Supporting Information

Titanocene Selenide Sulfides Revisited: Formation, Stabilities, and NMR Spectroscopic Properties

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Contents

1. Site occupation factors of selenium in chalcogen atom positions and interatomic distances

Table S1. The site occupancy factors of selenium in the disordered chalcogen atom sites of the crystals of phases ***B***-***E***.

Phase	E1	E2	E3	E4	E5
B	19.8(3)	51.5(3)	57.0(3)	43.0(3)	12.9(3)
C	23.1(4)	69.0(5)	84.6(6)	77.1(6)	34.5(5)
D [a]	45	82	82	71	32
E	82.1(5)	100.0	100.0	100.0	83.1(5)

[a] The data are taken from Pekonen, P.; Hiltunen, Y.; Laitinen, R. S.; Valkonen, J. ^{77}Se NMR Spectroscopic and X-ray Crystallographic Characterization of Bis(cyclopentadienyl)titanium Selenide Sulfides Mixtures [$Ti(C_5H_5)_2Se_xS_{5-x}$]. *Inorg. Chem.* **1991**, *30*, 1874-1878.

Table S2. The interatomic chalcogen-chalcogen and chalcogen-titanium distances.

Phase	Ti1-E1	Ti1-E5	E1-E2	E2-E3	E3-E4	E4-E5
B	2.4508(12)	2.4475(9)	2.1929(9)	2.2633(8)	2.2711(11)	2.1649(9)
C	2.4592(12)	2.4698(14)	2.2316(11)	2.3234(12)	2.3131(9)	2.2616(11)
D [a]	2.469(2)	2.469(2)	2.266(2)	2.312(1)	2.311(1)	2.239(2)
E	2.5191(13)	2.5545(13)	2.3207(15)	2.3373(11)	2.3353(10)	2.3199(15)

[a] The data are taken from Pekonen, P.; Hiltunen, Y.; Laitinen, R. S.; Valkonen, J. ^{77}Se NMR Spectroscopic and X-ray Crystallographic Characterization of Bis(cyclopentadienyl)titanium Selenide Sulfides Mixtures [$Ti(C_5H_5)_2Se_xS_{5-x}$]. *Inorg. Chem.* **1991**, *30*, 1874-1878.

2. The molecular composition of solid phases

All phases ***B***-***E*** are solid solutions of different [$TiCp_2Se_xS_{5-x}$] (x = 0-5) complexes. The identity of the complexes in different phases is based on the NMR assignment in the corresponding CS_2 solutions. The relative contents in the crystalline phases was estimated from the disorder scheme in chalcogen atom positions. However, in the solid state, the relative contents of individual [$TiCp_2Se_xS_{5-x}$] complexes can be different from those in solution because of the differing solubilities of the complexes. The results of the computations are shown in Table S3.

Table S3. The composition of the solid solution of phase ***B***-***E*** based on the site occupancy factors of selenium in different chalcogen atom positions (for numbering of chalcogen atom positions, see Figure 2 in the main text).

Complex		E1	E2	E3	E4	E5	Content [a]
(a) Phase ***B*** (Se:S = 1:4)							
[$TiCp_2Se_4S$] (**4**$_1$)	-Se-Se-Se-Se-S-	20	20	20	20	-	33
	-S-Se-Se-Se-Se-	-	13	13	13	13	
[$TiCp_2SSe_3S$] (**3**$_6$)	-S-Se-Se-Se-S-	-	1	1	1	-	1
[$TiCp_2SSe_2S_2$] (**2**$_5$)	-S-Se-Se-S-S-	-	15	15	-	-	23
	-S-S-Se-Se-S-	-	-	8	8		
[$TiCp_2SSeS_3$] (**1**$_2$)	-S-Se-S-S-S-	-	2	-	-	-	2
[$TiCp_2S_5$] (**0**$_1$) [b]	-S-S-S-S-S-	-	-	-	-	-	41
Total							100
Site occupancy factors of selenium	s.o.f(Calc.)	20	51	57	44	13	
(mol %)	s.o.f.(Exptl.) [c]	20	51	57	43	13	
(b) Phase ***C*** (Se:S = 2:3)							
[$TeCp_2Se_5$] (**5**$_1$)	-Se-Se-Se-Se-Se-	12	12	12	12	12	12
[$TiCp_2Se_4S$] (**4**$_1$)	-Se-Se-Se-Se-S-	8	8	8	8	-	25
	-S-Se-Se-Se-Se-	-	17	17	17	17	
[$TiCp_2Se_3S_2$] (**3**$_1$)	-Se-Se-Se-S-S-	3	3	3	-	-	9
	-S-S-Se-Se-Se-	-	-	6	6	6	

