

Supporting Information

for

From weak to strong interactions: Structural and electron topology analysis of the of the continuum from the supramolecular chalcogen bonding to covalent bonds

Daniel K. Miller,^a Ivan Yu. Chernyshov,^b Yury V. Torubaev,^{c*} Sergiy V. Rosokha^{a*}

a) Chemistry Department, Ball State University, Muncie, IN, 47306, USA. E-mail: svrosokha@bsu.edu

b) TheoMat group, ChemBio Cluster, ITMO University, Lomonosova 9, St. Petersburg, 191002, Russia

c) N.S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, GSP-1,
Leninsky prospect, 31, Moscow, 119991, Russia

Content	Pages
Distance and angle distributions in the Ch...X contacts (from CSD analysis, Figures S1 – S6)	S2-S7
Refcodes and structures of the solid-state associations comprising Se...Br and Te...I contacts chosen for the QTAIM analysis (Figures S7, S8)	S8,S9
The dependencies of the kinetic (G(r)) and potential (V(r)) energy densities at BCPs on the interatomic separations (Figure S9)	S10
Distance distribution of all and line-of-sight C-H...Te and C _{sp2} ...Te contacts (Figures S10, S11)	S10-S11
Comparison of G, V, and H values for promolecules with those in the bonded systems (Figures S12)	S11
CSD Refcodes, experimental and calculated Ch... Hal distances (Tables S1 and S2)	S12, S13
Characteristics of BCPs in the experimental and calculated structures containing Se...Br and Te...I contacts (Tables S3 – S8)	S13-S19
CSD refcodes, energies and coordinates of the experimental and calculated structures containing Se...Br and Te...I contacts (Tables S9-S14)	S20-S74

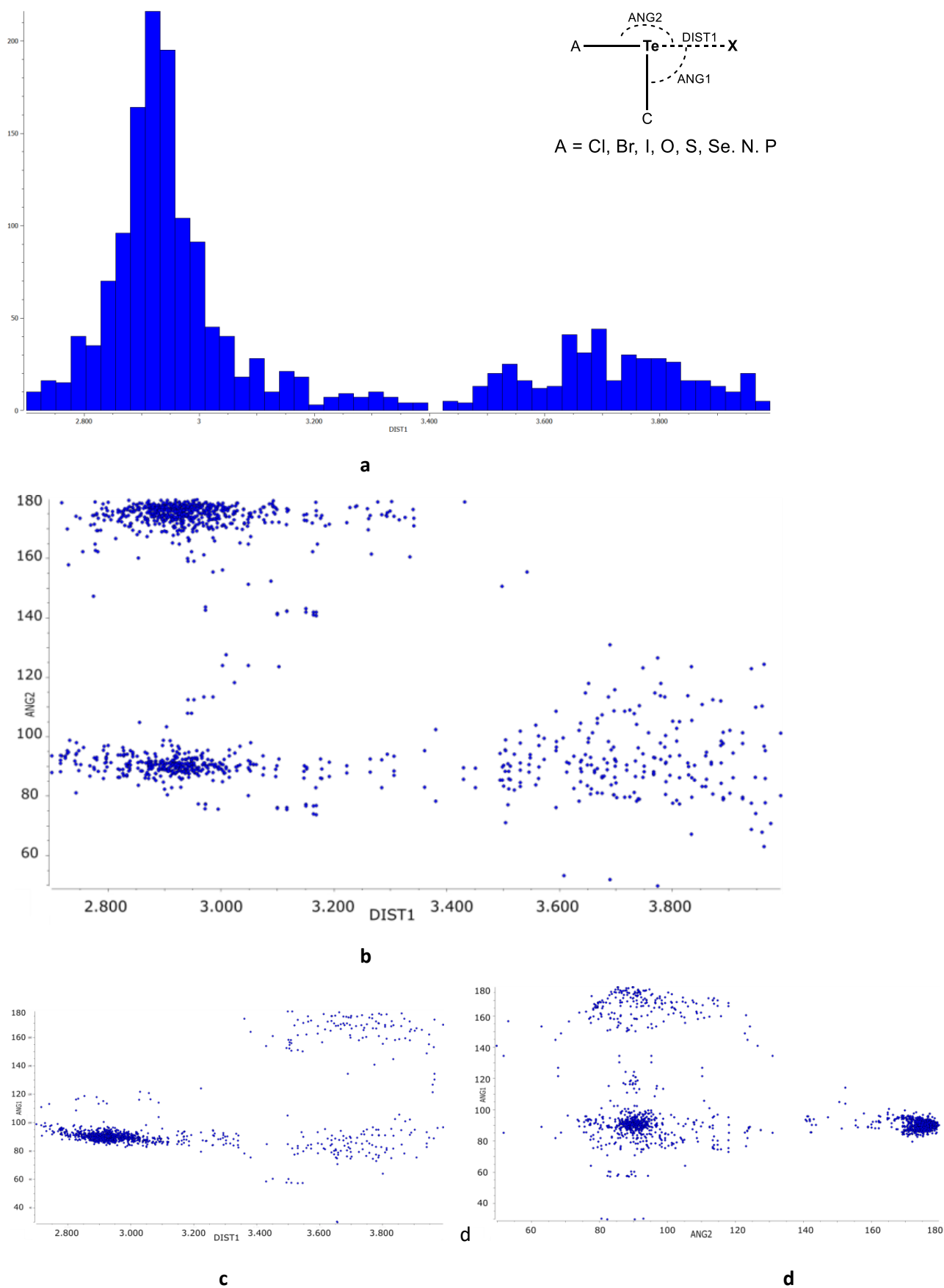
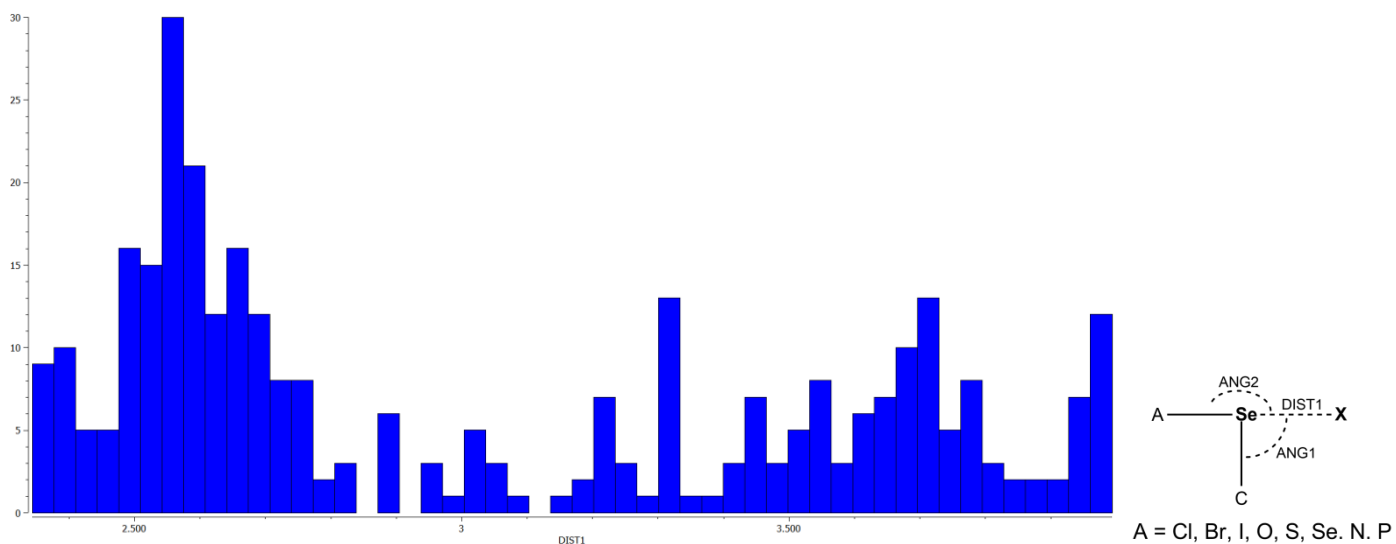
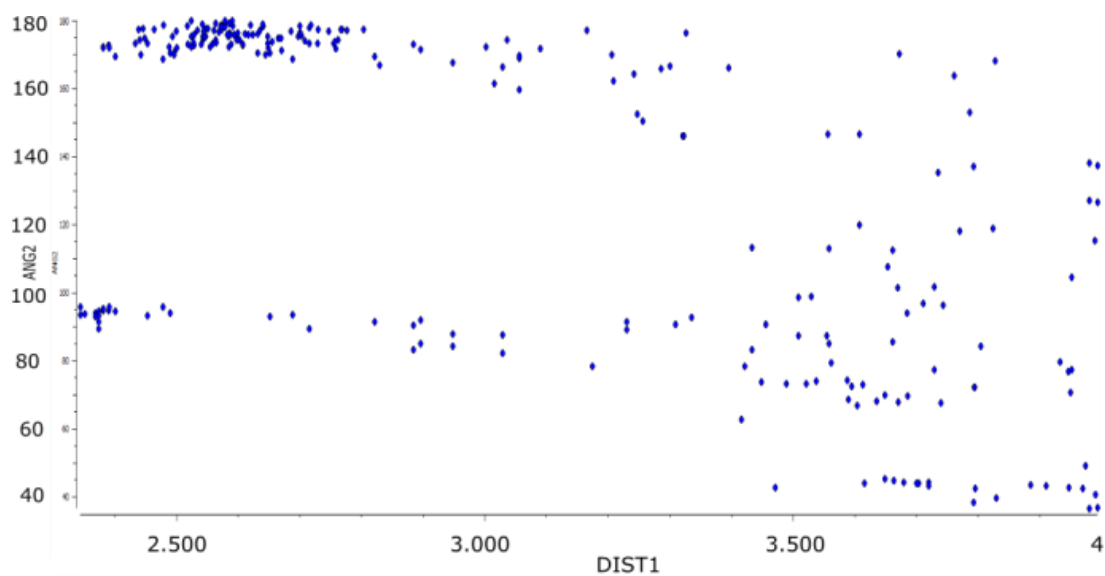


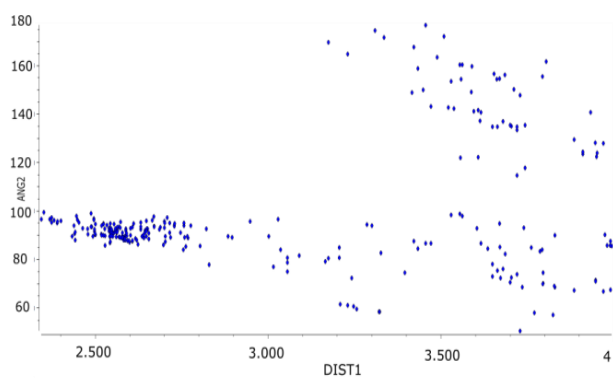
Figure S1. X = I: a) Te---I distance distribution; b) scattering of the Te---I distance (DIST1) with the and A-Te-I angles (ANG2); c) scattering of the Te---I distance (DIST1) with the and C-Te-I angles (ANG1); d) scattering of the C-Te-I angles (ANG1) with the C-Te-I angles (ANG2).



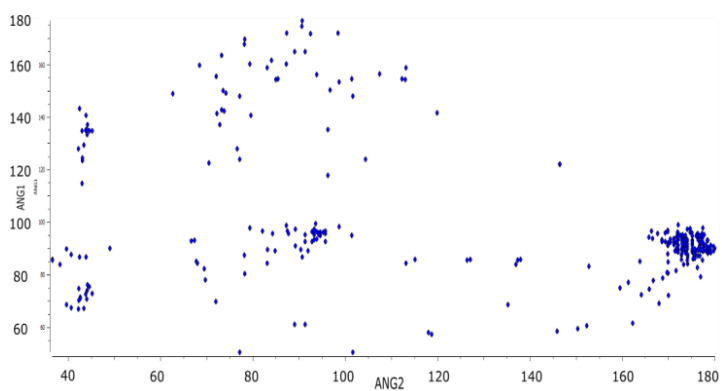
a



b



c



d

Figure S2. X = Br, 122 entry: a) Se...Br distance distribution; b) scattering of the Se---Br distance (DIST1) with the and A-Se-Br angles (ANG2); c) scattering of the Se---Br distance (DIST1) with the and C-Se-Br angles (ANG1); d) scattering of the C-Se-Br angles (ANG1) with the C-Se-Br angles (ANG1).

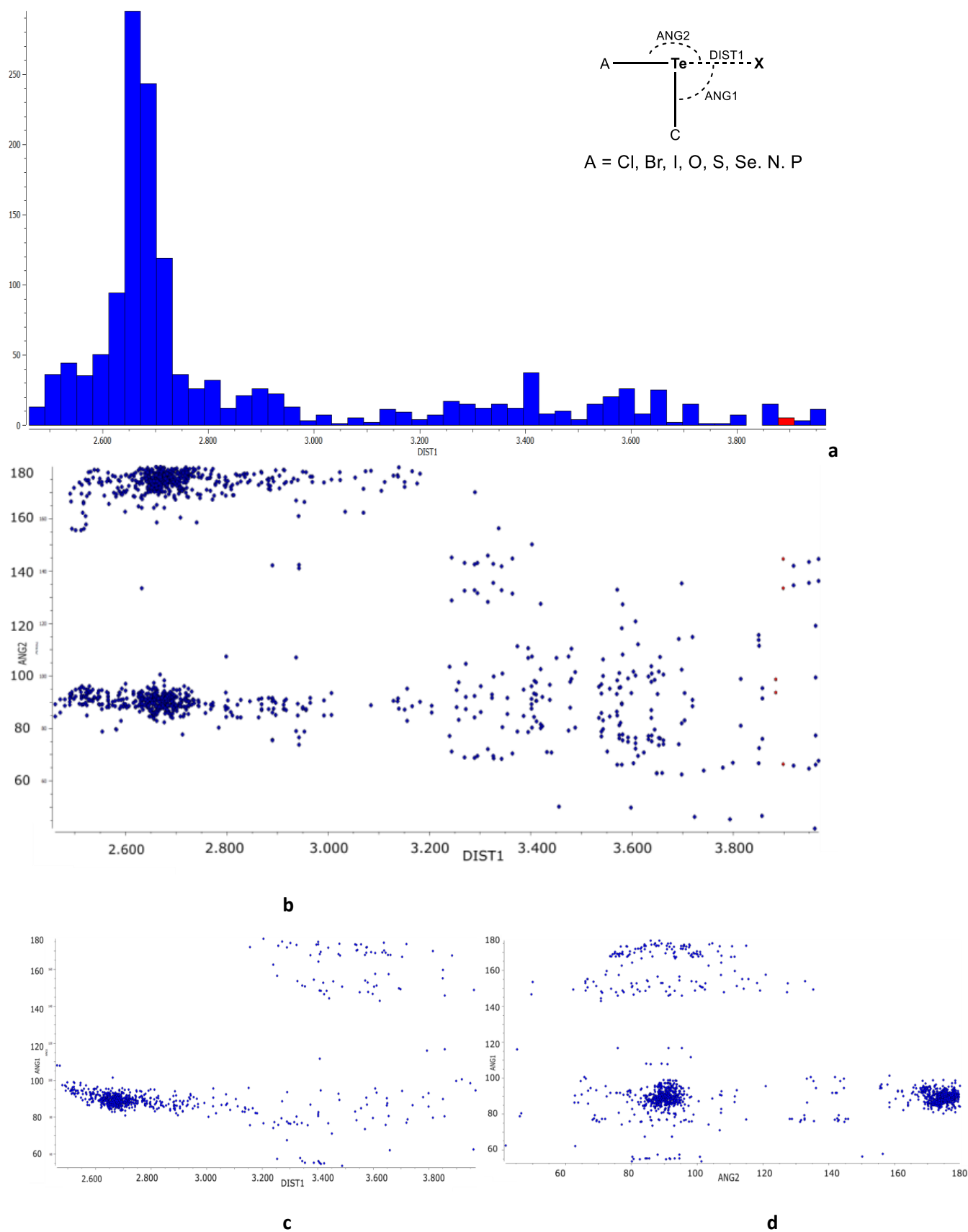
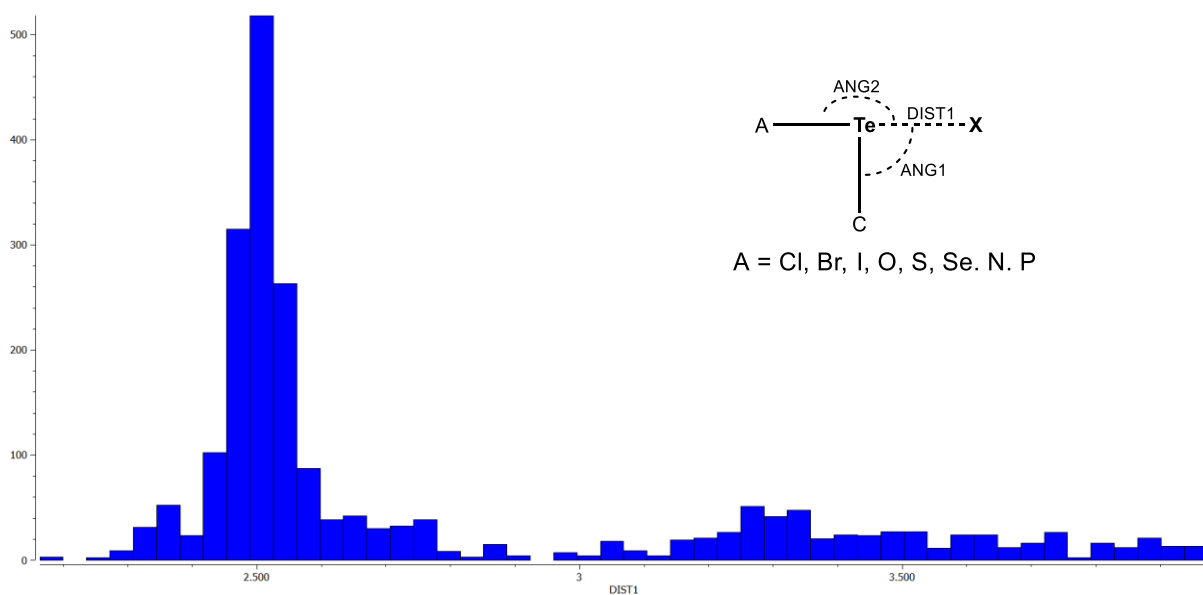
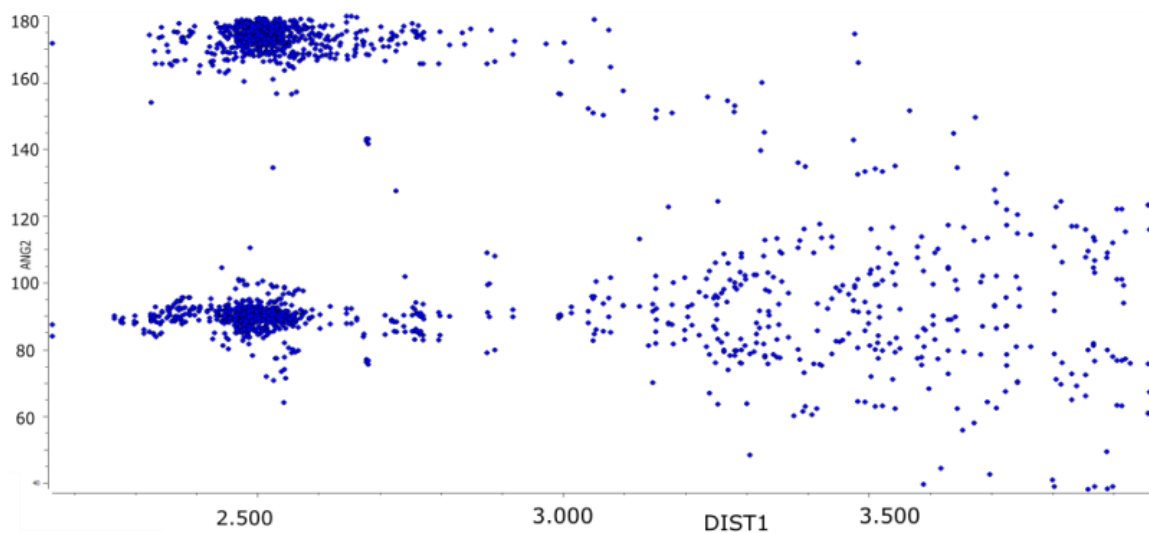


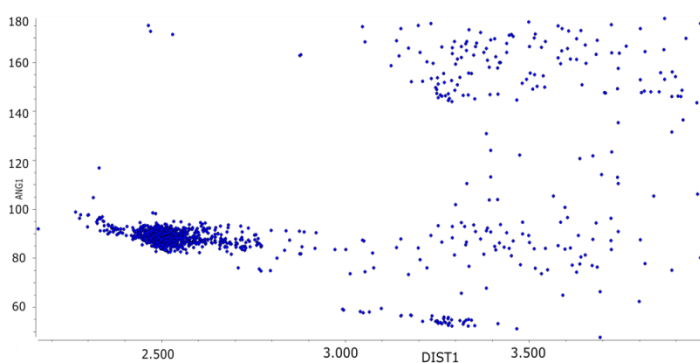
Figure S3. X = Br, 227 entries a) Te...Br distance distribution; b) scattering of the Te...Br distance (DIST1) with the and A-Te-Br angles (ANG2); c) scattering of the Te...Br distance (DIST1) with the and C-Te-Br angles (ANG1); d) scattering of the C-Te-Br angles (ANG1) with the C-Te-Br angles (ANG1).



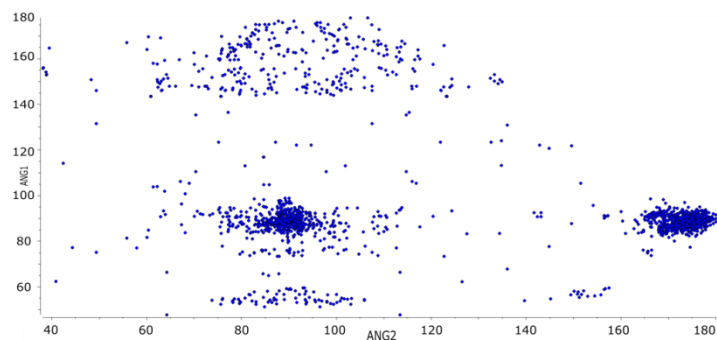
a



b

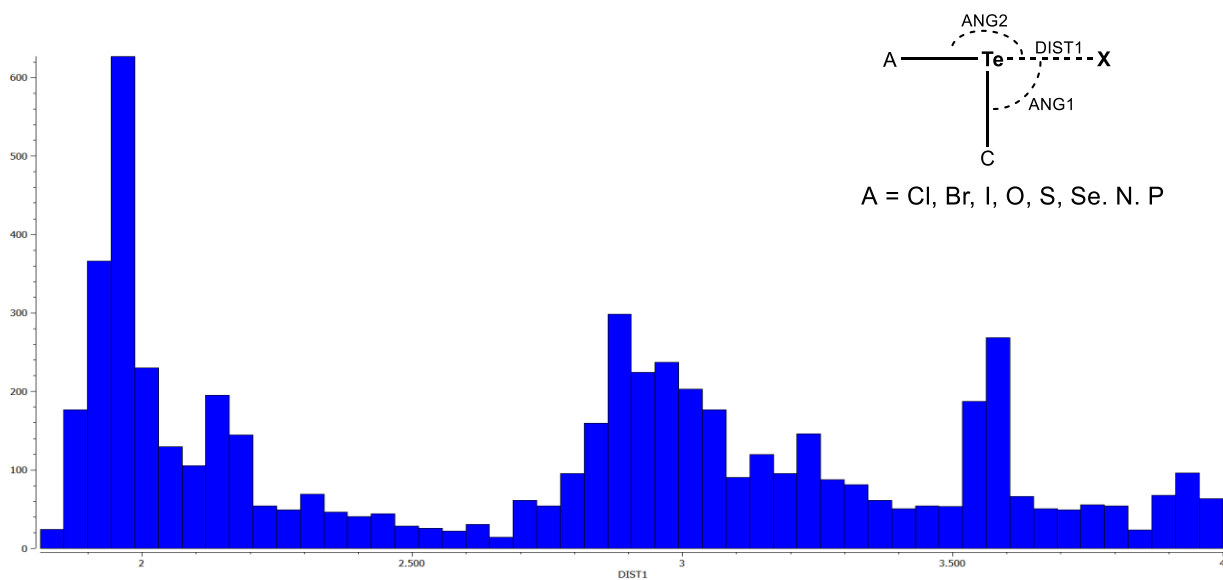


c

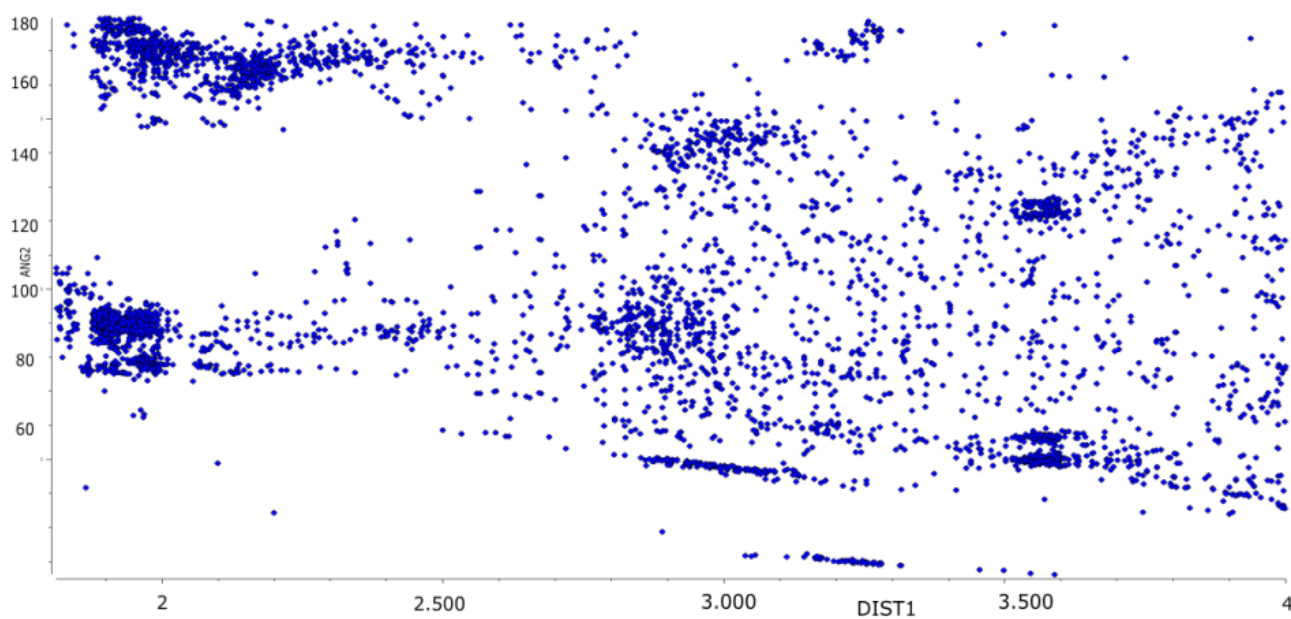


d

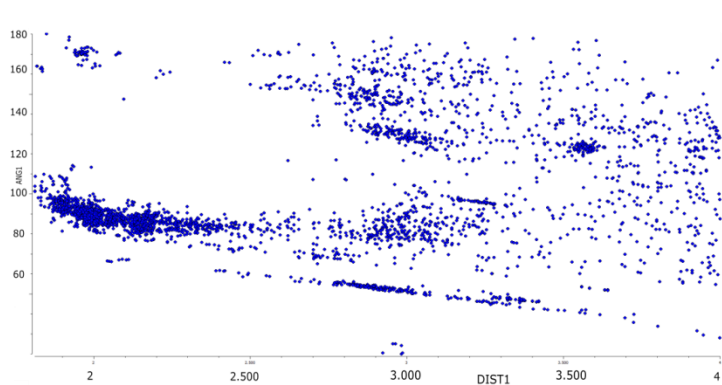
Figure S4. X = Cl, 357 entries: a) Te...Cl distance distribution; b) scattering of the Te-Cl distance (DIST1) with the and A-Te-Cl angles (ANG2); c) scattering of the Te...Cl distance (DIST1) with the and C-Te-Cl angles (ANG1); d) scattering of the C-Te-Cl angles (ANG1) with the C-Te-Cl angles (ANG1).



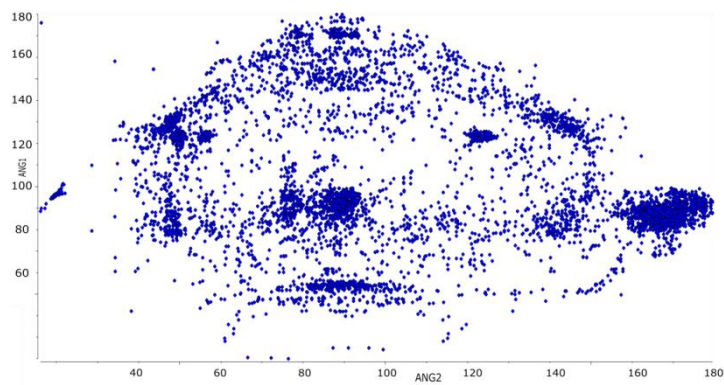
a



b

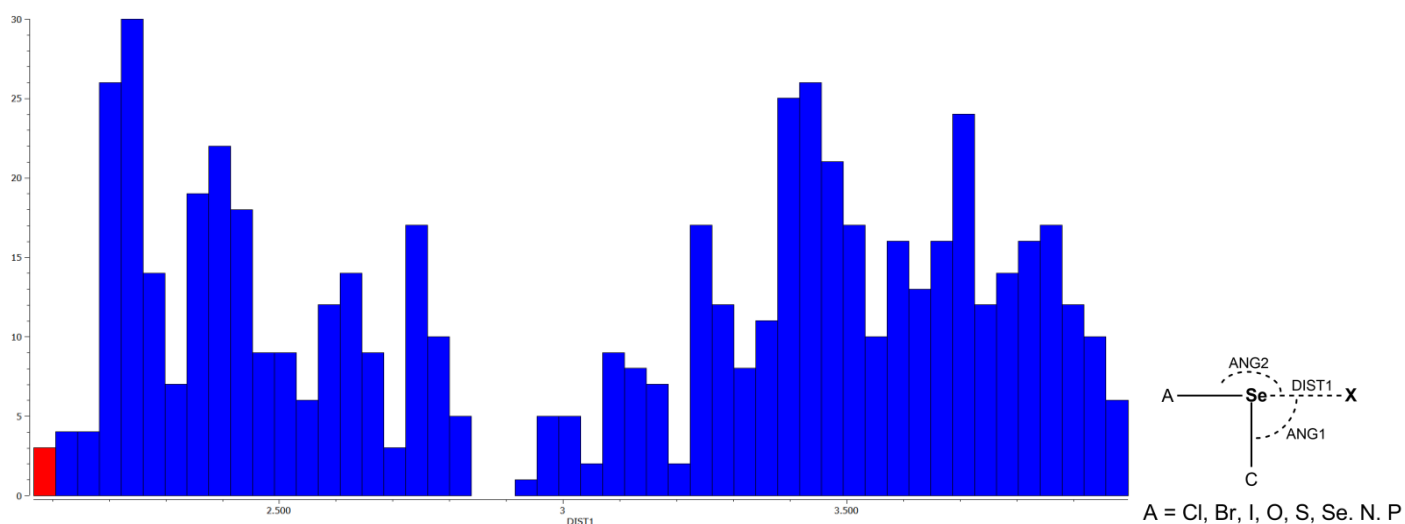


c

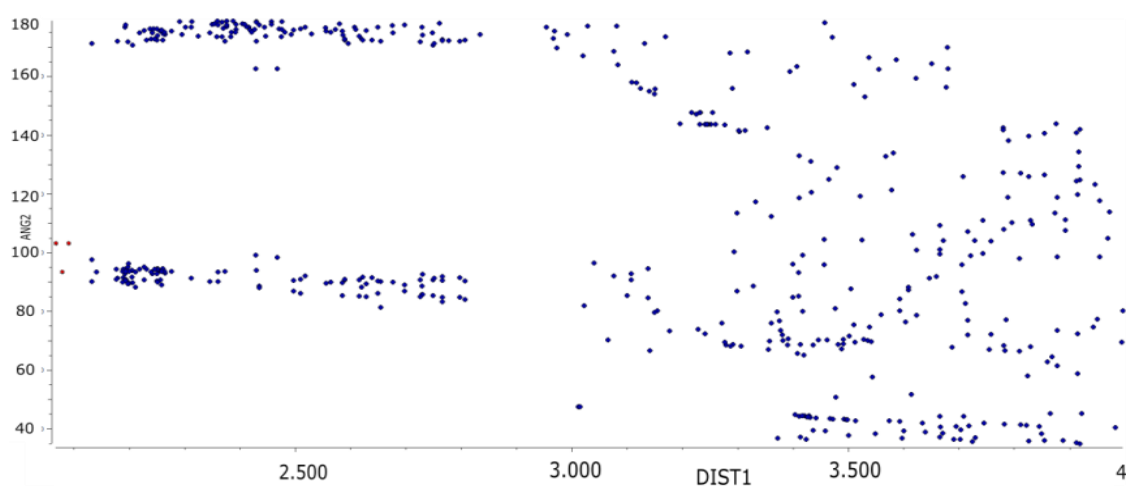


d

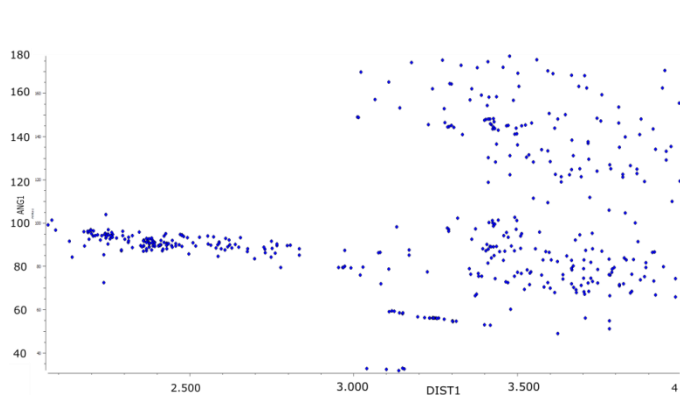
Figure S5. X = O, 576 entries: a) Te...O distance distribution; b) scattering of the Te...O distance (DIST1) with the and A-Te-O angles (ANG2); c) scattering of the Te...O distance (DIST1) with the and C-Te-O angles (ANG1); d) scattering of the C-Te-O angles (ANG1) with the C-Te-O angles (ANG1).



