

Exploring the Reactivity Trends

in the E2 and S_N2 Reactions of X⁻ + CH₃CH₂Cl

(X = F, Cl, Br, HO, HS, HSe, NH₂, PH₂, AsH₂, CH₃, SiH₃, and GeH₃)

Xiao-Peng Wu,^{1,2} Xiao-Ming Sun,² Xi-Guang Wei,² Yi Ren,²

Ning-Bew Wong,¹ Wai-Kee Li,³

¹ Department of Biology and Chemistry, City University of Hong Kong, Kowloon, Hong Kong ² College of Chemistry, Key Laboratory of Green Chemistry and Technology, Ministry of Education, and Key State Laboratory of Biotherapy, Sichuan University, Chengdu 610064, P. R. China

³ Department of Chemistry, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong

*Corresponding authors: Y. Ren, fax: +86-28-85412907; e-mail: yiren57@hotmail.com;

N. B. Wong, +852-2788 7406; e-mail: bhnbwong@cityu.edu.hk;

Supporting Information

MP2/6-31+G* Optimized Geometries and G2(+) enthalpies (hartree, 298.15K)

G2(+) enthalpies (hartree, 298.15K)

Reactants and Products			
F ⁻	-99.758239	NH ₃	-56.453339
Cl ⁻	-459.806636	PH ₃	-342.673982
Br ⁻	-2572.656049	AsH ₃	-2236.073445
HO ⁻	-75.708872	CH ₄	-40.404636
HS ⁻	-398.367905	SiH ₄	-291.413199
HSe ⁻	-2400.623758	GeH ₄	-2077.793461
NH ₂ ⁻	-55.812456	CH ₃ CH ₂ ⁺	-78.666142
PH ₂ ⁻	-342.090182	CH ₂ =CH ₂	-78.410093
AsH ₂ ⁻	-2235.504253	CH ₃ CH ₂ F	-178.776965
CH ₃ ⁻	-39.741760	CH ₃ CH ₂ Br	-2651.609922
SiH ₃ ⁻	-290.820317	CH ₃ CH ₂ OH	-154.756140
GeH ₃ ⁻	-2077.217760	CH ₃ CH ₂ SH	-477.365272
CH ₃ CH ₂ Cl	-538.774210	CH ₃ CH ₂ SeH	-2479.606759
HF	-100.346490	CH ₃ CH ₂ NH ₂	-134.885172
HCl	-460.336571	CH ₃ CH ₂ PH ₂	-421.120784
HBr	-2573.169607	CH ₃ CH ₂ AsH ₂	-2314.519273
H ₂ O	-76.327843	CH ₃ CH ₂ CH ₃	-118.845190
H ₂ S	-398.926224	CH ₃ CH ₂ SiH ₃	-369.867252
H ₂ Se	-2401.165731	CH ₃ CH ₂ GeH ₃	-2156.242734

E2 and S _N 2 TS			
<i>anti</i> -E2 TS	[X...H...CH ₂ CH ₂ ...Cl] ^{-‡}	backside-S _N 2 TS	[X...Et...Cl] ^{-‡}
X=F	-638.555943	X=F	-638.552556
Cl	-998.557500	Cl	-998.573960
Br	-3111.394656	Br	-3111.416930
HO	-614.507260	HO	-614.504710
HS	-937.124731	HS	-937.141071
HSe	-2939.370572	HSe	-2939.391321
NH ₂	-594.605888	NH ₂	-594.605824
PH ₂	-880.850951	PH ₂	-880.866725
AsH ₂	-2774.257672	AsH ₂	-2774.276526
CH ₃	-578.529779	CH ₃	-578.532491
SiH ₃	-829.5745947	SiH ₃	-829.592552
GeH ₃	-2615.966175	GeH ₃	-2615.985560
<i>syni</i> -E2 TS		frontside-S _N 2 TS	
X = F	-638.538799	X = F	-638.488112

