

Supplementary Information for:

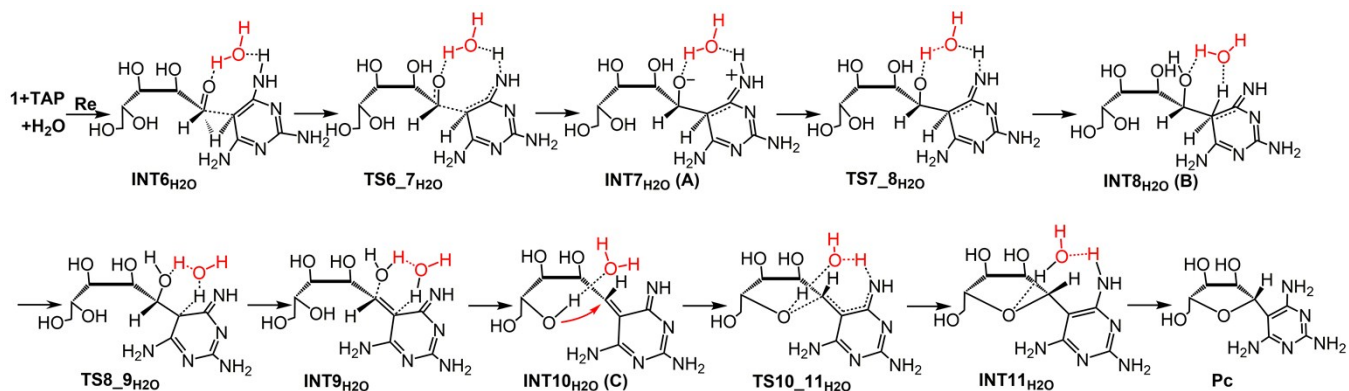
A Theoretical Insight into the Formation Mechanisms of C/N- ribonucleosides with Pyrimidine and Ribose

Wenjuan Wang, Fang Huang, Chuanzhi Sun, Jianbiao Liu, Xiehuang Sheng, Dezhan Chen**

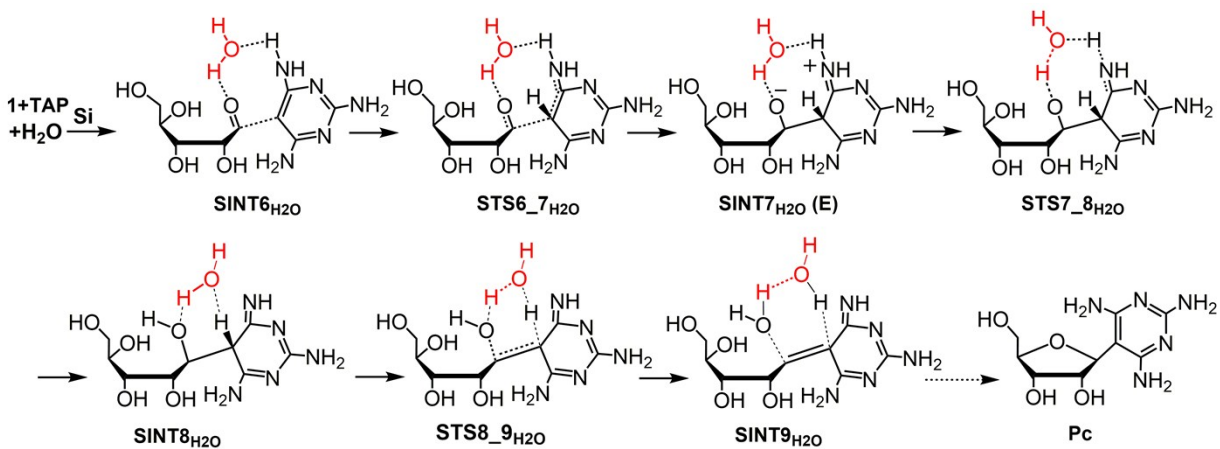
College of Chemistry, Chemical Engineering and Materials Science, Collaborative Innovation Center of Functionalized Probes for Chemical Imaging in Universities of Shandong, Key Laboratory of Molecular and Nano Probes, Ministry of Education, Shandong Provincial Key Laboratory of Clean Production of Fine Chemicals, Shandong Normal University, Jinan 250014, P. R. China.

Table of Contents

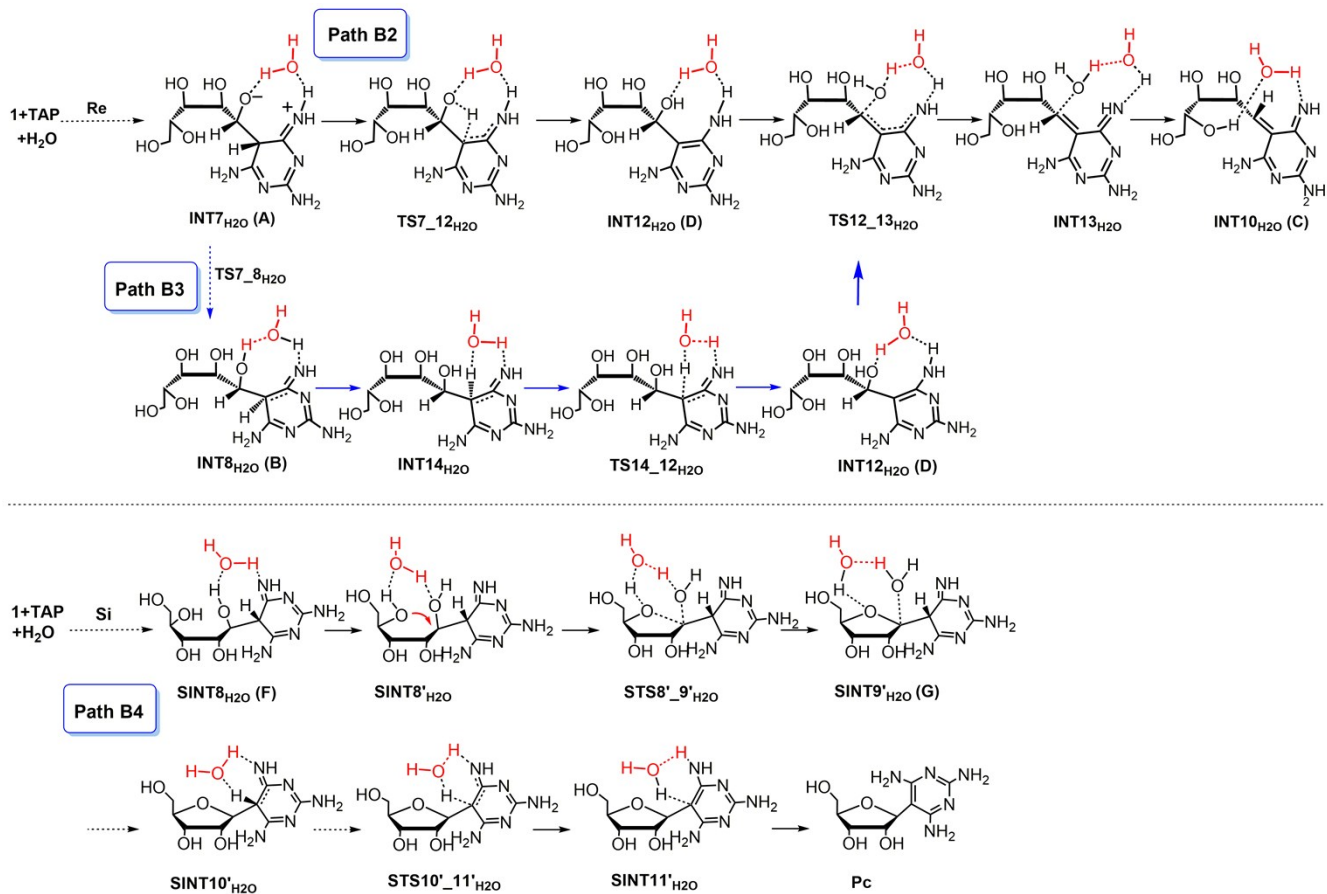
■ Scheme S1-S5 Detailed formation mechanisms of C/N-nucleosides	1-5
■ Fig. S1-S2 Optimized structures of key intermediates involved in the reactions	6
■ Cartesian Coordinates (Å), Absolute enthalpies and Gibbs free energies at 298.15 K and 1 atm for the Optimized Structures	7-138



Scheme S1 Detailed formation mechanisms of **P_C** from Re-face attack of aldehyde **1** in Path B1.

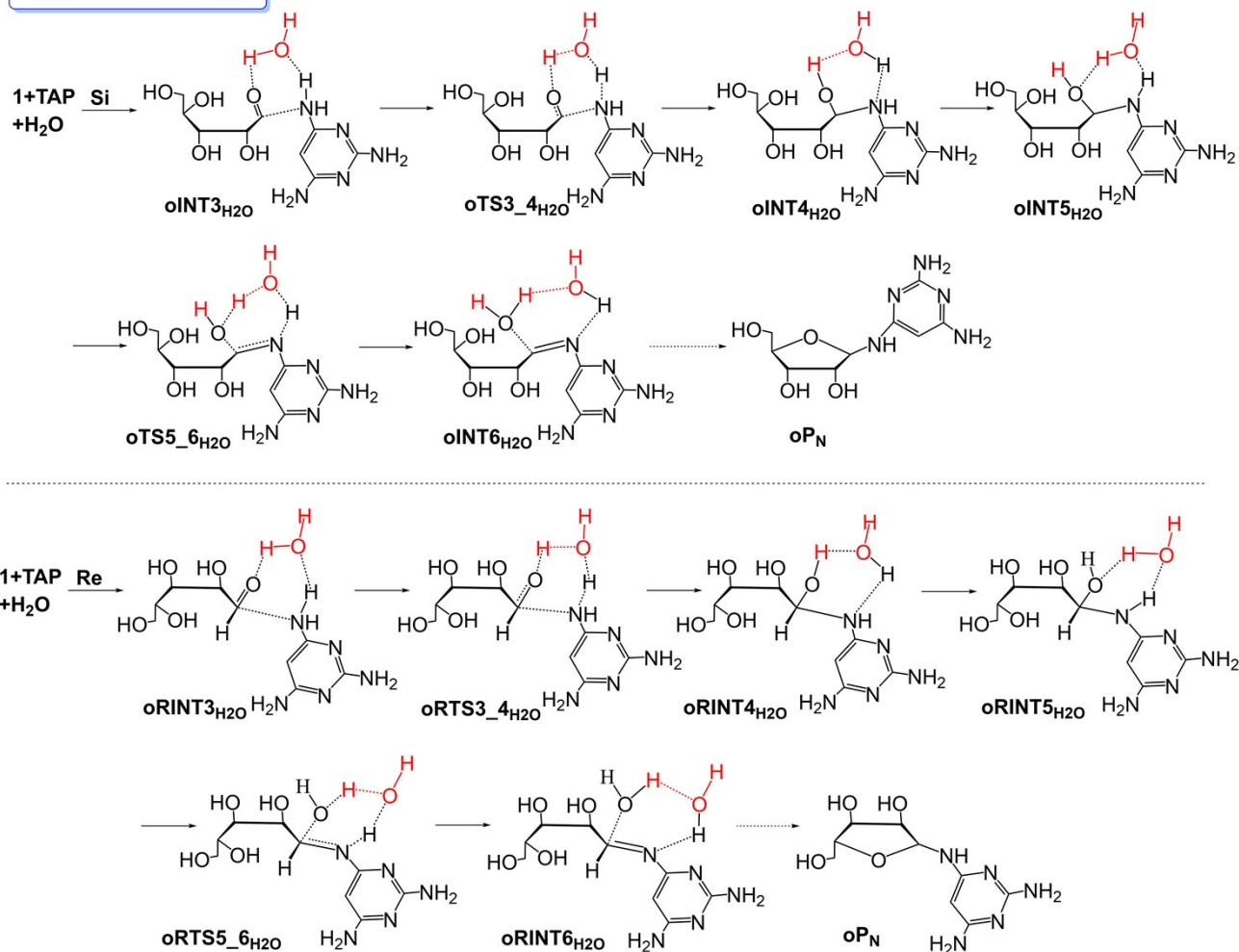


Scheme S2 Detailed formation mechanisms of **P_C** from Si-face attack of aldehyde **1** in Path B1.

