cl-_clono2_cjp_supp_info.txt

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A Theoretical Study of ClONO₂ + Cl- --> Cl₂ + NO₃- on Ice
 Roberto Bianco and James T Hynes

Supporting information

The model reaction system Cl-.ClONO₂.(H₂O)₈.(EFP)₂₉ comprises a core reaction system Cl-.ClONO₂.(H₂O)₈ modelled ab initio and an embedding lattice made of 29 water effective fragment potentials (EFPs).

This file contains structures, energies and vibrational frequencies for
 - transition state (TS)
 - reactant complex (RC)
 - product complex (PC)

The structure is given in cartesian coordinates (angstrom) as:
 atom label / nuclear charge / x / y / z.

Frequencies (cm⁻¹) are unscaled.

The internal modes of the fragment water molecules (whose internal structure is frozen) are excluded from the frequency calculation.

Each water effective fragment potential is described below as:

FRAGNAME=H2OEF2

ZO1	x1	y1	z1
ZH2	x2	y2	z2
ZH3	x3	y3	z3

Transition state (TS)

ENERGY= -221.183959 hartree

CL1	17.0	0.9709116379	0.4519755978	0.4863737292
CL2	17.0	2.3865414483	-0.4993482709	-1.0280548135
O3	8.0	3.4561284620	-1.2292377618	-2.4856857878
N4	7.0	3.7104356907	-2.5067291179	-2.4826666240
O5	8.0	3.6732719168	-3.1135233069	-1.4309268641
O6	8.0	3.9771665151	-3.0022903002	-3.5491878902
O	8.0	-0.4415425264	-2.4860098458	1.3726675743
H	1.0	-0.1498586218	-1.5617148742	1.3166837930
H	1.0	-1.4021204445	-2.5545494056	1.2075106570
O	8.0	-0.6219563661	1.0866872700	-2.5418992340
H	1.0	-0.3710080553	0.9279552364	-1.6175548472
H	1.0	-1.5798084098	0.9297347234	-2.6798970848
O	8.0	-0.5222829306	2.6627765629	2.5100124414
H	1.0	0.0764228014	2.0447950495	2.0610914873
H	1.0	-1.4301129503	2.5539261998	2.1609705799
O	8.0	0.9829276695	-3.9416807545	-0.4316546246
H	1.0	0.5317590809	-3.4610191004	0.3001511455
H	1.0	1.9371640527	-3.7675013241	-0.4450841290
O	8.0	0.8023699440	-0.7768279800	-4.0456319534
H	1.0	0.3379091561	-0.0270807454	-3.6152278289
H	1.0	1.7631499928	-0.6562180806	-4.0165500485
O	8.0	0.2554253699	5.1857128777	1.6823624978
H	1.0	0.0182840462	4.3212662808	2.0796109210
H	1.0	1.0573064117	5.5508049027	2.0730347617
O	8.0	0.0821917755	-3.2123714379	-2.9398566644
H	1.0	0.3771685515	-3.4540876079	-2.0349919533
H	1.0	0.3610406581	-2.3129785978	-3.2145214526
O	8.0	0.6172888575	-4.7429125143	-5.0802454039

