

**Enhanced Reactivity of $\text{RC}\equiv\text{CZ}^-$ ($\text{R} = \text{H}$ and Cl ; $\text{Z} = \text{O}, \text{S}$, and Se)
and the Influence of Leaving Group on the α -Effect in the E2 Reaction**

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Supporting Information Available:

Table S1: MP2/6-31+G (d) optimized structures and NPA charges of all E2 TS structures.

Table S1. Optimized E2 TS geometries by MP2/6-31+G(d) and NPA charges

$[\text{HO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.81341	0.140408	0.744705	-0.035773
H	0.13444	0.047182	1.369349	0.862829
H	0.13936	0.017563	1.356453	-0.937824
H	0.44948	1.477635	0.182485	-0.057285
C	0.17016	-0.76803	-0.397495	-0.007277
H	0.11762	-0.703831	-1.021829	-0.902865
H	0.11637	-0.658057	-1.014826	0.888925
O	-1.1576	2.601606	-0.295091	-0.070779
H	0.4033	3.053173	0.112804	0.69105
F	-0.55972	-2.25342	-0.078551	0.031078

$[\text{HS}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76815	-0.619082	0.894683	0.052401
H	0.15696	-0.593338	1.423359	1.005588
H	0.15619	-0.596066	1.534176	-0.830779
H	0.22982	1.131253	0.300908	-0.010589
C	0.07291	-1.318965	-0.305192	-0.020359
H	0.14073	-1.309467	-0.838648	-0.968257
H	0.13883	-1.310592	-0.949160	0.856631
S	-0.46098	2.516075	-0.094833	-0.033182
H	0.09070	2.235450	-1.328159	0.416126
F	-0.75701	-3.131795	-0.240233	-0.014452

$[\text{HSe}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.67800	-1.420415	0.882524	-0.000066
H	0.16399	-1.330793	1.453039	0.923106
H	0.16400	-1.330674	1.452706	-0.923430
H	0.18341	0.326856	0.262480	0.000227
C	0.02155	-2.116518	-0.300086	0.000103
H	0.15779	-2.214585	-0.866252	-0.918835
H	0.15779	-2.214706	-0.865916	0.919235
Se	-0.36103	1.869236	-0.039895	0.000007
H	0.04637	1.600630	-1.495603	-0.000400
F	-0.85587	-4.129906	-0.230963	-0.000041

$[\text{CH}_3\text{O}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.83731	0.461680	0.624208	0.000364
F	-0.57062	2.946543	0.083219	-0.000024
H	0.13847	0.490923	1.248726	-0.901348
H	0.13848	0.491074	1.248061	0.902531
H	0.47101	-0.837664	-0.168234	0.000223
C	0.16460	1.491146	-0.402362	-0.000111
H	0.11680	1.486138	-1.027271	0.897532
H	0.11680	1.485933	-1.026609	-0.898218
O	-0.95327	-1.858625	-0.715534	0.000021
C	-0.07527	-2.846756	0.276628	-0.000215
H	0.09039	-3.502813	0.209828	-0.887697
H	0.09036	-3.501909	0.211300	0.888063
H	0.10956	-2.397989	1.288653	-0.001266

$[\text{CH}_3\text{CH}_2\text{O}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.84856	-1.039753	0.286623	0.549420
F	-0.57692	-3.511166	0.288094	-0.077733
H	0.13915	-1.190028	0.024367	1.603926
H	0.13817	-0.896414	1.368442	0.433955
H	0.47970	0.251813	-0.424064	0.044037
C	0.16030	-2.080287	-0.236335	-0.315607
H	0.11705	-1.948619	0.025062	-1.369471
H	0.11709	-2.244729	-1.312029	-0.205677
O	-0.94446	1.238675	-0.898086	-0.270845
C	0.06928	2.241333	-0.264168	0.474530
H	0.11117	1.793338	0.309201	1.309043
H	0.09257	2.915534	-1.013952	0.927838
C	-0.51429	3.075220	0.688137	-0.384401
H	0.16484	2.428699	1.466265	-0.802853
H	0.13821	3.876982	1.166809	0.198502
H	0.15670	3.525442	0.136204	-1.216600

