Calculated Structures and Complete Energies

Guide to Structures and Structure Titles

The structure titles below are in most cases self-explanatory. PCM and SMD refer to structures optimized with the PCM and SMD implicit solvent model. TS refers to transition structures in which the 1,3-pentadiene is being protonated at C1, and this was explored with both one HCl and two HCl molecules present. When two HCl molecules are present, the second HCl may be located in varying positions and these are designated as "Conf A", "Conf B", etc. Not every conformation was located for every computational method / solvent model combination, despite careful searches in each case. For the product (E)-4-chloropent-2-ene, three conformations were located but only the lowest-energy conformation is presented here. Bichloride refers to the Cl—H—Cl anion, which was generally unsymmetrical in implicit solvent but was symmetrical for M06-2X calculations in the gas phase.

Tables of Energies

	Pot. E.	E+zpe	H	G	S (E.U.)	G 1 M
MP2/6-31+G structures**						
HCl-gas phase	-460.207617	-460.200527	-460.197223	-460.218391	44.55	-460.215373
HCl SMD	-460.213106	-460.206156	-460.202851	-460.224030	44.58	-460.221012
HCl PCM	-460.211164	-460.204120	-460.200815	-460.221987	44.56	-460.218969
HCl Dimer-gas phase	-920.418518	-920.402724	-920.396567	-920.430797	72.04	-920.427779
HCl Dimer SMD	-920.427032	-920.411759	-920.405431	-920.440047	72.86	-920.437029
HCl Dimer PCM	-920.424550	-920.408716	-920.402680	-920.436479	71.14	-920.433461
Chloride anion – gas phase	-459.671145	-459.671145	-459.668785	-459.686168	36.59	-459.683150
Chloride anion – SMD	-459.775357	-459.775357	-459.772996	-459.790380	36.59	-459.787362
Chloride anion – PCM	-459.780255	-459.780255	-459.777895	-459.795278	36.59	-459.792260
Bichloride anion SMD	-920.000061	-919.991806	-919.987619	-920.015845	59.41	-920.012827
Bichloride anion PCM	-920.002148	-919.995235	-919.990657	-920.014395	49.96	-920.011377
Pentadienyl cation – gas phase	-194.998888	-194.871875	-194.864144	-194.901797	79.25	-194.898779
Pentadienyl cation – SMD	-195.095043	-194.968443	-194.960645	-194.998474	79.62	-194.995456
Pentadienyl cation – PCM	-195.078935	-194.951888	-194.944081	-194.981965	79.73	-194.978947
1,3-pentadiene – gas phase	-194.669694	-194.554659	-194.547457	-194.583755	76.40	-194.580737
1,3-pentadiene – SMD	-194.674749	-194.559992	-194.552815	-194.589016	76.19	-194.585998
1,3-pentadiene – PCM	-194.671881	-194.557010	-194.549798	-194.586133	76.47	-194.583115
(E)-4-chloropent-2-ene – gas phase	-654.910587	-654.779735	-654.771254	-654.811787	85.31	-654.808769
(E)-4-chloropent-2-ene – SMD	-654.919429	-654.788938	-654.780450	-654.820975	85.29	-654.817957
(E)-4-chloropent-2-ene – PCM	-654.914356	-654.783702	-654.775207	-654.815754	85.34	-654.812736
TS / one HCl SMD	-654.867425	-654.744800	-654.735952	-654.778580	89.72	-654.775562
TS / one HCl PCM	-654.859761	-654.736546	-654.727737	-654.770334	89.65	-654.767316
TS / two HCl conf B SMD	-1115.090018	-1114.958685	-1114.947012	-1114.998187	107.71	-1114.995169
TS / two HCl conf C SMD	-1115.090006	-1114.958721	-1114.947045	-1114.999134	109.63	-1114.996116
TS / two HCl conf A PCM	-1115.079533	-1114.947843	-1114.936062	-1114.988721	110.83	-1114.985703
TS / two HCl conf B PCM	-1115.081097	-1114.949254	-1114.937593	-1114.988789	107.75	-1114.985771

M06-2X/6-31+G structures**

HCl-gas phase	-460.762018	-460.755187	-460.751882	-460.773067	44.59	-460.770049
HCl SMD	-460.767806	-460.761125	-460.757820	-460.779017	44.61	-460.775999
HCl PCM	-460.765738	-460.758967	-460.755662	-460.776851	44.60	-460.773833
(HCl)2 dimer-gas phase	-921.527331	-921.512445	-921.505984	-921.542172	76.16	-921.539154
(HCl)2 dimer SMD	-921.536203	-921.521639	-921.515214	-921.550656	74.59	-921.547638
(HCl)2 dimer PCM	-921.533574	-921.518915	-921.513401	-921.546204	69.04	-921.543186
Chloride anion – gas phase	-460.235297	-460.235297	-460.232937	-460.250320	36.59	-460.247302
Chloride anion – SMD	-460.339779	-460.339779	-460.337419	-460.354802	36.59	-460.351784
Chloride anion – PCM	-460.344843	-460.344843	-460.342483	-460.359866	36.59	-460.356848
Bichloride anion – SMD	-921.124048	-921.121093	-921.116239	-921.141285	52.71	-921.138267
Bichloride anion – PCM	-921.125594	-921.120193	-921.115949	-921.144165	59.39	-921.141147
Pentadienyl cation – gas phase	-195.547125	-195.422385	-195.414674	-195.452204	78.99	-195.449186
Pentadienyl cation – SMD	-195.642802	-195.518575	-195.510778	-195.548562	79.52	-195.545544
Pentadienyl cation – PCM	-195.626628	-195.501984	-195.494175	-195.531989	79.59	-195.528971
1,3-pentadiene – gas phase	-195.218451	-195.104296	-195.097236	-195.133135	75.56	-195.130117
1,3-pentadiene – SMD	-195.224268	-195.110463	-195.103413	-195.139270	75.47	-195.136252
1,3-pentadiene – PCM	-195.221028	-195.107071	-195.099997	-195.135938	75.65	-195.132920
(E)-4-chloropent-2-ene – gas phase	-656.014201	-655.885432	-655.876904	-655.917521	85.49	-655.914503
(E)-4-chloropent-2-ene – SMD	-656.023907	-655.895665	-655.887090	-655.927814	85.71	-655.924796
(E)-4-chloropent-2-ene – PCM	-656.018604	-655.890154	-655.881580	-655.922305	85.71	-655.919287
TS / one HCl SMD	-655.982855	-655.862594	-655.853735	-655.896236	89.45	-655.893218
TS / one HCl PCM	-655.975058	-655.853624	-655.844840	-655.887373	89.52	-655.884355
TS / two HCl conf B SMD	-1116.759071	-1116.630941	-1116.619259	-1116.669501	105.74	-1116.666483
TS / two HCl conf C SMD	-1116.759414	-1116.630610	-1116.619177	-1116.668316	103.42	-1116.665298
TS / two HCl conf A PCM	-1116.749085	-1116.620164	-1116.608466	-1116.660238	108.96	-1116.657220
TS / two HCl conf B PCM	-1116.750429	-1116.621518	-1116.609867	-1116.660794	107.19	-1116.657776

MP2/6-31+G** structures

HCl-gas phase

MP2/6-31+G**
EUMP2 = -0.46020761713804D+03

Zero-point correction= 0.007090 (Hartree/Particle)
Thermal correction to Energy= 0.009450
Thermal correction to Enthalpy= 0.010394
Thermal correction to Gibbs Free Energy= -0.010774
Sum of electronic and ZPE= -460.200527
Sum of electronic and thermal Energies= -460.198167
Sum of electronic and thermal Enthalpies= -460.197223
Sum of electronic and thermal Free Energies= -460.218391

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	5.930	4.968	44.553

Cl,0,-0.3873357934,-3.152125816,0.7128749805
H,0,-1.2288842066,-2.308634184,0.2732650195

HCl SMD

MP2/6-31+G**
EUMP2 = -0.46021310572512D+03

Zero-point correction= 0.006950 (Hartree/Particle)
Thermal correction to Energy= 0.009311
Thermal correction to Enthalpy= 0.010255
Thermal correction to Gibbs Free Energy= -0.010924
Sum of electronic and ZPE= -460.206156
Sum of electronic and thermal Energies= -460.203795
Sum of electronic and thermal Enthalpies= -460.202851
Sum of electronic and thermal Free Energies= -460.224030

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	5.843	4.968	44.575

Cl,0,-0.3850243313,-3.1544426155,0.7140824473
H,0,-1.2311956687,-2.3063173845,0.2720575527

HCl PCM

MP2/6-31+G**
EUMP2 = -0.46021116360143D+03

Zero-point correction= 0.007044 (Hartree/Particle)
Thermal correction to Energy= 0.009404
Thermal correction to Enthalpy= 0.010348
Thermal correction to Gibbs Free Energy= -0.010824
Sum of electronic and ZPE= -460.204120
Sum of electronic and thermal Energies= -460.201760
Sum of electronic and thermal Enthalpies= -460.200815
Sum of electronic and thermal Free Energies= -460.221987

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	5.901	4.968	44.560

Cl,0,-0.3865779149,-3.1528854445,0.7132708828
H,0,-1.2296420851,-2.3078745555,0.2728691172

