Online supplementary data for:

Isomorphic Substitution in Molecular Crystals and Geometry of Hypervalent Tellurium: Comments Inspired by the Case Study of $RMeTeI_2$ (R=Ph, Fc).

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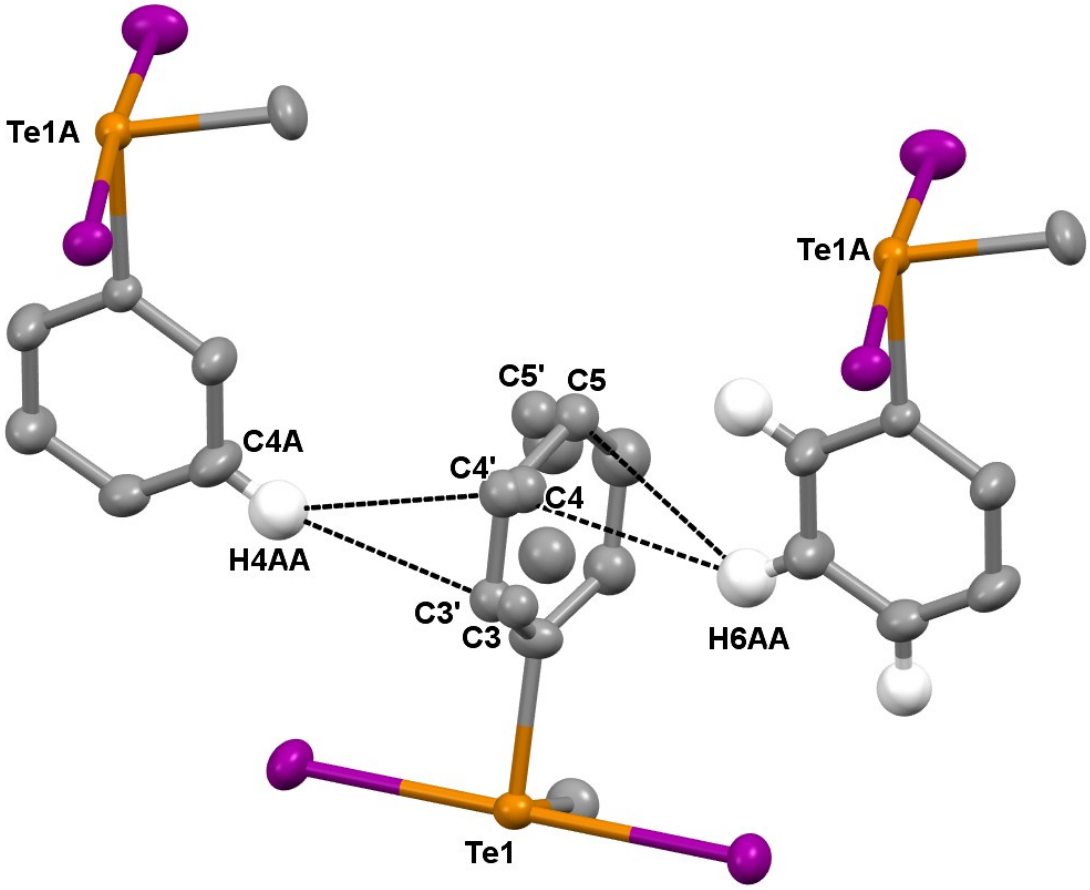
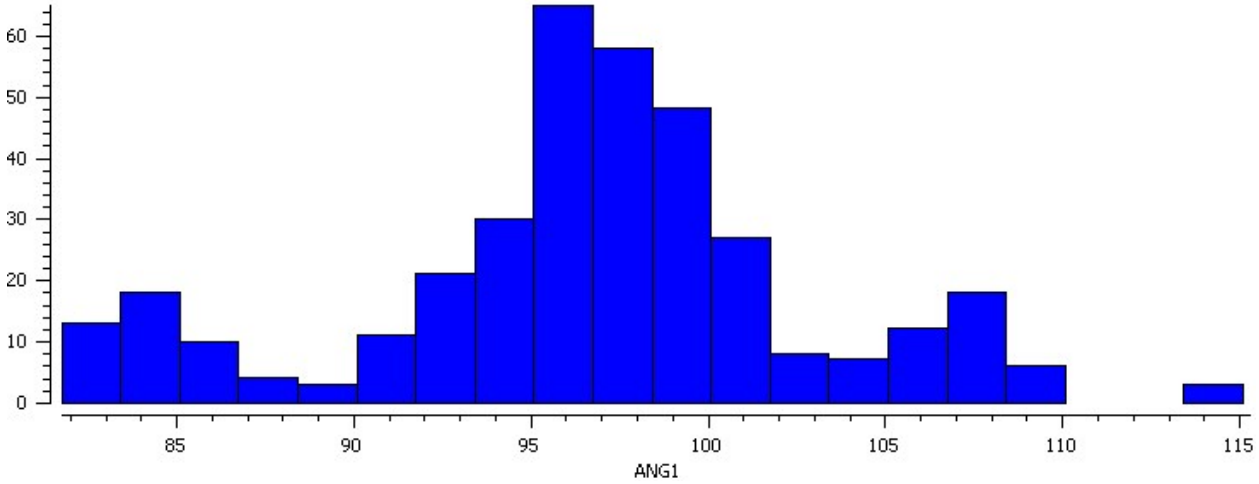


Figure S1. Disorder of Ph-ring in the solid state structure of **1**

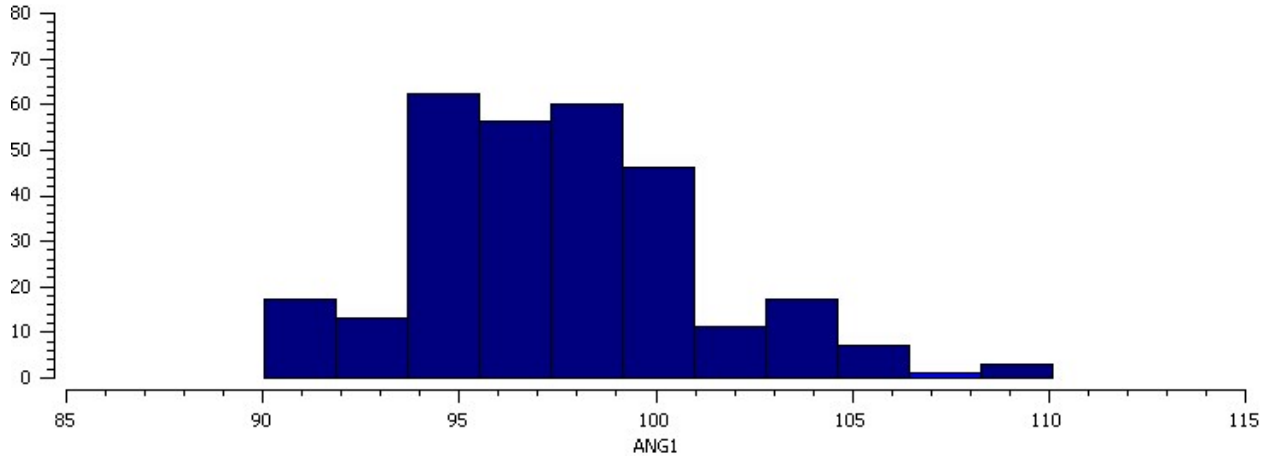
Selected distances, Å

H4AA C4	2.98
H4AA C3	2.88
H6AA C4'	2.89
H6AA C3'	2.84
H6AA C7	3.18
H6AA C6	3.13

~95 -100° - the most frequent angles between the equatorial organic fragments R in $R_2Te_2X_2$ (X = halogen).



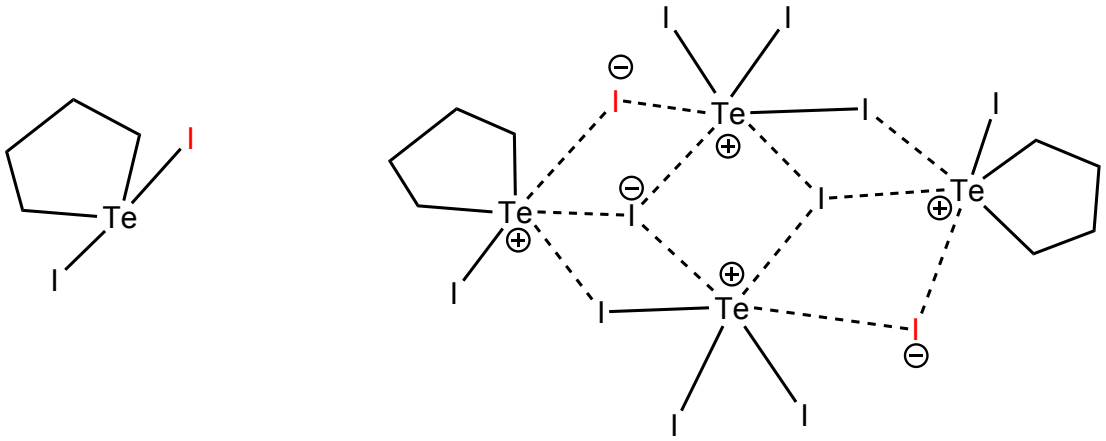
a



b

Scheme S1 C-Te-C angles in R_2TeX_2. **a**) all structures; **b**) excluding Te-heterocyclic structures, which has rigid C-Te-C angle.

Out of R_2TeX_2 289 structures found in CSD, in 149 of them Te atom forms two short contacts (Σ(vdW)+0.1Å).



Scheme S2. Schematic structure of neutral cyclic diorganoditellurium diiodide $C_4H_8TeI_2$ [1] and ionic telluronium salt $C_4H_8TeI]^+[TeI_5]^-$ [2]). See figures S3-4 below for the solid state structures.

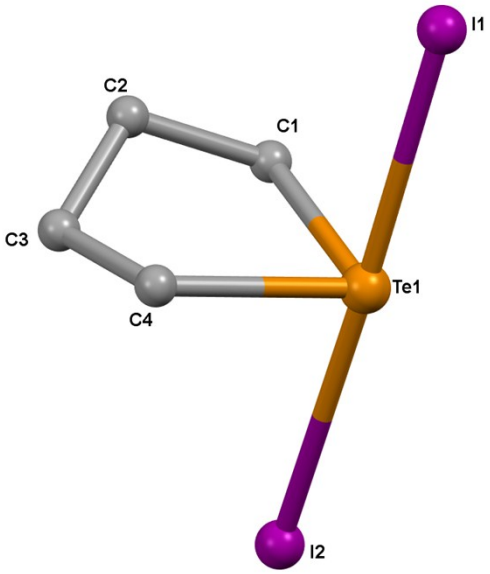


Figure S2. Molecular structure of neutral cyclic diorganoditellurium diiodide $C_4H_8TeI_2$
Selected distances, Å

Te1 I1	2.891(1)
Te1 I2	2.993(1)
angle	
I1 Te1 I2	176.49(3)°

1 . Garcia-Montalvo, A. Marcelo-Polo, R. Montoya, R. A. Toscano, S. Hernandez-Ortega, R. Cea-Olivares, *J. Organomet. Chem.,* 2001, **623**, 74.

2 . S. M. Narhi, R. Oilunkaniemi, R. S. Laitinen, M. Ahlgren, *Inorg. Chem,* 2004, **43**, 3742.