Table S1. *Cont.*

[$TiCp_2SSe_3S$] (**3**$_6$)	-S-Se-Se-Se-S-	-	18	18	18	-	18
[$TiCp_2SSe_2S_2$] (**2**$_5$)	-S-Se-Se-S-S-	-	6	6	-	-	21
	-S-S-Se-Se-S-	-	-	15	15		
[$TiCp_2SSeS_3$] (**1**$_2$)	-S-Se-S-S-S-	-	5	-	-	-	6
	-S-S-S-Se-S	-	-	-	1	-	
[$TiCp_2S_5$] (**0**$_1$) [b]	-S-S-S-S-S-	-	-	-	-	-	9
Total							100
Site occupancy factors of selenium	s.o.f(Calc.)	22	69	85	75	32	
(mol %)	s.o.f.(Exptl.) [c]	23	69	85	77	34	
Phase ***D*** (Se:S = 3:2)							
[$TeCp_2Se_5$] (**5**$_1$)	-Se-Se-Se-Se-Se-	25	25	25	25	25	25
[$TiCp_2Se_4S$] (**4**$_1$)	-Se-Se-Se-Se-S-	16	16	16	16	-	23
	-S-Se-Se-Se-Se-	-	7	7	7	7	
[$TiCp_2Se_3S_2$] (**3**$_1$)	-Se-Se-Se-S-S-	4	4	4	-	-	4
[$TiCp_2SSe_3S$] (**3**$_6$)	-S-Se-Se-Se-S-	-	24	24	24	-	24
[$TiCp_2SSe_2S_2$] (**2**$_5$)	-S-Se-Se-S-S-	-	6	6	-	-	6
[$TiCp_2S_5$] (**0**$_1$) [d]	-S-S-S-S-S-	-	-	-	-	-	18
Total							100
Site occupancy factors of selenium	s.o.f(Calc.)	45	82	82	72	35	
(mol %)	s.o.f.(Exptl.) [c,d]	45	82	82	71	32	
(d) Phase ***E*** (Se:S = 4:1)							
[$TeCp_2Se_5$] (**5**$_1$)	-Se-Se-Se-Se-Se-	65	65	65	65	65	65
[$TiCp_2Se_4S$] (**4**$_1$)	-Se-Se-Se-Se-S-	17	17	17	17	-	35
	-S-Se-Se-Se-Se-	-	18	18	18	18	
Total							100
Site occupancy factors of selenium	s.o.f. (Calc.)	82	100	100	100	83	
(mol %)	s.o.f. (Exptl.) [c]	82	100	100	100	83	

[a] in mol%. [b] Phases ***B***-***D*** also contain [$TiCp_2S_5$] the amount of which was estimated by completing the relative contents of the complexes to 100 %. [c] The experimental site occupancy factors of selenium in chalcogen atom positions have been taken from the refined crystal structures (see Table S1). The numerical values have been truncated to show only full integers. [d] Data are taken from Pekonen, P.; Hiltunen, Y.; Laitinen, R. S.; Valkonen, J. ^{77}Se NMR Spectroscopic and X-ray Crystallographic Characterization of Bis(cyclopentadienyl)titanium Selenide Sulfides Mixtures [$Ti(C_5H_5)_2Se_xS_{5-x}$]. *Inorg. Chem.* **1991**, *30*, 1874-1878.

3. Energetics of the twenty isomers of [$TiCp_2Se_xS_{5-x}$] (x = 0-5)

Table S4. Energy terms of atoms (in Hartree) used in the DLPNO-CCSD(T)/CBS enthalpy of formation calculations.

	def2-TZVPP		def2-QZVPP				
	HF	**CCSD(T)**	**HF**	**CCSD(T)**	**Total CBS**	**ΔE(C+R)**	**ΔH(0→298K)**
0_1	-3220.81910	-3224.03662	-3220.90464	-3224.31691	-3224.47296	-12.02420	0.19777
1_1	-5223.12788	-5226.43329	-5223.24930	-5226.80093	-5227.00005	-39.18928	0.19736
1_2	-5223.13017	-5226.43503	-5223.25160	-5226.80172	-5227.00011	-39.18932	0.19735
1_3	-5223.12991	-5226.43475	-5223.25134	-5226.80173	-5227.00034	-39.18951	0.19738
2_1	-7225.44076	-7228.83271	-7225.59810	-7229.28723	-7229.52903	-66.35444	0.19703
2_2	-7225.43897	-7228.83186	-7225.59630	-7229.28596	-7229.52746	-66.35454	0.19700
2_3	-7225.43901	-7228.83185	-7225.59634	-7229.28586	-7229.52729	-66.35441	0.19702
2_4	-7225.43630	-7228.83001	-7225.59360	-7229.28480	-7229.52684	-66.35434	0.19706
2_5	-7225.44322	-7228.83445	-7225.60060	-7229.28818	-7229.52938	-66.35472	0.19705
2_6	-7225.44141	-7228.83311	-7225.59876	-7229.28695	-7229.52825	-66.35435	0.19702
3_1	-9227.75417	-9231.23239	-9227.94745	-9231.77393	-9232.05852	-93.51984	0.19671
3_2	-9227.75231	-9231.23156	-9227.94554	-9231.77248	-9232.05665	-93.51953	0.19665
3_3	-9227.74963	-9231.22975	-9227.94284	-9231.77119	-9232.05575	-93.51950	0.19668
3_4	-9227.75237	-9231.23163	-9227.94564	-9231.77249	-9232.05657	-93.51978	0.19669
3_5	-9227.74784	-9231.22871	-9227.94105	-9231.77007	-9232.05458	-93.51957	0.19669
3_6	-9227.75666	-9231.23391	-9227.94999	-9231.77505	-9232.05932	-93.51990	0.19671
4_1	11230.06785	11233.63236	11230.29707	11234.26080	11234.58808	-120.68506	0.19637
4_2	11230.06327	11233.62977	11230.29243	11234.25802	11234.58520	-120.68490	0.19639
4_3	11230.06299	11233.62914	11230.29212	11234.25779	11234.58529	-120.68469	0.19638
5_1	13232.37891	13236.03047	13232.64400	13236.74626	13237.11664	-147.85022	0.19614
S_2	-795.08548	-795.44394	-795.10877	-795.49526	-795.51923	-2.75729	0.00511
Se_2	-4799.70605	-4800.23902	-4799.80138	-4800.46468	-4800.57435	-57.08803	0.004532

Table S5. Energy terms of atoms (in Hartree) used in the DLPNO-CCSD(T)/CBS enthalpy of formation calculations.