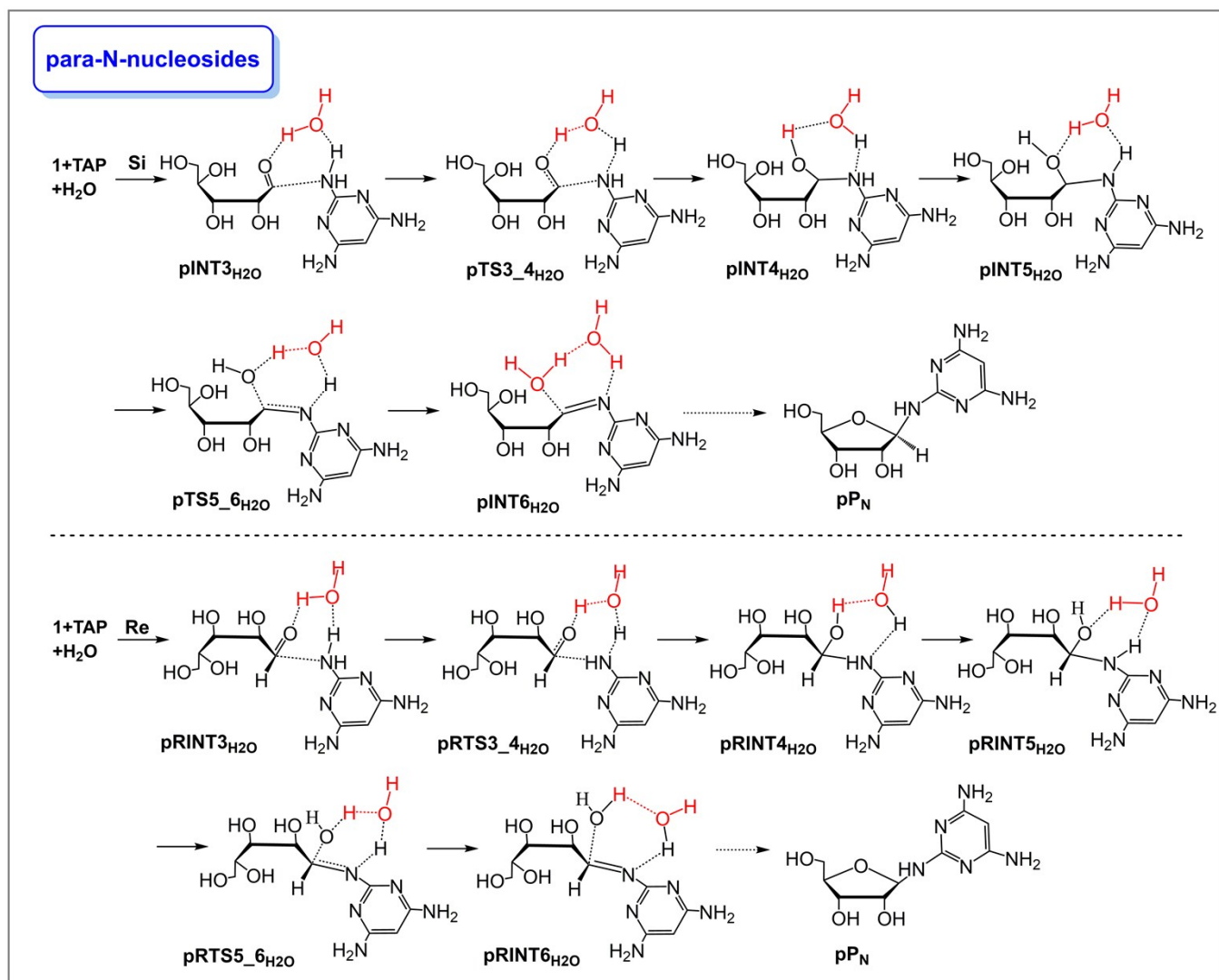


Scheme S3 Detailed formation mechanisms of **P_C** in Path B2, B3 and B4, respectively.

ortho-N-nucleosides



Scheme S4 Formation mechanisms of oP_N from Si- and Re-face of aldehyde **1** with one- H_2O assistance, respectively. Two- H_2O assisted paths are similar to one- H_2O assisted ones.



Scheme S5 Formation mechanisms of **pP_N** from Si- and Re-face of aldehyde **1** with one-H₂O assistance, respectively. Two-H₂O assisted paths are similar to one-H₂O assisted ones.

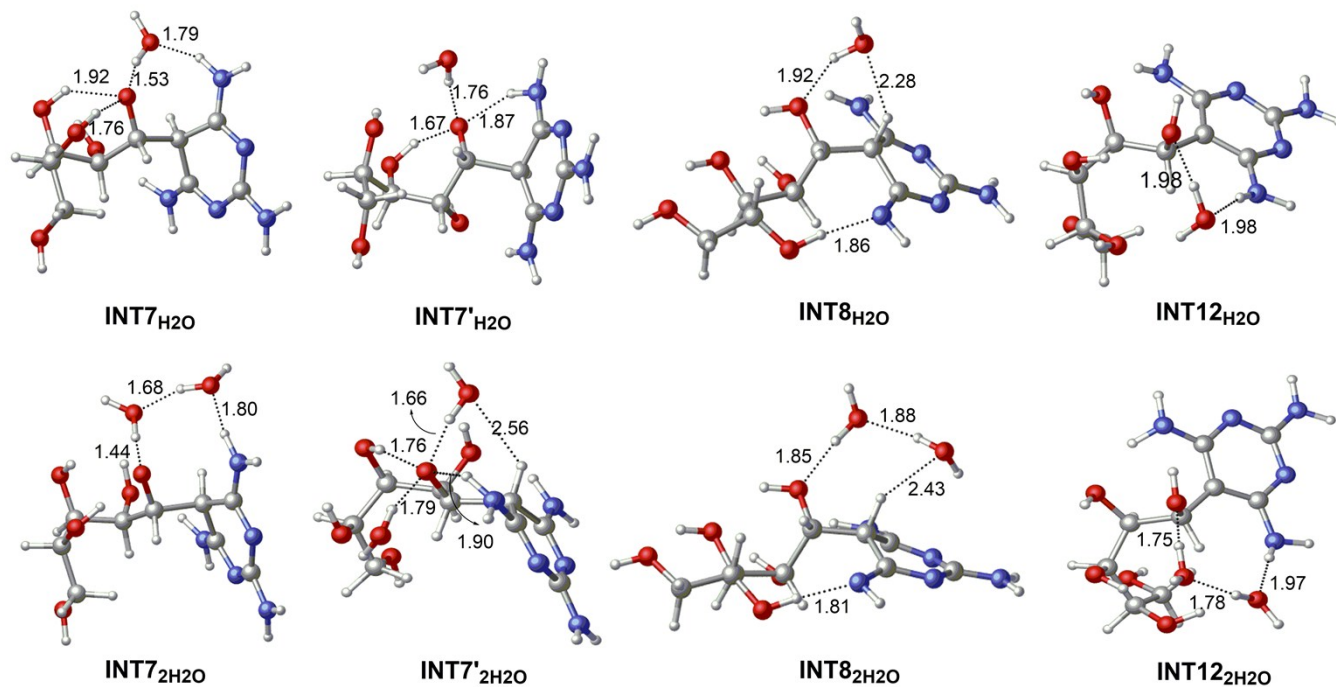


Fig. S1 Optimized structures of key intermediates involved in the reactions.

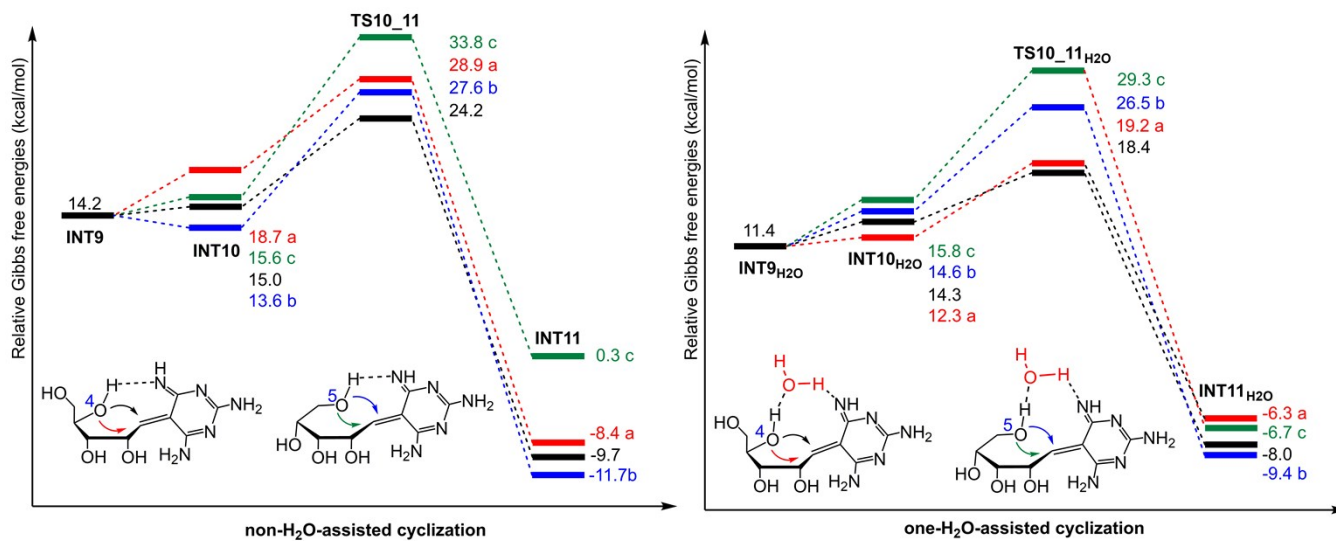


Fig. S2 Free energy profile of cyclization step which controls the formation of other isomers of **P_c**. a, b, c represent the formation of α -ribofuranoside, β -ribofuranoside and α -ribofuranoside, respectively.

1. Cartesian coordinates (Å), Absolute enthalpies and Gibbs free energies of optimized geometries at M06-2X/6-311++G(d,p) level.