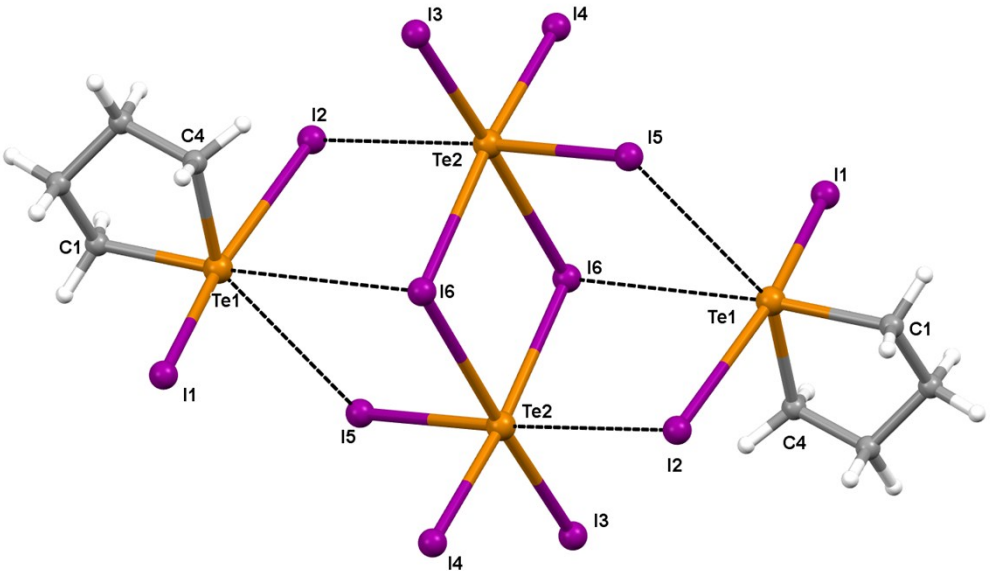


Figure S3. Solid state structure of ionic telluronium salt $C_4H_8TeI]^+[TeI_5]^-$

Selected distances, Å

I1 Te1	2.755(2)
I2 Te1	3.261(2)
Te1 I6	3.676(1)
Te1 I5	3.900(2)
Te2 I2	3.328(1)
Angles	
I2 Te1 I1	169.65(5)°
C1 Te1 I6	174.7(4)°
C4 Te1 I5	152.9(5)°

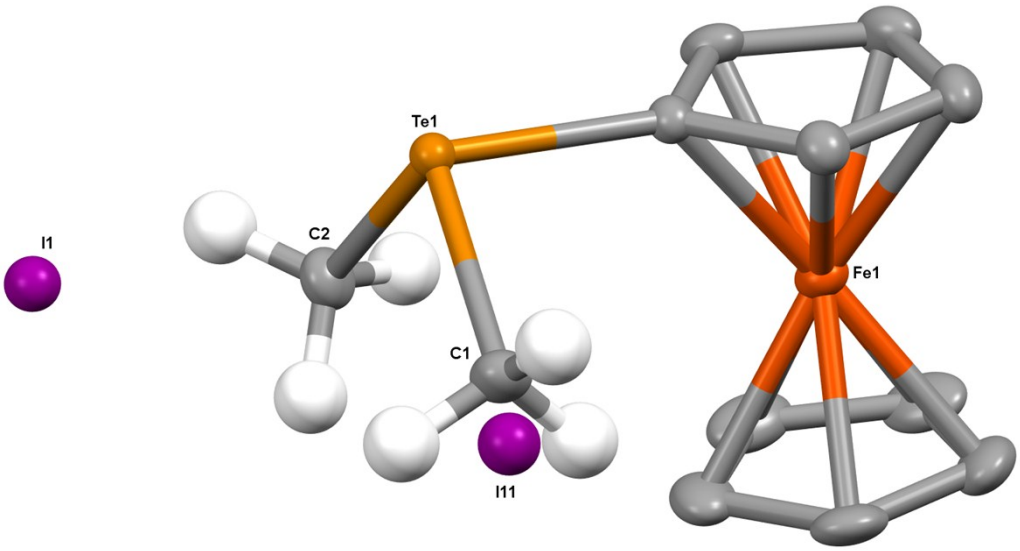


Figure S4. Me/I positional disorder in crystals of **3** obtained from reaction mixture**.** Hydrogen atoms at Cp rings of ferrocenyl fragment are omitted for clarity.

Selected distances, Å

I11	Te1	2.61(2)
Te1	C1	2.123(6)
Te1	C2	2.128(4)
Te1	I1	3.5939(9)

NBO Computations

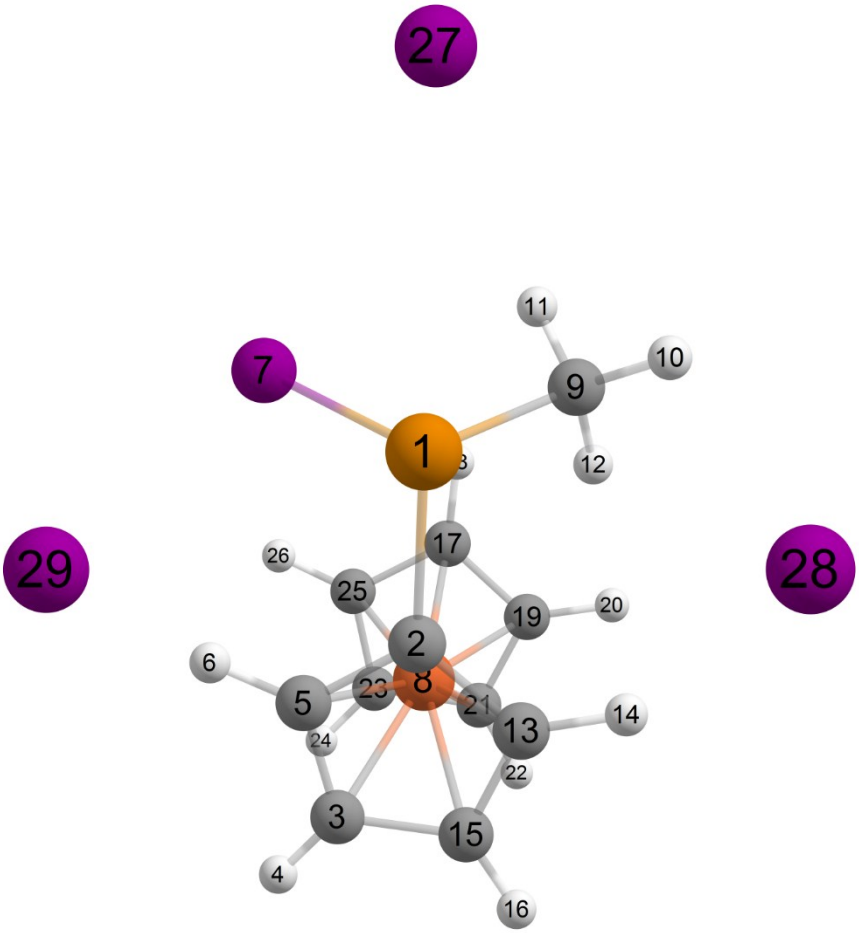


Figure S5

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
69. LP (2) I 7	121. BD*(1)Te 1- C 9	2.52	0.34	0.026
70. LP (3) I 7	119. BD*(1)Te 1- C 2	3.24	0.35	0.030
82. LP (4) I 28	120. BD*(1)Te 1- I 7	10.60	0.20	0.041
86. LP (4) I 29	121. BD*(1)Te 1- C 9	6.18	0.31	0.039

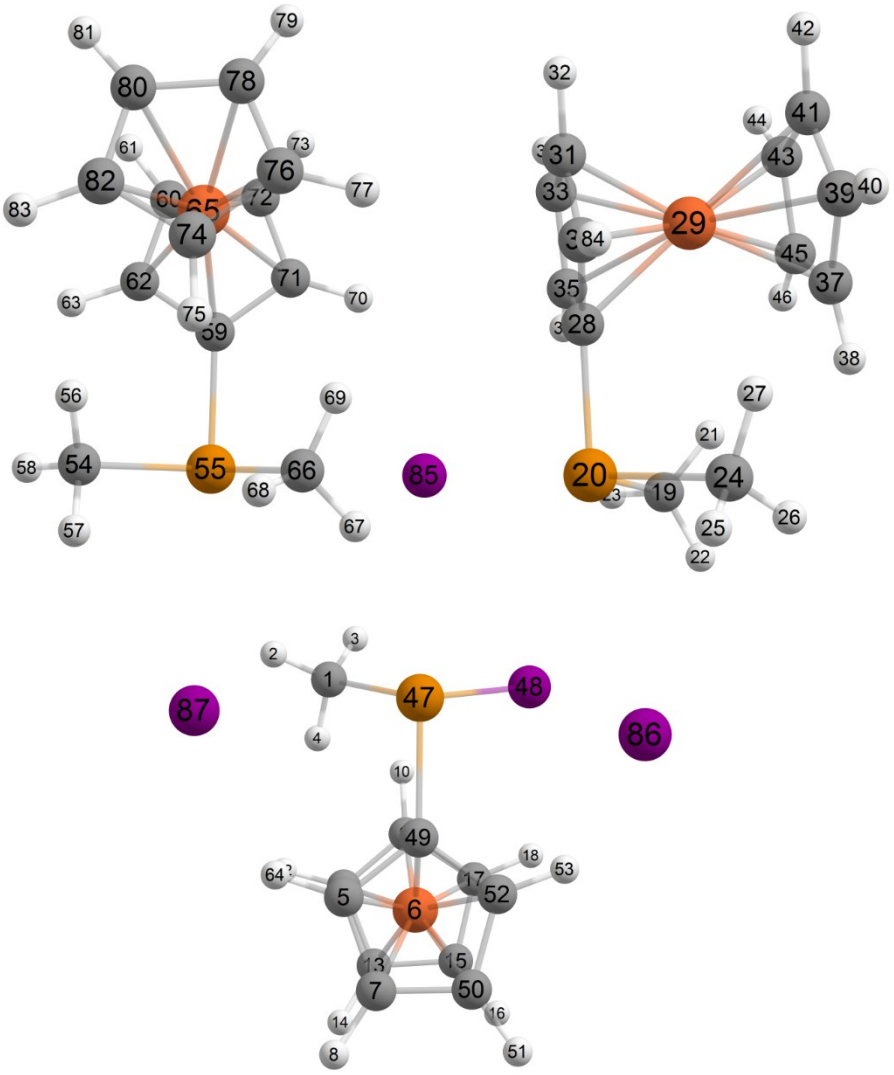


Figure S6

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
138. LP (2) I 48	264. BD*(1) C 1-Te 47	2.77	0.34	0.027
139. LP (3) I 48	316. BD*(1)Te 47- C 49	3.53	0.35	0.031
150. LP (4) I 85	316. BD*(1)Te 47- C 49	8.84	0.34	0.049
148. LP (2) I 85	287. BD*(1)Te 20- C 24	2.68	0.33	0.026
149. LP (3) I 85	286. BD*(1) C 19- H 23	1.52	0.63	0.028
149. LP (3) I 85	322. BD*(1) C 54-Te 55	3.87	0.31	0.031
153. LP (3) I 86	264. BD*(1) C 1-Te 47	3.68	0.29	0.029
154. LP (4) I 86	264. BD*(1) C 1-Te 47	2.88	0.32	0.027
154. LP (4) I 86	288. BD*(1)Te 20- C 28	5.62	0.35	0.040
158. LP (4) I 87	315. BD*(1)Te 47- I 48	10.28	0.21	0.042
157. LP (3) I 87	326. BD*(1)Te 55- C 59	5.51	0.34	0.038

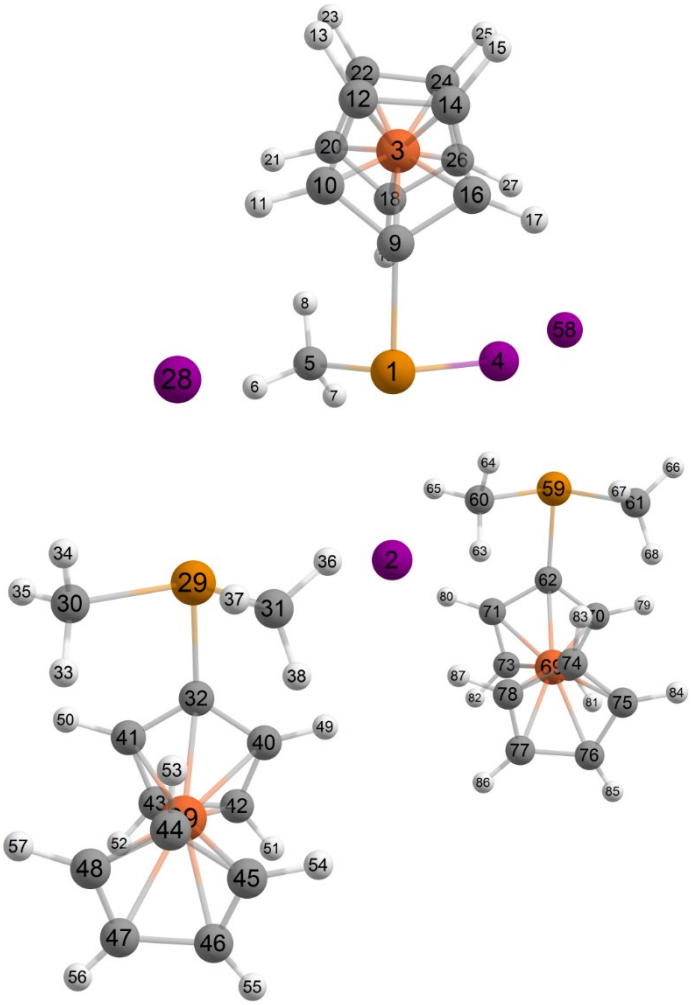


Figure S7

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
135. LP (2) I 4	262. BD*(1)Te 1- C 5	2.09	0.34	0.024
135. LP (2) I 4	355. RY (2)Te 1	1.30	0.94	0.031
136. LP (3) I 4	262. BD*(1)Te 1- C 5	1.06	0.34	0.017
136. LP (3) I 4	263. BD*(1)Te 1- C 9	2.41	0.36	0.026
136. LP (3) I 4	326. BD*(1) C 60- H 64	2.02	0.68	0.033
130. LP (4) I 2	263. BD*(1)Te 1- C 9	6.56	0.33	0.041
129. LP (3) I 2	290. BD*(1)Te 29- C 30	3.34	0.31	0.029
130. LP (4) I 2	290. BD*(1)Te 29- C 30	1.54	0.33	0.020
142. LP (4) I 28	261. BD*(1)Te 1- I 4	7.24	0.22	0.036
141. LP (3) I 28	292. BD*(1)Te 29- C 32	4.84	0.33	0.036
142. LP (4) I 28	292. BD*(1)Te 29- C 32	1.30	0.35	0.019
149. LP (1) I 58	261. BD*(1)Te 1- I 4	1.31	0.57	0.024
152. LP (4) I 58	261. BD*(1)Te 1- I 4	17.35	0.21	0.054
152. LP (4) I 58	458. RY (1) I 4	1.50	1.08	0.036
151. LP (3) I 58	324. BD*(1)Te 59- C 62	5.21	0.35	0.038

