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The Facile Coupling of Carbon Monochalcogenides to Ethenedichalcogenone Ligands in Binuclear Iron Carbonyl Derivatives: A Theoretical Study

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Supporting Information

Figure S1: All of the optimized $Fe_2(CO)_8(CE)_2$ structures.

Figure S2: Proposed $Fe_2(CO)_8(CE)_2$ formation mechanisms.

Figure S3: All of the optimized $Fe_2(CO)_7(CE)_2$ structures.

Figure S4: The predicted intermediates and transition states for coupling $Fe(CO)_4(CE)$ and $Fe(CO)_3(CE)$.

Figure S5: Several important orbitals for **8S-I**, **7S-I**, and **6S-I**.

Figure S6: Several important orbitals for **7S-II**.

Figure S7: Several important orbitals for **7S-VI** and **6S-VI**.

Figure S8: The predicted spin density for **6S-XT**.

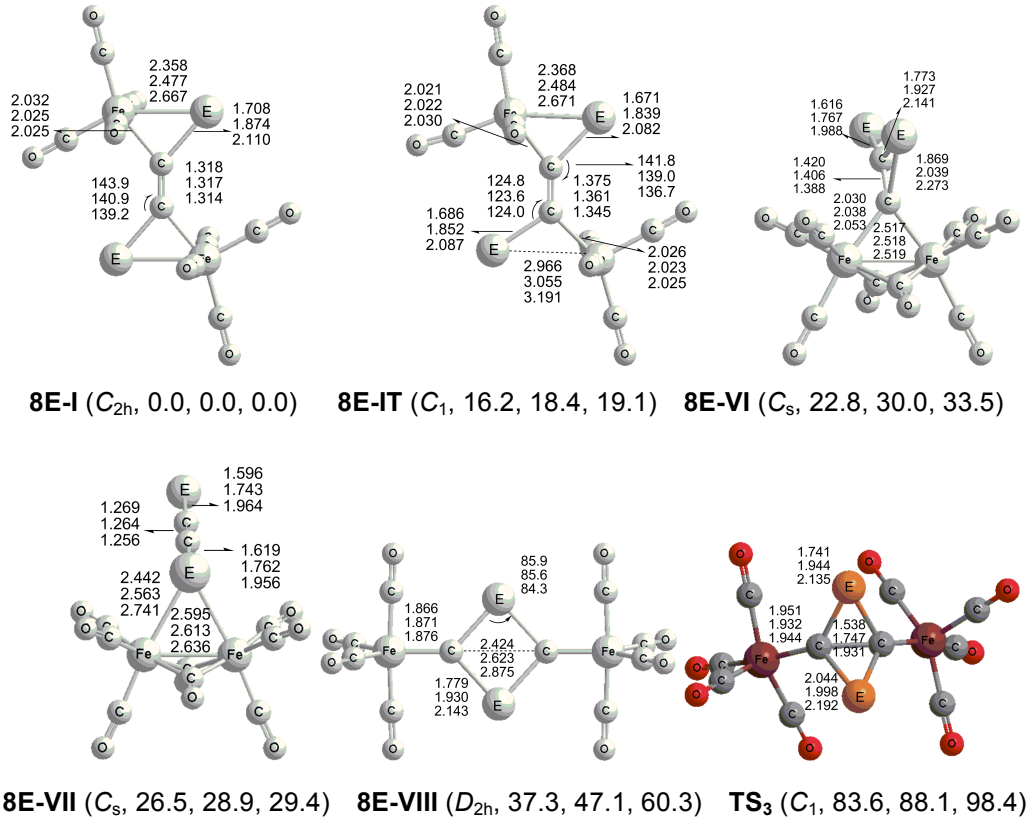
Table S1: $Fe_2(CO)_n(EC_2E)$ (n = 8, 7, 6; E = S, Se, Te) reaction energies.

Tables S2 to S16: Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CO)_n(EC_2E)$ (n = 8, 7, 6; E = S, Se, Te) structures.

Table S17 to S37: the theoretical harmonic vibrational frequencies for $Fe_2(CO)_8(EC_2E)$ (4*3 isomers), $Fe_2(CO)_7(EC_2E)$ (4*3 isomers), $Fe_2(CO)_6(EC_2E)$ (8*3 isomers).

Table S38 to S82: the theoretical Cartesian coordinates for $Fe_2(CO)_8(EC_2E)$ (18 isomers), $Fe_2(CO)_7(EC_2E)$ (21 isomers), $Fe_2(CO)_6(EC_2E)$ (24 isomers).

Complete Gaussian 09 reference (Reference 49)



8E-I (C_{2h}, 0.0, 0.0, 0.0) **8E-IT** (C_1, 16.2, 18.4, 19.1) **8E-VI** (C_s, 22.8, 30.0, 33.5)

8E-VII (C_s, 26.5, 28.9, 29.4) **8E-VIII** (D_{2h}, 37.3, 47.1, 60.3) **TS$_3$** (C_1, 83.6, 88.1, 98.4)

Figure S1. Optimized $Fe_2(CO)_8(CE)_2$ structures using the B3LYP method. Symmetry point groups and relative energies (in kcal/mol) are given in parentheses. The first, second, and third relative energies listed are for E = S, Se, and Te, respectively.

Five $Fe_2(CO)_8(CE)_2$ structures with coupled EC_2E ligands were found for each chalcogen (Figure 2). The lowest energy structures **8E-I** are found to have an EC_2E ligand bridging two $Fe(CO)_4$ fragments through a dihapto η^2-(EC)CE-Fe bond to each iron atom.

The analogous triplet $Fe_2(CO)_8(CE)_2$ structures **8E-IT** are found to lie at least 16 kcal/mol above the corresponding global minima **8E-I** (Figure 2). The upper η^2-EC(CE)-Fe interactions (Figure 2) are quite similar to those in the **8E-I** structures. However, the lower η^2-EC(CE)-Fe interactions are weakened owing to the longer Fe-E distances (2.966 Å for Fe-S, 3.055 Å for Fe-Se, and 3.191 Å for Fe-Te). The central C=C bond lengths in the triplet **8E-1T** structures average ~0.04 Å longer than those in the corresponding singlet structures **8E-I**.

The remaining $Fe_2(CO)_8(CE)_2$ structures **8E-VI** and **8E-VII** are similar to the well-known $Fe_2(CO)_6(\mu\text{-}CO)_3$[1] structure but with one of the bridging CO groups replaced by a two-electron donor μ-C(CE)E or a μ-E(CCE) ligand bonded to the central Fe_2 unit through a carbon or chalcogen atom, respectively (Figure 2). This gives each iron atom in these structures the favored 18-electron configuration similar to each iron atom in $Fe_2(CO)_6(\mu\text{-}CO)_3$. Structures **8E-VI** and **8E-VII** structures are

relatively high energy structures, lying at least 22 kcal/mol above the corresponding global minima **8E-I**.

The other structure **8E-VIII** (Figure S1) was found to have a head to tail four member ring C_2E_2 motif. This structure should be originated from dimerization of $Fe(CO)_4(CE)$ by using one the positively charged E atom attaching to the other negatively charged C atom. The analogue $[(PCy_3)_4(Pt^{II})_2(B_2O_2)]^{2+}$ complex[2] has been prepared and characterized by X-ray diffraction since the BO^- is more polarized. The polarized Fe-C-E bond will lead to the negatively charged carbon atom as well as the positively charged chalcongen atom. The C-Te bond should be the most polarized bond among the CE (E= S, Se, Te) series because of the Te atom with the largest atomic radius in corporate with smallest electrophilicity. Therefore, **8Te-VIII** is the most stable structure for its smallest dissociation energy of 5.0 kcal/mol with respect to dissociation into two $Fe(CO)_4(CE)$ monomers (Figure S2).

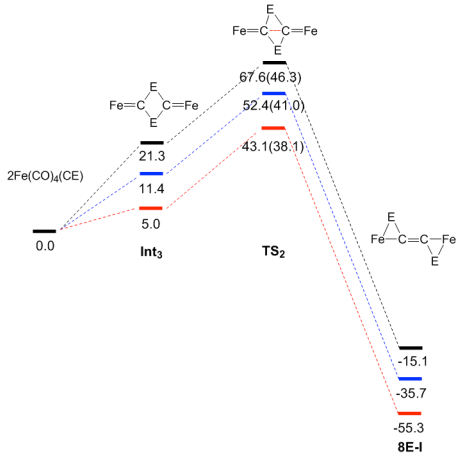
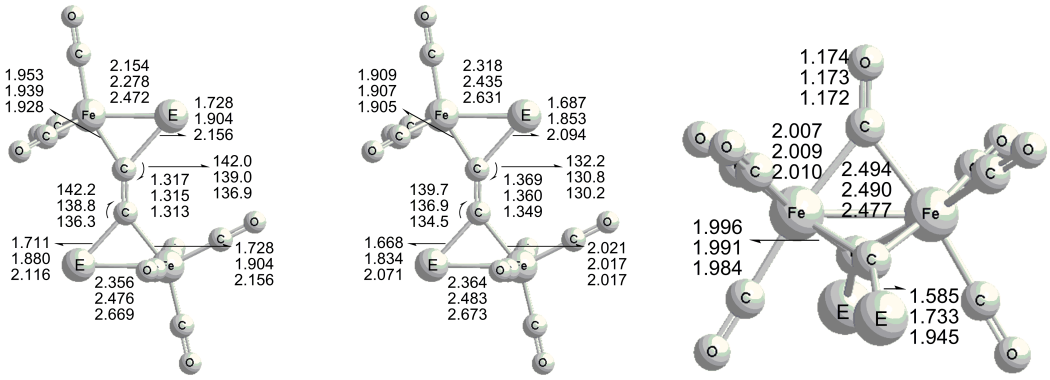
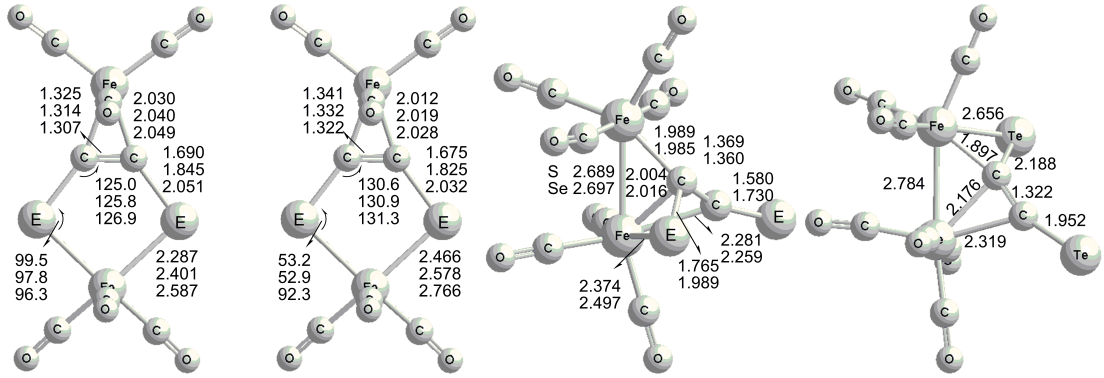


Figure S2. Proposed $Fe_2(CO)_8(CE)_2$ formation mechanisms. The relative energies as well as the activation energies (in parentheses) are given in kcal/mol.

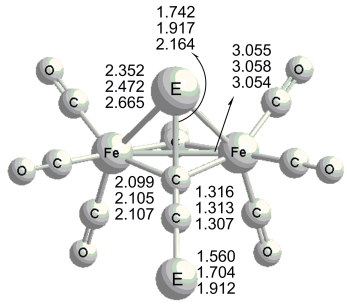
Two free monomers $Fe(CO)_4(CE)$ as starting materials dimerized into the predicted ring structure **Int$_3$** (identical to **8E-VIII** in Figure S1). Such dimerization processes are endothermic by 21.3 (S), 11.4 (Se), and 5.0 kcal/mo (Te), respectively. This is reasonable since the polarity of chalcogen atoms follows the rule of S < Se < Te. The **Int3** structures further convert to the transition states **TS$_2$** (in Figure S1) by drawing together two carbon atoms of the CE ligands. Thus, the activation energies are predicted to be 46.3 (S), 41.0 (Se), and 38.1 (Te) kcal/mol, respectively, indicating the coupling possibilities gradually increased from S to Te. However, these predicted activation energies are always more than 38.0 kcal/mol, thus the coupling processes are unlikely in the ambient conditions. The **TS2** will lead to the lowest energy structure **8E-I**, meanwhile releasing 82.7 (S), 88.2 (Se), and 98.4 kcal/mol (Te), respectively.



7E-I(C_s, 0.0, 0.0, 0.0) **7E-IT**(C_1, 0.5, 2.8, 3.8) **7E-IV**(C_{2v}, 10.9, 28.0, 42.4)

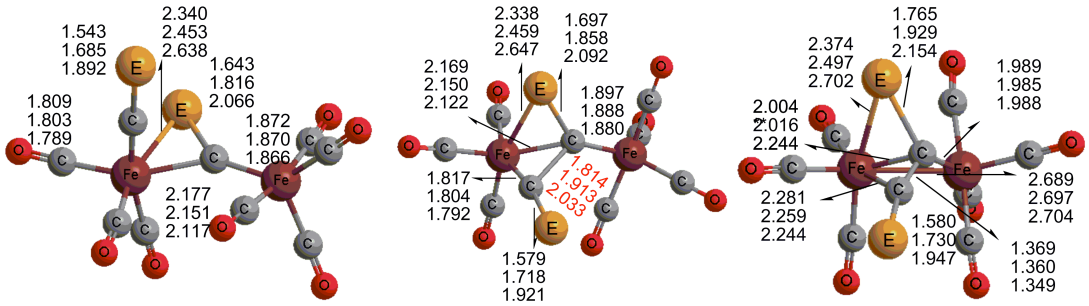


7E-II(C_s, 4.1, 3.3, 1.3)**7E-IIT**(C_s, 12.4, 13.5, 12.2) **7E-VII**(C_1, 2.9, 8.4, 14.3)



7E-VI(C_s, 8.3, 13.7, 16.0)

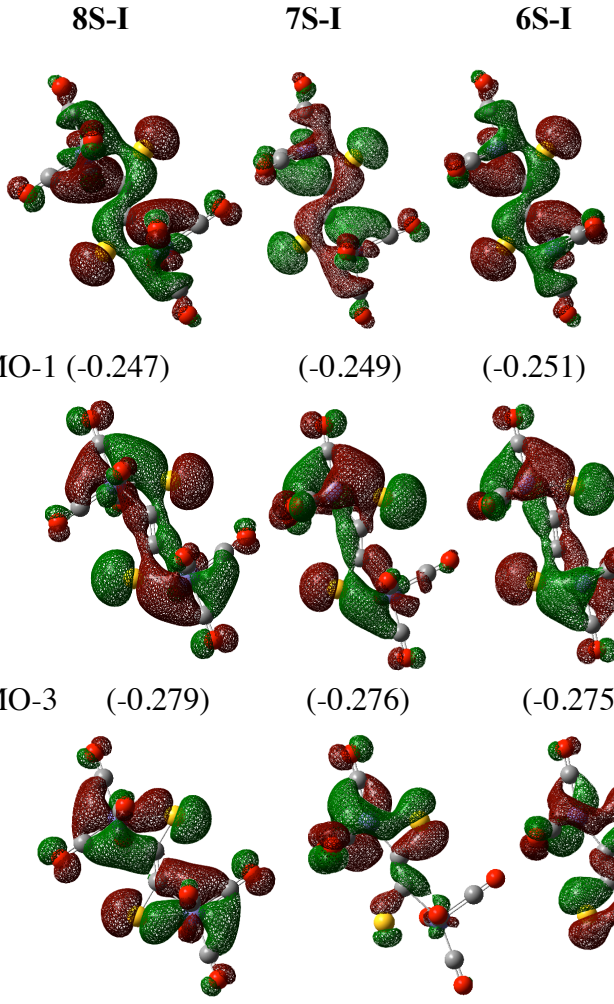
Figure S3: All of the optimized $Fe_2(CO)_7(CE)_2$ structures.



Int_1	TS	Int_2
-4193.6121	-4193.5924	-4193.6362
-8200.2834	-8200.2714	-8200.3242
-3413.2842	-3413.2789	-3413.3460

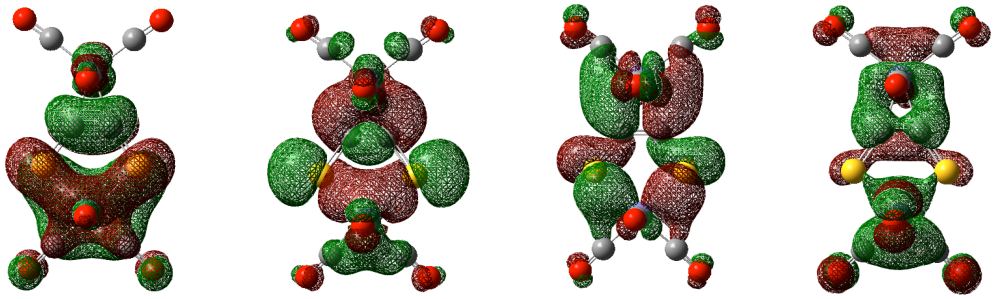
Figure S4. The predicted intermediates and transition states for coupling $Fe(CO)_4(CE)$ and $Fe(CO)_3(CE)$. The calculated energies are given in three lines, the first one for S, the second line for Se, and the last line for Te complexes, respectively.

Figure S5: Several important orbitals for **8S-I**, **7S-I**, and **6S-I**.



The two identical Fe-S distances in **8SI-1** are found to be 2.358 Å, which is elongated ~0.2 Å for the η^2-(EC)CE-Fe(CO)$_3$ in **7SI-1** and in **6SI-1**. For **7SI-1**, the Wiberg bond index of the upper contracted Fe-S is found to be 1.19, which is nearly twice the value in **8S-1** (0.70). This indicates a Fe=S double bond originating from C_2E_2 donating two occupied π^* electrons between EC(CE) to the vacant d orbital (HOMO-4 in Fig S5) as well as accepting a pair of occupied d electrons of the Fe(CO)$_3$ fragment though the vacant π^* orbital of EC(CE). Furthermore, the numbers of $d_{Fe}\rightarrow LP_{S(C2S)}$ (HOMO-6 in Fig S5) in **8SI-1**, **7SI-1**, and **6SI-1**, are none, one, and two, respectively. The natural charges of C_2E_2 in **8SI-1**, **7SI-1**, and **6SI-1**, are therefore increased to -0.108, 0.014, and 0.140, respectively.

Figure S6: Several important orbitals for **7S-II**.



HOMO HOMO-1 HOMO-3 HOMO-5

The HOMO orbital of **7S-II** is a three center S-Fe-S π bond originating from each sulfur atom donating electrons from a perpendicular lone pair to the $Fe(CO)_3$ fragment. The HOMO-1 orbital is a three centered S-Fe-S σ bond consisting of each sulfur atom donating a planar lone-pair electrons to the $Fe(CO)_3$ fragment. The HOMO-3 orbital has two different parts, one for the upper $Fe(CO)_4$ fragment donating two electrons to the C=C π-anti bond, and the other for the occupied orbital donating two electrons to the low $Fe(CO)_3$ fragment. The formal Fe-S bond order in **7S-II** therefore is 1.5, indicating by the Wiberg bond index of 1.006, which is larger than the singly bonded Fe-S (0.696) in **8S-I** but smaller than the doubly bonded Fe=S (1.192) in **7S-I**. The HOMO-5 orbital obviously presents $\pi(C_2E_2)\rightarrow$d(Fe) donating to the upper iron.

Figure S7: Several important orbitals for **7S-VI** and **6S-VI**.