1	C	-0.6313140	-0.3318200	0.5650280			
H = -572.451665 a.u.	O	0.4154010	-1.2785590	0.7653750			
G = -572.499927 a.u.	C	1.8166500	-0.6616030	0.0203840			
C	-0.7617480	-0.4467190	0.5380310	C	1.3485290	0.7473820	-0.2910860
O	0.0342320	-1.5700690	0.8605750	C	-0.1527820	0.6121490	-0.5500440
C	2.2497800	-0.4589250	-0.1167980	H	-0.7507330	0.2421150	1.4873340
C	1.3698160	0.7727380	-0.1327020	H	2.5688570	-0.7299370	0.8139010
C	-0.0823850	0.4607440	-0.4992410	H	1.8776950	1.1067030	-1.1805740
H	-0.8726370	0.1198310	1.4651900	H	-0.3097560	0.1477840	-1.5310220
H	2.8308040	-0.6060130	0.8112330	O	-0.7440680	1.8868100	-0.4825360
H	1.7560820	1.4282760	-0.9269020	H	-1.7006020	1.7620840	-0.4880260
H	-0.0868250	-0.0334330	-1.4824500	O	1.5881800	1.5575790	0.8325950
O	-0.7098640	1.7279550	-0.5603190	H	1.0123770	2.3275110	0.7563880
H	-1.6640790	1.5901600	-0.6153390	O	1.7796730	-1.5590170	-0.9269660
O	1.4612630	1.3965020	1.1239060	H	0.7270870	-1.8578300	-0.1997150
H	0.8567140	2.1468820	1.1080150	C	-1.9234290	-1.0412710	0.2103420
O	2.3298730	-1.2064240	-1.0559890	H	-2.2780960	-1.6402190	1.0541450
H	0.2315680	-2.0658580	0.0572730	H	-1.7477540	-1.6991210	-0.6501930
C	-2.1281610	-0.9378910	0.0693710	O	-2.8450870	-0.0092070	-0.1196200
H	-2.5799600	-1.5314600	0.8691360	H	-3.6977900	-0.3889700	-0.3407650
H	-1.9913040	-1.5786120	-0.8127880	2			
O	-2.9351720	0.1883380	-0.2546960	H = -572.461761 a.u.			
H	-3.8068210	-0.0998670	-0.5331390	G = -572.507355 a.u.			
1TS1	C	0.6436860	-0.2807950	-0.5926500			
H = -572.399014 a.u.	O	-0.4534950	-1.1398390	-0.8767240			
G = -572.443837 a.u.	C	-1.6006510	-0.7160220	-0.1635510			

C -1.3205380 0.7101440 0.2897300
C 0.1821900 0.6314100 0.5506120
H 0.8601800 0.3364550 -1.4718500
H -2.4543880 -0.7865920 -0.8408580
H -1.9007090 0.9645650 1.1802530
H 0.3596830 0.1469630 1.5177030
O 0.7499730 1.9190770 0.5114040
H 1.7074960 1.8072310 0.4934820
O -1.5925890 1.5797680 -0.7821800
H -1.0000650 2.3352700 -0.6901250
O -1.7837640 -1.4922310 0.9910150
H -1.8455100 -2.4131710 0.7221490
C 1.8699790 -1.0851400 -0.2180860
H 2.2097450 -1.6933130 -1.0617590
H 1.6247270 -1.7402840 0.6258690
O 2.8452660 -0.1129410 0.1493130
H 3.6677180 -0.5453780 0.3861810

1TS2

H = -572.398479 a.u.

G = -572.443498 a.u.

C -0.9840930 -0.2365710 0.5829910
O -0.0595010 -1.3490850 0.5585790
C 1.1093690 -1.0706650 -0.4762920
C 0.8383210 0.3941070 -0.9044010
C -0.1786180 0.9672610 0.1230960
H -1.3368340 -0.1036970 1.6054770
H 0.4294560 0.4475170 -1.9158250
H -0.8313460 1.7211340 -0.3272810
O 0.4899600 1.4757250 1.2501100
H 1.2811160 1.9250840 0.9279990

O 2.0489180 1.1012520 -0.8622470
H 2.6418960 0.5490450 -0.3209490
C -2.1336130 -0.6035540 -0.3397370
H -2.5773310 -1.5405770 0.0113160
H -1.7537340 -0.7618790 -1.3587200
O -3.0491030 0.4695140 -0.2908640
H -3.8368670 0.2427170 -0.7893640
O 2.0915650 -1.2057990 0.3899630
H 0.9097540 -1.2824690 1.1435070
H 0.9909780 -1.8332040 -1.2544280

2'

H = -572.462880 a.u.

G = -572.508408 a.u.

C 0.9707020 0.3596500 0.4491430
O 0.1168300 1.4826080 0.1767300
C -1.1204440 1.0650350 -0.3309330
C -0.8542240 -0.3378390 -0.9066990
C 0.1653640 -0.8853590 0.1047730
H 1.2392910 0.3523280 1.5081240
H -0.3942160 -0.2487220 -1.8946190
H 0.7998490 -1.6808030 -0.2932150
O -0.5152650 -1.3125900 1.2755780
H -1.1295300 -2.0054260 1.0069650
O -2.0069220 -1.1321610 -1.0080650
H -2.7032110 -0.6856920 -0.5094080
C 2.2246330 0.5131090 -0.3938690
H 2.6584680 1.4971670 -0.1894540
H 1.9600530 0.4677890 -1.4589100
O 3.1008410 -0.5373480 -0.0334210
H 3.9381070 -0.4235520 -0.4870360

O -2.1243860 1.0212460 0.6487120
H -1.7958890 0.4733040 1.3757240
H -1.4578920 1.7919890 -1.0689290

1TS3

H = -572.398206 a.u.

G = -572.442220 a.u.

C 0.7539970 1.1735350 -0.3410820
O 1.3686170 1.2362940 0.9401880
C -1.4466930 -0.7782830 0.2811710
C -0.0176670 -1.2160260 0.0255000
C 0.7647280 -0.2579300 -0.8786070
H 1.3043140 1.8075590 -1.0466300
H -0.1008120 -2.1832840 -0.4803960
H 0.3106640 -0.2652860 -1.8741830
O 2.1062800 -0.6922530 -0.9866150
H 2.2746840 -1.3017440 -0.2579390
O 0.6814360 -1.4615270 1.2297960
H 0.7997050 -0.6121370 1.6773770
C -0.6462500 1.7334540 -0.2342840
H -1.0463060 1.8665170 -1.2440340
H -0.6208850 2.6974330 0.2741540
O -1.5385360 0.8853590 0.5100490
H 2.3012930 1.0285440 0.8167700
O -2.3111780 -0.7614810 -0.6984070
H -2.3396630 0.4688730 -0.2213300
H -1.7846420 -1.0861190 1.2799280

3

H = -572.471266 a.u.

G = -572.514607 a.u.

C 0.7848990 1.0927540 -0.4894400

O 1.5549730 1.2693920 0.6921370
C -1.4883650 -0.4714520 0.3489300
C -0.1435520 -1.1647770 0.1463690
C 0.7126870 -0.3939600 -0.8630560
H 1.2386830 1.6503040 -1.3179380
H -0.3213410 -2.1785710 -0.2182750
H 0.2605880 -0.4867400 -1.8542970
O 2.0190970 -0.9353750 -0.9123220
H 2.1506150 -1.4321510 -0.0954090
O 0.5357690 -1.2955810 1.3797340
H 0.7048250 -0.4028170 1.7144620
C -0.6035780 1.6475270 -0.2270090
H -1.1609060 1.6937470 -1.1680260
H -0.5272370 2.6471710 0.1986660
O -1.3150410 0.8693620 0.7289760
H 2.4373200 0.9321090 0.5025140
O -2.2005520 -0.5935350 -0.8540180
H -3.0924900 -0.2611450 -0.7174100
H -2.0165750 -0.9365660 1.1848960

1TS4

H = -572.400114 a.u.

G = -572.443538 a.u.

C 1.1015060 0.9527030 -0.2615790
O 1.8841710 0.9361310 0.9181270
C -1.5587470 -0.5433370 -0.5078410
C -0.2508260 -1.1482870 -0.0277060
C 0.8981590 -0.4822100 -0.7807290
H 1.6921780 1.5068430 -0.9917210
H -0.2640470 -2.2188330 -0.2657220
H 0.6132340 -0.4440600 -1.8376190

O 2.0955380 -1.2075010 -0.7060780
H 2.5844380 -0.8818500 0.0594680
O -0.1122170 -0.9506460 1.3649760
H -1.0141780 -0.9385140 1.7233500
C -0.2373460 1.6638510 0.0111010
H -0.2059530 2.7099660 -0.2898980
H -0.4488370 1.6053710 1.0814610
O -1.3368910 1.0641120 -0.7067160
H 1.3818830 0.4338840 1.5762120
O -2.5308270 -0.3976630 0.3665680
H -2.2366550 0.8544620 -0.0181060
H -1.8167310 -0.8390610 -1.5319070

3'

H = -572.463854 a.u.

G = -572.507255 a.u.

C 1.1117790 0.9839480 -0.1586790
O 1.8521570 0.8596680 1.0423930
C -1.5314940 -0.2638090 -0.5590580
C -0.2797580 -1.0810180 -0.1882610
C 0.9243850 -0.3957820 -0.8246160
H 1.7228270 1.6099030 -0.8103460
H -0.3824690 -2.1012160 -0.5705980
H 0.7042430 -0.2531740 -1.8864790
O 2.0925380 -1.1657140 -0.7397710
H 2.5350270 -0.9225840 0.0825310
O -0.0728840 -1.1103300 1.2165550
H -0.9291930 -1.2552520 1.6360310
C -0.2653650 1.6287140 0.1001780
H -0.2480350 2.7008250 -0.0862190
H -0.5498280 1.4594050 1.1438920

O -1.2579800 1.0942710 -0.7704330
H 1.3228390 0.3087520 1.6359610
O -2.4559910 -0.4535690 0.4837570
H -3.2532940 0.0462020 0.2861150
H -1.9421230 -0.6197880 -1.5082840

1INT1_{H2O}

H = -648.866680 a.u.

G = -648.920281 a.u.

C 0.8212730 0.0073340 0.7291150
O -0.0968670 0.8295050 1.4156070
C -2.1908520 -0.2053210 0.2140720
C -1.1696340 -1.1971710 -0.2914470
C 0.2017270 -0.5675780 -0.5541790
H 1.0570000 -0.8271110 1.3946880
H -2.6217980 -0.4331380 1.2027540
H -1.5371550 -1.5623230 -1.2612310
H 0.0807050 0.2346250 -1.2958660
O 0.9776010 -1.6324180 -1.0746090
H 1.9035650 -1.3564000 -1.0643130
O -1.0817160 -2.2454610 0.6412890
H -0.3572060 -2.8118000 0.3512640
O -2.5519770 0.7449470 -0.4383030
H -1.4157560 2.2271350 -0.8770840
C 2.0872980 0.8089790 0.4432160
H 2.4993300 1.1615650 1.3933240
H 1.8208430 1.6729600 -0.1781170
O 3.0175610 -0.0328290 -0.2349370
H 3.8047210 0.4664930 -0.4615200
O -0.6010730 2.6964880 -0.6409190
H -0.8048400 3.6331910 -0.6853570

H -0.2365090 1.6354860 0.8917670

1TS1_{H2O}

H = -648.839239 a.u.

G = -648.888168 a.u.