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H          1.0    1.5645717098  -4.7911465544  -5.2719580490
H          1.0    0.4590632302  -4.2643183619  -4.2285821383
FRAGNAME=H2OEF2
ZO1        -3.2098735499  -2.5087393711   0.6032775647
ZH2        -3.4230178753  -1.6637384176   0.2407567525
ZH3        -3.4090371973  -3.1475758154  -0.0623802250
FRAGNAME=H2OEF2
ZO1        -0.2544418078  -3.1082545533   4.2559559337
ZH2        -0.2092432709  -2.9811290116   3.3217853695
ZH3        -0.5260903374  -4.0013666664   4.3953700069
FRAGNAME=H2OEF2
ZO1        -3.3923671656   0.8971489592  -2.9500274482
ZH2        -3.6646004434   0.3729604853  -3.6862298255
ZH3        -3.6735259822   1.7805603624  -3.1272630730
FRAGNAME=H2OEF2
ZO1        -0.6143357133   3.9115414110  -2.9667487432
ZH2        -0.4935866792   2.9842626900  -2.8384822301
ZH3        -0.0887920622   4.1529281353  -3.7126808944
FRAGNAME=H2OEF2
ZO1        -3.1192586291   2.3956324253   1.3348406712
ZH2        -3.4346037871   3.1795201006   0.9141792897
ZH3        -3.8210926413   2.0799040278   1.8813048076
FRAGNAME=H2OEF2
ZO1        -0.5315608259   1.7294388252   5.2429037234
ZH2        -0.4939063332   2.0855764089   4.3696187672
ZH3        -0.9511667138   2.3797272677   5.7832131666
FRAGNAME=H2OEF2
ZO1        -3.8165701627   0.0659803909  -0.2757414170
ZH2        -3.8305659540   0.2612007074  -1.1990894554
ZH3        -3.3965652728   0.7964122879   0.1496332301
FRAGNAME=H2OEF2
ZO1        -4.7147276572  -3.2895247616   2.8953952774
ZH2        -4.2286045510  -3.0092650560   2.1364372568
ZH3        -4.6069600593  -2.6179370105   3.5497915576
FRAGNAME=H2OEF2
ZO1        -5.0735002934   0.7450872772   2.4679923792
ZH2        -4.8327879668   0.1741450949   3.1800043555
ZH3        -5.1418136248   0.2040378781   1.6976176064
FRAGNAME=H2OEF2
ZO1        -4.2743891212  -1.0149562247   4.6601277897
ZH2        -3.3644772542  -0.9806282486   4.9086442649
ZH3        -4.7759437004  -0.9472374545   5.4568307622
FRAGNAME=H2OEF2
ZO1        -1.6845340089  -0.9762763766   5.5138128553
ZH2        -1.1825995549  -0.1813622909   5.4298375364
ZH3        -1.1438490762  -1.6749048285   5.1814628232
FRAGNAME=H2OEF2
ZO1        -4.1126654692  -5.9217396351   3.5398440100
ZH2        -4.3368153038  -5.0353751976   3.3053373157
ZH3        -4.7475505562  -6.2019078370   4.1796136240
FRAGNAME=H2OEF2
ZO1        -3.6028924762   3.6992368237  -2.9246388859
ZH2        -3.8579249910   3.9936201121  -2.0648858109
ZH3        -2.7053870614   3.9645197373  -3.0470621691
FRAGNAME=H2OEF2
ZO1        -3.7170300553   4.7975035224  -0.1567571245
ZH2        -2.8737546509   5.2044984419  -0.2755854967
ZH3        -4.3159351742   5.4825255315   0.0941132796
FRAGNAME=H2OEF2
ZO1        -1.2014343073   5.7079234104  -0.6444788290
ZH2        -0.6336313954   5.6160055985   0.1038723073
ZH3        -0.8331445294   5.1756493243  -1.3314470894
FRAGNAME=H2OEF2
ZO1        -3.9547878352  -1.0953130274  -4.7770551383
ZH2        -3.7464983038  -1.2180655257  -5.6894288278

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ZH3      -3.5846135797  -1.8292405542  -4.3131587489
FRAGNAME=H2OEF2
ZO1      -2.8705190836  -2.2550268218  -7.2161616638
ZH2      -1.9443100082  -2.0987584587  -7.1234502766
ZH3      -3.0057069048  -3.1779394975  -7.0718186696
FRAGNAME=H2OEF2
ZO1      -0.0726522970  -2.1506164649  -6.5003215190
ZH2      0.1533646108   -1.5901991708  -5.7752509928
ZH3      0.1253691886   -3.0337810444  -6.2325785999
FRAGNAME=H2OEF2
ZO1      0.1793758811   -6.6325957075  -0.4518269237
ZH2      0.4906347546   -5.7418055406  -0.4739458389
ZH3      0.7286772640   -7.1265633653  -1.0393151346
FRAGNAME=H2OEF2
ZO1      -1.2346257536   -5.8605587558   4.2385794894
ZH2      -2.1664557032   -5.8852244330   4.0903802876
ZH3      -0.8398620869   -6.4027131859   3.5744193616
FRAGNAME=H2OEF2
ZO1      -0.2999012782   -7.6805685981   2.0827830253
ZH2      -0.0755902740   -7.3015621144   1.2479674092
ZH3      0.3820962952   -8.2985569616   2.2921825156
FRAGNAME=H2OEF2
ZO1      -3.1769562231   -7.9281083202   1.5617766383
ZH2      -3.5832295070   -7.2853775658   2.1209882710
ZH3      -2.2954496971   -8.0447292643   1.8783587826
FRAGNAME=H2OEF2
ZO1      -2.5932584536   -6.9193481722   -1.0497978643
ZH2      -2.9139610942   -7.4071270177   -0.3081105526
ZH3      -1.6652323887   -6.8066429133   -0.9196302742
FRAGNAME=H2OEF2
ZO1      -3.9292324542   -4.5608887620   -1.2555352875
ZH2      -3.4863030483   -5.3877951228   -1.1510466946
ZH3      -4.8530347625   -4.7508000402   -1.2929713076
FRAGNAME=H2OEF2
ZO1      -2.6828019453   -3.3016736672   -3.4556016827
ZH2      -3.1362890637   -3.6868833286   -2.7229070640
ZH3      -1.7752357108   -3.2309960619   -3.2061890523
FRAGNAME=H2OEF2
ZO1      -2.3931311578   -5.0297849811   -5.6744271830
ZH2      -2.5750232315   -4.3984988535   -4.9967314159
ZH3      -1.4545194511   -5.0652111286   -5.7673330834
FRAGNAME=H2OEF2
ZO1      -2.6127057269   -7.5592508671   -4.0418627797
ZH2      -2.8222249963   -6.7835672960   -4.5371355603
ZH3      -2.7556205222   -7.3477530591   -3.1331700415
FRAGNAME=H2OEF2
ZO1      0.1931215942   -7.6218018316   -4.6101784015
ZH2      -0.7246561851   -7.7885614829   -4.4661172314
ZH3      0.2692944567   -6.7118123470   -4.8489152587
FRAGNAME=H2OEF2
ZO1      1.6302732931   -8.1749471090   -2.3163485894
ZH2      1.2146591441   -8.0247922655   -3.1503730832
ZH3      1.7286800473   -9.1093674478   -2.2266089929