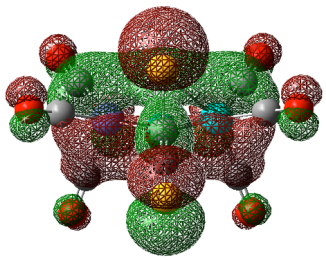
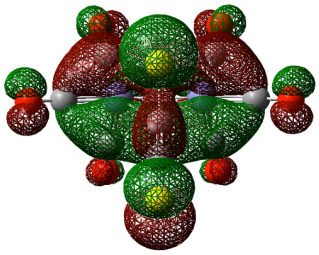
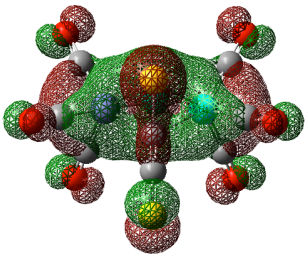
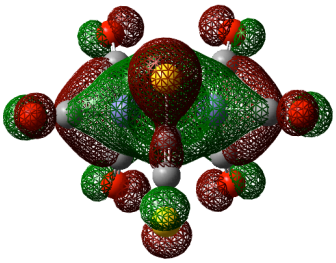
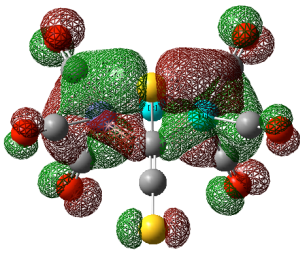
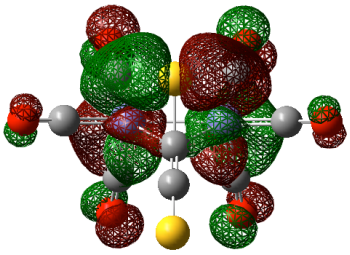
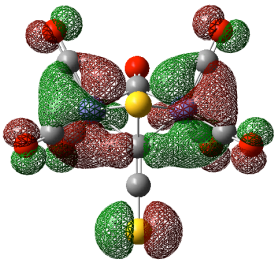
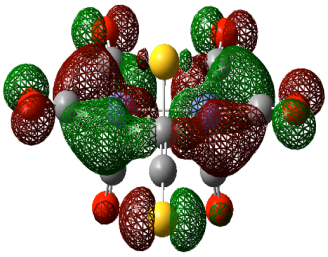
7S-VI	**6S-VI**	
		
HOMO-2 (-0.272)	HOMO-2(-0.269)	$d_{Fe} \rightarrow \pi^*_{SC(CS)}$
		
HOMO-4 (-0.284)	HOMO-5 (-0.282)	$\pi_{SC(CS)} \rightarrow d_{Fe}$
		
HOMO-7 (-0.297)	HOMO-7 (-0.291)	$LP_S \rightarrow d_{Fe}$
		
HOMO-5(-0.288)	HOMO-3(-0.280)	$LP_C \rightarrow d_{Fe}$

Figure S8: The predicted spin density for **6S-XT**.

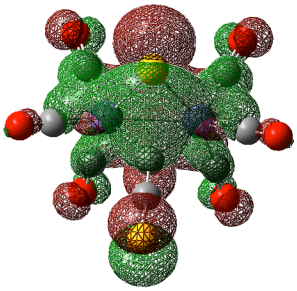


Table S1. Some dissociation energies are calculated for $Fe_2(CO)_n(CE)_2$. The first, second, and third values refer to the sulfur, selenium, and tellurium complexes, respectively.

Reactions	Energies (kcal/mol)
$Fe_2(CO)_8(CE)_2$à $Fe_2(CO)_7(CE)_2$+CO	14.3, 13.9, 14.5
$Fe_2(CO)_7(CE)_2$à $Fe_2(CO)_6(CE)_2$+CO	-6.6, -0.8, 2.7
$Fe_2(CO)_8(CE)_2$à $2Fe(CO)_4(CE)$	15.1, 35.7, 55.3
$Fe_2(CO)_7(CE)_2$à $Fe(CO)_4(CE)$+ $Fe(CO)_3(CE)$	33.2, 54.1, 69.9
$Fe_2(CO)_6(CE)_2$à $2Fe(CO)_3(CE)$	71.2, 87.1, 96.2
$Fe_2(CO)_8(CE)_2$à $Fe(CO)_4(C_2E_2)$+ $Fe(CO)_4$	35.8, 39.4, 39.8
$Fe_2(CO)_7(CE)_2$à $Fe(CO)_4(C_2E_2)$+ $Fe(CO)_3$	56.3, 60.6, 60.5
$Fe_2(CO)_6(CE)_2$à $Fe(CO)_3(C_2E_2)$+ $Fe(CO)_3$	72.3, 71.9, 69.3
2CEàEC_2E(T)	-61.4, -78.4, -112.7

In order to evaluate the stability of these coupled $Fe_2(CO)_n(EC_2E)$ (n = 8, 7, 6; E = S, Se, Te) structures, several possible dissociation reactions (Table S1) are calculated as following lists:

$$Fe_2(CO)_n(EC_2E) \rightarrow Fe_2(CO)_{n-1}(EC_2E) + CO \quad (1)$$

$$Fe_2(CO)_n(EC_2E) \rightarrow Fe(CO)_x(EC_2E) + Fe(CO)_y \quad (n = x + y) \quad (2)$$

$$Fe_2(CO)_n(EC_2E) \rightarrow Fe(CO)_x(CE) + Fe(CO)_y(CE) \quad (n = x + y) \quad (3)$$

Table S2. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CS)_2(CO)_8$ structures.

	8S-I	**8S-IT**	**8S-VI**	**8S-VII**	**8S-VIII**	**8S-TS3**
E	-4307.0064	-4306.9805	-4306.9701	-4306.9642	-4306.9469	-4306.8732
ΔE	0.0	16.2	22.8	26.5	37.3	83.6
N_{img}	0	0	0	0	0	1(229i)
$<S>^2$		2.04				

Table S3. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CSe)_2(CO)_8$ structures.

	8Se-I	**8Se-IT**	**8Se-VI**	**8Se-VII**	**8Se-VIII**	**8Se-TS3**
E	-8313.7025	-8313.6732	-8313.6565	-8313.6548	-8313.6275	-8313.5621
ΔE	0.0	18.4	30.0	28.9	47.1	88.1
N_{img}	0	0	0	0	0	1(287i)
$<S>^2$	0	2.04				

Table S4. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CTe)_2(CO)_8$ structures.

	8Te-I	**8Te-IT**	**8Te-VI**	**8Te-VII**	**8Te-VIII**	**8Te-TS3**
E	-3526.7291	-3526.6987	-3526.6758	-3526.6824	-3526.6331	-3526.5728
ΔE	0.0	19.1	33.5	29.4	60.3	98.4
N_{img}	0	0	0	0	0	1(385i)
$<S>^2$		2.04				

Table S5. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CS)_2(CO)_7$ structures.

	7S-I	**7S-II**	**7S-VI**	**7S-IV**	**7S-VII**	**7S-IT**	**7S-IIT**
E	-4193.6408	-4193.6343	-4193.6276	-4193.6235	-4193.6362	-4193.6400	-4193.6211
ΔE	0	4.1	8.3	10.9	2.9	0.5	12.4
N_{img}	0	0	0	0	0	0	0
$<S>^2$						2.10	2.07

Table S6. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CSe)_2(CO)_7$ structures.

	7Se-I	**7Se-II**	**7Se-VII**	**7Se-VI**	**7Se-IV**	**7Se-IT**	**7Se-IIT**
E	-8200.33755	-8200.33228	-8200.32418	-8200.31572	-8200.29296	-8200.33311	-8200.31600
ΔE	0.0	3.3	8.4	13.7	28.0	2.8	13.5
N_{img}	0	0	0	0	0	0	0
$<S>^2$	0.00	0.00	0.00	0.00	0.00	2.05	2.03

Table S7. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CTe)_2(CO)_7$ structures.

	7Te-I	**7Te-II**	**7Te-VII**	**7Te-VI**	**7Te-IV**	**7Te-IT**	**7Te-IIT**
E	-3413.3632	-3413.3612	-3413.3404	-3413.3377	-3413.2956	-3413.3438	-3413.3572
ΔE	0.0	1.3	14.3	16.0	42.4	12.2	3.8
N_{img}	0	0	0	0	0	0	0
$<S>^2$						2.03	2.05

Table S8. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CS)_2(CO)_6$ structures.

	6S-VI	**6S-I**	**6S-II**	**6S-III**	**6S-V**	**6S-IT**	**6S-XT**	**6S-IIT**
E	-4080.3085	-4080.2756	-4080.2878	-4080.2816	-4080.2598	-4080.2900	-4080.2758	-4080.2571
ΔE	0.0	20.6	13.0	16.8	30.5	11.6	20.5	32.2
N_{img}	0	0	0	0	0	0	0	0
$<S>^2$						2.06	2.05	2.10

Table S9. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequencies (N_{img}) for the optimized $Fe_2(CSe)_2(CO)_6$ structures.

	6Se-VI	**6Se-I**	**6Se-II**	**6Se-III**	**6Se-V**	**6Se-IT**	**6Se-XT**	**6Se-IIT**
E	-8086.9960	-8086.9731	-8086.9841	-8086.9751	-8086.9345	-8086.9813	-8086.9751	-8086.9565
ΔE	0.0	14.4	7.5	13.1	38.6	9.2	13.1	24.8
N_{img}	0	0	0	0	0	0	0	0
$<S>^2$						2.06	2.05	2.11

Table S10. Total energies (E, in Hartree), relative energies (ΔE, in kcal/mol), spin contamination ($\langle S \rangle^2$), and numbers of imaginary frequecncies (N_{img}) for the optimized $Fe_2(CTe)_2(CO)_6$ structures.

	6Te-VI	**6Te-I**	**6Te-II**	**6Te-III**	**6Te-V**	**6Te-IT**	**6Te-XT**	**6Te-IIT**
E	-3300.0161	-3299.9980	-3300.0106	-3300.0019	-3299.9422	-3300.0050	-3300.0066	-3299.9865
ΔE	0.0	11.3	3.5	8.9	46.4	6.9	6.0	18.6
N_{img}	0	0	0	0	0	0	0	0
$<S>^2$						2.07	2.04	2.37

Table S11. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2S_2)(CO)_8$ (infrared intensities in parentheses are in km/mol).

8S-I (C_{2h})	**8S-IT** (C_1)	**8S-VI** (C_s)	**8S-VII** (C_s)	**8S-VIII** (D_{2h})
21(au, 0)	16(a, 0)	14(a", 0)	24(a', 0)	8(b1u, 0)
31(au, 0)	25(a, 0)	42(a', 0)	29(a", 0)	11(b2g, 0)
34(bu, 0)	34(a, 0)	59(a", 0)	54(a", 0)	17(au, 0)
40(bg, 0)	40(a, 0)	59(a', 0)	56(a', 0)	48(b1u, 0)
45(ag, 0)	49(a, 0)	71(a", 0)	58(a', 0)	52(b3g, 0)
69(bu, 1)	68(a, 0)	76(a', 0)	68(a", 0)	55(b2u, 0)
70(ag, 0)	70(a, 1)	79(a", 0)	78(a", 0)	64(ag, 0)
72(ag, 0)	71(a, 0)	86(a', 0)	80(a', 0)	66(b3u, 2)
75(bu, 1)	80(a, 0)	88(a", 0)	83(a", 0)	86(ag, 0)
89(bg, 0)	83(a, 0)	89(a', 0)	85(a', 0)	87(b1g, 0)
89(au, 0)	88(a, 0)	92(a', 0)	90(a', 0)	91(b3g, 0)
101(au, 0)	90(a, 0)	95(a', 0)	90(a', 0)	91(au, 0)
101(bg, 0)	98(a, 1)	102(a", 0)	99(a", 0)	98(b2g, 0)
107(bu, 1)	101(a, 2)	107(a", 0)	107(a', 3)	99(b2u, 0)
109(ag, 0)	101(a, 0)	108(a', 1)	108(a", 0)	102(b1g, 0)
120(bg, 0)	105(a, 1)	149(a', 2)	109(a', 1)	108(b3u, 0)
132(bu, 1)	128(a, 1)	160(a", 0)	130(a", 0)	111(b1u, 0)
143(au, 4)	131(a, 1)	169(a", 0)	176(a", 0)	144(b2u, 1)
164(ag, 0)	142(a, 11)	225(a", 3)	182(a', 6)	204(ag, 0)
243(au, 1)	183(a, 8)	227(a', 2)	223(a", 0)	240(b1g, 0)
288(ag, 0)	248(a, 3)	264(a', 3)	235(a', 2)	331(b3u, 3)
316(bu, 5)	292(a, 3)	308(a", 0)	260(a", 0)	350(b2g, 0)
352(bg, 0)	335(a, 0)	359(a", 18)	299(a', 11)	368(b1u, 9)
390(bu, 21)	347(a, 1)	373(a', 0)	309(a", 0)	376(b3g, 0)
390(au, 0)	368(a, 16)	376(a', 1)	371(a', 0)	377(au, 0)
392(ag, 0)	381(a, 0)	386(a', 2)	383(a', 2)	406(b2g, 0)
396(ag, 0)	386(a, 11)	398(a', 3)	388(a', 7)	415(b3u, 85)
397(bg, 0)	389(a, 7)	429(a", 12)	398(a', 5)	419(ag, 0)
416(au, 12)	406(a, 0)	432(a", 7)	415(a", 7)	433(b1g, 0)
420(bg, 0)	412(a, 2)	434(a', 4)	419(a", 3)	436(b2u, 1)
421(bu, 6)	414(a, 12)	439(a', 5)	425(a', 10)	453(b1u, 0)
429(ag, 0)	424(a, 7)	443(a", 13)	432(a', 13)	454(ag, 0)
440(bu, 10)	439(a, 7)	450(a', 36)	433(a", 1)	457(b3u, 21)
456(ag, 0)	442(a, 1)	451(a", 1)	440(a", 8)	461(b3u, 340)
460(au, 21)	445(a, 4)	464(a', 8)	444(a", 32)	472(b2g, 0)
464(bu, 18)	455(a, 2)	465(a", 11)	446(a', 24)	477(b1u, 23)
466(bg, 0)	475(a, 29)	474(a', 42)	454(a', 20)	482(ag, 0)
471(ag, 0)	475(a, 52)	501(a", 3)	471(a', 21)	514(b1g, 0)
474(bu, 38)	482(a, 11)	507(a", 10)	472(a", 17)	518(b2u, 40)
490(ag, 0)	503(a, 3)	534(a', 16)	492(a", 0)	546(ag, 0)

508(bu, 4)	517(a, 27)	542(a', 37)	499(a", 14)	555(b3g, 0)
553(bg, 0)	518(a, 3)	551(a', 28)	526(a', 112)	556(au, 0)
554(au, 6)	551(a, 6)	582(a", 31)	535(a', 32)	588(b2u, 129)
595(bg, 0)	578(a, 46)	598(a", 85)	543(a', 16)	589(b1g, 0)
598(au, 133)	584(a, 73)	604(a', 27)	580(a", 152)	647(b3u, 456)
603(ag, 0)	591(a, 246)	617(a', 31)	593(a', 141)	650(b1u, 174)
613(bu, 368)	593(a, 42)	623(a", 1)	598(a', 41)	656(ag, 0)
623(bu, 266)	610(a, 83)	625(a', 71)	613(a", 70)	658(b2g, 0)
628(ag, 0)	625(a, 128)	653(a", 562)	617(a', 78)	758(b1g, 0)
661(ag, 0)	791(a, 10)	678(a', 187)	634(a", 280)	803(b3u, 992)
897(bu, 96)	940(a, 59)	872(a', 135)	1135(a', 18)	819(b2u, 59)
1729(ag, 0)	1458(a, 99)	1435(a', 217)	1908(a', 932)	984(ag, 0)
2092(bu, 1611)	2064(a, 736)	1924(a', 915)	1950(a', 837)	2069(b2g, 0)
2093(ag, 0)	2080(a, 995)	1964(a', 264)	1977(a', 1602)	2069(b1u, 2212)
2113(bu, 1181)	2083(a, 612)	2101(a", 30)	2099(a", 13)	2081(b1g, 0)
2115(bg, 0)	2103(a, 749)	2106(a', 1312)	2104(a', 1384)	2084(b3u, 1328)
2116(ag, 0)	2122(a, 890)	2110(a", 16)	2110(a", 310)	2087(b2u, 2376)
2126(au, 2073)	2127(a, 688)	2113(a', 1165)	2116(a', 1265)	2087(ag, 0)
2152(bu, 1058)	2127(a, 1301)	2132(a", 1908)	2130(a", 1947)	2120(b3u, 2509)
2174(ag, 0)	2173(a, 261)	2165(a', 167)	2161(a', 301)	2151(ag, 0)

Table S12. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2Se_2)(CO)_8$ (infrared intensities in parentheses are in km/mol).

8Se-I (C_{2h})	**8Se-IT** (C_1)	**8Se-VI** (C_s)	**8Se-VII** (C_s)	**8Se-VIII** (D_{2h})
20(au, 0)	16(a", 0)	18(a", 0)	18(a', 0)	8(b1u, 0)
28(au, 0)	23(a", 0)	36(a', 0)	21(a", 0)	11(b2g, 0)
34(bg, 0)	34(a", 0)	59(a", 0)	50(a', 1)	17(au, 0)
34(bu, 0)	35(a', 0)	59(a', 0)	55(a", 0)	31(b3g, 0)
45(ag, 0)	49(a', 0)	60(a", 0)	56(a', 0)	36(b1u, 0)
60(bu, 1)	62(a', 0)	74(a', 0)	70(a", 0)	52(b2u, 0)
71(ag, 0)	66(a', 1)	77(a", 0)	75(a', 0)	64(ag, 0)
71(ag, 0)	70(a', 1)	82(a', 0)	78(a", 0)	65(b3u, 2)
73(bu, 0)	77(a", 0)	86(a", 0)	84(a", 0)	84(b1g, 0)
87(bg, 0)	81(a", 0)	86(a', 0)	85(a', 0)	85(ag, 0)
87(au, 0)	83(a', 1)	89(a", 0)	90(a', 0)	91(b3g, 0)
97(bg, 0)	87(a", 0)	91(a', 0)	91(a', 0)	91(au, 0)
100(au, 0)	90(a', 2)	94(a', 0)	96(a", 0)	93(b2u, 0)
104(ag, 0)	96(a", 0)	103(a', 1)	100(a', 2)	97(b2g, 0)
105(bu, 1)	97(a", 0)	103(a", 0)	107(a', 1)	99(b1g, 0)
106(bg, 0)	102(a', 1)	117(a', 1)	112(a", 0)	102(b3u, 0)
111(au, 2)	109(a", 1)	153(a", 0)	114(a", 0)	105(b1u, 0)
120(bu, 0)	115(a', 0)	155(a', 2)	151(a', 6)	121(b2u, 1)
153(ag, 0)	122(a', 3)	162(a", 0)	169(a", 1)	162(b1g, 0)
199(ag, 0)	169(a', 1)	224(a", 3)	184(a", 0)	192(ag, 0)
223(au, 3)	208(a', 2)	238(a', 0)	209(a', 4)	238(b3u, 3)
236(bu, 2)	237(a", 4)	262(a', 2)	231(a', 3)	315(ag, 0)
269(ag, 0)	255(a', 2)	308(a", 0)	236(a", 1)	342(b2g, 0)
358(bg, 0)	335(a", 0)	342(a", 15)	301(a', 49)	361(b1u, 12)
389(au, 0)	347(a', 1)	373(a', 4)	311(a", 0)	376(b3g, 0)
392(bu, 18)	368(a', 14)	379(a', 2)	360(a', 1)	376(au, 0)
394(bg, 0)	379(a", 0)	387(a', 3)	371(a', 0)	397(b2g, 0)
395(ag, 0)	391(a', 11)	416(a", 0)	381(a", 1)	402(b1u, 1)
415(au, 11)	402(a", 0)	428(a", 4)	383(a', 0)	416(b3u, 83)
423(bu, 4)	403(a', 5)	432(a', 5)	397(a', 2)	420(ag, 0)
424(bg, 0)	414(a", 12)	434(a", 35)	416(a", 2)	429(b1g, 0)
424(ag, 0)	420(a', 6)	437(a', 3)	419(a", 1)	432(b2u, 0)
429(bu, 4)	436(a', 7)	446(a', 58)	423(a', 12)	453(b3u, 30)
450(ag, 0)	439(a", 0)	446(a", 1)	432(a', 11)	455(ag, 0)
463(au, 15)	442(a', 1)	449(a', 28)	439(a", 19)	462(b3u, 306)
465(bu, 9)	454(a', 3)	454(a", 0)	447(a", 32)	468(b1u, 16)
470(ag, 0)	477(a', 15)	466(a', 9)	449(a', 27)	471(b2g, 0)
473(bg, 0)	477(a", 23)	498(a', 8)	459(a', 16)	481(ag, 0)
474(bu, 24)	483(a', 31)	499(a", 1)	472(a', 25)	501(b1g, 0)

492(ag, 0)	501(a", 1)	505(a", 6)	473(a", 12)	507(b2u, 38)
505(bu, 1)	508(a', 12)	536(a', 4)	492(a", 1)	555(b3g, 0)
552(bg, 0)	515(a", 6)	542(a', 36)	500(a", 12)	555(au, 0)
553(au, 3)	551(a", 5)	562(a', 28)	536(a', 26)	584(b2u, 105)
567(ag, 0)	575(a', 37)	571(a", 1)	538(a', 10)	585(b1g, 0)
595(bg, 0)	583(a", 66)	592(a", 142)	583(a", 147)	645(b1u, 171)
598(au, 136)	592(a', 252)	608(a', 54)	591(a', 112)	645(b3u, 406)
607(bu, 197)	593(a", 51)	621(a", 0)	597(a', 35)	653(ag, 0)
621(bu, 395)	598(a', 28)	623(a', 149)	615(a", 91)	656(b2g, 0)
627(ag, 0)	623(a', 156)	627(a', 33)	617(a', 122)	670(b1g, 0)
647(ag, 0)	718(a', 39)	648(a", 518)	633(a", 261)	714(b2u, 74)
743(bu, 102)	763(a', 24)	743(a', 146)	923(a', 6)	738(b3u, 890)
1693(ag, 0)	1451(a', 181)	1367(a', 133)	904(a', 937)	901(ag, 0)
2092(bu, 1525)	2063(a', 692)	1924(a', 895)	1941(a', 1559)	2068(b2g, 0)
2093(ag, 0)	2080(a", 947)	1964(a', 283)	1953(a', 314)	2069(b1u, 2210)
2112(bu, 1051)	2083(a', 624)	2101(a", 40)	97(a", 1)	2076(b1g, 0)
2113(bg, 0)	2102(a', 675)	2106(a', 1266)	2102(a', 1305)	2082(b2u, 2271)
2115(ag, 0)	2120(a', 700)	2111(a", 17)	2107(a", 419)	2083(b3u, 1209)
2124(au, 2052)	2124(a", 1302)	2114(a', 1067)	114(a', 226)	2085(ag, 0)
2150(bu, 1149)	2125(a', 922)	2132(a", 1878)	2129(a", 1867)	2118(b3u, 2656)
2170(ag, 0)	2168(a', 286)	2163(a', 255)	2156(a', 563)	2146(ag, 0)

Table S13. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2Te_2)(CO)_8$ (infrared intensities in parentheses are in km/mol).