C -0.6082300 -0.4091190 0.6133660

O 0.7781880 -0.3750470 0.9497650

C 1.5153350 0.8612810 0.0464870

C 0.2597430 1.6465340 -0.2857270

C -0.7911500 0.5738310 -0.5520580

H -1.1775150 -0.0445930 1.4725590

H 2.1104370 1.2916840 0.8606700

H 0.4492860 2.2547400 -1.1756730

H -0.5664230 0.0780890 -1.5038190

O -2.0673430 1.1683280 -0.5676470

H -2.7156470 0.4546570 -0.5913280

O -0.1030200 2.4305630 0.8245400

H -1.0362730 2.6505080 0.7233890

O 2.1237670 0.3124420 -0.9569610

H 2.3851560 -0.9007310 -0.6600520

C -1.0545380 -1.8126020 0.2452330

H -0.9789800 -2.4836320 1.1071370

H -0.4232480 -2.1953480 -0.5651570

O -2.4060230 -1.6662280 -0.1776290

H -2.7549770 -2.5165190 -0.4522940

O 2.2192110 -1.9022360 -0.1346060

H 3.0153760 -2.2265510 0.2928660

H 1.4076090 -1.2644270 0.5882020

2_{H2O}

H = -648.874993 a.u.

G = -648.927363 a.u.

C -0.4938650 0.5807460 -0.5649930

O 0.8407610 0.1218120 -0.7646860

C 1.0772130 -1.0482310 0.0279790

C -0.3024010 -1.6324030 0.2881100

C -1.1146610 -0.3537330 0.4837720

H -1.0482840 0.4812910 -1.5039940

H 1.7195250 -1.7005850 -0.5675490

H -0.2972620 -2.2756980 1.1714770

H -0.9404290 0.0379650 1.4915680

O -2.4822180 -0.6099510 0.2658600

H -2.9344550 0.2409870 0.2600140

O -0.7258860 -2.3188850 -0.8641730

H -1.6885010 -2.2653600 -0.8889720

O 1.6375190 -0.7162650 1.2569640

H 2.4706280 -0.2517730 1.0861920

C -0.5049990 2.0239620 -0.1063390

H -0.0992260 2.6851450 -0.8789800

H 0.1018050 2.1142520 0.8024580

O -1.8759140 2.3113010 0.1524100

H -1.9661910 3.2097510 0.4757070

O 3.3599700 0.9938460 -0.1450320

H 4.1151270 1.0717580 -0.7304210

H 2.5657010 0.9753400 -0.6994230

1INT2_{H2O}

H = -648.865852 a.u.

G = -648.919765 a.u.

C 1.1554420 0.8771310 0.1901780

O 0.3608560 1.6249130 -0.6998180

C -1.0689990 -0.6503770 -1.2368230

C -0.1772390 -1.3243050 -0.2083610

C	0.4281670	-0.3177450	0.7975690	O	0.4028830	0.4338060	1.7843150
H	1.4905880	1.4935470	1.0337170	H	1.0094160	1.1866420	1.8168530
H	0.6411100	-1.8364060	-0.7284970	O	1.3371510	2.0844010	-0.0463150
H	1.1457520	-0.8760270	1.4065650	H	2.1429510	1.5933790	-0.2934060
O	-0.6129390	0.1791790	1.6272690	C	-2.2979560	-0.4722500	-0.6280070
H	-1.0244220	-0.5915480	2.0361410	H	-2.5813520	-1.4713870	-0.9738980
O	-0.9260160	-2.2532730	0.5417260	H	-2.0694620	0.1429380	-1.5081470
H	-1.8405150	-2.1940790	0.2316930	O	-3.3039900	0.1182880	0.1695930
C	2.3672280	0.4455820	-0.6252700	H	-4.1306140	0.1357850	-0.3168600
H	2.9367050	1.3411340	-0.8902780	O	2.1338350	-0.1765880	-0.9971780
H	2.0199430	-0.0211790	-1.5565350	H	2.2766560	-1.1672850	0.0639030
O	3.1317680	-0.4588200	0.1506280	H	0.5364790	-0.0870030	-2.2561350
H	3.9670160	-0.6284020	-0.2891230	O	1.8718840	-1.8802480	0.7250590
O	-2.2703850	-0.7252740	-1.1458680	H	1.7679820	-1.4147080	1.5664780
H	-2.7756970	1.7371260	-0.2467110	H	0.8122660	-1.6872060	0.1565730
H	-0.5826510	-0.1091400	-2.0583330				
O	-2.1670980	2.1407990	0.3789210	2' _{H2O}			
H	-1.9240680	1.4279720	0.9879710	H =	-648.876998	a.u.	
H	-0.4108440	2.0151090	-0.2532400	G =	-648.928846	a.u.	
				C	1.0401890	0.4982810	-0.2084480
				O	0.1573840	0.4248690	-1.3302980
				C	-0.7893500	-0.6084380	-1.1969220
				C	-0.3701980	-1.4059670	0.0661360
				C	0.4513100	-0.3877810	0.8788250
				H	1.0993510	1.5356930	0.1322600
				H	0.2650560	-2.2483410	-0.2204940
				H	1.2371690	-0.8519410	1.4795560
				O	-0.4050610	0.3795680	1.7089430
				H	-1.0409690	-0.2400950	2.0927620
				O	-1.4750870	-1.8845750	0.7861040
				H	-2.2560130	-1.4806670	0.3770690

1TS₂H_{2O}

H = -648.840798 a.u.

G = -648.889263 a.u.

C	-1.0616710	-0.6021500	0.2462390
O	-0.0116850	-1.1797690	-0.5377300
C	0.8708940	0.0198480	-1.2175590
C	0.2827220	1.2647640	-0.4770000
C	-0.5036640	0.7227620	0.7325960
H	-1.2747030	-1.2598330	1.0927430
H	-0.3790220	1.8327710	-1.1364610
H	-1.2931740	1.3989290	1.0687940

C 2.4224250 0.0429890 -0.6509260
H 2.7106730 0.6264790 -1.5309010
H 2.3878170 -1.0174610 -0.9365650
O 3.2996330 0.2570350 0.4374620
H 4.1944570 0.0326790 0.1749880
O -2.0901640 -0.1207180 -1.0786380
H -2.0754530 0.7638280 -0.6583940
H -0.7689980 -1.2243250 -2.0980220
O -1.9217590 2.2426470 0.3405000
H -1.2955710 1.8573560 0.9746050
H -1.5033390 3.0216740 -0.0314230

1INT3_{H2O}

H = -648.8640734 a.u.

G = -648.9181304 a.u.

C 0.9026410 1.2587810 -0.0968920
O 1.7404940 1.3183800 1.0592500
C -0.7530110 -1.4663770 0.2839750
C 0.7287660 -1.3292020 -0.0085210
C 1.0843370 -0.0774420 -0.8288730
H 1.1924680 2.0409040 -0.8070030
H 0.9819730 -2.1902030 -0.6378440
H 0.4600000 -0.0667950 -1.7241750
O 2.4417360 -0.1791150 -1.2342000
H 2.9164510 -0.6787070 -0.5607790
O 1.5024970 -1.4424610 1.1654860
H 1.5796240 -0.5637760 1.5654990
C -0.5126020 1.5433140 0.3730570
H -0.5197380 2.5242160 0.8622800
H -0.8127320 0.8101700 1.1363280
O -1.3553960 1.5090840 -0.7495330

H 2.6402790 1.4925100 0.7686210
O -1.5797760 -1.5967220 -0.5816150
H -3.2376640 -0.7121220 -0.0684580
H -1.0286680 -1.4744510 1.3564720
O -3.5188640 0.1234490 0.3311840
H -2.2408820 1.2410690 -0.4646090
H -4.4774280 0.1418190 0.3126240

1TS3_{H2O}

H = -648.836257 a.u.

G = -648.884539 a.u.

C 1.1123020 1.3182420 -0.0031740
O 1.4819760 1.0391140 1.3471640
C -0.8691240 -0.7375800 0.2612250
C 0.4958880 -1.1323090 -0.3045690
C 1.3009270 0.0665350 -0.8599200
H 1.7584950 2.1098670 -0.3948030
H 0.3294730 -1.8658170 -1.0941670
H 0.9573560 0.2807140 -1.8758060
O 2.6773770 -0.2469380 -0.9005880
H 2.7972140 -1.0668870 -0.4048630
O 1.2406710 -1.8024440 0.7008100
H 1.2681610 -1.2225860 1.4723760
C -0.3446700 1.7840910 -0.0298430
H -0.4689030 2.6227400 -0.7160090
H -0.6459160 2.0889120 0.9771950
O -1.1717890 0.7260220 -0.5083420
H 2.4397020 0.9355790 1.3588550
O -1.8711180 -1.4957080 0.0111680
H -2.9170630 -0.6829710 0.1189790
H -0.7718560 -0.3403420 1.2901940

O -3.4193310 0.3128970 0.0721430
H -2.3003010 0.7729560 -0.3096180
H -4.1205960 0.3104260 -0.5834850

3_{H2O}

H = -648.874886 a.u.

G = -648.925915 a.u.

C -1.1283870 -1.3374820 -0.0573200
O -1.4019300 -1.1458060 1.3309940
C 0.8318520 0.6019800 0.0908090
C -0.5723940 1.1036680 -0.2665750
C -1.4410080 -0.0511990 -0.8147090
H -1.7521100 -2.1515180 -0.4396150
H -0.4688770 1.8823800 -1.0236140
H -1.2095760 -0.1985470 -1.8736560
O -2.8140430 0.2464580 -0.6791560
H -2.8807880 1.0533940 -0.1529010
O -1.1982410 1.7213300 0.8436070
H -1.1759460 1.0877880 1.5717280
C 0.3529440 -1.6888190 -0.2194370
H 0.4844640 -2.4573550 -0.9804880
H 0.7326340 -2.0605470 0.7399440
O 1.1261320 -0.5781290 -0.6613520
H -2.3572470 -1.0500830 1.4144770
O 1.7479710 1.5767580 -0.2238510
H 2.6184250 1.2821710 0.0840050
H 0.8691680 0.3296310 1.1591550
O 3.6966000 -0.3391120 0.3124480
H 3.0579300 -0.7503890 -0.2876320
H 4.5719780 -0.5877960 0.0104740

1INT4_{H2O}

H = -648.868434 a.u.

G = -648.921319 a.u.

C -1.1187500 -1.2127290 -0.0038740
O -1.8840530 -1.1914650 1.1879320
C 0.8575580 1.3572050 -0.5737260
C -0.6064020 1.3014130 -0.2122430
C -1.3360750 0.0825810 -0.8038230
H -1.5312330 -2.0272930 -0.6043990
H -1.0597360 2.1802920 -0.6994150
H -0.9608540 -0.0634180 -1.8198720
O -2.7155140 0.3479020 -0.9015890
H -3.1212930 0.0465770 -0.0790410
O -0.7787930 1.3764540 1.1853470
H 0.0501030 1.7046330 1.5608600
C 0.3490050 -1.4918290 0.2915900
H 0.4527800 -2.5148470 0.6663740
H 0.7015890 -0.8094130 1.0765270
O 1.0730190 -1.2953390 -0.9086950
H -1.5673350 -0.4438990 1.7117810
O 1.7013740 1.5706230 0.2667900
H 3.2759310 0.3699020 0.2818430
H 1.1103570 1.2546690 -1.6394130
O 3.5149910 -0.5576060 0.1527570
H 2.0187200 -1.3035550 -0.6969650
H 4.4707590 -0.6180380 0.1938420

1TS4_{H2O}

H = -648.843082 a.u.

G = -648.889682 a.u.