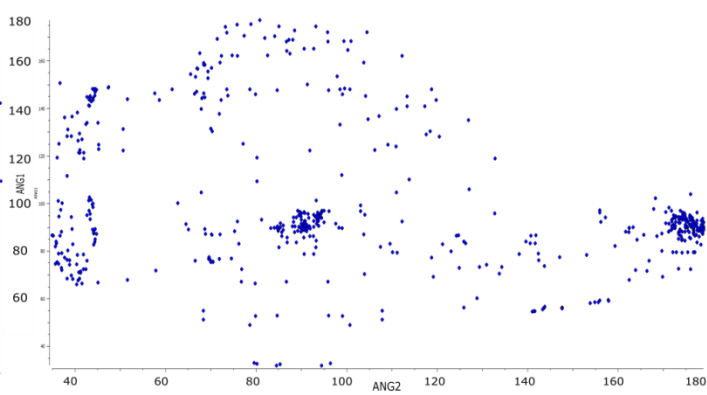
a



b



c



d

Figure S6. X = Cl, 140 entries: a) Se...Cl distance distribution; b) scattering of the Se...Cl distance (DIST1) with the and A-Se-Cl angles (ANG2); c) scattering of the Se...Cl distance (DIST1) with the and C-Se-Cl angles (ANG1); d) scattering of the C-Se-Cl angles (ANG1) with the C-Se-Cl angles (ANG2).

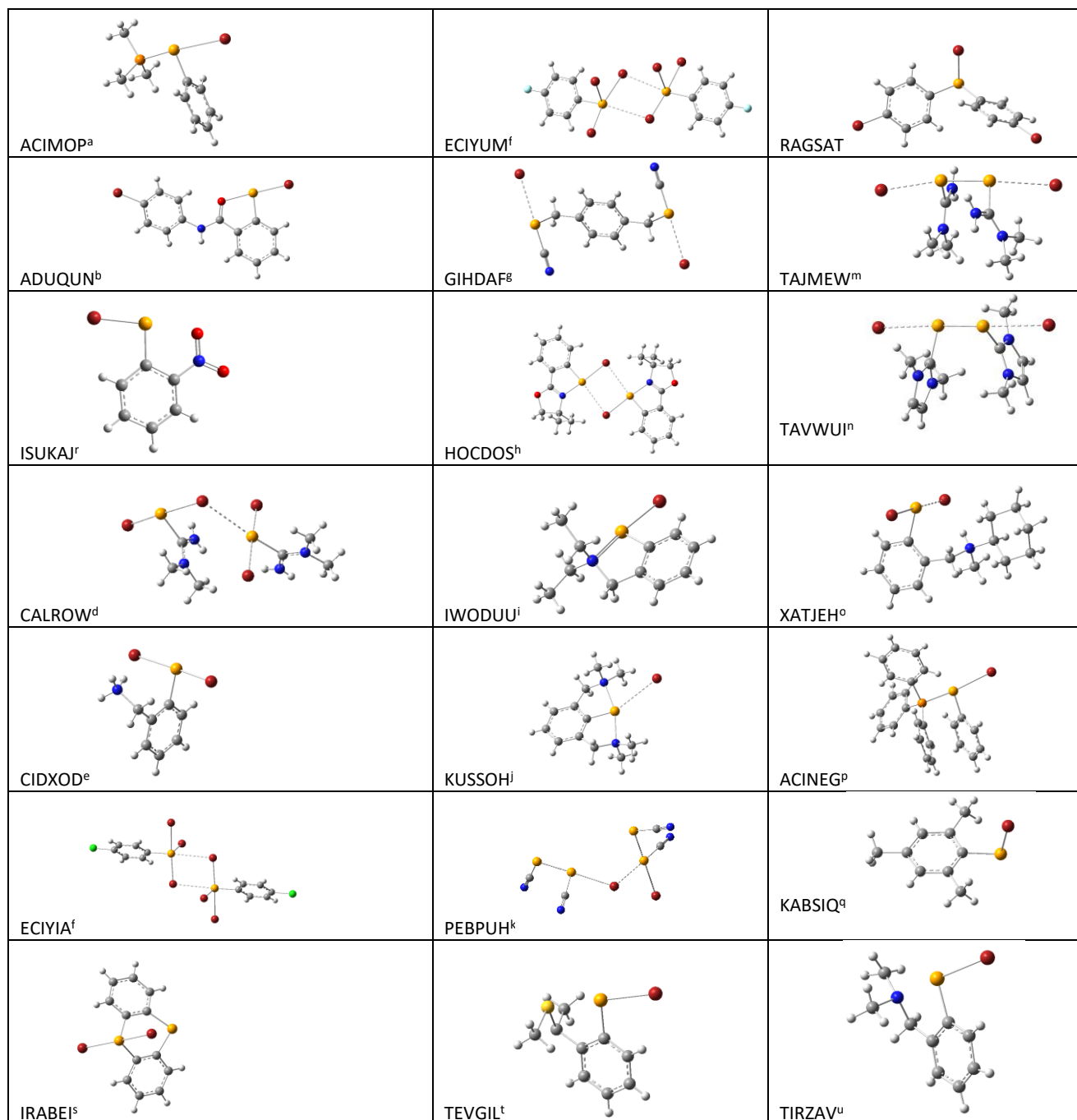


Figure S7. Refcodes and structures of the solid-state associations comprising Se...Br contacts which were chosen for the QTAIM analysis: a) Bromo(phenyl)(trimethylphosphino)selenane, b) (2-((4-bromophenyl)-carbonyl)phenyl)-bromo-selenium, c) bis(3-methylimidazolium-2-yl) diselenide dibromide d) N,N-Dimethylselenourea-dibromide, e) (R)-Dibromo-(2-(4-morpholinyl)phenyl)selenide, f) 1-Chloro-4-(tribromo- λ^4 -selanyl)benzene, g) tetrabutylammonium bromide (1,4-phenylene)bis(methylene) bis(selenocyanate), h) (2-(4,4-Dimethyl-2-oxazolonyl)phenyl)selanyl bromide, i) 1-bromo-2,2-diethyl-3H- $1\lambda^4,2\lambda^5$ -benzoselenazole, j) (2,6-bis(Dimethylaminomethyl)phenyl)selenium bromide, k) Phenyltrimethylammonium bromodiselenocyanate, l) bis(p-Bromophenyl)-bromo-selenide hexachloro-antimony, m) N1,N1,N3,N3-Tetramethyl- α,α' -diselenobisformamidinium dibromide, n) Se,Se'-bis(1,3-Dimethyl-4-imidazolin-2-yl)diselenium dibromide, o) N-(2-(Bromoseleno)benzyl)-N-cyclohexyl-N-methylammonium bromide, p) Bromo(phenyl)-(triphenylphosphino)selenane, q) Bromo(mesityl)selenium; r) 2-Nitrobenzeneselenenyl bromide; s) 5,5-dibromoselenanthrene; t) 1-(Bromoselenyl)-2-(1-methylthioethyl)benzene; u) (2-(Dimethylaminomethyl)phenyl)-selenium(ii) bromide.

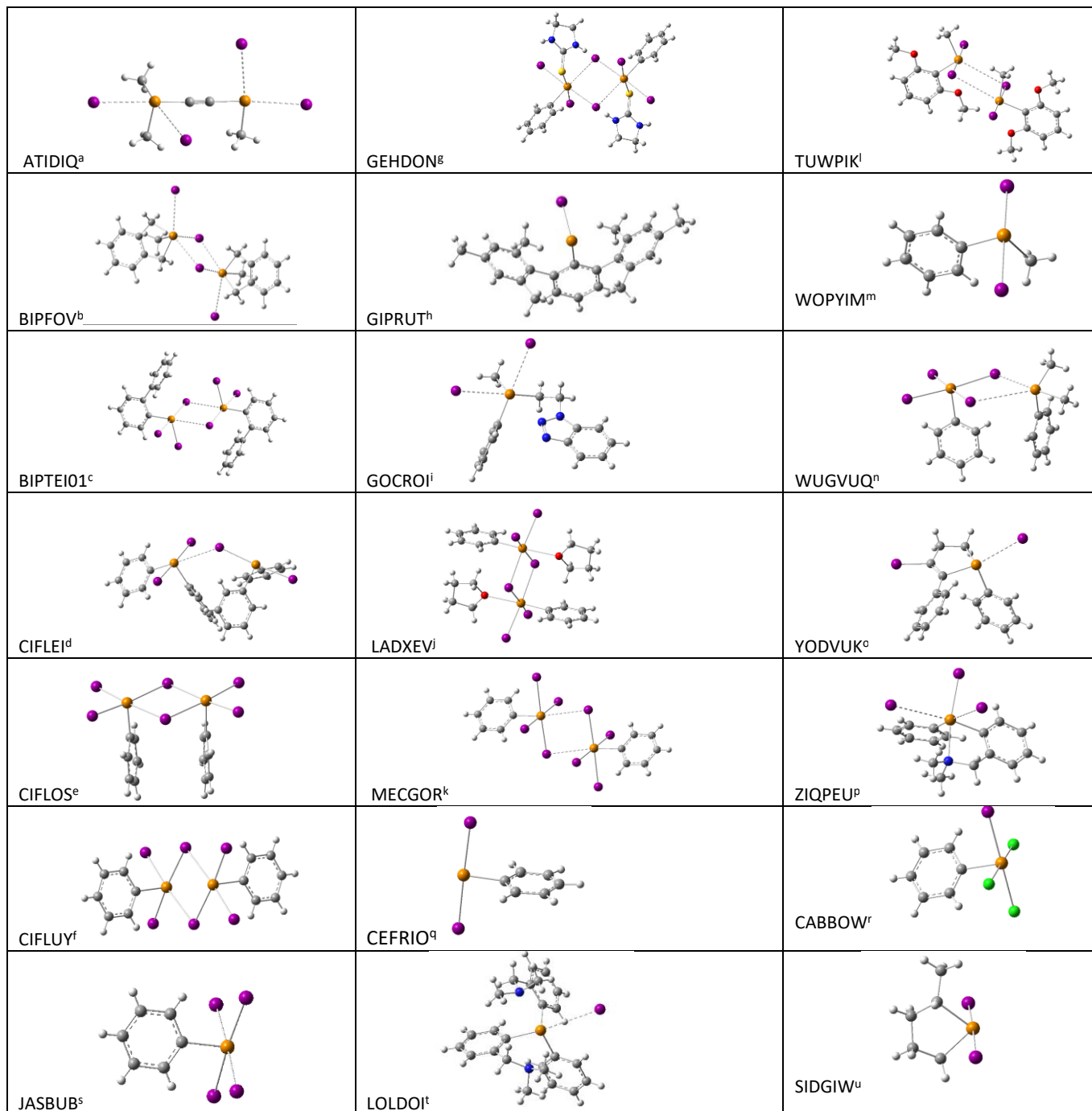


Figure S8. Refcodes and structures of the solid-state associations comprising Te...I contacts which were chosen for the QTAIM analysis: a) Dimethyl-((methyltelluro)ethynyl)telluronium iodide, b) 1-Trideuteromethyl-3,4-benzo-1-telluracyclopentane iodide, c) 2-Biphenyltellurium tri-iodide, d) Di-iodo-diphenyl-tellurium(iv), e) cis-bis(m2-Iodo)-tetraiodo-diphenyl-di-tellurium(iv), f) trans-bis(m2-Iodo)-tetraiodo-diphenyl-di-tellurium(iv), g) Tri-iodo-phenyl-(imidazolidine-2-thione)-tellurium(iv), h) (2,6-bis(2,4,6-trimethylphenyl)phenyl)tellurenyl iodide, i) [2-(1H-benzotriazol-1-yl)ethyl](methyl)phenyltellanium iodide, j) bis(m2-Iodo)-tetrakis(iodo)-diphenyl-bis(tetrahydrofuran)-di-tellurium, k) Phenyl-(thiourea-S)-selenium(ii) tetrakis(iodo)-phenyl-tellurium, l) Diiodo-methyl-(2,6-dimethoxyphenyl)-tellurium, m) diiodo-methyl-phenyl-tellurium, n) Dimethyl-phenyl-tellurium(iv) tetrakis(iodo)-phenyl-tellurium(iv), o) 4-iodo-1,5-diphenyl-2,3-dihydrotellurophenium iodide, p) (2-(Dimethylaminomethyl)phenyl)-iodo-phenyl-tellurium(iv) iodide ; q) Tetraphenylarsonium di-iodo-phenyl-tellurium(ii); r) Tetra-n-butylammonium trichloro-iodo-phenyl-tellurium; s) Tetraethylammonium tetraiodo-tellurium(iv); t) bis{2-[(dimethylamino)methyl]phenyl}(phenyl)tellanium iodide; u) 2-methyl-1,1-di-iodo-1-telluracyclopentane

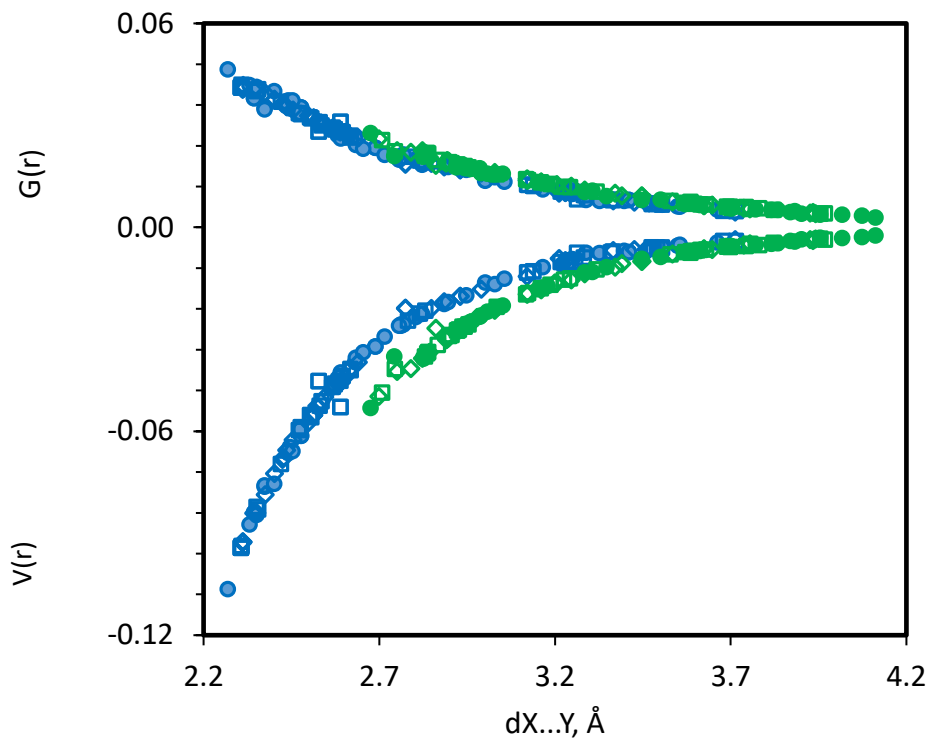


Figure S9. The dependencies of the kinetic ($G(r)$) and potential ($V(r)$) energy densities at BCPs on the Se...Br (blue) and Te...I (green) bond paths on the interatomic separations (legends are the same as in Figure 2).

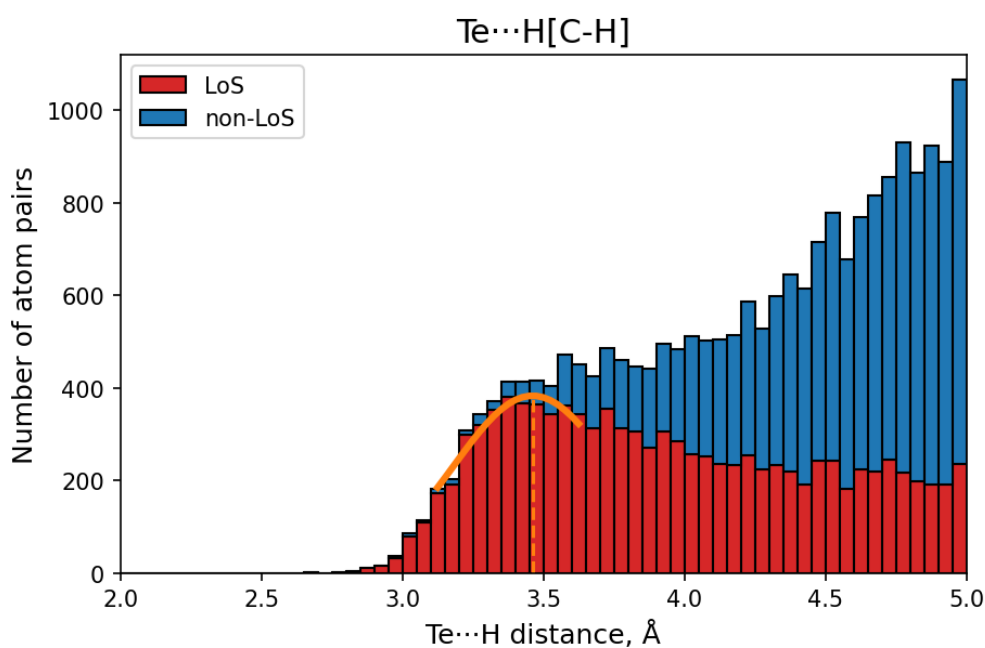


Figure S10. Distance distribution of all and line-of-sight C-H...Te contacts. Orange curve is a probability density function of the normal distribution, fitted to the histogram of distances of line-of-sight contacts, and the dotted orange line shows its maximum, which is treated as sum of van der Waals radii of the corresponding atoms.

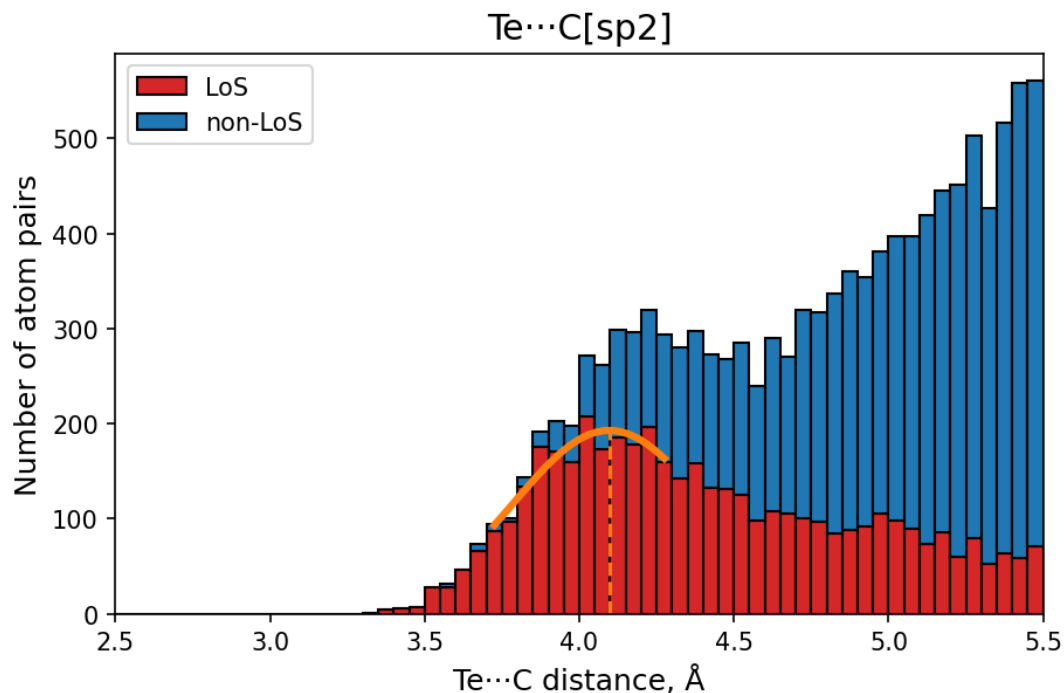


Figure S11. Distance distribution of all and line-of-sight $C_{sp^2}\cdots Te$ contacts. Distance distribution of all and line-of-sight $C-H\cdots Te$ contacts. Orange curve is a probability density function of the normal distribution, fitted to the histogram of distances of line-of-sight contacts, and the dotted orange line shows its maximum, which is treated as sum of van der Waals radii of the corresponding atoms.

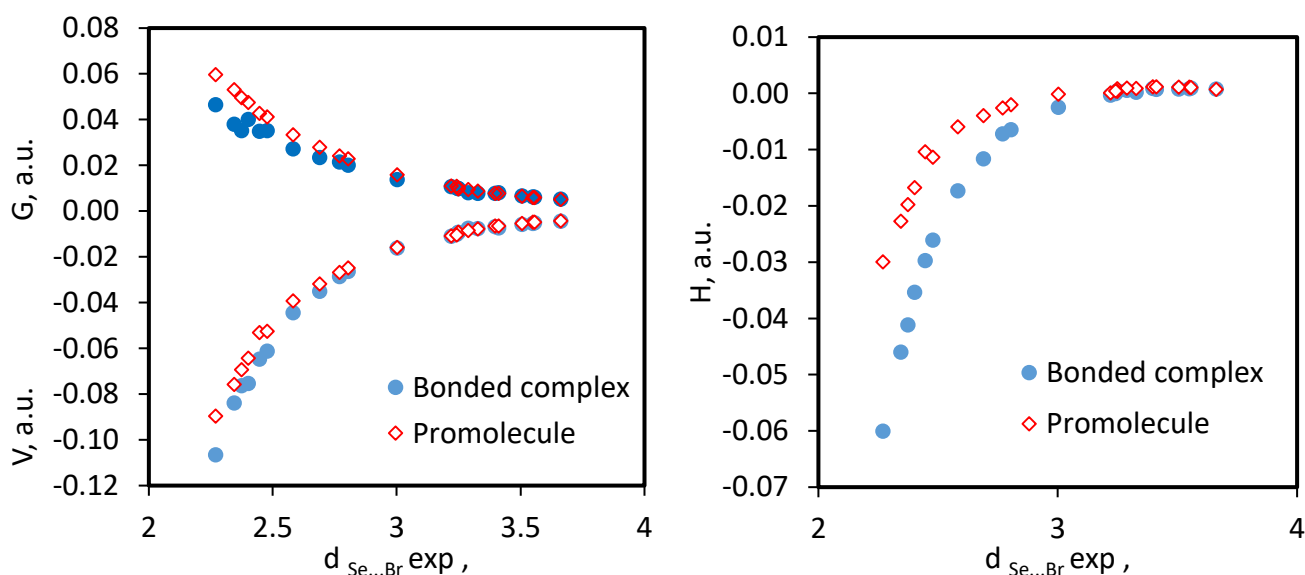


Figure S12. Variations of kinetic and potential energies (left) and energies (right) at BCP along Se-Br bonds in the experimental structures (bonded complexes) containing Se-Br contacts and in the corresponding promolecules constructed by the superposition of the non-interacting fragments extracted from these experimental structures.

Table S1. Experimental (solid-state) and calculated Se...Br distances ($d_{\text{Se}\cdots\text{Br}}$, in Å).^a

CSD Refcode	$d_{\text{Se}\cdots\text{Br}}^{\text{exp}}$	$d_{\text{Se}\cdots\text{Br}}^{\text{calc}}$ (vacuum)	$d_{\text{Se}\cdots\text{Br}}^{\text{calc}}$ (CH ₂ Cl ₂)
ACIMOP	3.327	2.573	3.282
ACINEG	3.002	2.522	3.216
ADUQUN	2.446	2.376	2.420
CALROW	3.397	3.427	3.475
	2.762	2.641	2.592
	2.441	2.534	2.574
CIDXOD	2.804	2.885	2.816
	2.439	2.437	2.477
ECIYIA	3.411	3.468	3.504
	2.344	2.311	2.306
	2.478	2.513	2.528
	2.689	2.584	2.590
	2.948	2.780	3.138
	3.029	2.780	3.138
ECIYUM	2.374	2.312	2.307
	2.401	2.514	2.507
	2.453	2.499	2.531
	2.716	2.585	2.619
	2.822	2.603	2.590
	3.505	3.459	3.481
	3.549	3.461	3.491
	2.885	2.930	3.121
	2.896	2.931	3.123
GIHDAF	3.249	3.230	3.359
HOCDOS	3.556	3.713	3.679
	2.632	2.569	2.782
IWODUU	2.582	2.428	2.574
KUSSOH	3.662	3.212	3.715
PEBPUH	3.289	3.366	3.364
	3.036	2.705	2.739
RAGSAT	2.269	2.313	2.308
TAJMEW	3.220	3.145	3.235
	3.056	3.134	3.234
TAVWUI	3.242	3.121	3.258
	3.166	2.991	3.247
XATJEH ^o	2.475	2.455	2.472
	2.769	2.849	2.832
KABSIQ	2.331	2.343	2.351
ISUKAJ	2.351	2.352	2.356
TEVGIL	2.591	2.402	2.503
TIRZAV	2.634	2.425	2.566
IRABEI	2.655	2.526	2.536
	2.757	2.589	2.618

a) See structures and names in Figure S7.

Table S2. Experimental and calculated Te...I distances ($d_{\text{Te}\cdots\text{I}}$, in Å).^a

CSD Refcode	$d_{\text{Se}\cdots\text{Br}}^{\text{exp}}$	$d_{\text{Se}\cdots\text{Br}}^{\text{calc}}$ (vacuum)	$d_{\text{Se}\cdots\text{Br}}^{\text{calc}}$ (CH ₂ Cl ₂)
ATIDIQ	3.447	3.201	3.319
	3.701	3.391	3.529
BIPFOV	3.688	3.624	3.614
	3.870	3.738	3.690
	4.112	3.625	3.587
BIPTEI01	3.028	2.862	2.943
CIFLEI	3.955	3.755	3.756
CIFLOS	3.179	3.161	3.187
	3.152	3.122	3.124
CIFLUY	3.285	3.161	3.160
GEHDON	3.883	3.934	3.969
GIPRUT	2.676	2.699	2.708
GOCROI	3.501	3.535	3.597
	3.570	3.285	3.571
LADXEV	2.743	2.751	2.745
	3.307	3.205	3.244
	3.052	3.121	3.119
MECGOR	2.961	2.891	2.922
	2.922	2.979	2.937
	3.834	3.926	3.743
TUWPIK	4.034	3.942	4.190
	4.018	3.942	4.190
WOPYIM	2.990	2.887	2.906
WUGVUQ	2.920	2.790	2.844
	2.986	2.790	2.844
	3.902	3.448	3.630
	4.074	3.448	3.823
YODVUK	3.347	3.029	3.226
ZIQPEU	3.816	3.648	3.781
	3.613	3.372	3.585
	2.825	2.843	2.830
CEFRI0	2.946	2.823	2.837
	2.963	2.823	2.840
CABBOW	2.837	2.958	2.954
JASBUB	2.925	2.924	2.925
	2.947	2.924	2.927
LOLDOI	3.772	3.247	3.699
SIDGIW	2.826	2.894	2.900
	3.008	2.898	2.923

a) See structures and names in Figure S8.

Table S3. CSD refcodes, interatomic distances $d_{x...y}$ (in Å) and characteristics of the BCPs along $Te...I$ bonds in the experimental structures containing $Te...I$ contacts: electron density, $\rho(\mathbf{r})$, the Laplacian of density, $\nabla^2\rho(\mathbf{r})$, kinetic, $G(\mathbf{r})$, and potential, $V(\mathbf{r})$ energy densities, and energy density, $H(\mathbf{r})$ (all in atomic units)

CSD Refcode	$d_{x...y}$	$\rho(\mathbf{r})$	$G(\mathbf{r})$	$V(\mathbf{r})$	$H(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
ATIDIQ	3.447	0.0203584656	0.0080807502	-0.0093145726	-0.0012338223	0.0273877207
	3.701	0.0134069855	0.0055169868	-0.0054636865	0.0000533004	0.0222811494
BIPFOV	3.688	0.0130151632	0.0056809606	-0.0055226423	0.0001583183	0.0233571160
	3.87	0.0097715638	0.0044643587	-0.0040144533	0.0004499054	0.0196570566
	4.112	0.0065670845	0.0028914056	-0.0024301808	0.0004612247	0.0134105212
BIPTEIO	3.028	0.0439280471	0.0156126109	-0.0240217407	-0.0084091297	0.0288141058
CIFLEI	3.955	0.0076842734	0.0037163859	-0.0030997076	0.0006166783	0.0173322569
CIFLOS	3.179	0.0336850209	0.0127668982	-0.0172670310	-0.0045001327	0.0330671124
	3.152	0.0349513294	0.0133258550	-0.0182559449	-0.0049300898	0.0335831264
CIFLUY	3.285	0.0283424288	0.0103968003	-0.0132576853	-0.0028608850	0.0301436808
GEHDON	3.883	0.0095024501	0.0047555799	-0.0042211861	0.0005343938	0.0211598946
GIPRUT	2.676	0.0729688864	0.0277550575	-0.0531248354	-0.0253697780	0.0095446916
GOCROI	3.501	0.0185631785	0.0081854701	-0.0087527661	-0.0005672960	0.0304726992
	3.57	0.0164776048	0.0068578997	-0.0072202473	-0.0003623475	0.0259822108
LADXEV	2.743	0.0608806637	0.0209329587	-0.0380004035	-0.0170674448	0.0154629122
	3.307	0.0267195388	0.0108023375	-0.0130959483	-0.0022936108	0.0340349202
	3.052	0.0414276278	0.0157367069	-0.0230285200	-0.0072918130	0.0337797216
MECGOR	2.922	0.0517907070	0.0186112872	-0.0307500190	-0.0121387318	0.0258906827
	2.961	0.0489191244	0.0171808275	-0.0278688973	-0.0106880698	0.0259713619
	3.834	0.0102948189	0.0051689094	-0.0046201783	0.0005487311	0.0228705619
TUWPIK	4.018	0.0076532317	0.0037157073	-0.0031634532	0.0005522542	0.0170718459
WOPYIM	2.99	0.0466567559	0.0159890756	-0.0258973257	-0.0099082500	0.0243235972
WUGVUQ	2.92	0.0527571089	0.0176103085	-0.0301231700	-0.0125128615	0.0203902028
	2.986	0.0454377487	0.0173330006	-0.0263065222	-0.0089735216	0.0334381754
	3.902	0.0088151024	0.0039862738	-0.0035186203	0.0004676535	0.0178157092
	4.074	0.0073634916	0.0034062997	-0.0028681959	0.0005381038	0.0157776137
YODVUK	3.347	0.0261552485	0.0091355806	-0.0117120472	-0.0025764666	0.0262364712
ZIQPEU	3.613	0.0152774847	0.0065064727	-0.0065627680	-0.0000562952	0.0265061226
	3.816	0.0118550005	0.0051232835	-0.0048204680	0.0003028156	0.0217043966
	2.825	0.0608876627	0.0207914688	-0.0383377426	-0.0175462738	0.0129818430
CEFRIO	2.946	0.0491510274	0.0180658844	-0.0289240231	-0.0108581387	0.0288313804
	2.963	0.0477840028	0.0174940075	-0.0277183254	-0.0102243179	0.0290791051
CABBOW	2.837	0.0590195862	0.0216044942	-0.0378459688	-0.0162414746	0.0214530195
JASBUB	2.925	0.0515184492	0.0180709432	-0.0300093892	-0.0119384461	0.0245304186
	2.947	0.0496943800	0.0173637964	-0.0283630570	-0.0109992607	0.0254584930
LOLDOI	3.772	0.0124840206	0.0053049438	-0.0051055406	0.0001994033	0.0220173887
SIDGIW	2.826	0.0593025147	0.0221363218	-0.0386868140	-0.0165504922	0.0223444536
	3.008	0.0449499249	0.0157339048	-0.0248552945	-0.0091213896	0.0264503231

Table S4. CSD refcodes, interatomic distances $d_{x...y}$ (in Å) and characteristics of the BCPs along $Te...I$ bonds in the optimized in vacuum structures containing $Te...I$ contacts: electron density, $\rho(r)$, the Laplacian of density, $\nabla^2\rho(r)$, kinetic, $G(r)$, and potential, $V(r)$ energy densities, and energy density, $H(r)$ (all in atomic units)

CSD Refcode	$d_{x...y}$	$\rho(r)$	$G(r)$	$V(r)$	$H(r)$	$\nabla^2\rho(r)$
ATIDIQ	3.20053	0.0309176369	0.0123205362	-0.0163004245	-0.0039798883	0.0333626578
	3.39107	0.0222595254	0.0092790910	-0.0106811194	-0.0014020285	0.0315082599
BIPFOV	3.62402	0.0142052614	0.0063827545	-0.0063601884	0.0000225661	0.0256212840
	3.7377	0.0115213110	0.0055611722	-0.0051892679	0.0003719044	0.0237323068
	3.62462	0.0142200782	0.0063908372	-0.0063695975	0.0000212397	0.0256483089
BIPTEIO	2.86176	0.0503310218	0.0182438181	-0.0296768082	-0.0114329901	0.0272437041
CIFLEI	3.75478	0.0108123622	0.0053763551	-0.0048241790	0.0005521761	0.0237141247
CIFLOS	3.16136	0.0344210441	0.0133154662	-0.0180171106	-0.0047016444	0.0344553452
	3.12245	0.0366555492	0.0140101871	-0.0195654839	-0.0055552968	0.0338196482
CIFLUY	3.16094	0.0352927622	0.0133610535	-0.0184450450	-0.0050839915	0.0331083115
GEHDON	3.93443	0.0088468356	0.0043994927	-0.0038687419	0.0005307508	0.0197209741
GIPRUT	2.69911	0.0707583729	0.0259999766	-0.0497452144	-0.0237452378	0.0090218842
GOCROI	3.28475	0.0270568226	0.0110079254	-0.0136887530	-0.0026808277	0.0333084171
	3.53463	0.0169473917	0.0075009733	-0.0078901673	-0.0003891940	0.0284471202
LADXEV	2.75109	0.0654580853	0.0225503376	-0.0424652707	-0.0199149331	0.0105428280
	3.20542	0.0318524429	0.0125523381	-0.0164003271	-0.0038479890	0.0348174340
	3.12144	0.0368739307	0.0142206016	-0.0197373704	-0.0055167689	0.0348154084
MECGOR	2.89091	0.0547200762	0.0188600869	-0.0324294142	-0.0135693273	0.0211635834
	2.97875	0.0470190061	0.0167763306	-0.0265052742	-0.0097289436	0.0281898246
	3.92626	0.0084521070	0.0041985332	-0.0035934387	0.0006050945	0.0192145107
TUWPIK	3.94187	0.0078662694	0.0040293645	-0.0034103423	0.0006190223	0.0185935474
WOPYIM	2.89167	0.0540386376	0.0195178944	-0.0331274414	-0.0136095470	0.0236340465
WUGVUQ	2.79031	0.0647714447	0.0220584166	-0.0415524578	-0.0194940412	0.0102586725
	3.12172	0.0367148300	0.0137835953	-0.0193117603	-0.0055281650	0.0330218037
	3.44767	0.0203153758	0.0092267851	-0.0100433846	-0.0008165995	0.0336407468
	3.44835	0.0202913916	0.0092162855	-0.0100284056	-0.0008121202	0.0336166653
YODVUK	3.02898	0.0428353773	0.0161367617	-0.0244578758	-0.0083211141	0.0312628280
ZIQPEU	3.64802	0.0152774847	0.0065064727	-0.0065627680	-0.0000562952	0.0258007107
	3.37193	0.0239642296	0.0099985199	-0.0116910604	-0.0016925406	0.0332239260
	2.84344	0.0586263024	0.0205698523	-0.0367630184	-0.0161931661	0.0175076761
CEFRIO	2.823	0.0589818701	0.0225047033	-0.0385298259	-0.0160251226	0.0259192870
CABBOW	2.958	0.0486329812	0.0174626738	-0.0281819817	-0.0107193080	0.0269738210
JASBUB	2.924	0.0515876886	0.0182801628	-0.0302394054	-0.0119592425	0.0252841135
LOLDOI	3.247	0.0296075433	0.0121396489	-0.0154608736	-0.0033212247	0.0352737279
SIDGIW	2.894	0.0533386434	0.0196119042	-0.0328508435	-0.0132389393	0.0254925409
	2.898	0.0530437972	0.0194128033	-0.0325435878	-0.0131307845	0.0251287411