8Te-I (C_{2h})	**8Te-IT** (C_1)	**8Te-VI** (C_s)	**8Te-VII** (C_s)	**8Te-VIII** (D_{2h})
21(au, 0)	15(a, 0)	25(a", 0)	15(a', 0)	3(b1u, 0)
27(au, 0)	22(a, 0)	34(a', 0)	18(a", 0)	5(b2g, 0)
31(bg, 0)	32(a, 0)	57(a", 0)	47(a', 0)	16(au, 0)
39(bu, 0)	36(a, 0)	60(a', 0)	55(a', 0)	25(b3g, 0)
48(ag, 0)	49(a, 0)	62(a", 0)	56(a", 0)	33(b1u, 0)
55(bu, 1)	57(a, 0)	69(a', 0)	74(a", 0)	51(b2u, 0)
70(ag, 0)	62(a, 0)	74(a", 0)	74(a', 0)	63(ag, 0)
74(ag, 0)	70(a, 0)	79(a', 0)	76(a", 0)	64(b3u, 2)
75(bu, 0)	73(a, 0)	84(a", 0)	84(a', 0)	79(b1g, 0)
85(au, 0)	80(a, 1)	84(a', 0)	86(a", 0)	87(ag, 0)
86(bg, 0)	82(a, 0)	92(a", 0)	90(a", 0)	88(b2u, 0)
98(ag, 0)	85(a, 0)	93(a', 0)	91(a', 0)	91(b3g, 0)
98(bg, 0)	89(a, 0)	95(a', 0)	91(a', 0)	91(au, 0)
98(au, 0)	95(a, 0)	97(a', 0)	99(a', 2)	95(b1g, 0)
103(au, 1)	97(a, 0)	105(a", 0)	104(a', 1)	99(b2g, 0)
104(bu, 1)	100(a, 1)	108(a', 0)	107(a", 0)	100(b3u, 0)
104(bg, 0)	105(a, 0)	124(a', 1)	119(a", 0)	104(b1u, 0)
116(bu, 0)	111(a, 0)	148(a", 0)	134(a', 3)	114(b2u, 1)
135(ag, 0)	115(a, 1)	166(a", 0)	137(a", 2)	135(b1g, 0)
160(ag, 0)	152(a, 1)	177(a', 2)	172(a', 11)	181(ag, 0)
201(bu, 1)	164(a, 1)	224(a", 3)	185(a", 0)	195(b3u, 2)
215(au, 5)	211(a, 2)	254(a', 1)	207(a', 14)	222(ag, 0)
223(ag, 0)	227(a, 6)	308(a", 2)	226(a', 10)	337(b2g, 0)
353(bg, 0)	337(a, 0)	319(a", 10)	236(a", 1)	345(b1u, 19)
388(au, 1)	341(a, 1)	362(a', 21)	310(a', 1)	376(b3g, 0)
391(bg, 0)	369(a, 17)	377(a', 1)	314(a", 0)	377(au, 0)
394(bu, 18)	375(a, 0)	382(a', 0)	330(a", 1)	381(b1u, 0)
396(ag, 0)	394(a, 12)	390(a", 1)	371(a', 0)	390(b2g, 0)
413(bu, 5)	398(a, 0)	426(a", 4)	383(a', 2)	419(b3u, 74)
416(au, 10)	402(a, 2)	426(a', 49)	399(a', 2)	422(ag, 0)
422(ag, 0)	415(a, 9)	430(a', 6)	417(a", 2)	425(b1g, 0)
424(bu, 4)	417(a, 3)	432(a", 30)	418(a", 0)	429(b2u, 0)
428(bg, 0)	430(a, 8)	434(a', 13)	421(a', 17)	450(b3u, 46)
449(ag, 0)	436(a, 0)	442(a', 11)	433(a', 8)	454(ag, 0)
458(bu, 18)	442(a, 3)	443(a", 1)	442(a", 17)	463(b3u, 256)
469(bu, 2)	458(a, 3)	449(a", 3)	451(a', 27)	468(b1u, 15)
470(ag, 0)	473(a, 26)	465(a', 24)	451(a", 36)	471(b2g, 0)
471(au, 16)	478(a, 10)	466(a', 4)	462(a', 21)	479(ag, 0)
478(bg, 0)	482(a, 23)	497(a", 0)	475(a', 26)	489(b1g, 0)
491(ag, 0)	494(a, 2)	503(a", 3)	479(a", 12)	498(b2u, 29)

502(bu, 1)	497(a, 0)	510(a', 55)	493(a", 1)	555(b3g, 0)
530(ag, 0)	518(a, 6)	537(a', 29)	503(a", 17)	556(au, 0)
553(bg, 0)	551(a, 4)	546(a', 1)	539(a', 33)	579(b1g, 0)
554(au, 3)	562(a, 15)	556(a", 28)	540(a', 16)	579(b2u, 51)
588(bu, 40)	574(a, 5)	589(a", 150)	586(a", 149)	619(b1g, 0)
594(bg, 0)	578(a, 56)	593(a', 23)	591(a', 112)	639(b2u, 122)
598(au, 137)	592(a, 62)	616(a', 80)	597(a', 27)	644(b3u, 275)
622(bu, 432)	596(a, 234)	621(a", 0)	619(a", 93)	646(b1u, 170)
624(ag, 0)	620(a, 181)	622(a', 66)	622(a', 148)	652(ag, 0)
641(ag, 0)	626(a, 34)	639(a', 170)	634(a", 265)	656(b2g, 0)
650(bu, 195)	659(a, 60)	645(a", 477)	769(a', 4)	692(b3u, 893)
1669(ag, 0)	1481(a, 305)	335(a', 95)	1900(a', 946)	815(ag, 0)
2090(bu, 1309)	2060(a, 604)	1922(a', 863)	1944(a', 789)	2066(b1g, 0)
2091(ag, 0)	2079(a, 867)	1962(a', 335)	1949(a', 618)	2068(b2g, 0)
2109(bg, 0)	2083(a, 688)	100(a", 38)	2093(a", 55)	2068(b1u, 2230)
2110(bu, 983)	2097(a, 537)	2106(a', 1171)	2097(a', 1223)	2070(b2u, 2121)
2113(ag, 0)	2115(a, 489)	2112(a", 21)	2103(a", 388)	2079(b3u, 846)
2120(au, 2093)	2117(a, 1403)	114(a', 939)	2110(a', 1184)	2081(ag, 0)
2147(bu, 1305)	2122(a, 1229)	2132(a", 1934)	2126(a", 1883)	2114(b3u, 3012)
2164(ag, 0)	2160(a, 329)	2159(a', 482)	2150(a', 1038)	2138(ag, 0)

Table S14. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2S_2)(CO)_7$ (infrared intensities in parentheses are in km/mol).

7S-I (C_s)	**7S-II** (C_s)	**7S-VI** (C_s)	**7S-IV** (C_{2v})
21(a", 0)	22(a, 0)	34(a', 0)	49(a1, 0)
28(a", 0)	28(a, 0)	37(a", 0)	54(b1, 0)
34(a', 0)	33(a, 0)	42(a", 0)	56(a2, 0)
42(a", 0)	60(a, 0)	45(a', 0)	73(b1, 0)
51(a', 0)	64(a, 0)	57(a', 0)	78(b2, 0)
70(a', 0)	68(a, 0)	68(a", 1)	78(a2, 0)
71(a', 0)	74(a, 0)	75(a', 0)	83(b2, 1)
73(a", 0)	84(a, 1)	79(a", 0)	83(a1, 0)
83(a', 0)	88(a, 0)	80(a', 0)	85(a1, 0)
84(a", 0)	89(a, 0)	90(a', 0)	89(b1, 0)
89(a", 0)	91(a, 0)	91(a", 0)	91(a1, 0)
100(a', 0)	101(a, 0)	99(a", 0)	97(a2, 0)
101(a", 0)	106(a, 1)	101(a', 1)	97(b2, 0)
108(a', 0)	108(a, 0)	115(a", 2)	102(b1, 1)
136(a', 0)	156(a, 4)	144(a', 0)	156(b2, 1)
137(a", 3)	193(a, 0)	175(a', 3)	178(a2, 0)
167(a', 0)	194(a, 5)	246(a', 10)	188(b2, 3)
233(a", 2)	217(a, 2)	260(a", 3)	254(a1, 0)
295(a', 1)	281(a, 1)	270(a", 0)	298(a2, 0)
347(a', 15)	313(a, 15)	281(a', 10)	303(b2, 3)
353(a", 0)	347(a, 19)	313(a", 7)	320(b1, 0)
382(a", 1)	382(a, 1)	348(a', 0)	325(a1, 0)
383(a', 20)	383(a, 0)	366(a", 19)	352(b1, 4)
393(a', 4)	391(a, 8)	377(a', 10)	378(a1, 2)
395(a", 0)	406(a, 11)	385(a', 3)	415(a1, 44)
418(a", 7)	418(a, 0)	402(a", 2)	426(b2, 40)
424(a', 9)	426(a, 0)	418(a", 4)	434(b1, 5)
435(a', 16)	443(a, 0)	434(a", 1)	435(a2, 0)
442(a", 1)	455(a, 16)	435(a', 0)	438(a1, 17)
448(a', 4)	455(a, 6)	441(a', 2)	440(b1, 49)
456(a', 11)	470(a, 29)	463(a", 1)	441(a2, 0)
465(a", 9)	472(a, 0)	471(a", 2)	442(b2, 0)
471(a', 3)	479(a, 10)	472(a', 3)	460(a1, 0)
474(a", 1)	485(a, 0)	478(a', 28)	497(a2, 0)
478(a', 22)	504(a, 7)	483(a', 6)	500(b2, 0)
484(a', 20)	511(a, 24)	498(a", 0)	504(b1, 2)
510(a', 10)	543(a, 3)	528(a', 10)	533(a1, 1)
548(a", 35)	551(a, 1)	540(a", 19)	544(b1, 7)
554(a", 7)	566(a, 82)	546(a", 152)	576(b2, 38)
567(a', 73)	588(a, 68)	582(a', 12)	591(a2, 0)

597(a", 71)	599(a, 52)	593(a", 66)	601(b2, 116)
608(a', 146)	619(a, 442)	595(a', 11)	607(a1, 104)
625(a', 180)	631(a, 51)	614(a', 98)	618(b1, 101)
644(a', 42)	633(a, 41)	628(a', 72)	622(a1, 5)
664(a', 0)	855(a, 27)	686(a", 173)	647(b2, 522)
885(a', 97)	948(a, 13)	1041(a', 25)	1180(b1, 827)
1738(a', 1)	1569(a, 626)	1776(a', 1491)	1220(a1, 249)
2088(a", 575)	2077(a, 801)	1799(a', 259)	1939(a1, 633)
2090(a', 675)	2078(a, 637)	2081(a", 0)	2099(a2, 0)
2091(a', 851)	2100(a, 928)	2086(a", 11)	2102(b2, 18)
2114(a', 701)	2113(a, 2421)	2089(a', 1484)	2104(b1, 1343)
2121(a", 1287)	2118(a, 889)	2118(a, 889)	2118(a, 889)
2134(a', 1265)	2121(a, 601)	2121(a, 601)	2121(a, 601)
2166(a', 171)	2169(a, 265)	2169(a, 265)	2169(a, 265)
2113(bu, 1181)	2169(a, 265)	2101(a", 30)	2099(a", 13)

Table S15. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2Se_2)(CO)_7$ (infrared intensities in parentheses are in km/mol).

7Se-I (C_s)	**7Se-II** (C_s)	**7Se-VI** (C_s)	**7Se-IV** (C_{2v})
21(a", 0)	20(a", 0)	27(a", 0)	35(a1, 0)
27(a", 0)	26(a', 0)	28(a', 0)	49(b1, 0)
34(a", 0)	32(a", 0)	42(a', 0)	57(a2, 0)
36(a', 0)	42(a", 0)	42(a", 0)	65(b1, 0)
49(a', 0)	60(a', 0)	56(a', 0)	71(a2, 0)
65(a", 0)	68(a', 0)	68(a", 1)	71(b2, 1)
69(a', 0)	69(a", 0)	70(a', 0)	75(a1, 0)
73(a', 0)	82(a', 1)	79(a", 0)	80(b2, 0)
79(a', 0)	85(a", 0)	80(a', 0)	85(a1, 0)
83(a", 0)	88(a", 0)	88(a', 0)	85(a2, 0)
87(a", 0)	88(a', 0)	88(a", 0)	89(a1, 0)
96(a', 0)	101(a', 0)	95(a", 0)	90(b1, 0)
99(a", 0)	102(a", 0)	97(a', 0)	95(b2, 0)
105(a', 0)	103(a', 0)	114(a", 2)	98(b1, 1)
109(a", 1)	124(a', 2)	118(a', 0)	132(b2, 1)
120(a', 0)	158(a', 1)	152(a', 7)	167(a2, 0)
157(a', 0)	158(a", 2)	170(a', 2)	182(b2, 4)
196(a', 0)	196(a', 5)	196(a", 1)	206(a1, 0)
214(a", 4)	201(a", 1)	242(a', 6)	243(b1, 0)
249(a', 5)	228(a', 8)	261(a", 2)	279(a1, 0)
287(a', 9)	256(a', 5)	294(a", 6)	300(b2, 5)
357(a", 0)	373(a", 0)	342(a', 0)	301(a2, 0)
382(a", 1)	384(a", 1)	359(a', 0)	334(b1, 5)
391(a", 1)	392(a', 11)	368(a", 19)	373(a1, 4)
393(a', 7)	408(a', 12)	379(a', 8)	399(a1, 41)
415(a', 10)	414(a', 0)	386(a', 4)	423(b2, 39)
418(a", 6)	417(a", 2)	401(a", 2)	429(b1, 11)
426(a', 0)	435(a", 0)	412(a", 2)	434(a2, 0)
442(a', 3)	442(a", 0)	433(a", 5)	436(a1, 16)
445(a", 1)	450(a', 11)	438(a', 4)	437(b1, 38)
453(a', 3)	452(a", 1)	445(a', 0)	439(a2, 0)
469(a", 7)	474(a', 18)	454(a", 2)	440(b2, 1)
470(a', 2)	479(a", 8)	466(a", 2)	456(a1, 1)
474(a', 9)	480(a', 10)	477(a', 15)	496(a2, 0)
479(a', 12)	488(a", 13)	482(a', 5)	497(b1, 3)
480(a", 1)	502(a', 7)	498(a", 1)	500(b2, 1)
505(a', 1)	511(a', 24)	514(a', 6)	529(a1, 0)
552(a", 7)	553(a", 7)	530(a', 13)	542(b1, 8)
554(a", 35)	554(a", 32)	535(a", 47)	571(b2, 16)
557(a', 13)	589(a', 71)	547(a", 113)	585(a2, 0)

590(a', 141)	597(a', 38)	582(a', 12)	597(b2, 140)
597(a", 73)	619(a', 446)	593(a", 70)	599(a1, 99)
624(a', 216)	625(a", 64)	608(a', 86)	612(b1, 86)
632(a', 41)	632(a', 38)	625(a', 84)	618(a1, 8)
652(a', 14)	746(a', 48)	684(a", 172)	639(b2, 451)
746(a', 97)	817(a", 10)	847(a', 17)	996(b1, 716)
1699(a', 3)	1607(a', 516)	1716(a', 1233)	1039(a1, 195)
2088(a", 540)	2072(a", 614)	1798(a', 417)	1943(a1, 664)
2090(a', 780)	74(a', 853)	80(a", 1)	2102(a2, 0)
2092(a', 677)	2096(a", 915)	2086(a", 4)	2106(b2, 34)
2114(a', 597)	2109(a', 2549)	2088(a', 1421)	2106(b1, 1273)
2118(a, 889)	2118(a, 889)	2118(a, 889)	2118(a, 889)
2121(a, 601)	2121(a, 601)	2121(a, 601)	2121(a, 601)
2169(a, 265)	2169(a, 265)	2169(a, 265)	2169(a, 265)
2113(bu, 1181)	2169(a, 265)	2101(a", 30)	2099(a", 13)

Table S16. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2Te_2)(CO)_7$ (infrared intensities in parentheses are in km/mol).