C 1.2270290 1.1639290 -0.1436210
O 1.9884830 1.2187990 1.0462310

C	-1.0195360	-0.8987340	-0.4917770	H	0.5063290	-2.1142650	-0.7927140
C	0.4448770	-1.2176680	-0.1656330	H	0.9675990	0.0826650	-1.9228950
C	1.3775330	-0.2094900	-0.8267140	O	2.6631770	-0.5945120	-1.0637150
H	1.6519160	1.9272430	-0.7972280	H	3.1383320	-0.3647750	-0.2558660
H	0.6608540	-2.2191690	-0.5559860	O	0.8081430	-1.3022720	1.0825440
H	1.0783160	-0.1208200	-1.8754450	H	0.0519300	-1.6715140	1.5552990
O	2.7181400	-0.6237920	-0.8178400	C	-0.1340090	1.4296200	0.3981210
H	3.1117100	-0.3165000	0.0077310	H	-0.3788880	2.4904030	0.3799480
O	0.6298870	-1.1927000	1.2374580	H	-0.2468470	1.0622010	1.4229550
H	-0.2336720	-1.4316600	1.6130240	O	-1.0781210	0.7837290	-0.4530410
C	-0.2520010	1.4547630	0.1510140	H	1.8924780	0.3629610	1.5656530
H	-0.4965240	2.5082280	0.0179930	O	-1.7304680	-1.1379060	0.6943630
H	-0.4919600	1.1583100	1.1760820	H	-2.6620850	-0.8911460	0.5873510
O	-1.0811610	0.7067210	-0.7562850	H	-1.4658340	-0.9591190	-1.3402950
H	1.6428510	0.5231880	1.6239010	O	-3.7895870	0.4299770	-0.2294460
O	-1.8496360	-1.1986680	0.4707640	H	-3.0484370	1.0021160	-0.4736240
H	-2.8640440	-0.3452280	0.3426450	H	-4.5697360	0.7373000	-0.6930000
H	-1.2923150	-1.2046890	-1.5111310				
O	-3.3007070	0.6328750	0.0481690	1INT1₂H₂O			
H	-2.1924150	0.8740930	-0.5068400	H =	-725.280300	a.u.	
H	-4.0821790	0.5443240	-0.5023330	G =	-725.341643	a.u.	
				C	1.0906390	0.4677340	0.6534230
3'_{H2O}				O	-0.0886030	0.4667560	1.4237100
H =	-648.876797	a.u.		C	-0.9990840	-1.7262180	0.4060330
G =	-648.926860	a.u.		C	0.3759450	-1.8054820	-0.2113750
C	1.3063630	1.1702160	-0.0838220	C	0.9255330	-0.4237850	-0.5856590
O	2.2027960	1.0905720	1.0092470	H	1.8815210	0.0386060	1.2748800
C	-1.0222230	-0.6350060	-0.3944620	H	-1.0681420	-2.0104640	1.4671470
C	0.4233450	-1.1528940	-0.2763540	H	0.2759290	-2.3690920	-1.1492140
C	1.3493920	-0.1269350	-0.9195150	H	0.2216090	0.0483160	-1.2872100
H	1.6704320	1.9964750	-0.6962300	O	2.1677350	-0.7001950	-1.2063350

H	2.6660180	0.1263130	-1.2539920	O	1.3134610	-2.2014170	1.0003670
O	1.2281250	-2.4663730	0.6906600	H	2.2684100	-2.0771430	0.9560960
H	2.1191290	-2.3952570	0.3286630	O	-1.3371120	-1.0425370	-1.0594680
O	-1.9669690	-1.4127490	-0.2463490	H	-2.5481150	-0.6984690	-0.8881960
H	-3.4725350	-0.3548850	-0.4458140	C	0.6451820	2.0231710	-0.0101150
C	1.4572550	1.9024780	0.2872140	H	0.2724530	2.7084200	0.7580350
H	1.5921510	2.4742730	1.2105520	H	-0.0637340	2.0039740	-0.8462580
H	0.6367480	2.3433480	-0.2912750	O	1.9504950	2.3905200	-0.4437190
O	2.6624240	1.8812050	-0.4766290	H	1.9309440	3.2695180	-0.8270400
H	2.8733620	2.7678240	-0.7755350	O	-3.5443080	-0.2247050	-0.6077760
O	-3.9477740	0.4729490	-0.6203810	H	-4.0202440	0.0445550	-1.3956130
H	-4.3037950	0.3902030	-1.5073570	H	-3.0710470	0.7191470	0.1398950
H	-2.6711810	1.6250240	-0.2041200	O	-2.4368380	1.3675200	0.8003920
O	-1.9068650	2.1274430	0.1431770	H	-2.8693100	1.4945900	1.6486670
H	-2.2827830	2.8338660	0.6732510	H	-1.3709640	0.7227700	0.8948040
H	-0.7543430	1.0412780	0.9993830				

1TS1_{2H2O}

H = -725.263167 a.u.

G = -725.317619 a.u.

C	0.8091780	0.6173510	0.5368350
O	-0.4388450	0.0445280	0.9179110
C	-0.6931240	-1.3304510	0.0234130
C	0.7721380	-1.6772450	-0.1878380
C	1.4016700	-0.3301570	-0.5203360
H	1.4684330	0.6258690	1.4094000
H	-1.1963340	-1.9216450	0.7982240
H	0.8546250	-2.3814600	-1.0209580
H	1.0837890	-0.0247070	-1.5225400
O	2.8043890	-0.4290070	-0.4338120
H	3.1608920	0.4593580	-0.5474150

2_{2H2O}

H = -725.291817 a.u.

G = -725.351454 a.u.

C	0.8509850	0.6403370	0.4201190
O	-0.5101920	0.2325120	0.5223330
C	-0.6999210	-1.0232790	-0.1556890
C	0.6787270	-1.6673360	-0.1382700
C	1.5601860	-0.4488510	-0.3993430
H	1.2904190	0.6737750	1.4226810
H	-1.4452660	-1.5741590	0.4233950
H	0.7656030	-2.4335600	-0.9122240
H	1.5304110	-0.2003740	-1.4655060
O	2.8785360	-0.7000260	0.0286160
H	3.3603000	0.1326420	-0.0297160
O	0.9187750	-2.1860660	1.1481180

H	1.8716620	-2.1572520	1.2932570	O	0.5414200	-0.4492240	-1.3209730
O	-1.0784780	-0.8300610	-1.4697920	H	-0.3750960	-0.5245950	-1.0203840
H	-2.0108540	-0.5474240	-1.4686340	C	1.7917490	1.8639790	0.9810900
C	0.9625680	1.9985560	-0.2402480	H	2.5805630	2.6171590	1.0616400
H	0.4870810	2.7731350	0.3700190	H	1.2202490	1.8692350	1.9174080
H	0.4733940	1.9583380	-1.2201410	O	0.9640980	2.2251960	-0.1091460
O	2.3641380	2.2234080	-0.3651630	H	0.6233610	1.4189530	-0.5259490
H	2.5227090	3.0552860	-0.8153290	C	-3.8057320	-0.4968750	-0.3719170
O	-3.6618380	-0.0802740	-0.8764650	N	-3.0905800	-1.3630150	0.3534430
H	-4.3632320	0.3157350	-1.3959400	C	-1.9996290	-0.8581160	0.9436150
H	-3.5947310	0.4308580	-0.0483830	C	-1.6230440	0.4798730	0.8044000
O	-2.9021020	1.1830070	1.4300150	C	-2.4402300	1.2732110	-0.0079460
H	-3.1037330	0.8857850	2.3193160	N	-3.5399680	0.7920330	-0.6008450
H	-1.9697350	0.9506650	1.2664910	H	-0.7661690	0.8820690	1.3223910
INT1				N	-4.9152100	-1.0026310	-0.9899880
H = -1002.756116 a.u.				H	-5.2620550	-1.8802420	-0.6398500
G = -1002.824138 a.u.				H	-5.5824520	-0.3304670	-1.3307280
C	2.4315340	0.4955020	0.8143180	N	-1.2568020	-1.7157730	1.7025650
O	1.4187380	-0.5206580	0.8284160	H	-1.4927890	-2.6927560	1.6383570
C	1.3636090	-1.1605850	-0.4301890	H	-0.3042260	-1.4620510	1.9213250
C	2.7843300	-1.0905770	-0.9667770	N	-2.1511170	2.5901280	-0.2137340
C	3.1910780	0.3223550	-0.5132810	H	-2.6680010	3.0391920	-0.9532400
H	3.1165570	0.3062720	1.6454370	H	-1.1983220	2.8936330	-0.0617940
H	1.0035990	-2.1772670	-0.2667140	TS1_2			
H	2.8062830	-1.2188250	-2.0526880	H = -1002.664186 a.u.			
H	2.8567520	1.0634080	-1.2434200	G = -1002.732694 a.u.			
O	4.5839400	0.4310300	-0.2754950	C	2.3490890	-0.4352160	-1.0112990
H	5.0142680	0.7999090	-1.0502060	O	0.8584960	-0.3363670	-1.1137520
O	3.5566650	-2.0622220	-0.3111120	C	0.4067270	0.6788540	-0.5393250
H	4.4223320	-1.6743960	-0.1350670	C	1.4332150	1.5279980	0.1566440

C	2.7542630	0.7411810	-0.1176370	H	-3.3617350	2.7256950	1.2867510
H	2.6508280	-0.2330060	-2.0406440	H	-2.2124230	2.2003800	2.4398090
H	-0.6164640	0.9687380	-0.7521710	INT2			
H	1.2082760	1.5822030	1.2200470	H =	-1002.741050	a.u.	
H	3.1751380	0.3703110	0.8120810	G =	-1002.807324	a.u.	
O	3.6635810	1.5651430	-0.8316000	C	2.1702950	-0.1275040	-1.2926390
H	4.4444140	1.7198690	-0.2958290	O	0.8929870	-0.6160830	-0.8585030
O	1.4001080	2.7928480	-0.4524430	C	0.2051660	0.4292920	-0.2112170
H	2.2326730	2.8918920	-0.9365530	C	1.3363890	1.1294230	0.5618270
O	1.2870140	-0.8017490	1.7849980	C	2.4328020	1.1677330	-0.5025270
H	1.3820300	-0.7128870	2.7363190	H	2.1170200	0.1004110	-2.3648790
C	2.7892680	-1.8509320	-0.5887170	H	-0.2233850	1.1204990	-0.9541040
H	3.6380580	-2.1124840	-1.2294480	H	1.6444920	0.4707350	1.3778880
H	1.9593360	-2.5216610	-0.8662430	H	3.4324500	1.1881230	-0.0649890
O	3.1756990	-1.9661940	0.7280910	O	2.1813920	2.3465230	-1.2657780
H	2.3947490	-1.5557910	1.2984020	H	2.9403410	2.5441420	-1.8182550
C	-3.2857480	-0.3839540	-0.8119330	O	1.0210950	2.3918970	1.0968410
N	-2.4852510	-1.4126350	-0.5382350	H	1.1573310	3.0359850	0.3889260
C	-1.6456090	-1.2476480	0.4999670	O	1.3570230	-2.1107250	1.8107470
C	-1.6259160	-0.0534770	1.2529350	H	1.4548360	-2.7249980	2.5410470
C	-2.5303620	0.9351470	0.8659250	C	3.2064380	-1.2066340	-1.0233450
N	-3.3503300	0.7990570	-0.1811020	H	4.1298100	-0.9516810	-1.5528930
H	-0.9504690	0.0563780	2.0881270	H	2.8310980	-2.1538870	-1.4293810
N	-4.1156260	-0.5294080	-1.8869110	O	3.5206490	-1.3050850	0.3402950
H	-4.2567180	-1.4683900	-2.2207740	H	2.7540080	-1.6683010	0.8246580
H	-4.8780150	0.1233720	-1.9598280	C	-3.2834420	-0.2378090	-0.6852500
N	-0.7877630	-2.2387980	0.7974600	N	-2.5907670	-1.3436100	-0.7150450
H	-0.7555880	-3.0070560	0.1458190	C	-1.5141100	-1.4198850	0.1313560
H	0.0643660	-1.9417360	1.3126160	C	-0.9249500	-0.1329750	0.6880420
N	-2.5563430	2.1550740	1.4944760	C	-2.0131470	0.9086790	0.8160060

N	-3.1170480	0.8643350	0.1387420	O	-1.9056050	-1.8271760	-1.3619330
H	-0.5015840	-0.3548750	1.6702600	H	-0.9556080	-2.0835320	-1.2671060
N	-4.3277490	-0.1070840	-1.5287820	C	3.2425390	-0.2005600	0.4359520
H	-4.5894210	-0.8936060	-2.0985250	N	2.5743580	-1.3154320	0.3132000
H	-4.9392630	0.6836290	-1.4246900	C	1.3734910	-1.2622470	-0.3457880
N	-0.9549880	-2.5203640	0.4640100	C	0.7323760	0.0860690	-0.6248160
H	-1.4173020	-3.2961020	-0.0084660	C	1.7424540	1.2014410	-0.5425030
H	0.5380360	-2.3858460	1.3129850	N	2.9237180	1.0662860	-0.0308000
N	-1.7946810	1.9268710	1.6627000	H	0.3547560	0.0404750	-1.6490050
H	-2.4685350	2.6783500	1.6434110	N	4.4219750	-0.2296450	1.0876490
H	-0.8411150	2.1522420	1.9232940	H	4.7728900	-1.1111650	1.4208610

INT3

H = -926.324434 a.u.