Table S5. CSD refcodes, interatomic distances $d_{x...y}$ (in Å) and characteristics of the BCPs along $Te...I$ bonds in the optimized in CH_2Cl_2 structures containing $Te...I$ contacts: electron density, $\rho(\mathbf{r})$, the Laplacian of density, $\nabla^2\rho(\mathbf{r})$, kinetic, $G(\mathbf{r})$, and potential, $V(\mathbf{r})$ energy densities, and energy density, $H(\mathbf{r})$ (all in atomic units)

CSD Refcode	$d_{x...y}$	$\rho(\mathbf{r})$	$G(\mathbf{r})$	$V(\mathbf{r})$	$H(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$
ATIDIQ	3.319	0.0242860741	0.0104945639	-0.0124114931	-0.0019169293	0.0343105608
	3.529	0.0168297258	0.0077599772	-0.0079755322	-0.0002155550	0.0301776910
BIPFOV	3.614	0.0141988588	0.0067438916	-0.0065955804	0.0001483112	0.0275688120
	3.690	0.0123619595	0.0060801422	-0.0057305670	0.0003495753	0.0257188705
	3.587	0.0149264830	0.0070821848	-0.0070052138	0.0000769710	0.0286366244
BIPTEIO	2.943	0.0498262326	0.0180003744	-0.0292045381	-0.0112041637	0.0271852330
CIFLEI	3.756	0.0108230568	0.0054172524	-0.0048611782	0.0005560742	0.0238933065
CIFLOS	3.187	0.0327718003	0.0127805166	-0.0169089215	-0.0041284049	0.0346084921
	3.124	0.0364242081	0.0139216807	-0.0193734695	-0.0054517888	0.0338796535
CIFLUY	3.160	0.0343405752	0.0132385349	-0.0179159986	-0.0046774636	0.0342443459
GEHDON	3.969	0.0083441291	0.0041387061	-0.0035990999	0.0005396063	0.0187132495
GIPRUT	2.708	0.0695821948	0.0256738827	-0.0486645773	-0.0229906946	0.0107356306
GOCROI	3.597	0.0146624815	0.0069493854	-0.0068916000	0.0000577854	0.0280286848
	3.571	0.0154330606	0.0072487237	-0.0072592980	-0.0000105743	0.0289525992
LADXEV	2.745	0.0645522589	0.0223240996	-0.0416996652	-0.0193755657	0.0117952975
	3.244	0.0296581255	0.0118259101	-0.0149949247	-0.0031690145	0.0346276092
	3.119	0.0370147371	0.0142065210	-0.0197495620	-0.0055430410	0.0346539990
MECGOR	2.937	0.0503968621	0.0179123089	-0.0292742797	-0.0113619708	0.0262017376
	2.922	0.0516991445	0.0183189533	-0.0303470141	-0.0120280608	0.0251640077
	3.743	0.0118935282	0.0059824201	-0.0054828869	0.0004995332	0.0259278135
TUWPIK	3.956	0.0078514102	0.0039538157	-0.0033700187	0.0005837969	0.0181504505
WOPYIM	2.906	0.0524130289	0.0188540324	-0.0316521004	-0.0127980680	0.0242244750
WUGVUQ	2.867	0.0568947831	0.0197918811	-0.0346271472	-0.0148352661	0.0198271430
	3.034	0.0425023665	0.0156274093	-0.0233865554	-0.0077591461	0.0314732286
	3.630	0.0138931927	0.0067241363	-0.0065017206	0.0002224157	0.0277862086
	3.823	0.0104381762	0.0050883959	-0.0045783971	0.0005099988	0.0223935791
YODVUK	3.226	0.0297764608	0.0119074237	-0.0153716025	-0.0034641788	0.0337730244
ZIQPEU	3.781	0.0119902092	0.0055985450	-0.0052239032	0.0003746418	0.0238927472
	3.585	0.0159612464	0.0074649439	-0.0074513788	0.0000135651	0.0299140369
	2.830	0.0596758863	0.0210855760	-0.0379612065	-0.0168756306	0.0168408717
CEFRIO	2.837	0.0576224532	0.0218586334	-0.0370666466	-0.0152080132	0.0266033520
	2.840	0.05712369	0.0217263190	-0.0367103849	-0.0149840659	0.0269698942
CABBOW	2.954	0.0489427013	0.0176965432	-0.0285974567	-0.0109009135	0.0271828965
JASBUB	2.925	0.0514134290	0.0182520772	-0.0301550051	-0.0119029279	0.0253970320
	2.927	0.0513240017	0.0182304711	-0.0300765845	-0.0118461134	0.0255378581
LOLDOI	3.699	0.0128706312	0.0060937933	-0.0057929771	0.0003008161	0.0255784381
SIGDIW	2.900	0.0523217696	0.0191918026	-0.0319281348	-0.0127363322	0.0258225515

Table S6. CSD refcodes, interatomic distances Se...Br distances $d_{x...y}$ (in Å) and characteristics of the BCPs along Se...Br bonds in the experimental structures containing Se...Br contacts (all in atomic units)

CSD Refcode	$d_{x...y}$	$\rho(r)$	$G(r)$	$V(r)$	$H(r)$	$\nabla^2\rho(r)$
ACIMOP	3.327	0.0168335958	0.0077909585	-0.0076162090	0.0001747495	0.0318628322
ACINEG	3.002	0.0306251284	0.0137393510	-0.0162149070	-0.0024755560	0.0450551801
ADUQUN	2.446	0.0829467828	0.0349364559	-0.0646650715	-0.0297286156	0.0208313611
CALROW	2.441	0.0825917844	0.0373409729	-0.0664747948	-0.0291338219	0.0328286041
	2.762	0.0467590387	0.0206054463	-0.0285929490	-0.0079875026	0.0504717747
	3.397	0.0130595544	0.0077286535	-0.0068767937	0.0008518598	0.0343220531
	2.762	0.0466114347	0.0210227583	-0.0289245746	-0.0079018162	0.0524837685
	2.441	0.0830037803	0.0369110045	-0.0661760283	-0.0292650239	0.0305839224
CIDXOD	2.804	0.0423381016	0.0200004358	-0.0264478784	-0.0064474426	0.0542119727
	2.439	0.0827242142	0.0365856477	-0.0660652145	-0.0294795668	0.0284243235
ECIYIA2	3.411	0.0132480928	0.0080242176	-0.0073152337	0.0007089839	0.0349328060
	3.411	0.0132480628	0.0080241413	-0.0073151460	0.0007089953	0.0349325465
	2.344	0.1056365102	0.0379567199	-0.0839575155	-0.0460007957	-0.0321763032
	2.344	0.1056481690	0.0379631265	-0.0839752184	-0.0460120920	-0.0321958620
	2.478	0.0809714810	0.0352166049	-0.0613051322	-0.0260885274	0.0365123099
	2.478	0.0809714165	0.0352169170	-0.0613055949	-0.0260886779	0.0365129562
	2.689	0.0566767801	0.0234172484	-0.0350441594	-0.0116269110	0.0471613495
	2.689	0.0566832036	0.0234208746	-0.0350507322	-0.0116298576	0.0471640680
ECIYUM2	2.374	0.1004561637	0.0351293008	-0.0762998619	-0.0411705612	-0.0241650416
	2.374	0.1006925033	0.0347026243	-0.0759841804	-0.0412815560	-0.0263157268
	2.401	0.0930104491	0.0400815184	-0.0754344294	-0.0353529110	0.0189144295
	2.716	0.0547937123	0.0212906531	-0.0321713312	-0.0108806782	0.0416398997
	2.822	0.0454767444	0.0183878168	-0.0255029109	-0.0071150941	0.0450908908
	2.453	0.0841268027	0.0373018284	-0.0658268752	-0.0285250468	0.0351071263
	3.5494	0.0105351212	0.0062027775	-0.0054067023	0.0007960752	0.0279954110
	3.5055	0.0113859160	0.0066358776	-0.0058878888	0.0007479888	0.0295354655
GIHDAF	3.249	0.0170555672	0.0098119109	-0.0093830397	0.0004288712	0.0409631287
	3.249	0.0170585581	0.0098132952	-0.0093847925	0.0004285027	0.0409671914
HOCDOS	3.556	0.0102150354	0.0060731429	-0.0051638944	0.0009092484	0.0279295653
	2.632	0.0577929145	0.0262587185	-0.0396518830	-0.0133931645	0.0514622159
IWODUU	2.582	0.0648975383	0.0271326029	-0.0444473497	-0.0173147468	0.0392714244
KUSSOH	3.662	0.0095881693	0.0051774214	-0.0044377514	0.0007396700	0.0236683656
PEBPUH	3.289	0.0163235060	0.0080161828	-0.0074694952	0.0005466876	0.0342514819
RAGSAT	2.269	0.1186880707	0.0464580811	-0.1064984120	-0.0600403308	-0.0543289987
TAJMEW	3.22	0.0210270621	0.0106357608	-0.0109812772	-0.0003455164	0.0411609776
	3.056	0.0279170933	0.0133836202	-0.0151548312	-0.0017712110	0.0464496366
TAVWUI	3.242	0.0196183827	0.0101520848	-0.0101868316	-0.0000347468	0.0404693520
	3.166	0.0225888100	0.0111576474	-0.0117541646	-0.0005965172	0.0422445207
XATJEH	2.475	0.0777793734	0.0336701867	-0.0594576228	-0.0257874361	0.0315310024
	2.769	0.0445190765	0.0213859338	-0.0286030935	-0.0072171597	0.0566750966
KABSIQ	2.331	0.1015754352	0.0418477979	-0.0874247656	-0.0455769677	-0.0149166794
ISUKAJ	2.351	0.0992926198	0.0413203812	-0.0845854174	-0.0432650362	-0.0077786202
TEVGIL	2.591	0.0646538249	0.0261226420	-0.0427099893	-0.0165873473	0.0381411787
TIRZAV	2.634	0.0594288807	0.0242509595	-0.0383890531	-0.0141380936	0.0404514634
IRABEI	2.655	0.0597338001	0.0231543958	-0.0367718535	-0.0136174576	0.0381477528
KABSIQ	2.757	0.0506369122	0.0198697323	-0.0289933247	-0.0091235924	0.0429845597
	2.331	0.1015754352	0.0418477979	-0.0874247656	-0.0455769677	-0.0149166794

Table S7. CSD refcodes, interatomic distances Se...Br distances $d_{x...y}$ (in Å) and characteristics of the BCPs along Se...Br bonds in the optimized in vacuum structures (all in atomic units)

CSD Refcode	$d_{x...y}$	$\rho(r)$	$G(r)$	$V(r)$	$H(r)$	$\nabla^2\rho(r)$
ACIMOP	2.573	0.0654976690	0.0289831915	-0.0464186560	-0.0174354646	0.0461909077
ACINEG	2.522	0.0717912410	0.0311841679	-0.0525440168	-0.0213598489	0.0392972762
ADUQUN	2.376	0.0943749531	0.0395123227	-0.0786296597	-0.0391173371	0.0015799424
CALROW	2.761	0.0688178480	0.0302529597	-0.0499647461	-0.0197117864	0.0421646934
	2.427	0.0604440117	0.0272458356	-0.0420934467	-0.0148476111	0.0495928981
	2.821	0.0123820984	0.0074147672	-0.0065246454	0.0008901218	0.0332195560
	2.545	0.0706186437	0.0307671147	-0.0513606536	-0.0205935389	0.0406943031
	2.614	0.0580863227	0.0262928849	-0.0396441332	-0.0133512483	0.0517665461
CIDXOD	3.427	0.0358069101	0.0177631733	-0.0218698504	-0.0041066771	0.0546259849
	2.534	0.0836350030	0.0354082050	-0.0656272591	-0.0302190541	0.0207566034
ECIYIA2	2.641	0.0121626624	0.0071913254	-0.0064602373	0.0007310882	0.0316896545
	2.885	0.0121623084	0.0071910954	-0.0064599888	0.0007311066	0.0316888080
	2.437	0.1118118766	0.0407264228	-0.0927985873	-0.0520721644	-0.0453829663
	3.468	0.1118122108	0.0407262788	-0.0927987439	-0.0520724651	-0.0453847451
	3.468	0.0766714444	0.0321607603	-0.0553647223	-0.0232039620	0.0358271932
	2.311	0.0766692856	0.0321594318	-0.0553619547	-0.0232025229	0.0358276355
	2.311	0.0673720564	0.0286974781	-0.0462374931	-0.0175400150	0.0446298524
	2.513	0.0673721316	0.0286972227	-0.0462373237	-0.0175401010	0.0446284865
ECIYUM2	2.513	0.1116521090	0.0406867274	-0.0926335801	-0.0519468527	-0.0450405013
	2.584	0.1116168203	0.0406420789	-0.0925590595	-0.0519169806	-0.0450996069
	2.584	0.0765610191	0.0321213101	-0.0552527752	-0.0231314651	0.0359593799
	2.312	0.0787767372	0.0327830490	-0.0574779973	-0.0246949483	0.0323524027
	2.312	0.0672286864	0.0286366689	-0.0460852955	-0.0174486266	0.0447521692
	2.514	0.0650570285	0.0278928497	-0.0440634127	-0.0161705630	0.0468891470
	2.499	0.0123482563	0.0073185276	-0.0065874373	0.0007310903	0.0321984713
	2.585	0.0122676190	0.0072762618	-0.0065363684	0.0007398933	0.0320646203
GIHDAF	2.603	0.0176619736	0.0101698705	-0.0098087909	0.0003610796	0.0421238006
	3.459	0.0176734064	0.0101760700	-0.0098163526	0.0003597174	0.0421431497
HOCDOS	3.461	0.0078590766	0.0044857727	-0.0036414239	0.0008443487	0.0213204856
	3.230	0.0649475757	0.0293196731	-0.0468186205	-0.0174989474	0.0472829027
IWODUU	3.230	0.0854338286	0.0361658348	-0.0677077795	-0.0315419448	0.0184955601
KUSSOH	3.713	0.0160768024	0.0100241232	-0.0091618338	0.0008622894	0.0435456503
PEBPUH	2.569	0.0128470034	0.0077367470	-0.0068400534	0.0008966937	0.0345337628
RAGSAT	2.428	0.1101535076	0.0417764773	-0.0926227507	-0.0508462734	-0.0362791843
TAJMEW	3.212			not ChB		
TAVWUI	3.366	0.0242639244	0.0138228666	-0.0144509693	-0.0006281027	0.0527790556
	2.705	0.0305967998	0.0159553289	-0.0182492383	-0.0022939094	0.0546456781
XATJEH	2.311	0.0806962410	0.0345245925	-0.0625264385	-0.0280018460	0.0260909858
	2.313	0.0386737577	0.0187856869	-0.0238379718	-0.0050522849	0.0549336078
KABSIQ	2.343	0.0996253100	0.0405714478	-0.0841620295	-0.0435905818	-0.0120765360
ISUKAJ	2.352	0.0990726558	0.0409529067	-0.0840049674	-0.0430520607	-0.0083966161
TEVGIL	2.402	0.0898072885	0.0377181690	-0.0724404826	-0.0347223136	0.0119834217
TIRZAV	2.425	0.0859309990	0.0363689655	-0.0683172504	-0.0319482849	0.0176827224
IRABEI	2.526	0.0742154056	0.0309229334	-0.0530858768	-0.0221629434	0.0350399600
KABSIQ	2.589	0.0664765323	0.0280375947	-0.0454164254	-0.0173788307	0.0426350561
	2.343	0.0996253100	0.0405714478	-0.0841620295	-0.0435905818	-0.0120765360

Table S8. CSD refcodes, interatomic distances Se...Br distances $d_{x...y}$ (in Å) and characteristics of the BCPs along Se...Br bonds in the optimized in CH₂Cl₂ structures containing Se...Br contacts (all in atomic units)

CSD Refcode	$d_{x...y}$	$\rho(r)$	$G(r)$	$V(r)$	$H(r)$	$\nabla^2\rho(r)$
ACIMOP	3.282	0.0162726986	0.0094842345	-0.0089356846	0.0005485498	0.0401311374
ACINEG	3.216	0.0184854122	0.0105251048	-0.0102332481	0.0002918566	0.0432678456
ADUQUN	2.420	0.0862783023	0.0369651389	-0.0695954520	-0.0326303132	0.0173393027
CALROW	3.352	0.0648323613	0.0288769030	-0.0462057196	-0.0173288166	0.0461923456
	2.806	0.0625372304	0.0280952126	-0.0441056249	-0.0160104123	0.0483392012
	3.054	0.0112429543	0.0068522905	-0.0059175591	0.0009347313	0.0311480872
	2.574	0.0656859437	0.0292902420	-0.0469503533	-0.0176601114	0.0465205223
	2.592	0.0623683326	0.0280530115	-0.0437659274	-0.0157129159	0.0493603823
CIDXOD	3.475	0.0405693757	0.0196376905	-0.0253848709	-0.0057471803	0.0555620407
	2.568	0.0771502979	0.0332857720	-0.0588164850	-0.0255307130	0.0310202363
ECIYIA2	2.596	0.0114322307	0.0067576411	-0.0060082109	0.0007494302	0.0300282853
	2.816	0.0114309742	0.0067568090	-0.0060073275	0.0007494815	0.0300251617
	2.477	0.1129955770	0.0412103613	-0.0943034949	-0.0530931336	-0.0475310892
	3.504	0.1129981954	0.0412105031	-0.0943063595	-0.0530958564	-0.0475414133
	3.504	0.0664119060	0.0281912113	-0.0452441551	-0.0170529438	0.0445530700
	2.306	0.0664128341	0.0281912649	-0.0452448296	-0.0170535647	0.0445508008
	2.306	0.0744494338	0.0310449579	-0.0528675451	-0.0218225872	0.0368894831
	2.528	0.0744431998	0.0310418975	-0.0528604344	-0.0218185369	0.0368934423
ECIYUM2	2.528	0.1129052682	0.0412162323	-0.0942431376	-0.0530269053	-0.0472426918
	2.590	0.1127429601	0.0411108569	-0.0939772551	-0.0528663982	-0.0470221651
	2.590	0.0740642994	0.0309339496	-0.0525032391	-0.0215692894	0.0374586408
	2.307	0.0774615691	0.0320198205	-0.0559005432	-0.0238807227	0.0325563914
	2.307	0.0663382478	0.0281668086	-0.0451579966	-0.0169911881	0.0447024821
	2.531	0.0629670758	0.0269680808	-0.0420384192	-0.0150703384	0.0475909697
	2.507	0.0119058610	0.0070551772	-0.0063126203	0.0007425570	0.0311909369
	2.590	0.0116547537	0.0069126384	-0.0061575740	0.0007550644	0.0306708114
GIHDAF	2.619	0.0135343214	0.0081834993	-0.0074002810	0.0007832183	0.0358668706
	3.481	0.0136266636	0.0082499315	-0.0074703520	0.0007795795	0.0361180438
HOCDOS	3.491	0.0084443216	0.0048384997	-0.0039970118	0.0008414879	0.0227199507
	3.359	0.0431066677	0.0207873921	-0.0274261000	-0.0066387080	0.0565947365
IWODUU	3.263	0.0643850268	0.0288344916	-0.0460370027	-0.0172025112	0.0465279218
KUSSOH	3.679	0.0085200181	0.0047420516	-0.0040080259	0.0007340257	0.0219043092
PEBPUH	2.782	0.0133485832	0.0079676375	-0.0071528326	0.0008148048	0.0351297692
RAGSAT	2.574	0.1111266525	0.0419193366	-0.0937835469	-0.0518642103	-0.0397794946
TAJMEW	3.715	0.0184736300	0.0107353911	-0.0104345032	0.0003008879	0.0441451157
	3.364	0.0185294626	0.0107637445	-0.0104699939	0.0002937506	0.0442299805
TAVWUI	2.739	0.0176141499	0.0104463467	-0.0099989034	0.0004474433	0.0435751603
	2.304	0.0179325450	0.0105767393	-0.0101751385	0.0004016008	0.0439133606
XATJEH	2.308	0.0779099613	0.0336106399	-0.0596972157	-0.0260865759	0.0300962561
	2.979	0.0394631813	0.0191612176	-0.0244857544	-0.0053245368	0.0553467231
ISUKAJ	2.351	0.0978946154	0.0400927339	-0.0822870427	-0.0421943088	-0.0084062997
TEVGIL	2.356	0.0981992462	0.0406544227	-0.0830077098	-0.0423532871	-0.0067954575
TIRZAV	2.503	0.0740476387	0.0323069560	-0.0552615383	-0.0229545823	0.0374094946
IRABEI	2.566	0.0652683694	0.0291854326	-0.0469256651	-0.0177402325	0.0457808008
KABSIQ	2.536	0.0725192112	0.0299813443	-0.0511735849	-0.0211922406	0.0351564148
ISUKAJ	2.618	0.0626335141	0.0263861507	-0.0416913038	-0.0153051531	0.0443239907

Table S9. CSD refcodes, energies (from single point calculations, in Hartree) and coordinates of the solid-state (experimental) structures containing Se...Br contacts.

	CSD refcode	E(RM062X)	Coordinates			
1	ACIMOP	-5668.308815	C	1.48530000	14.56020000	5.19490000
			H	0.68540000	14.23670000	5.66270000
			H	1.47650000	15.54020000	5.17810000
			H	2.28580000	14.24720000	5.66090000
			C	2.96670000	14.56590000	2.74190000
			H	3.00330000	14.25100000	1.81360000
			H	3.75620000	14.24440000	3.22650000
			H	2.95400000	15.54590000	2.75310000
			C	0.00920000	14.51840000	2.63010000
			H	-0.79500000	14.17210000	3.07000000
			H	0.04220000	14.19110000	1.70550000
			H	-0.01000000	15.49640000	2.63190000
			C	1.82450000	11.50240000	1.75030000
			C	3.16090000	11.50910000	1.23950000
			H	3.90470000	11.64130000	1.81920000
			C	0.77900000	11.25700000	0.88540000
			H	-0.11550000	11.21320000	1.19480000
			C	3.35570000	11.32170000	-0.11930000
			H	4.23080000	11.34640000	-0.48280000
			C	2.28770000	11.10280000	-0.93760000
H	2.41700000	10.95630000	-1.86770000			
C	1.08100000	11.08190000	-0.43240000			
H	0.35910000	10.93630000	-1.03080000			
Br	1.49000000	8.38090000	3.55380000			
Se	1.50270000	11.70750000	3.62360000			
P	1.48570000	13.93900000	3.52850000			
2	ACINEG	-6243.229759	C	7.95950000	7.93070000	-3.92720000
			C	7.50660000	9.00690000	-3.18420000
			C	7.80950000	9.08730000	-1.83400000
			C	8.55550000	8.09640000	-1.22690000
			C	9.02530000	7.03680000	-1.95910000
			C	8.73080000	6.94310000	-3.31650000
			C	6.47030000	6.30870000	-5.81920000
			C	5.74110000	5.86510000	-4.71740000
			C	4.91090000	4.77040000	-4.84970000
			C	4.80430000	4.10260000	-6.03670000
			C	5.51530000	4.53110000	-7.15310000
			C	6.35110000	5.63750000	-7.04610000
			C	6.74930000	9.16760000	-6.33390000
			C	5.50970000	9.04380000	-6.98820000
			C	4.91230000	10.12340000	-7.57170000
			C	5.54750000	11.36040000	-7.53550000
			C	6.75210000	11.52270000	-6.87760000
			C	7.35650000	10.41460000	-6.27050000
			C	10.25090000	8.78260000	-6.64560000
			C	10.85950000	9.17430000	-5.46040000
			C	11.39800000	10.44310000	-5.38610000
			C	11.34750000	11.30180000	-6.46440000
			H	11.71210000	12.15540000	-6.40820000
			C	10.74450000	10.86820000	-7.62970000
			C	10.17100000	9.64630000	-7.72940000
			P	7.56320000	7.71270000	-5.66590000
			Se	9.41400000	7.05020000	-6.78120000
			Br	11.95340000	5.93840000	-7.93330000
			H	6.95550000	9.57440000	-3.53390000
			H	7.54440000	9.82540000	-1.34110000
H	8.79250000	8.25200000	-0.29000000			
H	9.53570000	6.34390000	-1.55860000			
H	9.14310000	6.15970000	-3.80580000			

			H	5.80560000	6.31040000	-3.86020000
			H	4.41730000	4.36870000	-3.93260000
			H	4.24900000	3.41460000	-6.14360000
			H	5.42690000	4.13440000	-8.02840000
			H	6.89940000	5.94210000	-7.73840000
			H	5.17450000	8.26880000	-7.01350000
			H	4.08070000	9.99280000	-7.99220000
			H	5.13250000	12.11860000	-7.88340000
			H	7.20790000	12.28600000	-6.85040000
			H	8.13340000	10.52850000	-5.78120000
			H	10.92400000	8.50310000	-4.65760000
			H	11.82150000	10.74610000	-4.63940000
			H	10.71360000	11.46580000	-8.24590000
			H	9.70400000	9.28980000	-8.59020000
3	ADUQUN	-8180.57579	Se	7.25880000	1.74730000	4.37760000
			Br	9.26030000	0.46570000	3.79740000
			Br	-0.75700000	4.58420000	7.29560000
			O	5.46520000	2.91130000	4.80080000
			N	4.48170000	4.88390000	4.30350000
			H	4.57690000	5.61410000	3.85900000
			C	7.69970000	3.34330000	3.46050000
			C	6.72370000	4.35790000	3.50870000
			C	1.54070000	3.47170000	6.05960000
			H	1.18660000	2.65310000	6.32150000
			C	5.52150000	4.01830000	4.23580000
			C	8.89180000	3.60010000	2.79550000
			H	9.54490000	2.93890000	2.75650000
			C	6.97900000	5.57540000	2.89660000
			H	6.33470000	6.24630000	2.92190000
			C	3.26570000	4.74860000	5.00300000
			C	2.72740000	3.52970000	5.37170000
			H	3.17290000	2.74420000	5.15230000
			C	1.40660000	5.86390000	5.98380000
			H	0.95620000	6.65080000	6.19400000
			C	8.17560000	5.80460000	2.25110000
			H	8.34410000	6.62870000	1.85260000
			C	9.12000000	4.80240000	2.20290000
			H	9.92300000	4.95010000	1.75840000
			C	0.88620000	4.64370000	6.35480000
			C	2.59480000	5.90950000	5.30270000
			H	2.94890000	6.72810000	5.04090000
4	CALROW	-15556.89928	Se	1.75550000	5.01350000	0.68040000
			Br	3.59350000	3.22120000	-0.33930000
			Br	-0.03420000	6.49880000	1.42080000
			N	0.24710000	4.78610000	-1.64480000
			H	-0.29800000	4.30100000	-1.11870000
			H	0.09290000	4.89750000	-2.36550000
			N	2.03530000	6.19250000	-1.91380000
			C	1.31710000	5.37940000	-1.17760000
			C	1.60840000	6.51280000	-3.28350000
			H	0.76700000	6.05130000	-3.47990000
			H	2.29720000	6.22240000	-3.91720000
			H	1.47640000	7.48130000	-3.36720000
			C	3.28320000	6.83300000	-1.50210000
			H	3.49280000	6.57560000	-0.57980000
			H	3.18410000	7.80620000	-1.55510000
			H	4.00850000	6.54570000	-2.09390000
			Se	0.82840000	2.83510000	4.95020000
			Br	2.66640000	4.62740000	3.93060000
			Br	-0.96130000	1.34980000	5.69070000
			N	-0.68000000	3.06250000	2.62510000
			H	-1.22510000	3.54760000	3.15120000
			H	-0.83420000	2.95110000	1.90440000

			N	1.10820000	1.65610000	2.35610000
			C	0.39000000	2.46920000	3.09220000
			C	0.68140000	1.33580000	0.98630000
			H	-0.16010000	1.79730000	0.78990000
			H	1.37010000	1.62620000	0.35270000
			H	0.54930000	0.36730000	0.90260000
			C	2.35610000	1.01560000	2.76770000
			H	2.56570000	1.27300000	3.69000000
			H	2.25700000	0.04240000	2.71480000
			H	3.08140000	1.30290000	2.17590000
5	CIDXOD	-7876.73927	C	13.29700000	1.55910000	4.07080000
			C	13.04840000	2.75020000	3.43760000
			C	13.42120000	3.94010000	4.02870000
			H	13.25340000	4.75440000	3.61180000
			C	14.05720000	3.88700000	5.27220000
			H	14.30740000	4.67860000	5.69250000
			C	14.32190000	2.68450000	5.88540000
			H	14.76260000	2.66170000	6.70520000
			C	13.93290000	1.52240000	5.27850000
			H	14.10240000	0.70430000	5.68910000
			C	12.39950000	2.82230000	2.08830000
			H	12.83210000	2.19010000	1.49240000
			H	12.52380000	3.71120000	1.72050000
			N	10.93070000	2.51630000	2.15260000
			Se	12.75990000	-0.10530000	3.24510000
			Br	14.84210000	-0.35320000	1.99980000
			Br	10.32930000	0.27100000	4.59220000
			H	10.83060000	1.83350000	2.63370000
			H	10.55814306	2.27906492	1.25542619
			H	10.39612647	3.26057331	2.55296031
6	ECIYIA2	-21630.68073	C	1.24170000	15.11600000	7.74250000
			C	1.26400000	16.39370000	8.31210000
			H	1.30000000	16.50010000	9.25540000
			C	1.23320000	17.51920000	7.46250000
			H	1.26090000	18.40390000	7.81060000
			C	1.15940000	17.28090000	6.09430000
			C	1.18850000	16.03880000	5.54820000
			H	1.20630000	15.93740000	4.60380000
			C	1.19390000	14.90820000	6.36900000
			H	1.16480000	14.03110000	6.00280000
			Se	1.25000000	13.57020000	8.93910000
			Br	-0.29560000	14.41970000	10.48240000
			Br	-0.63520000	12.27330000	7.52760000
			Br	3.26430000	14.37020000	10.14020000
			Cl	1.07720000	18.68400000	5.04880000
			C	3.39930000	10.23370000	13.55150000
			C	3.37700000	8.95600000	12.98190000
			H	3.34100000	8.84960000	12.03860000
			C	3.40770000	7.83050000	13.83150000
			H	3.38010000	6.94580000	13.48340000
			C	3.48160000	8.06880000	15.19970000
			C	3.45240000	9.31090000	15.74590000
			H	3.43460000	9.41230000	16.69020000
			C	3.44710000	10.44150000	14.92500000
			H	3.47620000	11.31860000	15.29120000
			Se	3.39090000	11.77950000	12.35490000
			Br	4.93660000	10.93000000	10.81160000
			Br	5.27620000	13.07640000	13.76640000
			Br	1.37660000	10.97950000	11.15380000
			Cl	3.56380000	6.66570000	16.24520000
7	ECIYUM2	-20909.96787	C	4.10690000	3.99370000	9.18500000
			C	4.44920000	4.12390000	7.80060000
			H	4.73020000	4.95500000	7.44400000

			C	4.3650000	3.0151000	6.9989000
			H	4.5728000	3.0715000	6.0736000
			C	3.9733000	1.8152000	7.5582000
			C	3.7089000	1.6386000	8.9007000
			H	3.4850000	0.7875000	9.2549000
			C	3.7864000	2.7802000	9.7141000
			H	3.6151000	2.7056000	10.6440000
			Br	5.3355000	4.3990000	12.1887000
			Br	6.2846000	6.4052000	9.4696000
			Br	2.8972000	7.0682000	8.5082000
			F	3.8769000	0.7729000	6.7262000
			Se	4.2372000	5.5704000	10.3345000
			C	5.4975000	8.9588000	15.2027000
			C	5.1162000	8.8167000	16.5172000
			H	4.9729000	7.9437000	16.8644000
			C	4.9314000	9.9137000	17.3585000
			H	4.6878000	9.8281000	18.2721000
			C	5.1344000	11.1572000	16.7502000
			C	5.4584000	11.3402000	15.4824000
			H	5.5911000	12.2151000	15.1351000
			C	5.6045000	10.1987000	14.6527000
			H	5.7740000	10.2988000	13.7227000
			Br	6.6060000	5.9555000	15.6961000
			Br	7.7630000	8.0448000	13.1357000
			Br	4.2948000	8.6930000	11.9265000
			F	4.9904000	12.2597000	17.5496000
			Se	5.6605000	7.4114000	14.0374000
8	GIHDAF	-10446.95511	Br	6.0140000	1.2607000	16.1762000
			Se	5.0447000	2.0966000	13.1897000
			N	4.0168000	2.6410000	10.4144000
			C	6.6667000	0.1361000	11.7749000
			C	5.5627000	0.2302000	12.7910000
			H	5.8566000	-0.2096000	13.6277000
			H	4.7713000	-0.2599000	12.4534000
			C	7.9863000	0.3750000	12.1259000
			H	8.1921000	0.6277000	13.0184000
			C	4.4127000	2.4093000	11.4608000
			C	9.0066000	0.2534000	11.2051000
			H	9.8996000	0.4396000	11.4716000
			Se	10.3722000	-2.0966000	8.4754000
			N	11.4002000	-2.6410000	11.2506000
			C	8.7502000	-0.1361000	9.8901000
			C	9.8542000	-0.2302000	8.8740000
			H	9.5603000	0.2096000	8.0373000
			H	10.6457000	0.2599000	9.2116000
			C	7.4306000	-0.3750000	9.5391000
			H	7.2248000	-0.6277000	8.6467000
			C	11.0043000	-2.4093000	10.2042000
			C	6.4104000	-0.2534000	10.4599000
			H	5.5173000	-0.4396000	10.1934000
			Br	9.4029000	-1.2607000	5.4888000
9	HOCDOS2	-11063.84211	Se	3.5608000	8.8091000	0.2472000
			Br	4.7208000	10.9864000	1.1635000
			O	0.5935000	6.0749000	-0.3711000
			N	2.5346000	7.1440000	-0.4080000
			C	1.8831000	9.1123000	1.1447000
			C	1.5772000	10.1918000	1.9832000
			H	2.2098000	10.8788000	2.1062000
			C	0.3233000	10.2588000	2.5589000
			H	0.1267000	10.9382000	3.1358000
			C	-0.6457000	9.3030000	2.3241000
			H	-1.4155000	9.3832000	2.8227000
			C	-0.3538000	8.2329000	1.4913000