HCl Dimer-gas phase

MP2/6-31+G**
EUMP2 = -0.92041851838371D+03

Zero-point correction= 0.015795 (Hartree/Particle)
Thermal correction to Energy= 0.021008
Thermal correction to Enthalpy= 0.021952
Thermal correction to Gibbs Free Energy= -0.012278
Sum of electronic and ZPE= -920.402724
Sum of electronic and thermal Energies= -920.397511
Sum of electronic and thermal Enthalpies= -920.396567
Sum of electronic and thermal Free Energies= -920.430797

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	13.183	13.288	72.044

H,0,-2.0505141611,0.4812496329,-0.2640794703
Cl,0,-2.7018667446,-0.5920673714,-0.4630106611
Cl,0,-0.2658837139,-3.33122548,0.7701505738
H,0,-1.1237053804,-2.4929567815,0.3448895576

HCl Dimer SMD

MP2/6-31+G**
EUMP2 = -0.92042703189231D+03

Zero-point correction= 0.015272 (Hartree/Particle)
Thermal correction to Energy= 0.020657
Thermal correction to Enthalpy= 0.021601
Thermal correction to Gibbs Free Energy= -0.013016
Sum of electronic and ZPE= -920.411759
Sum of electronic and thermal Energies= -920.406375
Sum of electronic and thermal Enthalpies= -920.405431
Sum of electronic and thermal Free Energies= -920.440047

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	12.962	13.493	72.856

H,0,-2.0312533251,0.4508446608,-0.2538150919
Cl,0,-2.7070689877,-0.6140037846,-0.4632445705
Cl,0,-0.2892845415,-3.3257858407,0.7603474654
H,0,-1.1143631457,-2.4460550356,0.344662197

HCl Dimer PCM

MP2/6-31+G**
EUMP2 = -0.92042455018430D+03

Zero-point correction= 0.015834 (Hartree/Particle)
Thermal correction to Energy= 0.020926
Thermal correction to Enthalpy= 0.021870
Thermal correction to Gibbs Free Energy= -0.011928
Sum of electronic and ZPE= -920.408716

Sum of electronic and thermal Energies= -920.403624
Sum of electronic and thermal Enthalpies= -920.402680
Sum of electronic and thermal Free Energies= -920.436479

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	13.131	13.200	71.135

H,0,-2.041580278,0.4577644712,-0.2412473748
Cl,0,-2.6902031624,-0.6141177003,-0.4680085383
Cl,0,-0.3078017666,-3.3447098615,0.7523475298
H,0,-1.1023847929,-2.4339369094,0.3448583833

Chloride anion – gas phase

MP2/6-31+G**
EUMP2 = -0.45967114538099D+03

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and zero-point Energies= -459.671145
Sum of electronic and thermal Energies= -459.669729
Sum of electronic and thermal Enthalpies= -459.668785
Sum of electronic and thermal Free Energies= -459.686168

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	0.889	2.981	36.586

Chloride anion – SMD

MP2/6-31+G**
EUMP2 = -0.45977535694708D+03

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and ZPE= -459.775357
Sum of electronic and thermal Energies= -459.773941
Sum of electronic and thermal Enthalpies= -459.772996
Sum of electronic and thermal Free Energies= -459.790380

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	0.889	2.981	36.586

Chloride anion – PCM

MP2/6-31+G**
EUMP2 = -0.45978025499771D+03

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and ZPE= -459.780255
Sum of electronic and thermal Energies= -459.778839
Sum of electronic and thermal Enthalpies= -459.777895
Sum of electronic and thermal Free Energies= -459.795278

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	0.889	2.981	36.586

Bichloride anion SMD

MP2/6-31+G**
EUMP2 = -0.92000006107913D+03

Zero-point correction= 0.008255 (Hartree/Particle)
Thermal correction to Energy= 0.011498
Thermal correction to Enthalpy= 0.012442
Thermal correction to Gibbs Free Energy= -0.015784
Sum of electronic and ZPE= -919.991806
Sum of electronic and thermal Energies= -919.988563
Sum of electronic and thermal Enthalpies= -919.987619
Sum of electronic and thermal Free Energies= -920.015845

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	7.215	8.601	59.407

Cl,0,-2.6308407661,-1.0085694525,-0.4012935497
Cl,0,-0.3881788666,-3.1343659994,0.7031350289
H,0,-1.3009646093,-2.2691456198,0.253621591

Bichloride anion PCM

MP2/6-31+G**
EUMP2 = -0.92000214785299D+03

Zero-point correction= 0.006913 (Hartree/Particle)
Thermal correction to Energy= 0.010546
Thermal correction to Enthalpy= 0.011491
Thermal correction to Gibbs Free Energy= -0.012247
Sum of electronic and ZPE= -919.995235
Sum of electronic and thermal Energies= -919.991601
Sum of electronic and thermal Enthalpies= -919.990657
Sum of electronic and thermal Free Energies= -920.014395

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	6.618	8.842	49.961

Cl,0,-2.6500252448,-0.9911983622,-0.4102938476
Cl,0,-0.3826060758,-3.1396919337,0.7059033626
H,0,-1.2873886794,-2.2812197041,0.2598704851

Pentadienyl cation – gas phase

MP2/6-31+G**
EUMP2 = -0.19499888809994D+03

Zero-point correction= 0.127013 (Hartree/Particle)
Thermal correction to Energy= 0.133800
Thermal correction to Enthalpy= 0.134744
Thermal correction to Gibbs Free Energy= 0.097091
Sum of electronic and ZPE= -194.871875

Sum of electronic and thermal Energies= -194.865088
Sum of electronic and thermal Enthalpies= -194.864144
Sum of electronic and thermal Free Energies= -194.901797

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	83.961	22.384	79.248

C,0,1.8922072426,-0.3592629232,-0.3156541599
H,0,1.9704872805,-0.1696073453,-1.3844503717
C,0,0.7921813258,0.1617612585,0.3488755183
H,0,0.6634572611,0.0039675293,1.4126860519
C,0,-0.1398492157,0.8886460229,-0.3764383141
H,0,0.0402499333,1.0157547051,-1.4421914459
C,0,2.9622054018,-1.1472709532,0.3049755035
H,0,2.8211363827,-1.2982709435,1.3705883157
H,0,3.0330442831,-2.1114770751,-0.2093841909
H,0,3.9200266129,-0.6515125108,0.1149611672
C,0,-1.3521104082,1.5021292415,0.1759167385
H,0,-1.4691654808,1.3366428992,1.242286995
H,0,-1.3345185265,2.575115914,-0.0424477519
H,0,-2.2211320925,1.1148341804,-0.3663840556

Pentadienyl cation – SMD

MP2/6-31+G**
EUMP2 = -0.19509504268429D+03

Zero-point correction= 0.126600 (Hartree/Particle)
Thermal correction to Energy= 0.133453
Thermal correction to Enthalpy= 0.134397
Thermal correction to Gibbs Free Energy= 0.096569
Sum of electronic and ZPE= -194.968443
Sum of electronic and thermal Energies= -194.961590
Sum of electronic and thermal Enthalpies= -194.960645
Sum of electronic and thermal Free Energies= -194.998474

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	83.743	22.572	79.616

C,0,1.8855777759,-0.3554186563,-0.3138988269
H,0,1.9587723979,-0.1629717222,-1.3808446868
C,0,0.7913421715,0.1608449452,0.3577561851
H,0,0.6627246681,0.0032114035,1.4211226818
C,0,-0.133524327,0.8845053221,-0.3743198572
H,0,0.0512044424,1.0082367345,-1.4379603146
C,0,2.9558465366,-1.1431508474,0.3029074732
H,0,2.8104838746,-1.2917168963,1.3687863733
H,0,3.0190861659,-2.1047257121,-0.215922096
H,0,3.9088415292,-0.6408891464,0.109538107
C,0,-1.3454647418,1.4982843933,0.1742248529
H,0,-1.4582946283,1.3302577554,1.2411566279
H,0,-1.3197705079,2.5697917439,-0.0472650745
H,0,-2.208605357,1.1051906828,-0.3719414451

Pentadienyl cation – PCM

MP2/6-31+G**
EUMP2 = -0.19507893460018D+03

Zero-point correction= 0.127046 (Hartree/Particle)
Thermal correction to Energy= 0.133910
Thermal correction to Enthalpy= 0.134854
Thermal correction to Gibbs Free Energy= 0.096970
Sum of electronic and ZPE= -194.951888
Sum of electronic and thermal Energies= -194.945025
Sum of electronic and thermal Enthalpies= -194.944081
Sum of electronic and thermal Free Energies= -194.981965

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	84.030	22.488	79.734

C,0,1.8876442894,-0.3558291203,-0.3163777163
H,0,1.9641465504,-0.1646832651,-1.3830496589
C,0,0.7918846738,0.1614659291,0.3528438278
H,0,0.6630209482,0.0032563173,1.4155065605
C,0,-0.1346847067,0.886242671,-0.3767207843
H,0,0.0472936501,1.0125079017,-1.4402614572
C,0,2.9574546451,-1.1446310544,0.3039346781
H,0,2.81081572,-1.2938399124,1.3685099993
H,0,3.0234211848,-2.1063741031,-0.2125019259
H,0,3.9112855791,-0.6440261604,0.1149506794
C,0,-1.3475030292,1.4990932933,0.17548495
H,0,-1.4598750651,1.3299887447,1.2412532945
H,0,-1.3246045809,2.5705969669,-0.0422700073
H,0,-2.212079859,1.1076817916,-0.3679624397