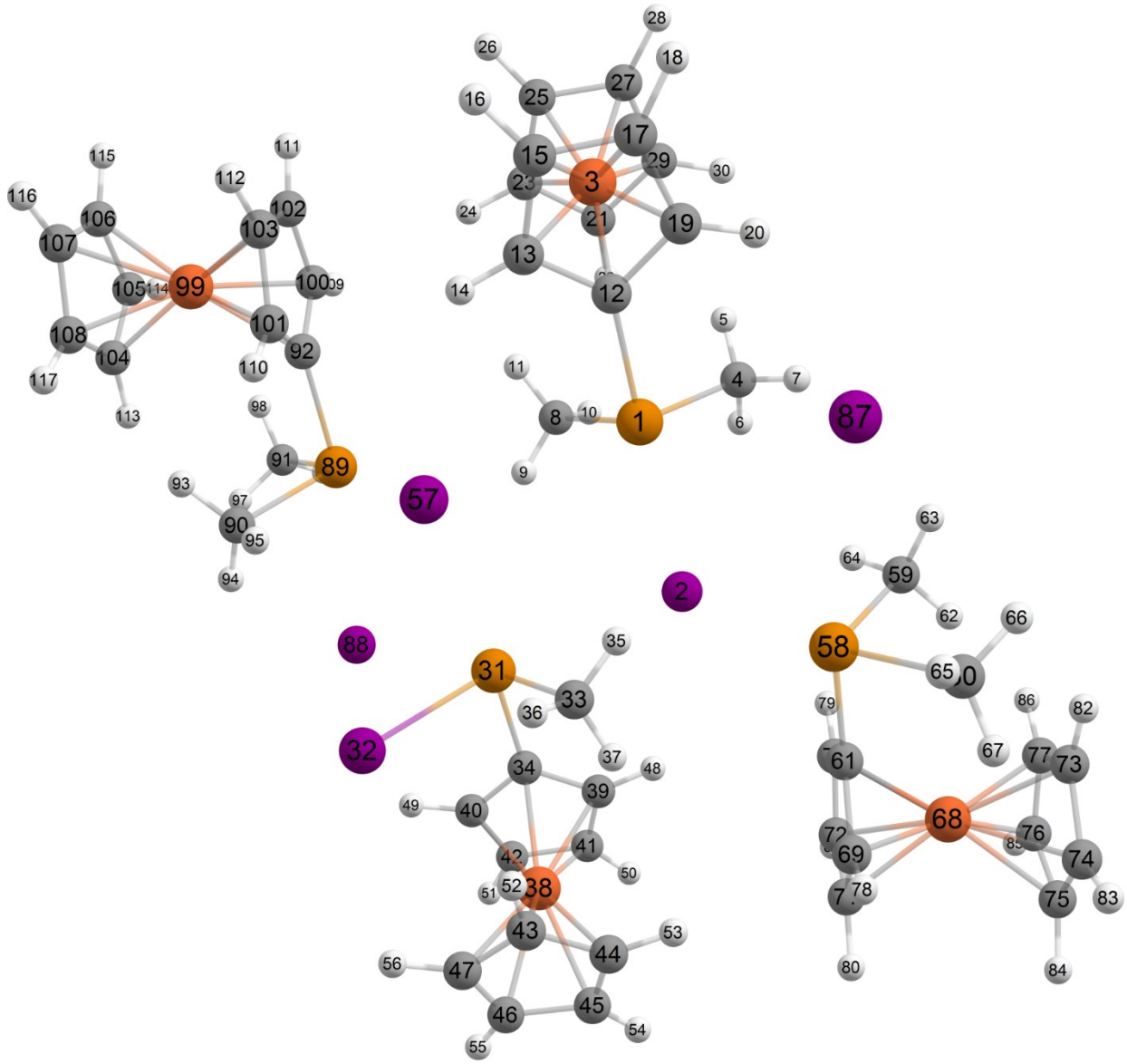


Figure S8

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
168. LP (3) I 2	347. BD*(1)Te 1- C 12	6.12	0.35	0.041
169. LP (4) I 2	377. BD*(1)Te 31- I 32	9.94	0.21	0.041
167. LP (2) I 2	407. BD*(1)Te 58- C 60	2.84	0.33	0.027
186. LP (3) I 57	345. BD*(1)Te 1- C 4	4.44	0.31	0.033
187. LP (4) I 57	379. BD*(1)Te 31- C 34	8.81	0.34	0.049
185. LP (2) I 57	439. BD*(1)Te 89- C 91	2.84	0.33	0.027
186. LP (3) I 57	443. BD*(1) C 90- H 95	1.47	0.63	0.027
196. LP (3) I 87	346. BD*(1)Te 1- C 8	3.55	0.32	0.030
197. LP (4) I 87	346. BD*(1)Te 1- C 8	1.33	0.33	0.019
197. LP (4) I 87	408. BD*(1)Te 58- C 61	6.14	0.35	0.041
200. LP (3) I 88	378. BD*(1)Te 31- C 33	3.52	0.29	0.029
201. LP (4) I 88	378. BD*(1)Te 31- C 33	3.11	0.32	0.028
201. LP (4) I 88	440. BD*(1)Te 89- C 92	5.49	0.35	0.039

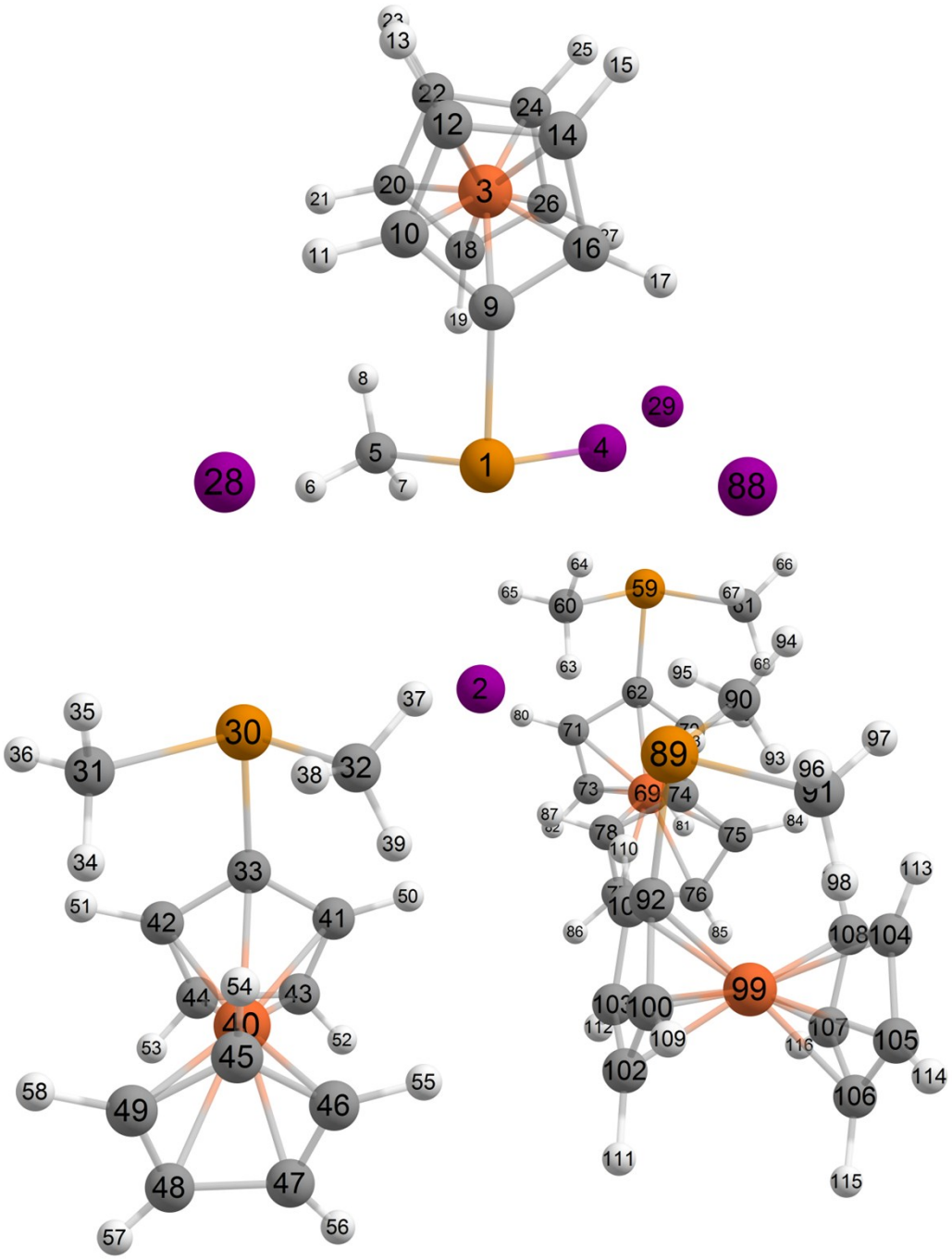


Figure S9

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
174. LP (2) I 4	346. BD*(1)Te 1- C 5	2.68	0.34	0.027
175. LP (3) I 4	347. BD*(1)Te 1- C 9	3.16	0.35	0.030
175. LP (3) I 4	410. BD*(1) C 60- H 64	2.11	0.67	0.034
169. LP (4) I 2	347. BD*(1)Te 1- C 9	7.89	0.34	0.046
168. LP (3) I 2	374. BD*(1)Te 30- C 31	3.63	0.31	0.030
169. LP (4) I 2	374. BD*(1)Te 30- C 31	1.08	0.34	0.017
167. LP (2) I 2	439. BD*(1)Te 89- C 91	2.86	0.31	0.027
168. LP (3) I 2	443. BD*(1) C 90- H 95	1.46	0.62	0.027
181. LP (4) I 28	345. BD*(1)Te 1- I 4	8.24	0.23	0.039
180. LP (3) I 28	376. BD*(1)Te 30- C 33	4.98	0.33	0.036
181. LP (4) I 28	376. BD*(1)Te 30- C 33	1.19	0.35	0.018
182. LP (1) I 29	345. BD*(1)Te 1- I 4	1.35	0.57	0.025
185. LP (4) I 29	**345. BD*(1)Te 1- I 4**	**17.09**	**0.22**	**0.054**
185. LP (4) I 29	574. RY (1) I 4	1.50	1.09	0.036
184. LP (3) I 29	408. BD*(1)Te 59- C 62	5.23	0.35	0.038
200. LP (3) I 88	346. BD*(1)Te 1- C 5	4.13	0.31	0.032
201. LP (4) I 88	346. BD*(1)Te 1- C 5	2.01	0.32	0.023

201. LP (4) I 88	440. BD*(1)Te 89- C 92	6.01	0.35	0.041

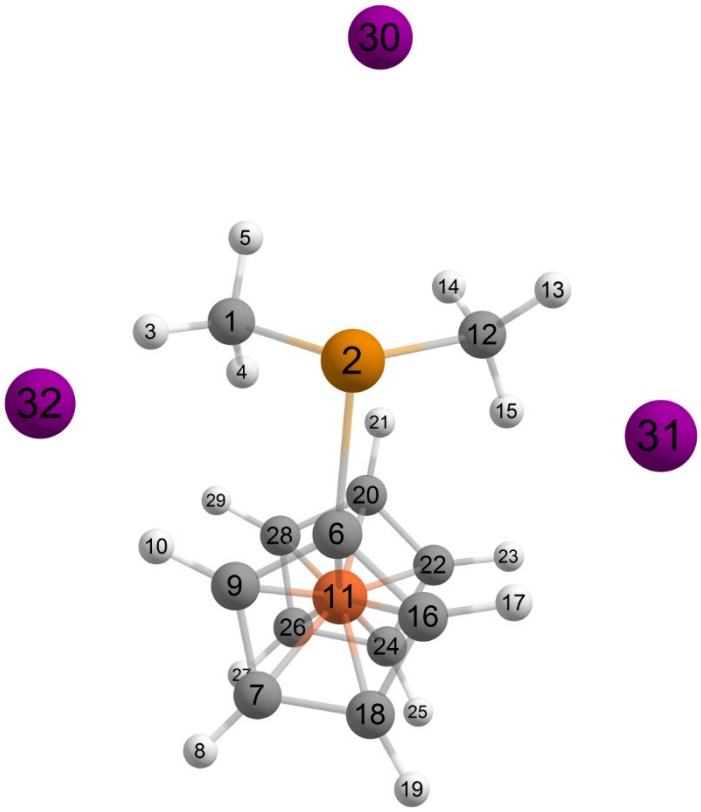


Figure S10

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
67. LP (4) I 30	115. BD*(1)Te 2- C 6	6.95	0.35	0.044
71. LP (4) I 31	111. BD*(1) C 1-Te 2	5.35	0.33	0.038
75. LP (4) I 32	116. BD*(1)Te 2- C 12	4.55	0.33	0.035