	def2-TZVPP		def2-QZVPP				
	HF	**CCSD(T)**	**HF**	**CCSD(T)**	**Total CBS**	**Δ*E*(SO)**	**Δ*E*(C+R)**
Ti	-848.39721	-848.72007	-848.413344	-848.753473	-848.768486	-0.00101	-4.51783
C	-37.69248	-37.78070	-37.693627	-37.786404	-37.789935	-0.00014	-0.05955
H	-0.49981	-	-0.499983	-	-0.500007	0.00000	-0.00001
S	-397.50200	-397.64607	-397.512996	-397.668363	-397.678243	-0.00089	-1.37824
Se	-2399.82719	-2400.05819	-2399.874606	-2400.167742	-2400.220298	-0.00431	-28.54398

Table S6. The DLPNO-CCSD(T)/CBS formation enthalpies (298 K) of $TiCp_2Se_xS_{5-x}$ molecules calculated at non-relativistic $\Delta_f H_{non-rel.}$ and relativistic level $\Delta_f H$ with core-correlation and scalar relativistic [ΔE(C+R)] and spin-orbit [ΔE (SO)] energy corrections included.

Complex	**$\Delta_f H_{nonrel.}$**	**Δ_fH**	**Complex**	**$\Delta_f H_{nonrel.}$**	**Δ_fH**
0_1	–25.2	–58.6	**3_1**	–38.9	–41.3
1_1	–26.2	–48.9	**3_2**	–34.2	–35.7
1_2	–26.4	–49.2	**3_3**	–31.7	–33.2
1_3	–26.9	–50.2	**3_4**	–33.9	–36.0
2_1	–31.9	–44.1	**3_5**	–28.6	–30.2
2_2	–27.9	–40.3	**3_6**	–41.0	–43.5
2_3	–27.4	–39.5	**4_1**	–46.2	–38.2
2_4	–26.1	–38.0	**4_2**	–38.6	–30.2
2_5	–32.8	–45.7	**4_3**	–38.9	–29.9
2_6	–29.9	–41.8	**5_1**	–50.6	–32.0

Table S7. Isotropic ^{77}Se-NMR shielding values calculated at PBE0/def2-TZVPP level of theory.

	Atom 1	**Atom 2**	**Atom 3**	**Atom 4**	**Atom 5**
1_1	657.8				
1_2		980.6			
1_3			1073.7		
2_1	701.4	1079.9			
2_2	628.7		1100.5		
2_3	645.9			979.3	
2_4	626.6				626.6
2_5		1043.7	1101.6		
2_6		1024.8		1024.8	
3_1	683.8	1151.9	1124.9		
3_2	696.4	1111.0		1019.2	
3_3	680.3	1064.1			614.8
3_4	619.0		1127.8	1041.8	
3_5	604.1		1135.3		604.1
3_6		1066.9	1143.0	1066.9	

Table S7. *Cont.*

4_1	676.4	1164.2	1159.6	1060.9	
4_2	664.3	1139.0	1158.7		590.3
4_3	665.0	1106.5		1106.5	665.0
5_1	648.0	1157.6	1190.3	1157.6	648.0

4. Quantitative details in syntheses

Table S8. The amounts of reagents and solvents in syntheses

Phase	Se:S	m_{Se} (g)	n_{Se} (mmol)	m_S (g)	n_S (mmol)
A				0.64	20.0
B	1 : 4	0.32	4.0	0.51	15.9
C	2 : 3	0.63	8.0	0.38	11.9
D	3 : 2	0.95	12.0	0.26	8.1
E	4 : 1	1.26	16.0	0.13	4.0
F		1.59	20.1		

The 0.1 M solution of lithium triethylhydridoborate in THF (8 ml, 8 mmol) was added into solid sulfur, selenium or their mixtures (see Table S8 for the quantities involved). The solution was stirred upon mild heating for 20 minutes, after which a solution of titanocene dichloride (1.00 g, 4.0 mmol) in 100 ml of THF was added dropwise during 30 minutes. The solution was filtered, the solvent THF was evaporated under dynamic vacuum, and the residue was extracted in 100 ml of CS_2. The NMR spectra were recorded from the saturated solutions thus obtained. The solid phases, which were used for crystal structure determinations, were obtained by recrystallization from these CS_2 solutions.

5. PBE0/def2-TZVPP optimized geometries of [$TiCp_2Se_xS_{5-x}$] (x = 0-5)

Cartesian X,Y,Z coordinates in Å units.

0_1 [$Ti(C_5H_5)_2S_5$] (C_s)

Ti	0.056104000	-0.931529000	0.000000000
S	0.727116000	0.470172000	1.797972000
S	-0.221400000	2.279067000	1.647879000
S	0.628288000	3.145016000	0.000000000
S	-0.221400000	2.279067000	-1.647879000
S	0.727116000	0.470172000	-1.797972000
C	-2.150980000	0.210661000	0.000000000
C	-2.121042000	-0.614048000	1.141448000
C	-2.062141000	-1.949046000	0.708911000
C	-2.062141000	-1.949046000	-0.708911000
C	-2.121042000	-0.614048000	-1.141448000
C	2.246694000	-1.545311000	0.000000000
C	1.655297000	-2.126736000	1.139452000
C	0.693649000	-3.059155000	0.705496000
C	0.693649000	-3.059155000	-0.705496000
C	1.655297000	-2.126736000	-1.139452000
H	-2.180086000	1.285377000	0.000000000
H	-2.117107000	-0.276305000	2.164112000
H	-2.045393000	-2.818902000	1.344464000

1_2 [$Ti(C_5H_5)_2SSeS_3$] (C_1)