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Saddle point single imaginary frequency: 249.21 I cm⁻¹.

Translations and rotations:

20.09 12.66 10.83 7.66 5.92 4.85

Vibrations:

7.69 15.59 18.74

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20.46	25.00	25.87	27.36	31.05
31.63	34.02	35.73	36.85	37.88
39.52	41.31	41.68	42.61	45.63
45.94	47.84	51.13	51.49	53.72
55.07	56.16	56.96	58.84	59.90
60.51	62.00	63.53	63.97	66.72
69.63	70.86	72.39	76.10	76.43
77.28	78.38	81.15	82.18	83.14
85.76	88.80	90.16	91.87	96.76
97.49	100.31	101.45	103.18	105.32
109.33	111.95	118.11	120.19	121.18
123.30	128.13	129.18	131.70	132.10
135.35	138.01	139.49	141.75	146.07
151.62	152.20	154.83	155.55	158.53
160.69	161.77	166.96	168.52	171.51
172.88	179.49	182.49	182.74	188.16
190.67	193.65	196.42	199.23	201.83
204.63	209.84	212.06	214.47	217.96
219.61	222.65	224.78	225.59	227.70
232.44	237.02	238.79	241.99	242.81
245.57	247.12	251.70	253.73	255.90
260.91	264.58	266.75	267.90	273.31
275.03	277.65	283.67	284.98	287.55
297.08	313.41	319.15	331.41	335.32
338.80	351.85	357.32	376.21	393.66
400.27	402.07	407.02	411.09	416.51
420.33	424.41	428.58	432.22	438.63
441.47	451.82	452.83	458.25	460.14
467.49	472.46	476.64	486.56	492.26
498.01	505.67	510.29	514.48	520.29
527.40	533.60	542.20	544.69	548.18
556.43	559.73	562.72	567.37	568.60
579.65	582.19	588.86	597.96	599.28
610.85	614.74	620.34	623.34	629.38
637.23	642.43	644.39	653.19	666.16
666.71	671.01	679.72	682.62	694.55
702.72	709.97	712.07	717.29	725.35
740.05	742.99	751.44	753.27	758.23
764.95	769.49	773.91	777.63	777.77
791.98	797.00	802.10	805.31	813.91
817.54	826.90	835.93	842.03	846.09
848.82	865.99	872.00	876.31	891.01
897.43	902.97	908.61	914.92	944.51
946.84	960.04	969.25	978.92	992.27
1001.89	1003.92	1029.91	1030.29	1050.76
1109.16	1132.66	1155.71	1534.03	1730.08
1734.87	1736.75	1738.45	1747.36	1750.08
1754.52	1759.39	1773.39	3503.54	3593.77
3644.16	3675.00	3723.29	3742.35	3771.38
3817.51	3826.61	3938.27	3939.27	3953.72
3967.78	3977.80	3983.42	4051.87	

Reactant complex (RC)

ENERGY= -221.194492 hartree

CL1	17.0	0.7268251495	0.3498150881	0.0866641048
CL2	17.0	3.1246024876	-0.7825729842	-1.1074002475
O3	8.0	4.4951130878	-1.3812192517	-1.9013309567
N4	7.0	4.7521373034	-2.7054905529	-1.7486614052
O5	8.0	4.0307216456	-3.3673367929	-1.0639905734
O6	8.0	5.7199144450	-3.0492156333	-2.3536688741
O	8.0	-0.5798360449	-2.3996566081	1.1534894627