1,3-pentadiene – gas phase

MP2/6-31+G**
EUMP2 = -0.19466969392284D+03

Zero-point correction= 0.115035 (Hartree/Particle)
Thermal correction to Energy= 0.121293
Thermal correction to Enthalpy= 0.122237
Thermal correction to Gibbs Free Energy= 0.085939
Sum of electronic and ZPE= -194.554659
Sum of electronic and thermal Energies= -194.548401
Sum of electronic and thermal Enthalpies= -194.547457
Sum of electronic and thermal Free Energies= -194.583755

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	76.112	21.281	76.396

C,0,1.8986175416,-0.3063618261,-0.3530631927
H,0,2.0545875479,-0.0835808938,-1.4058816623
C,0,0.844621285,0.2551048761,0.2739797037
H,0,0.6773123759,0.0404229432,1.3270872652
C,0,-0.1042572819,1.1477603725,-0.3767771216
H,0,0.0650305416,1.3606054755,-1.4286168364
C,0,2.8836892478,-1.2256332597,0.299160429
H,0,2.6361369662,-1.3812924108,1.3490783945
H,0,2.9000585455,-2.1983968283,-0.1963343313
H,0,3.8957366431,-0.8198806311,0.2428044867
C,0,-1.1576259486,1.709470842,0.2481003164
H,0,-1.3558506296,1.5189436999,1.2954884082
H,0,-1.8378868345,2.3671776406,-0.2741558594

1,3-pentadiene – SMD

MP2/6-31+G**
EUMP2 = -0.19467474942796D+03

Zero-point correction= 0.114757 (Hartree/Particle)
Thermal correction to Energy= 0.120991
Thermal correction to Enthalpy= 0.121935
Thermal correction to Gibbs Free Energy= 0.085733
Sum of electronic and ZPE= -194.559992
Sum of electronic and thermal Energies= -194.553759
Sum of electronic and thermal Enthalpies= -194.552815
Sum of electronic and thermal Free Energies= -194.589016

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	75.923	21.287	76.193

C,0,1.8986506177,-0.3068394863,-0.351625699
H,0,2.0542324707,-0.0836117741,-1.4049379043
C,0,0.8440547099,0.2542024714,0.278082517
H,0,0.6757571333,0.0400645379,1.3316978647
C,0,-0.103605015,1.1473584644,-0.3770015171
H,0,0.0679136855,1.3588301033,-1.4295386438
C,0,2.8832163327,-1.2255035634,0.2998315953
H,0,2.637888906,-1.383003695,1.3505698919
H,0,2.8999091636,-2.1963702869,-0.2005848917
H,0,3.8950936022,-0.8185722467,0.2382925317
C,0,-1.1581536098,1.7099159741,0.2478946605
H,0,-1.3575182837,1.5199021249,1.2962135764
H,0,-1.8372697131,2.3679673764,-0.2780239816

1,3-pentadiene – PCM

MP2/6-31+G**
EUMP2 = -0.19467188131503D+03

Zero-point correction= 0.114872 (Hartree/Particle)
Thermal correction to Energy= 0.121139
Thermal correction to Enthalpy= 0.122083
Thermal correction to Gibbs Free Energy= 0.085748
Sum of electronic and ZPE= -194.557010
Sum of electronic and thermal Energies= -194.550742
Sum of electronic and thermal Enthalpies= -194.549798
Sum of electronic and thermal Free Energies= -194.586133

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	76.016	21.298	76.473

C,0,1.8987457869,-0.3067875372,-0.3520884305
H,0,2.0546869952,-0.0839042488,-1.4050086382
C,0,0.8443065787,0.2544989767,0.276609854
H,0,0.6764521076,0.0400996601,1.3298921265
C,0,-0.1041795484,1.147775429,-0.376736048
H,0,0.0661963138,1.3600299947,-1.4288493043
C,0,2.8841335986,-1.2262002102,0.299735835
H,0,2.6377617847,-1.3831025606,1.3497488521
H,0,2.9008604977,-2.1970934331,-0.1992080587
H,0,3.895560725,-0.8196140232,0.2400276397
C,0,-1.1587257348,1.7103701202,0.2478487224
H,0,-1.3576946048,1.5201979866,1.29547575
H,0,-1.8379345001,2.368069846,-0.2765783

(E)-4-chloropent-2-ene – gas phase

Two alternative conformations were located but they were higher in energy by >1.2 kcal/mol.
MP2/6-31+G**
EUMP2 = -0.65491058652331D+03

Zero-point correction= 0.130852 (Hartree/Particle)
Thermal correction to Energy= 0.138388
Thermal correction to Enthalpy= 0.139332
Thermal correction to Gibbs Free Energy= 0.098800
Sum of electronic and ZPE= -654.779735
Sum of electronic and thermal Energies= -654.772199
Sum of electronic and thermal Enthalpies= -654.771254
Sum of electronic and thermal Free Energies= -654.811787

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	86.840	26.015	85.307

C,0,-3.2925531327,-0.1071523078,-0.0091588398
H,0,-2.5605937451,-0.0937028347,-0.8186151747
H,0,-4.2265807461,0.31062227,-0.3834741079
H,0,-3.4645175151,-1.152555433,0.2532777581
C,0,-2.7966995236,0.6632648295,1.1751779092
H,0,-1.8676690195,0.3261809732,1.628360819
C,0,-3.4214341268,1.7261102179,1.7076960031
H,0,-4.3589435812,2.0790701119,1.2852918924
C,0,-2.8874755406,2.4931577298,2.8687114528
H,0,-1.9393669411,2.0607303071,3.1891939089
C,0,-2.7184178154,3.9735610308,2.5699137514
H,0,-3.6705072634,4.415299463,2.2767005455
H,0,-2.3419529373,4.5067953905,3.4415327799
H,0,-2.0099247095,4.0914538259,1.7488830912
Cl,0,-4.0036831926,2.3016632958,4.283032291

(E)-4-chloropent-2-ene – SMD

MP2/6-31+G**
EUMP2 = -0.65491942935983D+03

Zero-point correction= 0.130492 (Hartree/Particle)
Thermal correction to Energy= 0.138035
Thermal correction to Enthalpy= 0.138980
Thermal correction to Gibbs Free Energy= 0.098454
Sum of electronic and ZPE= -654.788938
Sum of electronic and thermal Energies= -654.781394
Sum of electronic and thermal Enthalpies= -654.780450
Sum of electronic and thermal Free Energies= -654.820975

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	86.619	26.111	85.293

C,0,-3.2958154036,-0.1112620922,-0.0068775017
H,0,-2.5497911896,-0.1094332105,-0.8043007435
H,0,-4.2203797265,0.3158539832,-0.395569642
H,0,-3.4789346601,-1.1550284534,0.2572507902
C,0,-2.8043555629,0.654939887,1.1803677641
H,0,-1.8839704289,0.3088699057,1.644993285
C,0,-3.4192522198,1.7326501455,1.6982006271
H,0,-4.3427323616,2.104366653,1.2599578159

C,0,-2.8744162842,2.4960141781,2.8548555887
H,0,-1.9244836283,2.0677834946,3.1722834743
C,0,-2.7280402243,3.9792573617,2.5755564114
H,0,-3.6851322261,4.4156951977,2.2889223744
H,0,-2.3439440637,4.5074391135,3.447631781
H,0,-2.0240789492,4.1089862365,1.75185107
Cl,0,-3.9849928612,2.2783664694,4.2914009854

(E)-4-chloropent-2-ene – PCM

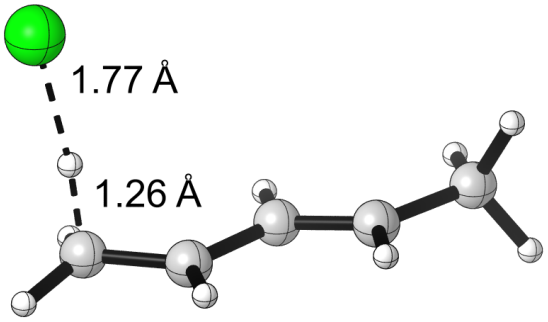
MP2/6-31+G**
EUMP2 = -0.65491435631652D+03

Zero-point correction= 0.130654 (Hartree/Particle)
Thermal correction to Energy= 0.138205
Thermal correction to Enthalpy= 0.139149
Thermal correction to Gibbs Free Energy= 0.098603
Sum of electronic and ZPE= -654.783702
Sum of electronic and thermal Energies= -654.776151
Sum of electronic and thermal Enthalpies= -654.775207
Sum of electronic and thermal Free Energies= -654.815754