$[\text{FO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\#}$	NPA Charge	X	Y	Z
C	-0.75473	-0.495401	0.718449	0.362705
H	0.16146	-0.496676	1.010499	1.412210
H	0.16584	-0.271360	1.516558	-0.344496
H	0.51357	1.100139	-0.207981	0.245648
C	0.04872	-1.289304	-0.335716	-0.042319
H	0.15170	-1.278313	-0.629693	-1.086771
H	0.14966	-1.503641	-1.133168	0.661893
O	-0.35263	2.010930	-0.700723	0.256307
F	-0.81097	-3.171535	-0.029711	-0.192150
F	-0.27261	2.846051	0.335618	-0.347990

$[\text{ClO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\#}$	NPA Charge	X	Y	Z
C	-0.72496	1.152992	1.143504	0.220273
H	0.16397	1.313331	1.922738	-0.523436
H	0.16372	1.157054	1.472965	1.257956
H	0.52801	-0.645081	0.894441	-0.074241
C	0.03485	1.490498	-0.156120	-0.077959
H	0.15858	1.343764	-0.931435	0.664718
H	0.15707	1.488356	-0.486069	-1.110415
O	-0.77520	-1.663886	0.954037	-0.233389
F	-0.84167	3.409026	-0.632819	-0.043552
Cl	0.13561	-2.228736	-0.631404	0.070036

$[\text{BrO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\#}$	NPA Charge	X	Y	Z
C	-0.70162	-1.854366	1.252695	0.000381
H	0.16584	-1.998665	1.811368	0.923430
H	0.16584	-1.998937	1.812120	-0.922170
H	0.52793	-0.024432	1.185731	-0.000080
C	0.01905	-2.016959	-0.109252	-0.000154
H	0.16256	-1.901803	-0.670161	-0.919126
H	0.16258	-1.901565	-0.670928	0.918316
O	-0.83989	0.996281	1.337090	-0.000382
F	-0.86676	-3.922219	-0.829855	-0.000074
Br	0.20447	1.668088	-0.387337	0.000057

$[\text{HOO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.85701	0.589190	0.998298	0.238891
H	0.14826	0.804236	1.838624	-0.426508
H	0.15129	0.631037	1.260888	1.298557
H	0.50481	-1.134331	0.698973	-0.058646
C	0.11377	1.166429	-0.243302	-0.120601
H	0.12928	0.941547	-1.080480	0.541892
H	0.12361	1.098855	-0.511531	-1.177000
O	-0.56071	-2.148082	0.550268	-0.307527
O	-0.53045	-2.392573	-0.784133	0.275828
H	0.44392	-1.995530	-1.342634	-0.420556
F	-0.66677	2.827301	-0.391433	-0.023766

$[\text{HSO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{F}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76316	1.144287	1.094730	0.298674
H	0.16072	1.356052	1.939617	-0.356504
H	0.16012	1.128430	1.324184	1.363591
H	0.53213	-0.623395	0.922030	-0.117335
C	0.05849	1.526302	-0.173927	-0.103370
H	0.15056	1.316171	-1.011879	0.553563
H	0.14582	1.522240	-0.405716	-1.164508
H	0.04601	-1.827047	-1.379050	-0.793133
F	-0.79800	3.361761	-0.598068	-0.042530
S	0.28728	-2.260760	-0.545124	0.175895
O	-0.97997	-1.622459	0.898824	-0.386131

$[\text{HO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.74769	0.733449	0.756968	-0.037999
Cl	-0.37821	-2.095483	-0.042497	0.017407
H	0.14612	0.648320	1.384955	0.856590
H	0.15071	0.634287	1.366170	-0.942343
H	0.43302	1.984222	0.215864	-0.040875
C	-0.13638	-0.152111	-0.394075	-0.014558
H	0.16190	-0.090547	-1.015985	-0.906815
H	0.16112	-0.060626	-1.003676	0.883644
O	-1.19396	3.167528	-0.314643	-0.060167
H	0.40336	3.679294	0.114910	0.650562

$[\text{HS}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.71132	0.148921	0.768263	0.085701
Cl	-0.68223	-2.934751	-0.062514	-0.001858
H	0.18163	0.172299	1.239678	1.068170
H	0.18108	0.159085	1.477977	-0.742235
H	0.27054	1.504749	0.279107	-0.016995
C	-0.01132	-0.649955	-0.367415	-0.059527
H	0.17206	-0.713065	-0.826783	-1.040019
H	0.16983	-0.705377	-1.065571	0.768997
S	-0.65260	3.095067	-0.095931	-0.072013
H	0.08231	2.958215	-0.911850	0.988829