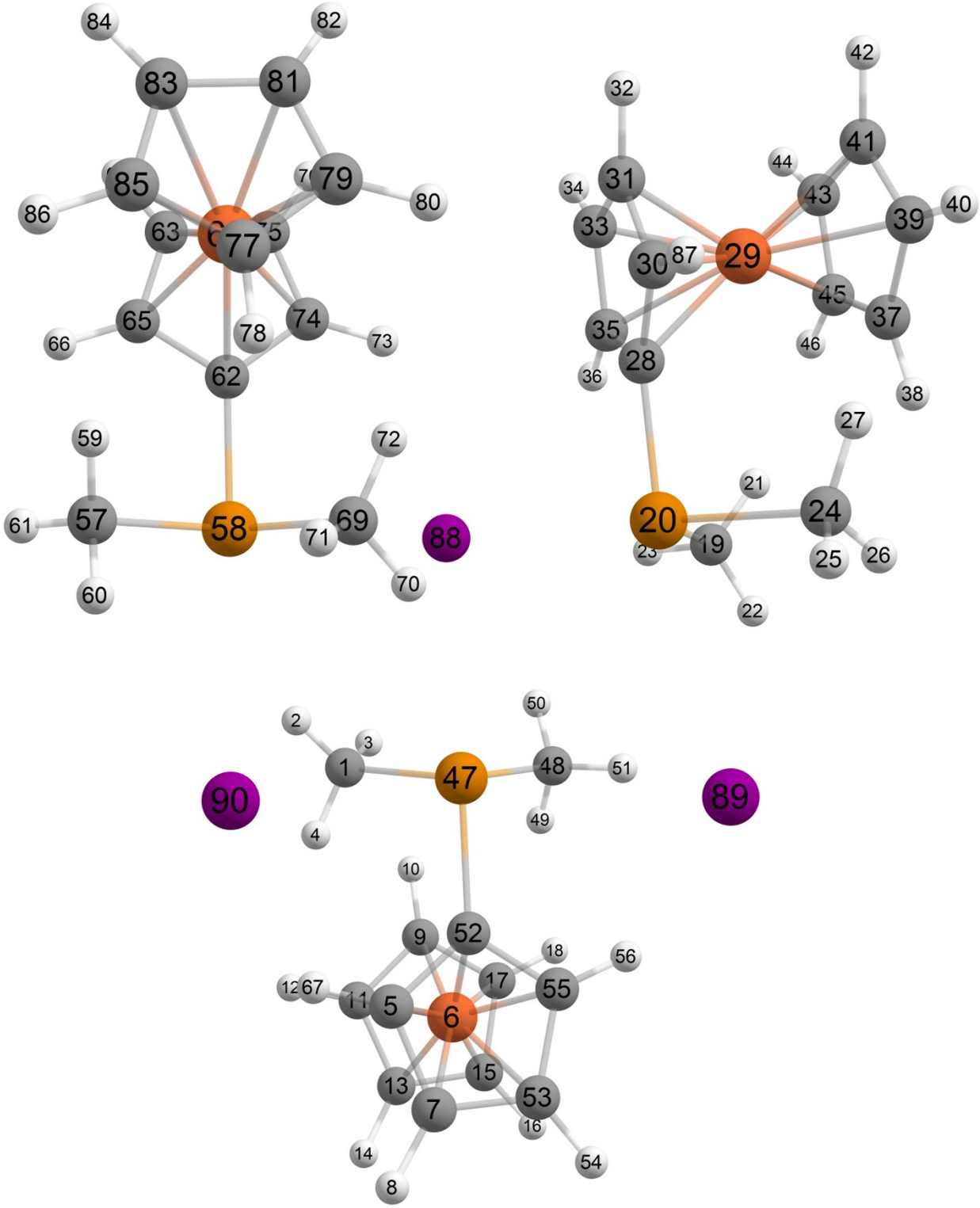


Figure S11

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
139. LP (4) I 88	308. BD*(1)Te 47- C 52	6.77	0.36	0.044
137. LP (2) I 88	279. BD*(1)Te 20- C 24	2.71	0.32	0.026
138. LP (3) I 88	278. BD*(1) C 19- H 23	1.51	0.63	0.028
138. LP (3) I 88	317. BD*(1) C 57-Te 58	3.89	0.31	0.031
142. LP (3) I 89	256. BD*(1) C 1-Te 47	3.56	0.32	0.030
143. LP (4) I 89	256. BD*(1) C 1-Te 47	1.27	0.33	0.018
143. LP (4) I 89	280. BD*(1)Te 20- C 28	6.15	0.35	0.041
146. LP (3) I 90	307. BD*(1)Te 47- C 48	4.13	0.32	0.032
147. LP (4) I 90	307. BD*(1)Te 47- C 48	1.52	0.34	0.020
147. LP (4) I 90	321. BD*(1)Te 58- C 62	5.65	0.35	0.040

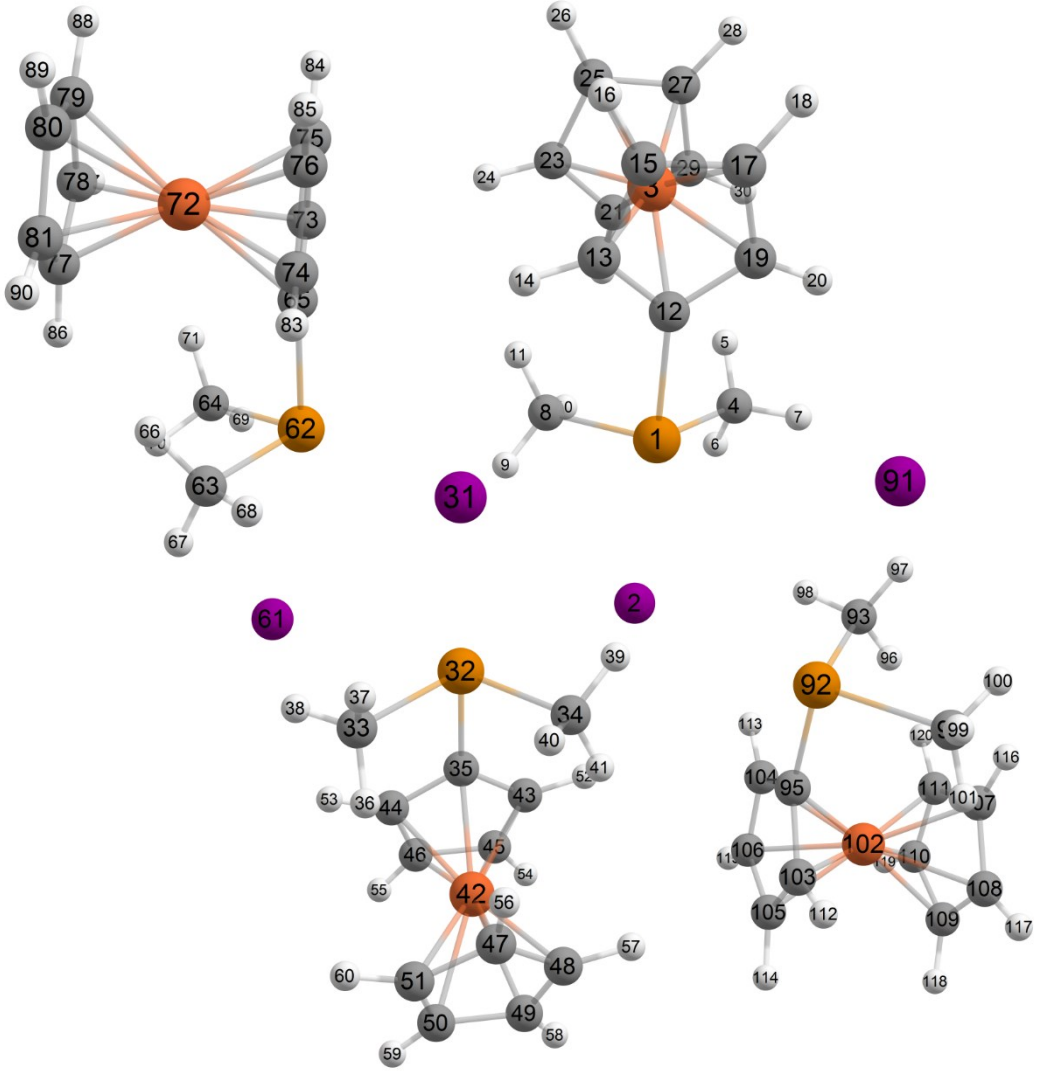


Figure S12

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
161. LP (4) I 2	339. BD*(1)Te 1- C 12	6.68	0.36	0.044
160. LP (3) I 2	369. BD*(1)Te 32- C 33	4.30	0.32	0.033
161. LP (4) I 2	369. BD*(1)Te 32- C 33	1.06	0.34	0.017
159. LP (2) I 2	434. BD*(1)Te 92- C 94	2.81	0.32	0.027
160. LP (3) I 2	438. BD*(1) C 93- H 98	1.48	0.63	0.027
169. LP (3) I 31	337. BD*(1)Te 1- C 4	4.31	0.32	0.033
170. LP (4) I 31	337. BD*(1)Te 1- C 4	1.06	0.34	0.017
170. LP (4) I 31	371. BD*(1)Te 32- C 35	6.68	0.36	0.044
168. LP (2) I 31	402. BD*(1)Te 62- C 64	2.81	0.32	0.027
169. LP (3) I 31	406. BD*(1) C 63- H 68	1.48	0.63	0.027
179. LP (3) I 61	370. BD*(1)Te 32- C 34	3.55	0.32	0.030
180. LP (4) I 61	370. BD*(1)Te 32- C 34	1.32	0.33	0.019
180. LP (4) I 61	403. BD*(1)Te 62- C 65	6.12	0.35	0.041
189. LP (3) I 91	338. BD*(1)Te 1- C 8	3.54	0.32	0.030
190. LP (4) I 91	338. BD*(1)Te 1- C 8	1.33	0.33	0.019
190. LP (4) I 91	435. BD*(1)Te 92- C 95	6.12	0.35	0.041