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	86.725	26.098	85.337

C,0,-3.2950014165,-0.1105234363,-0.0081159605
H,0,-2.554252851,-0.1015271968,-0.8094250695
H,0,-4.2233971105,0.3126422715,-0.3902797175
H,0,-3.471788296,-1.1552089504,0.2536881272
C,0,-2.802403249,0.6565279307,1.1795580916
H,0,-1.8788937772,0.3136286269,1.6393420352
C,0,-3.4206615768,1.7294477402,1.7018374183
H,0,-4.3478275523,2.0953322431,1.2675766272
C,0,-2.8787365547,2.4952933424,2.8586973003
H,0,-1.9304828625,2.0654359228,3.1791457347
C,0,-2.7243065714,3.9783939704,2.5735879207
H,0,-3.6794441152,4.4162473399,2.2846276642
H,0,-2.3427682363,4.5071664827,3.4455872317
H,0,-2.0190619973,4.1039922083,1.7512834774
Cl,0,-3.9912936231,2.2876503745,4.2894131994

TS / one HCl SMD



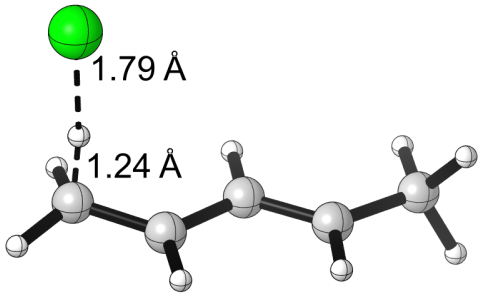
MP2/6-31+G**
EUMP2 = -0.65486742472659D+03

Zero-point correction= 0.122625 (Hartree/Particle)
Thermal correction to Energy= 0.130529
Thermal correction to Enthalpy= 0.131473
Thermal correction to Gibbs Free Energy= 0.088845
Sum of electronic and ZPE= -654.744800
Sum of electronic and thermal Energies= -654.736896
Sum of electronic and thermal Enthalpies= -654.735952
Sum of electronic and thermal Free Energies= -654.778580

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	81.908	26.505	89.718

C,0,1.906869462,-0.3190801909,-0.3194016219
H,0,2.0149998658,-0.0892567782,-1.3764309099
C,0,0.854930977,0.2271148658,0.3490388147
H,0,0.7001471122,0.029881773,1.404111111
C,0,-0.0541343529,1.0734417814,-0.3393885819
H,0,0.1438576185,1.2484760914,-1.3945142704
C,0,2.9329931043,-1.194995172,0.2931624372
H,0,2.7352042206,-1.3762003363,1.3477262782
H,0,2.9698857681,-2.1473097106,-0.2411300043
H,0,3.9185422011,-0.7362634465,0.1808836563
C,0,-1.2466169259,1.5512056289,0.1981354329
H,0,-1.3520199066,1.5426736473,1.2784619132
H,0,-1.7436571403,2.3583884618,-0.3284557787
H,0,-1.9043565594,0.5427435719,-0.1577078187
Cl,0,-3.0022254444,-0.8007201873,-0.4918106577

TS / one HCl PCM



MP2/6-31+G**
EUMP2 = -0.65485976096748D+03

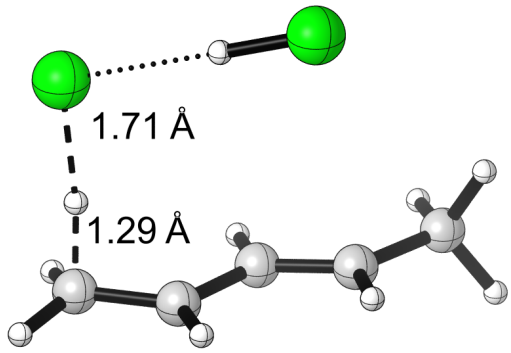
Zero-point correction= 0.123215 (Hartree/Particle)
Thermal correction to Energy= 0.131079
Thermal correction to Enthalpy= 0.132023
Thermal correction to Gibbs Free Energy= 0.089427
Sum of electronic and ZPE= -654.736546
Sum of electronic and thermal Energies= -654.728682
Sum of electronic and thermal Enthalpies= -654.727737
Sum of electronic and thermal Free Energies= -654.770334

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	82.253	26.280	89.653

C,0,1.9053438602,-0.3207654083,-0.3155452003
H,0,2.0086385871,-0.0953106519,-1.3735165429
C,0,0.854755916,0.2276361288,0.3558172977
H,0,0.7050131926,0.0341752085,1.4114256405
C,0,-0.0542544822,1.0696033955,-0.3332852798

H,0,0.1429490573,1.2417846401,-1.3884855908
C,0,2.9366793534,-1.1949735983,0.2920551463
H,0,2.7522390318,-1.3696641763,1.3491393074
H,0,2.9648689059,-2.1500124074,-0.2363562098
H,0,3.9210080199,-0.7396311126,0.1646069372
C,0,-1.253462111,1.5493425714,0.1982267781
H,0,-1.3575762392,1.5514736059,1.2779981007
H,0,-1.736317885,2.3643382112,-0.3281025515
H,0,-1.9100175876,0.5578519989,-0.1549120869
Cl,0,-3.0054476191,-0.8157484055,-0.516385746

TS / two HCl conf B SMD



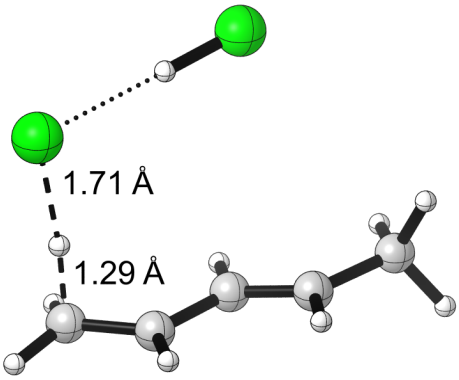
MP2/6-31+G**
EUMP2 = -0.11150900183123D+04

Zero-point correction= 0.131333 (Hartree/Particle)
Thermal correction to Energy= 0.142062
Thermal correction to Enthalpy= 0.143007
Thermal correction to Gibbs Free Energy= 0.091832
Sum of electronic and ZPE= -1114.958685
Sum of electronic and thermal Energies= -1114.947956
Sum of electronic and thermal Enthalpies= -1114.947012
Sum of electronic and thermal Free Energies= -1114.998187

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	89.145	34.972	107.707

C,0,-2.0107804706,-0.9201827246,-0.503670501
H,0,-2.0217408152,-1.4310822536,-1.4632457834
C,0,-0.9803310121,-1.1763020941,0.3437232003
H,0,-0.9164253433,-0.6907380421,1.311513035
C,0,0.0439093856,-2.0866585645,-0.0458354138
H,0,-0.0669511138,-2.5586604843,-1.019565269
C,0,-3.138034121,-0.001551897,-0.2125429905
H,0,-3.0332891434,0.4719321184,0.7618407433
H,0,-3.1963782109,0.7674959041,-0.9865085978
H,0,-4.0807118297,-0.5531313468,-0.2482632639
C,0,1.2333506459,-2.2685093537,0.6409269644
H,0,1.293541434,-1.9334124397,1.6712970917
H,0,1.8695190372,-3.0983022524,0.3558549996
H,0,1.7596733093,-1.2762413854,0.0009625348
Cl,0,2.6201567556,0.045608343,-0.6565187022
Cl,0,0.1388080885,1.3028695631,-2.7145468288
H,0,1.0641544037,0.8321489096,-1.9361102185

TS / two HCl conf C SMD



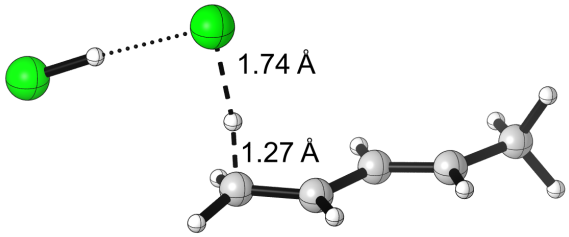
MP2/6-31+G**
EUMP2 = -0.11150900058283D+04

Zero-point correction= 0.131285 (Hartree/Particle)
Thermal correction to Energy= 0.142016
Thermal correction to Enthalpy= 0.142961
Thermal correction to Gibbs Free Energy= 0.090871
Sum of electronic and ZPE= -1114.958721
Sum of electronic and thermal Energies= -1114.947989
Sum of electronic and thermal Enthalpies= -1114.947045
Sum of electronic and thermal Free Energies= -1114.999134

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	89.117	34.996	109.631

6 -2.151880 -0.706361 -0.458131
1 -2.156234 -1.020974 -1.498821
6 -1.158560 -1.168524 0.345303
1 -1.105716 -0.881550 1.390098
6 -0.159135 -2.032745 -0.186809
1 -0.252846 -2.303218 -1.236154
6 -3.247419 0.189134 -0.014132
1 -3.143596 0.466749 1.033183
1 -3.261945 1.090816 -0.630842
1 -4.209856 -0.306882 -0.163392
6 0.996981 -2.395374 0.485513
1 1.030767 -2.272626 1.563239
1 1.616369 -3.176092 0.059985
1 1.570567 -1.312903 0.078930
17 2.484218 0.098418 -0.245441
17 0.061035 2.535975 0.149755
1 0.963271 1.615231 -0.000020