MP2/6-31+G* Optimized Geometries

HO ⁻	8	0.000000	0.000000	0.108608
	1	0.000000	0.000000	-0.868864
HS ⁻	16	0.000000	0.000000	0.079563
	1	0.000000	0.000000	-1.273010
HSe ⁻	34	0.000000	0.000000	-0.042570
	1	0.000000	0.000000	1.447368
NH ₂ ⁻	7	0.000000	0.000000	0.141139
	1	0.000000	0.814787	-0.493987
	1	0.000000	-0.814787	-0.493987
PH ₂ ⁻	15	0.000000	0.000000	0.116565
	1	0.000000	1.035486	-0.874235
	1	0.000000	-1.035486	-0.874235
AsH ₂ ⁻	33	0.000000	0.000000	0.061894
	1	0.000000	1.110584	-1.021259
	1	0.000000	-1.110584	-1.021259
CH ₃ ⁻	6	0.000000	0.000000	0.114631
	1	0.000000	1.046151	-0.229262
	1	0.905994	-0.523076	-0.229262
	1	-0.905994	-0.523076	-0.229262
SiH ₃ ⁻	14	0.000000	0.000000	0.138234
	1	0.000000	1.323913	-0.645090
	1	-1.146542	-0.661956	-0.645090
	1	1.146542	-0.661956	-0.645090
GeH ₃ ⁻	32	0.000000	0.000000	0.074013
	1	0.000000	1.376826	-0.789469
	1	-1.192366	-0.688413	-0.789469
	1	1.192366	-0.688413	-0.789469

CH ₃ CH ₂ ⁺	6	0.000000	0.691114	-0.062399
	1	-0.936037	1.245855	-0.074087
	1	0.936037	1.245855	-0.074087
	1	0.000000	0.000000	1.045142
	6	0.000000	-0.691114	-0.062399
	1	0.936037	-1.245855	-0.074087
	1	-0.936037	-1.245855	-0.074087
HF	9	0.000000	0.000000	0.094089
	1	0.000000	0.000000	-0.846797
HCl	17	0.000000	0.000000	0.071168
	1	0.000000	0.000000	-1.209856
HBr	35	0.000000	0.000000	0.039875
	1	0.000000	0.000000	-1.395626
H ₂ O	8	0.000000	0.000000	0.117643
	1	0.000000	0.772406	-0.470573
	1	0.000000	-0.772406	-0.470573
H ₂ S	16	0.000000	0.000000	0.102090
	1	0.000000	0.974867	-0.816723
	1	0.000000	-0.974867	-0.816723
H ₂ Se	34	0.000000	0.000000	0.057385
	1	0.000000	1.058494	-0.975549
	1	0.000000	-1.058494	-0.975549
NH ₃	7	0.000000	0.000000	-0.109146
	1	0.000000	0.949635	0.254675
	1	0.822408	-0.474817	0.254675
	1	-0.822408	-0.474817	0.254675
PH ₃	15	0.000000	0.000000	0.124033
	1	0.000000	1.202340	-0.620164
	1	-1.041257	-0.601170	-0.620164
	1	1.041257	-0.601170	-0.620164

AsH ₃	33	0.000000	0.000000	0.070897
	1	0.000000	1.276258	-0.779870
	1	-1.105271	-0.638129	-0.779870
	1	1.105271	-0.638129	-0.779870
CH ₄	6	0.000000	0.000000	0.000000
	1	0.630065	0.630065	0.630065
	1	-0.630065	-0.630065	0.630065
	1	-0.630065	0.630065	-0.630065
	1	0.630065	-0.630065	-0.630065
SiH ₄	14	0.000000	0.000000	0.000000
	1	0.855825	0.855825	0.855825
	1	-0.855825	-0.855825	0.855825
	1	-0.855825	0.855825	-0.855825
	1	0.855825	-0.855825	-0.855825
GeH ₄	32	0.000000	0.000000	0.000000
	1	0.894039	0.894039	0.894039
	1	-0.894039	-0.894039	0.894039
	1	-0.894039	0.894039	-0.894039
	1	0.894039	-0.894039	-0.894039
CH ₃ CH ₂ F	6	1.192368	-0.228134	0.000000
	1	2.045820	0.458343	-0.000012
	1	1.253788	-0.860876	-0.888623
	1	1.253796	-0.860856	0.888636
	6	-0.095816	0.557639	0.000000
	1	-0.205324	1.178236	-0.892771
	1	-0.205321	1.178230	0.892774
	9	-1.191341	-0.341123	0.000000
	CH ₃ CH ₂ Cl	6	-1.601579	-0.355747
1		-2.562532	0.170140	-0.000235
1		-1.554825	-0.992519	0.886760
1		-1.554565	-0.992850	-0.886510