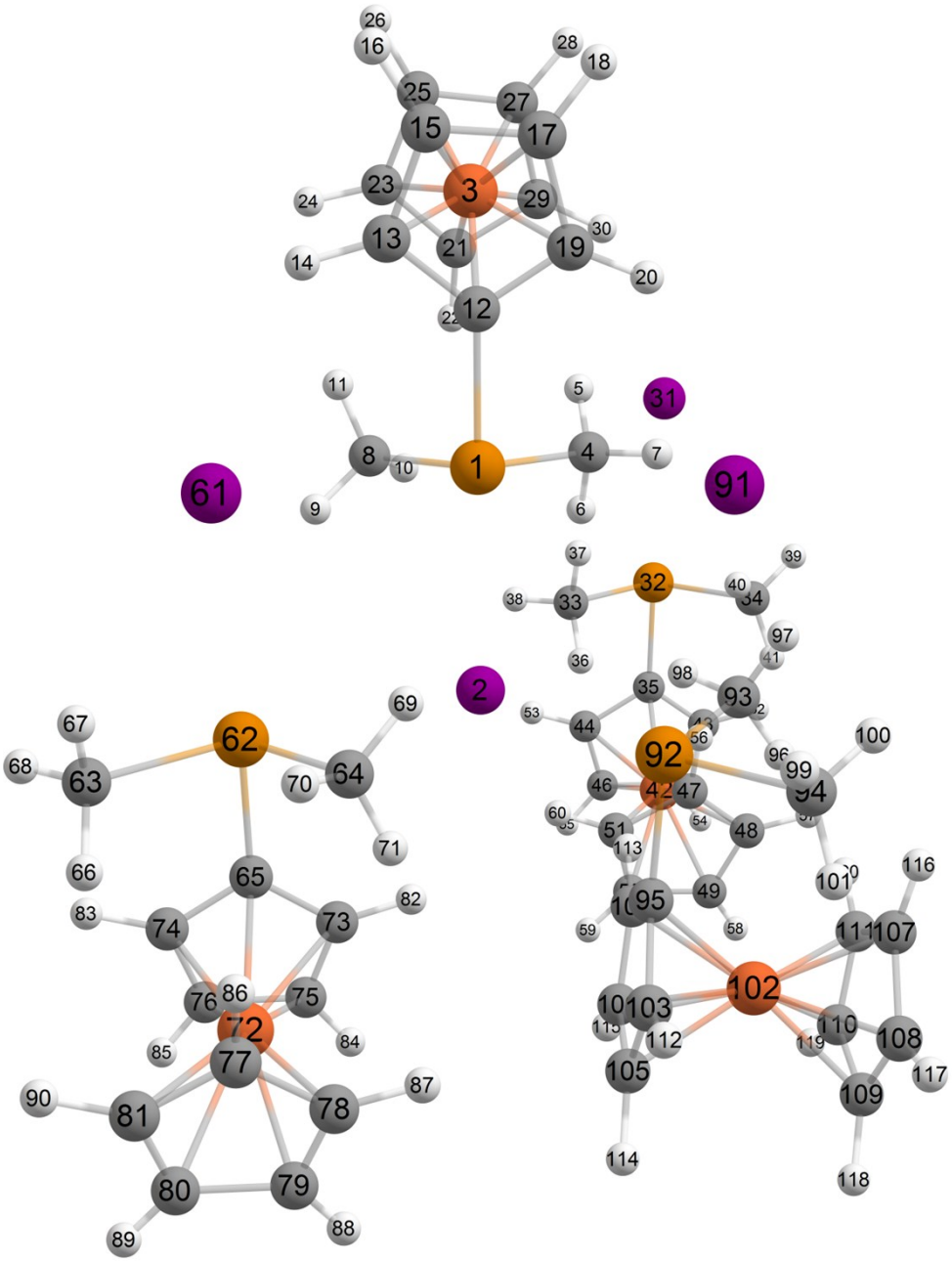


Figure S13

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
161. LP (4) I 2	339. BD*(1)Te 1- C 12	6.53	0.35	0.043
160. LP (3) I 2	401. BD*(1)Te 62- C 63	3.58	0.31	0.030
161. LP (4) I 2	401. BD*(1)Te 62- C 63	1.00	0.34	0.016
159. LP (2) I 2	434. BD*(1)Te 92- C 94	2.87	0.31	0.027
160. LP (3) I 2	438. BD*(1) C 93- H 98	1.48	0.62	0.027
170. LP (4) I 31	371. BD*(1)Te 32- C 35	5.82	0.33	0.039
179. LP (3) I 61	337. BD*(1)Te 1- C 4	4.22	0.32	0.033
180. LP (4) I 61	337. BD*(1)Te 1- C 4	1.40	0.34	0.020
180. LP (4) I 61	403. BD*(1)Te 62- C 65	5.72	0.35	0.040
189. LP (3) I 91	338. BD*(1)Te 1- C 8	3.59	0.32	0.030
190. LP (4) I 91	338. BD*(1)Te 1- C 8	1.26	0.33	0.018
190. LP (4) I 91	435. BD*(1)Te 92- C 95	6.16	0.35	0.041

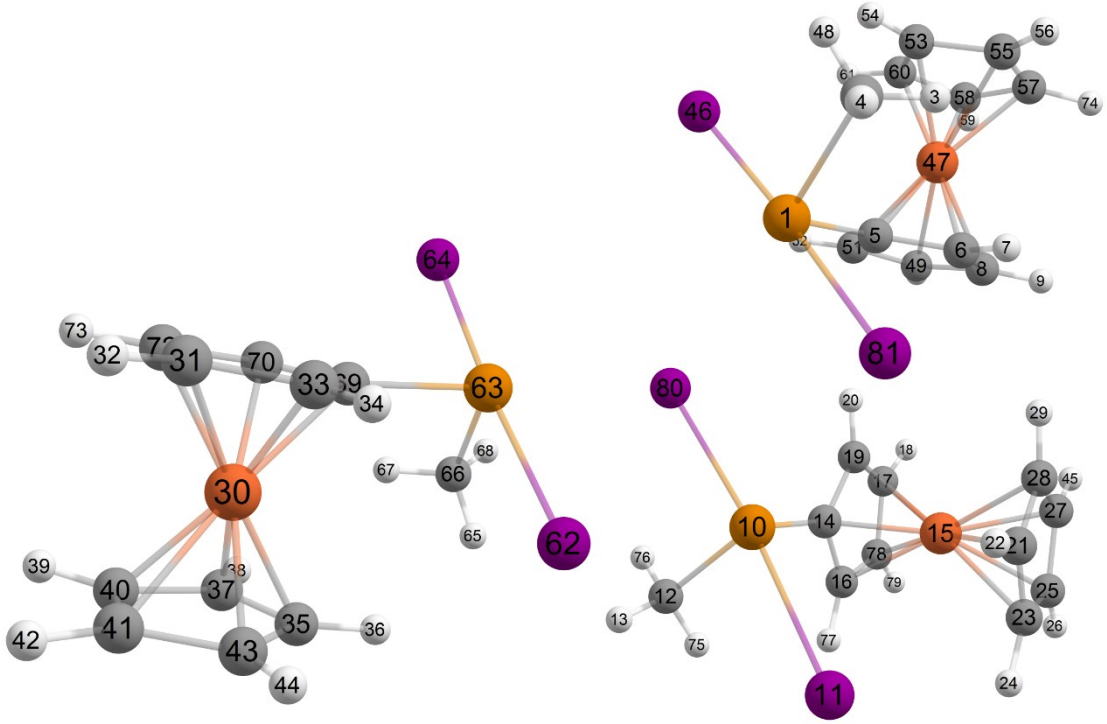


Figure S14

1.	I 46:-Te 1-: I 81	54.1/45.9	3.9534	177	174	179	180	174
2.	I 11:-Te 10-: I 80	59.3/40.7	3.9637	188	170	201	202	170
3.	I 64:-Te 63-: I 62	52.0/48.0	3.9543	250	162	325	326	162

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
154. LP (2) I 46	274. BD*(1)Te 1- C 2	1.07	0.29	0.016
155. LP (3) I 46	275. BD*(1)Te 1- C 5	1.35	0.32	0.019
145. LP (2) I 11	288. BD*(1)Te 10- C 12	1.21	0.32	0.018
146. LP (3) I 11	289. BD*(1)Te 10- C 14	1.88	0.33	0.022
165. LP (2) I 64	350. BD*(1)Te 63- C 66	1.06	0.29	0.016
166. LP (3) I 64	351. BD*(1)Te 63- C 69	1.39	0.32	0.019
161. LP (3) I 62	289. BD*(1)Te 10- C 14	7.23	0.35	0.045
159. LP (1) I 62	349. BD*(1)Te 63- I 64	6.27	0.51	0.050
160. LP (2) I 62	350. BD*(1)Te 63- C 66	1.48	0.30	0.019
161. LP (3) I 62	349. BD*(1)Te 63- I 64	1.65	0.17	0.015
161. LP (3) I 62	351. BD*(1)Te 63- C 69	1.30	0.35	0.019
162. LP (4) I 62	349. BD*(1)Te 63- I 64	98.29	0.16	0.112
162. LP (4) I 62	350. BD*(1)Te 63- C 66	1.39	0.30	0.018
162. LP (4) I 62	351. BD*(1)Te 63- C 69	1.24	0.33	0.018
162. LP (4) I 62	1497. RY (1)Te 63	4.48	0.92	0.057
162. LP (4) I 62	1502. RY (6)Te 63	1.12	1.20	0.033
162. LP (4) I 62	1532. RY (36)Te 63	1.04	37.92	0.177
162. LP (4) I 62	1460. RY (1) I 62	1.80	0.95	0.037
168. LP (2) I 80	274. BD*(1)Te 1- C 2	5.25	0.33	0.037
167. LP (1) I 80	287. BD*(1)Te 10- I 11	5.16	0.49	0.045
168. LP (2) I 80	287. BD*(1)Te 10- I 11	1.80	0.20	0.017
170. LP (4) I 80	287. BD*(1)Te 10- I 11	71.12	0.17	0.099
170. LP (4) I 80	288. BD*(1)Te 10- C 12	1.63	0.32	0.020
170. LP (4) I 80	289. BD*(1)Te 10- C 14	1.02	0.34	0.017
170. LP (4) I 80	525. RY (1)Te 10	3.42	0.96	0.051
169. LP (3) I 80	351. BD*(1)Te 63- C 69	6.02	0.33	0.040
170. LP (4) I 80	1751. RY (1) I 80	1.29	0.92	0.031
171. LP (1) I 81	276. BD*(1)Te 1- I 46	5.65	0.51	0.048
172. LP (2) I 81	275. BD*(1)Te 1- C 5	1.45	0.33	0.019
173. LP (3) I 81	276. BD*(1)Te 1- I 46	1.34	0.18	0.014
174. LP (4) I 81	274. BD*(1)Te 1- C 2	1.49	0.30	0.019
174. LP (4) I 81	275. BD*(1)Te 1- C 5	1.34	0.33	0.019
174. LP (4) I 81	276. BD*(1)Te 1- I 46	88.48	0.16	0.107
174. LP (4) I 81	364. RY (1)Te 1	4.42	0.93	0.057
173. LP (3) I 81	288. BD*(1)Te 10- C 12	5.28	0.33	0.037

174. LP (4) I 81	1788. RY (1) I 81	1.62	0.99	0.036

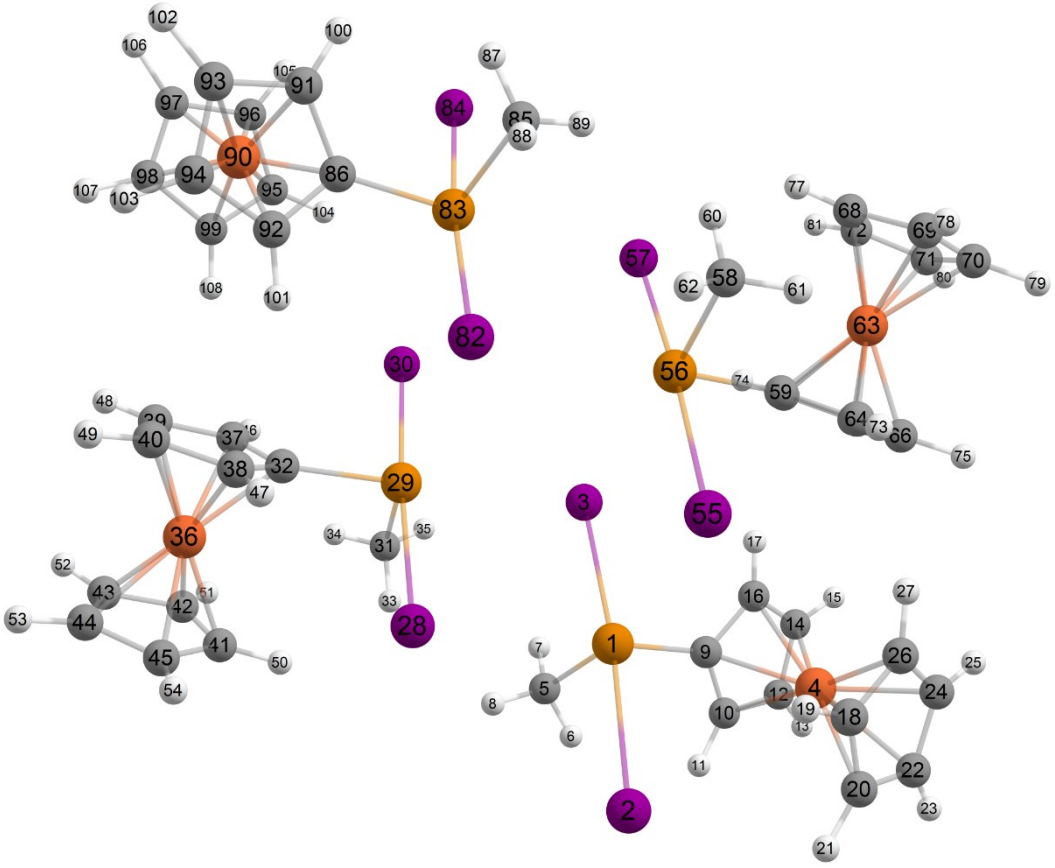


Figure S15

1.	I 2:-Te 1-: I 3	59.2/40.8	3.9629	241	196	241	242	196
6.	I 28:-Te 29-: I 30	52.2/47.8	3.9572	270	209	299	300	209
11.	I 57:-Te 56-: I 55	52.2/47.8	3.9572	299	218	357	358	218
16.	I 84:-Te 83-: I 82	59.2/40.8	3.9630	328	231	415	416	231