Ti	1.177707000	0.030566000	-0.053434000
S	0.070822000	-2.075581000	0.378729000
S	-1.760345000	-2.069396000	-0.536954000
S	-2.894828000	-0.816258000	0.603772000
Se	-2.355255000	1.243869000	0.049356000
S	-0.423322000	1.443488000	1.053507000
C	2.271158000	-0.085424000	-2.142612000
C	1.983453000	1.278331000	-1.882160000
C	0.587158000	1.432768000	-1.884007000
C	0.010913000	0.173018000	-2.128287000
C	1.051736000	-0.764226000	-2.292922000
C	3.263082000	0.805529000	0.751191000
C	2.320331000	1.052055000	1.767280000
C	1.840221000	-0.191840000	2.228556000
C	2.493344000	-1.204805000	1.500535000
C	3.366851000	-0.591399000	0.582130000
H	3.253167000	-0.521536000	-2.223878000
H	2.704469000	2.065626000	-1.735795000

H	0.050136000	2.348490000	-1.702516000
H	-1.042192000	-0.041102000	-2.170391000
H	0.928425000	-1.818557000	-2.476623000
H	3.819243000	1.553527000	0.211488000
H	2.012894000	2.021905000	2.125432000
H	1.072760000	-0.340257000	2.970296000
H	2.348624000	-2.266519000	1.624463000
H	4.014857000	-1.105651000	-0.108134000

1_3 [$Ti(C_5H_5)_2S_2SeS_2$] (C_s)

Ti	0.036826000	-1.252643000	0.000000000
S	-0.663005000	0.186140000	1.802393000
S	0.424775000	1.917759000	1.730605000
Se	-0.399612000	2.984633000	0.000000000
S	0.424775000	1.917759000	-1.730605000
S	-0.663005000	0.186140000	-1.802393000
C	1.981662000	-2.382977000	0.708950000
C	1.981662000	-2.382977000	-0.708950000
C	2.113836000	-1.053274000	-1.141361000
C	2.187831000	-0.231143000	0.000000000
C	2.113836000	-1.053274000	1.141361000
C	-0.838791000	-3.331586000	-0.705511000
C	-1.743234000	-2.343658000	-1.139740000
C	-2.298891000	-1.727531000	0.000000000
C	-1.743234000	-2.343658000	1.139740000
C	-0.838791000	-3.331586000	0.705511000
H	1.915074000	-3.250550000	1.344426000
H	1.915074000	-3.250550000	-1.344426000
H	2.129996000	-0.715538000	-2.164087000
H	2.271645000	0.840857000	0.000000000
H	2.129996000	-0.715538000	2.164087000
H	-0.266628000	-3.984694000	-1.342917000
H	-1.968346000	-2.097561000	-2.165621000
H	-2.987176000	-0.898301000	0.000000000
H	-1.968346000	-2.097561000	2.165621000
H	-0.266628000	-3.984694000	1.342917000

1_1 [$Ti(C_5H_5)_2SeS_4$] (C_1)

Ti	1.027647000	-0.155964000	-0.055525000
S	-0.293118000	-1.543780000	1.394355000
S	-2.082478000	-1.944436000	0.475896000
S	-3.129930000	-0.193878000	0.621237000
S	-2.464895000	1.051682000	-0.854441000
Se	-0.568910000	1.828619000	-0.042854000
C	2.050327000	-1.613493000	-1.588879000
C	2.066642000	-0.317323000	-2.164405000
C	0.737772000	0.065683000	-2.406495000
C	-0.100677000	-0.986605000	-1.982153000
C	0.710614000	-2.025117000	-1.490349000
C	3.216787000	-0.314111000	0.807393000
C	3.042486000	1.004011000	0.336163000
C	2.063812000	1.624686000	1.137519000
C	1.624626000	0.689507000	2.095875000
C	2.340580000	-0.508397000	1.892953000
H	2.911363000	-2.195919000	-1.305214000
H	2.945212000	0.264986000	-2.3888330000

2_1

[$Ti(C_5H_5)_2Se_2S_3$] (C_1)

Ti	1.271188000	-0.099345000	-0.102873000
S	0.214454000	-1.903359000	1.096215000
S	-1.589802000	-2.352060000	0.232647000
S	-2.839444000	-0.853718000	0.822928000
Se	-2.473207000	0.882356000	-0.477571000
Se	-0.479142000	1.668022000	0.433317000
C	2.346007000	-0.994573000	-1.995946000
C	2.067103000	0.369167000	-2.267918000
C	0.671555000	0.522783000	-2.320208000
C	0.087468000	-0.733956000	-2.069442000
C	1.121454000	-1.671598000	-1.878330000
C	3.270777000	1.064238000	0.368654000
C	2.308071000	1.540051000	1.279920000
C	1.934419000	0.470030000	2.119933000
C	2.675057000	-0.663821000	1.732262000
C	3.497378000	-0.300152000	0.648251000
H	3.324271000	-1.439098000	-1.917712000
H	2.794805000	1.146697000	-2.432117000
H	0.139383000	1.441500000	-2.500098000
H	-0.967137000	-0.939666000	-2.022542000
H	0.991530000	-2.717257000	-1.654528000
H	3.762034000	1.649191000	-0.390750000
H	1.934507000	2.550991000	1.335190000
H	1.181231000	0.501929000	2.890115000
H	2.618529000	-1.641406000	2.184535000
H	4.195552000	-0.946956000	0.144046000

2_2 [$Ti(C_5H_5)_2SeSSeS_2$] (C_1)