Continued:	6	-0.473394	0.656760	0.000000
	1	-0.506298	1.291232	0.887036
	1	-0.506279	1.291171	-0.887078
	17	1.125549	-0.151368	0.000001
CH ₃ CH ₂ Br	6	2.075465	-0.400514	0.000000
	1	3.068610	0.063965	-0.000022
	1	1.988028	-1.032762	-0.886998
	1	1.988055	-1.032736	0.887019
	6	1.020413	0.686688	0.000000
	1	1.076507	1.315235	-0.889573
	1	1.076510	1.315240	0.889570
	35	-0.793514	-0.067028	0.000000
CH ₃ CH ₂ OH	6	1.217173	-0.226848	0.000008
	1	1.271750	-0.862440	0.887535
	1	2.075966	0.452298	-0.000043
	1	1.271718	-0.862533	-0.887459
	6	-0.076376	0.557406	-0.000005
	1	-0.139030	1.197643	-0.890091
	1	-0.139063	1.197700	0.890040
	8	-1.148773	-0.398313	-0.000011
	1	-1.995945	0.080482	0.000089
CH ₃ CH ₂ SH	6	1.628460	-0.334224	0.000087
	1	2.588329	0.191192	-0.000117
	1	1.589748	-0.973632	-0.886543
	1	1.589835	-0.973177	0.887041
	6	0.483738	0.671418	-0.000106
	1	0.542936	1.306968	-0.887505
	1	0.542844	1.307169	0.887156
	16	-1.101458	-0.232796	-0.000053
	1	-1.903554	0.843048	0.000932

CH ₃ CH ₂ SeH	6	-2.077468	-0.375912	-0.000122
	1	-3.070620	0.084945	-0.000259
	1	-1.998469	-1.010818	0.887418
	1	-1.998221	-1.010682	-0.887756
	6	-1.007808	0.709227	0.000160
	1	-1.099250	1.338262	0.888857
	1	-1.099057	1.338556	-0.888344
	34	0.771832	-0.114557	0.000033
	1	1.534985	1.154773	-0.001259
CH ₃ CH ₂ NH ₂	6	1.241005	-0.241258	-0.029192
	1	2.118366	0.407692	0.058038
	1	1.286471	-0.774118	-0.982590
	1	1.288892	-0.979934	0.778754
	6	-0.044819	0.566819	0.056282
	1	-0.075932	1.299979	-0.756183
	1	-0.063010	1.129856	1.003207
	7	-1.201731	-0.321430	-0.115910
	1	-2.072646	0.207374	-0.101252
	1	-1.247135	-0.994207	0.648862
CH ₃ CH ₂ PH ₂	6	-1.524446	0.747034	0.000000
	1	-1.979262	1.744027	0.000000
	1	-1.884989	0.211659	0.883958
	1	-1.884989	0.211659	-0.883958
	6	0.000000	0.839187	0.000000
	1	0.346531	1.400891	0.875645
	1	0.346531	1.400891	-0.875645
	1	0.189173	-1.401824	-1.042742
	1	0.189173	-1.401824	1.042742
	15	0.921634	-0.778854	0.000000