TS / two HCl conf A PCM



MP2/6-31+G**

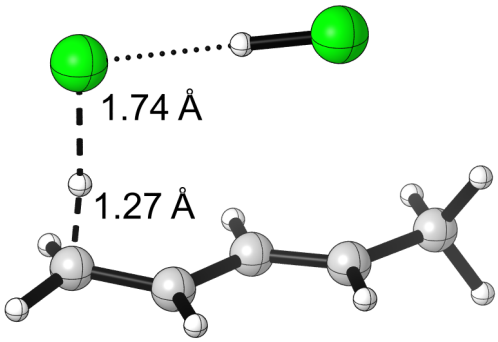
EUMP2 = -0.11150795326429D+04

Zero-point correction= 0.131690 (Hartree/Particle)
Thermal correction to Energy= 0.142527
Thermal correction to Enthalpy= 0.143471
Thermal correction to Gibbs Free Energy= 0.090812
Sum of electronic and ZPE= -1114.947843
Sum of electronic and thermal Energies= -1114.937006
Sum of electronic and thermal Enthalpies= -1114.936062
Sum of electronic and thermal Free Energies= -1114.988721

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	89.437	34.899	110.830

C,0,-2.0704254843,-0.9266551322,-0.4392028426
H,0,-2.0731717953,-1.4214147928,-1.4066872948
C,0,-0.9699224797,-1.0668206591,0.3477432148
H,0,-0.917343687,-0.5940408728,1.3216606471
C,0,0.125791589,-1.8531940428,-0.1018670474
H,0,0.0280458435,-2.3138599937,-1.0818411384
C,0,-3.2849969593,-0.158697425,-0.0698332636
H,0,-3.1899241743,0.3060535619,0.9086424106
H,0,-3.4767823863,0.6104100916,-0.8205261834
H,0,-4.1525646918,-0.8216898345,-0.073102717
C,0,1.3552193007,-1.9370393402,0.5417713931
H,0,1.4083507595,-1.6395666061,1.583464315
H,0,2.0375719539,-2.7177099905,0.2278024326
H,0,1.7985932237,-0.916474155,-0.0669252
Cl,0,2.6183015696,0.4852957599,-0.697382034
Cl,0,5.1325002674,-0.7013146321,1.3838269065
H,0,4.2232671505,-0.2242249367,0.5936984016

TS / two HCl conf B PCM



MP2/6-31+G**
EUMP2 = -0.11150810974363D+04

Zero-point correction= 0.131844 (Hartree/Particle)
Thermal correction to Energy= 0.142560
Thermal correction to Enthalpy= 0.143504
Thermal correction to Gibbs Free Energy= 0.092309
Sum of electronic and ZPE= -1114.949254
Sum of electronic and thermal Energies= -1114.938537
Sum of electronic and thermal Enthalpies= -1114.937593
Sum of electronic and thermal Free Energies= -1114.988789

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	89.458	34.800	107.751

C,0,-1.99801667,-0.9298981363,-0.4945802059
H,0,-2.0382869642,-1.4934653878,-1.4227662017
C,0,-0.9594464203,-1.1638295776,0.351633377
H,0,-0.869439683,-0.622929368,1.2867488451
C,0,0.0389961716,-2.1111607598,-0.0032284919
H,0,-0.1008164796,-2.6397677663,-0.9430873265
C,0,-3.0958840142,0.0348187303,-0.2429651299
H,0,-2.9621689005,0.5658945629,0.6965485479
H,0,-3.1472083118,0.7533892517,-1.0632411634
H,0,-4.0518717202,-0.4928037128,-0.2279225075
C,0,1.2502926837,-2.2662189262,0.6612825737
H,0,1.3330683643,-1.8852564305,1.6732668729
H,0,1.8566587941,-3.1299451961,0.4179784022
H,0,1.7730104118,-1.3349289997,-0.0289220752
Cl,0,2.6133497389,-0.0236772815,-0.8056008281
Cl,0,-0.0278910682,1.3304659237,-2.613954134
H,0,0.9641250677,0.834595074,-1.9418795547

M06-2X/6-31+G** structures

HCl-gas phase

M062X/6-31+G**
E(RM062X) = -460.762018131

Zero-point correction= 0.006832 (Hartree/Particle)
Thermal correction to Energy= 0.009192
Thermal correction to Enthalpy= 0.010136
Thermal correction to Gibbs Free Energy= -0.011048
Sum of electronic and ZPE= -460.755187
Sum of electronic and thermal Energies= -460.752826
Sum of electronic and thermal Enthalpies= -460.751882
Sum of electronic and thermal Free Energies= -460.773067

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	5.768	4.968	44.587

H,0,0.,0.,0.
Cl,0,0.,0.,1.2809

HCl SMD

M062X/6-31+G**
E(RM062X) = -460.767806264

Zero-point correction= 0.006681 (Hartree/Particle)
Thermal correction to Energy= 0.009042
Thermal correction to Enthalpy= 0.009986
Thermal correction to Gibbs Free Energy= -0.011210
Sum of electronic and ZPE= -460.761125
Sum of electronic and thermal Energies= -460.758765
Sum of electronic and thermal Enthalpies= -460.757820
Sum of electronic and thermal Free Energies= -460.779017

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 5.674 4.968 44.612

Cl,0,-0.3810752433,-3.1584008224,0.7161453808
H,0,-1.2351447567,-2.3023591776,0.2699946192

HCl PCM

M062X/6-31+G**
E(RM062X) = -460.765738082

Zero-point correction= 0.006771 (Hartree/Particle)
Thermal correction to Energy= 0.009132
Thermal correction to Enthalpy= 0.010076
Thermal correction to Gibbs Free Energy= -0.011113
Sum of electronic and ZPE= -460.758967
Sum of electronic and thermal Energies= -460.756606
Sum of electronic and thermal Enthalpies= -460.755662
Sum of electronic and thermal Free Energies= -460.776851

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 5.730 4.968 44.595

Cl,0,-0.3828436838,-3.1566282983,0.7152215788
H,0,-1.2333763162,-2.3041317017,0.2709184212

(HCl)2 dimer-gas phase

M062X/6-31+G**
E(RM062X) = -921.527330709

Zero-point correction= 0.014886 (Hartree/Particle)
Thermal correction to Energy= 0.020402
Thermal correction to Enthalpy= 0.021346
Thermal correction to Gibbs Free Energy= -0.014841
Sum of electronic and ZPE= -921.512445
Sum of electronic and thermal Energies= -921.506929
Sum of electronic and thermal Enthalpies= -921.505984
Sum of electronic and thermal Free Energies= -921.542172

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 12.803 13.392 76.163

1 1.902832 1.215626 0.004412
17 1.868993 -0.066067 -0.000619
17 -1.939857 0.013197 -0.000735
1 -0.698142 -0.316830 0.018600

(HCl)2 dimer SMD

M062X/6-31+G**
E(RM062X) = -921.536203447

Zero-point correction= 0.014564 (Hartree/Particle)
Thermal correction to Energy= 0.020045
Thermal correction to Enthalpy= 0.020989
Thermal correction to Gibbs Free Energy= -0.014453
Sum of electronic and ZPE= -921.521639
Sum of electronic and thermal Energies= -921.516158
Sum of electronic and thermal Enthalpies= -921.515214
Sum of electronic and thermal Free Energies= -921.550656

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 12.578 13.481 74.594

H,0,-1.9774656865,0.4064149934,-0.2062048138
Cl,0,-2.7073344093,-0.6191137879,-0.4911642161
Cl,0,-0.2632137611,-3.2608088049,0.7402692635
H,0,-1.193955143,-2.4614924006,0.3450507665

(HCl)2 dimer PCM

M062X/6-31+G**
E(RM062X) = -921.533573966

Zero-point correction= 0.014659 (Hartree/Particle)
Thermal correction to Energy= 0.019228
Thermal correction to Enthalpy= 0.020172
Thermal correction to Gibbs Free Energy= -0.012630
Sum of electronic and ZPE= -921.518915
Sum of electronic and thermal Energies= -921.514346
Sum of electronic and thermal Enthalpies= -921.513401
Sum of electronic and thermal Free Energies= -921.546204

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 12.066 11.444 69.039

H,0,-2.0054861315,0.4129814016,-0.2168371338
Cl,0,-2.6994177596,-0.6357041248,-0.4772544091
Cl,0,-0.31361205,-3.3123082894,0.749124104
H,0,-1.1234540589,-2.3999689874,0.3329174389

Chloride anion – gas phase

M062X/6-31+G**
E(RM062X) = -460.235297359

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and zero-point Energies= -460.235297
Sum of electronic and thermal Energies= -460.233881
Sum of electronic and thermal Enthalpies= -460.232937
Sum of electronic and thermal Free Energies= -460.250320

E (Thermal) CV S
KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin
Total 0.889 2.981 36.586

Chloride anion – SMD

M062X/6-31+G**
E(RM062X) = -460.339779210

Zero-point correction= 0.000000 (Hartree/Particle)

Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and ZPE= -460.339779
Sum of electronic and thermal Energies= -460.338363
Sum of electronic and thermal Enthalpies= -460.337419
Sum of electronic and thermal Free Energies= -460.354802