$[\text{HSe}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.68639	-0.706011	0.745727	-0.000044
Cl	-0.76238	-3.894648	-0.048739	-0.000004
H	0.18869	-0.662855	1.331009	0.917528
H	0.18869	-0.662850	1.330854	-0.917714
H	0.23862	0.674528	0.262551	0.000015
C	0.00310	-1.498350	-0.391331	0.000047
H	0.17482	-1.612055	-0.958602	-0.916306
H	0.17482	-1.612061	-0.958450	0.916494
Se	-0.55523	2.388336	-0.024262	0.000010
H	0.03526	2.107054	-1.480259	-0.000307

$[\text{CH}_3\text{O}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.75707	-0.138112	0.592507	0.000055
Cl	-0.39154	2.764016	0.065981	-0.000012
H	0.15143	-0.106653	1.215557	-0.900089
H	0.15143	-0.106630	1.215455	0.900268
H	0.43685	-1.335029	-0.103746	0.000041
C	-0.12942	0.847419	-0.468911	-0.000018
H	0.16132	0.838285	-1.087157	0.896861
H	0.16132	0.838263	-1.087055	-0.896967
O	-0.97766	-2.446925	-0.692834	0.000044
C	-0.06799	-3.434609	0.291540	-0.000044
H	0.08473	-4.095729	0.231507	-0.887463
H	0.08473	-4.095579	0.231817	0.887506
H	0.09188	-2.997979	1.313802	-0.000261

$[\text{CH}_3\text{CH}_2\text{O}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76214	-0.460790	-0.328571	0.492179
Cl	-0.40941	-3.363050	-0.176178	-0.072506
H	0.15272	-0.368945	-1.375548	0.184608
H	0.15315	-0.578178	-0.251875	1.578052
H	0.44279	0.727861	0.320192	0.145182
C	-0.11975	-1.454152	0.408943	-0.253544
H	0.16110	-1.568559	1.447899	0.052727
H	0.16123	-1.357005	0.328184	-1.335379
O	-0.96856	1.821719	0.852046	-0.130413
C	0.07847	2.813864	0.111432	0.508898
H	0.08184	3.419310	0.746214	1.188138
H	0.08930	2.365759	-0.681766	1.146725
C	-0.51181	3.763658	-0.557818	-0.488587
H	0.15610	4.228965	0.206076	-1.121001
H	0.13592	4.556016	-1.129297	0.019730
H	0.15905	3.197399	-1.235327	-1.136544

$[\text{FO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.77227	0.127489	0.978347	0.264664
Cl	-0.49889	-2.649755	-0.191005	0.003826
H	0.16454	0.098545	1.143811	1.344431
H	0.16076	-0.081082	1.894149	-0.295482
H	0.44157	1.506555	0.663236	-0.041166
C	-0.07796	-0.565583	-0.180509	-0.192288
H	0.16975	-0.385932	-1.092844	0.370873
O	-0.40817	2.677574	0.504272	-0.297250
F	-0.34278	2.851633	-0.870393	0.196299
H	0.16345	-0.548976	-0.348924	-1.266641

$[\text{ClO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76532	0.420336	1.122763	0.240548
Cl	-0.51759	3.088836	-0.301497	-0.011231
H	0.16585	0.681408	1.959591	-0.411768
H	0.16490	0.499128	1.382594	1.298564
H	0.45338	-0.990153	0.945913	-0.018672
C	-0.07169	0.986235	-0.131554	-0.123131
H	0.16525	0.912525	-0.402593	-1.173363
O	-0.82157	-2.167609	0.933338	-0.250419
Cl	0.05780	-2.675428	-0.659298	0.073902
H	0.16898	0.770606	-0.965951	0.538678

$[\text{BrO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76201	-1.144455	1.322207	0.000109
Cl	-0.54028	-3.640341	-0.424780	-0.000014
H	0.16712	-1.385027	1.879315	0.908158
H	0.16712	-1.385105	1.879523	-0.907792
H	0.45507	0.300022	1.262585	0.000003
C	-0.06253	-1.540540	-0.042368	-0.000031
H	0.16847	-1.337073	-0.607565	0.904855
O	-0.87700	1.495511	1.330041	-0.000113
H	0.16847	-1.337129	-0.607358	-0.905059
Br	0.11557	2.033600	-0.425846	0.000015

