,83758975	-3,00918104	H	1,725133725	-3,502367923	-3,203744842
C	-0,33396910	-0,94409023	-2,88438186	C	0,938731842	-1,407033812	-3,235905843
H	-0,67332558	0,07883381	-2,99619437	H	0,783884016	1,899652170	-3,352479549
C	1,70255317	2,11119032	-2,82109539	H	2,512633451	1,555480700	-3,310947115
C	1,97070830	3,61357893	-2,73801141	C	0,927299663	-2,811217886	-2,976250485
C	-0,30756152	-3,19816506	-2,45029484	C	-0,350780764	-0,889972604	-2,852043299
C	-1,10635306	-2,02998086	-2,39608444	H	-0,686004565	0,124811229	-3,002320681
H	-0,61668317	-4,19420559	-2,15233835	C	1,704085039	2,077056413	-2,779130259
H	2,91004003	3,82849920	-2,21008404	C	2,010408567	3,590934891	-2,697708591
H	-2,13817584	-1,98746819	-2,07100135	C	-0,347954108	-3,163402099	-2,418813583
H	1,17369556	4,14550143	-2,20045774	C	-1,146956776	-1,981626739	-2,375560064
H	-0,68665712	2,98704467	-2,03019558	H	-0,668073667	-4,155904348	-2,132093785
H	4,55103842	2,09109603	-1,99558427	H	2,952982027	3,782085979	-2,167874269
H	4,67327587	0,38314973	-1,56246666	H	-2,183884815	-1,936998172	-2,083732170
H	-2,30916705	0,85494259	-1,72004970	H	1,222175567	4,141313659	-2,166520417
H	3,16487704	-3,68341633	-1,48250532	H	-0,707958608	2,980773500	-2,067794844
C	-1,39128114	2,83467167	-1,22334494	H	4,538104909	2,061397264	-2,036128659
C	4,66790141	1,40145218	-1,14881537	H	4,668953009	0,367385637	-1,546418420
C	-2,24792142	1,71183026	-1,05904909	H	-2,320803849	0,829691718	-1,773590299
Ti	0,81010522	-1,72914706	-0,88499682	H	3,160234708	-3,611176471	-1,481268074
H	-3,73859034	-0,94626825	-0,76430412	C	-1,385539945	2,800369839	-1,248926117
Sb	1,48348491	1,08296139	-0,82540416	C	4,646726554	1,398357514	-1,168358040
H	3,87177289	-1,31181646	-0,44256835	C	-2,248520357	1,665312733	-1,093679031
H	5,66442999	1,58521472	-0,71589342	H	-3,719973193	-1,011672047	-0,764028029
C	2,70077851	-3,20393702	-0,62903116	H	3,877704433	-1,257489635	-0,408603620
C	-1,65549301	3,74472567	-0,17269366	H	5,630337130	1,607259605	-0,720988863
C	3,06912357	-1,94692041	-0,09057514	C	2,698268348	-3,144539024	-0,623950819
H	-1,16450256	4,69990567	-0,01898465	C	-1,643896943	3,703916847	-0,175778915
H	-3,53140015	-2,62817296	-0,24773011	C	3,071709493	-1,886365161	-0,066535057
C	3,56671279	1,59154167	-0,10666339	H	-1,161232660	4,659107056	-0,019476695
C	-3,56554996	-1,58960701	0,10869473	H	-3,498622146	-2,666941284	-0,185260693
H	3,53215412	2,63087447	0,24749339	C	3,517730678	1,613709912	-0,133617866
H	1,16041471	-4,70225984	0,01291604	C	-3,517722789	-1,613724937	0,133612385
C	-3,06919259	1,94243047	0,08792529	H	3,498640808	2,666928737	0,185257658
C	1,65285236	-3,74798287	0,16790368	H	1,161250868	-4,659108039	0,019495746
C	-2,70345026	3,20092415	0,62439824	C	-3,071697026	1,886367700	0,066539236
H	-5,66299162	-1,58391982	0,71848278	C	1,643907533	-3,703911210	0,175794333
H	-3,87111644	1,30672708	0,44042514	C	-2,698255780	3,144536936	0,623964017
Sb	-1,48183865	-1,08299877	0,82734229	H	-5,630327915	-1,607342599	0,720982214
H	3,73946885	0,95013707	0,76783138	H	-3,877692264	1,257492220	0,408605456
Ti	-0,81041274	1,72934637	0,88442968	H	3,719981305	1,011670598	0,764028123
C	2,24917723	-1,71733474	1,05753033	C	2,248530625	-1,665302546	1,093680216
C	-4,66630728	-1,40173675	1,15165509	C	-4,646733835	-1,398322672	1,168326552
C	1,39097842	-2,83933754	1,22059653	C	1,385545476	-2,800355132	1,248933680
H	-3,16891595	3,68114003	1,47670613	H	-3,160215181	3,611176944	1,481280732
H	2,31217966	-0,86168135	1,72004977	H	2,320811407	-0,829679043	1,773589867
H	-4,67123979	-0,38449748	1,56792772	H	-4,668955852	-0,367373372	1,546424168

H	-4,54960041	-2,09362744	1,99665322	H	-4,538118359	-2,061374886	2,036101054
H	0,68711123	-2,99224883	2,02807427	H	0,707957945	-2,980753913	2,067799736
H	-1,17338310	-4,14607828	2,19554937	H	-1,222161107	-4,141340928	2,166484410
H	2,13637999	1,99707999	2,07326707	H	2,183897381	1,936986181	2,083738407
H	-2,90961030	-3,82836046	2,20611704	H	-2,953015405	-3,782046512	2,167937342
H	0,60858511	4,19973044	2,14992610	H	0,668091441	4,155897280	2,132103424
C	1,10401076	2,03714512	2,39684742	C	1,146968812	1,981616269	2,375564181
C	0,30196901	3,20326659	2,44885264	C	0,347970776	3,163394416	2,418819849
C	-1,97020081	-3,61541892	2,73467299	C	-2,010343851	-3,590943243	2,697696289
C	-1,70138612	-2,11345574	2,82168739	C	-1,704121730	-2,077049844	2,779124973
H	0,67584208	-0,07212459	2,99956867	H	0,686007648	-0,124825315	3,002315847
C	0,33398293	0,94985494	2,88579548	C	0,350789668	0,889961047	2,852039677
C	-0,95736273	2,84008883	3,00703199	C	-0,927284934	2,811212031	2,976253897
H	-2,51965040	-1,59244633	3,33676417	H	-2,512658064	-1,555452699	3,310935316
H	-0,78261815	-1,90018698	3,38390717	H	-0,783907864	-1,899668044	3,352477872
C	-0,95100231	1,44571777	3,26592224	C	-0,938721377	1,407026530	3,235903042
H	-1,77040909	3,52080552	3,22736321	H	-1,725116940	3,502364881	3,203749301
H	-2,04943236	-4,06896389	3,73621301	H	-2,102804615	-4,030275046	3,702722453
H	-1,74874902	0,87323745	3,72297556	H	-1,735283309	0,853229497	3,710931641