7Te-I (C_s)	**7Te-II** (C_s)	**7Te-VI** (C_s)	**7Te-IV** (C_{2v})
20(a", 0)	24(a, 0)	25(a', 0)	28(a1, 0)
25(a", 0)	24(a, 0)	25(a", 0)	47(b1, 0)
28(a", 0)	30(a, 0)	42(a", 0)	60(a2, 0)
39(a', 0)	36(a, 0)	42(a', 0)	65(b1, 0)
51(a', 0)	56(a, 0)	55(a', 0)	65(a2, 0)
59(a", 0)	66(a, 0)	69(a', 0)	66(b2, 1)
67(a', 0)	67(a, 0)	69(a", 1)	75(a1, 0)
76(a', 0)	78(a, 1)	79(a', 0)	83(b2, 0)
80(a', 0)	84(a, 0)	79(a", 0)	86(a1, 0)
82(a", 0)	86(a, 0)	85(a", 0)	88(a2, 0)
86(a", 0)	89(a, 0)	85(a', 0)	90(a1, 0)
91(a', 0)	98(a, 0)	92(a', 0)	92(b1, 0)
97(a", 0)	100(a, 0)	93(a", 0)	94(b2, 1)
101(a', 0)	102(a, 0)	105(a', 0)	97(b1, 0)
104(a", 0)	112(a, 1)	114(a", 1)	124(b2, 1)
114(a', 0)	126(a, 1)	128(a', 7)	166(a2, 0)
131(a', 0)	140(a, 0)	147(a', 1)	169(a1, 0)
160(a', 1)	169(a, 1)	168(a", 1)	180(b2, 7)
207(a", 5)	190(a, 7)	220(a', 2)	208(b1, 0)
208(a', 3)	200(a, 5)	262(a", 3)	275(a1, 0)
242(a', 5)	213(a, 4)	279(a", 6)	300(b2, 8)
355(a", 0)	357(a, 0)	294(a', 4)	312(a2, 0)
381(a", 1)	384(a, 8)	347(a', 0)	325(b1, 8)
389(a", 1)	387(a, 1)	370(a", 19)	370(a1, 10)
394(a', 11)	394(a, 12)	384(a', 3)	388(a1, 46)
396(a', 21)	410(a, 2)	387(a', 5)	421(b2, 39)
420(a", 5)	412(a, 9)	389(a", 2)	425(b1, 15)
422(a', 1)	418(a, 0)	402(a", 1)	432(a2, 0)
439(a', 4)	424(a, 0)	428(a', 0)	434(b1, 31)
447(a", 0)	446(a, 1)	437(a", 6)	436(a1, 15)
454(a', 2)	451(a, 9)	449(a', 1)	438(a2, 0)
457(a', 5)	464(a, 14)	451(a", 11)	440(b2, 1)
470(a', 1)	480(a, 11)	455(a', 13)	454(a1, 2)
474(a", 8)	485(a, 15)	467(a", 1)	491(b1, 4)
476(a', 4)	487(a, 1)	480(a', 17)	497(a2, 0)
487(a", 1)	499(a, 13)	485(a', 2)	501(b2, 1)
502(a', 6)	516(a, 24)	493(a", 13)	523(a1, 0)
531(a', 13)	556(a, 1)	527(a", 45)	541(b1, 7)
554(a", 0)	558(a, 30)	527(a', 8)	561(b2, 0)
559(a", 40)	590(a, 75)	551(a", 84)	575(a2, 0)

580(a', 119)	593(a, 34)	582(a', 11)	592(a1, 94)
597(a", 75)	618(a, 427)	592(a", 83)	593(b2, 177)
617(a', 85)	625(a, 65)	604(a', 65)	604(b1, 72)
625(a', 133)	630(a, 24)	625(a', 100)	616(a1, 14)
640(a', 72)	677(a, 94)	684(a", 168)	629(b2, 363)
669(a', 76)	732(a, 10)	700(a', 28)	862(b1, 752)
1667(a', 4)	1640(a, 438)	1683(a', 1106)	908(a1, 170)
2086(a", 510)	2064(a, 565)	1797(a', 496)	1948(a1, 716)
88(a', 795)	68(a, 906)	77(a", 2)	104(a2, 0)
2092(a', 521)	2089(a, 892)	2085(a", 2)	2108(b1, 1176)
2112(a', 527)	2101(a, 2607)	2087(a', 1279)	2109(b2, 50)
2118(a, 889)	2118(a, 889)	2118(a, 889)	2118(a, 889)
2121(a, 601)	2121(a, 601)	2121(a, 601)	2121(a, 601)
2169(a, 265)	2169(a, 265)	2169(a, 265)	2169(a, 265)
2113(bu, 1181)	2169(a, 265)	2101(a", 30)	2099(a", 13)

Table S17. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2S_2)(CO)_6$ (infrared intensities in parentheses are in km/mol).

6S-VI (C_s)	**6S-XT** (C_s)	**6S-IT** (C_2)	**6S-I** (C_{2h})	**6S-II** (C_s)	**6S-III** (C_2)	**6S-IIIT** (C_2)	**6S-V** (C_1)
25(a", 0)	25(a", 0)	17(a, 0)	22(au, 0)	23(a", 0)	39(a, 0)	15(b, 0)	31(a, 0)
29(a", 0)	26(a', 0)	21(b, 0)	28(au, 0)	30(a', 0)	56(b, 0)	16(a, 0)	42(a, 0)
39(a', 0)	35(a", 0)	22(a, 0)	36(bu, 0)	51(a", 0)	61(a, 0)	31(a, 0)	54(a, 0)
59(a', 0)	42(a', 0)	44(b, 0)	41(bg, 0)	57(a", 0)	76(a, 0)	62(a, 0)	70(a, 0)
69(a", 0)	57(a', 0)	56(a, 0)	60(ag, 0)	60(a', 0)	80(b, 0)	67(a, 0)	73(a, 0)
69(a', 0)	74(a", 0)	66(b, 0)	61(bg, 0)	81(a', 0)	83(a, 0)	68(b, 0)	76(a, 0)
77(a", 0)	77(a", 0)	68(a, 0)	74(au, 0)	82(a", 0)	86(b, 0)	71(b, 0)	86(a, 0)
86(a', 0)	78(a', 0)	73(b, 0)	76(ag, 0)	84(a', 0)	98(a, 0)	75(b, 0)	90(a, 0)
91(a', 0)	86(a', 0)	74(a, 0)	80(bg, 0)	88(a", 0)	102(b, 0)	79(a, 0)	93(a, 0)
97(a", 0)	94(a', 0)	89(a, 0)	85(bu, 0)	91(a', 0)	102(a, 0)	93(a, 0)	95(a, 0)
97(a', 0)	99(a", 0)	89(b, 0)	98(bu, 0)	104(a', 0)	105(b, 0)	93(b, 0)	101(a, 0)
99(a", 0)	107(a", 1)	93(b, 0)	103(ag, 0)	106(a", 0)	113(b, 0)	98(b, 0)	104(a, 0)
110(a", 2)	112(a", 0)	105(a, 0)	113(au, 2)	144(a', 2)	166(a, 0)	100(a, 0)	112(a, 0)
137(a', 2)	119(a', 2)	118(a, 0)	142(bu, 0)	205(a', 1)	181(a, 2)	114(a, 0)	177(a, 3)
192(a', 1)	178(a', 0)	135(b, 2)	172(ag, 0)	220(a", 5)	205(a, 1)	147(b, 6)	203(a, 1)
269(a', 10)	229(a', 3)	181(a, 0)	225(au, 3)	271(a', 7)	215(b, 4)	208(a, 0)	212(a, 1)
271(a", 0)	270(a", 3)	278(b, 15)	320(ag, 0)	300(a", 0)	268(b, 0)	231(b, 37)	295(a, 9)
333(a', 14)	285(a', 8)	302(a, 4)	353(bg, 0)	323(a', 24)	357(a, 5)	267(a, 2)	313(a, 1)
338(a", 6)	358(a", 1)	325(b, 7)	360(bu, 44)	378(a', 21)	397(b, 3)	310(b, 25)	332(a, 7)
401(a', 0)	360(a', 8)	330(a, 1)	380(ag, 0)	388(a", 0)	402(a, 6)	317(b, 4)	377(a, 8)
405(a", 0)	380(a', 1)	349(b, 2)	382(au, 2)	395(a", 1)	411(b, 0)	319(a, 2)	384(a, 11)
435(a", 6)	387(a", 1)	369(a, 0)	383(bg, 0)	419(a', 0)	432(a, 7)	368(a, 2)	403(a, 10)
440(a", 0)	416(a", 19)	387(b, 10)	431(bu, 35)	432(a", 0)	432(b, 0)	372(b, 6)	408(a, 14)
444(a', 3)	420(a', 1)	399(a, 9)	435(au, 0)	437(a', 9)	434(a, 0)	380(b, 15)	419(a, 9)
449(a', 1)	437(a', 0)	414(b, 1)	445(bu, 14)	452(a", 2)	452(b, 0)	386(a, 16)	425(a, 2)
456(a", 1)	444(a", 0)	424(a, 0)	449(ag, 0)	455(a', 19)	454(a, 3)	401(a, 0)	447(a, 10)
470(a', 3)	458(a", 2)	437(b, 1)	454(bg, 0)	467(a', 2)	461(a, 6)	423(b, 0)	449(a, 12)
483(a", 1)	463(a', 1)	441(a, 1)	464(ag, 0)	477(a", 4)	476(b, 11)	431(a, 0)	456(a, 1)
487(a", 1)	467(a', 2)	461(a, 13)	474(bg, 0)	483(a", 0)	484(a, 19)	438(b, 1)	467(a, 2)
488(a', 3)	468(a", 16)	465(b, 9)	477(au, 0)	499(a', 5)	486(b, 14)	446(b, 4)	478(a, 24)
493(a', 14)	486(a", 0)	472(b, 15)	478(bu, 37)	500(a", 5)	493(b, 40)	449(a, 6)	488(a, 17)
497(a", 3)	492(a', 16)	497(a, 0)	483(ag, 0)	508(a', 15)	512(a, 0)	478(a, 7)	504(a, 10)
499(a', 0)	524(a', 10)	529(b, 100)	503(bu, 29)	548(a", 36)	557(b, 112)	480(b, 8)	519(a, 11)
572(a', 114)	543(a", 0)	531(a, 2)	550(au, 88)	585(a', 14)	564(a, 1)	521(a, 1)	541(a, 13)
574(a", 0)	569(a", 5)	537(b, 3)	550(bg, 0)	589(a", 60)	576(b, 62)	525(b, 88)	572(a, 12)
577(a", 190)	576(a', 57)	552(a, 42)	568(ag, 0)	591(a', 59)	587(a, 86)	550(b, 32)	586(a, 96)
595(a', 33)	584(a", 14)	577(b, 76)	572(bu, 165)	619(a', 262)	588(b, 38)	553(a, 5)	593(a, 150)
615(a', 23)	584(a', 67)	591(a, 6)	643(ag, 0)	623(a", 0)	622(a, 25)	574(a, 51)	607(a, 129)
626(a", 78)	605(a", 234)	601(b, 54)	647(bu, 75)	628(a', 60)	632(b, 230)	591(b, 66)	613(a, 95)
629(a', 50)	615(a', 14)	656(a, 16)	671(ag, 0)	891(a', 3)	734(a, 7)	618(a, 9)	626(a, 48)

1051(a', 23)	965(a', 42)	1001(b, 94)	870(bu, 106)	969(a", 22)	966(b, 89)	952(b, 90)	1168(a, 433)
1771(a', 1506)	1732(a', 441)	1450(a, 123)	1750(ag, 0)	1442(a', 2)	1410(a, 16)	1812(a, 24)	1211(a, 309)
2054(a", 1)	2070(a", 17)	60(a, 132)	2084(bg, 0)	2079(a', 709)	83(a, 33)	67(b, 538)	70(a, 88)
2058(a", 0)	2081(a", 3)	2061(b, 1257)	2089(au, 1641)	2084(a", 794)	2083(b, 9)	2073(a, 409)	2083(a, 371)
2075(a', 883)	2087(a', 1178)	2067(b, 1005)	2089(bu, 1448)	2099(a', 1023)	2098(a, 876)	2080(b, 1039)	2093(a, 969)
2080(a', 1424)	2092(a', 1286)	76(a, 564)	2090(ag, 0)	2101(a", 747)	102(b, 197)	80(a, 112)	96(a, 136)
2093(a", 2474)	2108(a", 2297)	2108(b, 1864)	2130(bu, 2028)	2118(a', 3186)	2113(b, 2293)	2120(b, 1544)	2113(a, 1946)
2139(a', 500)	2143(a', 429)	2129(a, 411)	2144(ag, 0)	2149(a', 120)	2153(a, 409)	2138(a, 150)	2146(a, 340)

Table S18. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2Se_2)(CO)_6$ (infrared intensities in parentheses are in km/mol).

6Se-VI (C_s)	**6Se-XT** (C_s)	**6Se-IT** (C_2)	**6Se-I** (C_{2h})	**6Se-II** (C_s)	**6Se-III** (C_2)	**6Se-IIIT** (C_2)	**6Se-V** ($C_{1,}$)
18(a", 0)	22(a", 0)	9(a, 0)	20(au, 0)	20(a", 0)	39(a, 0)	17(b, 0)	30(a, 0)
27(a", 0)	23(a", 0)	16(b, 0)	27(au, 0)	27(a', 0)	52(b, 0)	18(a, 0)	41(a, 0)
32(a', 0)	23(a', 0)	20(a, 0)	30(bg, 0)	38(a", 0)	57(a, 0)	30(a, 0)	42(a, 0)
54(a', 0)	36(a', 0)	36(b, 0)	33(bu, 0)	49(a", 0)	75(a, 0)	59(b, 0)	63(a, 0)
68(a", 0)	52(a', 0)	43(a, 0)	58(ag, 0)	55(a', 0)	76(a, 0)	60(a, 0)	73(a, 0)
68(a', 0)	73(a", 0)	62(b, 0)	58(bg, 0)	79(a", 0)	79(b, 0)	69(a, 0)	74(a, 0)
76(a", 0)	77(a", 0)	66(a, 0)	70(au, 0)	79(a', 0)	85(b, 0)	71(a, 0)	78(a, 0)
86(a', 0)	77(a', 0)	70(a, 0)	77(ag, 0)	82(a', 0)	90(b, 0)	71(b, 0)	81(a, 0)
90(a', 0)	84(a', 0)	71(b, 0)	81(bu, 0)	87(a", 0)	91(a, 0)	72(b, 0)	84(a, 0)
92(a", 0)	90(a', 0)	84(a, 0)	82(bg, 0)	90(a', 0)	98(b, 0)	90(a, 0)	88(a, 0)
97(a", 0)	95(a', 0)	84(b, 0)	86(au, 0)	101(a', 0)	99(a, 0)	91(b, 0)	93(a, 0)
99(a', 0)	97(a", 0)	87(a, 0)	95(bu, 0)	101(a", 0)	104(b, 0)	96(b, 0)	97(a, 0)
104(a", 2)	102(a", 1)	88(b, 0)	96(ag, 0)	116(a', 1)	122(a, 0)	98(a, 0)	105(a, 0)
111(a', 1)	108(a", 0)	107(a, 0)	121(bu, 0)	162(a', 2)	163(a, 2)	110(a, 0)	154(a, 2)
175(a', 1)	158(a', 0)	113(b, 1)	161(ag, 0)	180(a", 3)	168(b, 2)	132(b, 0)	173(a, 1)
182(a', 3)	202(a", 2)	141(a, 0)	194(ag, 0)	209(a", 0)	176(a, 0)	164(a, 0)	194(a, 1)
202(a", 0)	206(a', 3)	213(b, 8)	206(au, 5)	230(a', 6)	207(b, 0)	178(b, 13)	234(a, 1)
275(a', 8)	224(a', 3)	253(a, 2)	273(bu, 23)	248(a', 3)	247(a, 0)	222(a, 1)	273(a, 2)
320(a", 6)	265(a', 7)	325(b, 5)	296(ag, 0)	283(a', 12)	386(b, 3)	277(a, 0)	292(a, 2)
365(a', 2)	343(a", 0)	327(a, 1)	357(bg, 0)	385(a", 0)	401(a, 6)	297(b, 41)	353(a, 13)
402(a', 0)	380(a', 1)	342(b, 1)	383(au, 2)	393(a", 1)	410(b, 1)	319(b, 3)	381(a, 14)
405(a", 0)	387(a", 1)	347(a, 0)	384(bg, 0)	414(a', 1)	417(a, 0)	321(a, 2)	399(a, 4)
417(a", 0)	405(a', 2)	391(a, 5)	409(bu, 18)	420(a", 0)	424(b, 3)	372(b, 8)	405(a, 3)
434(a", 5)	416(a", 16)	391(b, 9)	431(ag, 0)	429(a', 15)	430(a, 4)	377(a, 0)	408(a, 18)
442(a', 5)	433(a', 0)	407(b, 0)	437(au, 0)	436(a", 2)	451(b, 0)	381(b, 10)	418(a, 6)
447(a', 0)	439(a", 0)	420(a, 2)	450(bu, 4)	442(a", 0)	455(a, 0)	393(a, 16)	435(a, 19)
449(a", 0)	454(a", 0)	427(b, 2)	457(ag, 0)	453(a', 0)	461(a, 15)	421(a, 1)	443(a, 6)
480(a", 2)	463(a', 0)	431(a, 0)	457(bg, 0)	462(a', 21)	475(b, 20)	421(b, 1)	450(a, 3)
481(a', 2)	464(a', 2)	462(b, 9)	469(bu, 11)	481(a", 0)	478(a, 25)	427(b, 1)	466(a, 3)
485(a", 0)	469(a", 20)	463(a, 9)	477(ag, 0)	483(a", 14)	479(b, 3)	440(b, 1)	468(a, 11)
491(a', 9)	486(a", 0)	471(a, 7)	480(bg, 0)	497(a', 3)	491(b, 25)	442(a, 12)	485(a, 18)
493(a', 4)	492(a', 15)	472(b, 15)	482(au, 1)	510(a', 12)	506(a, 0)	473(a, 6)	502(a, 7)
496(a", 5)	511(a", 1)	523(a, 2)	488(bu, 21)	530(a", 1)	550(b, 66)	481(b, 6)	514(a, 13)
535(a', 6)	520(a', 13)	525(b, 54)	555(bg, 0)	556(a", 44)	558(a, 5)	504(a, 1)	534(a, 9)
568(a', 112)	562(a", 0)	533(b, 39)	555(au, 91)	579(a', 39)	565(b, 64)	524(b, 81)	566(a, 12)
572(a", 1)	574(a', 59)	546(a, 62)	560(ag, 0)	590(a', 46)	582(a, 86)	532(a, 2)	581(a, 113)
578(a", 181)	583(a', 57)	570(b, 43)	570(bu, 131)	594(a", 40)	585(b, 48)	554(b, 39)	586(a, 82)
595(a', 33)	583(a", 23)	582(a, 0)	619(ag, 0)	614(a', 258)	619(b, 251)	557(a, 10)	601(a, 70)
625(a", 88)	603(a", 228)	590(a, 15)	644(bu, 93)	625(a', 73)	619(a, 23)	588(b, 78)	608(a, 187)
627(a', 59)	615(a', 22)	591(b, 86)	655(ag, 0)	812(a', 3)	664(a, 0)	596(a, 47)	617(a, 16)

865(a', 20)	806(a', 29)	807(b, 69)	744(bu, 108)	886(a", 19)	812(b, 69)	774(b, 46)	982(a, 339)
1711(a', 1382)	1693(a', 237)	1374(a, 53)	1710(ag, 0)	1482(a', 0)	1407(a, 4)	1774(a, 9)	1060(a, 273)
53(a", 0)	67(a", 12)	59(b, 69)	2084(bg, 0)	2079(a', 634)	81(b, 11)	66(b, 512)	71(a, 110)
2056(a", 0)	2076(a", 0)	2060(a, 178)	2089(au, 1609)	2083(a", 701)	2082(a, 63)	2073(a, 336)	2085(a, 301)
2073(a', 799)	2083(a', 1088)	2067(b, 1064)	2089(bu, 1396)	2091(a", 804)	2095(a, 798)	2078(b, 1049)	2095(a, 1046)
79(a', 362)	88(a', 237)	75(a, 519)	2090(ag, 0)	2092(a', 1119)	100(b, 109)	78(a, 152)	98(a, 1)
2092(a", 2479)	2104(a", 2332)	2106(b, 1912)	2129(bu, 2015)	2116(a', 3275)	2110(b, 2306)	2118(b, 1539)	2115(a, 1892)
2135(a', 645)	2137(a', 557)	2126(a, 488)	2142(ag, 0)	2142(a', 18)	2149(a, 497)	2134(a, 179)	2145(a, 427)

Table S19. The theoretical harmonic vibrational frequencies (in cm^{-1}) for $Fe_2(C_2Te_2)(CO)_6$ (infrared intensities in parentheses are in km/mol).