			H	-0.97140000	7.60450000	1.27670000
			C	0.90180000	8.14890000	0.91450000
			C	1.33710000	7.10530000	0.02790000
			C	1.42460000	5.32660000	-1.33140000
			H	0.88350000	5.35020000	-2.58240000
			H	1.33250000	4.47550000	-1.10450000
			C	2.83410000	5.98620000	-1.29450000
			C	3.87970000	5.11150000	-0.67190000
			H	4.84490000	5.69650000	-0.61930000
			H	3.57070000	4.76710000	0.23030000
			H	4.02170000	4.33020000	-1.25650000
			C	3.25160000	6.45610000	-2.67410000
			H	4.26190000	6.94110000	-2.57340000
			H	3.45760000	5.70500000	-3.18720000
			H	2.62860000	7.07130000	-2.96360000
			Se	7.85120000	10.06290000	-0.24720000
			Br	6.69120000	7.88560000	-1.16350000
			O	10.81850000	12.79710000	0.37110000
			N	8.87740000	11.72800000	0.40800000
			C	9.52890000	9.75970000	-1.14470000
			C	9.83480000	8.68020000	-1.98320000
			H	9.20220000	7.99320000	-2.10620000
			C	11.08870000	8.61320000	-2.55890000
			H	11.28530000	7.93380000	-3.13580000
			C	12.05770000	9.56900000	-2.32410000
			H	12.82750000	9.48880000	-2.82270000
			C	11.76580000	10.63910000	-1.49130000
			H	12.38340000	11.26750000	-1.27670000
			C	10.51020000	10.72310000	-0.91450000
			C	10.07490000	11.76670000	-0.02790000
			C	9.98740000	13.54540000	1.33140000
			H	10.52850000	13.52180000	2.58240000
			H	10.07950000	14.39650000	1.10450000
			C	8.57790000	12.88580000	1.29450000
			C	7.53230000	13.76050000	0.67190000
			H	6.56710000	13.17550000	0.61930000
			H	7.84130000	14.10490000	-0.23030000
			H	7.39030000	14.54180000	1.25650000
			C	8.16040000	12.41590000	2.67410000
			H	7.15010000	11.93090000	2.57340000
			H	7.95440000	13.16700000	3.18720000
			H	8.78340000	11.80070000	2.96360000
10	IWODUU	-5459.067703	Br	11.09710000	2.48180000	6.73350000
			C	8.55600000	3.20940000	8.76590000
			C	7.56270000	3.98340000	9.31940000
			C	6.30410000	3.41220000	9.54020000
			H	5.62180000	3.91560000	9.92290000
			C	6.08130000	2.09430000	9.18480000
			H	5.24250000	1.71490000	9.31490000
			C	7.07880000	1.35900000	8.65090000
			H	6.91820000	0.47020000	8.42860000
			C	8.32670000	1.89010000	8.43010000
			H	9.00450000	1.37110000	8.06110000
			C	7.87780000	5.40210000	9.62340000
			H	7.67180000	5.95970000	8.85660000
			H	7.34440000	5.70650000	10.37510000
			C	9.55460000	5.08170000	11.36270000
			H	9.17790000	4.19700000	11.48370000
			H	9.07450000	5.68620000	11.95100000
			C	10.98560000	5.04830000	11.78760000
			H	11.47910000	4.46710000	11.20390000
			H	11.04500000	4.72290000	12.68900000
			H	11.35350000	5.93350000	11.74230000

			C	9.88540000	6.83990000	9.61890000
			H	9.75980000	7.00210000	8.67060000
			H	10.83970000	6.82530000	9.78980000
			C	9.27340000	7.98240000	10.38870000
			H	8.32300000	7.98520000	10.25710000
			H	9.64270000	8.81290000	10.07860000
			H	9.46620000	7.87810000	11.32330000
			N	9.32020000	5.50710000	9.95310000
			Se	10.22250000	4.12130000	8.52690000
11	KUSSOH	-5553.659052	Br	2.64040000	8.35410000	13.21510000
			C	-1.10090000	10.52590000	16.48760000
			C	-0.95040000	10.55870000	17.85760000
			C	-1.95660000	11.37030000	15.80120000
			C	-2.06340000	11.12350000	14.32650000
			H	-2.79720000	10.51460000	14.14540000
			H	-2.23900000	11.95770000	13.86350000
			C	0.07440000	9.62390000	18.41970000
			H	0.92540000	10.08000000	18.50990000
			H	-0.20340000	9.31710000	19.29750000
			C	-0.85680000	7.47450000	17.70820000
			H	-0.76060000	7.08180000	18.57860000
			H	-0.79160000	6.78980000	17.03860000
			H	-1.71330000	7.90460000	17.64480000
			C	1.53860000	7.81630000	17.61830000
			H	2.23050000	8.46830000	17.47740000
			H	1.61560000	7.12370000	16.95760000
			H	1.63120000	7.43610000	18.49400000
			C	0.22290000	11.58420000	13.58330000
			H	1.06940000	11.17330000	13.38950000
			H	0.31190000	12.14780000	14.35510000
			H	-0.05520000	12.11270000	12.83090000
			C	-0.98410000	9.69970000	12.65300000
			H	-1.27370000	10.24980000	11.92350000
			H	-1.65310000	9.03420000	12.83800000
			H	-0.15860000	9.26850000	12.42220000
			C	-2.68600000	12.29160000	16.52940000
			H	-3.26730000	12.87330000	16.09420000
			C	-2.54860000	12.34930000	17.90200000
			H	-3.03940000	12.97290000	18.38480000
			C	-1.69270000	11.49360000	18.57160000
			H	-1.61390000	11.54230000	19.49660000
			N	0.21250000	8.47050000	17.49800000
			N	-0.78390000	10.53720000	13.85010000
			Se	-0.06280000	9.30190000	15.49590000
12	PEBPUH	-15125.88935	Br	6.79500000	10.11090000	1.60270000
			Se	2.14250000	7.40370000	0.86770000
			Se	4.23190000	8.57500000	1.06250000
			C	2.87430000	5.88210000	0.12700000
			C	4.69530000	7.63860000	2.61910000
			N	3.26840000	4.93240000	-0.31850000
			N	4.96040000	7.05650000	3.55740000
			Br	3.39750000	10.31310000	-1.60270000
			Se	-1.25500000	13.02030000	-0.86770000
			Se	0.83440000	11.84900000	-1.06250000
			C	-0.52320000	14.54190000	-0.12700000
			C	1.29780000	12.78540000	-2.61910000
			N	-0.12910000	15.49160000	0.31850000
			N	1.56290000	13.36750000	-3.55740000
13	RAGSAT	-10585.78522	Se	2.49720000	9.93530000	2.88310000
			Br	0.70050000	6.94140000	8.32290000
			Br	-2.74830000	10.50060000	-0.79710000
			Br	3.53590000	8.24530000	1.78110000
			C	1.92530000	8.97830000	4.41380000

			C	2.71910000	8.00350000	4.95550000
			H	3.51830000	7.75860000	4.55040000
			C	2.29570000	7.39130000	6.13040000
			H	2.78750000	6.68740000	6.48730000
			C	1.17990000	7.81220000	6.75250000
			C	0.38350000	8.80990000	6.21080000
			H	-0.40710000	9.06400000	6.62710000
			C	0.78100000	9.40680000	5.06320000
			H	0.28290000	10.10760000	4.70790000
			C	0.90930000	10.09540000	1.86940000
			C	0.77960000	11.20330000	1.10260000
			H	1.43170000	11.86750000	1.10590000
			C	-0.35170000	11.31810000	0.31500000
			H	-0.48410000	12.08170000	-0.19930000
			C	-1.25930000	10.32950000	0.29090000
			C	-1.12520000	9.21700000	1.04000000
			H	-1.78050000	8.55740000	1.02390000
			C	0.01150000	9.06700000	1.84360000
			H	0.15070000	8.29270000	2.34190000
14	TAJMEW	-10408.57517	Se	-0.39340000	1.94680000	2.27830000
			Se	1.17060000	2.66660000	3.92940000
			C	0.89450000	1.00520000	1.27560000
			N	1.85650000	1.76130000	0.65370000
			N	0.84280000	-0.27890000	1.01160000
			C	-0.24870000	-1.12970000	1.54310000
			C	1.72090000	-0.96110000	0.03720000
			C	0.89690000	1.04800000	4.94280000
			N	-0.14350000	1.05190000	5.73640000
			N	1.69230000	0.01040000	4.78860000
			C	1.45280000	-1.21790000	5.55400000
			C	2.93710000	0.10770000	4.03570000
			H	1.86020000	2.64850000	0.74580000
			H	2.49750000	1.34890000	0.16650000
			H	-0.84470000	-0.60310000	2.06570000
			H	0.10880000	-1.83530000	2.06570000
			H	-0.73820000	-1.50580000	0.79900000
			H	2.58750000	-0.57460000	0.05310000
			H	1.77930000	-1.89230000	0.25510000
			H	1.34510000	-0.87160000	-0.83970000
			H	-0.67320000	1.77690000	5.79140000
			H	-0.32720000	0.32680000	6.24840000
			H	0.59780000	-1.17510000	5.98270000
			H	2.13080000	-1.33850000	6.21480000
			H	1.45880000	-1.98050000	4.96230000
			H	3.66440000	-0.14530000	4.58490000
			H	2.88850000	-0.47730000	3.27570000
			H	3.05140000	1.00520000	3.73100000
			Br	3.21620000	3.00770000	6.17400000
			Br	-2.68052278	0.56736202	0.47979500
15	TAVWUI	-10561.01744	Br	-0.67840000	-0.02370000	2.58940000
			Br	6.20010000	3.47750000	-1.52240000
			Se	2.16430000	1.00210000	1.41690000
			Se	3.88330000	2.04150000	0.08750000
			N	0.61820000	3.25160000	2.30740000
			N	0.15170000	2.75110000	0.26010000
			N	3.89950000	4.69430000	1.21400000
			N	5.21460000	3.35890000	2.29460000
			C	0.95850000	2.43250000	1.31430000
			C	-0.68530000	3.79270000	0.64700000
			C	-0.38510000	3.91140000	1.90930000
			C	1.23570000	3.24930000	3.66620000
			C	0.15550000	2.10930000	-1.03760000
			C	4.32420000	3.42890000	1.26680000

			C	5.34340000	4.61640000	2.86620000
			C	4.52380000	5.44450000	2.17240000
			C	2.96400000	5.23100000	0.20210000
			C	5.97920000	2.16920000	2.70410000
			H	-1.35350000	4.21300000	0.10100000
			H	-0.78080000	4.81520000	2.43260000
			H	0.83030000	3.93960000	4.19560000
			H	2.18120000	3.40520000	3.60590000
			H	1.07800000	2.39630000	4.07720000
			H	-0.50630000	2.52960000	-1.59180000
			H	-0.05630000	1.17840000	-0.93730000
			H	1.01920000	2.19970000	-1.44480000
			H	5.89940000	4.85480000	3.61190000
			H	4.39910000	6.38560000	2.31800000
			H	2.80470000	6.16310000	0.36500000
			H	2.13550000	4.74970000	0.25940000
			H	3.33800000	5.11910000	-0.67490000
			H	6.52990000	2.38050000	3.46110000
			H	6.53390000	1.88000000	1.97560000
			H	5.36810000	1.46650000	2.93930000
16	XATJEH	-8150.470163	Br	7.34180000	-2.05770000	4.85220000
			Se	7.33850000	0.08210000	3.60950000
			N	4.40690000	2.25980000	3.88330000
			C	7.16650000	1.09920000	5.25710000
			C	8.32930000	1.38370000	5.98340000
			C	8.25020000	2.03020000	7.15500000
			C	7.06700000	2.45380000	7.67290000
			C	5.89660000	2.18220000	6.94040000
			C	5.94260000	1.51300000	5.72820000
			C	4.65210000	1.26410000	4.98330000
			C	4.25850000	3.63540000	4.45060000
			C	3.26140000	1.90900000	2.96830000
			C	3.60510000	0.73390000	2.06440000
			C	2.48190000	0.50430000	1.04570000
			C	1.15590000	0.29260000	1.76960000
			C	0.82500000	1.43050000	2.70810000
			C	1.94650000	1.64880000	3.67740000
			H	9.07860000	1.06690000	5.69980000
			H	9.05110000	2.19190000	7.63100000
			H	7.05210000	2.94520000	8.51150000
			H	5.04080000	2.43760000	7.28570000
			H	4.54990000	0.40250000	4.70460000
			H	3.92670000	1.32390000	5.59870000
			H	5.18980000	2.25980000	3.35060000
			H	3.45520000	3.71940000	4.92290000
			H	4.99840000	3.80990000	5.04870000
			H	4.24300000	4.25610000	3.61320000
			H	3.13500000	2.66070000	2.40600000
			H	3.71550000	-0.04360000	2.57490000
			H	4.40320000	0.92950000	1.58220000
			H	2.40610000	-0.52700000	0.26880000
			H	2.39480000	1.27210000	0.48710000
			H	0.62920000	0.27320000	0.95450000
			H	1.23170000	-0.52530000	2.27150000
			H	0.73480000	2.23230000	2.18640000
			H	0.04570000	1.25270000	3.17180000
			H	1.73410000	2.38260000	4.21870000
			H	2.02840000	0.85990000	4.19900000
			Br	7.21290000	2.46230000	2.20000000

Table S10. CSD refcodes of the starting structures, energies (in Hartree) and coordinates of the optimized structures containing Se...Br contacts (from calculation with CH₂Cl₂ as a medium)

	CSD refcode	E(RM062X)	Coordinates			
1	ACIMOP	-5668.533717	C	3.25004200	-2.12783800	-0.10579700
			H	2.94671500	-2.73620400	0.74411500
			H	4.32932000	-1.98411300	-0.08689000
			H	2.95941000	-2.61993600	-1.03184700
			C	2.94540300	0.48183800	-1.40263400
			H	2.44562800	1.44733700	-1.34287900
			H	2.66551000	-0.01942500	-2.32673200
			H	4.02486800	0.62577400	-1.36456600
			C	2.98512300	0.30591200	1.49274200
			H	2.73047500	-0.30425600	2.35679800
			H	2.48554800	1.27077500	1.56398900
			H	4.06355700	0.45490500	1.44260500
			C	-0.19811800	0.94896000	0.00108900
			C	-0.40027000	1.60309100	-1.20800600
			H	-0.29641600	1.06545900	-2.14059600
			C	-0.35459400	1.61773500	1.20867500
			H	-0.21851500	1.09138000	2.14364200
			C	-0.74933200	2.94664900	-1.20473700
			H	-0.91130600	3.45893200	-2.14313400
			C	-0.89839600	3.62554600	-0.00225200
			H	-1.17496000	4.67096100	-0.00366600
			C	-0.70319500	2.96195500	1.20172500
			H	-0.82953400	3.48606500	2.13905500
Br	-3.01606000	-1.27536200	0.00703600			
Se	0.24748400	-0.92812900	-0.00067800			
P	2.44449200	-0.52644500	-0.00386200			
2	ACINEG	-6243.712125	C	-1.56148600	0.74890000	1.48142900
			C	-2.43141100	1.83773300	1.42035100
			C	-2.86181500	2.43806800	2.59457700
			C	-2.43096100	1.95438600	3.82250400
			C	-1.57080700	0.86487000	3.88327300
			C	-1.13430700	0.25970900	2.71568100
			C	-2.18329900	-1.49209000	-0.29001700
			C	-3.42219400	-1.52059100	0.34899600
			C	-4.28850400	-2.57864900	0.11774800
			C	-3.92183700	-3.60384300	-0.74354100
			C	-2.68637600	-3.57728100	-1.37787200
			C	-1.81298800	-2.52472800	-1.15365400
			C	-1.17820400	1.04803700	-1.39480900
			C	-1.75343700	0.65351500	-2.60175000
			C	-1.78318300	1.53775700	-3.67011000
			C	-1.24135700	2.80872100	-3.53721800
			C	-0.66831000	3.20285600	-2.33424000
			C	-0.63149800	2.32693600	-1.26197800
			C	1.85554500	0.69188700	0.06916200
			C	1.95032600	1.47756400	1.21087900
			C	2.54308300	2.73101900	1.12531700
			C	3.04570200	3.18294000	-0.08803100
			H	3.50901300	4.15819300	-0.14999300
			C	2.96428400	2.38070100	-1.21935600
			C	2.36542000	1.13144500	-1.14562000
			P	-1.06571600	-0.10771000	-0.02199700
			Se	0.98728100	-1.02531800	0.14872800
Br	3.99366300	-2.16198600	0.27076900			
H	-2.77451700	2.21503600	0.46658500			
H	-3.53328300	3.28390500	2.54745900			
H	-2.76534300	2.42810500	4.73530100			
H	-1.23567200	0.48797700	4.83931300			

			H	-0.45962000	-0.58541200	2.76261400
			H	-3.70865200	-0.72830500	1.02742600
			H	-5.24795900	-2.60234600	0.61509200
			H	-4.59884500	-4.42885900	-0.91795300
			H	-2.39896300	-4.37755000	-2.04511400
			H	-0.85094200	-2.50904600	-1.64924600
			H	-2.18286900	-0.33303800	-2.70995900
			H	-2.23325200	1.23216200	-4.60417400
			H	-1.26661900	3.49535500	-4.37232200
			H	-0.24482000	4.19209300	-2.22985200
			H	-0.17895400	2.63915100	-0.32856000
			H	1.56705500	1.11812900	2.15594200
			H	2.61649800	3.34899700	2.00966200
			H	3.36280400	2.72784200	-2.16280500
			H	2.29061700	0.50441400	-2.02346500
3	ADUQUN	-8180.778678	Se	-2.58803700	-1.08023100	0.01269000
			Br	-4.94996200	-1.60064000	-0.08080300
			Br	6.58441100	-0.77061500	-0.02758000
			O	-0.39782400	-0.47584600	0.08180300
			N	0.90461400	1.37885700	0.03274800
			H	0.88554000	2.38271100	-0.04078100
			C	-2.72540000	0.83517500	0.02216700
			C	-1.52413200	1.56066900	0.05258500
			C	3.76021400	-0.99702000	0.25235800
			H	3.95902100	-2.04172900	0.44307200
			C	-0.28724700	0.75804400	0.05918500
			C	-3.93218700	1.52832200	0.00655200
			H	-4.86745500	0.99238800	-0.01985800
			C	-1.55124100	2.95535300	0.07977400
			H	-0.63633500	3.53074100	0.12073500
			C	2.19494300	0.81238800	0.02320300
			C	2.45168500	-0.53433600	0.26937200
			H	1.64703400	-1.21895700	0.47339300
			C	4.55922700	1.21957500	-0.24561600
			H	5.37459600	1.89970500	-0.44435700
			C	-2.75267600	3.63445900	0.06667600
			H	-2.76609900	4.71444500	0.08913800
			C	-3.94018600	2.91263600	0.02693600
			H	-4.88843900	3.43267000	0.01511300
			C	4.80217100	-0.12393200	-0.00473500
			C	3.25623200	1.68124900	-0.23120900
			H	3.06154200	2.72907800	-0.42166800
4	CALROW	-15557.30359	Se	-1.72495300	-0.19705700	0.18709000
			Br	-1.75260500	2.35634300	0.46117900
			Br	-1.91009300	-2.72372500	-0.38028200
			N	-3.27548100	-0.11975000	-2.14030000
			H	-2.40988700	-0.45658300	-2.52801700
			H	-4.08251300	-0.12604900	-2.74464400
			N	-4.50285400	0.35558000	-0.26583200
			C	-3.36906200	0.03251600	-0.82837600
			C	-5.67149000	0.61451600	-1.10882500
			H	-5.99362900	-0.30236400	-1.60324600
			H	-5.43607700	1.37704700	-1.85134900
			H	-6.47536000	0.97538600	-0.47796600
			C	-4.69573200	0.55344600	1.16899500
			H	-3.83918500	0.18606800	1.71969300
			H	-5.58655100	0.00637100	1.46861400
			H	-4.83050900	1.61553200	1.36737800
			Se	3.09578300	-0.23075000	0.74574900
			Br	1.02734400	-0.42769800	2.29612300
			Br	4.79924500	0.09246400	-1.15625600
			N	1.30749800	-1.25731100	-1.11781200
			H	1.62397600	-2.10861800	-0.68257200

			H	0.45855500	-1.31764600	-1.66157500
			N	1.40095300	1.05303900	-1.13067800
			C	1.77069000	-0.10734100	-0.65849400
			C	0.59634500	1.17462200	-2.34486400
			H	0.64608400	0.26234500	-2.93193600
			H	-0.43529700	1.41096200	-2.08514300
			H	1.01205500	1.98520200	-2.93887300
			C	1.82627100	2.31814500	-0.52357900
			H	1.73593400	2.26041200	0.55666600
			H	2.85476300	2.53930300	-0.80811000
			H	1.16027700	3.09328900	-0.88894600
5	CIDXOD	-7876.924274	C	-0.08602000	0.87111300	-0.37280200
			C	0.14873400	1.66022700	0.75822400
			C	0.30545100	3.03336500	0.60206800
			H	0.48070200	3.64969400	1.47489100
			C	0.23142000	3.61909500	-0.65402500
			H	0.35267500	4.68837700	-0.75750700
			C	-0.00136000	2.82971600	-1.76993700
			H	-0.06171100	3.27814400	-2.75202100
			C	-0.16075300	1.45767300	-1.62861200
			H	-0.34493600	0.83741100	-2.49482600
			C	0.24316300	1.06067600	2.13160700
			H	-0.50324000	0.28665900	2.28643400
			H	0.14306000	1.82024000	2.90114500
			N	1.58385300	0.41024500	2.32618400
			Se	-0.32434300	-1.03721900	-0.22716700
			Br	-2.76251300	-0.76881200	0.11835800
			Br	2.47770800	-1.23449700	-0.42427400
			H	1.80987300	-0.23643300	1.54195400
			H	1.62199000	-0.11461600	3.19943000
			H	2.32666000	1.10888700	2.34880600
6	ECIYIA2	-21630.82416	C	3.90175500	-0.00331400	0.06004000
			C	4.43189800	0.67277400	-1.02549600
			H	3.85665600	0.82283900	-1.92791800
			C	5.72240200	1.16596700	-0.93878800
			H	6.16512900	1.68821200	-1.77408700
			C	6.44128800	0.98978100	0.23580400
			C	5.89886000	0.32543200	1.32530100
			H	6.47530800	0.19944800	2.22983400
			C	4.61369100	-0.18525400	1.23610300
			H	4.19128900	-0.72345400	2.07319200
			Se	2.07659600	-0.64159200	0.06795400
			Br	1.76352400	-1.13289100	-2.16348000
			Br	2.81897800	-3.00203500	0.58709000
			Br	1.23024800	1.77930300	-0.29219000
			Cl	8.04977600	1.61090300	0.34050400
			C	-3.90177700	0.00339000	-0.06001000
			C	-4.43176200	-0.67211700	1.02595200
			H	-3.85642300	-0.82154000	1.92842200
			C	-5.72223500	-1.16545400	0.93965300
			H	-6.16485700	-1.68721400	1.77530900
			C	-6.44120600	-0.99008100	-0.23501100
			C	-5.89891300	-0.32636100	-1.32495700
			H	-6.47542500	-0.20101500	-2.22953800
			C	-4.61381400	0.18457300	-1.23613400
			H	-4.19152900	0.72229500	-2.07358500
			Se	-2.07664500	0.64169500	-0.06827900
			Br	-1.76350500	1.13285900	2.16316600
			Br	-2.81905200	3.00223300	-0.58716800
			Br	-1.23024900	-1.77918400	0.29181100
			Cl	-8.04963400	-1.61144000	-0.33923200
7	ECIYUM2	-20910.12638	C	3.90639700	-0.33148800	-0.43066900
			C	4.93300200	0.05651500	0.41608900

			H	4.76736800	0.78350200	1.19862000
			C	6.18785500	-0.49975300	0.24314000
			H	7.01483600	-0.23525600	0.88569900
			C	6.37378800	-1.40803500	-0.78448300
			C	5.35967400	-1.78928900	-1.64201600
			H	5.55475600	-2.50350000	-2.42837800
			C	4.09881500	-1.24570100	-1.45695700
			H	3.28383300	-1.54648300	-2.09993300
			Br	1.03794600	-1.89279000	-0.12868000
			Br	1.95028200	0.78574100	1.95134000
			Br	3.09565000	2.76418100	-0.68075400
			F	7.58734500	-1.94007600	-0.95255000
			Se	2.15357500	0.46849800	-0.32517600
			C	-3.90814600	0.27368300	-0.43446000
			C	-4.61626500	-0.09684700	-1.56922700
			H	-4.23826700	-0.85037700	-2.24588400
			C	-5.83689900	0.50657700	-1.82434600
			H	-6.42103300	0.24879000	-2.69548200
			C	-6.30692300	1.44740500	-0.92806900
			C	-5.60706000	1.82008500	0.20593600
			H	-6.01807900	2.56232800	0.87445500
			C	-4.37979500	1.22945400	0.45134300
			H	-3.80497800	1.51962200	1.31933400
			Br	-3.11976000	-2.86589500	-0.29460900
			Br	-1.95518000	-0.57096600	2.06428900
			Br	-1.06556800	1.81984100	-0.34763800
			F	-7.48928700	2.02199900	-1.16549700
			Se	-2.16138600	-0.52424700	-0.23252700
8	GIHDAF	-10447.25115	Br	5.09666300	1.74337300	-0.07902500
			Se	3.86082300	-1.36815900	0.18920100
			N	2.44508400	-4.02252900	0.36364600
			C	1.24168700	-0.32454800	-0.53181900
			C	2.57811100	-0.61582000	-1.12634100
			H	3.10157000	0.28636800	-1.43267100
			H	2.52864300	-1.32393000	-1.94782400
			C	1.05237800	0.82485800	0.23304700
			H	1.88976100	1.49510700	0.39230400
			C	2.97773200	-3.00384800	0.28680500
			C	-0.18704700	1.10305000	0.78575100
			H	-0.32537900	1.99946800	1.37774400
			Se	-3.83124400	1.39569200	-0.12946900
			N	-2.37660800	4.03425200	-0.09258100
			C	-1.26175000	0.23713200	0.58703800
			C	-2.60053700	0.53646400	1.17154100
			H	-3.15551400	-0.36380700	1.42246300
			H	-2.54854000	1.20146900	2.02819600
			C	-1.07260500	-0.91239400	-0.17673400
			H	-1.91106700	-1.58049500	-0.34021100
			C	-2.92408400	3.02052600	-0.09485200
			C	0.16866200	-1.19213200	-0.72693500
			H	0.30774300	-2.08972800	-1.31701000
			Br	-5.13116300	-1.70572600	-0.10829900
9	HOCDOS2	-11064.32501	Se	-2.24513200	-0.68214200	0.24383100
			Br	-0.96820400	1.53895400	1.32843100
			O	-5.13222900	-3.39068100	-0.39575000
			N	-3.24929500	-2.22891300	-0.44591200
			C	-3.90061900	-0.35461200	1.15153800
			C	-4.19492000	0.70805100	2.00328500
			H	-3.45138700	1.46129100	2.21185600
			C	-5.45216600	0.78062100	2.57767200
			H	-5.67471600	1.60760500	3.23864100
			C	-6.43643100	-0.18035800	2.32816000
			H	-7.40777100	-0.09349500	2.79346600

			C	-6.16107200	-1.23560100	1.48664100
			H	-6.89862900	-1.99614500	1.26960700
			C	-4.89586300	-1.31437300	0.90410500
			C	-4.44992100	-2.33676500	0.00811300
			C	-4.28831900	-4.08667800	-1.35474400
			H	-4.75887600	-3.99000000	-2.33052300
			H	-4.24374200	-5.13055500	-1.05846000
			C	-2.90203200	-3.38432100	-1.29849900
			C	-1.84844700	-4.23370600	-0.60040800
			H	-0.92520800	-3.66518800	-0.48669000
			H	-2.19792200	-4.55067900	0.38231700
			H	-1.63963200	-5.11857900	-1.20170000
			C	-2.43749900	-2.91964800	-2.66929700
			H	-1.49431200	-2.38039100	-2.58192800
			H	-2.28202700	-3.78638600	-3.31192200
			H	-3.18219700	-2.27038600	-3.12858400
			Se	2.24513200	0.68214200	-0.24383100
			Br	0.96820400	-1.53895400	-1.32843100
			O	5.13222900	3.39068100	0.39575000
			N	3.24929500	2.22891300	0.44591200
			C	3.90061900	0.35461200	-1.15153800
			C	4.19492000	-0.70805100	-2.00328500
			H	3.45138700	-1.46129100	-2.21185600
			C	5.45216600	-0.78062100	-2.57767200
			H	5.67471600	-1.60760500	-3.23864100
			C	6.43643100	0.18035800	-2.32816000
			H	7.40777100	0.09349500	-2.79346600
			C	6.16107200	1.23560100	-1.48664100
			H	6.89862900	1.99614500	-1.26960700
			C	4.89586300	1.31437300	-0.90410500
			C	4.44992100	2.33676500	-0.00811300
			C	4.28831900	4.08667800	1.35474400
			H	4.75887600	3.99000000	2.33052300
			H	4.24374200	5.13055500	1.05846000
			C	2.90203200	3.38432100	1.29849900
			C	1.84844700	4.23370600	0.60040800
			H	0.92520800	3.66518800	0.48669000
			H	2.19792200	4.55067900	-0.38231700
			H	1.63963200	5.11857900	1.20170000
			C	2.43749900	2.91964800	2.66929700
			H	1.49431200	2.38039100	2.58192800
			H	2.28202700	3.78638600	3.31192200
			H	3.18219700	2.27038600	3.12858400
10	IWODUU	-5459.320549	Br	-2.79899400	-1.32256300	-0.13350900
			C	-0.46154600	1.08110000	-0.00934100
			C	0.67366800	1.79024400	-0.40218800
			C	0.67315500	3.17560500	-0.36177500
			H	1.56211300	3.71728300	-0.65977600
			C	-0.46040300	3.86023800	0.05675700
			H	-0.46077000	4.94103200	0.08526600
			C	-1.58567000	3.14911700	0.44765000
			H	-2.46892400	3.67439800	0.78507600
			C	-1.59167400	1.75898900	0.42217700
			H	-2.47038000	1.21369200	0.73172700
			C	1.84703800	0.98152500	-0.87113600
			H	1.72470600	0.72746400	-1.92675700
			H	2.78644600	1.52527300	-0.75217700
			C	2.36052900	-0.04666300	1.26856800
			H	1.68195700	0.67470000	1.72297100
			H	3.34253300	0.43013200	1.20204600
			C	2.43816200	-1.30168200	2.11563400
			H	1.48885500	-1.83563200	2.11635900
			H	2.66579700	-1.01583700	3.14104400

			H	3.22258000	-1.97724100	1.77783800
			C	2.57606300	-1.36569600	-0.82103900
			H	2.10562700	-1.45507200	-1.79941000
			H	2.37752200	-2.29294500	-0.28521500
			C	4.07124600	-1.13749700	-0.96622900
			H	4.28416100	-0.21280300	-1.50196100
			H	4.50010800	-1.95947400	-1.53691500
			H	4.57448500	-1.10339100	-0.00069100
			N	1.86351200	-0.28049600	-0.11102600
			Se	-0.27176500	-0.83735600	-0.08599700
11	KUSSOH	-5553.976918	Br	3.76929700	0.18193100	-0.37672400
			C	-1.67189000	-0.25123100	-0.04986200
			C	-2.55855600	0.71137000	-0.49653100
			C	-2.02904200	-1.57548700	0.11684200
			C	-0.94524100	-2.45993400	0.66709400
			H	-0.99784800	-2.46513200	1.75737600
			H	-1.02023000	-3.49030300	0.31442000
			C	-1.96942700	2.08060200	-0.70244900
			H	-1.58426700	2.15948500	-1.72090500
			H	-2.69745100	2.87997000	-0.54721900
			C	-1.29120900	2.58535300	1.57343500
			H	-1.76456400	3.56966200	1.56425600
			H	-0.43950000	2.59516000	2.24886900
			H	-2.00942800	1.83993900	1.90942000
			C	0.15804900	3.21352100	-0.26165800
			H	0.52264500	2.90269900	-1.23757000
			H	0.99261000	3.24593000	0.43577500
			H	-0.29306300	4.20516200	-0.33216500
			C	0.73530400	-2.27376900	-1.09069100
			H	1.65815800	-1.76040000	-1.35348400
			H	-0.06204500	-1.97544600	-1.76867700
			H	0.87609700	-3.35509100	-1.14343500
			C	1.42992200	-2.28646500	1.22832300
			H	1.53441000	-3.37297200	1.22538800
			H	1.16472300	-1.94510700	2.22604700
			H	2.36060600	-1.81748100	0.91454000
			C	-3.33171600	-1.95428300	-0.17523800
			H	-3.63723600	-2.98582700	-0.05654600
			C	-4.24468400	-0.99834900	-0.61037300
			H	-5.26133600	-1.29263300	-0.83059800
			C	-3.86501200	0.33146900	-0.76900200
			H	-4.58218800	1.06488500	-1.11467100
			N	-0.82811900	2.23805800	0.22138600
			N	0.36787600	-1.89100400	0.28614200
			Se	0.11874200	0.24893400	0.31066200
12	PEBPUH	-15126.03856	Br	-3.92724600	-1.27565300	0.30909400
			Se	-1.14864600	1.20054500	0.74196500
			Se	-2.36443300	-0.05921300	-0.86783200
			C	-2.19757500	2.73107800	0.78252200
			C	-3.69550400	1.31197800	-1.25836100
			N	-2.79686000	3.70755100	0.87686700
			N	-4.45016700	2.08556900	-1.64619900
			Br	-0.39322400	-1.75045700	0.00225500
			Se	5.06180400	-0.06356100	0.03762700
			Se	2.83513800	-0.81308800	-0.12914600
			C	4.88562000	1.43667400	-1.02757800
			C	2.17767400	0.18862500	1.28098200
			N	4.81377300	2.37927900	-1.68224900
			N	1.73951100	0.81395500	2.14137200
13	RAGSAT	-10586.0226	Se	-0.00646900	1.70192600	0.91513300
			Br	5.14582200	-2.15621000	-0.21902700
			Br	-5.14270000	-2.09391300	-0.35833800
			Br	0.00258800	3.11673700	-0.90856800