CH ₃ CH ₂ AsH ₂	6	0.400238	-2.130805	0.000000
	1	-0.073714	-3.119285	0.000000
	1	1.040731	-2.063865	0.884979
	1	1.040731	-2.063865	-0.884979
	6	-0.651902	-1.025702	0.000000
	1	-1.304204	-1.115823	0.876990
	1	-1.304204	-1.115823	-0.876990
	1	1.055323	0.625331	-1.099262
	1	1.055323	0.625331	1.099262
	33	0.000000	0.823244	0.000000
	CH ₃ CH ₂ CH ₃	6	1.268272	-0.260719
1		2.169755	0.360486	-0.000611
1		1.303504	-0.906164	-0.884479
1		1.304010	-0.905155	0.885200
6		-0.000022	0.589699	-0.000001
1		-0.000071	1.245998	-0.878753
1		-0.000060	1.246372	0.878469
6		-1.268253	-0.260746	0.000005
1		-2.169759	0.360424	-0.000749
1		-1.304000	-0.905073	0.885278
1		-1.303364	-0.906297	-0.884405
CH ₃ CH ₂ SiH ₃	6	-1.705430	-0.350519	0.000003
	1	-2.683453	0.141557	0.000381
	1	-1.660005	-0.995912	0.883360
	1	-1.660237	-0.995109	-0.883913
	6	-0.563259	0.675260	0.000063
	1	-0.648353	1.329049	0.877212
	1	-0.648345	1.328801	-0.877354
	14	1.148071	-0.122099	0.000004
	1	2.220525	0.908027	-0.000776
	1	1.309140	-0.978220	-1.205813

Continued:	1	1.309872	-0.977254	1.206455
CH ₃ CH ₂ GeH ₃	6	-2.148793	-0.358782	-0.000029
	1	-3.127758	0.132066	0.000657
	1	-2.100224	-1.002839	0.884278
	1	-2.101026	-1.002069	-0.884911
	6	-1.018330	0.674915	-0.000086
	1	-1.108116	1.327498	0.877359
	1	-1.108607	1.328051	-0.877053
	32	0.771941	-0.058400	-0.000015
	1	1.836945	1.081407	0.000116
	1	1.005329	-0.946397	-1.260475
	1	1.004093	-0.945705	1.261216
H ₂ C=CH ₂	6	0.000000	0.000000	0.669983
	6	0.000000	0.000000	-0.669983
	1	0.000000	0.924580	1.239408
	1	0.000000	-0.924580	1.239408
	1	0.000000	-0.924580	-1.239408
	1	0.000000	0.924580	-1.239408

<i>syn</i> -E2-TS	6	0.019339	0.157929	0.019241
X = F	17	0.059042	0.500882	2.980714
	1	1.448198	-0.153471	0.263506
	1	0.174023	0.980913	-0.681940
	1	-0.245957	-0.780606	-0.472335
	6	-0.822859	0.491714	1.136756
	1	-1.190838	1.515253	1.189145
	1	-1.604668	-0.220671	1.395717
	9	2.529956	-0.414011	0.240430

front-side-S _N 2 TS X = F	1	-1.060661	0.327412	1.453187
	6	-0.648031	-0.313745	0.680907
	1	-0.093684	-1.133879	1.131784
	9	-0.681865	1.484199	-0.102393
	17	1.544449	-0.172779	-0.098802
	6	-1.600000	-0.812272	-0.364243
	1	-1.044422	-1.048643	-1.275293
	1	-2.074798	-1.742916	-0.008303
	1	-2.357100	-0.066414	-0.600186
<i>anti</i> -E2 TS [F···H···CH ₂ CH ₂ ···Cl] [‡]	6	-0.677049	-0.866248	0.000000
	17	2.113531	0.347006	0.000000
	1	-0.556846	-1.462971	0.907000
	1	-0.556846	-1.462971	-0.907000
	1	-2.046374	-0.452229	0.000000
	6	0.000000	0.384612	0.000000
	1	-0.097115	0.980202	-0.903950
	1	-0.097115	0.980202	0.903950
	9	-3.168158	-0.176835	0.000000
[Cl···H···CH ₂ CH ₂ ···Cl] [‡]	6	-0.223860	0.825741	0.000003
	17	2.998348	-0.081440	-0.000007
	1	-0.283313	1.405325	-0.919212
	1	-0.283296	1.405362	0.919197
	1	-1.588317	0.218268	0.000030
	6	0.522475	-0.332409	0.000021
	1	0.647352	-0.893487	0.917410
	1	0.647335	-0.893526	-0.917347
	17	-3.053140	-0.165732	-0.000006
[Br···H···CH ₂ CH ₂ ···Cl] [‡]	6	0.633018	0.873322	0.000002
	17	3.993129	-0.106903	-0.000004
	1	0.539081	1.442739	-0.921801
	1	0.539084	1.442752	0.921797