6Te-VI (C_s)	**6Te-XT** (C_s)	**6Te-IT** (C_2)	**6Te-I** (C_{2h})	**6Te-II** (C_s)	**6Te-III** (C_2)	**6Te-IIIT** (C_2)	**6Te-V** (C_1)
30(a, 0)	16(a", 0)	7(b, 0)	19(au, 0)	18(a, 0)	38(a, 0)	14(b, 0)	31(a, 0)
36(a, 0)	23(a", 0)	11(a, 0)	23(bg, 0)	24(a, 0)	49(b, 0)	18(a, 0)	36(a, 0)
47(a, 0)	24(a', 0)	25(a, 0)	25(au, 0)	34(a, 0)	54(a, 0)	28(a, 0)	40(a, 0)
58(a, 0)	31(a', 0)	34(b, 0)	34(bu, 0)	46(a, 0)	72(a, 0)	55(b, 0)	58(a, 0)
67(a, 0)	54(a', 0)	40(a, 0)	57(?a, 0)	51(a, 0)	76(a, 0)	57(a, 0)	66(a, 0)
75(a, 0)	73(a", 0)	61(b, 0)	57(?a, 0)	76(a, 0)	77(b, 0)	67(a, 0)	71(a, 0)
79(a, 0)	74(a', 1)	66(a, 0)	57(bg, 0)	78(a, 0)	85(b, 0)	69(a, 0)	78(a, 0)
84(a, 0)	79(a", 0)	70(a, 0)	80(ag, 0)	80(a, 0)	88(b, 0)	69(b, 0)	79(a, 0)
88(a, 0)	83(a', 0)	71(b, 0)	80(au, 0)	86(a, 0)	90(a, 0)	73(b, 0)	82(a, 0)
90(a, 1)	84(a', 0)	78(a, 0)	80(bu, 0)	90(a, 0)	94(b, 0)	87(a, 0)	87(a, 0)
95(a, 0)	94(a", 0)	80(b, 0)	84(bg, 0)	98(a, 0)	95(a, 0)	89(b, 0)	90(a, 0)
99(a, 0)	97(a', 0)	85(a, 0)	90(ag, 0)	100(a, 0)	105(b, 1)	93(a, 0)	95(a, 0)
102(a, 1)	99(a", 1)	87(b, 0)	93(bu, 0)	108(a, 1)	107(a, 0)	95(b, 0)	108(a, 0)
118(a, 6)	104(a", 0)	97(a, 0)	111(bu, 0)	127(a, 1)	147(b, 1)	114(a, 0)	143(a, 1)
141(a, 1)	140(a', 0)	105(b, 0)	126(ag, 0)	158(a, 1)	149(a, 1)	119(b, 0)	158(a, 0)
166(a, 1)	174(a", 1)	135(a, 0)	161(ag, 0)	170(a, 1)	168(a, 1)	140(a, 0)	173(a, 2)
178(a, 1)	184(a', 1)	184(b, 5)	199(au, 5)	200(a, 2)	176(b, 0)	157(b, 4)	203(a, 0)
225(a, 4)	195(a', 1)	221(a, 2)	226(bu, 15)	220(a, 3)	191(a, 0)	180(a, 1)	235(a, 3)
280(a, 15)	231(a', 9)	328(a, 1)	253(ag, 0)	240(a, 8)	373(b, 6)	252(a, 2)	275(a, 3)
357(a, 12)	331(a", 0)	328(b, 3)	358(bg, 0)	376(a, 0)	398(a, 8)	296(b, 45)	335(a, 11)
405(a, 8)	384(a', 2)	334(a, 0)	377(bu, 62)	384(a, 4)	407(b, 1)	324(b, 2)	362(a, 9)
406(a, 0)	390(a", 1)	336(b, 1)	382(bg, 0)	393(a, 1)	411(a, 0)	326(a, 1)	387(a, 14)
425(a, 12)	405(a', 2)	393(a, 1)	382(au, 2)	405(a, 3)	419(b, 6)	367(b, 9)	402(a, 2)
427(a, 8)	418(a", 12)	398(b, 4)	420(ag, 0)	410(a, 0)	428(a, 4)	381(a, 0)	407(a, 6)
435(a, 10)	429(a", 0)	403(b, 4)	438(au, 0)	423(a, 17)	450(b, 1)	383(b, 6)	421(a, 4)
445(a, 1)	433(a', 0)	421(a, 0)	447(bu, 1)	440(a, 1)	457(a, 1)	395(a, 13)	426(a, 16)
464(a, 7)	450(a", 1)	422(b, 2)	457(bg, 0)	449(a, 0)	466(a, 21)	416(b, 7)	440(a, 7)
467(a, 5)	465(a', 1)	431(a, 0)	458(bu, 9)	469(a, 8)	471(b, 14)	418(a, 1)	446(a, 4)
481(a, 13)	471(a', 0)	448(a, 15)	459(ag, 0)	476(a, 19)	472(a, 24)	422(b, 0)	459(a, 6)
485(a, 15)	476(a", 17)	458(b, 16)	478(ag, 0)	483(a, 2)	477(b, 6)	438(a, 14)	470(a, 3)
489(a, 1)	480(a", 2)	469(a, 12)	481(bu, 28)	496(a, 2)	493(b, 18)	439(b, 2)	486(a, 14)
499(a, 3)	491(a", 0)	475(b, 13)	488(bg, 0)	509(a, 4)	506(a, 0)	459(a, 0)	498(a, 7)
508(a, 9)	494(a', 16)	514(b, 2)	488(au, 4)	516(a, 13)	523(b, 28)	483(b, 5)	512(a, 9)
525(a, 26)	524(a', 15)	517(a, 6)	541(ag, 0)	557(a, 37)	548(a, 10)	488(a, 1)	529(a, 4)
564(a, 30)	562(a", 0)	526(b, 79)	559(bg, 0)	573(a, 52)	561(b, 98)	521(a, 0)	561(a, 12)
579(a, 107)	572(a', 52)	539(a, 45)	561(au, 91)	588(a, 40)	573(a, 57)	523(b, 71)	574(a, 105)
585(a, 49)	583(a", 36)	562(b, 6)	571(bu, 124)	593(a, 40)	583(b, 60)	557(b, 47)	582(a, 64)
597(a, 31)	584(a', 48)	566(a, 14)	601(ag, 0)	610(a, 233)	610(a, 4)	560(a, 6)	593(a, 39)
617(a, 107)	606(a", 220)	577(b, 116)	639(bu, 105)	623(a, 108)	612(b, 238)	586(b, 86)	609(a, 228)
627(a, 109)	615(a', 45)	585(a, 25)	644(ag, 0)	756(a, 4)	623(a, 44)	590(a, 62)	613(a, 6)

702(a, 83)	700(a', 26)	686(b, 68)	676(bu, 66)	826(a, 19)	713(b, 80)	656(b, 22)	853(a, 295)
1583(a, 253)	1689(a', 79)	1352(a, 13)	1668(ag, 0)	1513(a, 0)	1448(a, 1)	1766(a, 6)	958(a, 279)
2061(a, 12)	62(a", 8)	2056(b, 829)	83(bg, 0)	76(a, 322)	74(b, 16)	2064(b, 596)	71(a, 132)
2066(a, 21)	2068(a", 8)	2060(a, 207)	2087(bu, 1308)	2077(a, 260)	2074(a, 106)	2069(a, 73)	2085(a, 143)
2084(a, 729)	2077(a', 1067)	2067(b, 1127)	2088(au, 1589)	2080(a, 1169)	2088(a, 687)	2072(b, 906)	2094(a, 1160)
2087(a, 1177)	83(a', 34)	2075(a, 392)	88(ag, 0)	81(a, 456)	93(b, 971)	2075(a, 1417)	100(a, 880)
2100(a, 2300)	2097(a", 2400)	2104(b, 2003)	2125(bu, 2139)	2108(a, 3290)	2102(b, 2388)	2114(b, 1573)	2116(a, 1850)
2139(a, 801)	2128(a', 858)	2121(a, 725)	2135(ag, 0)	2132(a, 99)	2139(a, 700)	2127(a, 246)	2142(a, 657)

Table S20. The theoretical Cartesian coordinates (in Å) for the structure **8S-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.963847	2.374844	0.000000
2	16	0	2.239867	0.393687	0.000000
3	6	0	0.531794	0.389467	0.000000
4	6	0	-0.531794	-0.389467	0.000000
5	16	0	-2.239867	-0.393687	0.000000
6	26	0	-0.963847	-2.374844	0.000000
7	6	0	-0.966918	-2.213732	1.840061
8	6	0	-0.966918	-2.213732	-1.840061
9	6	0	0.673905	-3.130695	0.000000
10	6	0	-2.141090	-3.778747	0.000000
11	6	0	2.141090	3.778747	0.000000
12	6	0	0.966918	2.213732	1.840061
13	6	0	-0.673905	3.130695	0.000000
14	6	0	0.966918	2.213732	-1.840061
15	8	0	-0.966918	-2.084101	2.980856
16	8	0	-2.890914	-4.653287	0.000000
17	8	0	1.727229	-3.598748	0.000000
18	8	0	-0.966918	-2.084101	-2.980856
19	8	0	2.890914	4.653287	0.000000
20	8	0	0.966918	2.084101	2.980856
21	8	0	-1.727229	3.598748	0.000000
22	8	0	0.966918	2.084101	-2.980856

Table S21. The theoretical Cartesian coordinates (in Å) for the structure **8S-IT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.485125	0.000000	-0.077580
2	16	0	-0.938791	0.000000	-1.871146
3	6	0	-0.472711	0.000000	-0.266606
4	6	0	0.645502	0.000000	0.533602
5	16	0	0.622703	0.000000	2.219474
6	26	0	2.603478	0.000000	0.011722
7	6	0	2.446095	1.830509	0.191257
8	6	0	2.446116	-1.830506	0.191295
9	6	0	2.605425	0.000000	-1.842487
10	6	0	4.395626	0.000000	0.358930
11	6	0	-4.175454	0.000000	-0.800361
12	6	0	-2.361314	1.845304	-0.072080
13	6	0	-2.776146	0.000000	1.715384
14	6	0	-2.361324	-1.845305	-0.072163
15	8	0	2.327601	2.974479	0.265897
16	8	0	5.525200	0.000000	0.600456
17	8	0	2.570635	0.000000	-2.996859
18	8	0	2.327636	-2.974476	0.265961
19	8	0	-5.226278	0.000000	-1.269802
20	8	0	-2.264055	2.988294	-0.067706
21	8	0	-3.043000	0.000000	2.834699
22	8	0	-2.264072	-2.988296	-0.067842

Table S22. The theoretical Cartesian coordinates (in Å) for the structure **8S-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.494204	-0.042580	1.258411
2	6	0	2.009789	-0.559750	2.144282
3	6	0	0.221350	1.487944	2.214608
4	6	0	-0.624271	-1.094131	2.250794
5	8	0	2.949663	-0.878840	2.727245
6	8	0	-1.292133	-1.733512	2.933699
7	8	0	0.032303	2.433245	2.841683
8	26	0	0.494204	-0.042580	-1.258411
9	6	0	2.009789	-0.559750	-2.144282
10	6	0	0.221350	1.487944	-2.214608
11	6	0	-0.624271	-1.094131	-2.250794
12	8	0	2.949663	-0.878840	-2.727245
13	8	0	-1.292133	-1.733512	-2.933699
14	8	0	0.032303	2.433245	-2.841683
15	6	0	1.613758	1.051395	0.000000
16	6	0	0.707673	-1.592308	0.000000
17	8	0	2.462304	1.861117	0.000000
18	8	0	0.884629	-2.752002	0.000000
19	16	0	-2.210181	1.889806	0.000000
20	6	0	-1.022292	0.446652	0.000000
21	6	0	-2.406382	0.127204	0.000000
22	16	0	-3.549217	-1.014773	0.000000

Table S23. The theoretical Cartesian coordinates (in Å) for the structure **8S-VII** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.025697	-0.633222	1.297680
2	6	0	-1.099520	-1.882479	2.063219
3	6	0	1.433632	-1.011849	2.330482
4	6	0	-0.606902	0.780938	2.321366
5	8	0	-1.770489	-2.663241	2.578764
6	8	0	-0.958590	1.642995	2.993375
7	8	0	2.321781	-1.261188	3.018038
8	26	0	-0.025697	-0.633222	-1.297680
9	6	0	-1.099520	-1.882479	-2.063219
10	6	0	1.433632	-1.011849	-2.330482
11	6	0	-0.606902	0.780938	-2.321366
12	8	0	-1.770489	-2.663241	-2.578764
13	8	0	-0.958590	1.642995	-2.993375
14	8	0	2.321781	-1.261188	-3.018038
15	6	0	0.629185	-2.008139	0.000000
16	6	0	-1.495192	-0.170672	0.000000
17	8	0	1.121783	-3.077270	0.000000
18	8	0	-2.618624	0.163318	0.000000
19	16	0	1.397269	0.868521	0.000000
20	6	0	0.918755	2.415709	0.000000
21	6	0	0.423860	3.583916	0.000000
22	16	0	-0.132171	5.080097	0.000000

Table S24. The theoretical Cartesian coordinates (in Å) for the structure **8S-VIII** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.212075	0.000000	0.000000
2	6	0	-1.212075	0.000000	0.000000
3	16	0	0.000000	1.301652	0.000000
4	16	0	0.000000	-1.301652	0.000000
5	26	0	3.078311	0.000000	0.000000
6	26	0	-3.078311	0.000000	0.000000
7	6	0	3.010517	-1.818849	0.000000
8	6	0	4.146713	0.000000	1.470097
9	6	0	3.010517	1.818849	0.000000
10	6	0	4.146713	0.000000	-1.470097
11	6	0	-3.010517	-1.818849	0.000000
12	6	0	-4.146713	0.000000	-1.470097
13	6	0	-3.010517	1.818849	0.000000
14	6	0	-4.146713	0.000000	1.470097
15	8	0	2.981299	-2.971298	0.000000
16	8	0	2.981299	2.971298	0.000000
17	8	0	4.793075	0.000000	2.427967
18	8	0	4.793075	0.000000	-2.427967
19	8	0	-2.981299	-2.971298	0.000000
20	8	0	-4.793075	0.000000	-2.427967
21	8	0	-4.793075	0.000000	2.427967
22	8	0	-2.981299	2.971298	0.000000

Table S25. The theoretical Cartesian coordinates (in Å) for the structure **8S-TS$_3$** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.156573	1.368125	0.934242
2	6	0	0.363764	1.135082	0.956169
3	26	0	-2.691582	0.946855	-0.194380
4	6	0	-3.290413	2.641505	0.147132
5	6	0	-3.705246	0.032397	0.982217
6	6	0	-1.649881	-0.369872	-0.941368
7	6	0	-3.773729	0.882129	-1.663452
8	6	0	0.892610	2.758971	-1.009268
9	6	0	3.029119	1.467984	-1.616083
10	6	0	2.910665	2.477241	0.971993
11	8	0	-3.673119	3.703524	0.378718
12	8	0	-0.992776	-1.159226	-1.464556
13	8	0	-4.342574	-0.558119	1.741117
14	8	0	-4.452338	0.854022	-2.597144
15	8	0	0.244968	3.514845	-1.590466
16	8	0	3.724461	1.440517	-2.537402
17	8	0	3.532583	3.114364	1.705557
18	26	0	1.920459	1.490732	-0.165621
19	6	0	2.514845	-0.178451	0.290065
20	8	0	2.894290	-1.223512	0.593088
21	16	0	-0.253108	-0.181379	1.913950
22	16	0	-0.557397	2.737882	1.826356

Table S26. The theoretical Cartesian coordinates (in Å) for the structure **8Se-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.121378	2.563292	0.000000
2	6	0	0.304586	0.583598	0.000000
3	6	0	-0.304586	-0.583598	0.000000
4	26	0	0.121378	-2.563292	0.000000
5	6	0	0.028301	-2.415798	1.838103
6	6	0	0.028301	-2.415798	-1.838103
7	6	0	1.923001	-2.532958	0.000000
8	6	0	-0.307048	-4.346014	0.000000
9	6	0	0.307048	4.346014	0.000000
10	6	0	-0.028301	2.415798	1.838103
11	6	0	-1.923001	2.532958	0.000000
12	6	0	-0.028301	2.415798	-1.838103
13	8	0	-0.028301	-2.298549	2.979264
14	8	0	-0.592350	-5.461990	0.000000
15	8	0	3.074897	-2.495505	0.000000
16	8	0	-0.028301	-2.298549	-2.979264
17	8	0	0.592350	5.461990	0.000000
18	8	0	0.028301	2.298549	2.979264
19	8	0	-3.074897	2.495505	0.000000
20	8	0	0.028301	2.298549	-2.979264
21	34	0	-2.025080	-1.327361	0.000000
22	34	0	2.025080	1.327361	0.000000

Table S27. The theoretical Cartesian coordinates (in Å) for the structure **8Se-IT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.163046	-2.630447	0.000000
2	6	0	-0.436166	-0.698383	0.000000
3	6	0	0.251989	0.476181	0.000000
4	26	0	-0.047794	2.475731	0.000000
5	6	0	-0.025541	2.334181	1.841932
6	6	0	-0.025541	2.334181	-1.841932
7	6	0	-1.851166	2.682921	0.000000
8	6	0	0.553082	4.213178	0.000000
9	6	0	-0.121060	-4.434021	0.000000
10	6	0	-0.015686	-2.485503	1.830465
11	6	0	2.016134	-2.558309	0.000000
12	6	0	-0.015686	-2.485503	-1.830465
13	8	0	-0.015686	2.224524	2.984309
14	8	0	0.954896	5.291708	0.000000
15	8	0	-2.979296	2.910628	0.000000
16	8	0	-0.015686	2.224524	-2.984309
17	8	0	-0.323140	-5.571286	0.000000
18	8	0	-0.090763	-2.371335	2.974843
19	8	0	3.168193	-2.475920	0.000000
20	8	0	-0.090763	-2.371335	-2.974843
21	34	0	1.995465	1.062506	0.000000
22	34	0	-2.284899	-0.802006	0.000000

Table S28. The theoretical Cartesian coordinates (in Å) for the structure **8Se-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.106871	-0.933264	1.258765
2	6	0	-0.625480	-2.452713	2.134911
3	6	0	1.422442	-0.670285	2.222697
4	6	0	-1.158547	0.174684	2.265454
5	8	0	-0.947461	-3.396156	2.710491
6	8	0	-1.795065	0.827966	2.964551
7	8	0	2.364129	-0.496791	2.859211
8	26	0	-0.106871	-0.933264	-1.258765
9	6	0	-0.625480	-2.452713	-2.134911
10	6	0	1.422442	-0.670285	-2.222697
11	6	0	-1.158547	0.174684	-2.265454
12	8	0	-0.947461	-3.396156	-2.710491
13	8	0	-1.795065	0.827966	-2.964551
14	8	0	2.364129	-0.496791	-2.859211
15	6	0	0.990891	-2.048360	0.000000
16	6	0	-1.657362	-1.140573	0.000000
17	8	0	1.802759	-2.894898	0.000000
18	8	0	-2.817110	-1.316200	0.000000
19	6	0	0.383635	0.592738	0.000000
20	6	0	0.061348	1.961748	0.000000
21	34	0	1.985512	1.854716	0.000000
22	34	0	-1.238617	3.158362	0.000000

Table S29. The theoretical Cartesian coordinates (in Å) for the structure **8Se-VII** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.137047	-1.109383	1.306630
2	6	0	-1.304341	-2.283177	2.044908
3	6	0	1.273912	-1.598586	2.355072
4	6	0	-0.625296	0.337625	2.331744
5	8	0	-2.033616	-3.019679	2.546617
6	8	0	-0.927023	1.214671	3.008925
7	8	0	2.128172	-1.920460	3.056525
8	26	0	-0.137047	-1.109383	-1.306630
9	6	0	-1.304341	-2.283177	-2.044908
10	6	0	1.273912	-1.598586	-2.355072
11	6	0	-0.625296	0.337625	-2.331744
12	8	0	-2.033616	-3.019679	-2.546617
13	8	0	-0.927023	1.214671	-3.008925
14	8	0	2.128172	-1.920460	-3.056525
15	6	0	0.438445	-2.511185	0.000000
16	6	0	-1.557692	-0.532192	0.000000
17	8	0	0.877628	-3.603968	0.000000
18	8	0	-2.650886	-0.109280	0.000000
19	6	0	0.956693	2.061185	0.000000
20	6	0	0.405117	3.198846	0.000000
21	34	0	1.487721	0.381395	0.000000
22	34	0	-0.280507	4.801873	0.000000