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
191. LP (2) I 2	370. BD*(1)Te 1- C 5	1.20	0.32	0.017
192. LP (3) I 2	371. BD*(1)Te 1- C 9	1.88	0.34	0.022
193. LP (1) I 3	369. BD*(1)Te 1- I 2	5.04	0.48	0.044
194. LP (2) I 3	369. BD*(1)Te 1- I 2	1.93	0.20	0.018
196. LP (4) I 3	369. BD*(1)Te 1- I 2	71.21	0.17	0.099
196. LP (4) I 3	370. BD*(1)Te 1- C 5	1.63	0.32	0.020
196. LP (4) I 3	371. BD*(1)Te 1- C 9	1.03	0.34	0.017
196. LP (4) I 3	485. RY (1)Te 1	3.40	0.97	0.051
196. LP (4) I 3	559. RY (1) I 3	1.21	0.94	0.030
195. LP (3) I 3	400. BD*(1)Te 29- C 32	7.24	0.34	0.044
194. LP (2) I 3	428. BD*(1)Te 56- C 58	6.47	0.33	0.041
204. LP (3) I 28	371. BD*(1)Te 1- C 9	7.18	0.35	0.045
203. LP (2) I 28	399. BD*(1)Te 29- C 31	1.76	0.30	0.021
204. LP (3) I 28	400. BD*(1)Te 29- C 32	1.69	0.35	0.022
206. LP (1) I 30	398. BD*(1) I 28-Te 29	6.89	0.50	0.052
207. LP (2) I 30	400. BD*(1)Te 29- C 32	1.65	0.33	0.021
208. LP (3) I 30	398. BD*(1) I 28-Te 29	1.77	0.17	0.016
208. LP (3) I 30	399. BD*(1)Te 29- C 31	1.09	0.31	0.017
209. LP (4) I 30	398. BD*(1) I 28-Te 29	96.39	0.16	0.111
209. LP (4) I 30	399. BD*(1)Te 29- C 31	1.55	0.30	0.019
209. LP (4) I 30	400. BD*(1)Te 29- C 32	1.13	0.34	0.017
209. LP (4) I 30	1009. RY (1)Te 29	4.14	0.96	0.056
209. LP (4) I 30	1046. RY (1) I 30	1.71	1.04	0.038
208. LP (3) I 30	457. BD*(1)Te 83- C 85	5.25	0.33	0.037
217. LP (3) I 55	370. BD*(1)Te 1- C 5	5.24	0.33	0.037
218. LP (4) I 55	1459. RY (1) I 55	1.71	1.04	0.038

215. LP (1) I 55	427. BD*(1)Te 56- I 57	6.89	0.50	0.052
216. LP (2) I 55	429. BD*(1)Te 56- C 59	1.65	0.33	0.021
217. LP (3) I 55	427. BD*(1)Te 56- I 57	1.76	0.17	0.016
217. LP (3) I 55	428. BD*(1)Te 56- C 58	1.09	0.31	0.017
218. LP (4) I 55	427. BD*(1)Te 56- I 57	96.33	0.16	0.111
218. LP (4) I 55	428. BD*(1)Te 56- C 58	1.55	0.30	0.019
218. LP (4) I 55	429. BD*(1)Te 56- C 59	1.13	0.34	0.017
218. LP (4) I 55	1496. RY (1)Te 56	4.14	0.96	0.056
221. LP (2) I 57	428. BD*(1)Te 56- C 58	1.76	0.30	0.021
222. LP (3) I 57	429. BD*(1)Te 56- C 59	1.68	0.35	0.022
222. LP (3) I 57	458. BD*(1)Te 83- C 86	7.19	0.35	0.045
229. LP (2) I 82	399. BD*(1)Te 29- C 31	6.46	0.33	0.041
230. LP (3) I 82	429. BD*(1)Te 56- C 59	7.23	0.34	0.044
231. LP (4) I 82	1946. RY (1) I 82	1.22	0.94	0.030
228. LP (1) I 82	456. BD*(1)Te 83- I 84	5.03	0.48	0.044
229. LP (2) I 82	456. BD*(1)Te 83- I 84	1.98	0.20	0.018
231. LP (4) I 82	456. BD*(1)Te 83- I 84	71.07	0.17	0.099
231. LP (4) I 82	457. BD*(1)Te 83- C 85	1.63	0.32	0.020
231. LP (4) I 82	458. BD*(1)Te 83- C 86	1.02	0.34	0.017
231. LP (4) I 82	1983. RY (1)Te 83	3.39	0.97	0.051
234. LP (2) I 84	457. BD*(1)Te 83- C 85	1.21	0.32	0.018
235. LP (3) I 84	458. BD*(1)Te 83- C 86	1.88	0.34	0.022

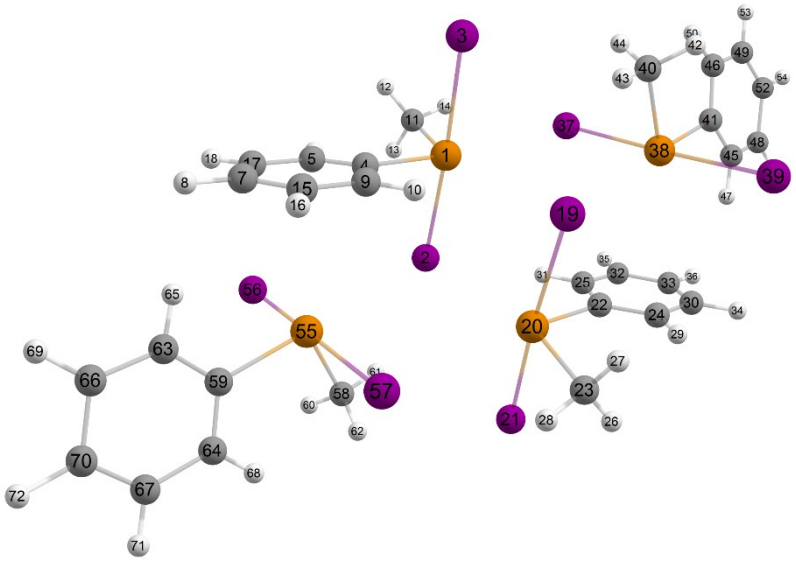


Figure S16

1.	I 3:-Te 1-: I 2	59.5/40.5	3.9505	169	141	169	170	141
2.	I 21:-Te 20-: I 19	59.5/40.5	3.9505	189	148	209	210	148
3.	I 39:-Te 38-: I 37	56.5/43.5	3.9532	209	156	249	250	156
4.	I 56:-Te 55-: I 57	56.5/43.5	3.9532	229	168	289	290	168

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
144. LP (3) I 3	250. BD*(1)Te 1- C 4	1.22	0.33	0.018
138. LP (1) I 2	249. BD*(1)Te 1- I 3	5.29	0.51	0.046
141. LP (4) I 2	249. BD*(1)Te 1- I 3	71.24	0.17	0.099
141. LP (4) I 2	250. BD*(1)Te 1- C 4	1.30	0.33	0.019
141. LP (4) I 2	251. BD*(1)Te 1- C 11	1.83	0.32	0.022
141. LP (4) I 2	329. RY (1)Te 1	3.80	0.91	0.052
141. LP (4) I 2	366. RY (1) I 2	1.30	0.95	0.031
139. LP (2) I 2	271. BD*(1)Te 20- C 23	3.06	0.32	0.028
139. LP (2) I 2	280. BD*(1) C 25- H 31	1.12	0.68	0.025
140. LP (3) I 2	311. BD*(1)Te 55- C 59	4.47	0.35	0.035
146. LP (2) I 19	251. BD*(1)Te 1- C 11	3.06	0.32	0.028
146. LP (2) I 19	261. BD*(1) C 9- H 10	1.12	0.68	0.025
148. LP (4) I 19	662. RY (1) I 19	1.30	0.95	0.031
145. LP (1) I 19	269. BD*(1)Te 20- I 21	5.29	0.51	0.046
148. LP (4) I 19	269. BD*(1)Te 20- I 21	71.22	0.17	0.099

148. LP (4) I 19	270. BD*(1)Te 20- C 22	1.30	0.33	0.019
148. LP (4) I 19	271. BD*(1)Te 20- C 23	1.83	0.32	0.022
148. LP (4) I 19	699. RY (1)Te 20	3.80	0.91	0.052
147. LP (3) I 19	291. BD*(1)Te 38- C 41	4.47	0.35	0.035
152. LP (3) I 21	270. BD*(1)Te 20- C 22	1.22	0.33	0.018
155. LP (3) I 37	250. BD*(1)Te 1- C 4	5.48	0.34	0.039
156. LP (4) I 37	995. RY (1) I 37	1.56	0.94	0.034
153. LP (1) I 37	289. BD*(1)Te 38- I 39	5.67	0.51	0.048
155. LP (3) I 37	289. BD*(1)Te 38- I 39	1.25	0.18	0.013
155. LP (3) I 37	291. BD*(1)Te 38- C 41	1.07	0.35	0.017
156. LP (4) I 37	290. BD*(1)Te 38- C 40	1.96	0.32	0.022
156. LP (4) I 37	291. BD*(1)Te 38- C 41	1.21	0.33	0.018
156. LP (4) I 37	1032. RY (1)Te 38	4.11	0.91	0.055
167. LP (3) I 57	270. BD*(1)Te 20- C 22	5.48	0.34	0.039
165. LP (1) I 57	309. BD*(1)Te 55- I 56	5.67	0.51	0.048
167. LP (3) I 57	309. BD*(1)Te 55- I 56	1.25	0.18	0.013
167. LP (3) I 57	311. BD*(1)Te 55- C 59	1.08	0.35	0.017
168. LP (4) I 57	310. BD*(1)Te 55- C 58	1.96	0.32	0.022
168. LP (4) I 57	311. BD*(1)Te 55- C 59	1.21	0.33	0.018
168. LP (4) I 57	1328. RY (1)Te 55	4.11	0.91	0.055
168. LP (4) I 57	1402. RY (1) I 57	1.56	0.94	0.034
193. BD (2) C 22- C 24	269. BD*(1)Te 20- I 21	5.23	0.19	0.028

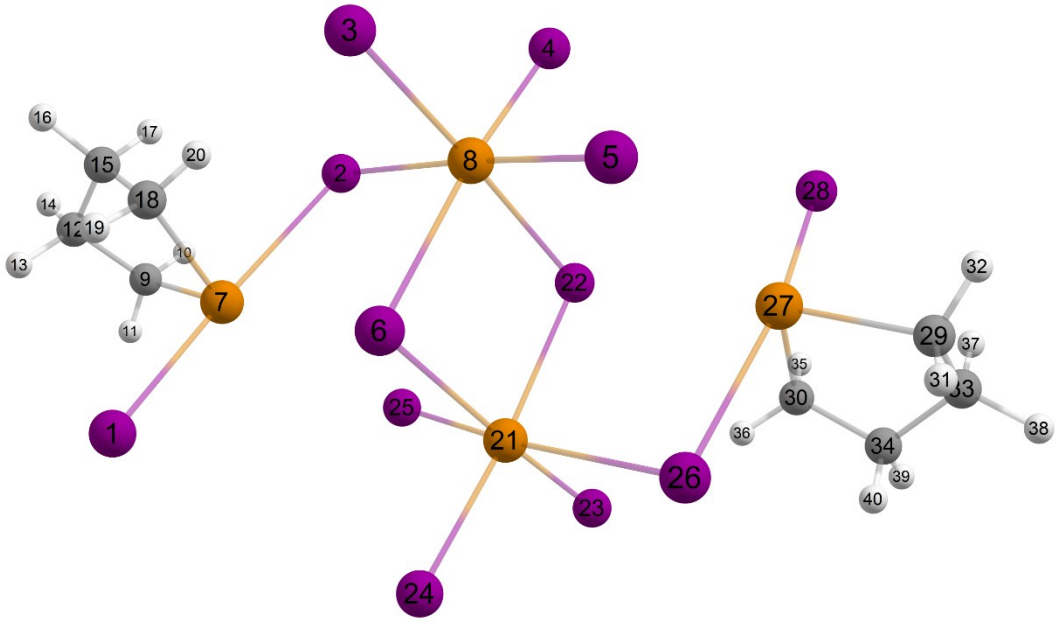


Figure S17

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
154. LP (2) I 1	236. BD*(1)Te 7- C 18	1.56	0.32	0.020
154. LP (2) I 1	489. RY (3)Te 7	1.05	0.87	0.027
155. LP (3) I 1	235. BD*(1)Te 7- C 9	1.88	0.31	0.022
155. LP (3) I 1	236. BD*(1)Te 7- C 18	1.14	0.32	0.017
155. LP (3) I 1	488. RY (2)Te 7	1.13	0.84	0.027
156. LP (1) I 2	231. BD*(1) I 1-Te 7	2.27	0.53	0.031
158. LP (3) I 2	231. BD*(1) I 1-Te 7	26.20	0.21	0.067
158. LP (3) I 2	487. RY (1)Te 7	1.52	0.93	0.033
159. LP (4) I 2	231. BD*(1) I 1-Te 7	2.49	0.19	0.019
156. LP (1) I 2	234. BD*(1) I 5-Te 8	3.64	0.50	0.038
158. LP (3) I 2	234. BD*(1) I 5-Te 8	6.38	0.18	0.030
159. LP (4) I 2	234. BD*(1) I 5-Te 8	32.61	0.15	0.063
159. LP (4) I 2	524. RY (1)Te 8	2.83	0.67	0.039
160. LP (1) I 3	530. RY (7)Te 8	1.46	1.05	0.035
161. LP (2) I 3	234. BD*(1) I 5-Te 8	4.61	0.17	0.025
161. LP (2) I 3	528. RY (5)Te 8	1.38	0.64	0.026