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H	1.0	-0.2731689758	-1.4872687089	0.9831473925
H	1.0	-1.5517220320	-2.4567225362	1.0887099839
O	8.0	-0.8954695840	1.0521270266	-2.5693301792
H	1.0	-0.5279342670	0.8824148489	-1.6769457400
H	1.0	-1.8619516428	0.9049932062	-2.6007549001
O	8.0	-0.6073939583	2.3822454041	2.1901162897
H	1.0	-0.1283992167	1.7389040459	1.6304613643
H	1.0	-1.5599483634	2.3520958071	1.9807370357
O	8.0	0.9322572932	-3.8791358429	-0.4640627277
H	1.0	0.3730250207	-3.3795727202	0.1862693203
H	1.0	1.8726514133	-3.7511169224	-0.2767952008
O	8.0	0.5836036354	-0.5950473975	-4.0900021610
H	1.0	0.0107256927	0.0469421607	-3.5977550138
H	1.0	1.4488725372	-0.2046550653	-4.2663583704
O	8.0	0.2904450643	4.8742775303	1.5118933773
H	1.0	0.0106919815	3.9855399389	1.8278622793
H	1.0	1.2197726074	5.0388053405	1.7079965151
O	8.0	0.2666265390	-3.1380669672	-3.0407240345
H	1.0	0.5292694197	-3.3777300670	-2.1243811437
H	1.0	0.4776459939	-2.2093228590	-3.2752298913
O	8.0	0.3686057092	-4.6895296674	-5.1917803284
H	1.0	1.2606119409	-4.8054429644	-5.5447260294
H	1.0	0.3811693647	-4.1907304601	-4.3323893285
FRAGNAME=H2OEF2				
ZO1		-3.4229890028	-2.4505191653	0.6547578282
ZH2		-3.6809837503	-1.6005810254	0.3355050714
ZH3		-3.6293880440	-3.0703251646	-0.0265045391
FRAGNAME=H2OEF2				
ZO1		-0.1364007431	-3.0171638217	4.0102288078
ZH2		-0.1891804037	-2.8513275462	3.0825483180
ZH3		-0.4013504100	-3.9135794735	4.1410688142
FRAGNAME=H2OEF2				
ZO1		-3.7268841086	0.9272693115	-2.8338731856
ZH2		-3.9969388230	0.4269285582	-3.5872708468
ZH3		-3.9923488895	1.8192581191	-2.9912354151
FRAGNAME=H2OEF2				
ZO1		-0.9556141396	3.8711324213	-2.9847953932
ZH2		-0.8270824968	2.9474129602	-2.8395355290
ZH3		-0.4678516845	4.0940581968	-3.7615001892
FRAGNAME=H2OEF2				
ZO1		-3.4014765875	2.3954556739	1.3992601278
ZH2		-3.6977423260	3.2077626836	1.0207599451
ZH3		-4.0638481632	2.1256464956	2.0151703137
FRAGNAME=H2OEF2				
ZO1		-0.3235225632	1.6993788259	4.9395730188
ZH2		-0.3406729459	1.9224607150	4.0226113025
ZH3		-0.7186506524	2.4212378745	5.4018194478
FRAGNAME=H2OEF2				
ZO1		-4.1773954508	0.0932723848	-0.1564102827
ZH2		-4.1823888868	0.2745121835	-1.0826962294
ZH3		-3.7462706576	0.8222071705	0.2603197798
FRAGNAME=H2OEF2				
ZO1		-4.7135908625	-3.2681911154	3.0513898350
ZH2		-4.3034120343	-2.9820657662	2.2509124353
ZH3		-4.5471267601	-2.5989237694	3.6957882958
FRAGNAME=H2OEF2				
ZO1		-5.2462275452	0.7454327007	2.7264894690
ZH2		-4.8960392433	0.1805569439	3.3966849529
ZH3		-5.3633833196	0.2124155122	1.9563948934
FRAGNAME=H2OEF2				
ZO1		-4.1375080420	-1.0112262985	4.7963096457
ZH2		-3.2087811823	-0.9597660982	4.9566116166
ZH3		-4.5611021431	-0.9658131055	5.6385590942
FRAGNAME=H2OEF2				
ZO1		-1.4890348785	-0.9400310159	5.4317290241