Table S30. The theoretical Cartesian coordinates (in Å) for the structure **8Se-VIII** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.311705	0.000000	0.000000
2	6	0	1.311705	0.000000	0.000000
3	26	0	-3.182711	0.000000	0.000000
4	26	0	3.182711	0.000000	0.000000
5	6	0	-3.107456	1.816808	0.000000
6	6	0	-4.250790	0.000000	1.469942
7	6	0	-3.107456	-1.816808	0.000000
8	6	0	-4.250790	0.000000	-1.469942
9	6	0	3.107456	1.816808	0.000000
10	6	0	4.250790	0.000000	-1.469942
11	6	0	3.107456	-1.816808	0.000000
12	6	0	4.250790	0.000000	1.469942
13	8	0	-3.062672	2.969246	0.000000
14	8	0	-3.062672	-2.969246	0.000000
15	8	0	-4.896650	0.000000	2.428209
16	8	0	-4.896650	0.000000	-2.428209
17	8	0	3.062672	2.969246	0.000000
18	8	0	4.896650	0.000000	-2.428209
19	8	0	4.896650	0.000000	2.428209
20	8	0	3.062672	-2.969246	0.000000
21	34	0	0.000000	-1.415541	0.000000
22	34	0	0.000000	1.415541	0.000000

Table S31. The theoretical Cartesian coordinates (in Å) for the structure **8Se-TS$_3$** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.265745	1.227548	1.115767
2	6	0	0.477284	1.339133	1.123383
3	26	0	-2.706285	0.886900	-0.125812
4	6	0	-3.092769	2.674217	-0.082259
5	6	0	-3.946324	0.201879	0.990418
6	6	0	-1.764742	-0.576210	-0.700014
7	6	0	-3.627677	0.803653	-1.695331
8	6	0	0.987876	2.927605	-0.875998
9	6	0	2.884501	1.469233	-1.679191
10	6	0	3.151036	2.367259	0.926102
11	8	0	-3.357862	3.796835	-0.054748
12	8	0	-1.185046	-1.472322	-1.139028
13	8	0	-4.725515	-0.237573	1.721083
14	8	0	-4.199867	0.765538	-2.698074
15	8	0	0.403487	3.759664	-1.421997
16	8	0	3.474825	1.402679	-2.669854
17	8	0	3.914380	2.892623	1.615636
18	26	0	1.935082	1.550624	-0.126318
19	6	0	2.331680	-0.217585	0.121492
20	8	0	2.602602	-1.328238	0.277945
21	34	0	-0.243299	-0.178636	2.100249
22	34	0	-0.558595	2.840788	1.937411

Table S32. The theoretical Cartesian coordinates (in Å) for the structure **8Te-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.088660	2.564693	0.000000
2	52	0	2.279369	1.337427	0.000000
3	6	0	0.310150	0.579140	0.000000
4	6	0	-0.310150	-0.579140	0.000000
5	52	0	-2.279369	-1.337427	0.000000
6	26	0	0.088660	-2.564693	0.000000
7	6	0	0.010182	-2.421337	1.837556
8	6	0	0.010182	-2.421337	-1.837556
9	6	0	1.886762	-2.546782	0.000000
10	6	0	-0.338559	-4.348206	0.000000
11	6	0	0.338559	4.348206	0.000000
12	6	0	-0.010182	2.421337	1.837556
13	6	0	-1.886762	2.546782	0.000000
14	6	0	-0.010182	2.421337	-1.837556
15	8	0	-0.010182	-2.311688	2.981261
16	8	0	-0.627424	-5.463260	0.000000
17	8	0	3.039487	-2.530798	0.000000
18	8	0	-0.010182	-2.311688	-2.981261
19	8	0	0.627424	5.463260	0.000000
20	8	0	0.010182	2.311688	2.981261
21	8	0	-3.039487	2.530798	0.000000
22	8	0	0.010182	2.311688	-2.981261

Table S33. The theoretical Cartesian coordinates (in Å) for the structure **8Te-IT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.451483	0.334449	-0.000576
2	52	0	1.351533	-2.099692	-0.000669
3	6	0	0.494080	-0.201962	-0.000158
4	6	0	-0.749951	0.309929	0.000239
5	52	0	-1.169676	2.354427	0.000662
6	26	0	-2.608944	-0.493280	0.000591
7	6	0	-2.462897	-0.352856	1.830532
8	6	0	-2.463835	-0.352290	-1.829380
9	6	0	-2.413409	-2.336760	0.000256
10	6	0	-4.427771	-0.307706	0.001086
11	6	0	4.245045	-0.062102	-0.001095
12	6	0	2.302390	0.297979	1.837493
13	6	0	2.488379	2.144201	-0.000307
14	6	0	2.301450	0.298544	-1.838579
15	8	0	-2.340867	-0.306005	2.975841
16	8	0	-5.573738	-0.164071	0.001402
17	8	0	-2.267301	-3.482820	0.000000
18	8	0	-2.342392	-0.305085	-2.974738
19	8	0	5.361750	-0.342274	-0.001423
20	8	0	2.188634	0.297490	2.980595
21	8	0	2.631368	3.287046	-0.000168
22	8	0	2.187111	0.298407	-2.981623

Table S34. The theoretical Cartesian coordinates (in Å) for the structure **8Te-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.197046	1.288770	1.259426
2	6	0	0.766747	2.798466	2.117209
3	6	0	-1.331831	1.097471	2.243495
4	6	0	1.211903	0.165031	2.286985
5	8	0	1.123329	3.736791	2.680744
6	8	0	1.821914	-0.490294	3.007382
7	8	0	-2.266354	0.987464	2.904105
8	26	0	0.197046	1.288770	-1.259426
9	6	0	0.766747	2.798466	-2.117209
10	6	0	-1.331831	1.097471	-2.243495
11	6	0	1.211903	0.165031	-2.286985
12	8	0	1.123329	3.736791	-2.680744
13	8	0	1.821914	-0.490294	-3.007382
14	8	0	-2.266354	0.987464	-2.904105
15	6	0	-0.874477	2.425519	0.000000
16	6	0	1.752248	1.439445	0.000000
17	8	0	-1.668120	3.289444	0.000000
18	8	0	2.917343	1.575509	0.000000
19	6	0	-0.339649	-0.240695	0.000000
20	6	0	-0.056230	-1.598959	0.000000
21	52	0	1.393420	-2.959121	0.000000
22	52	0	-2.196411	-1.551697	0.000000

Table S35. The theoretical Cartesian coordinates (in Å) for the structure **8Te-VII** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.256354	-1.551733	1.317860
2	6	0	-1.485748	-2.681858	2.015349
3	6	0	1.106176	-2.119876	2.386230
4	6	0	-0.707921	-0.102473	2.353320
5	8	0	-2.254275	-3.390838	2.498209
6	8	0	-1.002604	0.765806	3.045667
7	8	0	1.924664	-2.497145	3.104044
8	26	0	-0.256354	-1.551733	-1.317860
9	6	0	-1.485748	-2.681858	-2.015349
10	6	0	1.106176	-2.119876	-2.386230
11	6	0	-0.707921	-0.102473	-2.353320
12	8	0	-2.254275	-3.390838	-2.498209
13	8	0	-1.002604	0.765806	-3.045667
14	8	0	1.924664	-2.497145	-3.104044
15	6	0	0.276302	-2.961092	0.000000
16	6	0	-1.633144	-0.901599	0.000000
17	8	0	0.690055	-4.064429	0.000000
18	8	0	-2.702835	-0.420802	0.000000
19	6	0	0.845633	1.828597	0.000000
20	6	0	0.378662	2.994656	0.000000
21	52	0	1.568661	0.011455	0.000000
22	52	0	-0.326482	4.827274	0.000000

Table S36. The theoretical Cartesian coordinates (in Å) for the structure **8Te-VIII** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.437522	0.000000	0.000000
2	6	0	1.437522	0.000000	0.000000
3	26	0	-3.313438	0.000000	0.000000
4	26	0	3.313438	0.000000	0.000000
5	6	0	-3.240863	1.812976	0.000000
6	6	0	-4.381618	0.000000	1.468829
7	6	0	-3.240863	-1.812976	0.000000
8	6	0	-4.381618	0.000000	-1.468829
9	6	0	3.240863	1.812976	0.000000
10	6	0	4.381618	0.000000	-1.468829
11	6	0	3.240863	-1.812976	0.000000
12	6	0	4.381618	0.000000	1.468829
13	8	0	-3.194644	2.966552	0.000000
14	8	0	-3.194644	-2.966552	0.000000
15	8	0	-5.026220	0.000000	2.428051
16	8	0	-5.026220	0.000000	-2.428051
17	8	0	3.194644	2.966552	0.000000
18	8	0	5.026220	0.000000	-2.428051
19	8	0	5.026220	0.000000	2.428051
20	8	0	3.194644	-2.966552	0.000000
21	52	0	0.000000	-1.589508	0.000000
22	52	0	0.000000	1.589508	0.000000

Table S37. The theoretical Cartesian coordinates (in Å) for the structure **8Te-TS$_3$** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.417280	0.906541	1.137736
2	6	0	0.490869	1.026336	1.332478
3	26	0	-2.679721	0.914051	-0.338326
4	6	0	-2.931225	2.707704	-0.132727
5	6	0	-3.895492	0.005731	0.624128
6	6	0	-1.598180	-0.226237	-1.256500
7	6	0	-3.684698	1.045534	-1.848474
8	6	0	1.022446	3.123139	-0.278018
9	6	0	1.933074	0.968010	-1.452850
10	6	0	3.490484	2.585615	0.322491
11	8	0	-3.130947	3.842543	-0.015641
12	8	0	-0.930874	-0.922820	-1.897641
13	8	0	-4.666523	-0.580887	1.258857
14	8	0	-4.314625	1.137073	-2.813132
15	8	0	0.503543	4.044858	-0.732862
16	8	0	1.941460	0.544408	-2.525737
17	8	0	4.454131	3.218232	0.395984
18	26	0	1.947786	1.608789	0.238505
19	6	0	2.778878	0.153820	0.931872
20	8	0	3.279821	-0.783047	1.381898
21	52	0	-0.363777	-0.867198	1.867852
22	52	0	-0.740122	2.443420	2.460971

Table S38. The theoretical Cartesian coordinates (in Å) for the structure **7S-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.677970	-2.595946	0.000000
2	16	0	-2.128469	-1.003745	0.000000
3	6	0	-0.435130	-0.657703	0.000000
4	6	0	0.419561	0.343938	0.000000
5	16	0	2.095045	0.691554	0.000000
6	26	0	0.444765	2.372623	0.000000
7	6	0	0.483525	2.213605	1.839859
8	6	0	0.483525	2.213605	-1.839859
9	6	0	-1.308554	2.790397	0.000000
10	6	0	1.320971	3.982197	0.000000
11	6	0	-1.705594	-4.133026	0.000000
12	6	0	0.510943	-2.984222	1.283233
13	6	0	0.510943	-2.984222	-1.283233
14	8	0	0.510943	2.085210	2.980517
15	8	0	1.883365	4.987522	0.000000
16	8	0	-2.434353	3.039640	0.000000
17	8	0	0.510943	2.085210	-2.980517
18	8	0	-2.337709	-5.095623	0.000000
19	8	0	1.240717	-3.170104	2.156671
20	8	0	1.240717	-3.170104	-2.156671

Table S39. The theoretical Cartesian coordinates (in Å) for the structure **7S-II** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	2.462046	0.000000	-0.022299
2	6	0	0.549771	0.662542	-0.186367
3	6	0	0.549771	-0.662526	-0.186440
4	16	0	-0.835175	-1.631196	-0.199119
5	16	0	-0.835174	1.631214	-0.198941
6	26	0	-2.435970	0.000000	-0.112043
7	6	0	-2.742497	0.000000	1.632165
8	6	0	-3.599608	-1.304249	-0.591616
9	6	0	-3.599607	1.304310	-0.591481
10	6	0	2.115676	-0.000103	1.788927
11	6	0	3.584344	-1.434633	0.072431
12	6	0	2.431577	0.000101	-1.873805
13	6	0	3.584331	1.434633	0.072590
14	8	0	-4.345078	2.132545	-0.892604
15	8	0	-2.941577	-0.000142	2.770313
16	8	0	-4.345081	-2.132451	-0.892823
17	8	0	2.368971	0.000163	-3.020152
18	8	0	1.852010	-0.000165	2.906895
19	8	0	4.255683	2.368229	0.129533
20	8	0	4.255707	-2.368227	0.129269

Table S40. The theoretical Cartesian coordinates (in Å) for the structure **7S-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.314380	-0.092427	1.527591
2	6	0	0.209375	1.595423	2.130950
3	6	0	-0.783417	-0.791912	2.893130
4	6	0	1.871716	-0.541055	2.308695
5	8	0	0.138888	2.687084	2.497173
6	8	0	2.876225	-0.839416	2.789982
7	8	0	-1.399144	-1.184375	3.782847
8	26	0	0.314380	-0.092427	-1.527591
9	6	0	0.209375	1.595423	-2.130950
10	6	0	-0.783417	-0.791912	-2.893130
11	6	0	1.871716	-0.541055	-2.308695
12	8	0	0.138888	2.687084	-2.497173
13	8	0	2.876225	-0.839416	-2.789982
14	8	0	-1.399144	-1.184375	-3.782847
15	6	0	-1.103374	-0.339994	0.000000
16	6	0	1.410509	0.640517	0.000000
17	8	0	2.392033	1.323941	0.000000
18	6	0	-2.379000	-0.016214	0.000000
19	16	0	-3.856269	0.485003	0.000000
20	16	0	-0.173756	-1.813336	0.000000

Table S41. The theoretical Cartesian coordinates (in Å) for the structure **7S-IV** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000000	1.246840	0.154016
2	6	0	1.367070	2.178979	0.941240
3	6	0	0.000000	2.169776	-1.420861
4	6	0	-1.367070	2.178979	0.941240
5	8	0	2.221810	2.789180	1.412390
6	8	0	-2.221810	2.789180	1.412390
7	8	0	0.000000	2.768557	-2.403370
8	26	0	0.000000	-1.246840	0.154016
9	6	0	1.367070	-2.178979	0.941240
10	6	0	0.000000	-2.169776	-1.420861
11	6	0	-1.367070	-2.178979	0.941240
12	8	0	2.221810	-2.789180	1.412390
13	8	0	-2.221810	-2.789180	1.412390
14	8	0	0.000000	-2.768557	-2.403370
15	6	0	1.340642	0.000000	-0.639894
16	6	0	-1.340642	0.000000	-0.639894
17	6	0	0.000000	0.000000	1.726248
18	8	0	0.000000	0.000000	2.900367
19	16	0	2.706842	0.000000	-1.442891
20	16	0	-2.706842	0.000000	-1.442891

Table S42. The theoretical Cartesian coordinates (in Å) for the structure **7S-Int$_1$** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.301117	-0.163764	-0.649587
2	6	0	-1.775201	1.511967	-0.084842
3	26	0	2.021216	0.001810	0.069688
4	6	0	1.300431	0.053567	1.732803
5	6	0	2.837183	1.597030	0.314001
6	6	0	2.590864	-0.084148	-1.652646
7	6	0	3.095058	-1.380462	0.532294
8	6	0	-2.021015	-0.211775	1.734064
9	6	0	-1.474234	-2.129887	0.069541
10	8	0	0.843938	0.087349	2.792760
11	8	0	2.935883	-0.141189	-2.752310
12	8	0	3.344537	2.627679	0.461664
13	8	0	3.771035	-2.274661	0.822488
14	8	0	-2.268830	-0.145339	2.859085
15	8	0	-1.253514	-3.254500	0.149065
16	26	0	-1.787094	-0.296798	-0.049403
17	6	0	-3.491782	-0.448073	-0.675425
18	8	0	-4.571816	-0.512923	-1.072381
19	16	0	-1.731277	3.054061	-0.116007
20	16	0	-0.560696	-0.297085	-2.042217

Table S43. The theoretical Cartesian coordinates (in Å) for the structure **7S-TS** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.511684	0.803251	-0.330574
2	6	0	0.244361	2.199438	0.546324
3	26	0	-2.123162	0.875392	-1.329050
4	6	0	-1.806732	2.647366	-1.646766
5	6	0	-3.908578	1.229348	-1.149727
6	6	0	-2.400947	-0.836021	-0.770990
7	6	0	-1.867720	0.398948	-3.045428
8	6	0	1.764528	3.054193	-1.409272
9	6	0	2.195673	0.496959	-1.954498
10	8	0	-1.614584	3.759534	-1.878304
11	8	0	-2.578201	-1.916795	-0.413831
12	8	0	-5.034207	1.454542	-1.018573
13	8	0	-1.676679	0.086707	-4.142039
14	8	0	1.928833	4.061066	-1.947383
15	8	0	2.585256	-0.153756	-2.820011
16	26	0	1.532019	1.502570	-0.530025
17	6	0	2.987993	1.597195	0.524208
18	8	0	3.886278	1.676041	1.243349
19	16	0	0.482539	-0.392431	0.349305
20	16	0	-0.497135	3.089964	1.618819

Table S44. The theoretical Cartesian coordinates (in Å) for the structure **7S-Int$_2$** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.163095	0.666667	-1.097616
2	6	0	-1.082882	1.575017	-0.648294
3	26	0	1.436240	0.171899	-0.024030
4	6	0	1.182842	1.584387	1.113245
5	6	0	2.700612	1.045845	-0.970331
6	6	0	1.644052	-1.380300	-1.031280
7	6	0	2.318037	-0.690005	1.326853
8	6	0	-1.196396	-0.049492	1.868233
9	6	0	-0.850914	-2.327141	0.428537
10	8	0	1.094106	2.474791	1.836150
11	8	0	1.938947	-2.352300	-1.569411
12	8	0	3.490443	1.606459	-1.594596
13	8	0	2.849655	-1.242783	2.187964
14	8	0	-1.277212	0.258067	2.979320
15	8	0	-0.692451	-3.456792	0.603691
16	26	0	-1.144612	-0.562082	0.145239
17	6	0	-2.942229	-0.636604	-0.067606
18	8	0	-4.084612	-0.674886	-0.209243
19	16	0	-1.882399	2.922864	-0.448702
20	16	0	-0.854695	-0.515733	-2.210853

Table S45. The theoretical Cartesian coordinates (in Å) for the structure **7Se-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.660386	-2.571711	0.000000
2	34	0	-2.296380	-0.986738	0.000000
3	6	0	-0.423339	-0.646958	0.000000
4	6	0	0.399273	0.379496	0.000000
5	34	0	2.249650	0.709301	0.000000
6	26	0	0.440701	2.399460	0.000000
7	6	0	0.500764	2.231325	1.837992
8	6	0	0.500764	2.231325	-1.837992
9	6	0	-1.317198	2.790193	0.000000
10	6	0	1.271595	4.034223	0.000000
11	6	0	-1.657690	-4.126755	0.000000
12	6	0	0.529301	-2.933918	1.287623
13	6	0	0.529301	-2.933918	-1.287623
14	8	0	0.529301	2.101280	2.978880
15	8	0	1.809696	5.052620	0.000000
16	8	0	-2.446834	3.020252	0.000000
17	8	0	0.529301	2.101280	-2.978880
18	8	0	-2.285732	-5.092236	0.000000
19	8	0	1.263636	-3.106517	2.159880
20	8	0	1.263636	-3.106517	-2.159880