			C	1.47575400	0.56057900	0.47206700
			C	2.64277700	1.12455000	-0.02196700
			H	2.70942000	2.17772000	-0.25652900
			C	3.73973500	0.30624400	-0.23205300
			H	4.65506300	0.72035200	-0.62805700
			C	3.64966000	-1.04623700	0.06967600
			C	2.48430600	-1.59924500	0.57944700
			H	2.43106100	-2.65272600	0.81064000
			C	1.37959100	-0.78807300	0.78681100
			H	0.47113400	-1.21697900	1.18571500
			C	-1.47739800	0.56888700	0.50040400
			C	-2.53259000	0.57682500	1.40215400
			H	-2.50803000	1.19137700	2.29144000
			C	-3.63256300	-0.22794200	1.14556300
			H	-4.46502700	-0.24542500	1.83296700
			C	-3.64846300	-1.00388800	-0.00341900
			C	-2.58947700	-0.99816400	-0.90799500
			H	-2.62804600	-1.60766400	-1.79843800
			C	-1.48885900	-0.20307200	-0.65615700
			H	-0.66031300	-0.18642600	-1.35176600
14	TAJMEW	-10408.88215	Se	1.16351200	-1.15389000	0.26547200
			Se	-1.16490000	-1.15334900	-0.26556500
			C	1.58117800	0.26035800	-0.99171800
			N	1.74102600	-0.11872700	-2.24625500
			N	1.63505800	1.52351700	-0.64762900
			C	1.65521800	2.00048300	0.73167100
			C	2.00726500	2.51389600	-1.65813400
			C	-1.58125700	0.26162600	0.99121800
			N	-1.74154400	-0.11695800	2.24582800
			N	-1.63392600	1.52475800	0.64676300
			C	-2.00555100	2.51565300	1.65698200
			C	-1.65303400	2.00134700	-0.73268700
			H	1.71155500	-1.09927900	-2.47120500
			H	2.01824600	0.51749100	-2.97735800
			H	1.31529400	1.22559100	1.40805900
			H	1.00728200	2.87234000	0.80548400
			H	2.67789700	2.27255400	0.99038300
			H	1.32532800	2.46787000	-2.50664100
			H	1.94137800	3.50038200	-1.21302600
			H	3.03289500	2.33966100	-1.98939200
			H	-1.71304900	-1.09746200	2.47109100
			H	-2.01765200	0.51981000	2.97687600
			H	-1.32308400	2.47007900	2.50509400
			H	-3.03094400	2.34151800	1.98900600
			H	-1.94007400	3.50191400	1.21133400
			H	-2.67547100	2.27317700	-0.99245600
			H	-1.00522000	2.87331800	-0.80613600
			H	-1.31219600	1.22641300	-1.40855800
			Br	-4.30164100	-0.38230800	-0.41787200
			Br	4.30186400	-0.38248000	0.41889100
15	TAVWUI	-10561.31011	Br	4.32587700	-0.42391700	-0.73717900
			Br	-4.32116800	-0.62464100	0.60093600
			Se	1.14741600	-1.10932700	-0.53868000
			Se	-1.15614500	-1.21598500	0.18049100
			N	1.68270800	1.58503500	0.33579900
			N	1.90304500	0.15864400	1.94384500
			N	-1.68182200	1.61917800	0.13782300
			N	-1.90413900	0.72803400	-1.81828300
			C	1.60257200	0.28666300	0.64823600
			C	2.20492000	1.39276000	2.45787500
			C	2.07251900	2.28727200	1.44677700
			C	1.56248900	2.13523800	-1.00871100
			C	1.97621100	-1.10885900	2.66046200

			C	-1.60690700	0.46903700	-0.54166300
			C	-2.19775700	2.06022600	-1.94818000
			C	-2.06359200	2.61867400	-0.71913900
			C	-1.55965700	1.75142800	1.58442600
			C	-1.97551300	-0.27146300	-2.87751300
			H	2.48309900	1.52718300	3.48681400
			H	2.21969500	3.35120600	1.42307800
			H	1.56483800	3.21725100	-0.93107900
			H	0.63400100	1.80064100	-1.46448200
			H	2.41020700	1.79077400	-1.59861900
			H	2.29673500	-0.90314300	3.67579600
			H	2.69851900	-1.75119700	2.16213400
			H	0.99744000	-1.58196800	2.66926900
			H	-2.47037800	2.49283300	-2.89301000
			H	-2.20646100	3.62951700	-0.38469100
			H	-1.52505600	2.80861400	1.82559300
			H	-0.64779400	1.26609700	1.92284100
			H	-2.42385100	1.27858700	2.04815300
			H	-2.30271300	0.22376200	-3.78504600
			H	-2.69184000	-1.03709800	-2.58956800
			H	-0.99468400	-0.71502500	-3.02999900
16	XATJEH	-8150.88308	Br	-1.56570300	-2.81421400	-0.27814300
			Se	-1.15083100	-0.72579900	0.97684100
			N	1.30205500	1.17350700	-0.55378800
			C	-1.80109100	0.34833800	-0.48568400
			C	-3.14137600	0.71069500	-0.49931300
			C	-3.65095900	1.46725000	-1.54570800
			C	-2.81913700	1.86067500	-2.58285800
			C	-1.47886800	1.50105900	-2.56681000
			C	-0.95179000	0.74670900	-1.52312800
			C	0.50517800	0.37378000	-1.54611900
			C	1.34850200	2.61063200	-0.92809100
			C	2.68195800	0.61100300	-0.27853000
			C	2.59815800	-0.61973100	0.61505700
			C	4.01152200	-1.08398800	0.97032100
			C	4.83899800	-1.35371900	-0.28346400
			C	4.87835100	-0.12471000	-1.18738800
			C	3.46493600	0.33224600	-1.55410100
			H	-3.78486800	0.39552800	0.31031700
			H	-4.69634700	1.74360600	-1.54910900
			H	-3.20937900	2.44599100	-3.40384600
			H	-0.83037000	1.80898300	-3.37764700
			H	0.63990400	-0.67673300	-1.30000500
			H	0.93332500	0.56934200	-2.52617400
			H	0.79512400	1.14350400	0.35062800
			H	1.87484500	2.71798200	-1.87213500
			H	0.33113100	2.97833700	-1.02057400
			H	1.86153300	3.15271400	-0.13985200
			H	3.18229800	1.40478000	0.28091000
			H	2.07161400	-1.42780100	0.10018200
			H	2.03124900	-0.38349900	1.51729700
			H	3.95149500	-1.97732400	1.59118300
			H	4.50173200	-0.31123300	1.56945300
			H	5.85149200	-1.65050300	-0.00888900
			H	4.39773000	-2.19017100	-0.83364200
			H	5.39878100	0.68916200	-0.67457800
			H	5.43637100	-0.33568500	-2.09919600
			H	3.50863500	1.21647900	-2.19116100
			H	2.97531300	-0.46386500	-2.12030500
			Br	-0.43755500	1.70940200	2.23345600

Table S11. CSD refcodes of the starting structures, energies (in Hartree) and coordinates of the optimized structures containing Se...Br contacts (from calculation in vacuum)

	CSD Refcode	E(RM062X)	Coordinates			
1	ACIMOP	-5668.498556	C	2.89475600	-2.39968100	0.48549400
			H	2.44938000	-2.72937600	1.42304500
			H	3.97900300	-2.36197500	0.58972500
			H	2.63154000	-3.11692700	-0.29111900
			C	3.15486500	-0.26980900	-1.42543500
			H	2.88080500	0.75148900	-1.68682000
			H	2.89761000	-0.92465800	-2.25656600
			H	4.22866100	-0.31923700	-1.24014600
			C	2.80145300	0.35276800	1.34859200
			H	2.32903200	0.08238800	2.29212000
			H	2.49961100	1.36862400	1.09283800
			H	3.88594600	0.30532300	1.45238600
			C	-0.21364800	0.94820900	-0.04666800
			C	0.12753000	1.65561200	-1.19247000
			H	0.31727900	1.12245600	-2.11490800
			C	-0.50948100	1.62540500	1.13044900
			H	-0.80799200	1.06651400	2.00712500
			C	0.20121200	3.04297100	-1.15245700
			H	0.46255900	3.59220100	-2.04719200
			C	-0.07697600	3.72077300	0.02573300
			H	-0.02479200	4.80066000	0.05479700
C	-0.44063200	3.01056200	1.16335100			
H	-0.67562100	3.53641700	2.07902300			
Br	-2.83133900	-0.92332800	-0.04966600			
Se	-0.25907500	-0.98199100	-0.06988100			
P	2.21452800	-0.77270400	0.04936100			
2	ACINEG	-6243.684807	C	-1.49120400	0.56632000	1.57522900
			C	-2.33044400	1.67289900	1.68492800
			C	-2.70705200	2.13865300	2.93756300
			C	-2.25418100	1.50189700	4.08419600
			C	-1.41914700	0.39666000	3.98030200
			C	-1.03357300	-0.06650400	2.73204800
			C	-2.10025500	-1.50801200	-0.33322100
			C	-3.32010100	-1.64162700	0.32753600
			C	-4.15221700	-2.71363800	0.04011500
			C	-3.77420100	-3.65589200	-0.90707500
			C	-2.55900100	-3.52978100	-1.56591800
			C	-1.72028300	-2.46315100	-1.27731000
			C	-1.36611500	1.13668900	-1.25614300
			C	-2.22884700	0.88929800	-2.32206400
			C	-2.45205500	1.86947800	-3.27989000
			C	-1.81936800	3.09964800	-3.18081300
			C	-0.95853400	3.35161000	-2.11954900
			C	-0.72680700	2.37640800	-1.16376700
			C	1.99722600	0.69592000	-0.00610600
			C	1.97124700	1.44207700	1.16622700
			C	2.34999800	2.77824900	1.14099800
			C	2.76640500	3.36211000	-0.04828500
			H	3.06566600	4.40153600	-0.06505700
			C	2.81101700	2.60653500	-1.21277400
			C	2.42426900	1.27400000	-1.19508200
			P	-0.96555300	-0.12832100	-0.01919700
			Se	1.41321500	-1.14121200	0.00219400
			Br	3.79700400	-1.96427200	0.04494800
			H	-2.69032500	2.17119300	0.79446100
			H	-3.35722200	2.99957700	3.01547300
			H	-2.54870800	1.86778000	5.05856000
			H	-1.06112500	-0.10034200	4.87162400
			H	-0.36744000	-0.91739700	2.65007200

			H	-3.61736500	-0.91117500	1.06885900
			H	-5.09663200	-2.81347100	0.55778700
			H	-4.42428000	-4.49193900	-1.12714700
			H	-2.25796200	-4.26621300	-2.29838100
			H	-0.76684700	-2.37108500	-1.78329600
			H	-2.73084900	-0.06552300	-2.40488900
			H	-3.12481100	1.66914300	-4.10278200
			H	-1.99479700	3.86098600	-3.92885300
			H	-0.45821500	4.30719500	-2.03746500
			H	-0.04858800	2.58133800	-0.34335400
			H	1.65544600	0.98061400	2.09205600
			H	2.32560200	3.35912300	2.05325800
			H	3.14290200	3.05525700	-2.13943500
			H	2.45372300	0.67985700	-2.09816900
3	ADUQUN	-8180.767901	Se	-2.67587800	-1.09776700	0.08139000
			Br	-4.99783400	-1.53551000	-0.16436700
			Br	6.62438900	-0.75756900	-0.03675500
			O	-0.36342000	-0.51448500	0.25418100
			N	0.92322200	1.33388200	-0.01337000
			H	0.88609400	2.31908900	-0.20817700
			C	-2.72273300	0.82086000	0.05443500
			C	-1.50293900	1.51798300	0.09069700
			C	3.80476600	-1.00047100	0.27071600
			H	4.01745200	-2.03584300	0.49469100
			C	-0.26821500	0.70248700	0.12158500
			C	-3.90931400	1.55031900	0.01267500
			H	-4.85630900	1.03538800	-0.02154700
			C	-1.50191600	2.91343200	0.11327500
			H	-0.57359500	3.46500200	0.18552200
			C	2.21805800	0.78157500	-0.00950100
			C	2.49134700	-0.55315500	0.28093400
			H	1.69141800	-1.23613000	0.50839100
			C	4.57802700	1.20045300	-0.31207100
			H	5.38669600	1.87897100	-0.54138700
			C	-2.68275100	3.62592500	0.07712300
			H	-2.66864200	4.70612700	0.09955300
			C	-3.88592900	2.93304300	0.02011500
			H	-4.82157900	3.47503400	-0.01020200
			C	4.83915900	-0.13006500	-0.02424000
			C	3.27062200	1.64847400	-0.30325600
			H	3.06462300	2.68775400	-0.52960800
4	CALROW	-15557.27013	Se	-1.70143100	-0.14844000	0.27954500
			Br	-1.72796900	2.32247100	-0.28386500
			Br	-1.85654400	-2.78467800	0.31359200
			N	-3.37863900	-0.89502400	-1.85357000
			H	-2.59769000	-1.51923700	-1.99762800
			H	-4.24088500	-1.15396200	-2.30645800
			N	-4.46920200	0.37136000	-0.28888600
			C	-3.38158000	-0.23319400	-0.69847700
			C	-5.64091000	0.40914700	-1.15884900
			H	-6.10009700	-0.57855800	-1.23568800
			H	-5.35939500	0.76582400	-2.15008800
			H	-6.36486600	1.09600800	-0.73423800
			C	-4.58683100	1.09857700	0.97348800
			H	-3.75688500	0.85323400	1.62497500
			H	-5.52303300	0.80308800	1.44346700
			H	-4.58351600	2.16953300	0.77673000
			Se	3.11975700	0.14117800	0.78171400
			Br	1.00649300	0.49284300	2.27896600
			Br	4.73248100	-0.27398300	-1.14280800
			N	1.35048600	-1.65358300	-0.38854800
			H	1.69406300	-2.18079000	0.39851700
			H	0.45227700	-1.95302000	-0.74619000

			N	1.33497000	0.43322700	-1.39533300
			C	1.77055700	-0.39983400	-0.48431500
			C	0.51183600	0.01131300	-2.52033700
			H	0.43760000	-1.07095500	-2.56462400
			H	-0.48036600	0.45656500	-2.43880300
			H	0.99101500	0.35722100	-3.43603800
			C	1.73877300	1.84234400	-1.40961000
			H	1.63554100	2.26262000	-0.41319900
			H	2.76887300	1.92818000	-1.75632900
			H	1.06376300	2.36631000	-2.08021400
5	CIDXOD	-7876.894515	C	-0.08953400	0.87000200	-0.36430900
			C	0.18883000	1.59845800	0.79618700
			C	0.39291500	2.97032700	0.71040800
			H	0.59863200	3.53790000	1.61042000
			C	0.32261100	3.61979700	-0.51389800
			H	0.47939000	4.68815100	-0.56830000
			C	0.04779600	2.89263400	-1.66111600
			H	-0.00813900	3.39073200	-2.61938500
			C	-0.15872500	1.52168400	-1.58607500
			H	-0.37344500	0.94934900	-2.47756400
			C	0.29009900	0.91062500	2.12512600
			H	-0.50129800	0.17558300	2.25076100
			H	0.25864400	1.62593200	2.94433800
			N	1.59303000	0.16688900	2.21473600
			Se	-0.39286500	-1.03436000	-0.29221500
			Br	-2.77046000	-0.69989800	0.12682600
			Br	2.48440700	-1.20314500	-0.42292000
			H	1.82098900	-0.38403700	1.30465500
			H	1.60664800	-0.49172900	2.99038300
			H	2.37264200	0.81347600	2.32217400
6	ECIYIA2	-21630.81053	C	-3.91731900	-0.00075100	-0.07179400
			C	-4.37613300	0.78929000	0.96929500
			H	-3.74737600	0.99995600	1.82265700
			C	-5.65229400	1.31888200	0.89837800
			H	-6.03900000	1.92930600	1.70121800
			C	-6.43437500	1.06955800	-0.22153000
			C	-5.96442600	0.29234700	-1.26849800
			H	-6.58981100	0.10905100	-2.12983600
			C	-4.69456500	-0.25778100	-1.19041900
			H	-4.33294500	-0.89224600	-1.98710600
			Se	-2.10590000	-0.69071200	-0.08645700
			Br	-1.82318000	-1.18147000	2.15434900
			Br	-2.90170800	-3.01747000	-0.60562800
			Br	-1.20548500	1.70629100	0.26242800
			Cl	-8.02271700	1.73854900	-0.30843200
			C	3.91731700	0.00073600	0.07179500
			C	4.37614000	-0.78913900	-0.96941400
			H	3.74740800	-0.99960900	-1.82284400
			C	5.65227600	-1.31880300	-0.89854400
			H	6.03899200	-1.92908600	-1.70148700
			C	6.43431100	-1.06974700	0.22145300
			C	5.96435200	-0.29271400	1.26855000
			H	6.58970600	-0.10962600	2.12995500
			C	4.69453200	0.25751600	1.19050600
			H	4.33291400	0.89184400	1.98729800
			Se	2.10590400	0.69076500	0.08650400
			Br	1.82317100	1.18155700	-2.15429200
			Br	2.90180400	3.01751800	0.60563700
			Br	1.20547600	-1.70622600	-0.26243100
			Cl	8.02261900	-1.73882700	0.30829400
7	ECIYUM2	-20910.11212	C	-3.91454700	0.34171200	-0.41339700
			C	-4.94877000	-0.09276700	0.40127700
			H	-4.78583100	-0.87264900	1.13173300

			C	-6.20043200	0.47847300	0.26119100
			H	-7.03213200	0.17775100	0.88148000
			C	-6.38307100	1.45023400	-0.70765500
			C	-5.36242800	1.87857200	-1.53397800
			H	-5.55346100	2.64296500	-2.27279900
			C	-4.10330400	1.32105800	-1.37749100
			H	-3.28144600	1.66499000	-1.98909000
			Br	-1.02580200	1.84723500	-0.17334900
			Br	-1.94059600	-0.80047600	1.93711700
			Br	-3.16231200	-2.75381600	-0.67943200
			F	-7.59253500	1.99501500	-0.84584700
			Se	-2.16762300	-0.48634000	-0.34235500
			C	3.91780900	-0.28611900	-0.42056900
			C	4.72243200	0.13491600	-1.46922200
			H	4.42617400	0.95974300	-2.10144300
			C	5.93334300	-0.50247200	-1.68802000
			H	6.58949700	-0.20698000	-2.49350500
			C	6.30483200	-1.52686700	-0.83900200
			C	5.50970500	-1.94914500	0.21208200
			H	5.84467100	-2.75689500	0.84630900
			C	4.29136100	-1.32665900	0.41575300
			H	3.63867100	-1.65654500	1.21138500
			Br	3.19188600	2.85994300	-0.28801800
			Br	1.94659000	0.58934300	2.04361600
			Br	1.04980400	-1.76120700	-0.41026700
			F	7.47653800	-2.13236000	-1.03790000
			Se	2.18265900	0.55758500	-0.25601300
8	GIHDAF	-10447.05204	Br	5.07022200	1.75613200	-0.00461200
			Se	3.93451400	-1.26077300	0.19588300
			N	2.79541800	-4.07057300	0.12915500
			C	1.27175900	-0.26570900	-0.52685600
			C	2.62295000	-0.53103800	-1.10423400
			H	3.13217200	0.38257700	-1.40362500
			H	2.58686100	-1.24110000	-1.92606500
			C	1.02947600	0.91961100	0.16499400
			H	1.84410800	1.62448200	0.29519400
			C	3.18920800	-2.98649900	0.14471000
			C	-0.23064100	1.18022800	0.68131700
			H	-0.41516300	2.10925900	1.20814400
			Se	-3.93405300	1.26088100	-0.19600600
			N	-2.79392400	4.07021500	-0.12933300
			C	-1.27142400	0.26525500	0.52654500
			C	-2.62263400	0.53048800	1.10389400
			H	-3.13202000	-0.38319900	1.40279800
			H	-2.58664000	1.24015800	1.92606800
			C	-1.02913900	-0.92005600	-0.16529900
			H	-1.84376100	-1.62493000	-0.29550900
			C	-3.18807600	2.98627400	-0.14489900
			C	0.23098200	-1.18067400	-0.68163400
			H	0.41551500	-2.10971400	-1.20844300
			Br	-5.07142100	-1.75573100	0.00505800
9	HOCDOS2	-11064.30265	Se	-2.10642700	-0.45216100	0.27245000
			Br	-1.03418000	1.63630700	1.31584600
			O	-5.01183400	-3.32384200	-0.35775000
			N	-3.13021700	-2.14362900	-0.48920100
			C	-3.79729800	-0.24186100	1.16266500
			C	-4.14582600	0.79538100	2.02716900
			H	-3.43811200	1.57925000	2.24583200
			C	-5.40308000	0.81230800	2.60516900
			H	-5.65524300	1.62435400	3.27441400
			C	-6.34641300	-0.18404400	2.34919400
			H	-7.32057000	-0.14529600	2.81560900
			C	-6.02187300	-1.21514400	1.49524800

			H	-6.72302400	-2.00679800	1.26774800
			C	-4.75700800	-1.23716200	0.90954500
			C	-4.30507200	-2.25274800	0.00316600
			C	-4.21901100	-3.99512300	-1.36477500
			H	-4.70897400	-3.84286400	-2.32631700
			H	-4.19410500	-5.05455700	-1.12197200
			C	-2.81909800	-3.32559600	-1.31165900
			C	-1.79762400	-4.18785800	-0.57907300
			H	-0.87198100	-3.63134600	-0.43500400
			H	-2.18218500	-4.49058300	0.39572700
			H	-1.58018400	-5.08219400	-1.16450700
			C	-2.32562700	-2.91345100	-2.68901500
			H	-1.37382800	-2.38978300	-2.60642300
			H	-2.18100200	-3.79837200	-3.31041400
			H	-3.04771800	-2.25710500	-3.17432500
			Se	2.10642700	0.45216100	-0.27245000
			Br	1.03418000	-1.63630700	-1.31584600
			O	5.01183400	3.32384200	0.35775000
			N	3.13021700	2.14362900	0.48920100
			C	3.79729800	0.24186100	-1.16266500
			C	4.14582600	-0.79538100	-2.02716900
			H	3.43811200	-1.57925000	-2.24583200
			C	5.40308000	-0.81230800	-2.60516900
			H	5.65524300	-1.62435400	-3.27441400
			C	6.34641300	0.18404400	-2.34919400
			H	7.32057000	0.14529600	-2.81560900
			C	6.02187300	1.21514400	-1.49524800
			H	6.72302400	2.00679800	-1.26774800
			C	4.75700800	1.23716200	-0.90954500
			C	4.30507200	2.25274800	-0.00316600
			C	4.21901100	3.99512300	1.36477500
			H	4.70897400	3.84286400	2.32631700
			H	4.19410500	5.05455700	1.12197200
			C	2.81909800	3.32559600	1.31165900
			C	1.79762400	4.18785800	0.57907300
			H	0.87198100	3.63134600	0.43500400
			H	2.18218500	4.49058300	-0.39572700
			H	1.58018400	5.08219400	1.16450700
			C	2.32562700	2.91345100	2.68901500
			H	1.37382800	2.38978300	2.60642300
			H	2.18100200	3.79837200	3.31041400
			H	3.04771800	2.25710500	3.17432500
10	IWODUU	-5459.309385	Br	-2.77901200	-1.28544300	-0.12470400
			C	-0.47891100	1.05668400	-0.01885500
			C	0.66844000	1.74329100	-0.42373600
			C	0.69129200	3.12913700	-0.38426000
			H	1.58945400	3.65166800	-0.69088600
			C	-0.42167800	3.84132300	0.03970500
			H	-0.39856400	4.92205800	0.06423700
			C	-1.55738400	3.15403400	0.43901100
			H	-2.42897700	3.69657200	0.77970100
			C	-1.58945400	1.76564300	0.41625100
			H	-2.47852800	1.23963500	0.73045200
			C	1.84099400	0.93681600	-0.90635600
			H	1.67028400	0.63472900	-1.94360000
			H	2.76216600	1.52980600	-0.87079000
			C	2.43760500	0.00979300	1.24708400
			H	1.75470200	0.74225400	1.67916800
			H	3.42192800	0.49168400	1.18179500
			C	2.50878800	-1.21380500	2.14211900
			H	1.55667100	-1.74359400	2.14444600
			H	2.72594300	-0.90077000	3.16211200
			H	3.29449300	-1.90336000	1.83436800

			C	2.63779200	-1.37602400	-0.78843100
			H	2.14044300	-1.51176700	-1.74934600
			H	2.46292600	-2.28854000	-0.21813600
			C	4.13096300	-1.15404300	-0.98921800
			H	4.32495800	-0.24502200	-1.55931300
			H	4.55676100	-1.99047800	-1.54187200
			H	4.65889500	-1.08027300	-0.03829300
			N	1.94157200	-0.28129400	-0.10605300
			Se	-0.38676000	-0.87182800	-0.07343900
11	KUSSOH	-5553.939258	Br	3.40563700	0.18477600	-0.30785600
			C	-1.60051500	-0.22121700	-0.00437800
			C	-2.48521000	0.77267900	-0.39354400
			C	-1.99837700	-1.53756000	0.14387100
			C	-0.91503200	-2.46612100	0.61813400
			H	-0.92130100	-2.50111000	1.70970900
			H	-1.03534400	-3.48529400	0.24272700
			C	-1.87009800	2.12659100	-0.64148500
			H	-1.55326700	2.18544500	-1.68526600
			H	-2.57157500	2.94567000	-0.45288000
			C	-1.00471100	2.63619500	1.56678200
			H	-1.42449900	3.64676500	1.59672400
			H	-0.10438700	2.59824000	2.17597200
			H	-1.73302500	1.93039800	1.96344100
			C	0.34740100	3.15603100	-0.37495200
			H	0.61560000	2.80859200	-1.36998300
			H	1.24257900	3.11159800	0.24371400
			H	-0.02329500	4.18414200	-0.42046500
			C	0.73095100	-2.30802800	-1.18747400
			H	1.65577600	-1.79864100	-1.45948400
			H	-0.08092900	-1.98889400	-1.83891700
			H	0.85340200	-3.39186300	-1.25300300
			C	1.47406000	-2.39194500	1.11445500
			H	1.50757100	-3.48420500	1.10423100
			H	1.25627000	-2.03576200	2.11886300
			H	2.41832800	-1.96439400	0.77818800
			C	-3.32416600	-1.87329600	-0.08882500
			H	-3.65478300	-2.89885700	0.01905500
			C	-4.23055200	-0.88251800	-0.45176000
			H	-5.26589200	-1.14079000	-0.62476100
			C	-3.81487900	0.43712100	-0.60299000
			H	-4.52637000	1.19786300	-0.89977300
			N	-0.66704000	2.26146400	0.19276100
			N	0.40421300	-1.93555100	0.20388800
			Se	0.23924700	0.19544000	0.23127400
12	PEBPUH	-15126.01906	Br	-3.67580000	1.52400000	-0.74879300
			Se	-1.31357300	-1.38577800	-0.35955000
			Se	-2.63730800	0.18694300	0.82499900
			C	-2.55880100	-2.74689600	-0.55504100
			C	-4.23974100	-0.91527800	0.95827900
			N	-3.26648200	-3.63544600	-0.73432300
			N	-5.18486800	-1.50948100	1.23015700
			Br	-0.29777000	1.46801200	0.37604700
			Se	5.17231600	0.06243100	-0.46727700
			Se	2.96178200	0.71759600	-0.00316000
			C	5.48184900	-0.92522300	1.06055400
			C	2.13161500	-0.75198500	-0.75759500
			N	5.71706900	-1.54771200	1.99785100
			N	1.58514500	-1.65659400	-1.21104900
13	RAGSAT	-10585.96079	Se	-0.00124200	1.66187600	0.90005000
			Br	5.18494000	-2.14071900	-0.21554200
			Br	-5.19342100	-2.05565100	-0.34286400
			Br	0.01911200	3.12353900	-0.89208300
			C	1.48039300	0.53104200	0.44965200

			C	2.68351500	1.12601600	0.09045800
			H	2.76672600	2.19596800	-0.04608900
			C	3.78911900	0.32090500	-0.11412300
			H	4.73262000	0.75843600	-0.40629400
			C	3.68130400	-1.05596400	0.05952400
			C	2.47678600	-1.63744100	0.43518700
			H	2.40845300	-2.70730400	0.56914100
			C	1.36083900	-0.84049500	0.63511500
			H	0.42522500	-1.29458500	0.93019400
			C	-1.48692000	0.55429000	0.49257500
			C	-2.50725100	0.51848500	1.43573300
			H	-2.44651000	1.09050800	2.35239400
			C	-3.61789500	-0.27218100	1.18650600
			H	-4.42264000	-0.32374300	1.90522100
			C	-3.69052300	-0.99298600	0.00115300
			C	-2.66552800	-0.93749700	-0.94497100
			H	-2.74838800	-1.49952400	-1.86386300
			C	-1.55246200	-0.15921700	-0.70110400
			H	-0.75358800	-0.10424000	-1.42952900
14	TAJMEW	-10408.83108	Se	1.13102500	-1.22374400	0.40163400
			Se	-1.13506800	-1.22683400	-0.36743700
			C	1.75403300	0.19971500	-0.74819200
			N	1.96454000	-0.14444900	-2.03423300
			N	1.60233800	1.48161100	-0.43131700
			C	1.57012700	1.91765800	0.95738800
			C	2.12991200	2.47131200	-1.36065300
			C	-1.75856900	0.20541000	0.76927100
			N	-2.00430600	-0.13386300	2.04882700
			N	-1.60017600	1.48402800	0.44846200
			C	-2.13412700	2.48173300	1.36548600
			C	-1.54375600	1.91458200	-0.94157000
			H	2.15332900	-1.12525800	-2.16985800
			H	2.56302300	0.45460400	-2.58322400
			H	1.07051400	1.17854100	1.57361300
			H	1.02653700	2.85994800	1.00736700
			H	2.59556400	2.04282400	1.31381500
			H	1.66981800	2.35680300	-2.34115500
			H	1.89478300	3.46193700	-0.98373500
			H	3.21851300	2.36580400	-1.43233900
			H	-2.19600800	-1.11387800	2.18544200
			H	-2.60901100	0.47057200	2.58476700
			H	-1.69706600	2.36192400	2.35572400
			H	-3.22528800	2.39117600	1.41348800
			H	-1.87688100	3.46852700	0.99300000
			H	-2.56328400	2.04931000	-1.31074900
			H	-0.98865500	2.85030600	-0.98746700
			H	-1.04506500	1.16728300	-1.54854400
			Br	-4.11407200	-0.25460300	-0.37693800
			Br	4.12276300	-0.25609800	0.32821200
15	TAVWUI	-10561.25923	Br	4.14768400	-0.34323000	-0.75450500
			Br	-4.10300000	-0.61473200	0.62740300
			Se	1.12350500	-1.10615200	-0.64765300
			Se	-1.20906100	-1.23425700	0.19351600
			N	1.65191100	1.56015100	0.32282500
			N	2.00232600	0.05911000	1.83828800
			N	-1.63249100	1.62038900	0.25508300
			N	-1.99902400	0.78660500	-1.70402800
			C	1.62968200	0.24205700	0.56634600
			C	2.34536700	1.27099400	2.38436500
			C	2.12967700	2.21036300	1.43448800
			C	1.52074200	2.14475800	-1.00173000
			C	2.25899200	-1.24731400	2.42365300
			C	-1.63637800	0.48321100	-0.45300400

			C	-2.29342400	2.12562200	-1.77530300
			C	-2.06743800	2.64723500	-0.54691700
			C	-1.48314500	1.68278400	1.70061200
			C	-2.25771800	-0.20757200	-2.73422200
			H	2.71086300	1.35781900	3.39066600
			H	2.27819200	3.27407000	1.45034600
			H	1.51939600	3.22601700	-0.89813800
			H	0.59097200	1.81652100	-1.46024900
			H	2.37143100	1.81064000	-1.59853200
			H	2.58548100	-1.10193200	3.44874600
			H	3.04246700	-1.72869100	1.83710500
			H	1.35064600	-1.84403800	2.40428400
			H	-2.63423400	2.58523300	-2.68439700
			H	-2.18053900	3.64899100	-0.17603700
			H	-1.45537400	2.72808600	1.99425000
			H	-0.55952800	1.19162400	1.99755400
			H	-2.33798100	1.17426200	2.14925200
			H	-2.57840800	0.31012000	-3.63287900
			H	-3.04475300	-0.86999200	-2.37334100
			H	-1.35084500	-0.77280700	-2.93431400
15	XATJEH	-8150.862313	Br	-1.51493300	-2.80007500	-0.24832200
			Se	-1.10913200	-0.73717900	1.01985300
			N	1.22666200	1.16376200	-0.58951500
			C	-1.83551700	0.32932800	-0.41328700
			C	-3.17421900	0.69120600	-0.36999900
			C	-3.73363100	1.43368400	-1.40036100
			C	-2.95579500	1.81501000	-2.48237000
			C	-1.61565500	1.45862100	-2.52379900
			C	-1.04141200	0.72007600	-1.49495300
			C	0.41552500	0.35779300	-1.56281200
			C	1.25474000	2.59761700	-0.96230900
			C	2.60630900	0.61285700	-0.32346800
			C	2.54412300	-0.61768200	0.57365800
			C	3.96441400	-1.07382100	0.90966400
			C	4.78043900	-1.34040300	-0.35205900
			C	4.80366400	-0.11143400	-1.25673000
			C	3.38384200	0.33939600	-1.60473400
			H	-3.77493200	0.38484200	0.47475300
			H	-4.77860500	1.70889700	-1.35725800
			H	-3.38771100	2.38692600	-3.29203900
			H	-1.00557600	1.75544200	-3.36903900
			H	0.56074700	-0.69298800	-1.32059600
			H	0.81409900	0.55892700	-2.55607500
			H	0.72622100	1.15597500	0.33878200
			H	1.78146200	2.71982200	-1.90572200
			H	0.23080800	2.94957200	-1.04896800
			H	1.74956400	3.14568500	-0.16568600
			H	3.10567300	1.40926400	0.23521300
			H	2.01024800	-1.42846900	0.07034600
			H	1.98761400	-0.37885900	1.48075200
			H	3.91746200	-1.96663500	1.53225900
			H	4.45884900	-0.30000500	1.50478000
			H	5.79769400	-1.63312500	-0.09072900
			H	4.33798000	-2.17947700	-0.89737700
			H	5.32691600	0.70446700	-0.74918700
			H	5.35463100	-0.31839500	-2.17419200
			H	3.41554400	1.22343200	-2.24436000
			H	2.89052100	-0.45816600	-2.16649300
			Br	-0.27867700	1.73999300	2.15500200

Table S12. CSD refcodes and coordinates of the solid-state (experimental) structures containing Te···I contacts.