Continued:	1	-0.770947	0.224926	0.000010
	6	1.355756	-0.288881	0.000010
	1	1.532195	-0.831420	0.919509
	1	1.532192	-0.831436	-0.919479
	35	-2.376784	-0.089624	-0.000001
[HO...H...CH ₂ CH ₂ ...Cl] ^{-#}	6	0.733449	0.756968	-0.037999
	17	-2.095483	-0.042497	0.017407
	1	0.648320	1.384955	0.856590
	1	0.634287	1.366170	-0.942343
	1	1.984222	0.215864	-0.040875
	6	-0.152111	-0.394075	-0.014558
	1	-0.090547	-1.015985	-0.906815
	1	-0.060626	-1.003676	0.883644
	8	3.167528	-0.314643	-0.060167
	1	3.679294	0.114910	0.650562
[HS...H...CH ₂ CH ₂ ...Cl] ^{-#}	6	0.148921	0.768263	0.085701
	17	-2.934751	-0.062514	-0.001858
	1	0.172299	1.239678	1.068170
	1	0.159085	1.477977	-0.742235
	1	1.504749	0.279107	-0.016995
	6	-0.649955	-0.367415	-0.059527
	1	-0.713065	-0.826783	-1.040019
	1	-0.705377	-1.065571	0.768997
	16	3.095067	-0.095931	-0.072013
	1	2.958215	-0.911850	0.988829
[HSe...H...CH ₂ CH ₂ ...Cl] ^{-#}	6	-0.706011	0.745727	-0.000044
	17	-3.894648	-0.048739	-0.000004
	1	-0.662855	1.331009	0.917528
	1	-0.662850	1.330854	-0.917714
	1	0.674528	0.262551	0.000015
	6	-1.498350	-0.391331	0.000047

Continued:	1	-1.612055	-0.958602	-0.916306
	1	-1.612061	-0.958450	0.916494
	34	2.388336	-0.024262	0.000010
	1	2.107054	-1.480259	-0.000307
[H ₂ N...H...CH ₂ CH ₂ ...Cl] ^{-#}	6	0.685400	0.763560	-0.035955
	17	-2.115013	-0.054545	0.015835
	1	0.591959	1.394432	0.855617
	1	0.584151	1.373322	-0.940415
	1	1.918824	0.279642	-0.022004
	6	-0.206312	-0.392500	-0.015440
	1	-0.124283	-1.016200	-0.906689
	1	-0.093634	-1.006224	0.879276
	1	3.472759	-0.935429	-0.639144
	1	3.617909	-0.437653	0.916261
	7	3.301857	-0.135854	-0.014820
[H ₂ P...H...CH ₂ CH ₂ ...Cl] ^{-#}	6	-0.093521	0.659921	0.000009
	17	2.950630	-0.009146	0.000000
	1	-0.105982	1.265471	-0.908281
	1	-0.105982	1.265461	0.908299
	1	-1.403320	0.166479	0.000000
	6	0.789320	-0.441278	0.000000
	1	0.834681	-1.036078	0.908219
	1	0.834681	-1.036068	-0.908231
	1	-3.501551	0.698007	-1.042471
	15	-3.159100	-0.211833	-0.000011
	1	-3.501531	0.697847	1.042589
[H ₂ As...H...CH ₂ CH ₂ ...Cl] ^{-#}	6	-0.001291	-0.021448	-0.001474
	6	0.000268	0.011548	1.400190
	1	1.317120	-0.016352	-0.467105
	17	-2.049310	0.002541	2.425069
	1	0.310179	-0.883316	1.930937