Table S46. The theoretical Cartesian coordinates (in Å) for the structure **7Se-II** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.087513	-2.679233	0.000000
2	6	0	0.173162	-0.749853	0.657017
3	6	0	0.173162	-0.749853	-0.657017
4	26	0	0.000000	2.398454	0.000000
5	6	0	-1.753618	2.623128	0.000000
6	6	0	0.426559	3.571643	-1.308470
7	6	0	0.426559	3.571643	1.308470
8	6	0	-1.737996	-2.418091	0.000000
9	6	0	0.039480	-3.796713	-1.437809
10	6	0	1.934612	-2.580723	0.000000
11	6	0	0.039480	-3.796713	1.437809
12	8	0	0.693800	4.334062	2.133994
13	8	0	-2.899955	2.770396	0.000000
14	8	0	0.693800	4.334062	-2.133994
15	8	0	3.078017	-2.474856	0.000000
16	8	0	-2.867107	-2.207067	0.000000
17	8	0	0.010449	-4.471634	2.370824
18	8	0	0.010449	-4.471634	-2.370824
19	34	0	0.141769	0.746279	-1.736536
20	34	0	0.141769	0.746279	1.736536

Table S47. The theoretical Cartesian coordinates (in Å) for the structure **7Se-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.079340	-0.660937	1.528897
2	6	0	1.782921	-0.483412	2.062494
3	6	0	-0.613751	0.450730	2.882126
4	6	0	-0.282729	-2.209877	2.368749
5	8	0	2.883519	-0.364310	2.387585
6	8	0	-0.526236	-3.210248	2.888126
7	8	0	-1.009226	1.089303	3.754335
8	26	0	0.079340	-0.660937	-1.528897
9	6	0	1.782921	-0.483412	-2.062494
10	6	0	-0.613751	0.450730	-2.882126
11	6	0	-0.282729	-2.209877	-2.368749
12	8	0	2.883519	-0.364310	-2.387585
13	8	0	-0.526236	-3.210248	-2.888126
14	8	0	-1.009226	1.089303	-3.754335
15	6	0	-0.214886	0.754998	0.000000
16	6	0	0.790977	-1.769267	0.000000
17	8	0	1.451949	-2.766032	0.000000
18	6	0	-0.033520	2.055762	0.000000
19	34	0	-1.826663	-0.283188	0.000000
20	34	0	0.320695	3.722094	0.000000

Table S48. The theoretical Cartesian coordinates (in Å) for the structure **7Se-IV** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000000	1.244758	0.405311
2	6	0	1.369846	2.176233	1.193658
3	6	0	0.000000	2.172947	-1.166274
4	6	0	-1.369846	2.176233	1.193658
5	8	0	2.227573	2.781804	1.664467
6	8	0	-2.227573	2.781804	1.664467
7	8	0	0.000000	2.772115	-2.147949
8	26	0	0.000000	-1.244758	0.405311
9	6	0	1.369846	-2.176233	1.193658
10	6	0	0.000000	-2.172947	-1.166274
11	6	0	-1.369846	-2.176233	1.193658
12	8	0	2.227573	-2.781804	1.664467
13	8	0	-2.227573	-2.781804	1.664467
14	8	0	0.000000	-2.772115	-2.147949
15	6	0	1.332273	0.000000	-0.393354
16	6	0	-1.332273	0.000000	-0.393354
17	6	0	0.000000	0.000000	1.982245
18	8	0	0.000000	0.000000	3.155505
19	34	0	2.820902	0.000000	-1.280025
20	34	0	-2.820902	0.000000	-1.280025

Table S49. The theoretical Cartesian coordinates (in Å) for the structure **7Se-Int$_1$** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.511369	-0.359377	-0.409770
2	6	0	-1.760528	0.995368	0.022424
3	26	0	2.205814	0.166360	0.181469
4	6	0	1.518897	0.353380	1.848590
5	6	0	2.792147	1.878376	0.174680
6	6	0	2.730104	-0.072975	-1.540655
7	6	0	3.496284	-0.954978	0.780800
8	6	0	-1.663352	-0.506797	2.059836
9	6	0	-0.837145	-2.494265	0.565715
10	8	0	1.085126	0.478075	2.911218
11	8	0	3.048398	-0.228976	-2.638705
12	8	0	3.142512	2.981913	0.156848
13	8	0	4.305311	-1.690747	1.160542
14	8	0	-1.880770	-0.348084	3.181382
15	8	0	-0.406137	-3.545331	0.737791
16	26	0	-1.482888	-0.766280	0.287286
17	6	0	-3.174159	-1.268829	-0.175382
18	8	0	-4.246571	-1.553562	-0.485721
19	34	0	-1.985358	2.648063	-0.218189
20	34	0	-0.392900	-0.841233	-1.909220

Table S50. The theoretical Cartesian coordinates (in Å) for the structure **7Se-TS** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505480	0.779475	-0.378053
2	6	0	0.259447	2.206805	0.639783
3	26	0	-2.087858	0.869440	-1.404240
4	6	0	-1.699170	2.618979	-1.737926
5	6	0	-3.842090	1.296184	-1.134084
6	6	0	-2.398313	-0.834836	-0.845082
7	6	0	-1.936308	0.388582	-3.136571
8	6	0	1.712540	3.074279	-1.352895
9	6	0	2.123943	0.511297	-1.906134
10	8	0	-1.458227	3.723242	-1.962733
11	8	0	-2.593263	-1.911529	-0.483616
12	8	0	-4.947310	1.569461	-0.935717
13	8	0	-1.808686	0.074853	-4.242034
14	8	0	1.873674	4.080127	-1.893495
15	8	0	2.462344	-0.142012	-2.790884
16	26	0	1.509895	1.523840	-0.466594
17	6	0	3.017653	1.612873	0.522367
18	8	0	3.944603	1.685702	1.204483
19	34	0	0.511359	-0.505222	0.498571
20	34	0	-0.622899	3.103383	1.810208

Table S51. The theoretical Cartesian coordinates (in Å) for the structure **7Se-Int$_2$** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.740951	1.313304	0.447513
2	6	0	-0.170900	2.446748	0.937465
3	26	0	-1.597074	1.191695	-1.339199
4	6	0	-1.665712	3.018690	-1.468284
5	6	0	-3.330195	1.083660	-0.844120
6	6	0	-1.418501	-0.663518	-1.354473
7	6	0	-1.577398	1.115170	-3.165022
8	6	0	1.292136	2.662002	-1.650122
9	6	0	1.554724	-0.038958	-1.725816
10	8	0	-1.770326	4.157182	-1.590332
11	8	0	-1.430089	-1.799267	-1.533279
12	8	0	-4.428822	1.007740	-0.505348
13	8	0	-1.538732	1.073549	-4.316821
14	8	0	1.540309	3.565761	-2.325620
15	8	0	1.937551	-0.859587	-2.441787
16	26	0	0.990836	1.245980	-0.582519
17	6	0	2.519711	1.422252	0.372590
18	8	0	3.489585	1.545011	0.981586
19	34	0	0.038271	3.903763	1.847313
20	34	0	0.096348	-0.251833	1.203686

Table S52. The theoretical Cartesian coordinates (in Å) for the structure **7Te-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.448772	-0.955989	0.000000
2	52	0	-2.266312	1.508838	0.000000
3	6	0	-0.757351	-0.031091	0.000000
4	6	0	0.554149	-0.088883	0.000000
5	52	0	2.016696	-1.617712	0.000000
6	26	0	2.223781	1.043241	0.000000
7	6	0	2.117517	0.912662	1.837752
8	6	0	2.117517	0.912662	-1.837752
9	6	0	1.521438	2.698730	0.000000
10	6	0	4.034702	1.334054	0.000000
11	6	0	-4.285535	-1.121641	0.000000
12	6	0	-2.021184	-2.110806	1.295204
13	6	0	-2.021184	-2.110806	-1.295204
14	8	0	2.016696	0.850576	2.980760
15	8	0	5.175311	1.493950	0.000000
16	8	0	1.069499	3.759242	0.000000
17	8	0	2.016696	0.850576	-2.980760
18	8	0	-5.433879	-1.219843	0.000000
19	8	0	-1.717829	-2.803240	2.166303
20	8	0	-1.717829	-2.803240	-2.166303

Table S53. The theoretical Cartesian coordinates (in Å) for the structure **7Te-II** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.909825	-0.000009	0.022780
2	6	0	-0.973886	-0.653339	-0.126588
3	6	0	-0.973885	0.653298	-0.126579
4	52	0	0.666877	1.883912	-0.156593
5	52	0	0.666900	-1.883927	-0.156594
6	26	0	2.436383	0.000003	-0.058014
7	6	0	2.673267	-0.000013	1.693241
8	6	0	3.601318	1.305162	-0.490433
9	6	0	3.601330	-1.305136	-0.490468
10	6	0	-2.597844	-0.000055	1.838302
11	6	0	-4.013576	1.442897	0.106902
12	6	0	-2.881258	-0.000031	-1.823127
13	6	0	-4.013759	-1.442776	0.106894
14	8	0	4.376973	-2.121046	-0.754964
15	8	0	2.848912	-0.000019	2.836352
16	8	0	4.376952	2.121088	-0.754908
17	8	0	-2.817537	-0.000051	-2.970231
18	8	0	-2.352890	-0.000090	2.960994
19	8	0	-4.689938	-2.375151	0.158434
20	8	0	-4.689610	2.375377	0.158440

Table S54. The theoretical Cartesian coordinates (in Å) for the structure **7Te-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.283717	-0.919869	1.526887
2	6	0	1.999529	-0.637419	1.957788
3	6	0	-0.393991	0.210418	2.866229
4	6	0	0.047353	-2.448311	2.445382
5	8	0	3.106262	-0.449040	2.225014
6	8	0	-0.114530	-3.436154	3.018029
7	8	0	-0.775629	0.880916	3.720786
8	26	0	0.283717	-0.919869	-1.526887
9	6	0	1.999529	-0.637419	-1.957788
10	6	0	-0.393991	0.210418	-2.866229
11	6	0	0.047353	-2.448311	-2.445382
12	8	0	3.106262	-0.449040	-2.225014
13	8	0	-0.114530	-3.436154	-3.018029
14	8	0	-0.775629	0.880916	-3.720786
15	6	0	-0.100449	0.480994	0.000000
16	6	0	0.976004	-2.041072	0.000000
17	8	0	1.619297	-3.049336	0.000000
18	6	0	-0.038308	1.786698	0.000000
19	52	0	-1.892512	-0.732644	0.000000
20	52	0	0.199752	3.683420	0.000000

Table S55. The theoretical Cartesian coordinates (in Å) for the structure **7Te-IV** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000000	1.238406	0.621620
2	6	0	1.370179	2.171599	1.411815
3	6	0	0.000000	2.167048	-0.946332
4	6	0	-1.370179	2.171599	1.411815
5	8	0	2.228430	2.774993	1.883834
6	8	0	-2.228430	2.774993	1.883834
7	8	0	0.000000	2.766873	-1.927320
8	26	0	0.000000	-1.238406	0.621620
9	6	0	1.370179	-2.171599	1.411815
10	6	0	0.000000	-2.167048	-0.946332
11	6	0	-1.370179	-2.171599	1.411815
12	8	0	2.228430	-2.774993	1.883834
13	8	0	-2.228430	-2.774993	1.883834
14	8	0	0.000000	-2.766873	-1.927320
15	6	0	1.325728	0.000000	-0.182239
16	6	0	-1.325728	0.000000	-0.182239
17	6	0	0.000000	0.000000	2.205293
18	8	0	0.000000	0.000000	3.377454
19	52	0	2.997632	0.000000	-1.176557
20	52	0	-2.997632	0.000000	-1.176557

Table S56. The theoretical Cartesian coordinates (in Å) for the structure **7Te-Int$_1$** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.749853	-0.338300	-0.192211
2	6	0	-1.707966	0.469557	0.149253
3	26	0	2.297916	0.631292	0.190052
4	6	0	1.462242	1.235443	1.680298
5	6	0	2.802248	2.330764	-0.201092
6	6	0	2.897479	0.082331	-1.432842
7	6	0	3.637465	-0.174249	1.102148
8	6	0	-1.155495	-0.510696	2.429667
9	6	0	0.075516	-2.506181	1.243061
10	8	0	0.932585	1.652399	2.617652
11	8	0	3.267432	-0.267308	-2.468716
12	8	0	3.096392	3.416103	-0.476055
13	8	0	4.471108	-0.716145	1.693825
14	8	0	-1.345742	-0.190939	3.521180
15	8	0	0.776846	-3.357831	1.565509
16	52	0	-0.110645	-1.420706	-1.726786
17	52	0	-2.427230	2.125841	-0.414955
18	26	0	-1.008924	-1.072217	0.729017
19	6	0	-2.554860	-2.031482	0.583848
20	8	0	-3.546525	-2.604536	0.459346

Table S57. The theoretical Cartesian coordinates (in Å) for the structure **7Te-TS** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.483281	0.742104	-0.419974
2	6	0	0.301016	2.225274	0.728905
3	26	0	-2.046483	0.837430	-1.460728
4	6	0	-1.620154	2.571439	-1.809538
5	6	0	-3.781011	1.320421	-1.175871
6	6	0	-2.406444	-0.842254	-0.866276
7	6	0	-1.934545	0.331566	-3.192425
8	6	0	1.630730	3.093410	-1.331361
9	6	0	2.044748	0.536100	-1.896869
10	8	0	-1.370454	3.674401	-2.033035
11	8	0	-2.636215	-1.903606	-0.478460
12	8	0	-4.873287	1.630370	-0.958712
13	8	0	-1.827861	0.002630	-4.295623
14	8	0	1.781405	4.101918	-1.870139
15	8	0	2.339755	-0.099841	-2.809568
16	52	0	0.575982	-0.658037	0.717831
17	52	0	-0.714572	3.203473	2.033280
18	26	0	1.480894	1.546256	-0.436005
19	6	0	3.045887	1.661048	0.466746
20	8	0	4.008456	1.752457	1.095142

Table S58. The theoretical Cartesian coordinates (in Å) for the structure **7Te-Int$_2$** using the B3LYP/DZP method

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.757400	1.308517	0.444061
2	6	0	-0.176868	2.422216	0.935635
3	26	0	-1.594463	1.164600	-1.353376
4	6	0	-1.693264	2.994706	-1.462461
5	6	0	-3.328467	1.031820	-0.865997
6	6	0	-1.407673	-0.683884	-1.423376
7	6	0	-1.554998	1.124914	-3.178464
8	6	0	1.262396	2.638832	-1.654165
9	6	0	1.575366	-0.050377	-1.697672
10	8	0	-1.823963	4.130243	-1.582164
11	8	0	-1.411610	-1.811334	-1.651503
12	8	0	-4.428206	0.937188	-0.536083
13	8	0	-1.510399	1.112284	-4.330859
14	8	0	1.498149	3.534699	-2.344282
15	8	0	1.972449	-0.863789	-2.414822
16	52	0	0.119510	-0.417333	1.387714
17	52	0	0.060981	4.054931	1.968431
18	26	0	0.991889	1.233461	-0.565837
19	6	0	2.528922	1.450163	0.364916
20	8	0	3.512855	1.616931	0.940565

Table S59. The theoretical Cartesian coordinates (in Å) for the structure **6S-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.127791	-0.323640	-1.268081
2	6	0	-1.636218	-0.522481	-1.513976
3	6	0	0.300166	1.233893	0.000000
4	6	0	0.535205	-2.044049	-1.580931
5	6	0	0.535205	0.343820	-2.896589
6	8	0	0.818630	-3.147624	-1.775353
7	8	0	-2.773052	-0.631667	-1.694493
8	8	0	0.779435	0.755463	-3.947782
9	26	0	0.127791	-0.323640	1.268081
10	6	0	-1.636218	-0.522481	1.513976
11	6	0	0.535205	0.343820	2.896589
12	6	0	0.535205	-2.044049	1.580931
13	8	0	-2.773052	-0.631667	1.694493
14	8	0	0.779435	0.755463	3.947782
15	8	0	0.818630	-3.147624	1.775353
16	6	0	-0.126730	2.483149	0.000000
17	16	0	-0.743254	3.911324	0.000000
18	16	0	1.862269	0.437360	0.000000

Table S60. The theoretical Cartesian coordinates (in Å) for the structure **6S-XT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.325784	0.165572	1.314198
2	6	0	-0.745454	-1.543169	1.745642
3	6	0	1.001481	-0.419419	0.000000
4	6	0	-1.868272	0.891585	1.956249
5	6	0	0.710246	0.525441	2.741674
6	8	0	-2.840042	1.378451	2.340785
7	8	0	-0.982901	-2.643276	1.999518
8	8	0	1.398877	0.768794	3.634531
9	26	0	-0.325784	0.165572	-1.314198
10	6	0	-0.745454	-1.543169	-1.745642
11	6	0	0.710246	0.525441	-2.741674
12	6	0	-1.868272	0.891585	-1.956249
13	8	0	-0.982901	-2.643276	-1.999518
14	8	0	1.398877	0.768794	-3.634531
15	8	0	-2.840042	1.378451	-2.340785
16	6	0	2.224848	-0.878111	0.000000
17	16	0	3.700737	-1.424161	0.000000
18	16	0	0.000000	1.963199	0.000000

Table S61. The theoretical Cartesian coordinates (in Å) for the structure **6S-IT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.026767	-2.345241	-0.091509
2	16	0	1.532258	-1.460788	-1.609921
3	6	0	0.270088	-0.628109	-0.950415
4	6	0	-0.270088	0.628109	-0.950415
5	16	0	-1.532258	1.460788	-1.609921
6	26	0	-0.026767	2.345241	-0.091509
7	6	0	1.772883	2.391501	0.127067
8	6	0	-0.548021	2.009772	1.674933
9	6	0	-0.270088	4.148609	-0.079529
10	6	0	0.270088	-4.148609	-0.079529
11	6	0	-1.772883	-2.391501	0.127067
12	6	0	0.548021	-2.009772	1.674933
13	8	0	2.920743	2.394788	0.267884
14	8	0	-0.442245	5.290530	-0.092392
15	8	0	-0.862567	1.789577	2.762713
16	8	0	0.442245	-5.290530	-0.092392
17	8	0	-2.920743	-2.394788	0.267884
18	8	0	0.862567	-1.789577	2.762713

Table S62. The theoretical Cartesian coordinates (in Å) for the structure **6S-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.534807	0.029703	0.000000
2	16	0	-1.355902	1.829960	0.000000
3	6	0	-0.598973	0.271171	0.000000
4	6	0	0.598973	-0.271171	0.000000
5	16	0	1.355902	-1.829960	0.000000
6	26	0	2.534807	-0.029703	0.000000
7	6	0	2.622774	1.216715	1.282820
8	6	0	2.622774	1.216715	-1.282820
9	6	0	4.274710	-0.655862	0.000000
10	6	0	-4.274710	0.655862	0.000000
11	6	0	-2.622774	-1.216715	1.282820
12	6	0	-2.622774	-1.216715	-1.282820
13	8	0	2.622774	1.970316	2.156274
14	8	0	5.360350	-1.039804	0.000000
15	8	0	2.622774	1.970316	-2.156274
16	8	0	-5.360350	1.039804	0.000000
17	8	0	-2.622774	-1.970316	2.156274
18	8	0	-2.622774	-1.970316	-2.156274

Table S63. The theoretical Cartesian coordinates (in Å) for the structure **6S-II** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000000	2.475242	0.000000
2	6	0	-0.004726	0.733839	-0.681695
3	6	0	-0.004726	0.733839	0.681695
4	16	0	0.102667	-0.666562	1.637256
5	16	0	0.102667	-0.666562	-1.637256
6	26	0	0.269813	-2.254341	0.000000
7	6	0	-1.455545	-2.635903	0.000000
8	6	0	0.777677	-3.403330	1.326656
9	6	0	0.777677	-3.403330	-1.326656
10	6	0	-1.633016	3.178719	0.000000
11	6	0	0.616481	3.435745	1.416130
12	6	0	0.616481	3.435745	-1.416130
13	8	0	1.093489	-4.123617	-2.166926
14	8	0	-2.582575	-2.877788	0.000000
15	8	0	1.093489	-4.123617	2.166926
16	8	0	-2.723136	3.561639	0.000000
17	8	0	1.031725	3.977608	-2.346148
18	8	0	1.031725	3.977608	2.346148