Ti	1.313770000	-0.166707000	-0.043508000
S	-0.110091000	-1.618029000	1.238023000
S	-1.836107000	-1.987401000	0.198157000
Se	-2.997900000	-0.138195000	0.398540000
S	-2.070893000	1.256817000	-1.011297000
Se	-0.223686000	1.860450000	0.023911000
C	2.398743000	-1.517333000	-1.632464000
C	2.439005000	-0.183536000	-2.113130000
C	1.120898000	0.219565000	-2.381886000
C	0.265434000	-0.855257000	-2.063464000
C	1.055899000	-1.929348000	-1.613989000
C	3.440347000	-0.456878000	0.934596000
C	3.340733000	0.891521000	0.532107000
C	2.337105000	1.502701000	1.309265000
C	1.808815000	0.532030000	2.184471000
C	2.494741000	-0.678268000	1.954652000
H	3.247689000	-2.121247000	-1.357553000
H	3.325865000	0.410244000	-2.262275000
H	0.811776000	1.184556000	-2.746949000
H	-0.807423000	-0.849048000	-2.139052000
H	0.689822000	-2.887987000	-1.286812000
H	4.131653000	-1.185983000	0.546836000
H	3.938961000	1.380325000	-0.218846000
H	2.042470000	2.539955000	1.260148000
H	0.993857000	0.678913000	2.874166000
H	0.410850000	1.003669000	-2.822978000
H	-1.175615000	-0.987900000	-2.017470000
H	0.362171000	-2.959376000	-1.083392000
H	3.911194000	-1.040025000	0.419091000
H	3.576276000	1.468756000	-0.476240000
H	1.727323000	2.646389000	1.048258000
H	0.844995000	0.847899000	2.822772000
H	2.229869000	-1.416790000	2.464109000

H	2.319464000	-1.612212000	2.465086000
H	-2.045393000	-2.818902000	-1.344464000
H	-2.117107000	-0.276305000	-2.164112000
H	2.981395000	-0.756984000	0.000000000
H	1.894661000	-1.894344000	2.165340000
H	0.084834000	-3.677922000	1.343157000
H	0.084834000	-3.677922000	-1.343157000
H	1.894661000	-1.894344000	-2.165340000

2_3 [$Ti(C_5H_5)_2SeS_2SeS$] (C_1)

Ti	-1.207850000	0.224946000	-0.068473000
S	0.386900000	1.488615000	1.205140000
Se	2.326904000	1.465151000	0.190104000
S	2.961960000	-0.614188000	0.514666000
S	1.940369000	-1.786689000	-0.800337000
Se	-0.035150000	-2.030878000	0.144727000
C	-1.969550000	1.685108000	-1.743800000
C	-2.288363000	0.367910000	-2.161490000
C	-1.085159000	-0.320148000	-2.381929000
C	-0.022089000	0.565726000	-2.103966000
C	-0.569603000	1.804115000	-1.724770000
C	-3.320091000	0.867109000	0.765604000
C	-3.379765000	-0.512695000	0.479048000
C	-2.501980000	-1.176018000	1.359341000
C	-1.890335000	-0.208313000	2.180323000
C	-2.399161000	1.055404000	1.814385000
H	-2.671791000	2.468660000	-1.511041000
H	-3.280637000	-0.031454000	-2.293338000
H	-0.985674000	-1.347903000	-2.688529000
H	1.025886000	0.328769000	-2.160793000
H	-0.012103000	2.680126000	-1.439488000
H	-3.890166000	1.640760000	0.279246000
H	-3.999748000	-0.986324000	-0.264211000
H	-2.347036000	-2.242780000	1.413986000
H	-1.133598000	-0.397486000	2.923782000
H	-2.123159000	2.000571000	2.254578000

2_4 [$Ti(C_5H_5)_2SeS_3Se$] (C_s)

Ti	0.175330000	-1.092623000	0.000000000
Se	-0.648195000	0.404514000	1.878018000
S	0.439793000	2.310592000	1.653608000
S	-0.405461000	3.158873000	0.000000000
S	0.439793000	2.310592000	-1.653608000
Se	-0.648195000	0.404514000	-1.878018000
C	2.178095000	-2.093671000	0.709386000
C	2.178095000	-2.093671000	-0.709386000
C	2.233203000	-0.758222000	-1.141792000
C	2.253562000	0.066755000	0.000000000
C	2.233203000	-0.758222000	1.141792000
C	-0.586324000	-3.204116000	0.705436000
C	-0.586324000	-3.204116000	-0.705436000
C	-1.548498000	-2.270793000	-1.140050000
C	-2.140275000	-1.689642000	0.000000000
C	-1.548498000	-2.270793000	1.140050000
H	2.166818000	-2.963957000	1.344564000
H	2.166818000	-2.963957000	-1.344564000
H	2.237215000	-0.420535000	-2.164418000
H	2.271092000	1.142055000	0.000000000
H	2.237215000	-0.420535000	2.164418000
H	0.020244000	-3.825384000	1.342770000
H	0.020244000	-3.825384000	-1.342770000
H	-1.800376000	-2.052775000	-2.166658000
H	-2.882360000	-0.907953000	0.000000000
H	-1.800376000	-2.052775000	2.166658000

2_5 [$Ti(C_5H_5)_2SSe_2S_2$] (C_1)