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ZH2	-1.0107132249	-0.1372504486	5.2989502211	
ZH3	-0.9749703880	-1.6295832998	5.0429697137	
FRAGNAME=H2OEF2				
ZO1	-4.0321235421	-5.8846822616	3.6215246572	
ZH2	-4.2847659778	-4.9995480151	3.4127481752	
ZH3	-4.6144747886	-6.1793554715	4.3033700790	
FRAGNAME=H2OEF2				
ZO1	-3.9220289629	3.7394961668	-2.8029980590	
ZH2	-4.1373023821	4.0388549809	-1.9341366722	
ZH3	-3.0206402340	3.9744030341	-2.9552990016	
FRAGNAME=H2OEF2				
ZO1	-3.8904869613	4.8661564260	-0.0360938183	
ZH2	-3.0225286270	5.2106606977	-0.1733657773	
ZH3	-4.4321108453	5.5926821610	0.2278803827	
FRAGNAME=H2OEF2				
ZO1	-1.3412977564	5.6426592268	-0.6107522444	
ZH2	-0.7336343682	5.4832033835	0.0936606279	
ZH3	-1.0542888446	5.1175987233	-1.3406945752	
FRAGNAME=H2OEF2				
ZO1	-4.1461176940	-1.0916083521	-4.7023913456	
ZH2	-4.0153287507	-1.2240918146	-5.6277133644	
ZH3	-3.6385768629	-1.7526275308	-4.2592949631	
FRAGNAME=H2OEF2				
ZO1	-3.1741961762	-2.2526623450	-7.1995883124	
ZH2	-2.2552946409	-2.0481489836	-7.1312311078	
ZH3	-3.2629505604	-3.1715668294	-7.0030796309	
FRAGNAME=H2OEF2				
ZO1	-0.3531475397	-2.0491968447	-6.4896731513	
ZH2	-0.1565362933	-1.4946059853	-5.7516681035	
ZH3	-0.1997947920	-2.9375137389	-6.2099331213	
FRAGNAME=H2OEF2				
ZO1	0.0957306362	-6.5616470448	-0.5586104156	
ZH2	0.4008248146	-5.6684624264	-0.5544590551	
ZH3	0.6365103351	-7.0301787678	-1.1741701575	
FRAGNAME=H2OEF2				
ZO1	-1.1140847965	-5.7798593986	4.1075528001	
ZH2	-2.0542453710	-5.8088112178	4.0292052385	
ZH3	-0.7686176536	-6.3530009660	3.4419405624	
FRAGNAME=H2OEF2				
ZO1	-0.3176578427	-7.6728418553	1.9621757659	
ZH2	-0.1137420595	-7.2868857054	1.1253157670	
ZH3	0.3649370640	-8.2982531278	2.1460327420	
FRAGNAME=H2OEF2				
ZO1	-3.2196891189	-7.8465711716	1.5597545910	
ZH2	-3.5965217374	-7.2122495692	2.1484070661	
ZH3	-2.3308401721	-7.9866433828	1.8447208689	
FRAGNAME=H2OEF2				
ZO1	-2.7146801033	-6.8301634419	-1.0567982300	
ZH2	-3.0218422496	-7.2993225960	-0.2975752337	
ZH3	-1.7823083540	-6.7265126010	-0.9527891995	
FRAGNAME=H2OEF2				
ZO1	-3.9981536954	-4.4406826053	-1.3299191247	
ZH2	-3.5905767229	-5.2806635255	-1.1913856659	
ZH3	-4.9044961678	-4.6090533283	-1.5325840611	
FRAGNAME=H2OEF2				
ZO1	-2.5911321219	-3.1578352207	-3.4025920984	
ZH2	-3.0195261913	-3.5264758688	-2.6466416715	
ZH3	-1.6716204601	-3.1074021878	-3.1956301042	
FRAGNAME=H2OEF2				
ZO1	-2.6070971317	-4.9153451630	-5.6047049956	
ZH2	-2.7154076433	-4.2799615824	-4.9151870534	
ZH3	-1.6785951786	-5.0015788704	-5.7507403505	
FRAGNAME=H2OEF2				
ZO1	-2.8461974434	-7.4725113515	-4.0175444160	
ZH2	-3.0526770729	-6.6824801597	-4.4909315014	