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	0.889	2.981	36.586

Chloride anion – PCM

M062X/6-31+G**
E(RM062X) = -460.344843251

Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and ZPE= -460.344843
Sum of electronic and thermal Energies= -460.343427
Sum of electronic and thermal Enthalpies= -460.342483
Sum of electronic and thermal Free Energies= -460.359866

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	0.889	2.981	36.586

Bichloride anion – SMD

M062X/6-31+G**
E(RM062X) = -921.124048470

Zero-point correction= 0.002956 (Hartree/Particle)
Thermal correction to Energy= 0.006865
Thermal correction to Enthalpy= 0.007810
Thermal correction to Gibbs Free Energy= -0.017237
Sum of electronic and ZPE= -921.121093
Sum of electronic and thermal Energies= -921.117183
Sum of electronic and thermal Enthalpies= -921.116239
Sum of electronic and thermal Free Energies= -921.141285

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	4.308	10.094	52.714

Cl,0,-2.5168414281,-1.1345281374,-0.3353119414
Cl,0,-0.3676479508,-3.1382948219,0.7047063261
H,0,-1.4355306211,-2.1392870407,0.1860856153

Bichloride anion – PCM

M062X/6-31+G**
E(RM062X) = -921.125593733

Zero-point correction= 0.005400 (Hartree/Particle)
Thermal correction to Energy= 0.008701
Thermal correction to Enthalpy= 0.009645
Thermal correction to Gibbs Free Energy= -0.018571
Sum of electronic and ZPE= -921.120193
Sum of electronic and thermal Energies= -921.116893
Sum of electronic and thermal Enthalpies= -921.115949
Sum of electronic and thermal Free Energies= -921.144165

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	5.460	9.134	59.385

Cl,0,-2.54443073,-1.1054689919,-0.35049718
Cl,0,-0.3836506949,-3.1243626452,0.6975054644
H,0,-1.3919414505,-2.1822807238,0.208473096

Pentadienyl cation – gas phase

M062X/6-31+G**
E(RM062X) = -195.547125325

Zero-point correction= 0.124740 (Hartree/Particle)
Thermal correction to Energy= 0.131507
Thermal correction to Enthalpy= 0.132451
Thermal correction to Gibbs Free Energy= 0.094921
Sum of electronic and ZPE= -195.422385
Sum of electronic and thermal Energies= -195.415618
Sum of electronic and thermal Enthalpies= -195.414674
Sum of electronic and thermal Free Energies= -195.452204

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	82.522	22.577	78.988

C,0,1.8915383279,-0.358632542,-0.3169984956
H,0,1.9757194848,-0.1717039753,-1.3896130202
C,0,0.7926973786,0.1623636768,0.3440068769
H,0,0.6634850011,0.0039660088,1.4117606751
C,0,-0.1389191421,0.8883121522,-0.3777310033
H,0,0.0362503051,1.0193440159,-1.4476266867
C,0,2.9573891473,-1.1449091423,0.3077394682
H,0,2.8167029241,-1.2969355972,1.3770206572
H,0,3.0343284854,-2.1125993527,-0.2093610679
H,0,3.9215739895,-0.6519583999,0.1150963386
C,0,-1.3479503874,1.4989817402,0.1789503529
H,0,-1.4662694187,1.3334433446,1.2489340931
H,0,-1.3356237132,2.5763011277,-0.0423711696
H,0,-2.2227023823,1.1154769431,-0.3664670185

Pentadienyl cation – SMD

M062X/6-31+G**
E(RM062X) = -195.642801576

Zero-point correction= 0.124227 (Hartree/Particle)
Thermal correction to Energy= 0.131079
Thermal correction to Enthalpy= 0.132024
Thermal correction to Gibbs Free Energy= 0.094240
Sum of electronic and ZPE= -195.518575
Sum of electronic and thermal Energies= -195.511722
Sum of electronic and thermal Enthalpies= -195.510778
Sum of electronic and thermal Free Energies= -195.548562

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 82.254 22.797 79.523

C,0,1.8857342176,-0.3556097727,-0.314578006
H,0,1.9648443651,-0.1660346004,-1.3852431976
C,0,0.7914350287,0.1609417811,0.3533074053
H,0,0.6620684635,0.002673198,1.4207400657
C,0,-0.1337131284,0.8843527075,-0.375513388
H,0,0.0463708416,1.0117697994,-1.4431578282
C,0,2.9515212147,-1.1411158729,0.3066547742
H,0,2.8071590866,-1.2916254783,1.375924924
H,0,3.0221642489,-2.1048669369,-0.216788163
H,0,3.9103558257,-0.6415863392,0.1092917045
C,0,-1.3418295532,1.4955515249,0.1773170704
H,0,-1.4576495315,1.3271869822,1.2474215751
H,0,-1.3201758401,2.5710756844,-0.0477236856
H,0,-2.2100652393,1.108737323,-0.3743132506

Pentadienyl cation – PCM

M062X/6-31+G**
E(RM062X) = -195.626628369

Zero-point correction= 0.124644 (Hartree/Particle)
Thermal correction to Energy= 0.131509
Thermal correction to Enthalpy= 0.132453
Thermal correction to Gibbs Free Energy= 0.094639
Sum of electronic and ZPE= -195.501984
Sum of electronic and thermal Energies= -195.495119
Sum of electronic and thermal Enthalpies= -195.494175
Sum of electronic and thermal Free Energies= -195.531989

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 82.523 22.734 79.587

C,0,1.8874873385,-0.355689829,-0.3173545985
H,0,1.9702339601,-0.1671380279,-1.3876057593
C,0,0.7920812296,0.1616609781,0.3481104029
H,0,0.6623878133,0.0025795226,1.4146939015
C,0,-0.1342879021,0.8861658469,-0.3780365471
H,0,0.0430297619,1.0165672984,-1.4454581998
C,0,2.9527200721,-1.142514578,0.3074755711
H,0,2.8062944213,-1.2934763795,1.3753367406
H,0,3.0260689927,-2.1065617473,-0.213164418
H,0,3.9124301986,-0.6444314246,0.1154482236
C,0,-1.3435680985,1.4961926235,0.1785569407
H,0,-1.4576912841,1.3271437519,1.2476593829
H,0,-1.3257287013,2.5715470506,-0.043225677
H,0,-2.2132378022,1.1094049144,-0.3690959637

1,3-pentadiene – gas phase

M062X/6-31+G**
E(RM062X) = -195.218450825

Zero-point correction= 0.114155 (Hartree/Particle)
Thermal correction to Energy= 0.120270
Thermal correction to Enthalpy= 0.121214
Thermal correction to Gibbs Free Energy= 0.085315
Sum of electronic and ZPE= -195.104296
Sum of electronic and thermal Energies= -195.098181
Sum of electronic and thermal Enthalpies= -195.097236
Sum of electronic and thermal Free Energies= -195.133135

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 75.471 21.056 75.556

C,0,1.8920441373,-0.3038310985,-0.3461098071
H,0,2.0463750967,-0.0787892503,-1.4023143613
C,0,0.845874336,0.2531205264,0.2773747453
H,0,0.675475632,0.0396722821,1.3336212811
C,0,-0.1062881338,1.1484533514,-0.3743436774
H,0,0.0692879901,1.3577620724,-1.429337583
C,0,2.8820196052,-1.2244298297,0.2991681633
H,0,2.6411412391,-1.3861758304,1.3530544546
H,0,2.8988270397,-2.1979173903,-0.2030427251
H,0,3.8967713926,-0.8162616565,0.2370981309
C,0,-1.1530207814,1.7078069548,0.2428802307
H,0,-1.3529634666,1.5172556349,1.2942365901
H,0,-1.8353740869,2.3676742338,-0.2814154419

1,3-pentadiene – SMD

M062X/6-31+G**
E(RM062X) = -195.224267908

Zero-point correction= 0.113805 (Hartree/Particle)
Thermal correction to Energy= 0.119911
Thermal correction to Enthalpy= 0.120855
Thermal correction to Gibbs Free Energy= 0.084998
Sum of electronic and ZPE= -195.110463
Sum of electronic and thermal Energies= -195.104357
Sum of electronic and thermal Enthalpies= -195.103413
Sum of electronic and thermal Free Energies= -195.139270

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 75.245 21.088 75.468

C,0,1.8916836388,-0.30485062,-0.3431683221
H,0,2.0445878668,-0.0795579002,-1.4000664538
C,0,0.8447817487,0.2519730063,0.2840235993
H,0,0.6732153543,0.0401274775,1.3410109021
C,0,-0.105635,1.1473209625,-0.3738801279
H,0,0.0737602688,1.3531480759,-1.4297296037
C,0,2.8822579715,-1.2243447162,0.2994516239
H,0,2.6465641848,-1.3892724789,1.3545315142
H,0,2.8992310299,-2.1949991154,-0.2092424635
H,0,3.8962784254,-0.8143819045,0.2293030073
C,0,-1.1544595666,1.7091821845,0.2418265075
H,0,-1.3569542747,1.5211041431,1.2943027524
H,0,-1.8351416561,2.3688908735,-0.2874929395