Table S64. The theoretical Cartesian coordinates (in Å) for the structure **6S-III** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.690769	-0.036318	-1.346155
2	6	0	0.690769	0.036318	-1.346155
3	16	0	1.833364	-1.191236	-1.437553
4	16	0	-1.833364	1.191236	-1.437553
5	26	0	0.116899	1.347283	0.010895
6	26	0	-0.116899	-1.347283	0.010895
7	6	0	1.634529	1.147755	0.945682
8	6	0	0.576851	2.918045	-0.744994
9	6	0	-0.893368	1.918764	1.430204
10	6	0	0.893368	-1.918764	1.430204
11	6	0	-1.634529	-1.147755	0.945682
12	6	0	-0.576851	-2.918045	-0.744994
13	8	0	2.625197	1.054263	1.527912
14	8	0	0.893368	3.913277	-1.232183
15	8	0	-1.517008	2.276497	2.330415
16	8	0	1.517008	-2.276497	2.330415
17	8	0	-0.893368	-3.913277	-1.232183
18	8	0	-2.625197	-1.054263	1.527912

Table S65. The theoretical Cartesian coordinates (in Å) for the structure **6S-IIIT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.634761	0.120894	-1.004445
2	6	0	0.634761	-0.120894	-1.004445
3	16	0	1.957044	-1.133770	-1.020380
4	16	0	-1.957044	1.133770	-1.020380
5	26	0	-0.007024	1.865286	0.039332
6	26	0	0.007024	-1.865286	0.039332
7	6	0	1.131249	1.509122	1.423137
8	6	0	1.131249	2.822432	-1.113692
9	6	0	-0.728483	3.308257	0.832747
10	6	0	0.728483	-3.308257	0.832747
11	6	0	-1.131249	-1.509122	1.423137
12	6	0	-1.131249	-2.822432	-1.113692
13	8	0	1.860923	1.277910	2.287289
14	8	0	1.825617	3.419631	-1.812259
15	8	0	-1.202047	4.233749	1.334591
16	8	0	1.202047	-4.233749	1.334591
17	8	0	-1.825617	-3.419631	-1.812259
18	8	0	-1.860923	-1.277910	2.287289

Table S66. The theoretical Cartesian coordinates (in Å) for the structure **6S-V** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.276962	0.104824	0.053215
2	26	0	-1.328728	0.272302	-0.085321
3	6	0	-1.974034	-0.428671	1.486049
4	6	0	-2.638729	-0.384584	-1.107672
5	6	0	-1.902956	1.976305	0.282201
6	8	0	-2.373735	-0.896245	2.460038
7	8	0	-2.264726	3.053933	0.476678
8	8	0	-3.453136	-0.798601	-1.812813
9	6	0	-0.049894	-1.325813	-0.105176
10	6	0	-0.149610	0.656438	-1.345806
11	6	0	1.064406	0.037489	1.819375
12	8	0	0.976450	-0.014126	2.970530
13	6	0	2.718918	-0.991199	-0.005610
14	8	0	3.614996	-1.713485	-0.050214
15	6	0	2.073678	1.794685	0.197756
16	8	0	2.590394	2.816292	0.319227
17	16	0	-0.193335	-2.910382	-0.194948
18	16	0	1.054168	0.573174	-2.392522

Table S67. The theoretical Cartesian coordinates (in Å) for the structure **6Se-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.106865	-0.709844	1.275857
2	6	0	1.879138	-0.605751	1.504470
3	6	0	-0.279335	0.806499	0.000000
4	6	0	0.002661	-2.474113	1.589578
5	6	0	-0.390400	-0.110874	2.904184
6	8	0	-0.085554	-3.610576	1.783138
7	8	0	3.018732	-0.520761	1.680984
8	8	0	-0.689847	0.260406	3.956431
9	26	0	0.106865	-0.709844	-1.275857
10	6	0	1.879138	-0.605751	-1.504470
11	6	0	-0.390400	-0.110874	-2.904184
12	6	0	0.002661	-2.474113	-1.589578
13	8	0	3.018732	-0.520761	-1.680984
14	8	0	-0.689847	0.260406	-3.956431
15	8	0	-0.085554	-3.610576	-1.783138
16	6	0	-0.120994	2.114194	0.000000
17	34	0	0.204635	3.781290	0.000000
18	34	0	-1.879490	-0.263307	0.000000

Table S68. The theoretical Cartesian coordinates (in Å) for the structure **6Se-XT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.189397	-0.635342	1.323433
2	6	0	1.908631	-0.236216	1.715036
3	6	0	0.091068	0.811670	0.000000
4	6	0	0.254630	-2.336615	1.959880
5	6	0	-0.570131	0.128964	2.763459
6	8	0	0.278055	-3.422710	2.348658
7	8	0	3.001497	0.047510	1.953305
8	8	0	-1.074335	0.634212	3.670209
9	26	0	0.189397	-0.635342	-1.323433
10	6	0	1.908631	-0.236216	-1.715036
11	6	0	-0.570131	0.128964	-2.763459
12	6	0	0.254630	-2.336615	-1.959880
13	8	0	3.001497	0.047510	-1.953305
14	8	0	-1.074335	0.634212	-3.670209
15	8	0	0.278055	-3.422710	-2.348658
16	6	0	-0.032131	2.105819	0.000000
17	34	0	-0.202178	3.817312	0.000000
18	34	0	-1.697918	-1.208046	0.000000

Table S69. The theoretical Cartesian coordinates (in Å) for the structure **6Se-IT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.006510	2.361473	0.217047
2	34	0	-1.608422	1.514633	-1.403426
3	6	0	-0.245789	0.635997	-0.595675
4	6	0	0.245789	-0.635997	-0.595675
5	34	0	1.608422	-1.514633	-1.403426
6	26	0	0.006510	-2.361473	0.217047
7	6	0	-1.804854	-2.399041	0.344866
8	6	0	0.451776	-2.029299	1.995728
9	6	0	0.245789	-4.164357	0.245233
10	6	0	-0.245789	4.164357	0.245233
11	6	0	1.804854	2.399041	0.344866
12	6	0	-0.451776	2.029299	1.995728
13	8	0	-2.957973	-2.395824	0.431027
14	8	0	0.417787	-5.306462	0.239535
15	8	0	0.718917	-1.806741	3.095984
16	8	0	-0.417787	5.306462	0.239535
17	8	0	2.957973	2.395824	0.431027
18	8	0	-0.718917	1.806741	3.095984

Table S70. The theoretical Cartesian coordinates (in Å) for the structure **6Se-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.346284	2.142270	0.000000
2	34	0	2.426541	0.139740	0.000000
3	6	0	0.533472	0.383139	0.000000
4	6	0	-0.533472	-0.383139	0.000000
5	34	0	-2.426541	-0.139740	0.000000
6	26	0	-1.346284	-2.142270	0.000000
7	6	0	-0.325022	-2.849326	1.287846
8	6	0	-0.325022	-2.849326	-1.287846
9	6	0	-2.772421	-3.315744	0.000000
10	6	0	2.772421	3.315744	0.000000
11	6	0	0.325022	2.849326	1.287846
12	6	0	0.325022	2.849326	-1.287846
13	8	0	0.325022	-3.234020	2.159711
14	8	0	-3.666953	-4.041281	0.000000
15	8	0	0.325022	-3.234020	-2.159711
16	8	0	3.666953	4.041281	0.000000
17	8	0	-0.325022	3.234020	2.159711
18	8	0	-0.325022	3.234020	-2.159711

Table S71. The theoretical Cartesian coordinates (in Å) for the structure **6Se-II** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.107878	2.675531	0.000000
2	6	0	-0.029251	0.928056	0.675424
3	6	0	-0.029251	0.928056	-0.675424
4	34	0	-0.075144	-0.585516	-1.743428
5	34	0	-0.075144	-0.585516	1.743428
6	26	0	-0.143026	-2.240379	0.000000
7	6	0	1.601061	-2.511011	0.000000
8	6	0	-0.581366	-3.406364	-1.326410
9	6	0	-0.581366	-3.406364	1.326410
10	6	0	1.484846	3.464166	0.000000
11	6	0	-0.758169	3.602995	-1.422749
12	6	0	-0.758169	3.602995	1.422749
13	8	0	-0.856110	-4.151266	2.161563
14	8	0	2.741528	-2.685272	0.000000
15	8	0	-0.856110	-4.151266	-2.161563
16	8	0	2.554885	3.899975	0.000000
17	8	0	-1.195642	4.124286	2.354378
18	8	0	-1.195642	4.124286	-2.354378

Table S72. The theoretical Cartesian coordinates (in Å) for the structure **6Se-III** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.668333	0.157242	-1.099910
2	6	0	0.668333	-0.157242	-1.099910
3	34	0	1.455073	-1.812732	-1.230483
4	34	0	-1.455073	1.812732	-1.230483
5	26	0	0.536571	1.252410	0.261641
6	26	0	-0.536571	-1.252410	0.261641
7	6	0	1.921692	0.596849	1.194840
8	6	0	1.455073	2.607802	-0.485981
9	6	0	-0.249627	2.095647	1.684880
10	6	0	0.249627	-2.095647	1.684880
11	6	0	-1.921692	-0.596849	1.194840
12	6	0	-1.455073	-2.607802	-0.485981
13	8	0	2.835390	0.210373	1.782157
14	8	0	2.069579	3.458435	-0.963635
15	8	0	-0.731608	2.621350	2.590324
16	8	0	0.731608	-2.621350	2.590324
17	8	0	-2.069579	-3.458435	-0.963635
18	8	0	-2.835390	-0.210373	1.782157

Table S73. The theoretical Cartesian coordinates (in Å) for the structure **6Se-IIIT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615097	0.197404	-0.793566
2	6	0	0.615097	-0.197404	-0.793566
3	34	0	1.853592	-1.531824	-0.844563
4	34	0	-1.853592	1.531824	-0.844563
5	26	0	0.347201	1.842251	0.198884
6	26	0	-0.347201	-1.842251	0.198884
7	6	0	1.345258	1.285913	1.629127
8	6	0	1.675073	2.525793	-0.937231
9	6	0	-0.072382	3.421037	0.943397
10	6	0	0.072382	-3.421037	0.943397
11	6	0	-1.345258	-1.285913	1.629127
12	6	0	-1.675073	-2.525793	-0.937231
13	8	0	1.984974	0.930693	2.521664
14	8	0	2.492438	2.953418	-1.627532
15	8	0	-0.347201	4.437672	1.417596
16	8	0	0.347201	-4.437672	1.417596
17	8	0	-2.492438	-2.953418	-1.627532
18	8	0	-1.984974	-0.930693	2.521664

Table S74. The theoretical Cartesian coordinates (in Å) for the structure **6Se-V** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.151485	0.070902	0.546160
2	26	0	1.215269	-0.881494	-0.047628
3	6	0	2.358742	-0.309735	1.279500
4	6	0	2.398725	-0.721168	-1.376765
5	6	0	1.361414	-2.658114	0.393695
6	8	0	3.074557	0.077191	2.094239
7	8	0	1.437621	-3.782938	0.635204
8	8	0	3.116566	-0.617080	-2.273788
9	6	0	0.461445	1.008956	-0.031349
10	6	0	-0.268535	-0.959873	-0.998409
11	6	0	-0.542981	0.142182	2.218978
12	8	0	-0.195200	0.215183	3.318569
13	6	0	-2.185533	1.555326	0.665119
14	8	0	-2.818403	2.515625	0.723066
15	6	0	-2.365568	-1.278633	1.009554
16	8	0	-3.118817	-2.090943	1.323071
17	34	0	1.072196	2.606759	-0.372996
18	34	0	-1.687938	-0.551893	-1.935435

Table S75. The theoretical Cartesian coordinates (in Å) for the structure **6Te-VI** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.606184	-0.901788	0.320777
2	6	0	1.238678	-1.438336	1.983041
3	6	0	-0.151725	-0.751744	-0.357886
4	6	0	3.244933	-0.197276	0.678004
5	6	0	2.138082	-2.500419	-0.306432
6	8	0	4.285675	0.257687	0.884129
7	8	0	0.996831	-1.815596	3.047953
8	8	0	2.460779	-3.539278	-0.692947
9	26	0	-0.008580	1.182982	0.396221
10	6	0	-0.534695	1.081285	2.110161
11	6	0	-1.186054	2.431288	-0.168456
12	6	0	1.381513	2.258122	0.764895
13	8	0	-0.895079	1.046008	3.206054
14	8	0	-1.932364	3.242576	-0.508454
15	8	0	2.252451	2.981002	1.000237
16	6	0	-1.443255	-0.503796	-0.157491
17	52	0	-3.355593	-0.835138	-0.040200
18	52	0	0.913114	0.316581	-1.910045

Table S75. The theoretical Cartesian coordinates (in Å) for the structure **6Te-XT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.684548	-0.616098	-1.322485
2	6	0	-2.063129	0.493904	-1.658361
3	6	0	0.056023	0.649274	0.000000
4	6	0	-1.524801	-2.093559	-1.946859
5	6	0	0.291607	-0.245621	-2.784434
6	8	0	-2.063107	-3.035525	-2.344197
7	8	0	-2.930984	1.223320	-1.876385
8	8	0	0.928298	0.004921	-3.714701
9	26	0	-0.684548	-0.616098	1.322485
10	6	0	-2.063129	0.493904	1.658361
11	6	0	0.291607	-0.245621	2.784434
12	6	0	-1.524801	-2.093559	1.946859
13	8	0	-2.930984	1.223320	1.876385
14	8	0	0.928298	0.004921	3.714701
15	8	0	-2.063107	-3.035525	2.344197
16	6	0	0.697125	1.767953	0.000000
17	52	0	1.667940	3.434635	0.000000
18	52	0	0.941400	-2.115549	0.000000

Table S77. The theoretical Cartesian coordinates (in Å) for the structure **6Te-IT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.376627	2.325380	0.494949
2	52	0	-1.463333	1.843915	-1.302339
3	6	0	-0.119726	0.666093	-0.302004
4	6	0	0.119726	-0.666093	-0.302004
5	52	0	1.463333	-1.843915	-1.302339
6	26	0	-0.376627	-2.325380	0.494949
7	6	0	-2.180801	-2.096823	0.506529
8	6	0	0.023267	-1.998600	2.269436
9	6	0	-0.404538	-4.139985	0.601761
10	6	0	0.404538	4.139985	0.601761
11	6	0	2.180801	2.096823	0.506529
12	6	0	-0.023267	1.998600	2.269436
13	8	0	-3.324290	-1.927157	0.525060
14	8	0	-0.404538	-5.294298	0.647932
15	8	0	0.262783	-1.777754	3.376834
16	8	0	0.404538	5.294298	0.647932
17	8	0	3.324290	1.927157	0.525060
18	8	0	-0.262783	1.777754	3.376834

Table S78. The theoretical Cartesian coordinates (in Å) for the structure **6Te-I** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	1.354364	2.123399	0.000000
2	52	0	2.661336	0.025495	0.000000
3	6	0	0.529909	0.385987	0.000000
4	6	0	-0.529909	-0.385987	0.000000
5	52	0	-2.661336	-0.025495	0.000000
6	26	0	-1.354364	-2.123399	0.000000
7	6	0	-0.328653	-2.801515	1.296051
8	6	0	-0.328653	-2.801515	-1.296051
9	6	0	-2.740842	-3.337803	0.000000
10	6	0	2.740842	3.337803	0.000000
11	6	0	0.328653	2.801515	1.296051
12	6	0	0.328653	2.801515	-1.296051
13	8	0	0.328653	-3.175204	2.167296
14	8	0	-3.610940	-4.093572	0.000000
15	8	0	0.328653	-3.175204	-2.167296
16	8	0	3.610940	4.093572	0.000000
17	8	0	-0.328653	3.175204	2.167296
18	8	0	-0.328653	3.175204	-2.167296

Table S79. The theoretical Cartesian coordinates (in Å) for the structure **6Te-II** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-2.894437	0.000004	-0.090449
2	6	0	-1.139461	-0.671015	-0.030916
3	6	0	-1.139458	0.671025	-0.030915
4	52	0	0.519068	1.892753	-0.093678
5	52	0	0.519061	-1.892750	-0.093679
6	26	0	2.288701	-0.000002	-0.118417
7	6	0	2.522607	-0.000001	1.630912
8	6	0	3.458235	1.319055	-0.529252
9	6	0	3.458232	-1.319061	-0.529254
10	6	0	-3.686867	-0.000041	1.497901
11	6	0	-3.818729	1.432470	-0.721119
12	6	0	-3.818729	-1.432432	-0.721180
13	8	0	4.227505	-2.141682	-0.782154
14	8	0	2.694741	-0.000006	2.773204
15	8	0	4.227509	2.141671	-0.782164
16	8	0	-4.122562	-0.000070	2.568298
17	8	0	-4.341627	-2.366555	-1.152646
18	8	0	-4.341630	2.366615	-1.152535

Table S80. The theoretical Cartesian coordinates (in Å) for the structure **6Te-III** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.557809	0.386918	-0.907038
2	6	0	0.557809	-0.386918	-0.907038
3	52	0	0.745528	-2.413272	-1.127703
4	52	0	-0.745528	2.413272	-1.127703
5	26	0	0.964043	0.958880	0.476635
6	26	0	-0.964043	-0.958880	0.476635
7	6	0	1.979142	-0.173763	1.423143
8	6	0	2.351923	1.841989	-0.249418
9	6	0	0.557809	2.027006	1.901738
10	6	0	-0.557809	-2.027006	1.901738
11	6	0	-1.979142	0.173763	1.423143
12	6	0	-2.351923	-1.841989	-0.249418
13	8	0	2.671749	-0.867221	2.031551
14	8	0	3.274406	2.371957	-0.696524
15	8	0	0.326417	2.686625	2.819661
16	8	0	-0.326417	-2.686625	2.819661
17	8	0	-3.274406	-2.371957	-0.696524
18	8	0	-2.671749	0.867221	2.031551

Table S81. The theoretical Cartesian coordinates (in Å) for the structure **6Te-IIIT** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.559378	0.320686	-0.629617
2	6	0	0.559378	-0.320686	-0.629617
3	52	0	1.604954	-2.056505	-0.772954
4	52	0	-1.604954	2.056505	-0.772954
5	26	0	0.780490	1.703435	0.352896
6	26	0	-0.780490	-1.703435	0.352896
7	6	0	1.604630	0.925463	1.788549
8	6	0	2.223660	2.049185	-0.788884
9	6	0	0.763361	3.335939	1.096943
10	6	0	-0.763361	-3.335939	1.096943
11	6	0	-1.604630	-0.925463	1.788549
12	6	0	-2.223660	-2.049185	-0.788884
13	8	0	2.139947	0.437269	2.687135
14	8	0	3.116926	2.258993	-1.486243
15	8	0	0.763361	4.387877	1.576153
16	8	0	-0.763361	-4.387877	1.576153
17	8	0	-3.116926	-2.258993	-1.486243
18	8	0	-2.139947	-0.437269	2.687135

Table S82. The theoretical Cartesian coordinates (in Å) for the structure **6Te-V** using the B3LYP/DZP method

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.843179	-0.261546	1.016763
2	26	0	-0.483959	1.574820	-0.298028
3	6	0	-1.960293	2.023790	0.720396
4	6	0	-1.292995	1.758960	-1.878627
5	6	0	0.338975	3.209018	-0.138308
6	8	0	-2.897997	2.269130	1.341239
7	8	0	0.893869	4.216605	-0.062506
8	8	0	-1.768850	1.840004	-2.926050
9	6	0	-0.882502	-0.357205	0.121563
10	6	0	0.890988	0.603097	-0.807134
11	6	0	0.037626	0.462147	2.432149
12	8	0	-0.461659	0.879005	3.387514
13	6	0	0.830419	-1.956130	1.664218
14	8	0	0.802134	-3.037497	2.058817
15	6	0	2.516391	0.339169	1.597644
16	8	0	3.532804	0.716302	1.986415
17	52	0	-2.355480	-1.601647	-0.246139
18	52	0	2.105215	-0.815865	-1.431591

Complete Gaussian 09 reference (Reference 49)

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