G = -926.385080 a.u.

C	-2.3272410	-0.8845080	0.8368860
O	-0.9319590	-0.6717630	1.0527160
C	-0.4686310	0.4373820	0.3192360
C	-1.6754650	0.9888310	-0.4771980
C	-2.8611620	0.4520350	0.3201170
H	-2.7786700	-1.1271090	1.8059680
H	-0.1400050	1.2001970	1.0363920
H	-1.6979440	0.5572290	-1.4758880
H	-3.7631910	0.3426140	-0.2887930
O	-3.0597940	1.3964280	1.3657670
H	-3.7702010	1.1071450	1.9423660
O	-1.6533710	2.3917090	-0.6190140
H	-2.0052260	2.7652160	0.1998020
C	-2.5210020	-2.0564630	-0.1212840
H	-3.5919700	-2.2191690	-0.2859570
H	-2.1113800	-2.9511670	0.3621990

H	4.9786180	0.6057970	1.1309800
N	0.7456660	-2.2988790	-0.7560060
H	1.2681270	-3.1355700	-0.4993740
N	1.3473960	2.3998020	-1.0032020
H	1.9652820	3.1811410	-0.8429460
H	0.3644190	2.5874990	-1.1692740

TS3_Pc

H = -926.240535 a.u.

G = -926.301920 a.u.

C	-2.3857080	-0.7446240	0.9390790
O	-0.9572850	-0.7079660	0.9401220
C	-0.4744990	0.4542390	0.2908200
C	-1.6390010	0.9382470	-0.5908900
C	-2.8595110	0.5351140	0.2360650
H	-2.7417920	-0.7489350	1.9764910
H	-0.2824430	1.2337890	1.0438790
H	-1.6419530	0.3897510	-1.5329880
H	-3.7459410	0.3659940	-0.3816310
O	-3.0730070	1.6072620	1.1489920

H	-3.8876560	1.4682050	1.6363220	C	2.8651210	0.4182780	0.3075310
O	-1.5699710	2.3153270	-0.8844710	H	3.3593190	-0.9534450	-1.2936390
H	-1.9927790	2.7758730	-0.1475230	H	0.6983220	1.3228870	-1.3573860
C	-2.8030040	-2.0320510	0.2428620	H	1.0738560	0.4551040	1.5137170
H	-3.8934590	-2.0971960	0.1925850	H	3.4364490	0.2079920	1.2158630
H	-2.4363360	-2.8794630	0.8341190	O	3.4887450	1.4379810	-0.4654350
O	-2.3142960	-2.0805120	-1.0767610	H	4.4152680	1.2295300	-0.6016940
H	-1.3463040	-2.1238380	-1.0285990	O	1.4393240	2.3369240	0.8329470
C	3.3574460	-0.2890260	0.4014300	H	2.1663430	2.7085480	0.3157060
N	2.6330410	-1.4035140	0.2430210	C	2.5347570	-2.1083260	0.3226870
C	1.4626560	-1.1829360	-0.3386340	H	3.5224970	-2.2981550	0.7539740
C	0.8198120	0.1494830	-0.4786340	H	2.2916110	-2.9537270	-0.3331580
C	1.8162510	1.1942460	-0.3920880	O	1.6177290	-2.0012160	1.3844350
N	3.0689830	0.9686070	-0.0094010	H	0.7304440	-2.1710210	1.0253640
H	0.4030010	-0.7800150	-1.5287530	C	-3.4443620	-0.1696110	0.1002130
N	4.5560340	-0.4331030	0.9999770	N	-2.6994770	-1.2641420	-0.0454720
H	4.8781270	-1.3585570	1.2247940	C	-1.3991790	-1.0712780	-0.2826140
H	5.1792070	0.3549580	1.0319500	C	-0.8119360	0.1968660	-0.3537690
N	0.7651350	-1.9874620	-1.1202110	C	-1.7127470	1.2662210	-0.1489760
H	1.0733600	-2.9464510	-1.2599400	N	-3.0197520	1.0910910	0.0630010
N	1.4542290	2.4640540	-0.6213600	H	0.0717130	-2.1809670	-1.1061310
H	2.1288070	3.1942150	-0.4586800	N	-4.7868370	-0.3610810	0.2789070
H	0.5140240	2.6825630	-0.9293080	H	-5.0750880	-1.2839920	0.5580830
Pc				H	-5.3076900	0.4240830	0.6322630
H =	-926.343990	a.u.		N	-0.6661720	-2.2529450	-0.4166210
G =	-926.406101	a.u.		H	-1.2908130	-3.0361990	-0.5594760
C	2.5950510	-0.8373010	-0.5167290	N	-1.2880590	2.5656530	-0.1923210
O	1.3403230	-0.6202530	-1.1668240	H	-1.9984890	3.2261560	0.0852030
C	0.6442200	0.5048740	-0.6256780	H	-0.3483970	2.7725570	0.1245180
C	1.4603690	0.9424680	0.6195620				

INT1_{H2O}

H = -1079.168142 a.u.	H 1.7194880 -2.5005040 0.9184180
G = -1079.245719 a.u.	H 3.3961000 -2.9005670 1.0923270
C -2.6712930 0.7796300 -0.5712870	N 1.3615400 1.8288480 -0.7525270
O -1.3085660 0.4603250 -0.8491110	H 0.4154180 1.4597020 -0.7784780
C -1.0695870 -0.9339000 -0.6411170	H -1.1104520 -0.3857170 2.1352570
C -2.4450410 -1.5865460 -0.6115700	N 6.0076040 0.6656540 -0.3007180
C -3.2845940 -0.4877060 0.0369070	H 6.6182850 -0.1264360 -0.1806040
H -3.1853820 1.0043630 -1.5127590	H 6.3248040 1.4073140 -0.9010570
H -0.4583510 -1.2798740 -1.4785850	O -1.5737000 0.1019100 2.8371150
H -2.4276530 -2.5129800 -0.0314170	H -1.1333380 -0.1355670 3.6549080
H -3.1423880 -0.4938910 1.1227130	H 1.5620750 2.6424130 -1.3079110
O -4.6435910 -0.6612170 -0.2980130	TS1_2_{H2O}
H -5.1037720 0.1358380 -0.0100820	H = -1079.069624 a.u.
O -2.8606210 -1.8090160 -1.9385940	G = -1079.142714 a.u.
H -3.8209420 -1.7153970 -1.9513260	C -2.0710440 -0.2896000 -0.9098670
O -0.4207270 -1.1378090 0.5769390	O -0.6097070 -0.4042690 -0.9486510
H 0.4859800 -0.7265780 0.4739690	C -0.1603890 -1.0623010 0.0197750
C -2.7659110 1.9602220 0.3731420	C -1.2286560 -1.6931930 0.8796580
H -2.3640620 2.8679520 -0.0898110	C -2.5031130 -0.9630180 0.4002140
H -2.2110890 1.7321150 1.2877740	H -2.4233020 -0.8660720 -1.7683670
O -4.1621270 2.1048220 0.6386660	H 0.9014670 -1.3013200 0.0321100
H -4.2784300 2.5984230 1.4524400	H -1.0449120 -1.5791210 1.9462120
C 3.0409440 -1.0139950 0.4446330	H -2.8016110 -0.2210790 1.1368460
N 2.0396230 -0.1914680 0.1028380	O -3.5105480 -1.9261480 0.1861770
C 2.3818230 0.9986370 -0.4249510	H -4.3338850 -1.4696720 -0.0132440
C 3.7202140 1.3548050 -0.5998730	O -1.1937260 -3.0452830 0.4821780
C 4.6697660 0.4117190 -0.2060150	H -2.0996320 -3.3048140 0.2621290
N 4.3427570 -0.7814710 0.3104950	O -0.9645390 0.8393230 1.9999910
H 4.0029560 2.3155550 -1.0069480	H -0.0608190 0.6665400 2.2792070
N 2.6781150 -2.2009160 1.0079010	C -2.4631410 1.1657180 -1.0353590

H	-2.1156560	1.5728960	-1.9889250	C	-2.0866730	-0.6625150	-0.3377050
H	-2.0303010	1.7504440	-0.2215900	H	-2.4442840	0.4253010	-2.1614540
O	-3.8835590	1.1154600	-0.9656660	H	0.8711180	-0.5663210	-1.7704040
H	-4.2151430	1.9945070	-0.7694820	H	-0.5504430	-2.2102290	-0.0868710
C	2.9064480	-0.5153200	-1.1305510	H	-1.9801200	-0.4020680	0.7229560
N	2.1678460	0.4969970	-1.5447480	O	-3.2640960	-1.4043380	-0.5584750
C	1.6177900	1.3125450	-0.5864240	H	-4.0015050	-0.7886450	-0.4683310
C	1.9086400	1.0337780	0.7905960	O	-1.1200560	-2.0331910	-2.0716580
C	2.7228150	-0.0509330	1.0780950	H	-2.0340450	-2.3428440	-2.0614800
N	3.1970780	-0.8803030	0.1373150	O	-0.6635860	-1.6877930	2.7311100
H	1.5988440	1.7360650	1.5545750	H	-1.5229020	-2.1148270	2.7509130
N	3.4047050	-1.3555560	-2.1010020	C	-2.6015940	1.8001300	-0.5092720
H	3.4369850	-0.9596980	-3.0270310	H	-2.5470760	2.6863550	-1.1482470
H	4.1913330	-1.9182660	-1.8185530	H	-2.0755480	1.9928860	0.4313790
N	0.8000440	2.2874020	-0.9142140	O	-3.9582380	1.4146100	-0.2764600
H	0.7256150	2.3404040	-1.9263850	H	-4.3952680	2.0839080	0.2529550
H	-0.9381490	1.7822110	1.7145620	C	3.3455280	0.4754900	-0.5939980
N	3.0184880	-0.4035660	2.3869570	N	2.6185580	1.5414010	-0.3559840
H	3.8013820	-1.0381670	2.4560620	C	1.4794790	1.3312250	0.3737730
H	3.0519770	0.3585640	3.0472280	C	0.9109750	-0.0652350	0.3628400
O	-0.7777760	3.2607500	0.8695750	C	2.0533800	-1.0313780	0.4994080
H	-0.5142980	4.1185280	1.2060020	N	3.2047710	-0.7927520	-0.0532970
H	-0.1042830	2.9784930	0.1228340	H	0.2133400	-0.1829090	1.1854580
INT₂H₂O				N	4.4195140	0.5962940	-1.3988390
H = -1079.153466 a.u.				H	4.6593180	1.5064670	-1.7530290
G = -1079.226626 a.u.				H	5.0576090	-0.1762270	-1.4780230
C	-1.9703100	0.6037610	-1.1882770	N	0.8461510	2.2292390	1.0334430
O	-0.5788890	0.8189420	-1.3592350	H	1.3073060	3.1316680	0.9212580
C	0.1573550	-0.3348180	-0.9759470	H	-0.8301890	-0.7358180	2.8711980
C	-0.8691770	-1.4549170	-0.8115020	N	1.8216770	-2.1637060	1.1701270

H 2.5891180 -2.8051490 1.3003500
H 0.9846750 -2.2432310 1.7422680
O -1.0034710 1.1004710 2.7104100
H -1.1210470 1.6102970 3.5147390
H -0.3618490 1.6179910 2.1447660

INT3_{H2O}

H = -1002.741065 a.u.