$[\text{HOO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76132	-0.117977	1.022676	0.221922
Cl	-0.44223	2.590973	-0.198368	0.005840
H	0.15603	0.131211	1.894685	-0.391153
H	0.15357	-0.038403	1.257816	1.288093
H	0.43392	-1.462287	0.746998	-0.043576
C	-0.09865	0.562493	-0.184199	-0.167728
H	0.16765	0.348669	-1.054248	0.448357
H	0.16351	0.500172	-0.424106	-1.227531
O	-0.61455	-2.675300	0.524604	-0.253324
O	-0.59234	-2.720359	-0.925910	0.067169
H	0.43442	-3.027729	-0.869315	0.990609

$[\text{HSO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76004	0.417908	1.106676	0.238345
Cl	-0.53154	3.106046	-0.294686	-0.002559
H	0.16705	0.685884	1.949959	-0.402943
H	0.16341	0.493295	1.356984	1.299240
H	0.45643	-0.970924	0.949573	-0.029038
C	-0.06151	0.990477	-0.142631	-0.131343
H	0.16991	0.780066	-0.983947	0.522023
H	0.16430	0.931743	-0.405631	-1.184356
O	-1.04097	-2.163553	0.908536	-0.257558
H	0.02734	-3.038502	-0.600161	1.303632
S	0.24561	-2.676639	-0.644355	-0.002913

$[\text{HCCO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.73213	0.253298	1.256344	0.037623
Cl	-0.72834	3.011716	-0.383269	-0.003813
H	0.18185	0.412213	1.868439	-0.849884
H	0.18193	0.384092	1.788937	0.979197
H	0.47833	-1.203434	1.052426	-0.001256
C	0.01183	0.681555	-0.067821	-0.013083
H	0.17538	0.615707	-0.605531	-0.951158
O	-0.83063	-2.382802	1.014007	-0.028506
H	0.17729	0.593409	-0.683215	0.873920
C	0.46320	-2.763833	-0.218992	-0.029461
C	-0.59592	-3.091263	-1.405318	0.065166
H	0.21720	-3.417278	-2.402820	-0.119407

$[\text{ClCCO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.72885	-1.659470	1.461917	0.017383
Cl	-0.74466	-3.720755	-1.020619	-0.004375
H	0.18327	-1.987692	1.947498	0.935844
H	0.18347	-1.974243	1.963853	-0.896789
H	0.48200	-0.201698	1.753923	0.037868
C	0.00907	-1.611815	0.073111	0.004907
H	0.17613	-1.359055	-0.456363	0.915427
O	-0.81056	0.912230	2.107964	0.047850
H	0.17823	-1.352779	-0.439692	-0.913248
C	0.45158	1.685516	1.075191	-0.006633
C	-0.41483	2.361247	0.064809	-0.222354
Cl	0.03516	3.422211	-1.196033	0.050156

$[\text{HCCS}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.67900	0.281190	-1.266547	0.000826
Cl	-0.89372	3.514305	0.110171	-0.000171
H	0.19602	0.349218	-1.843540	0.921544
H	0.19602	0.349497	-1.845107	-0.918888
H	0.25807	-1.148938	-1.044941	0.000233
C	0.05249	0.813881	0.004052	-0.000170
H	0.18557	0.942134	0.558540	0.918874
H	0.18556	0.942269	0.557051	-0.920094
C	-0.21097	-2.242590	0.916723	-0.000057
C	-0.35577	-1.622337	1.985662	0.000534
H	0.22496	-1.257663	2.989175	-0.000080
S	-0.15924	-2.706284	-0.692714	-0.000343

$[\text{ClCCS}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.66709	-0.854805	-1.827634	0.003116
Cl	-0.90844	-3.758466	0.199372	-0.000920
H	0.19684	-1.043694	-2.379256	-0.916088
H	0.19664	-1.039515	-2.374742	0.925821
H	0.24995	0.608350	-1.935306	-0.002370
C	0.03346	-1.091390	-0.472374	0.000174
H	0.18757	-1.122442	0.092567	-0.921486
H	0.18776	-1.121075	0.096694	0.919285
C	-0.21910	2.053920	-0.232215	-0.001371
C	-0.22184	1.569037	0.907271	0.021964
S	-0.12502	2.185401	-1.900531	-0.003728
Cl	0.08926	1.328548	2.545231	-0.004304

$[\text{HCCSe}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.65839	-0.996199	-1.199676	0.002193
Cl	-0.87963	-4.226145	0.108715	-0.000336
H	0.19248	-1.010707	-1.781446	-0.917574
H	0.19245	-1.010048	-1.776661	0.924974
H	0.22213	0.480575	-0.862824	0.000561
C	0.02033	-1.574387	0.046051	-0.000771
H	0.18376	-1.687962	0.603108	-0.921317
H	0.18376	-1.687673	0.607573	0.917083
C	-0.28559	1.682531	1.245645	-0.001093
C	-0.32857	1.392462	2.441278	-0.000343
H	0.22214	1.132747	3.476448	0.009680
Se	-0.06486	2.135326	-0.509240	-0.000223