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cl-_clono2_cjp_supp_info.txt      Mon Jan 06 14:57:30 2003      7
ZH3      -2.9541554997  -7.2755178762  -3.1008017679
FRAGNAME=H2OEF2
ZO1      -0.0702791769  -7.5516752673  -4.6722635508
ZH2      -0.9775882465  -7.7377489986  -4.4904799627
ZH3      -0.0196308026  -6.6344712554  -4.8891736632
FRAGNAME=H2OEF2
ZO1      1.5560065085   -8.0154127638  -2.4968734970
ZH2      1.0558732534   -7.9244383806  -3.2921525945
ZH3      1.7493258398   -8.9343411527  -2.4016017476

```

Translations and rotations:

	1.24	1.01	0.46	0.10	0.22	0.96
Vibrations:						
	8.10	13.91	18.61	21.41		
23.16	25.14	27.73	29.03	31.34		
33.86	36.35	37.43	37.82	38.99		
40.16	40.82	42.21	43.32	44.48		
46.54	47.60	49.40	53.14	55.45		
55.73	57.42	59.22	59.44	62.14		
63.31	63.85	65.29	66.71	67.84		
70.43	72.98	73.52	75.46	75.78		
78.56	79.83	80.91	83.28	84.87		
86.79	89.16	90.90	94.00	98.57		
100.99	102.14	104.14	105.14	105.65		
107.86	112.13	114.58	118.12	123.15		
127.90	130.34	131.44	134.48	136.56		
140.49	142.23	145.63	147.36	148.00		
150.82	152.52	154.19	158.87	161.59		
163.11	165.44	168.45	169.74	175.56		
179.46	180.90	182.78	184.06	187.38		
191.27	194.36	196.63	201.30	202.94		
204.48	206.19	207.50	212.87	214.43		
216.90	219.93	222.02	223.08	226.03		
229.31	231.68	235.75	239.06	239.56		
241.49	243.43	245.61	250.86	254.44		
257.45	262.28	270.17	274.31	277.42		
280.67	282.94	299.44	303.89	311.37		
316.05	320.65	325.11	328.89	331.53		
348.28	362.13	374.91	388.99	393.36		
403.51	409.11	411.51	417.86	423.69		
432.51	435.87	438.33	439.48	446.43		
455.95	458.37	461.93	465.10	468.02		
470.24	482.86	489.72	495.61	498.91		
509.53	512.18	513.32	517.64	525.60		
530.49	534.83	543.21	546.29	554.30		
557.83	560.61	568.62	571.82	577.60		
583.78	588.24	598.04	602.71	608.52		
619.32	625.91	635.22	637.31	644.90		
649.63	654.40	659.41	664.34	672.34		
679.90	681.35	687.49	696.36	708.79		
711.05	720.47	726.60	729.84	733.90		
736.65	745.07	750.70	754.45	763.48		
765.74	772.72	777.90	778.61	780.83		
785.53	795.60	800.65	809.22	823.34		
830.61	839.31	842.33	850.43	852.42		
860.47	869.64	878.60	886.23	895.66		
901.99	909.11	933.00	941.51	952.29		
968.69	978.38	988.60	992.37	1007.30		
1010.26	1015.44	1038.14	1040.61	1079.07		
1082.65	1131.79	1146.12	1545.43	1725.43		
1742.61	1744.67	1752.35	1760.50	1762.33		
1774.61	1781.83	1866.16	3443.48	3466.02		

cl1-clono2_cjp_supp_info.txt

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3500.10	3638.98	3657.22	3731.24	3759.42
3774.28	3782.43	3837.75	3881.27	3895.26
4017.58	4028.01	4039.97	4063.20	

Product complex (PC)

ENERGY= -221.210153 hartree

CL1	17.0	2.0179154194	1.6503201341	0.2757742064
CL2	17.0	2.7763869223	0.1026653966	-0.7267392284
O3	8.0	3.3486901772	-1.9403276720	-2.8379326441
N4	7.0	3.2601225900	-3.1088761535	-3.2370656511
O5	8.0	3.1770803216	-4.0374035588	-2.4084368470
O6	8.0	3.2297058407	-3.3589089072	-4.4382858042
O	8.0	-0.5545255449	-1.5651639570	1.3686312694
H	1.0	0.1773480828	-1.7600383428	0.7658007293
H	1.0	-1.3784216980	-1.9763329387	1.0400551468
O	8.0	-0.7438262419	1.1521417285	-2.6148531553
H	1.0	-0.9575115934	0.8222668736	-1.7270570240
H	1.0	-1.5571075873	1.0872716852	-3.1527781372
O	8.0	-1.2453020164	1.0642941604	2.1661106464
H	1.0	-0.9271078136	0.1742490481	1.9073973653
H	1.0	-2.1229457817	1.2465201394	1.7858615044
O	8.0	1.5242045110	-3.7955397800	-0.3356942695
H	1.0	1.9004603104	-3.6125647486	0.5337301830
H	1.0	2.2331013444	-3.8073472527	-1.0291124247
O	8.0	0.8628706134	-0.8211133162	-3.7770266267
H	1.0	0.4965310264	0.0160278869	-3.4360294959
H	1.0	1.8293164876	-0.8878962464	-3.6818307736
O	8.0	0.1410653293	3.4178688961	1.9862392840
H	1.0	-0.2821586591	2.5333870436	2.0499126463
H	1.0	0.5911243739	3.6444617083	2.8094015627
O	8.0	-0.2132702425	-2.9967269655	-2.5777579726