Ti	1.449246000	0.002671000	-0.033344000
S	0.195283000	-2.052009000	0.176010000
S	-1.558607000	-1.906477000	-0.866123000
Se	-2.816575000	-0.618355000	0.383179000
Se	-1.983913000	1.528659000	0.019643000
S	-0.098334000	1.434457000	1.125442000
C	2.617667000	-0.031393000	-2.084795000
C	2.426511000	1.325936000	-1.722177000
C	1.047788000	1.592055000	-1.757298000
C	0.385267000	0.406010000	-2.123759000
C	1.356050000	-0.594965000	-2.332824000
C	3.539585000	0.566738000	0.918987000
C	2.568901000	0.789211000	1.914108000
C	1.990329000	-0.454268000	2.245651000
C	2.611516000	-1.443861000	1.459285000
C	3.563031000	-0.814893000	0.633636000
H	3.565284000	-0.537466000	-2.168853000
H	3.200074000	2.038095000	-1.486616000
H	0.576271000	2.530294000	-1.518108000
H	-0.678946000	0.280292000	-2.215884000
H	1.158233000	-1.617357000	-2.608602000
H	4.165933000	1.318922000	0.469719000
H	2.307563000	1.743723000	2.342886000
H	1.182706000	-0.613129000	2.941104000
H	2.394910000	-2.500191000	1.484293000
H	4.207801000	-1.311248000	-0.072475000

2_6 [$Ti(C_5H_5)_2SSeSSeS$] (C_s)

Ti	1.510212971	0.064838241	0.000000000
S	0.167675479	-0.782967145	1.816542000
Se	-1.815806240	0.134627010	1.767851000
S	-2.688984101	-0.824621806	0.000000000
Se	-1.815806240	0.134627010	-1.767851000
S	0.167675479	-0.782967145	-1.816542000
C	2.444249310	2.112799662	0.709005000
C	2.444249310	2.112799662	-0.709005000
C	1.108327884	2.113813455	-1.141299000
C	0.282977160	2.106841970	0.000000000
C	1.108327884	2.113813455	1.141299000
C	3.672762028	-0.589664541	-0.705589000
C	2.786183885	-1.593412025	-1.139466000
C	2.231147437	-2.210171843	0.000000000
C	2.786183885	-1.593412025	1.139466000
C	3.672762028	-0.589664541	0.705589000
H	3.313933920	2.132355345	1.344638000
H	3.313933920	2.132355345	-1.344638000
H	0.771471384	2.095748278	-2.164182000
H	-0.792486543	2.089708290	0.000000000
H	0.771471384	2.095748278	2.164182000
H	4.263485057	0.046495134	-1.343119000
H	2.566153639	-1.843647209	-2.165191000
H	1.477251067	-2.980170414	0.000000000
H	2.566153639	-1.843647209	2.165191000
H	4.263485057	0.046495134	1.343119000

3_1 [$Ti(C_5H_5)_2Se_3S_2$] (C_1)

Ti	1.511787000	-0.131707000	-0.089687000
S	0.269646000	-1.986028000	0.814668000
S	-1.478274000	-2.255872000	-0.216599000
Se	-2.809401000	-0.683424000	0.528945000
Se	-2.116264000	1.257083000	-0.559123000
Se	-0.131909000	1.690618000	0.583747000
C	2.619130000	-0.878146000	-2.028270000
C	2.470865000	0.528218000	-2.136219000
C	1.098357000	0.812050000	-2.232241000
C	0.397880000	-0.408676000	-2.170783000
C	1.337623000	-1.451560000	-2.055912000
C	3.681050000	-0.575057000	0.724058000
C	3.543633000	0.826494000	0.635548000
C	2.561223000	1.225536000	1.562575000
C	2.084647000	0.071602000	2.219299000
C	2.782782000	-1.039007000	1.704451000
H	3.550548000	-1.415628000	-1.962501000
H	3.269391000	1.251221000	-2.164400000
H	0.655632000	1.790140000	-2.316239000
H	-0.671372000	-0.523275000	-2.195648000
H	1.108084000	-2.500918000	-1.975517000
H	4.369107000	-1.184529000	0.162772000
H	4.105101000	1.482993000	-0.007976000
H	2.243174000	2.239635000	1.749733000
H	1.295138000	0.040204000	2.952268000
H	2.648330000	-2.066068000	2.005126000

3_2 [$Ti(C_5H_5)_2Se_2SSeS$] (C_1)

Ti	1.416244000	-0.141268000	-0.104433000
S	0.096866000	-1.809503000	1.019887000
Se	-1.878690000	-1.985479000	0.093976000
S	-2.862605000	-0.148967000	0.772157000
Se	-2.128479000	1.503951000	-0.466812000
Se	-0.037857000	1.867745000	0.492859000
C	2.317390000	-1.177410000	-2.014274000
C	2.350027000	0.222911000	-2.237406000
C	1.024650000	0.682192000	-2.301270000
C	0.172910000	-0.425689000	-2.112977000
C	0.971318000	-1.572828000	-1.948579000
C	3.621400000	-0.632109000	0.585365000
C	3.522448000	0.769169000	0.454251000
C	2.617701000	1.232573000	1.429412000
C	2.147400000	0.119797000	2.155269000
C	2.773057000	-1.032144000	1.635793000
H	3.170817000	-1.830573000	-1.938125000
H	3.235458000	0.825726000	-2.354938000
H	0.710561000	1.702065000	-2.446627000
H	-0.902360000	-0.396046000	-2.090874000
H	0.611855000	-2.572804000	-1.773457000
H	4.251833000	-1.281691000	0.001898000
H	4.059632000	1.385264000	-0.247613000
H	2.349821000	2.263108000	1.604818000
H	1.406032000	0.141762000	2.937132000
H	2.621860000	-2.043560000	1.978316000

3_3 [$Ti(C_5H_5)_2Se_2S_2Se$] (C_1)