G = -1002.807443 a.u.

C 2.1702640 -0.1286900 -1.2922660
O 0.8936260 -0.6175510 -0.8565750
C 0.2056060 0.4289150 -0.2110550
C 1.3367660 1.1290860 0.5620870
C 2.4337740 1.1662210 -0.5017730
H 2.1155510 0.1001400 -2.3642150
H -0.2217500 1.1195800 -0.9551570
H 1.6440410 0.4706650 1.3786920
H 3.4331310 1.1852410 -0.0635710
O 2.1846460 2.3452780 -1.2654180
H 2.9477410 2.5464560 -1.8108390
O 1.0219970 2.3921040 1.0960860
H 1.1604570 3.0356730 0.3881400
O 1.3564470 -2.1076680 1.8125790
H 1.4525360 -2.7209580 2.5439060
C 3.2066330 -1.2080760 -1.0249960
H 4.1297910 -0.9524030 -1.5545060
H 2.8311890 -2.1548610 -1.4320280
O 3.5214210 -1.3084270 0.3384860
H 2.7530030 -1.6676440 0.8228770
C -3.2846970 -0.2384940 -0.6849530
N -2.5919990 -1.3442830 -0.7131170

C -1.5150680 -1.4193000 0.1330900
C -0.9256750 -0.1315750 0.6878340
C -2.0135490 0.9108410 0.8134260
N -3.1177570 0.8652820 0.1367780
H -0.5034570 -0.3521140 1.6708820
N -4.3296600 -0.1094240 -1.5278710
H -4.5914770 -0.8967400 -2.0964370
H -4.9405420 0.6819940 -1.4255460
N -0.9561960 -2.5194970 0.4672290
H -1.4193070 -3.2954810 -0.0041010
H 0.5385860 -2.3834110 1.3134790
N -1.7943730 1.9310350 1.6574300
H -2.4681150 2.6825600 1.6370510
H -0.8408960 2.1560530 1.9186020

TS3_4_{H2O}

H = -1002.712972 a.u.

G = -1002.775959 a.u.

C 2.4425010 -0.5255680 -1.0642430
O 1.0162280 -0.6889860 -1.0103910
C 0.3835340 0.4361630 -0.4458070
C 1.4975680 1.1051490 0.3987710
C 2.7285260 0.8513300 -0.4710990
H 2.7426150 -0.5600230 -2.1179880
H 0.0730600 1.1320060 -1.2406690
H 1.5980040 0.5792780 1.3482530
H 3.6497260 0.8698080 0.1138800
O 2.7144950 1.8880070 -1.4536690
H 3.5498800 1.8982530 -1.9248790
O 1.3093510 2.4786890 0.6653510
H 1.5963380 2.9592190 -0.1227160

O	0.6314690	-1.4965170	1.8776130	C	2.8277290	0.2896340	-0.6671620
H	0.4556140	-1.8111870	2.7671500	H	2.9437600	-1.8760660	-0.5958700
C	3.1200480	-1.6507310	-0.2859100	H	0.6088400	-0.5166420	-1.7919360
H	4.1686930	-1.7004020	-0.6018950	H	1.3821360	1.3952140	0.4576590
H	2.6390700	-2.5948640	-0.5798620	H	3.6238320	0.8480820	-0.1717760
O	3.1011280	-1.4492800	1.0950610	O	3.0791760	0.1581630	-2.0628800
H	2.1626250	-1.5348860	1.4408650	H	4.0081440	-0.0291790	-2.2112950
C	-3.5304400	-0.1049720	-0.3827180	O	1.3059140	2.0554300	-1.4599670
N	-2.8418750	-1.2185230	-0.6346430	H	1.7007980	1.7862440	-2.2987180
C	-1.5822930	-1.2303480	-0.2034840	O	0.1668280	0.3496440	2.5632210
C	-0.8765380	-0.0384190	0.3473830	H	-0.2232560	1.1672680	2.2264800
C	-1.8422070	1.0535800	0.5994590	C	3.1270820	-1.1341150	1.4263790
N	-3.1266510	0.9909520	0.2920870	H	4.2074470	-1.2907650	1.3531820
H	-0.3285640	-0.5498860	1.3233420	H	2.6933950	-2.0040920	1.9346380
N	-4.7968000	-0.0707020	-0.8283300	O	2.9333600	0.0514240	2.1546340
H	-5.1734610	-0.8759020	-1.2982530	H	1.9973940	0.1362340	2.4056780
H	-5.3682720	0.7299880	-0.6204620	C	-3.5978340	-0.0804310	0.0492280
N	-0.9450540	-2.3825070	-0.1728040	N	-3.0642770	-1.2272110	-0.3738970
H	-1.4447230	-3.2077430	-0.4660570	C	-1.7502710	-1.2066840	-0.5964700
H	-0.0878780	-2.4244090	0.3893160	C	-0.9444320	-0.0581680	-0.4166820
N	-1.4214650	2.1849060	1.1630960	C	-1.6423850	1.0775730	0.0201920
H	-2.1017960	2.9250370	1.2471870	N	-2.9549980	1.0666270	0.2700470
H	-0.4335760	2.4044240	1.2611100	H	-0.1253770	-0.3253500	1.9380670
INT4_{H2O}				N	-4.9449310	-0.0730390	0.2530480
H = -1002.762478 a.u.				H	-5.4079440	-0.9648040	0.2989280
G = -1002.828449 a.u.				H	-5.3282410	0.7008440	0.7686980
C	2.5511370	-1.0578490	0.0200880	N	-1.1969910	-2.3733950	-1.0474730
O	1.1192030	-1.1797000	0.0990730	H	-1.8198510	-3.1658220	-1.0065390
C	0.5164230	-0.1800340	-0.7469280	H	-0.2336200	-2.5469990	-0.7988340
C	1.4775430	0.9986650	-0.5530080	N	-1.0179620	2.2839960	0.3013770

H -1.7065940 3.0099270 0.4528260
H -0.2925380 2.5658320 -0.3493850

INT1'_{H₂O}

H = -1079.167743 a.u.

G = -1079.244123 a.u.

C -2.8711520 0.1688860 -0.0673160
C -0.7464320 -0.8132620 -0.1052590
C -1.7403420 -1.9198300 0.2089290
C -2.8892110 -1.0951920 0.8020320
H -3.5769850 0.0520340 -0.8949620
H -0.0280180 -1.0735010 -0.8843230
H -1.3153030 -2.6410720 0.9124910
H -2.6660310 -0.8495680 1.8450990
O -4.1504700 -1.7285230 0.6816000
H -4.3068110 -2.2747380 1.4557680
O -2.1424960 -2.5308260 -0.9903600
H -3.0763580 -2.7551940 -0.9057730
O -0.1329200 -0.4567600 1.0941570
H 0.6012610 0.1459890 0.9012910
C -3.2189680 1.4081580 0.7250920
H -2.4321900 1.5833850 1.4695950
H -4.1719710 1.2251220 1.2369480
O -3.3280530 2.5066120 -0.1684050
H -3.6794590 3.2600370 0.3110750
C 3.3605580 -1.1081460 -0.2007740
N 2.6463490 -0.6709170 -1.2405500
C 2.1381160 0.5649310 -1.1226850
C 2.2996600 1.3321000 0.0431840
C 3.1085360 0.7689830 1.0344550
N 3.6392300 -0.4545840 0.9305960

H 1.8857720 2.3289070 0.1183460
N 3.8389020 -2.3843790 -0.2923730
H 3.8523110 -2.7951750 -1.2108610
H 4.5632600 -2.6411640 0.3570720
N 1.4492340 1.0442210 -2.1865960
H 1.2312170 0.3878590 -2.9186740
H 0.8616620 1.8604710 -2.0667760
N 3.4209670 1.4602100 2.1731180
H 3.8005440 0.9131870 2.9292070
H 2.8642990 2.2613070 2.4190510
O -0.4404900 2.8180020 -0.8750140
H -1.2074840 3.3832070 -0.9970580
H -0.8420260 1.9437640 -0.7313400
O -1.5512030 0.2519340 -0.6096640

TS1'_{H₂O}

H = -1079.030820 a.u.

G = -1079.104845 a.u.

C -3.1433970 -0.1193910 -0.2800810
C -0.9644030 -0.4411590 -0.8128640
C -1.2749540 -1.6354450 0.0466080
C -2.6548960 -1.2509350 0.6333960
H -3.8795640 -0.4873990 -0.9970380
H -0.0503620 -0.2813500 -1.3731100
H -0.5142930 -1.8085330 0.8054090
H -2.5234990 -0.8946320 1.6540880
O -3.5738250 -2.3246700 0.5475890
H -3.6130630 -2.7815940 1.3916740
O -1.3636500 -2.7114490 -0.8622740
H -2.2228110 -3.1363460 -0.7304090
O -0.6767000 0.5430890 1.3471510