H	1.0	0.1797145908	-3.2102087513	-1.7154218850
H	1.0	0.1739646308	-2.1749949370	-2.9618409479
O	8.0	0.6048369913	-4.6905749710	-4.7182127269
H	1.0	1.5661166406	-4.5565213273	-4.8030914298
H	1.0	0.2995864849	-4.2379648370	-3.9058743132

FRAGNAME=H2OEF2

ZO1	-3.1329347023	-2.2927452533	0.3714223869
ZH2	-3.2243922589	-1.5448052961	-0.1969962879
ZH3	-3.3268188428	-3.0551604458	-0.1501238415

FRAGNAME=H2OEF2

ZO1	-0.2976696994	-2.4880145479	4.1784498171
ZH2	-0.3232182700	-2.1764245318	3.2878672064
ZH3	-0.5908995239	-3.3849950978	4.1605440325

FRAGNAME=H2OEF2

ZO1	-3.4275441806	1.0518807891	-3.5233809476
ZH2	-3.7673449634	0.5343677674	-4.2358373704
ZH3	-3.7779089595	1.9219350906	-3.6288725979

FRAGNAME=H2OEF2

ZO1	-0.5605743606	3.9641960975	-2.5732639572
ZH2	-0.4707520597	3.0248655811	-2.5516170340
ZH3	0.1046496725	4.2868763507	-3.1599775960

FRAGNAME=H2OEF2

ZO1	-3.8842682623	1.8194211650	1.1334073396
ZH2	-4.0483151087	2.7234787107	0.9174280806
ZH3	-4.5995581290	1.5371583558	1.6807340859

FRAGNAME=H2OEF2

ZO1	-1.0539650164	1.8656106583	4.8717024919
ZH2	-1.1148758839	1.5420937749	3.9871092823
ZH3	-1.7590925292	2.4829231982	4.9839471928

FRAGNAME=H2OEF2


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ZO1      -3.0416557991      0.1264144219      -0.9253790665
ZH2      -3.3819082844      0.3228897397      -1.7835772661
ZH3      -3.4163963982      0.7590687317      -0.3336050710
FRAGNAME=H2OEF2
ZO1      -4.7479571375      -2.7084574096      2.6689960534
ZH2      -4.1946612697      -2.4554329068      1.9473862297
ZH3      -4.4750188388      -2.1956540611      3.4129153131
FRAGNAME=H2OEF2
ZO1      -5.6810376877      0.4469417511      2.8376932625
ZH2      -5.2235428859      0.1709119709      3.6157578619
ZH3      -5.9713200221      -0.3377987234      2.4008900939
FRAGNAME=H2OEF2
ZO1      -4.3104271143      -0.9920010391      4.9803852461
ZH2      -3.4176366999      -0.8771206641      5.2642976083
ZH3      -4.8054916579      -1.2523675371      5.7406475946
FRAGNAME=H2OEF2
ZO1      -1.7591715397      -0.7656881026      5.8811876950
ZH2      -1.3818253460      0.0926487815      5.7728082799
ZH3      -1.1934548016      -1.3699685737      5.4276591529
FRAGNAME=H2OEF2
ZO1      -4.2548654711      -5.4036967897      3.2530470234
ZH2      -4.4872275339      -4.5307301330      2.9795227244
ZH3      -4.8743369316      -5.6528710514      3.9201645175
FRAGNAME=H2OEF2
ZO1      -3.5863097662      3.8473393651      -2.8751878930
ZH2      -3.8733880526      3.9765872112      -1.9853792024
ZH3      -2.6668613410      4.0594992702      -2.8971246681
FRAGNAME=H2OEF2
ZO1      -3.8492242934      4.4841260737      0.0932037141
ZH2      -2.9371382676      4.7193657561      0.1535346961
ZH3      -4.3437810234      5.2527812368      0.3287060181
FRAGNAME=H2OEF2
ZO1      -1.1768069572      5.0272591575      0.0965504256
ZH2      -0.6705401273      4.5720724759      0.7502915334
ZH3      -0.8339109275      4.7654600721      -0.7429506201
FRAGNAME=H2OEF2
ZO1      -4.1074341020      -1.0741110280      -5.1098952523
ZH2      -3.7825058449      -1.3056553450      -5.9652824810
ZH3      -3.7852962688      -1.7286630555      -4.5110068538
FRAGNAME=H2OEF2
ZO1      -2.6951849548      -2.3507379466      -7.2714278723
ZH2      -1.7977751275      -2.1332593410      -7.0758847516
ZH3      -2.7970627309      -3.2712837680      -7.0895082102
FRAGNAME=H2OEF2
ZO1      0.0091844743      -2.0992064274      -6.2984147942
ZH2      0.2565723732      -1.5422747548      -5.5776479848
ZH3      0.2800795084      -2.9741782892      -6.0705583137
FRAGNAME=H2OEF2
ZO1      0.2639987493      -6.3865048797      -0.3245091970
ZH2      0.6624324651      -5.5327538132      -0.3814138950
ZH3      0.7770201880      -6.9621233508      -0.8688903441
FRAGNAME=H2OEF2