Continued:	1	0.280541	0.939969	1.888063
	1	-0.370356	0.871121	-0.508150
	1	-0.341658	-0.947975	-0.465873
	1	2.502082	1.292705	-2.178533
	1	2.213708	-0.851141	-2.595751
	33	2.884422	-0.026796	-1.476950
[H ₃ C...H...CH ₂ CH ₂ ...Cl] [≠]	6	0.633380	0.792457	-0.000030
	17	-2.151792	-0.067093	0.000015
	1	0.536460	1.410024	0.900180
	1	0.536370	1.410080	-0.900192
	1	1.851768	0.342399	-0.000197
	6	-0.245824	-0.375522	-0.000031
	1	-0.132443	-0.992311	-0.892927
	1	-0.132415	-0.992346	0.892836
	6	3.391757	-0.229056	-0.000019
	1	3.960749	0.086598	-0.892135
	1	3.326712	-1.332410	-0.003433
	1	3.957380	0.081270	0.896095
[H ₃ Si...H...CH ₂ CH ₂ ...Cl] [≠]	6	-0.008998	0.717454	0.000011
	6	0.843013	-0.409848	0.000013
	1	-1.345312	0.302551	0.000027
	17	3.005489	-0.041669	-0.000006
	1	0.865578	-1.006846	0.907988
	1	0.865561	-1.006863	-0.907951
	1	-0.003206	1.323716	-0.908218
	1	-0.003186	1.323733	0.908229
	1	-4.067523	0.341517	1.173947
	1	-4.067971	0.343566	-1.172864
	1	-3.419781	-1.584308	-0.001265
	14	-3.208683	-0.083881	0.000005

[H ₃ Ge...H...CH ₂ CH ₂ ...Cl] [‡]	6	0.823023	0.677529	0.000059
	6	1.669169	-0.440385	0.000085
	1	-0.524724	0.257879	0.000188
	17	3.911046	-0.021160	-0.000042
	1	1.736948	-1.025534	0.912043
	1	1.736854	-1.025650	-0.911806
	1	0.807990	1.278248	-0.910654
	1	0.808103	1.278369	0.910695
	1	-3.454937	1.153081	-0.000536
	1	-2.918122	-0.906433	-1.226106
	1	-2.918934	-0.906085	1.226012
	32	-2.397316	-0.036469	0.000000
	backside-S _N 2 TS [F...Et...Cl] [‡]	6	-0.616447	1.273045
17		1.801977	-0.235534	0.000001
1		-0.159992	1.725670	-0.883997
1		-0.160039	1.725655	0.884024
1		-1.692706	1.454743	-0.000024
6		-0.408095	-0.213316	-0.000001
1		-0.452956	-0.767326	0.919146
1		-0.452936	-0.767349	-0.919143
9		-2.396414	-0.636188	0.000000
[Cl...Et...Cl] [‡]	6	-0.481336	-1.361603	0.000000
	17	2.312177	-0.505229	0.000000
	1	-0.102991	-1.880434	0.882877
	1	-0.102991	-1.880434	-0.882877
	1	-1.571669	-1.393934	0.000000
	6	0.000000	0.062823	0.000000
	1	0.204533	0.578980	-0.919085
	1	0.204533	0.578980	0.919085
	17	-2.061788	1.198730	0.000000

[Br...Et...Cl] ^{-‡}	6	1.493715	0.831304	0.000000
	17	-0.485989	2.989886	0.000000
	1	1.788978	1.402802	0.882198
	1	1.788978	1.402802	-0.882198
	1	2.013587	-0.127065	0.000000
	6	0.000000	0.635854	0.000000
	1	-0.556621	0.615319	-0.918479
	1	-0.556621	0.615319	0.918479
	35	-0.147965	-1.815434	0.000000
	[HO...Et...Cl] ^{-‡}	1	-0.203162	3.125752
8		-0.868443	2.408376	0.000000
6		-1.392092	-0.175139	0.000000
17		1.168574	-1.425568	0.000000
1		-1.554268	-0.797210	0.884812
1		-1.554268	-0.797210	-0.884812
1		-2.088000	0.667421	0.000000
6		0.000000	0.385089	0.000000
1		0.417017	0.754597	-0.918984
1		0.417017	0.754597	0.918984
[HS...Et...Cl] ^{-‡}	1	-2.730036	-1.244562	0.000000
	6	1.280693	-0.679780	0.000000
	17	0.942126	2.172647	0.000000
	1	1.871411	-0.425244	0.883046
	1	1.871411	-0.425244	-0.883046
	1	1.088173	-1.754270	0.000000
	6	0.000000	0.114161	0.000000
	1	-0.504371	0.336421	-0.921651
	1	-0.504371	0.336421	0.921651
	16	-1.549533	-1.897800	0.000000