	CSD Refcode	Coordinates
1	ATIDIQ	I 9.14550000 9.93500000 -8.98260000
		I 9.07740000 12.63910000 -3.81530000
		Te 10.91860000 12.24850000 -6.70260000
		Te 13.93130000 12.52960000 -11.06780000
		C 12.07120000 12.39920000 -8.41450000
		C 12.74790000 12.46990000 -9.37460000
		C 12.65990000 13.97940000 -12.01510000
		H 12.71230000 14.82820000 -11.52840000
		H 12.95250000 14.11480000 -12.94110000
		H 11.73490000 13.65580000 -12.01000000
		C 12.09410000 13.71000000 -5.68930000
		H 12.05550000 14.55730000 -6.17910000
		H 11.74420000 13.83940000 -4.78390000
		H 13.02420000 13.40450000 -5.63960000
		C 9.43690000 13.58510000 -7.46480000
		H 9.26960000 13.38190000 -8.40930000
		H 8.60730000 13.47670000 -6.95630000
H 9.75550000 14.50760000 -7.38100000		
2	BIPFOV	Te -0.62350000 5.93010000 0.18060000
		C 0.16240000 6.35050000 2.14850000
		C -0.71340000 5.62670000 3.10260000
		C -0.35060000 5.51650000 4.43700000
		C -1.20850000 4.86310000 5.33040000
		C -2.35760000 4.33590000 4.93850000
		C -2.74400000 4.45730000 3.58780000
		C -1.93540000 5.07880000 2.66640000
		C -2.32740000 5.19860000 1.25270000
		C 0.27330000 4.01800000 0.04200000
		Te -4.59140000 7.25850000 -2.17280000
		C -3.14500000 7.85860000 -3.59480000
		C -3.68480000 7.45920000 -4.94320000
		C -3.01840000 7.83940000 -6.11660000
		C -3.51790000 7.45120000 -7.34370000
		C -4.67040000 6.70830000 -7.45100000
		C -5.33790000 6.32970000 -6.25660000
		C -4.83620000 6.69710000 -5.04580000
		C -5.48130000 6.19710000 -3.75580000
		C -5.75230000 9.01530000 -2.48910000
		I -2.29210000 4.42140000 -2.62510000
		I -2.86480000 9.06750000 0.50900000
		I 2.86480000 6.90850000 -0.50900000
		I -8.33520000 6.90850000 -0.50900000
		H 0.03751257 7.39792544 2.32795217
		H 1.13573076 5.90995853 2.20724056
		H 0.57599324 5.92687408 4.78039202
		H -0.92684469 4.78783930 6.35991742
		H -2.98534272 3.82410306 5.63771597
		H -3.68558255 4.05756240 3.27390169
		H -3.08512270 5.95197754 1.19632104
		H -2.52762765 4.21054157 0.89416211
		H 0.82751035 3.81838928 0.93525609
		H -0.48730950 3.27526254 -0.07930233
H 0.93307711 3.99368449 -0.80002311		
H -2.26251119 7.27980565 -3.41841802		
H -3.09726504 8.92729651 -3.57223567		
H -2.12649444 8.42791563 -6.06133862		
H -2.99552122 7.73529897 -8.23325505		
H -5.05348433 6.42345382 -8.40860589		
H -6.23817699 5.75374693 -6.30836291		
H -5.20952350 5.16847953 -3.64188132		

		H	-6.51344607	6.47750644	-3.78656891
		H	-6.61569529	8.99076986	-1.85755678
		H	-5.16419221	9.87821742	-2.25585603
		H	-6.06036890	9.05971099	-3.51282907
3	BIPTEI	I	3.70140000	6.77880000	3.41190000
		I	0.87060000	9.76590000	3.62740000
		I	-0.70780000	8.19120000	6.99240000
		Te	1.56950000	7.55430000	5.10110000
		C	2.93930000	8.51440000	6.45710000
		C	3.50590000	9.69370000	6.10450000
		C	4.39590000	10.29790000	7.03490000
		C	4.62890000	9.72690000	8.26140000
		C	4.04030000	8.53930000	8.57410000
		C	3.17250000	7.88800000	7.70010000
		C	2.52790000	6.60890000	8.08180000
		C	1.76760000	6.52430000	9.24910000
		C	1.12660000	5.33950000	9.58510000
		C	1.25190000	4.24890000	8.77030000
		C	1.97120000	4.27380000	7.63700000
		C	2.63090000	5.47390000	7.26600000
		H	3.32130000	10.10250000	5.22470000
		H	4.82480000	11.15570000	6.81730000
		H	5.22830000	10.15790000	8.89560000
		H	4.23610000	8.12080000	9.45880000
		H	1.69060000	7.31700000	9.81810000
		H	0.60410000	5.30760000	10.38140000
		H	0.80450000	3.42290000	9.01210000
		H	2.05740000	3.46450000	7.06980000
		H	3.16200000	5.51550000	6.45800000
		I	-4.95580000	7.07920000	6.29940000
		I	-2.12500000	4.09210000	6.08390000
		I	-0.54660000	5.66680000	2.71890000
		Te	-2.82390000	6.30370000	4.61030000
		C	-4.19370000	5.34360000	3.25430000
		C	-4.76020000	4.16430000	3.60680000
		C	-5.65030000	3.56010000	2.67640000
		C	-5.88320000	4.13110000	1.44990000
		C	-5.29470000	5.31870000	1.13720000
		C	-4.42680000	5.97000000	2.01120000
		C	-3.78230000	7.24910000	1.62960000
		C	-3.02200000	7.33370000	0.46230000
		C	-2.38100000	8.51850000	0.12620000
		C	-2.50630000	9.60910000	0.94100000
		C	-3.22550000	9.58420000	2.07430000
		C	-3.88530000	8.38410000	2.44530000
		H	-4.57570000	3.75550000	4.48660000
		H	-6.07920000	2.70230000	2.89400000
		H	-6.48270000	3.70010000	0.81580000
		H	-5.49050000	5.73720000	0.25250000
		H	-2.94500000	6.54100000	-0.10680000
		H	-1.85850000	8.55040000	-0.67010000
		H	-2.05890000	10.43510000	0.69920000
		H	-3.31180000	10.39350000	2.64150000
		H	-4.41640000	8.34250000	3.25330000
4	CIFLEI	Te	5.84200000	0.00000000	0.00000000
		I	8.76380000	0.14870000	-0.11410000
		C	5.75900000	1.57500000	1.43660000
		C	6.71950000	1.60070000	2.46230000
		C	6.71710000	2.68380000	3.40950000
		C	5.79290000	3.65830000	3.27600000
		C	4.83720000	3.65710000	2.25130000
		C	4.85350000	2.59850000	1.33980000
		H	7.37730000	0.90900000	2.52350000

		H	7.32240000	2.69550000	4.13650000
		H	5.81750000	4.40490000	3.89080000
		H	4.16420000	4.33940000	2.18810000
		H	4.21910000	2.59150000	0.61380000
		I	2.92020000	-0.14870000	-0.11410000
		C	5.92500000	-1.57500000	1.43660000
		C	4.96450000	-1.60070000	2.46230000
		C	6.83050000	-2.59850000	1.33980000
		C	4.96690000	-2.68380000	3.40950000
		H	4.30670000	-0.90900000	2.52350000
		C	6.84680000	-3.65710000	2.25130000
		H	7.46490000	-2.59150000	0.61380000
		C	5.89110000	-3.65830000	3.27600000
		H	4.36160000	-2.69550000	4.13650000
		H	7.51980000	-4.33940000	2.18810000
		H	5.86650000	-4.40490000	3.89080000
		Te	5.84200000	5.84200000	-2.54900000
		I	5.69330000	8.76380000	-2.66310000
		C	4.26700000	5.75900000	-1.11240000
		C	4.24130000	6.71950000	-0.08670000
		C	3.15820000	6.71710000	0.86050000
		C	2.18370000	5.79290000	0.72700000
		C	2.18490000	4.83720000	-0.29770000
		C	3.24350000	4.85350000	-1.20920000
		H	4.93300000	7.37730000	-0.02550000
		H	3.14650000	7.32240000	1.58750000
		H	1.43710000	5.81750000	1.34180000
		H	1.50260000	4.16420000	-0.36090000
		H	3.25050000	4.21910000	-1.93520000
		I	5.99070000	2.92020000	-2.66310000
		C	7.41700000	5.92500000	-1.11240000
		C	7.44270000	4.96450000	-0.08670000
		C	8.44050000	6.83050000	-1.20920000
		C	8.52580000	4.96690000	0.86050000
		H	6.75100000	4.30670000	-0.02550000
		C	9.49910000	6.84680000	-0.29770000
		H	8.43350000	7.46490000	-1.93520000
		C	9.50030000	5.89110000	0.72700000
		H	8.53750000	4.36160000	1.58750000
		H	10.18140000	7.51980000	-0.36090000
		H	10.24690000	5.86650000	1.34180000
5	CIFLOS	Te	7.70030000	4.42240000	4.43350000
		I	9.95750000	2.56630000	5.61550000
		I	9.95750000	6.32620000	3.25510000
		I	5.78290000	2.86710000	5.70090000
		I	5.88170000	6.21850000	3.31130000
		C	7.78480000	3.20090000	2.65660000
		C	7.96000000	3.80020000	1.45060000
		C	8.05160000	3.02680000	0.29440000
		C	7.92220000	1.62890000	0.44960000
		C	7.68720000	1.05100000	1.67050000
		C	7.65530000	1.84710000	2.77980000
		H	7.93610000	4.75160000	1.37080000
		H	8.16710000	3.35860000	-0.63840000
		H	8.04960000	1.00310000	-0.27930000
		H	7.58160000	0.07950000	1.73700000
		H	7.44220000	1.45220000	3.67540000
		Te	12.21470000	4.42240000	4.43350000
		I	14.13210000	2.86710000	5.70090000
		I	14.03330000	6.21850000	3.31130000
		C	12.13020000	3.20090000	2.65660000
		C	11.95500000	3.80020000	1.45060000
		C	12.25970000	1.84710000	2.77980000

		C	11.86340000	3.02680000	0.29440000
		H	11.97890000	4.75160000	1.37080000
		C	12.22780000	1.05100000	1.67050000
		H	12.47280000	1.45220000	3.67540000
		C	11.99280000	1.62890000	0.44960000
		H	11.74790000	3.35860000	-0.63840000
		H	12.33340000	0.07950000	1.73700000
		H	11.86540000	1.00310000	-0.27930000
6	CIFLUY	Te	2.99020000	3.79870000	0.00000000
		I	4.45550000	5.77950000	2.17240000
		I	1.80020000	2.29740000	2.01480000
		C	4.74070000	2.59960000	0.00000000
		C	5.32160000	2.22280000	1.19530000
		C	6.52110000	1.49690000	1.20070000
		C	7.05220000	1.17090000	0.00000000
		H	4.90640000	2.46550000	2.02180000
		H	6.92740000	1.23100000	2.02450000
		H	7.86480000	0.67740000	0.00000000
		I	4.45550000	5.77950000	-2.17240000
		I	1.80020000	2.29740000	-2.01480000
		Te	5.92080000	7.76030000	0.00000000
		C	5.32160000	2.22280000	-1.19530000
		C	6.52110000	1.49690000	-1.20070000
		I	7.11080000	9.26160000	-2.01480000
		I	7.11080000	9.26160000	2.01480000
		C	4.17030000	8.95940000	0.00000000
		H	4.90640000	2.46550000	-2.02180000
		H	6.92740000	1.23100000	-2.02450000
		C	3.58940000	9.33620000	-1.19530000
		C	3.58940000	9.33620000	1.19530000
		C	2.38990000	10.06210000	-1.20070000
		H	4.00460000	9.09350000	-2.02180000
		C	2.38990000	10.06210000	1.20070000
		H	4.00460000	9.09350000	2.02180000
		C	1.85880000	10.38810000	0.00000000
		H	1.98360000	10.32800000	-2.02450000
		H	1.98360000	10.32800000	2.02450000
		H	1.04620000	10.88160000	0.00000000
7	GEHDON	I	3.82650000	6.79830000	8.30010000
		I	2.90720000	2.43950000	4.49980000
		Te	3.41180000	4.55310000	6.40930000
		I	1.45860000	3.50210000	8.21230000
		S	5.47230000	5.36790000	4.71700000
		C	2.78430000	5.90260000	1.87260000
		H	2.73360000	6.74320000	1.39160000
		H	1.89360000	5.52520000	1.94800000
		C	3.71290000	4.95320000	1.19490000
		H	3.27650000	4.10680000	1.00770000
		H	4.05530000	5.32540000	0.36780000
		C	4.94590000	3.42800000	7.40670000
		N	3.38140000	6.08280000	3.16720000
		H	3.03830000	6.57200000	3.78550000
		C	4.49430000	5.42630000	3.30320000
		C	6.83330000	2.06250000	8.84950000
		H	7.46630000	1.60000000	9.35060000
		C	5.66120000	1.42880000	8.45750000
		H	5.51170000	0.54120000	8.69320000
		C	6.11120000	4.06280000	7.76770000
		H	6.26760000	4.94780000	7.52520000
		C	4.72430000	2.10890000	7.72600000
		H	3.94650000	1.68380000	7.44710000
		C	7.05340000	3.34740000	8.50460000
		H	7.84530000	3.76230000	8.76060000

		N	4.77470000	4.79510000	2.18370000
		H	5.49460000	4.34450000	2.05170000
		I	-0.01690000	5.89020000	5.17150000
		I	0.90240000	10.24910000	8.97180000
		Te	0.39770000	8.13550000	7.06240000
		I	2.35090000	9.18650000	5.25930000
		S	-1.66280000	7.32060000	8.75470000
		C	1.02520000	6.78600000	11.59910000
		H	1.07600000	5.94540000	12.08000000
		H	1.91590000	7.16330000	11.52360000
		C	0.09660000	7.73530000	12.27670000
		H	0.53310000	8.58170000	12.46390000
		H	-0.24570000	7.36310000	13.10380000
		C	-1.13630000	9.26050000	6.06490000
		N	0.42820000	6.60570000	10.30440000
		H	0.77130000	6.11650000	9.68610000
		C	-0.68470000	7.26230000	10.16840000
		C	-3.02380000	10.62600000	4.62210000
		H	-3.65670000	11.08860000	4.12100000
		C	-1.85170000	11.25970000	5.01410000
		H	-1.70210000	12.14740000	4.77840000
		C	-2.30170000	8.62570000	5.70390000
		H	-2.45800000	7.74070000	5.94640000
		C	-0.91470000	10.57960000	5.74560000
		H	-0.13690000	11.00470000	6.02450000
		C	-3.24380000	9.34110000	4.96700000
		H	-4.03570000	8.92620000	4.71100000
		N	-0.96510000	7.89350000	11.28790000
		H	-1.68500000	8.34400000	11.41990000
8	GIPRUT	C	4.50100000	-0.08220000	3.94650000
		C	3.13830000	-0.35390000	4.18260000
		C	2.30790000	-0.58900000	3.08830000
		H	1.40770000	-0.76970000	3.22850000
		C	2.80350000	-0.55740000	1.79080000
		H	2.23690000	-0.72040000	1.07260000
		C	4.14570000	-0.27930000	1.56770000
		H	4.47070000	-0.24900000	0.69640000
		C	5.01460000	-0.04420000	2.63950000
		C	2.55130000	-0.36270000	5.56050000
		C	2.62030000	-1.51920000	6.35560000
		C	2.08770000	-1.48000000	7.64740000
		H	2.13190000	-2.24340000	8.17590000
		C	1.49560000	-0.33870000	8.16430000
		C	1.40790000	0.78110000	7.34550000
		H	0.99890000	1.54830000	7.67370000
		C	1.91550000	0.78740000	6.04310000
		C	3.25760000	-2.78060000	5.84400000
		H	3.56990000	-2.64030000	4.94740000
		H	2.61110000	-3.49090000	5.85010000
		H	3.99740000	-3.01700000	6.40840000
		C	0.96690000	-0.30840000	9.58380000
		H	0.59320000	0.55740000	9.76730000
		H	1.68450000	-0.48410000	10.19670000
		H	0.28640000	-0.97830000	9.68690000
		C	1.75500000	2.01720000	5.19170000
		H	2.15610000	1.86550000	4.33300000
		H	2.18620000	2.76040000	5.61950000
		H	0.82110000	2.20930000	5.07940000
		C	6.45490000	0.26290000	2.36400000
		C	6.82820000	1.57480000	2.05270000
		C	8.18050000	1.85790000	1.83730000
		H	8.43370000	2.73260000	1.64460000
		C	9.15190000	0.87840000	1.90080000

		C	8.75830000	-0.42340000	2.17560000
		H	9.39980000	-1.09580000	2.19990000
		C	7.42460000	-0.74820000	2.41420000
		C	5.80830000	2.67320000	1.96010000
		H	6.24690000	3.49850000	1.73860000
		H	5.35910000	2.76540000	2.80220000
		H	5.16770000	2.45830000	1.27740000
		C	10.61500000	1.22470000	1.72650000
		H	11.14460000	0.42590000	1.79930000
		H	10.88080000	1.84780000	2.40620000
		H	10.74980000	1.61910000	0.86170000
		C	7.04000000	-2.17010000	2.74300000
		H	6.09110000	-2.22200000	2.87950000
		H	7.49290000	-2.44690000	3.54400000
		H	7.29220000	-2.74650000	2.01780000
		Te	5.81920000	0.16860000	5.60080000
		I	5.40960000	2.77540000	6.04630000
9	GOCROI	Te	0.85750000	1.85230000	6.87260000
		N	0.59300000	4.36840000	9.23420000
		N	0.41450000	3.05900000	9.48980000
		N	0.16680000	2.90290000	10.76990000
		C	1.77840000	1.64350000	4.95520000
		H	1.78550000	0.69840000	4.69740000
		H	2.69830000	1.97840000	4.99650000
		H	1.27270000	2.15920000	4.29240000
		C	0.18520000	4.14630000	11.35570000
		C	-0.05590000	4.52040000	12.67870000
		H	-0.24440000	3.88010000	13.35340000
		C	-0.00430000	5.88890000	12.95240000
		H	-0.16720000	6.18950000	13.83950000
		C	0.28160000	6.83620000	11.94820000
		H	0.30870000	7.75700000	12.18180000
		C	0.52320000	6.47510000	10.64780000
		H	0.72450000	7.11540000	9.97540000
		C	0.45320000	5.09960000	10.37180000
		C	0.73290000	4.81050000	7.85460000
		H	1.13620000	5.71400000	7.84520000
		H	-0.16640000	4.87580000	7.44550000
		C	1.58130000	3.88620000	7.02690000
		H	2.49190000	3.86600000	7.41450000
		H	1.65470000	4.26250000	6.11420000
		C	2.39960000	0.91630000	7.99940000
		C	1.98380000	0.16410000	9.10990000
		H	1.06830000	0.14050000	9.36240000
		C	2.93650000	-0.54420000	9.83130000
		H	2.66860000	-1.06010000	10.58360000
		C	4.27820000	-0.50620000	9.46490000
		H	4.92050000	-0.99760000	9.96430000
		C	4.67910000	0.25210000	8.36800000
		H	5.59620000	0.27960000	8.12200000
		C	3.73600000	0.97330000	7.62850000
		H	4.00630000	1.49480000	6.88270000
		I	-1.70190000	3.39670000	5.05020000
		I	0.21110000	-1.60490000	6.25790000
10	LADXEV	Te	10.05590000	4.44810000	1.32000000
		I	12.88020000	5.56400000	1.62420000
		I	9.28040000	5.69590000	3.63630000
		I	7.47910000	3.41140000	0.78760000
		C	10.48400000	1.42610000	1.67330000
		H	10.03780000	1.39880000	0.85690000
		O	9.10970000	6.94010000	0.19660000
		C	10.69200000	2.60470000	2.28400000
		C	11.34970000	2.69720000	3.52210000

		H	11.48150000	3.51580000	3.94230000
		C	7.83010000	7.60300000	0.36320000
		H	7.87240000	8.24290000	1.09100000
		H	7.13540000	6.95510000	0.55980000
		C	10.92930000	0.25440000	2.25400000
		H	10.79400000	-0.56070000	1.82630000
		C	11.58460000	0.30280000	3.48460000
		H	11.87190000	-0.48500000	3.88680000
		C	11.80210000	1.48770000	4.09540000
		H	12.25770000	1.50790000	4.90570000
		C	7.54440000	8.29930000	-0.92740000
		H	7.29860000	9.22450000	-0.77140000
		H	6.82200000	7.85830000	-1.40160000
		C	8.84370000	8.21300000	-1.71980000
		H	8.66250000	8.03340000	-2.65620000
		H	9.34280000	9.04220000	-1.65230000
		C	9.56100000	7.14790000	-1.14050000
		H	10.50770000	7.36090000	-1.13600000
		H	9.43010000	6.34510000	-1.66130000
		Te	13.77850000	4.35470000	-1.32000000
		I	10.95420000	3.23880000	-1.62420000
		I	14.55400000	3.10690000	-3.63630000
		I	16.35530000	5.39140000	-0.78760000
		C	13.35040000	7.37670000	-1.67330000
		H	13.79660000	7.40400000	-0.85690000
		O	14.72470000	1.86270000	-0.19660000
		C	13.14240000	6.19810000	-2.28400000
		C	12.48470000	6.10560000	-3.52210000
		H	12.35290000	5.28700000	-3.94230000
		C	16.00430000	1.19980000	-0.36320000
		H	15.96200000	0.55990000	-1.09100000
		H	16.69900000	1.84770000	-0.55980000
		C	12.90510000	8.54840000	-2.25400000
		H	13.04040000	9.36350000	-1.82630000
		C	12.24980000	8.50000000	-3.48460000
		H	11.96250000	9.28780000	-3.88680000
		C	12.03230000	7.31510000	-4.09540000
		H	11.57670000	7.29490000	-4.90570000
		C	16.29000000	0.50350000	0.92740000
		H	16.53580000	-0.42170000	0.77140000
		H	17.01240000	0.94450000	1.40160000
		C	14.99070000	0.58980000	1.71980000
		H	15.17190000	0.76940000	2.65620000
		H	14.49160000	-0.23940000	1.65230000
		C	14.27340000	1.65490000	1.14050000
		H	13.32670000	1.44190000	1.13600000
		H	14.40430000	2.45770000	1.66130000
11	MECGOR	I	6.48410000	1.91920000	10.11250000
		I	3.12050000	-0.50500000	10.04410000
		I	4.07150000	5.28600000	10.43950000
		I	0.68690000	2.81170000	10.36780000
		Te	3.60580000	2.41330000	10.17770000
		C	3.51340000	2.58670000	8.02750000
		C	2.69490000	3.54290000	7.45750000
		H	2.20460000	4.12660000	7.98970000
		C	2.62280000	3.61060000	6.08610000
		H	2.05830000	4.23620000	5.69270000
		C	3.35720000	2.78560000	5.28950000
		H	3.31580000	2.86630000	4.36390000
		C	4.14850000	1.84750000	5.85830000
		H	4.63270000	1.26850000	5.31510000
		C	4.25330000	1.73180000	7.24190000
		H	4.80890000	1.09180000	7.62560000

		I	1.23380000	4.94370000	14.24650000
		I	4.59740000	7.36800000	14.31490000
		I	3.64640000	1.57700000	13.91940000
		I	7.03100000	4.05130000	13.99120000
		Te	4.11210000	4.44970000	14.18130000
		C	4.20450000	4.27620000	16.33150000
		C	5.02300000	3.32010000	16.90150000
		H	5.51330000	2.73640000	16.36920000
		C	5.09510000	3.25240000	18.27290000
		H	5.65960000	2.62680000	18.66630000
		C	4.36070000	4.07740000	19.06940000
		H	4.40210000	3.99670000	19.99510000
		C	3.56940000	5.01550000	18.50060000
		H	3.08520000	5.59450000	19.04380000
		C	3.46460000	5.13120000	17.11700000
		H	2.90900000	5.77110000	16.73340000
12	TUPWIK	I	5.50690000	-1.21500000	13.88450000
		I	0.81180000	-1.18100000	10.42430000
		Te	3.15090000	-1.22710000	12.13400000
		O	3.06130000	1.92170000	13.17570000
		O	4.44820000	-0.76800000	9.63470000
		C	3.75870000	0.63440000	11.35090000
		C	3.63080000	1.88720000	11.92870000
		C	4.07470000	3.00640000	11.25960000
		C	4.66300000	2.85780000	10.01880000
		C	4.81900000	1.63500000	9.42090000
		C	4.37420000	0.51240000	10.09470000
		C	2.91930000	3.18720000	13.80450000
		C	5.10330000	-1.01210000	8.39390000
		C	1.92300000	-0.64830000	13.75650000
		H	3.98040000	3.86540000	11.65460000
		H	4.96420000	3.63390000	9.56030000
		H	5.22820000	1.55210000	8.56590000
		H	2.51620000	3.07780000	14.65800000
		H	2.37220000	3.74560000	13.26550000
		H	3.77510000	3.58670000	13.90830000
		H	4.66770000	-0.52510000	7.70460000
		H	6.01030000	-0.73460000	8.45280000
		H	5.06910000	-1.94020000	8.19720000
		H	2.43830000	-0.14050000	14.37150000
		H	1.58320000	-1.42200000	14.19020000
		H	1.20020000	-0.12090000	13.43740000
		I	1.70580000	-4.54220000	13.88450000
		I	-2.98930000	-4.57610000	10.42430000
		Te	-0.65020000	-4.53010000	12.13400000
		O	-0.73970000	-7.67890000	13.17570000
		O	0.64710000	-4.98910000	9.63470000
		C	-0.04230000	-6.39160000	11.35090000
		C	-0.17020000	-7.64430000	11.92870000
		C	0.27370000	-8.76350000	11.25960000
		C	0.86190000	-8.61500000	10.01880000
		C	1.01800000	-7.39220000	9.42090000
		C	0.57320000	-6.26950000	10.09470000
		C	-0.88170000	-8.94430000	13.80450000
		C	1.30230000	-4.74500000	8.39390000
		C	-1.87800000	-5.10890000	13.75650000
		H	0.17940000	-9.62250000	11.65460000
		H	1.16310000	-9.39110000	9.56030000
		H	1.42720000	-7.30930000	8.56590000
		H	-1.28480000	-8.83490000	14.65800000
		H	-1.42890000	-9.50280000	13.26550000
		H	-0.02590000	-9.34390000	13.90830000
		H	0.86660000	-5.23210000	7.70460000

		H	2.20920000	-5.02250000	8.45280000
		H	1.26800000	-3.81700000	8.19720000
		H	-1.36270000	-5.61670000	14.37150000
		H	-2.21780000	-4.33510000	14.19020000
		H	-2.60090000	-5.63620000	13.43740000
13	WOPYIM	Te	16.57750000	1.62020000	13.03370000
		I	16.60420000	-1.28530000	12.33010000
		I	16.53060000	4.42360000	13.52020000
		C	14.48530000	1.66420000	12.65270000
		C	13.96410000	1.62850000	11.38650000
		H	14.53800000	1.54390000	10.63450000
		C	11.77170000	1.82780000	12.29140000
		H	10.83350000	1.90870000	12.16570000
		C	13.65570000	1.72820000	13.74370000
		H	14.01870000	1.70750000	14.62130000
		C	17.25740000	2.01590000	11.06410000
		H	16.89310000	2.87340000	10.76020000
		H	16.95550000	1.30320000	10.46510000
		H	18.23620000	2.05540000	11.05830000
		C	12.28780000	1.82220000	13.55860000
		H	11.70790000	1.88050000	14.30960000
		C	12.58520000	1.71870000	11.21120000
		H	12.21560000	1.70560000	10.33650000
14	WUGVUQ	Te	3.31200000	4.88940000	1.98800000
		I	6.27270000	5.19020000	1.74490000
		I	2.96750000	7.83360000	1.78540000
		I	0.45360000	4.50540000	2.03080000
		I	3.72930000	2.00320000	2.14300000
		C	3.37190000	5.07660000	4.13630000
		C	4.20720000	5.99590000	4.71360000
		H	4.77870000	6.51110000	4.19010000
		C	2.54730000	4.28090000	4.88880000
		H	2.00990000	3.63820000	4.48450000
		C	4.18440000	6.14510000	6.10870000
		H	4.74280000	6.76400000	6.52000000
		C	2.52860000	4.45290000	6.27460000
		H	1.96090000	3.93580000	6.80040000
		C	3.34170000	5.37980000	6.85650000
		H	3.32030000	5.49110000	7.77960000
		Te	6.85370000	9.04710000	1.64270000
		C	7.76310000	10.95740000	1.91390000
		H	7.13960000	11.55160000	2.33690000
		H	8.01610000	11.31580000	1.05860000
		H	8.54240000	10.86520000	2.46540000
		C	8.53680000	8.17010000	0.73850000
		H	8.51370000	8.33450000	-0.20800000
		H	8.53050000	7.22410000	0.89970000
		H	9.33550000	8.55220000	1.11000000
		C	7.25270000	8.48760000	3.64560000
		C	6.44990000	9.05230000	4.62010000
		H	5.72420000	9.58560000	4.38870000
		C	8.30760000	7.67480000	3.99150000
		H	8.83860000	7.28590000	3.33240000
		C	8.56610000	7.44560000	5.32350000
		H	9.28200000	6.90000000	5.55950000
		C	6.75910000	8.79940000	5.95910000
		H	6.24320000	9.18820000	6.62750000
		C	7.80630000	7.99130000	6.30500000
		H	7.99410000	7.81930000	7.20000000
15	YODVUK	I	0.03730000	-0.42520000	2.19980000
		Te	-0.44250000	4.51340000	2.31360000
		C	-0.85460000	2.44660000	2.77460000
		C	0.09490000	1.69060000	2.28640000

		C	1.32540000	2.22960000	1.61490000
		H	1.29730000	2.00360000	0.67150000
		H	2.10900000	1.80700000	1.99810000
		C	1.44820000	3.74620000	1.76540000
		H	1.73670000	4.14170000	0.92700000
		H	2.10340000	3.96090000	2.44710000
		C	-2.11930000	2.12460000	3.45500000
		C	-2.13310000	1.17980000	4.46290000
		H	-1.34250000	0.76730000	4.72840000
		C	-3.34790000	0.84530000	5.08130000
		H	-3.37180000	0.19780000	5.74770000
		C	-4.47160000	1.46800000	4.70310000
		H	-5.27560000	1.23070000	5.10660000
		C	-4.47390000	2.42400000	3.75970000
		H	-5.26220000	2.86590000	3.53970000
		C	-3.28450000	2.74610000	3.11480000
		H	-3.28430000	3.39140000	2.44450000
		C	0.02180000	5.08310000	4.29210000
		C	-0.43220000	6.29450000	4.76510000
		H	-0.95620000	6.84040000	4.22510000
		C	-0.10560000	6.69570000	6.05000000
		H	-0.40180000	7.51620000	6.37370000
		C	0.65100000	5.88430000	6.83400000
		H	0.86620000	6.15100000	7.69900000
		C	1.09200000	4.69660000	6.37370000
		H	1.61870000	4.15640000	6.91750000
		C	0.76320000	4.27740000	5.09770000
		H	1.04880000	3.44670000	4.79170000
		I	0.96610000	7.36070000	1.25840000
16	ZIQPEU	Te	1.33230000	2.09000000	15.18170000
		I	1.14040000	-0.71950000	15.39730000
		C	1.43270000	4.46210000	13.22390000
		C	0.58020000	5.21480000	15.37670000
		C	2.95970000	4.99420000	15.02000000
		N	1.63790000	4.46510000	14.70290000
		C	2.09010000	3.28410000	12.61200000
		C	2.67460000	3.37380000	11.28520000
		C	3.21550000	2.26330000	10.71610000
		C	3.28820000	1.06110000	11.34540000
		C	2.70710000	0.95730000	12.64370000
		C	2.15950000	2.07280000	13.26990000
		C	3.20330000	2.03150000	16.17720000
		C	3.17590000	2.19280000	17.55790000
		C	4.35960000	2.15040000	18.28550000
		C	5.56990000	1.94490000	17.63400000
		C	5.59730000	1.78360000	16.25330000
		C	4.41360000	1.82700000	15.52570000
		H	0.48310000	4.44190000	13.02740000
		H	1.80320000	5.27330000	12.84190000
		H	0.64180000	6.14190000	15.13570000
		H	0.67940000	5.12920000	16.32780000
		H	-0.27630000	4.86720000	15.11030000
		H	3.00530000	5.91620000	14.75840000
		H	3.62590000	4.49430000	14.54600000
		H	3.11380000	4.91760000	15.96480000
		H	2.68190000	4.18400000	10.82860000
		H	3.55370000	2.32880000	9.85220000
		H	3.70410000	0.33150000	10.94440000
		H	2.69050000	0.13400000	13.07650000
		H	2.36740000	2.32980000	17.99390000
		H	4.34220000	2.25830000	19.20970000
		H	6.36180000	1.91660000	18.12070000
		H	6.40580000	1.64660000	15.81730000

	H	4.43360000	1.71810000	14.60150000
	I	-1.74260000	2.23610000	13.29050000
	I	-0.56610000	2.80240000	18.41390000

Table S13. CSD refcodes of the starting structures, energies (in Hartree) and coordinates of the optimized structures containing Te···I contacts(from calculation in dichloromethane).