162. LP (3) I 3	233. BD*(1) I 4-Te 8	5.32	0.18	0.027
162. LP (3) I 3	526. RY (3)Te 8	1.89	0.61	0.030
163. LP (1) I 4	529. RY (6)Te 8	1.90	1.06	0.040
164. LP (2) I 4	232. BD*(1) I 3-Te 8	4.61	0.17	0.025
164. LP (2) I 4	526. RY (3)Te 8	1.22	0.60	0.024
165. LP (3) I 4	234. BD*(1) I 5-Te 8	4.46	0.17	0.024
165. LP (3) I 4	527. RY (4)Te 8	1.44	0.57	0.026
166. LP (1) I 5	531. RY (8)Te 8	1.33	1.04	0.033
167. LP (2) I 5	233. BD*(1) I 4-Te 8	4.45	0.17	0.025
167. LP (2) I 5	527. RY (4)Te 8	1.35	0.57	0.025
168. LP (3) I 5	232. BD*(1) I 3-Te 8	4.33	0.18	0.025
168. LP (3) I 5	528. RY (5)Te 8	1.34	0.64	0.026
168. LP (3) I 5	253. BD*(1)Te 27- C 30	2.41	0.33	0.025
170. LP (2) I 6	235. BD*(1)Te 7- C 9	6.18	0.33	0.040
169. LP (1) I 6	233. BD*(1) I 4-Te 8	4.32	0.48	0.041
172. LP (4) I 6	233. BD*(1) I 4-Te 8	44.17	0.19	0.081
172. LP (4) I 6	524. RY (1)Te 8	1.14	0.70	0.025
172. LP (4) I 6	525. RY (2)Te 8	2.77	0.72	0.040
169. LP (1) I 6	248. BD*(1)Te 21- I 23	3.87	0.48	0.039
171. LP (3) I 6	248. BD*(1)Te 21- I 23	37.91	0.17	0.072
171. LP (3) I 6	706. RY (2)Te 21	2.36	0.70	0.036
172. LP (4) I 6	248. BD*(1)Te 21- I 23	4.24	0.19	0.025
188. LP (3) I 25	236. BD*(1)Te 7- C 18	2.41	0.33	0.025
180. LP (1) I 23	711. RY (7)Te 21	1.46	1.05	0.035
181. LP (2) I 23	250. BD*(1)Te 21- I 25	4.61	0.17	0.025
181. LP (2) I 23	709. RY (5)Te 21	1.38	0.64	0.026
182. LP (3) I 23	249. BD*(1)Te 21- I 24	5.33	0.18	0.027
182. LP (3) I 23	707. RY (3)Te 21	1.89	0.61	0.030
183. LP (1) I 24	710. RY (6)Te 21	1.90	1.06	0.040
184. LP (2) I 24	248. BD*(1)Te 21- I 23	4.60	0.17	0.025
184. LP (2) I 24	707. RY (3)Te 21	1.22	0.60	0.024
185. LP (3) I 24	250. BD*(1)Te 21- I 25	4.45	0.17	0.024
185. LP (3) I 24	708. RY (4)Te 21	1.44	0.57	0.026
186. LP (1) I 25	712. RY (8)Te 21	1.33	1.04	0.033
187. LP (2) I 25	249. BD*(1)Te 21- I 24	4.45	0.17	0.025
187. LP (2) I 25	708. RY (4)Te 21	1.35	0.57	0.025
188. LP (3) I 25	248. BD*(1)Te 21- I 23	4.33	0.18	0.025
188. LP (3) I 25	709. RY (5)Te 21	1.35	0.64	0.026
176. LP (1) I 22	232. BD*(1) I 3-Te 8	3.87	0.48	0.039
178. LP (3) I 22	232. BD*(1) I 3-Te 8	37.91	0.17	0.072
178. LP (3) I 22	525. RY (2)Te 8	2.37	0.70	0.036
179. LP (4) I 22	232. BD*(1) I 3-Te 8	4.24	0.19	0.025
176. LP (1) I 22	249. BD*(1)Te 21- I 24	4.32	0.48	0.041
179. LP (4) I 22	249. BD*(1)Te 21- I 24	44.16	0.19	0.081
179. LP (4) I 22	705. RY (1)Te 21	1.12	0.70	0.025
179. LP (4) I 22	706. RY (2)Te 21	2.79	0.72	0.040
177. LP (2) I 22	252. BD*(1)Te 27- C 29	6.19	0.33	0.041
189. LP (1) I 26	250. BD*(1)Te 21- I 25	3.64	0.50	0.038
191. LP (3) I 26	250. BD*(1)Te 21- I 25	6.43	0.18	0.031
192. LP (4) I 26	250. BD*(1)Te 21- I 25	32.57	0.15	0.063
192. LP (4) I 26	705. RY (1)Te 21	2.83	0.67	0.039
189. LP (1) I 26	251. BD*(1)Te 27- I 28	2.27	0.53	0.031
191. LP (3) I 26	251. BD*(1)Te 27- I 28	26.18	0.21	0.067
191. LP (3) I 26	927. RY (1)Te 27	1.52	0.93	0.033
192. LP (4) I 26	251. BD*(1)Te 27- I 28	2.53	0.19	0.019
195. LP (2) I 28	253. BD*(1)Te 27- C 30	1.57	0.32	0.020
195. LP (2) I 28	929. RY (3)Te 27	1.05	0.87	0.027
196. LP (3) I 28	252. BD*(1)Te 27- C 29	1.89	0.31	0.022
196. LP (3) I 28	253. BD*(1)Te 27- C 30	1.14	0.32	0.017
196. LP (3) I 28	928. RY (2)Te 27	1.13	0.84	0.027

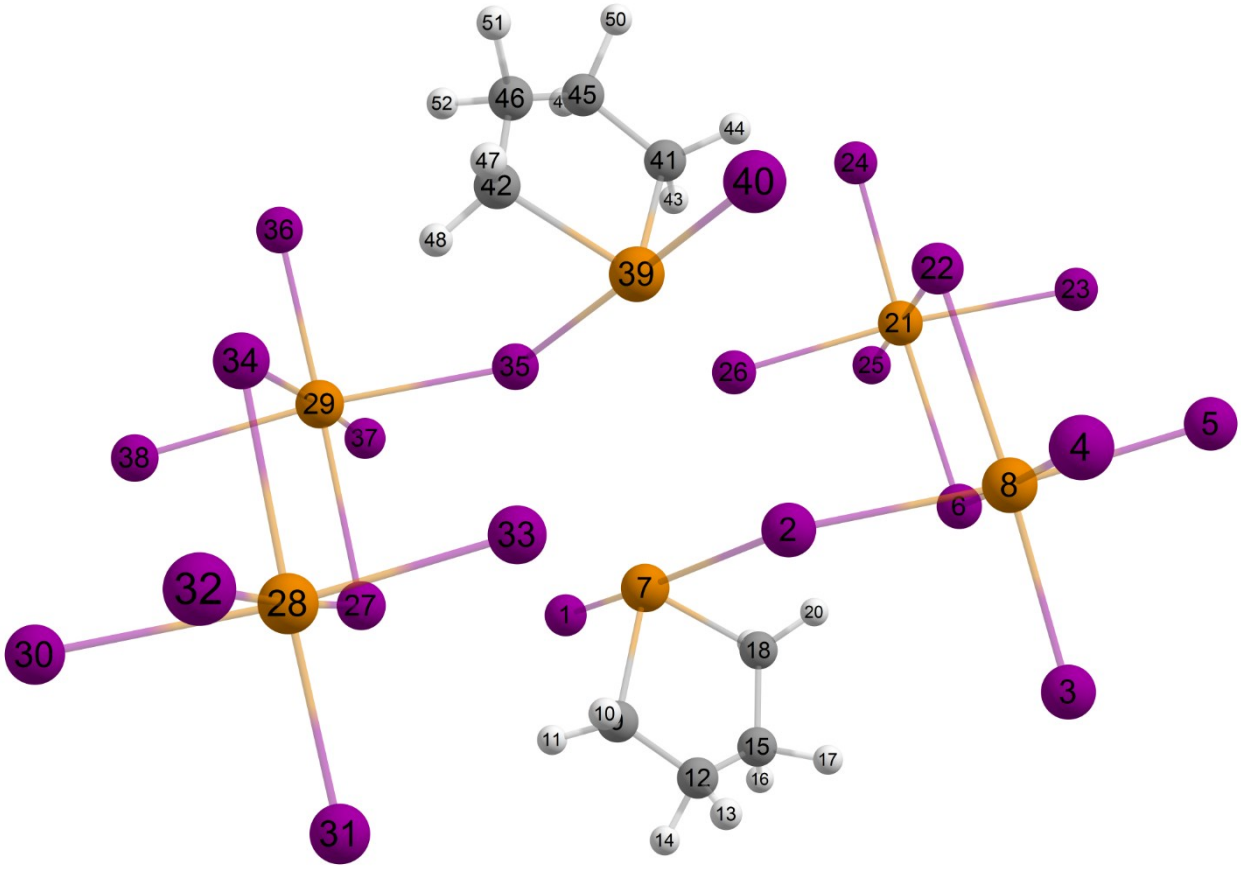


Figure S18

	Hyperbond A:-B-:C	%A-B/%B-C	occ	NBOs BD(A-B)	NBOs LP(C)	3-center hybrids h(A)	3-center hybrids h(B)	3-center hybrids h(C)
1.	I 5:-Te 8-: I 2	65.4/34.6	3.8109	343	267	346	347	267
2.	I 30:-Te 28-: I 33	51.9/48.1	3.7352	360	318	380	381	318
3.	I 38:-Te 29-: I 35	65.4/34.6	3.8088	365	326	390	391	326

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
262. LP (2) I 1	385. BD*(1)Te 7- C 9	2.00	0.32	0.023
262. LP (2) I 1	645. RY (3)Te 7	1.06	0.88	0.027
263. LP (3) I 1	385. BD*(1)Te 7- C 9	1.36	0.32	0.019
263. LP (3) I 1	386. BD*(1)Te 7- C 18	1.88	0.32	0.022
263. LP (3) I 1	644. RY (2)Te 7	1.25	0.83	0.029
264. LP (1) I 2	381. BD*(1) I 1-Te 7	1.24	0.33	0.018
265. LP (2) I 2	381. BD*(1) I 1-Te 7	2.49	0.45	0.030
266. LP (3) I 2	381. BD*(1) I 1-Te 7	16.56	0.22	0.054
267. LP (4) I 2	381. BD*(1) I 1-Te 7	3.37	0.20	0.023
264. LP (1) I 2	384. BD*(1) I 5-Te 8	5.91	0.28	0.036
265. LP (2) I 2	384. BD*(1) I 5-Te 8	9.03	0.40	0.054
265. LP (2) I 2	685. RY (6)Te 8	1.34	0.88	0.031
266. LP (3) I 2	383. BD*(1) I 4-Te 8	1.20	0.19	0.013
267. LP (4) I 2	384. BD*(1) I 5-Te 8	61.52	0.15	0.086
267. LP (4) I 2	680. RY (1)Te 8	2.52	0.72	0.038
267. LP (4) I 2	681. RY (2)Te 8	1.09	0.71	0.025
265. LP (2) I 2	409. BD*(1)Te 39- C 42	1.26	0.57	0.024
268. LP (1) I 3	687. RY (8)Te 8	1.04	1.02	0.029
269. LP (2) I 3	383. BD*(1) I 4-Te 8	2.72	0.16	0.019
269. LP (2) I 3	384. BD*(1) I 5-Te 8	2.40	0.15	0.017
269. LP (2) I 3	683. RY (4)Te 8	1.31	0.57	0.024
270. LP (3) I 3	383. BD*(1) I 4-Te 8	2.36	0.17	0.018
270. LP (3) I 3	384. BD*(1) I 5-Te 8	2.95	0.15	0.019
270. LP (3) I 3	682. RY (3)Te 8	1.26	0.58	0.024
271. LP (1) I 4	687. RY (8)Te 8	1.03	1.02	0.029