$[\text{ClCCSe}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.65126	-1.667175	-1.482167	0.000195
Cl	-0.87936	-4.436287	0.616303	-0.000035
H	0.19171	-1.828118	-2.038505	-0.921230
H	0.19171	-1.827953	-2.038149	0.921864
H	0.21691	-0.132285	-1.541160	0.000055
C	0.00726	-1.893764	-0.128898	-0.000046
H	0.18362	-1.855508	0.440326	-0.919664
H	0.18362	-1.855376	0.440678	0.919349
C	-0.28328	1.633795	0.149357	0.000012
C	-0.20741	1.710171	1.375676	-0.000092
Se	-0.04235	1.543196	-1.663117	-0.000027
Cl	0.08883	1.867605	3.018932	0.000042

$[\text{HCC}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Cl}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.76425	-0.177019	0.874931	-0.000533
C	-0.09966	0.600156	-0.325220	0.000613
H	0.32017	-1.531490	0.455437	0.001236
Cl	-0.45650	2.651257	-0.151229	-0.000227
H	0.16341	0.515514	-0.929534	0.902392
H	0.16342	0.514859	-0.931711	-0.899636
H	0.16055	-0.095232	1.481116	-0.907625
H	0.16055	-0.094442	1.483312	0.905022
C	-0.31765	-2.915485	0.118761	0.001669
C	-0.51710	-4.060554	-0.374145	-0.000843
H	0.18707	-5.063157	-0.753689	-0.002967

$[\text{HO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.71905	-1.441980	0.813495	0.031612
H	0.15327	-1.345122	1.435766	-0.864052
H	0.15618	-1.341152	1.418577	0.937185
H	0.42068	-2.628549	0.283948	0.024553
C	-0.14844	-0.591694	-0.359639	0.014983
H	0.17131	-0.648271	-0.975679	0.910140
H	0.17109	-0.666971	-0.964052	-0.886592
O	-1.22221	-3.838911	-0.364338	0.048827
H	0.39692	-4.473912	0.094558	-0.532731
Br	-0.37974	1.543352	-0.031473	-0.007391

$[\text{HS}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.70436	0.988957	0.770875	0.079030
Br	-0.65759	-2.234025	-0.030253	0.000670
H	0.18489	1.003067	1.245011	1.060388
H	0.18459	0.989957	1.481863	-0.747830
H	0.27969	2.295349	0.286851	-0.018359
C	-0.02888	0.187664	-0.366530	-0.065372
H	0.17590	0.118953	-0.825830	-1.045886
H	0.17376	0.127922	-1.063856	0.763939
S	-0.68866	3.925101	-0.102405	-0.072186
H	0.08065	3.794296	-0.852777	1.037334

$[\text{HSe}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.68924	-0.159078	0.734280	-0.000003
Br	-0.73107	3.162194	-0.020379	-0.000009
H	0.19204	-0.189046	1.322713	-0.916348
H	0.19204	-0.189011	1.322836	0.916266
H	0.25029	-1.491885	0.267651	0.000055
C	-0.00881	0.641983	-0.401774	0.000060
H	0.17741	0.754552	-0.970143	0.916619
H	0.17741	0.754520	-0.970266	-0.916428
Se	-0.59341	-3.243278	-0.022915	-0.000002
H	0.03334	-2.941887	-1.475430	-0.000137

$[\text{CH}_3\text{O}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.72477	-0.902732	-0.667797	0.000000
H	0.15732	-0.833324	-1.285110	0.900613
H	0.15732	-0.833324	-1.285110	-0.900613
H	0.41786	-2.064721	-0.055295	0.000000
C	-0.14767	0.000000	0.463410	0.000000
H	0.17037	-0.034509	1.075740	-0.899034
H	0.17037	-0.034509	1.075740	0.899034
O	-0.99780	-3.243661	0.574399	0.000000
C	-0.06248	-4.243320	-0.391549	0.000000
H	0.08011	-4.907395	-0.326824	0.887284
H	0.08011	-4.907395	-0.326824	-0.887284
H	0.08052	-3.828490	-1.426195	0.000000
Br	-0.38124	2.121979	0.043837	0.000000