1,3-pentadiene – PCM

M062X/6-31+G**
E(RM062X) = -195.221027859

Zero-point correction= 0.113957 (Hartree/Particle)
Thermal correction to Energy= 0.120087
Thermal correction to Enthalpy= 0.121031
Thermal correction to Gibbs Free Energy= 0.085089

Sum of electronic and ZPE= -195.107071
Sum of electronic and thermal Energies= -195.100941
Sum of electronic and thermal Enthalpies= -195.099997
Sum of electronic and thermal Free Energies= -195.135938

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	75.355	21.090	75.645

C,0,1.8918510865,-0.3046382317,-0.3440008932
H,0,2.0456856779,-0.0799405837,-1.4004668143
C,0,0.8452084093,0.2523834219,0.2816421112
H,0,0.6740074613,0.040183006,1.3382394255
C,0,-0.1063220985,1.1479496029,-0.3739260511
H,0,0.0714914636,1.3549922247,-1.4293287538
C,0,2.882947602,-1.224952695,0.2995346522
H,0,2.6456093375,-1.3886625134,1.3538372648
H,0,2.8997364018,-2.1959172391,-0.2070612694
H,0,3.8966059736,-0.8155789854,0.2316848205
C,0,-1.1546682344,1.7092813716,0.2420212202
H,0,-1.3561681131,1.5205058298,1.2937487044
H,0,-1.8358149675,2.3687347914,-0.2850544171

(E)-4-chloropent-2-ene – gas phase

M062X/6-31+G**
E(RM062X) = -656.014200700

Zero-point correction= 0.128769 (Hartree/Particle)
Thermal correction to Energy= 0.136352
Thermal correction to Enthalpy= 0.137296
Thermal correction to Gibbs Free Energy= 0.096680
Sum of electronic and ZPE= -655.885432
Sum of electronic and thermal Energies= -655.877848
Sum of electronic and thermal Enthalpies= -655.876904
Sum of electronic and thermal Free Energies= -655.917521

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	85.562	26.292	85.485

C,0,-3.2959339927,-0.1068581332,-0.0107816581
H,0,-2.565320829,-0.0901615549,-0.8261025845
H,0,-4.2382501887,0.3020389801,-0.3834492793
H,0,-3.4567059166,-1.1567918395,0.2551316836
C,0,-2.7980465646,0.668591427,1.171198102
H,0,-1.8609368187,0.3327158955,1.6176154996
C,0,-3.4179073148,1.7207029767,1.7064623863
H,0,-4.3631301162,2.0749601481,1.2930441184
C,0,-2.8806990104,2.4920472881,2.8680056759
H,0,-1.938979843,2.0547703763,3.2071366656
C,0,-2.713592095,3.9739618459,2.569269339
H,0,-3.6689268333,4.4111634072,2.2660533471
H,0,-2.3479476626,4.5111529045,3.4469053866
H,0,-1.9975346428,4.0963848463,1.7509489354
Cl,0,-4.0164079617,2.3098203017,4.2850864625

(E)-4-chloropent-2-ene – SMD

M062X/6-31+G**
E(RM062X) = -656.023907117

Zero-point correction= 0.128242 (Hartree/Particle)
Thermal correction to Energy= 0.135873
Thermal correction to Enthalpy= 0.136817
Thermal correction to Gibbs Free Energy= 0.096094
Sum of electronic and ZPE= -655.895665
Sum of electronic and thermal Energies= -655.888034
Sum of electronic and thermal Enthalpies= -655.887090
Sum of electronic and thermal Free Energies= -655.927814

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	85.261	26.473	85.709

C,0,-3.3007960436,-0.1137179762,-0.0078734143
H,0,-2.5522603706,-0.1161969454,-0.8078162664
H,0,-4.2295061055,0.3092242287,-0.4002848091
H,0,-3.47954401,-1.1604627606,0.2620643973
C,0,-2.8065775479,0.6574112566,1.1765187533
H,0,-1.8820377907,0.307938141,1.6391101481
C,0,-3.412133041,1.7304262094,1.6920489769
H,0,-4.339481199,2.1080542042,1.2578857957
C,0,-2.8627272356,2.4966818928,2.8490468938
H,0,-1.9181826309,2.0648598801,3.1841635077
C,0,-2.7264419539,3.9831457149,2.577958125
H,0,-3.6886392519,4.4129941202,2.2843083132
H,0,-2.3522380648,4.5128348721,3.4572351292
H,0,-2.0167357828,4.1241848267,1.7563204649
Cl,0,-3.9930187617,2.2771212053,4.2958380647

(E)-4-chloropent-2-ene – PCM

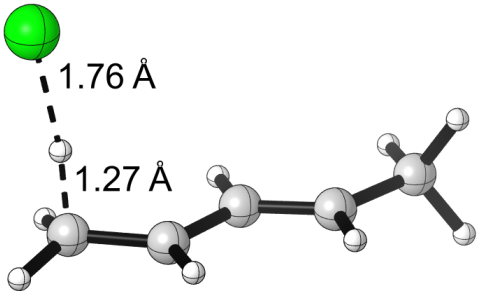
M062X/6-31+G**
E(RM062X) = -656.018604171

Zero-point correction= 0.128450 (Hartree/Particle)
Thermal correction to Energy= 0.136080
Thermal correction to Enthalpy= 0.137025
Thermal correction to Gibbs Free Energy= 0.096300
Sum of electronic and ZPE= -655.890154
Sum of electronic and thermal Energies= -655.882524
Sum of electronic and thermal Enthalpies= -655.881580
Sum of electronic and thermal Free Energies= -655.922305

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	85.392	26.443	85.713

C,0,-3.3000333938,-0.1128722242,-0.008982679
H,0,-2.5569007607,-0.1083847734,-0.81287881
H,0,-4.2324347921,0.3063800528,-0.3947359367
H,0,-3.4728772164,-1.1603027005,0.2589517677
C,0,-2.8045208078,0.659298202,1.1756310623
H,0,-1.8767012724,0.313029163,1.6330261973
C,0,-3.4134007094,1.7271695019,1.6957232804
H,0,-4.34449838,2.099089286,1.2658534282
C,0,-2.8671397924,2.4957848585,2.85301186
H,0,-1.9242125187,2.0627035552,3.1910807063
C,0,-2.7226784438,3.9821697822,2.5758954429
H,0,-3.6828870754,4.412887982,2.2791073839
H,0,-2.3521480011,4.5126137881,3.455395329
H,0,-2.0110925318,4.1188317791,1.756218388
Cl,0,-3.9987940941,2.2861006175,4.29322666

TS / one HCl SMD



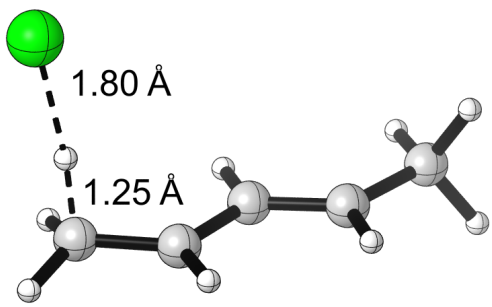
M06-2X/6-31+G**
E(RM062X) = -655.982854808

Zero-point correction= 0.120261 (Hartree/Particle)
Thermal correction to Energy= 0.128176
Thermal correction to Enthalpy= 0.129120
Thermal correction to Gibbs Free Energy= 0.086619
Sum of electronic and ZPE= -655.862594
Sum of electronic and thermal Energies= -655.854679
Sum of electronic and thermal Enthalpies= -655.853735
Sum of electronic and thermal Free Energies= -655.896236

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	80.431	26.878	89.451

C,0,1.9285979896,-0.3023708143,-0.3173152528
H,0,2.0557197106,-0.0562659872,-1.3722841561
C,0,0.86232593,0.2217621306,0.3368706081
H,0,0.690893148,0.0085126672,1.3904337167
C,0,-0.0486351997,1.0662935257,-0.3549853606
H,0,0.1581031586,1.2526948784,-1.4098584904
C,0,2.9485875617,-1.1837491249,0.297247169
H,0,2.7366956379,-1.3889811775,1.3481706756
H,0,3.0023512321,-2.127539007,-0.2583419309
H,0,3.9381825569,-0.7195876036,0.2065968361
C,0,-1.235605934,1.5540294206,0.1856587875
H,0,-1.3478931911,1.5368231813,1.2693855504
H,0,-1.7450880253,2.3556932636,-0.3446786149
H,0,-1.9275058816,0.5392938592,-0.1528576485
Cl,0,-3.0605106937,-0.779727212,-0.4244208892

TS / one HCl PCM



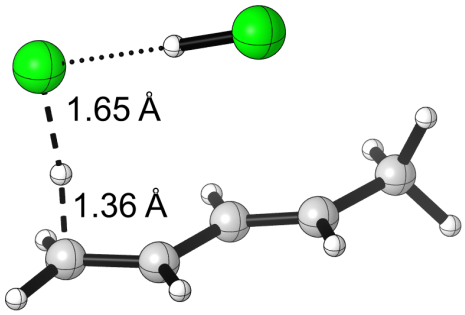
M062X/6-31+G**
E(RM062X) = -655.975058349