Ti	1.284293000	0.119236000	-0.182960000
Se	0.187631000	-2.065024000	0.527568000
S	-1.773488000	-2.164088000	-0.477761000
S	-2.920038000	-0.817269000	0.528846000
Se	-2.468335000	1.187194000	-0.252323000
Se	-0.462866000	1.644889000	0.844621000
C	2.349886000	-0.158572000	-2.262558000
C	1.989031000	1.207517000	-2.138401000
C	0.585570000	1.284203000	-2.132686000
C	0.078638000	-0.024615000	-2.228213000
C	1.168914000	-0.915393000	-2.319052000
C	3.333462000	1.050393000	0.511027000
C	2.396156000	1.364978000	1.514504000
C	1.971654000	0.157865000	2.109321000
C	2.652832000	-0.900253000	1.476179000
C	3.489516000	-0.351534000	0.483802000
H	3.354024000	-0.545509000	-2.318886000
H	2.666475000	2.044148000	-2.089527000
H	-0.000397000	2.183457000	-2.047526000
H	-0.961328000	-0.300386000	-2.224099000
H	1.102362000	-1.987741000	-2.395563000
H	3.853437000	1.759523000	-0.110915000
H	2.068307000	2.356352000	1.786520000
H	1.228240000	0.057860000	2.883255000
H	2.568359000	-1.947210000	1.724476000
H	4.149907000	-0.909481000	-0.158969000

3_4 [$Ti(C_5H_5)_2SeSSe_2S$] (C_1)

Ti	-1.471559000	0.189011000	-0.047827000
S	0.092105000	1.536839000	1.178217000
Se	1.983107000	1.700906000	0.084563000
Se	2.874239000	-0.432863000	0.368107000
S	1.714213000	-1.707884000	-0.979052000
Se	-0.178683000	-2.002383000	0.104936000
C	-2.387285000	1.597547000	-1.691984000
C	-2.621074000	0.261675000	-2.106859000
C	-1.377389000	-0.335462000	-2.365751000
C	-0.374351000	0.623684000	-2.110618000
C	-0.999978000	1.818008000	-1.709803000
C	-3.578830000	0.715808000	0.874547000
C	-3.581206000	-0.662136000	0.573009000
C	-2.637683000	-1.290085000	1.410033000
C	-2.043122000	-0.301703000	2.219455000
C	-2.628724000	0.938578000	1.890002000
H	-3.138065000	2.327283000	-1.436981000
H	-3.584843000	-0.208581000	-2.214002000
H	-1.211987000	-1.351555000	-2.682442000
H	0.686065000	0.462787000	-2.195954000
H	-0.499561000	2.731104000	-1.434979000
H	-4.205903000	1.465191000	0.421595000
H	-4.206348000	-1.158026000	-0.151084000
H	-2.428500000	-2.348441000	1.445036000
H	-1.250235000	-0.460677000	2.931707000
H	-2.384079000	1.891477000	2.331882000

3_5 [$Ti(C_5H_5)_2SeSSeSSe$] (C_s)

Ti	1.478382883	0.192090026	0.000000000
Se	-0.041608517	-0.572353510	1.883278000
S	-1.883876767	0.628199535	1.739582000
Se	-2.913937032	-0.210551925	0.000000000
S	-1.883876767	0.628199535	-1.739582000
Se	-0.041608517	-0.572353510	-1.883278000
C	2.555210137	2.155424780	0.709365000
C	2.555210137	2.155424780	-0.709365000
C	1.222646176	2.258855274	-1.141718000
C	0.398683508	2.307835483	0.000000000
C	1.222646176	2.258855274	1.141718000
C	3.558119362	-0.652164576	-0.705446000
C	2.587728553	-1.576751615	-1.140155000
C	1.983217550	-2.144993585	0.000000000
C	2.587728553	-1.576751615	1.140155000
C	3.558119362	-0.652164576	0.705446000
H	3.424555483	2.112271119	1.344545000
H	3.424555483	2.112271119	-1.344545000
H	0.885032817	2.275514744	-2.164257000
H	-0.675562677	2.361656397	0.000000000
H	0.885032817	2.275514744	2.164257000
H	4.202783427	-0.070495629	-1.342785000
H	2.360554679	-1.820047634	-2.166840000
H	1.174334138	-2.857419236	0.000000000
H	2.360554679	-1.820047634	2.166840000
H	4.202783427	-0.070495629	1.342785000

3_6 [$Ti(C_5H_5)_2SSe_3S$] (C_s)

Ti	1.794690391	-0.023290425	0.000000000
S	0.406952514	0.738432991	1.819605000
Se	-1.496652390	-0.337978171	1.842284000
Se	-2.568449789	0.600376957	0.000000000
Se	-1.496652390	-0.337978171	-1.842284000
S	0.406952514	0.738432991	-1.819605000
C	2.854375011	-2.010150212	-0.708976000
C	1.520960875	-2.091234339	-1.141184000
C	0.696335577	-2.132129541	0.000000000
C	1.520960875	-2.091234339	1.141184000
C	2.854375011	-2.010150212	0.708976000
C	3.910627218	0.767268037	0.705596000
C	3.910627218	0.767268037	-0.705596000
C	2.962490743	1.713023788	-1.139534000
C	2.369048543	2.293132200	0.000000000
C	2.962490743	1.713023788	1.139534000
H	3.723666729	-1.977034171	-1.344659000
H	1.183695127	-2.093614415	-2.164083000
H	-0.378576763	-2.175741264	0.000000000
H	1.183695127	-2.093614415	2.164083000
H	3.723666729	-1.977034171	1.344659000
H	4.539973775	0.169354823	1.343220000
H	4.539973775	0.169354823	-1.343220000
H	2.727787801	1.949273110	-2.165265000
H	1.569032835	3.015145532	0.000000000
H	2.727787801	1.949273110	2.165265000

4_1 [$Ti(C_5H_5)_2Se_4S$] (C_1)