$[\text{CH}_3\text{CH}_2\text{O}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.73022	0.375387	-0.338725	0.566000
H	0.15850	0.430872	-1.389555	0.266920
H	0.15898	0.244079	-0.245473	1.647893
H	0.42408	1.518843	0.247650	0.236767
C	-0.13923	-0.561006	0.440591	-0.207838
H	0.17010	-0.649979	1.483454	0.089897
H	0.17027	-0.464107	0.338930	-1.286932
O	-0.98817	2.665939	0.817635	-0.088620
C	0.08338	3.688293	0.081395	0.495371
H	0.07860	4.296243	0.698076	1.192167
H	0.07721	3.282528	-0.756374	1.109436
C	-0.51198	4.637717	-0.520635	-0.546472
H	0.15595	5.072176	0.282089	-1.152270
H	0.13458	5.452932	-1.093850	-0.077065
H	0.15692	4.076285	-1.183041	-1.214256
Br	-0.39897	-2.669421	-0.082821	-0.055599

$[\text{FO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.74729	0.933211	1.158612	0.000330
H	0.16609	0.789568	1.751274	0.906854
H	0.16608	0.789394	1.752055	-0.905656
H	0.42519	2.258566	0.776649	-0.000023
C	-0.08445	0.281481	-0.109149	-0.000169
H	0.17488	0.378417	-0.703732	-0.903984
H	0.17489	0.378556	-0.704518	0.903114
O	-0.42177	3.486573	0.446153	-0.000391
F	-0.35700	3.287246	-1.011730	0.000256
Br	-0.49662	-1.981727	-0.103776	-0.000013

$[\text{ClO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.74150	-0.421969	1.310456	0.000402
H	0.16873	-0.231052	1.889846	-0.905523
H	0.16872	-0.231190	1.889085	0.906842
H	0.43312	-1.777186	1.072212	0.000066
C	-0.09105	0.123503	-0.006742	-0.000103
H	0.17479	-0.014184	-0.592569	0.903952
H	0.17478	-0.014205	-0.591887	-0.904598
O	-0.83527	-3.030331	0.919475	-0.000454
Cl	0.04684	-3.243720	-0.766188	0.000126
Br	-0.49917	2.384129	-0.166274	-0.000030

$[\text{BrO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.74225	0.312822	1.459918	0.000271
H	0.17052	0.545697	2.022060	-0.906575
H	0.17050	0.546095	2.022104	0.906992
H	0.43644	-1.062305	1.344564	0.000346
C	-0.08511	0.751831	0.105701	0.000268
H	0.17516	0.579035	-0.467757	0.905807
H	0.17517	0.578672	-0.467903	-0.905111
O	-0.88881	-2.317254	1.319280	-0.000370
Br	0.10380	-2.696126	-0.472896	0.000022
Br	-0.51543	3.009352	-0.224276	-0.000071

$[\text{HOO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.73146	-0.916039	1.162082	0.045940
H	0.16305	-0.729654	1.797557	-0.824106
H	0.15932	-0.747308	1.707596	0.978698
H	0.41527	-2.198728	0.841265	0.001754
C	-0.09576	-0.267346	-0.118228	-0.012921
H	0.17009	-0.384728	-0.755903	0.858433
H	0.17713	-0.383629	-0.670899	-0.940513
O	-0.62797	-3.474535	0.462447	-0.044506
Br	-0.45645	1.959518	-0.104099	-0.002135
O	-0.60398	-3.215600	-1.000983	-0.082100
H	0.43074	-3.517704	-1.230996	0.815169

$[\text{HSO}\cdots\text{H}\cdots\text{CH}_2\text{CH}_2\cdots\text{Br}]^{-\ddagger}$	NPA Charge	X	Y	Z
C	-0.73665	-0.426748	1.271424	0.108794
H	0.17187	-0.205072	1.951873	-0.716345
H	0.16850	-0.267898	1.742267	1.081458
H	0.43499	-1.759422	1.063365	0.008054
C	-0.07166	0.125293	-0.034659	-0.024718
H	0.17455	-0.008119	-0.718488	0.807086
H	0.17407	0.022927	-0.518576	-0.990971
O	-1.05686	-3.025265	0.901254	-0.105823
Br	-0.52785	2.414421	-0.161175	-0.006412
H	0.02284	-3.527518	-0.931939	1.266461
S	0.24621	-3.296799	-0.723626	-0.055576