Zero-point correction= 0.121434 (Hartree/Particle)
Thermal correction to Energy= 0.129274
Thermal correction to Enthalpy= 0.130218
Thermal correction to Gibbs Free Energy= 0.087685
Sum of electronic and ZPE= -655.853624
Sum of electronic and thermal Energies= -655.845784
Sum of electronic and thermal Enthalpies= -655.844840
Sum of electronic and thermal Free Energies= -655.887373

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	81.121	26.344	89.519

C,0,1.9316417867,-0.304066703,-0.3141985805
H,0,2.0557272466,-0.0609354814,-1.3696688331
C,0,0.86342055,0.2179848962,0.342068
H,0,0.6965144075,0.0067155178,1.3957575754
C,0,-0.0480046773,1.054947995,-0.3499671722
H,0,0.1579100786,1.2408548705,-1.4044860271
C,0,2.9577927853,-1.1806590543,0.2970510573
H,0,2.7576036204,-1.3791339066,1.3504940982
H,0,3.005083023,-2.1272283507,-0.2530386745
H,0,3.945162235,-0.7167919655,0.1919141666
C,0,-1.2452263908,1.5427454131,0.1850384924
H,0,-1.3484989742,1.5417105385,1.2691055202
H,0,-1.7298397102,2.3618036267,-0.3408562493
H,0,-1.9410572793,0.5625050929,-0.148348369
Cl,0,-3.1020107014,-0.7835724892,-0.4512440046

TS / two HCl conf B SMD



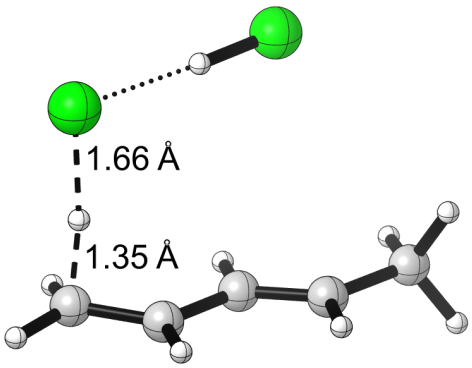
M062X/6-31+G**
E(RM062X) = -1116.75907127

Zero-point correction= 0.128130 (Hartree/Particle)
Thermal correction to Energy= 0.138868
Thermal correction to Enthalpy= 0.139812
Thermal correction to Gibbs Free Energy= 0.089570
Sum of electronic and ZPE= -1116.630941
Sum of electronic and thermal Energies= -1116.620203
Sum of electronic and thermal Enthalpies= -1116.619259
Sum of electronic and thermal Free Energies= -1116.669501

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	87.141	35.542	105.743

C,0,-2.0154141801,-0.9095808868,-0.5013475198
H,0,-2.0306020647,-1.3926960294,-1.4790679725
C,0,-0.9878018524,-1.187220195,0.3314570052
H,0,-0.9238528908,-0.7265507096,1.3160095345
C,0,0.056159735,-2.075952908,-0.0808926234
H,0,-0.0428098262,-2.5236420116,-1.0709971371
C,0,-3.1332953493,0.0162481049,-0.188700291
H,0,-3.0403332414,0.4470274346,0.81032846
H,0,-3.1590886152,0.8239893245,-0.9303434481
H,0,-4.0912583319,-0.5098310261,-0.2727866249
C,0,1.2247726162,-2.2804068144,0.6208201422
H,0,1.2893739816,-1.9510022271,1.6568502363
H,0,1.9125226432,-3.0571621619,0.2972193399
H,0,1.7462877782,-1.1902790165,0.0041558382
Cl,0,2.5563273998,0.1463714634,-0.5357793879
Cl,0,0.1565638286,1.0756579113,-2.7847140647
H,0,1.0609177293,0.7203134178,-1.8928999969

TS / two HCl conf C SMD



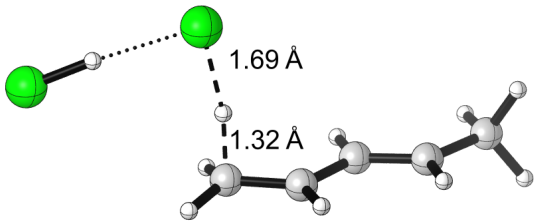
M062X/6-31+G**
E(RM062X) = -1116.75941400

Zero-point correction= 0.128804 (Hartree/Particle)
Thermal correction to Energy= 0.139293
Thermal correction to Enthalpy= 0.140237
Thermal correction to Gibbs Free Energy= 0.091098
Sum of electronic and ZPE= -1116.630610
Sum of electronic and thermal Energies= -1116.620121
Sum of electronic and thermal Enthalpies= -1116.619177
Sum of electronic and thermal Free Energies= -1116.668316

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	87.408	35.203	103.421

C	-2.049444	-0.893905	-0.470478
H	-2.048689	-1.304489	-1.480971
C	-1.025044	-1.215259	0.350414
H	-0.977671	-0.825300	1.366150
C	0.043115	-2.047213	-0.114459
H	-0.035211	-2.428044	-1.133662
C	-3.185211	-0.012370	-0.101232
H	-3.100254	0.357971	0.922501
H	-3.233572	0.838157	-0.791615
H	-4.131188	-0.555195	-0.214281
C	1.212934	-2.262755	0.582280
H	1.257687	-2.008596	1.640478
H	1.930872	-2.987919	0.208795
H	1.685364	-1.105731	0.060249
Cl	2.424439	0.322470	-0.338088
Cl	-0.196213	2.442676	0.217424
H	0.794715	1.600681	-0.005501

TS / two HCl conf A PCM



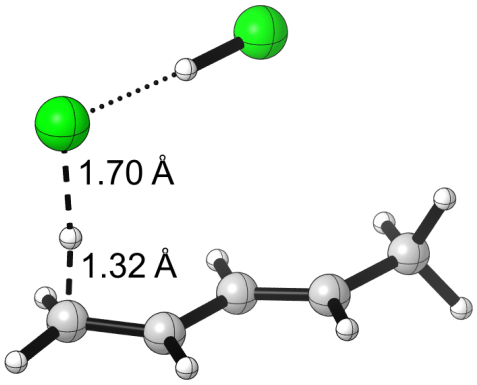
M062X/6-31+G**
E(RM062X) = -1116.74908508

Zero-point correction= 0.128921 (Hartree/Particle)
Thermal correction to Energy= 0.139675
Thermal correction to Enthalpy= 0.140619
Thermal correction to Gibbs Free Energy= 0.088847
Sum of electronic and ZPE= -1116.620164
Sum of electronic and thermal Energies= -1116.609410
Sum of electronic and thermal Enthalpies= -1116.608466
Sum of electronic and thermal Free Energies= -1116.660238

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	87.647	35.071	108.964

C,0,-2.078565247,-0.9425500974,-0.4429473568
H,0,-2.0728590675,-1.4440137253,-1.4109746742
C,0,-0.9834605971,-1.0556277268,0.3432299881
H,0,-0.943251916,-0.5736480852,1.3178282274
C,0,0.1401459347,-1.8220060301,-0.0916625417
H,0,0.0646534417,-2.2930052085,-1.0721937865
C,0,-3.3063530547,-0.1867813663,-0.0859511697
H,0,-3.2312859399,0.2748798842,0.8996076545
H,0,-3.4939090773,0.5885790323,-0.8368742237
H,0,-4.1735026068,-0.8556728574,-0.1094554839
C,0,1.3457124307,-1.9023767062,0.5829437028
H,0,1.3912249248,-1.5761610758,1.620561119
H,0,2.0743515686,-2.6446351452,0.2683418427
H,0,1.8092369468,-0.8248462587,-0.0298757166
Cl,0,2.6551792312,0.5305196236,-0.572918594
Cl,0,5.1606352939,-0.8722476561,1.2554882758
H,0,4.2345586838,-0.2913504211,0.5160950966

TS / two HCl conf B PCM



M062X/6-31+G**
E(RM062X) = -1116.75042899

Zero-point correction= 0.128911 (Hartree/Particle)
Thermal correction to Energy= 0.139618
Thermal correction to Enthalpy= 0.140562
Thermal correction to Gibbs Free Energy= 0.089635
Sum of electronic and ZPE= -1116.621518
Sum of electronic and thermal Energies= -1116.610811
Sum of electronic and thermal Enthalpies= -1116.609867
Sum of electronic and thermal Free Energies= -1116.660794

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	87.612	35.118	107.185

C	-2.015089	-0.931119	-0.477702
H	-1.998367	-1.340774	-1.487982
C	-0.988625	-1.229974	0.351613
H	-0.958640	-0.837657	1.366202
C	0.096270	-2.035220	-0.106812
H	0.028007	-2.422469	-1.123808
C	-3.171543	-0.073135	-0.117757
H	-3.110482	0.283990	0.911219
H	-3.213856	0.786855	-0.795813
H	-4.105976	-0.627135	-0.259351
C	1.280468	-2.215774	0.587375
H	1.309835	-1.976222	1.648744
H	1.998456	-2.945064	0.224515
H	1.733610	-1.084627	0.082955
Cl	2.430723	0.403724	-0.348585
Cl	-0.291288	2.389094	0.231860
H	0.738140	1.596516	-0.002656