ZO1      -1.3683814606      -5.1828831859      3.9819613958
ZH2      -2.2936928652      -5.2458179779      3.8067002465
ZH3      -0.9466957397      -5.8410625056      3.4529438252
FRAGNAME=H2OEF2
ZO1      -0.3349883601      -7.2906261864      2.2146507451
ZH2      -0.0749188606      -6.9805523080      1.3619512087
ZH3      0.3367230959      -7.8879246950      2.5026032855
FRAGNAME=H2OEF2
ZO1      -3.1751146847      -7.6370005013      1.5869044960
ZH2      -3.6103713909      -6.9292862116      2.0347555179
ZH3      -2.3118028248      -7.7053826041      1.9622642897
FRAGNAME=H2OEF2
ZO1      -2.4881276013      -6.7721771763      -1.0480814749

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ZH2	-2.7942236351	-7.2575274878	-0.2986692070
ZH3	-1.5740970909	-6.5902809160	-0.8986143195
FRAGNAME=H2OEF2			
ZO1	-3.9978949340	-4.5188068096	-1.1914475594
ZH2	-3.4910565173	-5.3142030767	-1.1548681694
ZH3	-4.9012194785	-4.7672229720	-1.0766754735
FRAGNAME=H2OEF2			
ZO1	-2.8915081832	-3.1288072528	-3.4217547276
ZH2	-3.3977176396	-3.5557650515	-2.7491943374
ZH3	-2.0208665284	-3.0155747397	-3.0752868921
FRAGNAME=H2OEF2			
ZO1	-2.2857218247	-4.9597725370	-5.5429173239
ZH2	-2.5419666299	-4.2980086045	-4.9205946169
ZH3	-1.3419912106	-4.9695392684	-5.5553910175
FRAGNAME=H2OEF2			
ZO1	-2.5165107630	-7.4996931723	-4.0118344429
ZH2	-2.6891255369	-6.7223557589	-4.5186175716
ZH3	-2.6460441122	-7.2674340386	-3.1062102050
FRAGNAME=H2OEF2			
ZO1	0.3417081402	-7.5856770552	-4.3964751377
ZH2	-0.5891884488	-7.7334973975	-4.3468854102
ZH3	0.4608866243	-6.6707270823	-4.5953255589
FRAGNAME=H2OEF2			
ZO1	1.4411808525	-8.3097650887	-1.9647770840
ZH2	1.2033239630	-8.0801384215	-2.8488439072
ZH3	1.1433162648	-9.1943867227	-1.8247781335

One imaginary frequency (16.94 I cm⁻¹) not included in the calculation of the zero point energy.

Translations and rotations:

0.51	0.42	0.15	0.08	1.26	1.58
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Vibrations:

		12.32	20.13	21.63
24.68	26.55	27.19	31.51	33.55
34.94	35.99	37.60	39.69	40.58
40.89	42.86	43.68	45.61	46.53
47.06	47.95	50.98	52.80	52.92
55.35	55.63	56.88	59.08	59.77
60.53	62.88	63.96	64.77	66.25
68.05	70.52	70.71	72.40	74.13
74.84	77.34	79.33	80.78	82.26
84.22	86.25	88.60	89.28	92.82
94.74	96.86	98.38	99.64	103.68
104.78	108.53	109.94	113.02	113.32
118.16	118.82	121.76	125.33	127.83
128.84	133.77	137.86	142.81	143.78
146.82	148.88	152.06	152.90	153.64
156.36	158.73	160.22	161.54	166.22
169.34	171.13	176.03	178.63	178.94
181.98	185.31	188.47	193.17	197.79
202.73	206.25	206.70	209.99	210.69
215.64	216.80	222.26	224.84	229.73
232.68	234.69	237.20	239.42	243.87
245.66	246.25	248.46	250.04	253.21
256.39	261.16	262.62	265.22	280.86
284.51	285.40	289.16	296.23	300.69
301.96	315.47	323.54	341.11	346.69
358.80	363.32	371.15	374.26	386.94
392.10	395.57	403.11	403.68	404.79
412.17	415.96	422.06	426.03	440.11
440.57	445.97	455.11	461.47	463.68

cl-_clqno2_cjp_supp_info.txt

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468.65	471.47	474.69	477.22	483.80
490.05	499.83	503.79	515.07	517.41
520.06	526.50	535.03	554.72	560.95
568.83	574.76	579.68	581.23	586.70
588.08	589.99	596.43	604.55	605.25
607.17	612.19	617.36	619.93	635.09
641.69	646.44	647.61	660.11	667.17
671.99	672.56	680.97	690.56	697.88
701.72	709.42	717.09	721.31	729.12
737.20	739.70	748.01	749.09	754.96
764.37	766.71	772.45	774.75	777.71
785.06	788.42	792.36	794.58	810.90
816.22	824.32	832.77	838.81	851.35
854.45	859.32	867.11	873.53	888.61
897.57	899.09	910.09	929.95	934.26
938.20	949.32	959.81	974.66	985.77
1001.28	1010.48	1016.09	1024.68	1030.75
1044.98	1102.95	1231.02	1568.95	1630.95
1716.58	1730.39	1745.46	1747.79	1766.21
1775.68	1781.83	1791.97	3489.78	3585.57
3657.63	3738.27	3762.64	3773.89	3806.19
3814.98	3903.49	3908.64	3919.69	3927.11
3979.76	4021.24	4025.52	4048.54	