	CSD Refcode	E(RM062X), Hartree	Coordinates
1	ATIDIQ	-1327.20188221	I -0.13746500 2.80479600 -0.00161300 I -4.19052300 -0.70427600 -0.11647800 Te -0.87303500 -0.64277400 -0.17420800 Te 4.43404300 -0.98173900 0.02653700 C 1.19038200 -0.79276100 -0.01467700 C 2.39948500 -0.87496300 -0.00870100 C 4.71967800 1.08999100 -0.40987300 H 4.26214600 1.68287400 0.37374200 H 5.79427900 1.25090300 -0.43095700 H 4.28357400 1.31321800 -1.37673600 C -1.01596300 -2.75810100 0.01206500 H -0.43683900 -3.06311800 0.87819200 H -2.06811300 -2.99822800 0.12467900 H -0.60957900 -3.19513600 -0.89549100 C -1.18092600 -0.22554500 1.87443700 H -0.20703600 -0.03548800 2.31377700 H -1.81505400 0.65235800 1.91957000 H -1.66838900 -1.09199400 2.31140400
2	BIPFOV	-2425.95354786	Te -2.10363500 -0.03871100 -0.56773900 C -3.63306900 1.17635700 0.27596300 C -3.32210600 2.59897000 -0.10625700 C -4.22871900 3.62199900 0.16852400 C -3.93744200 4.93120500 -0.17690200 C -2.73282400 5.23119300 -0.80490100 C -1.82870200 4.21982200 -1.08357700 C -2.11467400 2.89997400 -0.73682300 C -1.12782800 1.80094900 -1.02828300 C -3.06154000 -0.11631200 -2.45588400 Te 2.11164100 -0.00725500 0.57345200 C 1.34207400 -1.91671100 1.12648400 C 2.43790600 -2.91566400 0.86424100 C 2.31873800 -4.23425700 1.30081900 C 3.32645200 -5.15114100 1.05125900 C 4.46886200 -4.75597500 0.36298200 C 4.59542500 -3.44675700 -0.07143200 C 3.58362500 -2.51931900 0.17266700 C 3.71412300 -1.09692700 -0.30437300 C 3.14236600 0.23257700 2.40810700 I 0.70081500 -1.22899300 -2.59687500 I -0.69845300 0.99092200 2.68463100 I -4.63479300 -2.47849900 0.26796600 I 4.23549200 2.68322100 -0.48434500 H -3.61191800 1.01604400 1.35183600 H -4.58387300 0.82107100 -0.11701300 H -5.16490600 3.38417300 0.65766700 H -4.64721100 5.71766300 0.04173900 H -2.50053400 6.25210200 -1.07645900 H -0.88904800 4.44859100 -1.57030500 H -0.24045200 1.87156700 -0.40168600 H -0.82023800 1.76179500 -2.07181100 H -3.42235500 0.88391800 -2.68456800 H -2.32465800 -0.44592500 -3.18202500 H -3.88101100 -0.82361900 -2.37190600 H 0.46060700 -2.09929800 0.51301700

			H	1.04265800	-1.86680200	2.17164800
			H	1.42806000	-4.53662100	1.83688000
			H	3.22386100	-6.17199100	1.39383100
			H	5.25960700	-5.46786400	0.16808300
			H	5.48379400	-3.13495900	-0.60610100
			H	3.60525600	-1.00423400	-1.38317700
			H	4.64312700	-0.62080000	0.00368300
			H	3.86880300	1.02733000	2.26652800
			H	2.40716900	0.49712000	3.16197900
			H	3.62868900	-0.71152100	2.64238700
3	BIPTEI	-3247.17839335	I	-3.61373400	2.04518800	1.88517300
			I	-1.74992300	2.30479900	-1.64045200
			I	-0.88409100	-1.57474900	-1.76533000
			Te	-2.23325900	0.28862500	0.07036500
			C	-4.10518100	-0.40125000	-0.66097500
			C	-4.90080500	0.39886700	-1.46679100
			C	-6.08649900	-0.11416400	-1.97080600
			C	-6.46156300	-1.41699900	-1.67105900
			C	-5.66418400	-2.20225100	-0.85415600
			C	-4.47530500	-1.70617600	-0.32046000
			C	-3.64048300	-2.54897400	0.56668000
			C	-3.23296900	-3.81749900	0.15536100
			C	-2.39217000	-4.57449700	0.95400200
			C	-1.94584800	-4.07597400	2.17424200
			C	-2.36635000	-2.82787100	2.60571600
			C	-3.22173600	-2.07143100	1.81074400
			H	-4.60686300	1.41020600	-1.71180000
			H	-6.71026900	0.50417900	-2.60088200
			H	-7.38302100	-1.81993400	-2.06802500
			H	-5.96583200	-3.21087400	-0.60349800
			H	-3.54943500	-4.18984800	-0.81019900
			H	-2.06877500	-5.55019000	0.61800200
			H	-1.28046800	-4.66649400	2.78926600
			H	-2.04674900	-2.44351700	3.56465200
			H	-3.61078600	-1.13141300	2.18898800
			I	3.61373400	-2.04528300	-1.88515200
			I	1.74994500	-2.30472300	1.64044300
			I	0.88411000	1.57472800	1.76529300
			Te	2.23326500	-0.28864100	-0.07041000
			C	4.10516000	0.40121700	0.66091800
			C	4.90075600	-0.39892600	1.46673200
			C	6.08644100	0.11408600	1.97078200
			C	6.46150600	1.41693400	1.67109300
			C	5.66414000	2.20222000	0.85420900
			C	4.47527800	1.70616300	0.32046000
			C	3.64045500	2.54902600	-0.56662600
			C	3.23291700	3.81751300	-0.15521000
			C	2.39212500	4.57456900	-0.95380700
			C	1.94582300	4.07614100	-2.17409300
			C	2.36636300	2.82808500	-2.60566900
			C	3.22176500	2.07160300	-1.81075500
			H	4.60679100	-1.41026600	1.71171600
			H	6.71019400	-0.50427900	2.60085300
			H	7.38295200	1.81985800	2.06809900
			H	5.96578400	3.21085800	0.60360800
			H	3.54935700	4.18978400	0.81038800
			H	2.06870600	5.55022800	-0.61772900
			H	1.28044400	4.66669900	-2.78908100
			H	2.04678800	2.44380300	-3.56464200
			H	3.61087500	1.13165100	-2.18910100
4	CIFLEI	-2653.04495780	Te	2.77624200	0.05553900	-0.53954500
			I	1.80384300	2.78432400	-0.46996400
			C	1.70083600	-0.43487900	1.21693800

			C	1.76047800	0.40369000	2.32154000
			C	1.03292600	0.07655900	3.45917700
			C	0.24527500	-1.06667400	3.47957100
			C	0.19412500	-1.89711800	2.36718700
			C	0.92585300	-1.58779800	1.22992700
			H	2.35877400	1.30545300	2.30341000
			H	1.08111100	0.72194400	4.32578400
			H	-0.32788600	-1.31316600	4.36329400
			H	-0.41541500	-2.78940400	2.37873800
			H	0.88749200	-2.24486000	0.37236600
			I	3.81108800	-2.67170600	-0.68974000
			C	4.57222900	0.66474000	0.39590600
			C	5.00350100	0.05648400	1.56726000
			C	5.33018600	1.64672600	-0.22815200
			C	6.20857100	0.45439000	2.12901800
			H	4.41793400	-0.72276500	2.03736000
			C	6.54020900	2.02730700	0.33633700
			H	4.98536700	2.12328600	-1.13656500
			C	6.97572900	1.43571800	1.51423300
			H	6.54827500	-0.00874200	3.04512900
			H	7.13739600	2.78928600	-0.14498700
			H	7.91598000	1.73874500	1.95416100
			Te	-3.24973100	-0.11820700	-0.88326600
			I	-5.91771100	0.40138000	0.11015400
			C	-2.99261400	-1.65514900	0.54386400
			C	-3.31195400	-1.43190300	1.87735000
			C	-3.26125900	-2.49402600	2.76873700
			C	-2.91010800	-3.76292700	2.32464900
			C	-2.58365500	-3.97122700	0.99139800
			C	-2.61918500	-2.91381400	0.09096200
			H	-3.61238100	-0.45082300	2.22099200
			H	-3.50610400	-2.32815900	3.80879200
			H	-2.88443400	-4.58977200	3.02122800
			H	-2.30334500	-4.95624500	0.64507900
			H	-2.35967900	-3.07934800	-0.94631100
			I	-0.60299800	-0.61616000	-2.03527900
			C	-2.51598900	1.51525900	0.22664600
			C	-1.54814200	1.34779700	1.20774200
			C	-3.03546100	2.76716000	-0.07978500
			C	-1.11976200	2.46417600	1.91421600
			H	-1.12558000	0.37287800	1.42367100
			C	-2.58177900	3.87440600	0.62175000
			H	-3.79509300	2.88567300	-0.84150200
			C	-1.63340200	3.72018700	1.62407500
			H	-0.36964100	2.34826300	2.68360600
			H	-2.97763900	4.85310200	0.38886800
			H	-1.28707800	4.58341700	2.17572000
5	CIFLOS	-2785.09484875	Te	-0.01658200	-0.54155200	2.29064200
			I	-2.16049200	-0.76500700	0.02924300
			I	2.15841200	-0.76573400	-0.02862500
			I	-1.99133600	-0.64265800	4.21863000
			I	2.04747900	-0.33615000	4.13981900
			C	-0.13295700	1.56675800	2.02244200
			C	1.03364900	2.28600000	1.79929800
			C	0.95348800	3.66272300	1.64142900
			C	-0.27355700	4.30592500	1.71330000
			C	-1.43200400	3.57322900	1.92898600
			C	-1.36972900	2.19549800	2.07958900
			H	1.99647000	1.79676600	1.75329800
			H	1.85771800	4.22817000	1.46315700
			H	-0.32785300	5.37944800	1.59290500
			H	-2.39171300	4.06864400	1.97955400
			H	-2.27839100	1.63404200	2.24371700

			Te	0.01449800	-0.54201800	-2.29011100
			I	-2.04958600	-0.33640800	-4.13919300
			I	1.98916100	-0.64388900	-4.21814400
			C	0.13144300	1.56630200	-2.02226200
			C	1.36842200	2.19463200	-2.07949100
			C	-1.03494300	2.28597900	-1.79938300
			C	1.43113800	3.57237800	-1.92921600
			H	2.27691300	1.63284500	-2.24343600
			C	-0.95434100	3.66271100	-1.64181700
			H	-1.99792700	1.79707000	-1.75334000
			C	0.27291600	4.30550100	-1.71377100
			H	2.39101000	4.06747100	-1.97983900
			H	-1.85840100	4.22849300	-1.46374100
			H	0.32755100	5.37903600	-1.59363800
6	CIFLUY	-2785.09172990	Te	-0.05646600	2.29222900	-0.00001300
			I	0.07806000	-0.01221900	2.15694600
			I	-0.04261400	4.17848800	2.02620300
			C	-2.17594200	2.09217800	-0.00000700
			C	-2.85216800	2.01780200	1.21038900
			C	-4.23147600	1.86449900	1.20245200
			C	-4.92016700	1.78677800	0.00000000
			H	-2.32760100	2.07926000	2.15330200
			H	-4.76297300	1.80699400	2.14207100
			H	-5.99494600	1.66804800	0.00000200
			I	0.07805900	-0.01224100	-2.15694900
			I	-0.04263000	4.17847000	-2.02624500
			Te	0.07568500	-2.32216700	0.00001000
			C	-2.85217800	2.01784400	-1.21040000
			C	-4.23148600	1.86454100	-1.20245600
			I	-0.04247100	-4.20449700	-2.02720500
			I	-0.04245900	-4.20447500	2.02724700
			C	2.20274600	-2.24491100	0.00000600
			H	-2.32762000	2.07933500	-2.15331600
			H	-4.76299100	1.80706900	-2.14207300
			C	2.88193000	-2.20974900	-1.21029300
			C	2.88193500	-2.20977600	1.21030300
			C	4.26770800	-2.13598500	-1.20246700
			H	2.35391800	-2.24198600	-2.15266700
			C	4.26771300	-2.13601200	1.20247300
			H	2.35392700	-2.24203500	2.15267900
			C	4.95968300	-2.09779400	0.00000200
			H	4.80166500	-2.10931300	-2.14206400
			H	4.80167500	-2.10936100	2.14206900
			H	6.03948400	-2.04101500	0.00000000
7	GEHDON	-4036.41616351	I	-0.45360200	-1.89290100	-1.76903900
			I	-4.03331100	1.45824500	1.40422100
			Te	-2.27044700	-0.25937600	-0.15420500
			I	-1.67384900	-1.87322400	2.15794000
			S	-2.93395300	1.14956600	-2.38721200
			C	-1.81682200	4.42232300	-0.42272500
			H	-1.13804800	5.11832300	-0.91134500
			H	-1.60754100	4.40377400	0.64437800
			C	-3.29900100	4.73401400	-0.72936200
			H	-3.90815300	4.71964000	0.17256200
			H	-3.42884200	5.68362400	-1.24011400
			C	-3.90351900	-1.52730200	-0.67754300
			N	-1.65842900	3.08483900	-0.99216900
			H	-0.77157500	2.60018200	-1.04761400
			C	-2.73875100	2.68298200	-1.63314100
			C	-6.04916100	-3.12901800	-1.37112800
			H	-6.88762900	-3.75605300	-1.64170500
			C	-5.87636600	-2.73191600	-0.05251700
			H	-6.57694800	-3.04586500	0.70884900

			C	-4.06510800	-1.92011600	-1.99968800
			H	-3.35995800	-1.62518200	-2.76457100
			C	-4.80280700	-1.92630300	0.30144900
			H	-4.67884400	-1.61895700	1.33024900
			C	-5.14485900	-2.72236900	-2.34218000
			H	-5.27197800	-3.02919700	-3.37110700
			N	-3.68039900	3.61586100	-1.59700500
			H	-4.63355800	3.40180700	-1.84048800
			I	0.45360300	1.89290500	1.76903600
			I	4.03330900	-1.45825100	-1.40421400
			Te	2.27044800	0.25937600	0.15420400
			I	1.67385300	1.87322000	-2.15794400
			S	2.93394900	-1.14956400	2.38721200
			C	1.81682300	-4.42232300	0.42272500
			H	1.13805200	-5.11832200	0.91134800
			H	1.60754000	-4.40377700	-0.64437800
			C	3.29900300	-4.73401100	0.72935900
			H	3.90815400	-4.71963300	-0.17256600
			H	3.42884800	-5.68362100	1.24010900
			C	3.90351800	1.52730300	0.67754300
			N	1.65843000	-3.08483800	0.99216500
			H	0.77157500	-2.60018200	1.04761100
			C	2.73875100	-2.68297900	1.63313900
			C	6.04915500	3.12902500	1.37113100
			H	6.88762100	3.75606100	1.64170900
			C	5.87636700	2.73191600	0.05252100
			H	6.57695300	3.04586100	-0.70884300
			C	4.06509800	1.92012600	1.99968700
			H	3.35994200	1.62519900	2.76456700
			C	4.80281000	1.92630100	-0.30144600
			H	4.67885200	1.61894900	-1.33024600
			C	5.14484700	2.72238200	2.34218000
			H	5.27196000	3.02921600	3.37110600
			N	3.68040000	-3.61585800	1.59700300
			H	4.63355900	-3.40180200	1.84048600
8	GIPRUT	-1495.19030044	C	0.23280900	1.05578700	0.34399800
			C	-0.94929700	1.67139100	0.78530300
			C	-0.86021300	2.70807600	1.71081000
			H	-1.77241800	3.17799200	2.05621800
			C	0.36948800	3.14057800	2.18175300
			H	0.42168400	3.95183600	2.89544500
			C	1.53085500	2.53050900	1.73808600
			H	2.49538500	2.85994800	2.10324300
			C	1.48199800	1.48121500	0.82210400
			C	-2.30362000	1.24986200	0.32490700
			C	-2.81139400	1.72171700	-0.89317500
			C	-4.07668400	1.31401600	-1.29640200
			H	-4.47080700	1.67880300	-2.23844800
			C	-4.85207900	0.45637800	-0.52066100
			C	-4.34059900	0.02957300	0.69743700
			H	-4.93701500	-0.62370900	1.32449600
			C	-3.07895400	0.42018200	1.14040400
			C	-2.00937900	2.66038500	-1.75165800
			H	-1.63524100	3.50472200	-1.17142400
			H	-2.61209500	3.04255900	-2.57309100
			H	-1.13964300	2.15575500	-2.17933000
			C	-6.20073000	-0.00412000	-1.00104300
			H	-6.82102000	-0.34017200	-0.17174700
			H	-6.09588400	-0.83857100	-1.69699100
			H	-6.72489900	0.79419400	-1.52539100
			C	-2.58696900	-0.02459700	2.49196400
			H	-1.53040700	-0.29067800	2.46834900
			H	-3.15155200	-0.88729700	2.84169600

			H	-2.70228400	0.77590600	3.22620900
			C	2.76719700	0.85343600	0.39828500
			C	3.27736000	-0.22681500	1.12711500
			C	4.47485900	-0.80447400	0.72245100
			H	4.86722900	-1.64710800	1.28079300
			C	5.17765400	-0.33381600	-0.38253900
			C	4.65036100	0.74039200	-1.08913500
			H	5.18012600	1.11651100	-1.95706700
			C	3.45338800	1.34473200	-0.71512200
			C	2.52781300	-0.77038300	2.31260600
			H	3.05849700	-1.61084900	2.75513500
			H	1.53086000	-1.10913400	2.02026000
			H	2.39133900	-0.00479600	3.07806600
			C	6.48636800	-0.95753200	-0.78265400
			H	6.71071900	-0.76431700	-1.83041300
			H	6.47231600	-2.03516900	-0.62395400
			H	7.30518800	-0.54953400	-0.18696600
			C	2.89732300	2.49079600	-1.51684100
			H	2.71878100	3.36475600	-0.88916100
			H	1.93718600	2.22876300	-1.96918700
			H	3.57901100	2.77145300	-2.31687200
			Te	0.18354100	-0.45814800	-1.14727600
			I	-0.87102900	-2.51664000	0.26133000
9	GOCROI	-1608.82939033	Te	0.65560500	0.11555400	0.31023800
			N	-2.84033600	0.24341200	0.01549500
			N	-2.12358400	-0.68129500	-0.62421100
			N	-2.89477100	-1.47108900	-1.27820700
			C	2.14286600	0.57548400	1.74108000
			H	2.79634800	-0.28823200	1.81113900
			H	1.66610800	0.80331600	2.69098300
			H	2.67963900	1.44037200	1.36565100
			C	-4.18661200	-1.05622500	-1.07929400
			C	-5.40162000	-1.56473600	-1.55927200
			H	-5.42436900	-2.42996600	-2.20666700
			C	-6.54747000	-0.91442500	-1.17162500
			H	-7.50789700	-1.26945400	-1.51847900
			C	-6.50707100	0.21978500	-0.32553900
			H	-7.43779500	0.69809700	-0.05271100
			C	-5.32561400	0.73211500	0.15465800
			H	-5.30073200	1.60261700	0.79431900
			C	-4.16063200	0.06308400	-0.24130400
			C	-2.18221300	1.29362400	0.77862800
			H	-2.92184700	1.67890000	1.47978700
			H	-1.89274000	2.10628000	0.11082300
			C	-0.97951200	0.78296500	1.54770000
			H	-1.24077400	-0.04410600	2.20555700
			H	-0.56533000	1.60507700	2.12555700
			C	0.46399900	-1.90936000	0.89131800
			C	0.18379800	-2.85557200	-0.08660800
			H	0.07118400	-2.55754700	-1.12091300
			C	0.04924700	-4.18990600	0.26960400
			H	-0.16689300	-4.92800800	-0.49071900
			C	0.19560500	-4.57544100	1.59642700
			H	0.09364000	-5.61676400	1.87066800
			C	0.47527600	-3.62694200	2.57028700
			H	0.59161000	-3.92440700	3.60364300
			C	0.60997100	-2.28889300	2.21926000
			H	0.83132400	-1.55836100	2.98769200
			I	0.75142300	3.70278900	0.05900000
			I	3.61966800	-1.13820700	-1.23658900
10	LADXEV	-3249.99612199	Te	-1.87213500	0.08798900	1.32150300
			I	1.03163700	1.20622300	1.53141400
			I	-2.47571800	1.23494300	3.74089400

			I	-4.50800100	-0.69390200	0.84340300
			C	-1.77452400	-2.96256800	1.66282300
			H	-2.46623800	-2.96686400	0.83218000
			O	-2.50056000	2.81044500	0.46264000
			C	-1.29397200	-1.77068800	2.19203100
			C	-0.40247900	-1.77318200	3.25867000
			H	-0.02849400	-0.84851000	3.67662700
			C	-3.85972600	3.25534200	0.42039700
			H	-3.91040700	4.29561200	0.75412400
			H	-4.44054700	2.63570500	1.10400000
			C	-1.35938100	-4.16755500	2.21328000
			H	-1.73586000	-5.09512900	1.80475400
			C	-0.46422500	-4.18012800	3.27403600
			H	-0.14016900	-5.12116500	3.69722100
			C	0.01289100	-2.98453500	3.79433600
			H	0.70731500	-2.98811800	4.62328700
			C	-4.27507000	3.12326600	-1.03509800
			H	-5.11764300	3.76139300	-1.29164900
			H	-4.53817900	2.08621600	-1.25264800
			C	-2.97917000	3.50391500	-1.75145300
			H	-2.92194900	3.13222500	-2.77215400
			H	-2.86200800	4.58824000	-1.77140700
			C	-1.92360100	2.87038500	-0.85135300
			H	-0.99272600	3.43567400	-0.80434900
			H	-1.69072500	1.85154200	-1.17679600
			Te	1.87213500	-0.08798900	-1.32150300
			I	-1.03163700	-1.20622300	-1.53141400
			I	2.47571800	-1.23494300	-3.74089400
			I	4.50800100	0.69390200	-0.84340300
			C	1.77452400	2.96256800	-1.66282300
			H	2.46623800	2.96686400	-0.83218000
			O	2.50056000	-2.81044500	-0.46264000
			C	1.29397200	1.77068800	-2.19203100
			C	0.40247900	1.77318200	-3.25867000
			H	0.02849400	0.84851000	-3.67662700
			C	3.85972600	-3.25534200	-0.42039700
			H	3.91040700	-4.29561200	-0.75412400
			H	4.44054700	-2.63570500	-1.10400000
			C	1.35938100	4.16755500	-2.21328000
			H	1.73586000	5.09512900	-1.80475400
			C	0.46422500	4.18012800	-3.27403600
			H	0.14016900	5.12116500	-3.69722100
			C	-0.01289100	2.98453500	-3.79433600
			H	-0.70731500	2.98811800	-4.62328700
			C	4.27507000	-3.12326600	1.03509800
			H	5.11764300	-3.76139300	1.29164900
			H	4.53817900	-2.08621600	1.25264800
			C	2.97917000	-3.50391500	1.75145300
			H	2.92194900	-3.13222500	2.77215400
			H	2.86200800	-4.58824000	1.77140700
			C	1.92360100	-2.87038500	0.85135300
			H	0.99272600	-3.43567400	0.80434900
			H	1.69072500	-1.85154200	1.17679600
11	MECGOR	-3380.75220959	I	-2.43393300	2.89975000	0.25245200
			I	-4.22800500	0.24006100	-2.33869200
			I	-0.58586400	-0.22868400	2.22635100
			I	-2.36092800	-2.91034500	-0.44592900
			Te	-2.44259200	-0.01221000	-0.03940500
			C	-4.10425800	-0.20349100	1.29589200
			C	-4.08151500	-1.18439200	2.27921500
			H	-3.23969900	-1.85559800	2.37326000
			C	-5.15469800	-1.30060200	3.15195600
			H	-5.13438600	-2.06289300	3.91887700

			C	-6.24185100	-0.44474800	3.04180300
			H	-7.07527200	-0.53746700	3.72509100
			C	-6.25723800	0.53067000	2.05468300
			H	-7.10082400	1.20110200	1.96274900
			C	-5.18806300	0.65614300	1.17739500
			H	-5.20769100	1.41978000	0.41272300
			I	2.43382100	-2.89972700	-0.25242400
			I	4.22805200	-0.24012400	2.33864400
			I	0.58585800	0.22876200	-2.22633700
			I	2.36101900	2.91035900	0.44593100
			Te	2.44259100	0.01222300	0.03940600
			C	4.10423300	0.20344300	-1.29589100
			C	4.08157000	1.18442000	-2.27913800
			H	3.23982000	1.85571700	-2.37312400
			C	5.15475800	1.30059700	-3.15187800
			H	5.13450800	2.06294800	-3.91874000
			C	6.24183200	0.44463400	-3.04179800
			H	7.07525700	0.53733000	-3.72508400
			C	6.25713300	-0.53086400	-2.05475500
			H	7.10065600	-1.20138300	-1.96287600
			C	5.18795300	-0.65630600	-1.17746900
			H	5.20751000	-1.42001200	-0.41286300
12	TUPWIK	-2727.71630228	I	2.98078300	2.70392500	0.61004800
			I	0.88802500	-2.52031000	-0.93914700
			Te	1.92450400	0.10349700	-0.08269500
			O	4.77681300	0.37363600	-1.54668800
			O	2.79203900	-1.72522000	2.11382900
			C	3.81302700	-0.74782100	0.26125700
			C	4.93929300	-0.48238100	-0.52323200
			C	6.15380700	-1.09222200	-0.21367300
			C	6.22426900	-1.94183400	0.87770700
			C	5.12642700	-2.19502200	1.68471700
			C	3.91596000	-1.58100600	1.37786200
			C	5.90838000	0.72429600	-2.32691400
			C	2.84042100	-2.58493000	3.24264700
			C	2.01284000	0.53208800	-2.15938800
			H	7.03160200	-0.90713100	-0.81217900
			H	7.16764700	-2.41554100	1.11284800
			H	5.21878000	-2.85047500	2.53581100
			H	5.55177500	1.43905200	-3.06152900
			H	6.31802400	-0.15021300	-2.83321800
			H	6.67619400	1.18696100	-1.70612800
			H	3.07429500	-3.60536600	2.93857800
			H	3.57677100	-2.23189300	3.96462800
			H	1.85256800	-2.55576900	3.69066200
			H	2.45902900	1.51257600	-2.27908000
			H	0.98024200	0.51028800	-2.49320900
			H	2.60342200	-0.24541500	-2.62775600
			I	-1.06051700	2.48400500	-1.11820300
			I	-3.97840300	-2.51389500	-0.42889300
			Te	-2.50647400	-0.06768100	-0.80027200
			O	-4.73478400	1.98485300	0.41944200
			O	-1.24120000	-0.80569500	1.68531400
			C	-3.01567900	0.57282800	1.12540200
			C	-4.01874300	1.48825700	1.44366400
			C	-4.21805900	1.84245800	2.77733900
			C	-3.40594300	1.28932700	3.75493100
			C	-2.39174300	0.39303200	3.45315600
			C	-2.19847000	0.03997900	2.12285500
			C	-5.74608100	2.93979000	0.70169000
			C	-0.38277400	-1.41500500	2.63552500
			C	-4.08932300	0.64253000	-2.02055600
			H	-4.99031100	2.54358600	3.05156400

			H	-3.56517000	1.57167000	4.78669600
			H	-1.76708300	-0.01136000	4.23393900
			H	-6.17939500	3.20533700	-0.25714200
			H	-6.51414700	2.51182200	1.34645900
			H	-5.31930000	3.82658300	1.17091500
			H	-0.95925700	-1.98707600	3.36343000
			H	0.22229100	-0.66155100	3.14400900
			H	0.25812700	-2.07805000	2.06240500
			H	-3.98684800	1.71637700	-2.11657700
			H	-3.95261700	0.13402200	-2.97168500
			H	-5.02688300	0.36485700	-1.55586200
13	WOPYIM	-1134.79198672	Te	0.00041400	-0.67022800	-0.17738700
			I	2.90603800	-0.67215800	-0.17691900
			I	-2.90109600	-0.68863600	-0.03045600
			C	-0.00537100	1.42914400	-0.01814700
			C	0.57725200	2.05303900	1.07572000
			H	1.04595300	1.47979300	1.86469400
			C	-0.01354700	4.18313900	0.12371200
			H	-0.01787400	5.26293100	0.18068100
			C	-0.58686400	2.15992200	-1.04524300
			H	-1.04881800	1.66530700	-1.88987100
			C	0.00910300	-1.12488500	1.89217900
			H	-0.69207900	-0.44765900	2.36917600
			H	1.02147000	-1.00607300	2.26150400
			H	-0.32668000	-2.15381500	1.98050100
			C	-0.58490500	3.54594200	-0.96968100
			H	-1.03421300	4.12461100	-1.76470800
			C	0.56406900	3.43930700	1.14442200
			H	1.01037800	3.93522800	1.99519900
14	WUGVUQ	-2269.58837283	Te	-1.43823500	-0.05580900	-0.47303400
			I	0.70764900	-2.19093100	-0.26328900
			I	0.56666700	2.12365500	-0.88445200
			I	-3.50146500	1.87955600	-0.76210000
			I	-3.38592100	-2.13532100	-0.15514700
			C	-1.33235900	0.24625800	1.63712100
			C	-0.09696200	0.36540100	2.26086400
			H	0.82692100	0.31161800	1.69891100
			C	-2.51315500	0.31752000	2.36334000
			H	-3.47331700	0.22394000	1.87572100
			C	-0.05517200	0.55711500	3.63586500
			H	0.90387900	0.64893500	4.12577500
			C	-2.45593000	0.51114700	3.73628800
			H	-3.37500000	0.56755100	4.30302800
			C	-1.22885300	0.63037700	4.37283100
			H	-1.18662500	0.78051700	5.44302900
			Te	3.59442600	-0.19058100	-1.18272000
			C	5.31057800	0.99428600	-1.56890400
			H	5.01876500	2.03852300	-1.50459900
			H	5.64622500	0.76346000	-2.57599700
			H	6.07162900	0.75414400	-0.83318000
			C	4.66486200	-2.00813000	-1.06060300
			H	5.09593800	-2.18692400	-2.04185600
			H	3.96151100	-2.79631400	-0.80889800
			H	5.43875800	-1.90546400	-0.30564700
			C	3.58531900	0.21423400	0.88226600
			C	3.58379100	1.53932700	1.30041700
			H	3.57532900	2.35269400	0.58701200
			C	3.57231500	-0.82684700	1.80120600
			H	3.55401200	-1.85916800	1.47956200
			C	3.57042900	-0.53253800	3.15863000
			H	3.55939300	-1.33917200	3.87849600
			C	3.58202300	1.82258600	2.65946500
			H	3.58034400	2.85187600	2.99003200

			C	3.57900000	0.78834200	3.58589200
			H	3.57766100	1.01275800	4.64407300
15	YODVUK	-1481.29536949	I	-3.72570600	-1.53816900	0.55444700
			Te	0.91375200	-0.25212500	-0.66746800
			C	-1.22001500	-0.12992700	-0.39724300
			C	-1.67326700	-1.21137800	0.21733900
			C	-0.78009200	-2.33865900	0.66215700
			H	-0.97308400	-3.20237300	0.02361200
			H	-1.04226800	-2.63756500	1.67713500
			C	0.69871700	-1.94676900	0.60056000
			H	1.34315700	-2.72248900	0.20136600
			H	1.09421400	-1.62282700	1.56064300
			C	-1.93070500	1.06386600	-0.87550400
			C	-2.62887800	1.86979700	0.02475100
			H	-2.65773700	1.59577100	1.07148200
			C	-3.27727700	3.01299300	-0.41776500
			H	-3.81460700	3.63137100	0.28835100
			C	-3.23415700	3.36459700	-1.76085100
			H	-3.74041900	4.25638400	-2.10420300
			C	-2.53352100	2.57190400	-2.66065300
			H	-2.49492100	2.84194400	-3.70712800
			C	-1.87723900	1.43198600	-2.22028000
			H	-1.33100600	0.81640900	-2.92453500
			C	1.24915400	1.26853500	0.74974000
			C	2.17978700	2.25745600	0.45839900
			H	2.76053200	2.21905100	-0.45367900
			C	2.37393500	3.28989400	1.36548100
			H	3.09503700	4.06518500	1.14670400
			C	1.65093500	3.32157200	2.55089800
			H	1.80978200	4.12472000	3.25742500
			C	0.72473900	2.32625700	2.83299700
			H	0.16192000	2.35064000	3.75592600
			C	0.51266700	1.29649600	1.92588000
			H	-0.22315400	0.53128200	2.14222800
			I	4.04813600	-0.94916500	-0.35751100
16	ZIQPEU	-1797.60776447	Te	0.00820100	0.23201200	-0.04031600
			I	-0.17005900	0.47440100	2.77377000
			C	1.90581200	-0.01784000	-2.47881900
			C	-0.28622300	-0.93307100	-2.99990000
			C	0.09921300	1.45090100	-3.12600900
			N	0.44875800	0.20689800	-2.42375400
			C	2.59919600	0.79664200	-1.42503000
			C	3.88525400	1.28317700	-1.62278100
			C	4.54340700	1.96467600	-0.60922900
			C	3.91723200	2.16832900	0.61179700
			C	2.62956800	1.69209800	0.82228600
			C	1.97723700	1.01314800	-0.19593000
			C	-0.98267800	2.10020700	-0.28655100
			C	-2.36092400	2.07612800	-0.47069600
			C	-3.04632400	3.27263100	-0.64447500
			C	-2.36178400	4.47929200	-0.63024800
			C	-0.98565300	4.49491000	-0.43922000
			C	-0.29033200	3.30622100	-0.26644700
			H	2.08717100	-1.07468100	-2.27439800
			H	2.28284100	0.21551700	-3.47776300
			H	-0.00242200	-1.06526500	-4.04673300
			H	-1.35502100	-0.74422000	-2.92657000
			H	-0.04870100	-1.83432400	-2.43591600
			H	0.33555100	1.34477600	-4.18793200
			H	0.67013400	2.27961800	-2.71176400
			H	-0.96275500	1.65375500	-3.01020100
			H	4.37202200	1.12064600	-2.57597500
			H	5.54471500	2.33812200	-0.77434000

			H	4.42513600	2.69992400	1.40446100
			H	2.14582800	1.85391200	1.77497200
			H	-2.89856800	1.13591700	-0.48068600
			H	-4.11792900	3.25517800	-0.78960700
			H	-2.89878800	5.40842500	-0.76509500
			H	-0.44884400	5.43371200	-0.42380900
			H	0.78104400	3.33306300	-0.12207400
			I	1.85629500	-2.83700300	0.10519500
			I	-3.21335200	-1.70818400	-0.43644400

Table S14. CSD refcodes of the starting structures, energies (in Hartree) and coordinates of the optimized structures containing Te...I contacts(from calculation in vacuum).