272. LP (2) I 4	384. BD*(1) I 5-Te 8	4.72	0.15	0.024
272. LP (2) I 4	684. RY (5)Te 8	1.34	0.55	0.024
273. LP (3) I 4	382. BD*(1) I 3-Te 8	5.37	0.16	0.026
273. LP (3) I 4	682. RY (3)Te 8	1.87	0.57	0.029
274. LP (1) I 5	685. RY (6)Te 8	1.95	0.99	0.039
275. LP (2) I 5	382. BD*(1) I 3-Te 8	1.52	0.16	0.014
275. LP (2) I 5	383. BD*(1) I 4-Te 8	1.95	0.16	0.016
275. LP (2) I 5	684. RY (5)Te 8	1.38	0.54	0.024
276. LP (3) I 5	382. BD*(1) I 3-Te 8	1.79	0.17	0.016
276. LP (3) I 5	383. BD*(1) I 4-Te 8	1.13	0.17	0.012
276. LP (3) I 5	683. RY (4)Te 8	1.32	0.57	0.025
278. LP (2) I 6	397. BD*(1) C 18- H 20	1.86	0.67	0.031
277. LP (1) I 6	383. BD*(1) I 4-Te 8	4.73	0.50	0.043
279. LP (3) I 6	383. BD*(1) I 4-Te 8	30.95	0.20	0.071
279. LP (3) I 6	680. RY (1)Te 8	2.01	0.76	0.035
280. LP (4) I 6	383. BD*(1) I 4-Te 8	19.56	0.15	0.048
280. LP (4) I 6	680. RY (1)Te 8	1.69	0.71	0.031
277. LP (1) I 6	399. BD*(1)Te 21- I 24	4.64	0.49	0.043
278. LP (2) I 6	398. BD*(1)Te 21- I 23	1.30	0.12	0.011
279. LP (3) I 6	399. BD*(1)Te 21- I 24	25.20	0.20	0.064
279. LP (3) I 6	862. RY (2)Te 21	1.13	0.75	0.026
280. LP (4) I 6	399. BD*(1)Te 21- I 24	25.49	0.15	0.055
280. LP (4) I 6	862. RY (2)Te 21	2.07	0.70	0.034
288. LP (1) I 23	866. RY (6)Te 21	1.39	0.96	0.033
289. LP (2) I 23	399. BD*(1)Te 21- I 24	2.18	0.15	0.016
290. LP (3) I 23	400. BD*(1)Te 21- I 25	1.14	0.20	0.013
291. LP (1) I 24	868. RY (8)Te 21	1.83	1.06	0.039
292. LP (2) I 24	398. BD*(1)Te 21- I 23	6.23	0.12	0.024
292. LP (2) I 24	864. RY (4)Te 21	1.37	0.54	0.024
293. LP (3) I 24	400. BD*(1)Te 21- I 25	4.93	0.17	0.026
294. LP (1) I 25	867. RY (7)Te 21	1.74	1.13	0.040
295. LP (2) I 25	398. BD*(1)Te 21- I 23	5.21	0.12	0.022
295. LP (2) I 25	865. RY (5)Te 21	1.94	0.54	0.029
296. LP (3) I 25	399. BD*(1)Te 21- I 24	5.16	0.16	0.026
296. LP (3) I 25	863. RY (3)Te 21	1.44	0.56	0.025
290. LP (3) I 23	380. LV (1) I 26	2.70	0.03	0.009
284. LP (1) I 22	382. BD*(1) I 3-Te 8	4.53	0.49	0.042
286. LP (3) I 22	382. BD*(1) I 3-Te 8	37.49	0.20	0.078
286. LP (3) I 22	681. RY (2)Te 8	2.87	0.75	0.041
287. LP (4) I 22	382. BD*(1) I 3-Te 8	9.36	0.15	0.034
287. LP (4) I 22	681. RY (2)Te 8	1.21	0.70	0.026
284. LP (1) I 22	400. BD*(1)Te 21- I 25	4.79	0.49	0.043
285. LP (2) I 22	398. BD*(1)Te 21- I 23	1.76	0.14	0.014
285. LP (2) I 22	400. BD*(1)Te 21- I 25	1.09	0.18	0.012
286. LP (3) I 22	400. BD*(1)Te 21- I 25	16.81	0.20	0.052
287. LP (4) I 22	400. BD*(1)Te 21- I 25	35.96	0.15	0.066
287. LP (4) I 22	862. RY (2)Te 21	2.36	0.70	0.036
285. LP (2) I 22	409. BD*(1)Te 39- C 42	1.04	0.33	0.017
297. LP (1) I 26	385. BD*(1)Te 7- C 9	1.03	0.60	0.022
298. LP (2) I 26	385. BD*(1)Te 7- C 9	1.18	0.39	0.019
297. LP (1) I 26	398. BD*(1)Te 21- I 23	10.05	0.40	0.057
297. LP (1) I 26	866. RY (6)Te 21	1.26	0.92	0.030
298. LP (2) I 26	398. BD*(1)Te 21- I 23	4.94	0.19	0.027
298. LP (2) I 26	400. BD*(1)Te 21- I 25	1.68	0.23	0.018
298. LP (2) I 26	866. RY (6)Te 21	1.06	0.70	0.024
299. LP (3) I 26	398. BD*(1)Te 21- I 23	10.12	0.17	0.037
299. LP (3) I 26	399. BD*(1)Te 21- I 24	1.61	0.21	0.017
297. LP (1) I 26	380. LV (1) I 26	11.72	0.28	0.051
298. LP (2) I 26	380. LV (1) I 26	9.66	0.07	0.023
299. LP (3) I 26	380. LV (1) I 26	10.22	0.05	0.021
301. LP (2) I 27	386. BD*(1)Te 7- C 18	1.03	0.33	0.017
300. LP (1) I 27	403. BD*(1)Te 28- I 32	4.79	0.49	0.043
301. LP (2) I 27	401. BD*(1)Te 28- I 30	1.76	0.14	0.014
301. LP (2) I 27	403. BD*(1)Te 28- I 32	1.07	0.18	0.012
302. LP (3) I 27	403. BD*(1)Te 28- I 32	17.08	0.20	0.053
303. LP (4) I 27	403. BD*(1)Te 28- I 32	35.65	0.15	0.066
303. LP (4) I 27	1121. RY (2)Te 28	2.34	0.70	0.036
300. LP (1) I 27	404. BD*(1)Te 29- I 36	4.53	0.49	0.042
302. LP (3) I 27	404. BD*(1)Te 29- I 36	37.28	0.20	0.078
302. LP (3) I 27	1158. RY (2)Te 29	2.85	0.75	0.041
303. LP (4) I 27	404. BD*(1)Te 29- I 36	9.65	0.15	0.034

303. LP (4) I 27	1158. RY (2)Te 29	1.24	0.70	0.026
306. LP (1) I 30	1125. RY (6)Te 28	1.39	0.96	0.033
307. LP (2) I 30	402. BD*(1)Te 28- I 31	2.17	0.15	0.016
308. LP (3) I 30	403. BD*(1)Te 28- I 32	1.14	0.20	0.013
309. LP (1) I 31	1127. RY (8)Te 28	1.83	1.06	0.039
310. LP (2) I 31	401. BD*(1)Te 28- I 30	6.23	0.12	0.024
310. LP (2) I 31	1123. RY (4)Te 28	1.38	0.54	0.024
311. LP (3) I 31	403. BD*(1)Te 28- I 32	4.93	0.17	0.026
312. LP (1) I 32	1126. RY (7)Te 28	1.73	1.13	0.040
313. LP (2) I 32	401. BD*(1)Te 28- I 30	5.21	0.12	0.022
313. LP (2) I 32	1124. RY (5)Te 28	1.94	0.54	0.029
314. LP (3) I 32	402. BD*(1)Te 28- I 31	5.17	0.16	0.026
314. LP (3) I 32	1122. RY (3)Te 28	1.44	0.56	0.025
327. LP (1) I 36	1164. RY (8)Te 29	1.04	1.02	0.029
328. LP (2) I 36	405. BD*(1)Te 29- I 37	2.74	0.16	0.019
328. LP (2) I 36	406. BD*(1)Te 29- I 38	2.39	0.15	0.017
328. LP (2) I 36	1160. RY (4)Te 29	1.29	0.57	0.024
329. LP (3) I 36	405. BD*(1)Te 29- I 37	2.34	0.17	0.018
329. LP (3) I 36	406. BD*(1)Te 29- I 38	2.96	0.15	0.019
329. LP (3) I 36	1159. RY (3)Te 29	1.24	0.58	0.024
330. LP (1) I 37	1164. RY (8)Te 29	1.04	1.02	0.029
331. LP (2) I 37	406. BD*(1)Te 29- I 38	4.72	0.15	0.023
331. LP (2) I 37	1161. RY (5)Te 29	1.33	0.55	0.024
332. LP (3) I 37	404. BD*(1)Te 29- I 36	5.37	0.16	0.026
332. LP (3) I 37	1159. RY (3)Te 29	1.88	0.57	0.029
333. LP (1) I 38	1162. RY (6)Te 29	1.95	0.99	0.039
334. LP (2) I 38	404. BD*(1)Te 29- I 36	1.51	0.16	0.014
334. LP (2) I 38	405. BD*(1)Te 29- I 37	1.95	0.16	0.016
334. LP (2) I 38	1161. RY (5)Te 29	1.39	0.54	0.025
335. LP (3) I 38	404. BD*(1)Te 29- I 36	1.79	0.17	0.016
335. LP (3) I 38	405. BD*(1)Te 29- I 37	1.12	0.17	0.012
335. LP (3) I 38	1160. RY (4)Te 29	1.33	0.57	0.025
315. LP (1) I 33	401. BD*(1)Te 28- I 30	10.06	0.40	0.057
315. LP (1) I 33	1125. RY (6)Te 28	1.27	0.92	0.030
316. LP (2) I 33	401. BD*(1)Te 28- I 30	4.96	0.19	0.027
316. LP (2) I 33	403. BD*(1)Te 28- I 32	1.68	0.23	0.018
316. LP (2) I 33	1125. RY (6)Te 28	1.05	0.70	0.024
317. LP (3) I 33	401. BD*(1)Te 28- I 30	10.00	0.17	0.037
317. LP (3) I 33	402. BD*(1)Te 28- I 31	1.62	0.21	0.017
318. LP (4) I 33	401. BD*(1)Te 28- I 30	124.25	0.12	0.108
318. LP (4) I 33	1120. RY (1)Te 28	5.63	0.71	0.056
318. LP (4) I 33	1134. RY (15)Te 28	1.12	20.30	0.134
318. LP (4) I 33	1135. RY (16)Te 28	1.17	27.41	0.160
318. LP (4) I 33	1305. RY (1) I 33	1.40	1.03	0.034
315. LP (1) I 33	408. BD*(1)Te 39- C 41	1.03	0.60	0.022
316. LP (2) I 33	408. BD*(1)Te 39- C 41	1.18	0.39	0.019
319. LP (1) I 34	402. BD*(1)Te 28- I 31	4.64	0.49	0.043
320. LP (2) I 34	401. BD*(1)Te 28- I 30	1.30	0.12	0.011
321. LP (3) I 34	402. BD*(1)Te 28- I 31	25.52	0.20	0.064
321. LP (3) I 34	1121. RY (2)Te 28	1.16	0.75	0.026
322. LP (4) I 34	402. BD*(1)Te 28- I 31	25.05	0.15	0.055
322. LP (4) I 34	1121. RY (2)Te 28	2.05	0.70	0.034
319. LP (1) I 34	405. BD*(1)Te 29- I 37	4.73	0.50	0.043
321. LP (3) I 34	405. BD*(1)Te 29- I 37	30.62	0.20	0.070
321. LP (3) I 34	1157. RY (1)Te 29	1.98	0.76	0.035
322. LP (4) I 34	405. BD*(1)Te 29- I 37	19.98	0.15	0.049
322. LP (4) I 34	1157. RY (1)Te 29	1.71	0.71	0.031
320. LP (2) I 34	415. BD*(1) C 42- H 48	1.87	0.67	0.032
324. LP (2) I 35	386. BD*(1)Te 7- C 18	1.25	0.57	0.024
323. LP (1) I 35	380. LV (1) I 26	2.10	0.13	0.015
324. LP (2) I 35	380. LV (1) I 26	2.93	0.25	0.024
323. LP (1) I 35	406. BD*(1)Te 29- I 38	5.90	0.28	0.036
324. LP (2) I 35	406. BD*(1)Te 29- I 38	9.04	0.40	0.054
324. LP (2) I 35	1162. RY (6)Te 29	1.34	0.88	0.031
325. LP (3) I 35	405. BD*(1)Te 29- I 37	1.20	0.19	0.013
326. LP (4) I 35	406. BD*(1)Te 29- I 38	61.50	0.15	0.086
326. LP (4) I 35	1157. RY (1)Te 29	2.53	0.72	0.038
326. LP (4) I 35	1158. RY (2)Te 29	1.08	0.71	0.025
323. LP (1) I 35	407. BD*(1)Te 39- I 40	1.24	0.33	0.018
324. LP (2) I 35	407. BD*(1)Te 39- I 40	2.49	0.45	0.030
325. LP (3) I 35	407. BD*(1)Te 39- I 40	16.58	0.22	0.054

326. LP (4) I 35	407. BD*(1)Te 39- I 40	3.37	0.20	0.023
338. LP (2) I 40	408. BD*(1)Te 39- C 41	2.00	0.32	0.023
338. LP (2) I 40	1529. RY (3)Te 39	1.06	0.88	0.027
339. LP (3) I 40	408. BD*(1)Te 39- C 41	1.36	0.32	0.019
339. LP (3) I 40	409. BD*(1)Te 39- C 42	1.88	0.32	0.022
339. LP (3) I 40	1528. RY (2)Te 39	1.25	0.83	0.029