[HSe...Et...Cl] ^{-#}	6	0.000000	0.768893	0.000000
	17	-0.386488	2.988604	0.000000
	1	-1.640874	-1.959329	0.000000
	1	-0.542004	0.665786	0.921447
	1	-0.542004	0.665786	-0.921447
	34	-0.159352	-1.836556	0.000000
	6	1.507907	0.838604	0.000000
	1	1.967859	-0.151445	0.000000
	1	1.848926	1.385424	-0.882604
	1	1.848926	1.385424	0.882604
	[H ₂ N...Et...Cl] ^{-#}	17	-1.837788	-0.296878
6		0.261439	-0.173388	0.003077
1		0.437289	-0.725579	-0.904626
7		2.618581	-0.519033	-0.077840
1		2.888721	-1.507245	-0.208922
1		0.417164	-0.715631	0.918304
1		3.071753	-0.254863	0.812056
6		0.485344	1.314810	-0.024855
1		-0.095409	1.768389	-0.833609
1		0.162836	1.772494	0.915821
1		1.549280	1.494054	-0.193638
[H ₂ P...Et...Cl] ^{-#}	17	-2.387987	-0.387532	0.022153
	6	-0.216195	-0.108648	-0.058397
	1	-0.096912	-0.613324	-1.002297
	1	2.997089	-1.514304	0.429969
	1	-0.042099	-0.694052	0.825839
	1	2.587094	0.377971	1.177341
	6	-0.157392	1.398129	-0.009120
	1	-0.879056	1.814250	-0.716958
	1	-0.426474	1.749426	0.990928
	1	0.834294	1.782819	-0.261422

Continued:	15	2.524225	-0.270109	-0.094326
[H ₂ As...Et...Cl] ^{-#}	17	-3.029719	-0.436609	0.010958
	6	-0.897419	-0.061438	-0.019312
	1	-0.723162	-0.583078	-0.944783
	1	2.295133	-1.520583	0.492353
	1	-0.693273	-0.607852	0.884609
	1	1.943260	0.496114	1.358381
	6	-0.924011	1.450399	-0.006943
	1	-1.542472	1.809096	-0.834551
	1	-1.378816	1.801448	0.923850
	1	0.069500	1.894492	-0.099538
	33	1.892837	-0.127304	-0.054820
	[H ₃ C...Et...Cl] ^{-#}	17	1.594561	-1.043468
6		0.000000	0.260043	0.000000
1		0.209315	0.811306	0.902075
1		0.209315	0.811306	-0.902075
6		-1.671897	2.312172	0.000000
1		-2.245636	2.048657	-0.903605
1		-2.245636	2.048657	0.903605
1		-1.467343	3.395735	0.000000
6		-1.184473	-0.675325	0.000000
1		-1.153568	-1.320508	-0.883685
1		-1.153568	-1.320508	0.883685
1		-2.122204	-0.117037	0.000000
[H ₃ Si...Et...Cl] ^{-#}	1	-0.132867	-0.710477	-0.914814
	1	-0.132530	-0.711099	0.913490
	17	-2.448624	-0.362181	0.000095
	1	2.915003	0.575831	1.162989
	1	3.737987	-1.271105	0.000557
	1	2.916713	0.577142	-1.161493

Continued:	6	-0.267767	-0.158754	-0.000442
	6	-0.174493	1.348800	0.000063
	1	-0.684651	1.743106	-0.882957
	1	-0.683992	1.742529	0.883717
	1	0.851289	1.726420	-0.000211
	14	2.535229	-0.332538	-0.000043
[H ₃ Ge...Et...Cl] [‡]	17	-0.034100	3.074779	0.000000
	6	0.000000	0.895415	0.000000
	1	-0.560899	0.809654	0.914600
	1	-0.560899	0.809654	-0.914600
	1	0.578320	-2.248535	-1.203251
	1	0.578320	-2.248535	1.203251
	1	-1.357041	-3.096985	0.000000
	6	1.496874	0.689909	0.000000
	1	1.926433	1.169666	-0.883305
	1	1.926433	1.169666	0.883305
	1	1.797653	-0.361389	0.000000
	32	-0.397809	-1.805824	0.000000