	CSD refcode	E(RM062X)	Coordinates			
1	ATIDIQ	-1327.12696989	I	0.41567500	2.51459300	0.00410300
			I	-4.21803200	-0.40787300	-0.10728600
			Te	-1.02178000	-0.55052900	-0.19113200
			Te	4.24645700	-1.05279800	0.02302500
			C	1.02372000	-1.01680600	-0.01636300
			C	2.22336100	-1.18525100	0.00009200
			C	4.22846500	1.04354100	-0.41204900
			H	3.40053100	1.48236400	0.14069100
			H	5.18064500	1.45664100	-0.08910600
			H	4.08107400	1.19075200	-1.47579400
			C	-1.35999800	-2.65849200	0.05632900
			H	-0.79566500	-2.99092100	0.92343500
			H	-2.42733400	-2.80820100	0.17826200
			H	-0.99104800	-3.15681100	-0.83702100
			C	-1.24295200	-0.08863500	1.85612900
			H	-0.24329200	0.01200200	2.26665100
			H	-1.77755400	0.85392200	1.88951700
H	-1.82122400	-0.88908400	2.30879400			
2	BIPFOV	-2425.75563335	Te	-2.28071700	-0.05671900	-0.38218300
			C	-3.66818500	1.24681400	0.57873000
			C	-3.45512200	2.61405000	-0.00573900
			C	-4.39671300	3.62759100	0.15600300
			C	-4.18555400	4.88318500	-0.39196700
			C	-3.02609100	5.13557100	-1.11503000
			C	-2.08740200	4.13027200	-1.28658300
			C	-2.29075000	2.86707000	-0.73608500
			C	-1.28684100	1.76391500	-0.91562300
			C	-3.32644600	-0.06432000	-2.22621200
			Te	2.28056400	0.05613800	0.38556500
			C	1.29904500	-1.76921900	0.92479100
			C	2.30619900	-2.86801700	0.73672500
			C	2.10932500	-4.13386500	1.28359400
			C	3.05016300	-5.13568100	1.10415500
			C	4.20545300	-4.87719900	0.37652800
			C	4.41021200	-3.61902800	-0.16781800
			C	3.46641200	-2.60880500	0.00202500
			C	3.67353500	-1.23890900	-0.57846400
			C	3.33303900	0.07236000	2.22573600
			I	0.43693000	-1.06344900	-2.66695900
			I	-0.43670300	1.04413800	2.68004500
			I	-5.12101900	-2.18370700	0.35705600
			I	5.10344700	2.19982900	-0.36904700
			H	-3.41753700	1.20540200	1.63843700
			H	-4.66584200	0.84171900	0.42324500
			H	-5.30038600	3.42237900	0.71663900
H	-4.92510500	5.66257300	-0.25896300			
H	-2.85508200	6.11319700	-1.54717700			
H	-1.18229700	4.31939500	-1.85014900			

			H	-0.44255900	1.87087300	-0.23621800
			H	-0.92075700	1.66122300	-1.93504000
			H	-3.70395600	0.94225300	-2.39545600
			H	-2.60249800	-0.34993200	-2.98510000
			H	-4.13317900	-0.78461600	-2.13308800
			H	0.44951000	-1.87990400	0.25257300
			H	0.94084200	-1.66870000	1.94723600
			H	1.20735400	-4.32782000	1.85054300
			H	2.88402700	-6.11539100	1.53347500
			H	4.94662800	-5.65390700	0.23705500
			H	5.31051500	-3.40913900	-0.73214200
			H	3.42408700	-1.19537900	-1.63830700
			H	4.66925400	-0.82988900	-0.42075600
			H	4.13710700	0.79505500	2.12764600
			H	2.61106600	0.35771800	2.98662900
			H	3.71432900	-0.93258500	2.39641000
3	BIPTEI	-3247.16290484	I	-3.81478100	1.88154200	1.89880100
			I	-1.87456000	2.36194000	-1.55363500
			I	-0.80992500	-1.45817500	-1.76923800
			Te	-2.28263700	0.27521400	0.09272300
			C	-4.09277200	-0.50196500	-0.71213400
			C	-4.91188300	0.26571200	-1.52467600
			C	-6.04877800	-0.30440100	-2.07662400
			C	-6.35535200	-1.63256000	-1.81614900
			C	-5.53802500	-2.38622900	-0.99006900
			C	-4.39725800	-1.83261000	-0.41119400
			C	-3.54384100	-2.64364100	0.48879700
			C	-3.02514000	-3.86407900	0.05937800
			C	-2.17288600	-4.58731200	0.87592900
			C	-1.82599900	-4.10162600	2.13206500
			C	-2.35203600	-2.90005600	2.57807300
			C	-3.21847700	-2.17789700	1.76433200
			H	-4.67084600	1.29875200	-1.73488800
			H	-6.68964400	0.29037700	-2.71255900
			H	-7.23953000	-2.07962600	-2.24955300
			H	-5.78644300	-3.41541400	-0.76513900
			H	-3.25981100	-4.21813900	-0.93590100
			H	-1.76024200	-5.52329200	0.52499400
			H	-1.15250000	-4.66581200	2.76313400
			H	-2.10319300	-2.52384600	3.56095600
			H	-3.68231900	-1.27295700	2.14361600
			I	3.81480000	-1.88181300	-1.89874900
			I	1.87454000	-2.36186300	1.55366400
			I	0.80995900	1.45815700	1.76916700
			Te	2.28266800	-0.27526300	-0.09280300
			C	4.09283000	0.50198600	0.71199600
			C	4.91201400	-0.26569300	1.52446600
			C	6.04888700	0.30444800	2.07642600
			C	6.35535400	1.63265500	1.81607400
			C	5.53795300	2.38633900	0.99008500
			C	4.39722700	1.83268900	0.41115700
			C	3.54373700	2.64380400	-0.48870100
			C	3.02495900	3.86414300	-0.05909000
			C	2.17269100	4.58747500	-0.87554500
			C	1.82584300	4.10197700	-2.13176700
			C	2.35198100	2.90052600	-2.57797300
			C	3.21847700	2.17830200	-1.76435200
			H	4.67104700	-1.29876000	1.73462100
			H	6.68980600	-0.29033700	2.71230100
			H	7.23950400	2.07974800	2.24950800
			H	5.78628700	3.41556700	0.76525900
			H	3.25959200	4.21805200	0.93625200
			H	1.75998400	5.52336900	-0.52445800

			H	1.15232300	4.66622600	-2.76275800
			H	2.10318700	2.52445800	-3.56092200
			H	3.68245100	1.27351200	-2.14382900
4	CIFLEI	-2653.02766707	Te	2.78650700	0.04865700	-0.56018000
			I	1.90427200	2.81112000	-0.46899400
			C	1.72123600	-0.39605200	1.21957500
			C	1.80997400	0.46549900	2.30418400
			C	1.08428000	0.18389100	3.45469500
			C	0.26877700	-0.93820000	3.50839600
			C	0.19328100	-1.79519900	2.41897400
			C	0.92534400	-1.53251600	1.26998000
			H	2.42799300	1.35280600	2.25499700
			H	1.15554600	0.84820100	4.30565200
			H	-0.30513700	-1.14865300	4.40113700
			H	-0.43700700	-2.67222300	2.45591000
			H	0.87038000	-2.21101200	0.43031300
			I	3.70305100	-2.68919600	-0.72404400
			C	4.60501800	0.59824600	0.38121700
			C	5.05454200	-0.10228700	1.49235400
			C	5.35189100	1.63244800	-0.16520400
			C	6.26481300	0.25125800	2.07041600
			H	4.47683800	-0.92256600	1.89810700
			C	6.56963000	1.96685100	0.41167700
			H	4.98621800	2.19006800	-1.01735100
			C	7.02281100	1.28102600	1.52910000
			H	6.61763600	-0.28617900	2.93997800
			H	7.15787300	2.76939500	-0.01155000
			H	7.96904100	1.54860300	1.97948700
			Te	-3.25882100	-0.12329800	-0.87541600
			I	-5.92789300	0.37441200	0.07694800
			C	-2.99472600	-1.62151400	0.59638300
			C	-3.33797800	-1.36504600	1.91705000
			C	-3.28746100	-2.40006400	2.83961700
			C	-2.91424600	-3.67662200	2.43893500
			C	-2.56067200	-3.91765100	1.11867500
			C	-2.59257900	-2.88611700	0.18876300
			H	-3.66200800	-0.37877800	2.22278200
			H	-3.55616500	-2.20844700	3.86956000
			H	-2.89399500	-4.48399500	3.15854000
			H	-2.26131800	-4.90839500	0.80546400
			H	-2.30266100	-3.07247400	-0.83705300
			I	-0.61447400	-0.64874700	-1.99034300
			C	-2.54575600	1.54308900	0.20069800
			C	-1.50613300	1.41568200	1.11073800
			C	-3.13758500	2.77128900	-0.06384900
			C	-1.07215300	2.54945300	1.78420700
			H	-1.02943900	0.45907300	1.29315000
			C	-2.67835900	3.89666400	0.60314700
			H	-3.96030000	2.85430400	-0.76197300
			C	-1.65250400	3.78335100	1.53068800
			H	-0.25926200	2.46409200	2.49099900
			H	-3.12877400	4.85841700	0.40035700
			H	-1.29642700	4.66197000	2.05098100
5	CIFLOS	-2785.08614268	Te	-0.01007800	-0.54848500	2.27889700
			I	-2.15126800	-0.76880300	-0.03647400
			I	2.15148800	-0.76823700	0.03634000
			I	-2.08469900	-0.31892500	4.10260200
			I	1.95229300	-0.64279500	4.22491000
			C	0.12240500	1.56092300	2.00193900
			C	1.36019000	2.18370800	2.08105400
			C	1.43088100	3.56233500	1.94544900
			C	0.27945700	4.30259500	1.72186500
			C	-0.94798500	3.66505400	1.62310300

			C	-1.03616800	2.28745400	1.76602000
			H	2.26202300	1.61421100	2.25442900
			H	2.39179400	4.05311400	2.01846000
			H	0.33946600	5.37790400	1.61878100
			H	-1.84753700	4.23622100	1.43870700
			H	-1.99909000	1.80025700	1.70275600
			Te	0.01025600	-0.54836700	-2.27902400
			I	-1.95205400	-0.64316000	-4.22508000
			I	2.08484600	-0.31809600	-4.10268100
			C	-0.12282700	1.56099400	-2.00196300
			C	1.03553900	2.28784500	-1.76602300
			C	-1.36079200	2.18342700	-2.08103600
			C	0.94696400	3.66541400	-1.62305200
			H	1.99859900	1.80091400	-1.70278500
			C	-1.43187700	3.56202800	-1.94537300
			H	-2.26246600	1.61367800	-2.25440600
			C	-0.28066100	4.30260800	-1.72177500
			H	1.84635400	4.23683200	-1.43863800
			H	-2.39293100	4.05253700	-2.01835000
			H	-0.34097500	5.37789600	-1.61865200
6	CIFLUY	-2785.08851488	Te	-0.11621100	3.41094600	0.00077600
			I	1.06868600	1.33638000	2.07049100
			I	-1.03382400	5.04403600	2.03379400
			C	-1.86337200	2.18908100	0.00029200
			C	-2.38406100	1.74956900	1.21025300
			C	-3.42212100	0.82781000	1.20205100
			C	-3.93203000	0.35819400	-0.00045400
			H	-1.97964200	2.09373300	2.15151200
			H	-3.81786300	0.46825300	2.14160600
			H	-4.72655700	-0.37533800	-0.00076300
			I	1.06865100	1.33708700	-2.06959500
			I	-1.03332000	5.04477200	-2.03182100
			Te	-0.05912500	-0.75648300	0.00017100
			C	-2.38401300	1.75051000	-1.21002600
			C	-3.42208200	0.82877200	-1.20258000
			I	-1.05588700	-2.35532400	-2.03178300
			I	-1.05581300	-2.35601400	2.03161300
			C	1.84969700	-1.69083000	-0.00001200
			H	-1.97950500	2.09542800	-2.15097800
			H	-3.81778700	0.46994800	-2.14242800
			C	2.46756300	-1.97400700	-1.20976000
			C	2.46785000	-1.97402900	1.20958200
			C	3.72679800	-2.55594300	-1.20230600
			H	1.98268300	-1.75151000	-2.14996700
			C	3.72708100	-2.55596900	1.20181300
			H	1.98320200	-1.75153200	2.14990700
			C	4.35552500	-2.84673400	-0.00032400
			H	4.21300400	-2.77986300	-2.14165600
			H	4.21351100	-2.77991200	2.14104100
			H	5.33696200	-3.30103300	-0.00044700
7	GEHDON	-4036.39165599	I	-0.43381500	-1.91953100	-1.70559800
			I	-4.04354000	1.49732300	1.34795000
			Te	-2.26414000	-0.26967500	-0.14052100
			I	-1.70049600	-1.78317000	2.19188200
			S	-2.93636900	1.11575600	-2.45874600
			C	-1.76926300	4.33404800	-0.45491000
			H	-1.10660900	5.05880500	-0.92601000
			H	-1.53131200	4.26609900	0.60480400
			C	-3.26110800	4.64588000	-0.71015200
			H	-3.84266900	4.57278400	0.20787500
			H	-3.40966600	5.62450700	-1.15996200
			C	-3.89689300	-1.53853600	-0.66137200
			N	-1.61738000	3.02907000	-1.08698700

			H	-0.73880400	2.52719300	-1.13652800
			C	-2.71210600	2.62986300	-1.70406300
			C	-6.04050000	-3.14279300	-1.35120200
			H	-6.87852800	-3.77141700	-1.62038700
			C	-5.89047200	-2.70930300	-0.04193500
			H	-6.60847900	-2.99609400	0.71408600
			C	-4.03518300	-1.96822400	-1.97392200
			H	-3.30932900	-1.70101200	-2.72960000
			C	-4.81833700	-1.90200300	0.31000200
			H	-4.71107800	-1.56391400	1.33116300
			C	-5.11428500	-2.77120800	-2.31466600
			H	-5.22344200	-3.10712700	-3.33669400
			N	-3.65447400	3.57899600	-1.63365400
			H	-4.61566300	3.30574100	-1.75665700
			I	0.43382200	1.91954300	1.70558800
			I	4.04353800	-1.49734100	-1.34793200
			Te	2.26413500	0.26967600	0.14052000
			I	1.70052200	1.78317500	-2.19188300
			S	2.93634200	-1.11577900	2.45873600
			C	1.76928000	-4.33406600	0.45486600
			H	1.10664000	-5.05883400	0.92597100
			H	1.53132100	-4.26612300	-0.60484700
			C	3.26113200	-4.64587600	0.71009800
			H	3.84268800	-4.57275500	-0.20792900
			H	3.40970800	-5.62450800	1.15989100
			C	3.89688500	1.53853100	0.66139400
			N	1.61738200	-3.02909100	1.08694600
			H	0.73880100	-2.52722300	1.13648500
			C	2.71210000	-2.62987800	1.70403200
			C	6.04045600	3.14282300	1.35125400
			H	6.87847000	3.77146000	1.62045100
			C	5.89045500	2.70932900	0.04198500
			H	6.60846900	2.99613100	-0.71402500
			C	4.03513400	1.96824300	1.97393900
			H	3.30925900	1.70104300	2.72960000
			C	4.81833500	1.90201700	-0.30996900
			H	4.71109300	1.56393200	-1.33113200
			C	5.11422200	2.77123900	2.31470000
			H	5.22335200	3.10717100	3.33672800
			N	3.65447900	-3.57900000	1.63361600
			H	4.61566500	-3.30573300	1.75662500
8	GIPRUT	-1495.18367650	C	0.29907400	1.02155300	0.35045300
			C	-0.87333200	1.67935700	0.75259600
			C	-0.77012500	2.74400200	1.64494100
			H	-1.67745800	3.24392200	1.96016800
			C	0.46215700	3.16979600	2.11299800
			H	0.52304100	4.00323800	2.80012800
			C	1.61531400	2.52834700	1.69408200
			H	2.58541100	2.85447900	2.04772100
			C	1.55186300	1.44848100	0.81618100
			C	-2.23299200	1.29339300	0.27772700
			C	-2.68387900	1.71608400	-0.97905900
			C	-3.95971800	1.35281900	-1.39102600
			H	-4.30969200	1.67958900	-2.36387700
			C	-4.80029900	0.59166100	-0.58660700
			C	-4.34430800	0.21631400	0.66931000
			H	-4.99100600	-0.36448100	1.31745200
			C	-3.07480800	0.56131700	1.12065500
			C	-1.81748700	2.56275700	-1.87034300
			H	-1.36097500	3.38388000	-1.31669800
			H	-2.39996200	2.97852800	-2.69034200
			H	-1.00632500	1.97180700	-2.30126700
			C	-6.15891800	0.17087600	-1.07413300

			H	-6.84392900	0.00938100	-0.24300600
			H	-6.09237300	-0.76355800	-1.63465500
			H	-6.59039900	0.92118700	-1.73563300
			C	-2.63536700	0.16182200	2.50383700
			H	-1.59764800	-0.17099000	2.51484500
			H	-3.25780000	-0.64608000	2.88505900
			H	-2.71279300	1.00386100	3.19526300
			C	2.82847800	0.79978200	0.39815800
			C	3.31559000	-0.29822500	1.11555200
			C	4.50695100	-0.88636900	0.71284300
			H	4.88244200	-1.74208600	1.26279000
			C	5.22308700	-0.41425900	-0.38201300
			C	4.71637000	0.67327800	-1.08078800
			H	5.25660800	1.04951600	-1.94217400
			C	3.52751400	1.29208800	-0.70647600
			C	2.53770500	-0.85747800	2.27396400
			H	3.09229200	-1.65373400	2.76630600
			H	1.58310300	-1.26796100	1.93358100
			H	2.30906300	-0.08548400	3.00979400
			C	6.52398900	-1.05448200	-0.78064000
			H	6.76960800	-0.83566100	-1.81861500
			H	6.48303800	-2.13623700	-0.65774000
			H	7.34227900	-0.68441200	-0.15998100
			C	2.99726600	2.46143900	-1.49352900
			H	2.91617100	3.35384000	-0.87118400
			H	1.99474700	2.26174200	-1.88013400
			H	3.64678700	2.68750200	-2.33667600
			Te	0.26735500	-0.56995000	-1.06118200
			I	-1.15040400	-2.43435000	0.28015600
9	GOCROI	-1608.74639581	Te	0.74275700	0.18440400	0.20273600
			N	-2.77131000	-0.26845900	0.22396400
			N	-2.02005000	-1.27247600	-0.23668800
			N	-2.73611400	-2.09304600	-0.91473800
			C	2.22964100	1.03789900	1.43694700
			H	2.94795200	0.25483900	1.66029900
			H	1.75726600	1.45827300	2.32074200
			H	2.68529700	1.82333000	0.84415900
			C	-4.02330500	-1.62145500	-0.91751400
			C	-5.19083500	-2.12741100	-1.50103800
			H	-5.16836200	-3.04649300	-2.06959100
			C	-6.34798600	-1.40689100	-1.32256400
			H	-7.27205100	-1.76037300	-1.75945500
			C	-6.36251900	-0.20201900	-0.58305500
			H	-7.29630000	0.33400300	-0.47800700
			C	-5.22584800	0.31011600	-0.00273100
			H	-5.23518100	1.23905000	0.54983600
			C	-4.05266700	-0.43138600	-0.18376200
			C	-2.20508600	0.83669100	0.99223500
			H	-2.94287900	1.08713000	1.75794700
			H	-2.08219900	1.70785100	0.34529500
			C	-0.88335800	0.48328800	1.64194800
			H	-0.96549300	-0.41489600	2.25140200
			H	-0.57716500	1.33576800	2.24287700
			C	1.00225800	-1.79479400	0.94920700
			C	0.87939600	-2.87208100	0.08227400
			H	0.69821700	-2.70228000	-0.97078100
			C	1.01068100	-4.16475100	0.56659300
			H	0.91444000	-5.00163300	-0.11220200
			C	1.27597200	-4.38521500	1.91225600
			H	1.38690800	-5.39533200	2.28466600
			C	1.40380300	-3.30875300	2.77705800
			H	1.61616400	-3.47321400	3.82560700
			C	1.26091000	-2.01272600	2.29519700

			H	1.35955600	-1.17665500	2.97844500
			I	0.03115000	3.64666000	0.19935700
			I	3.43331200	-0.63654000	-1.49331100
10	LADXEV	-3249.98554157	Te	-1.88297800	0.06539800	1.27999400
			I	1.00498200	1.22544000	1.51957200
			I	-2.53177400	1.24169500	3.68080300
			I	-4.47837200	-0.81950200	0.80483100
			C	-1.63713200	-2.97572100	1.65461000
			H	-2.31089100	-3.01864800	0.81038900
			O	-2.76226900	2.59599900	0.25596800
			C	-1.24009000	-1.75658400	2.18982500
			C	-0.37563000	-1.70807600	3.27691200
			H	-0.06837700	-0.76165400	3.69985900
			C	-4.01616700	3.27778000	0.32620200
			H	-3.89169300	4.17592400	0.93643000
			H	-4.74114400	2.62147700	0.80843100
			C	-1.15729300	-4.15377900	2.21045900
			H	-1.46652500	-5.10207400	1.79284100
			C	-0.28641200	-4.11334900	3.28992500
			H	0.08805200	-5.03360700	3.71805700
			C	0.10000700	-2.89173200	3.82328100
			H	0.77261000	-2.85331200	4.66952500
			C	-4.37567300	3.62470800	-1.11359600
			H	-5.01058900	4.50522900	-1.18474800
			H	-4.88994200	2.78557100	-1.58433000
			C	-2.99391900	3.81147400	-1.74173900
			H	-2.99111800	3.71383800	-2.82535200
			H	-2.58291500	4.78785800	-1.47950000
			C	-2.20282800	2.70610200	-1.05822900
			H	-1.13677100	2.91637400	-0.96117900
			H	-2.32620000	1.75305000	-1.58402500
			Te	1.88297800	-0.06539800	-1.27999400
			I	-1.00498200	-1.22544000	-1.51957200
			I	2.53177400	-1.24169500	-3.68080300
			I	4.47837200	0.81950200	-0.80483100
			C	1.63713200	2.97572100	-1.65461000
			H	2.31089100	3.01864800	-0.81038900
			O	2.76226900	-2.59599900	-0.25596800
			C	1.24009000	1.75658400	-2.18982500
			C	0.37563000	1.70807600	-3.27691200
			H	0.06837700	0.76165400	-3.69985900
			C	4.01616700	-3.27778000	-0.32620200
			H	3.89169300	-4.17592400	-0.93643000
			H	4.74114400	-2.62147700	-0.80843100
			C	1.15729300	4.15377900	-2.21045900
			H	1.46652500	5.10207400	-1.79284100
			C	0.28641200	4.11334900	-3.28992500
			H	-0.08805200	5.03360700	-3.71805700
			C	-0.10000700	2.89173200	-3.82328100
			H	-0.77261000	2.85331200	-4.66952500
			C	4.37567300	-3.62470800	1.11359600
			H	5.01058900	-4.50522900	1.18474800
			H	4.88994200	-2.78557100	1.58433000
			C	2.99391900	-3.81147400	1.74173900
			H	2.99111800	-3.71383800	2.82535200
			H	2.58291500	-4.78785800	1.47950000
			C	2.20282800	-2.70610200	1.05822900
			H	1.13677100	-2.91637400	0.96117900
			H	2.32620000	-1.75305000	1.58402500
11	MECGOR	-3380.56798544	I	-2.48472400	2.56986800	-0.16006400
			I	-4.70224100	-0.24211800	-2.27762700
			I	-0.75315100	-0.39908900	2.06189700
			I	-2.97114000	-3.25504100	0.01051300

			Te	-2.69317000	-0.32762000	-0.08101500
			C	-4.28882100	-0.16827600	1.35044800
			C	-4.28912000	-0.98585100	2.47153300
			H	-3.49581800	-1.70313000	2.62632400
			C	-5.31873700	-0.88006700	3.39688400
			H	-5.31306100	-1.51863400	4.27063300
			C	-6.34331600	0.03491900	3.20319200
			H	-7.14485600	0.11515000	3.92696300
			C	-6.33593200	0.84740500	2.07873700
			H	-7.13006900	1.56482300	1.91721200
			C	-5.30893900	0.75016200	1.14924500
			H	-5.30779900	1.38684700	0.27603100
			I	3.34340300	-3.04545800	-0.03189500
			I	4.82219700	0.16912800	2.20207300
			I	0.74518100	-0.47465400	-1.97089300
			I	2.20230000	2.68532500	0.23087000
			Te	2.73465000	-0.15982700	0.10281700
			C	4.23639700	0.19359700	-1.39314600
			C	3.96792100	1.05731200	-2.44519300
			H	3.01056700	1.55402600	-2.51604200
			C	4.93938700	1.28219600	-3.41133100
			H	4.72456400	1.95492600	-4.23137800
			C	6.17148300	0.65027400	-3.32619700
			H	6.92674700	0.82763100	-4.08176000
			C	6.43125200	-0.21080600	-2.26988600
			H	7.38869200	-0.70970100	-2.19353400
			C	5.46517200	-0.44328000	-1.30018600
			H	5.67065800	-1.11764100	-0.48129900
12	TUPWIK	-2727.70283788	I	-2.18412800	-2.55793000	1.02738600
			I	-1.59590800	2.57089100	-1.65930200
			Te	-1.82712900	0.01042600	-0.26028400
			O	-4.75728200	-1.19879100	-0.84599100
			O	-2.70035200	2.19116200	1.60407200
			C	-3.77079300	0.54559500	0.35668000
			C	-4.92334100	-0.14357600	-0.02686400
			C	-6.16917000	0.28251200	0.42998200
			C	-6.24613600	1.39249500	1.25426200
			C	-5.11429000	2.08077800	1.65738700
			C	-3.87111500	1.63559100	1.21920600
			C	-5.84092200	-2.08590600	-1.03713100
			C	-2.72541100	3.50621300	2.12092600
			C	-2.26540800	-0.78848800	-2.17717500
			H	-7.06795600	-0.23712400	0.13714400
			H	-7.21605300	1.72609300	1.59750000
			H	-5.19760900	2.93387100	2.31247600
			H	-5.44412400	-2.92263900	-1.60405200
			H	-6.64543900	-1.61054500	-1.60125500
			H	-6.21986900	-2.44219800	-0.07788400
			H	-3.26160200	4.17325500	1.44423200
			H	-3.18147700	3.53196600	3.11237500
			H	-1.68878000	3.82278200	2.19215400
			H	-2.43041400	-1.85396800	-2.06222900
			H	-1.38995700	-0.56979900	-2.77973700
			H	-3.14324000	-0.27354500	-2.54899100
			I	1.15465000	-2.09551800	-1.74767400
			I	5.40087000	1.03566300	0.65307100
			Te	3.28358400	-0.44862700	-0.61626200
			O	1.77291500	-1.82850600	1.89777700
			O	2.12553400	2.21255900	-0.37202400
			C	1.92042900	0.23331900	0.81601300
			C	1.37803900	-0.54553200	1.83860500
			C	0.48097300	0.03781300	2.73323500
			C	0.15380100	1.37707300	2.58743300

			C	0.67965200	2.16014900	1.57210500
			C	1.56337300	1.57448600	0.67249900
			C	1.29663900	-2.63479700	2.96181600
			C	2.03038300	3.62587600	-0.43486900
			C	4.12544500	-2.17943100	0.27977600
			H	0.03485100	-0.54556900	3.52304500
			H	-0.54936400	1.81738300	3.28142000
			H	0.39316400	3.19408200	1.46087500
			H	1.74630900	-3.61228700	2.81581200
			H	1.61039300	-2.22416900	3.92360500
			H	0.21133500	-2.72394600	2.92210900
			H	2.42649700	4.06989400	0.47998800
			H	0.99699100	3.93243000	-0.59748900
			H	2.63896900	3.92660100	-1.28155500
			H	3.42326200	-2.99609100	0.16432900
			H	5.05285900	-2.35079700	-0.26131300
			H	4.32557000	-1.95031200	1.31939800
13	WOPYIM	-1134.78239442	Te	0.00997300	-0.64891400	-0.18758300
			I	2.89722500	-0.67748400	-0.18047000
			I	-2.87476800	-0.73563000	-0.00726200
			C	-0.02040800	1.45878600	-0.03470800
			C	0.76712200	2.10319200	0.90828300
			H	1.42029500	1.54326500	1.56440200
			C	-0.07336700	4.21386000	0.11602800
			H	-0.09494900	5.29339000	0.17665000
			C	-0.82956600	2.17282700	-0.90706200
			H	-1.45975200	1.66204500	-1.62294200
			C	0.02678000	-1.08097500	1.89055200
			H	-0.68341000	-0.40374800	2.35412700
			H	1.03969100	-0.94983500	2.25460300
			H	-0.30548300	-2.10974700	1.99643300
			C	-0.84631600	3.55830800	-0.83151700
			H	-1.47187900	4.12174300	-1.50993600
			C	0.72806400	3.48798700	0.98626000
			H	1.33280200	3.99757300	1.72371900
14	WUGVUQ	-2269.56572417	Te	-1.40569400	0.00014100	-0.42817700
			I	0.70484300	-2.29802400	-0.52397300
			I	0.70477200	2.29838200	-0.52387900
			I	-3.35213500	1.99942300	-0.43548600
			I	-3.35192000	-1.99939600	-0.43590100
			C	-1.24610100	-0.00005400	1.69603400
			C	0.00837300	-0.00019300	2.28841800
			H	0.90907400	0.00026500	1.69108500
			C	-2.40273900	-0.00040600	2.46140500
			H	-3.37811900	-0.00028600	1.99438200
			C	0.09875100	-0.00083500	3.67340200
			H	1.07615300	-0.00148100	4.13625900
			C	-2.29817600	-0.00093600	3.84466100
			H	-3.19755900	-0.00119900	4.44494400
			C	-1.05012800	-0.00124500	4.45067100
			H	-0.97373100	-0.00176900	5.52970600
			Te	3.16315600	-0.00028000	-1.27464200
			C	4.58383600	1.55104700	-1.62372600
			H	4.08613700	2.49715300	-1.42718800
			H	4.88144900	1.50310500	-2.66846900
			H	5.44005200	1.41526900	-0.96932900
			C	4.58379400	-1.55166100	-1.62333500
			H	4.88047600	-1.50459100	-2.66839900
			H	4.08686200	-2.49788500	-1.42545400
			H	5.44060700	-1.41487400	-0.96990600
			C	3.48996900	0.00007700	0.81091000
			C	3.59683400	1.20834200	1.48717700
			H	3.48348100	2.14947700	0.96707300

			C	3.59674400	-1.20782000	1.48781200
			H	3.48350600	-2.14925400	0.96818800
			C	3.81627400	-1.20195300	2.85868200
			H	3.89147200	-2.14100400	3.38939100
			C	3.81634400	1.20320900	2.85804000
			H	3.89159400	2.14255100	3.38822800
			C	3.92662100	0.00080900	3.54228200
			H	4.09350200	0.00109400	4.61114900
15	YODVUK	-1481.27853340	I	-3.75071200	-1.50900700	0.52908700
			Te	0.97417800	-0.29128600	-0.62123300
			C	-1.19355200	-0.10590200	-0.34059100
			C	-1.68195200	-1.17937700	0.25537600
			C	-0.81294000	-2.32009000	0.72074600
			H	-1.00645000	-3.18315000	0.08015600
			H	-1.10511500	-2.61732400	1.72872500
			C	0.66870000	-1.94709100	0.69001100
			H	1.32490100	-2.73880100	0.34342300
			H	1.04041300	-1.58973700	1.64849200
			C	-1.87433500	1.08881100	-0.85083900
			C	-2.64318800	1.88592000	-0.00159300
			H	-2.75688000	1.59895000	1.03564500
			C	-3.25583000	3.03345100	-0.47930200
			H	-3.84874800	3.64214500	0.18989700
			C	-3.10931500	3.40240600	-1.80959100
			H	-3.58850600	4.29799200	-2.18065400
			C	-2.34100000	2.62004700	-2.66032100
			H	-2.22242900	2.90123500	-3.69789200
			C	-1.72010100	1.47619500	-2.18296300
			H	-1.12381800	0.86771600	-2.85211800
			C	1.30470900	1.29332300	0.73721600
			C	2.35282400	2.17190900	0.49666800
			H	3.02620400	2.01047100	-0.33447400
			C	2.55176900	3.24002000	1.35874300
			H	3.36557200	3.92820000	1.17627200
			C	1.72070200	3.41588800	2.45690400
			H	1.88592800	4.24484700	3.13165000
			C	0.68072800	2.52873700	2.69296500
			H	0.03438300	2.66179800	3.54982500
			C	0.46131100	1.46696900	1.82507700
			H	-0.36248500	0.78641600	2.00101000
			I	3.90219400	-1.02101500	-0.35865100
16	ZIQPEU	-1797.52601733	Te	-0.00110100	-0.04041900	0.11570700
			I	0.29972300	1.21467400	2.64936400
			C	1.44745200	-0.66105700	-2.63512900
			C	-0.06470000	-2.45951400	-2.09421100
			C	-0.93682900	-0.41916900	-3.02800800
			N	0.09726900	-0.99479600	-2.15922000
			C	1.90300700	0.67504600	-2.12900300
			C	2.79274700	1.44513700	-2.86944000
			C	3.30190700	2.62704200	-2.35475300
			C	2.91849900	3.04650400	-1.08928900
			C	2.01879500	2.29378200	-0.34742100
			C	1.51388200	1.11039900	-0.86514300
			C	-1.43442500	1.51026800	-0.40165800
			C	-2.62903100	1.53664500	0.31251500
			C	-3.56505500	2.52874000	0.06474800
			C	-3.32194000	3.49866100	-0.89853400
			C	-2.13036100	3.47964700	-1.60557500
			C	-1.18313600	2.49318600	-1.35203200
			H	2.13145000	-1.41173300	-2.23217500
			H	1.47626900	-0.70287600	-3.73000400
			H	0.15071100	-2.88205500	-3.08221800
			H	-1.08477100	-2.69293200	-1.80129200

			H	0.63166900	-2.86253200	-1.36065900
			H	-0.91655600	-0.92460500	-4.00014400
			H	-0.74758800	0.64163600	-3.17545300
			H	-1.91206000	-0.55991000	-2.56097800
			H	3.09243600	1.10494100	-3.85352500
			H	3.99564300	3.21720200	-2.93887000
			H	3.31191600	3.96590300	-0.67660300
			H	1.71235000	2.63436500	0.63162700
			H	-2.83920400	0.77700900	1.05194000
			H	-4.49096200	2.53458400	0.62413400
			H	-4.05758900	4.26826700	-1.09384300
			H	-1.92557000	4.23525700	-2.35303100
			H	-0.25175500	2.51459900	-1.90119600
			I	2.75598900	-1.92620900	0.57629800
			I	-3.10637100	-1.94928900	-0.03117800