Ti	1.639174000	-0.151519000	-0.075791000
S	0.251592000	-1.829592000	0.944105000
Se	-1.660137000	-2.027027000	-0.104908000
Se	-2.790029000	-0.115980000	0.593693000
Se	-1.837673000	1.627882000	-0.619256000
Se	0.191955000	1.868014000	0.499418000
C	2.622032000	-1.143304000	-1.969775000
C	2.673256000	0.262053000	-2.154047000
C	1.354926000	0.732351000	-2.264514000
C	0.488510000	-0.373408000	-2.141716000
C	1.272019000	-1.530278000	-1.973743000
C	3.802955000	-0.685575000	0.704933000
C	3.724378000	0.719696000	0.606988000
C	2.779015000	1.167334000	1.550394000
C	2.263233000	0.040950000	2.222729000
C	2.901798000	-1.103825000	1.702791000
H	3.467268000	-1.804558000	-1.873996000
H	3.566742000	0.861344000	-2.215725000
H	1.053862000	1.757794000	-2.397449000
H	-0.586673000	-0.336212000	-2.162782000
H	0.898377000	-2.531639000	-1.841270000
H	4.453995000	-1.326753000	0.135012000
H	4.300100000	1.348150000	-0.052010000
H	2.514883000	2.196122000	1.741142000
H	1.486861000	0.050600000	2.970113000
H	2.724653000	-2.122162000	2.010261000

4_2 [$Ti(C_5H_5)_2Se_3SSe$] (C_1)

Ti	1.527140000	0.065610000	-0.159162000
Se	0.253967000	-2.049826000	0.449408000
S	-1.638166000	-2.042355000	-0.678867000
Se	-2.874790000	-0.579719000	0.376363000
Se	-2.121190000	1.502746000	-0.345116000
Se	-0.130817000	1.697157000	0.855626000
C	2.621711000	-0.269736000	-2.213954000
C	2.399774000	1.123337000	-2.064446000
C	1.012366000	1.344764000	-2.091821000
C	0.376187000	0.097382000	-2.234751000
C	1.370974000	-0.898244000	-2.323360000
C	3.600763000	0.840606000	0.645556000
C	2.647931000	1.165729000	1.630914000
C	2.131351000	-0.038744000	2.153462000
C	2.772906000	-1.107018000	1.495145000
C	3.676390000	-0.565601000	0.559088000
H	3.581589000	-0.757585000	-2.256019000
H	3.158541000	1.883491000	-1.977182000
H	0.519397000	2.297307000	-1.996498000
H	-0.686288000	-0.070130000	-2.261156000
H	1.196791000	-1.955505000	-2.432518000
H	4.184334000	1.544839000	0.076743000
H	2.371075000	2.161982000	1.939248000
H	1.355975000	-0.127670000	2.896865000
H	2.618244000	-2.157213000	1.690303000
H	4.327989000	-1.132285000	-0.084897000

4_3 [$Ti(C_5H_5)_2Se_2SSe_2$] (C_s)

Ti	-0.194925000	1.452920000	0.000000000
Se	0.731167000	0.036452000	1.899231000
Se	-0.278921000	-2.060983000	1.775631000
S	0.689809000	-2.902940000	0.000000000
Se	-0.278921000	-2.060983000	-1.775631000
Se	0.731167000	0.036452000	-1.899231000
C	-2.259121000	2.322965000	0.709341000
C	-2.259121000	2.322965000	-0.709341000
C	-2.225510000	0.987000000	-1.141758000
C	-2.191020000	0.162577000	0.000000000
C	-2.225510000	0.987000000	1.141758000
C	0.418592000	3.615906000	-0.705522000
C	1.443754000	2.752825000	-1.139927000
C	2.073893000	2.213031000	0.000000000
C	1.443754000	2.752825000	1.139927000
C	0.418592000	3.615906000	0.705522000
H	-2.305264000	3.191839000	1.344821000
H	-2.305264000	3.191839000	-1.344821000
H	-2.206535000	0.649923000	-2.164367000
H	-2.139492000	-0.912121000	0.000000000
H	-2.206535000	0.649923000	2.164367000
H	-0.228797000	4.194166000	-1.343123000
H	1.710232000	2.553907000	-2.166479000
H	2.869042000	1.485339000	0.000000000
H	1.710232000	2.553907000	2.166479000
H	-0.228797000	4.194166000	1.343123000

5_1 [$Ti(C_5H_5)_2Se_5$] (C_1)

Ti	-0.163486000	1.667386000	0.000000000
Se	0.703187000	0.221200000	1.903207000
Se	-0.432482000	-1.814837000	1.853517000
Se	0.538003000	-2.833458000	0.000000000
Se	-0.432482000	-1.814837000	-1.853517000
Se	0.703187000	0.221200000	-1.903207000
C	-2.191627000	2.620152000	0.709267000
C	-2.191627000	2.620152000	-0.709267000
C	-2.209029000	1.284032000	-1.141625000
C	-2.204276000	0.458691000	0.000000000
C	-2.209029000	1.284032000	1.141625000
C	0.539636000	3.802308000	-0.705432000
C	1.528312000	2.898039000	-1.139820000
C	2.135479000	2.332431000	0.000000000
C	1.528312000	2.898039000	1.139820000
C	0.539636000	3.802308000	0.705432000
H	-2.204384000	3.490532000	1.344188000
H	-2.204384000	3.490532000	-1.344188000
H	-2.203452000	0.946332000	-2.164119000
H	-2.190324000	-0.617267000	0.000000000
H	-2.203452000	0.946332000	2.164119000
H	-0.083660000	4.406060000	-1.343152000
H	1.786834000	2.689125000	-2.166214000
H	2.901623000	1.574419000	0.000000000
H	1.786834000	2.689125000	2.166214000
H	-0.083660000	4.406060000	1.343152000