H	-0.6539600	1.5079700	1.3424780	C	-3.0423980	0.7887090	-0.8010900
C	-3.6639630	1.0921540	0.4506720	O	-2.7721800	0.0108990	-1.9574670
H	-2.8963630	1.4644840	1.1340000	C	-0.7146770	-1.1316570	-0.4504580
H	-4.5405840	0.7677680	1.0226780	C	-1.2535050	-0.3006510	0.7072270
O	-4.0085170	2.0696680	-0.5207350	C	-2.7496000	-0.0087080	0.4715840
H	-4.5622200	2.7393680	-0.1116640	H	-4.1051140	1.0627620	-0.7723610
C	4.3460720	0.0926720	-0.0401710	H	-0.7066120	0.6408010	0.7908170
N	3.7071560	1.2592520	-0.0134760	H	-3.0929180	0.5587480	1.3382040
C	2.3690630	1.1703500	0.0812550	O	-3.4883850	-1.2180840	0.4711030
C	1.6292270	-0.0211450	0.1646160	H	-3.0538790	-1.8535530	-0.1118190
C	2.4570230	-1.1447360	0.0625860	O	-1.0931170	-0.9808670	1.9307560
N	3.7996200	-1.1196470	-0.0233320	H	-1.5791260	-1.8123070	1.8741300
H	0.3013100	0.2579710	0.9483290	C	-2.1889770	2.0463340	-0.9282700
N	5.7218810	0.1463540	-0.1520570	H	-2.5435690	2.6434070	-1.7735300
H	6.1325330	1.0165220	0.1469930	H	-1.1559500	1.7629020	-1.1458260
H	6.1981090	-0.6933560	0.1365990	O	-2.1669200	2.7869890	0.2768120
N	1.7223140	2.3943720	0.1495560	H	-2.9758720	3.2981400	0.3529630
H	2.2947700	3.1725560	-0.1422000	O	-0.8564320	-2.3334550	-0.4592040
H	0.7632030	2.4197630	-0.1671850	H	-3.5118370	-0.5801040	-2.1203410
N	1.9324010	-2.4426680	0.0839360	H	-0.2531670	-0.6009180	-1.2983160
H	2.6250260	-3.1256210	-0.1925010	C	3.1671580	0.9443760	-0.4727740
H	1.0582050	-2.5733810	-0.4044250	N	2.6510520	1.2344860	0.7243820
O	-1.3111150	3.0834540	-0.1462790	C	1.9938520	0.2377920	1.3298380
H	-1.2440500	4.0403900	-0.1869040	C	1.8551690	-1.0285210	0.7524260
H	-2.1078880	2.8491490	-0.6415020	C	2.4051990	-1.1860060	-0.5210270
O	-1.9845360	0.2684620	-1.0884270	N	3.0686330	-0.2051010	-1.1455900
INT6				H	1.3524300	-1.8338580	1.2685310
H = -1002.741910 a.u.				N	3.8301790	1.9601180	-1.1063620
G = -1002.813146 a.u.				H	4.1251020	2.7280020	-0.5261900
				H	4.4258280	1.6922770	-1.8722980

N 1.4594230 0.5074170 2.5569960
H 1.4349940 1.4825210 2.8121480
H 0.6844630 -0.0669400 2.8595470
N 2.2909300 -2.3720310 -1.1955390
H 1.5082570 -2.9646130 -0.9589140
H 2.5283890 -2.3253510 -2.1746770

TS6_8

H = -1002.722676 a.u.

G = -1002.788767 a.u.

C -3.0361910 0.1644440 -0.9502480
O -2.3592840 -0.5010910 -1.9962560
C -0.2365090 -0.7398300 -0.1465030
C -1.1372800 0.0123250 0.8452270
C -2.6135640 -0.2335370 0.4666420
H -4.1108780 -0.0683160 -1.0041300
H -0.9160280 1.0817740 0.8232480
H -3.2162380 0.3705820 1.1498360
O -2.9323760 -1.5875190 0.7457160
H -2.2278650 -2.1272840 0.3432280
O -0.9602010 -0.4261990 2.1839130
H -1.5377260 -1.1902480 2.3108350
C -2.8380650 1.6544480 -1.2169660
H -3.1799730 1.8726620 -2.2337980
H -1.7743430 1.8987140 -1.1728260
O -3.4844800 2.4693360 -0.2560700
H -4.4329570 2.4273400 -0.4007650
O -0.4936190 -1.9754500 -0.3357990
H -2.0261760 -1.3566540 -1.6977190
H 0.0249870 -0.1229360 -1.0234350
C 3.2674420 0.8818540 -0.5893320

N 2.6733090 1.4508790 0.4751990
C 1.8695730 0.6622200 1.1772490
C 1.5145560 -0.6679850 0.7465710
C 2.3384970 -1.1614740 -0.3260460
N 3.1702180 -0.3865470 -1.0139440
H 1.2099480 -1.3647070 1.5162070
N 4.0685500 1.6862580 -1.3099310
H 4.2014100 2.6384650 -1.0165130
H 4.5591140 1.3086940 -2.1020220
N 1.3609680 1.1477550 2.3181640
H 1.5606700 2.1079710 2.5494480
H 0.6075720 0.6530060 2.7800170
N 2.2113680 -2.4474560 -0.6892720
H 1.3061990 -2.8655740 -0.4780810
H 2.6303110 -2.6871130 -1.5766310

INT8

H = -1002.738442 a.u.

G = -1002.803078 a.u.

C 2.7451290 -0.8976500 -0.1589550
O 2.0542590 -2.0857830 0.1183130
C 0.1193240 0.5429820 -0.7786720
C 0.6791650 0.3855740 0.6484250
C 2.2030490 0.3011530 0.6422970
H 2.7015720 -0.6363890 -1.2263700
H 0.2928560 -0.5356560 1.0840470
H 2.5302020 0.2183320 1.6872850
O 2.6708970 1.5341220 0.0892150
H 3.6354720 1.4830670 0.0490370
O 0.2463590 1.4349880 1.4883800
H 0.7048920 2.2350430 1.2087510

C	4.1949450	-1.1795070	0.2072760	C	-1.0315980	0.9774680	-0.6268010
H	4.5883480	-1.9565820	-0.4532740	C	-2.4554690	0.5286170	-0.3380440
H	4.2221910	-1.5404290	1.2411560	H	-2.3845190	-1.2412440	0.8794340
O	4.9367580	0.0331890	0.0720730	H	-0.6933130	0.5208680	-1.5573440
H	5.8430700	-0.1086390	0.3512290	H	-3.0985410	0.8747090	-1.1569030
O	0.3206740	1.8651360	-1.2700020	O	-2.8199360	1.1923010	0.8735190
H	1.1660550	-2.0770260	-0.2980660	H	-3.7308970	0.9345690	1.0673600
H	0.6277590	-0.1645160	-1.4366580	O	-0.9673150	2.3797430	-0.7944670
C	-3.6561140	-0.7083510	0.3121730	H	-1.4762810	2.7761560	-0.0763480
N	-3.4477900	0.6503360	0.3687840	C	-3.9912100	-1.4458420	-0.5002160
C	-2.3573480	1.0935640	-0.1848840	H	-4.1174140	-2.5020080	-0.2486620
C	-1.3692210	0.1894270	-0.8950210	H	-4.1688340	-1.3079830	-1.5725790
C	-1.6141060	-1.2781710	-0.5507650	O	-4.8638030	-0.6191680	0.2723230
N	-2.8463870	-1.6545950	-0.0978210	H	-5.7769510	-0.8392910	0.0787820
H	-1.6253350	0.2966720	-1.9589090	O	-0.0153450	1.5005390	1.6130380
N	-4.8723520	-1.0760400	0.7625510	H	-0.8714560	-1.9467220	-0.5195010
H	-5.4689590	-0.3793500	1.1734310	H	-0.5629550	-0.4074540	0.9609040
H	-5.0826670	-2.0559040	0.8452900	C	3.8105160	-0.6724660	-0.0477460
N	-2.1519100	2.4094270	-0.2467210	N	3.5399830	0.6030980	-0.4462780
H	-2.8037560	3.0055990	0.2384450	C	2.2888260	0.9917550	-0.2891030
H	-1.2602940	2.7563360	-0.5746120	C	1.3186870	0.1525590	0.3614580
N	-0.6577980	-2.1143840	-0.7413970	C	1.6496680	-1.2810620	0.3772030
H	1.2645520	2.0561760	-1.1698520	N	2.9718660	-1.6228230	0.3078280
H	-1.0028050	-3.0472910	-0.5137770	H	1.0189660	1.0054420	1.6827170
TS8_9				N	5.1365370	-0.9821340	-0.0482930
H =	-1002.661286	a.u.		H	5.7536500	-0.3553370	-0.5362050
G =	-1002.726185	a.u.		H	5.3771880	-1.9571220	0.0152450
C	-2.5724350	-1.0083090	-0.1780340	N	1.9718500	2.2459010	-0.6837880
O	-1.6958940	-1.7072790	-1.0162010	H	2.7003090	2.7635550	-1.1489660
C	-0.1245990	0.4687620	0.4939100	H	1.0102550	2.5487000	-0.7735540

N 0.6881960 -2.1562040 0.4454060
H -0.6928410 1.3668080 2.2972980
H 1.0986420 -3.0864990 0.4827310

INT9

H = -1002.7226 a.u.

G = -1002.791279 a.u.

C 2.7125420 -1.0547210 -0.6409910
O 2.1510710 -2.3306550 -0.3837810
C 0.0158560 0.2142780 -0.0882480
C 1.0023890 -0.1263820 1.0013560
C 2.4397000 -0.0498240 0.4946570
H 2.3161360 -0.6278500 -1.5704930
H 0.8331900 -1.1385050 1.3789520
H 3.0950830 -0.2704230 1.3474670
O 2.6641320 1.2730660 0.0347530
H 3.5721380 1.3123260 -0.2910440
O 0.8129560 0.7437640 2.1087750
H 0.6877840 1.6441620 1.7497480
C 4.2034590 -1.3118700 -0.8034560
H 4.3723030 -1.9216460 -1.6954070
H 4.5485010 -1.8653750 0.0773270
O 4.8612600 -0.0537460 -0.9063060
H 5.8106100 -0.1843940 -0.9464390
O 0.3957180 3.0013240 0.4241370
H 1.2325450 -2.3377040 -0.6664010
H 0.4177600 0.6648160 -0.9922300
C -3.8200070 -0.6119200 -0.5156840
N -3.3411580 -0.9015020 0.7493920
C -2.1395540 -0.4815380 1.0272940
C -1.3192930 0.1671750 -0.0152210

C -2.1316680 0.8014460 -1.0926480
N -3.3410810 0.2256320 -1.3988360
H -0.2725860 2.8374350 -0.2637210
N -4.9626680 -1.2726130 -0.8105490
H -5.4320100 -1.7674970 -0.0717230
H -5.4636740 -1.0056590 -1.6411500
N -1.6306760 -0.6794830 2.2533760
H -2.2567060 -1.0761740 2.9380690
H -0.8270620 -0.1356400 2.5588830
N -1.6458540 1.8512900 -1.6467310
H 1.2412850 2.7863560 0.0110690
H -2.2868720 2.1726170 -2.3724400

INT10

H = -926.303913 a.u.

G = -926.367202 a.u.

C 2.3641630 0.8141460 -0.1579150
O 1.3404860 1.5587270 -0.7791020
C -0.0435800 -0.1995310 0.9547840
C 1.0575830 -1.1896050 0.8336400
C 2.0507530 -0.7002060 -0.2608830
H 2.5031200 1.0880010 0.8953830
H 0.7067650 -2.1913250 0.5581950
H 1.5992900 -0.8415160 -1.2537840
O 3.1738040 -1.5477460 -0.1185950
H 3.9886330 -1.0290810 -0.1864250
O 1.7200560 -1.2363600 2.0756590
H 2.5655330 -1.6711590 1.9064510
C 3.6235450 1.2037930 -0.9275500
H 3.6970290 2.2931620 -0.9089390
H 3.5250840 0.8732960 -1.9686840

O	4.7615500	0.6044840	-0.3077710	H	-4.0472480	0.9485410	-0.3499550
H	5.5616730	0.8905540	-0.7536850	O	-1.7410830	1.4371330	1.9993120
H	0.6532200	1.8808530	-0.1665890	H	-2.6411740	1.7296790	1.8001470
H	0.2077590	0.6190060	1.6265680	C	-3.4235170	-1.3922550	-0.9324570
C	-3.8321710	0.1294970	-0.1323770	H	-3.4908490	-2.4668710	-0.7470260
N	-3.2987240	1.2158180	0.3574430	H	-3.1220600	-1.2286540	-1.9736520
C	-1.9275270	1.2338240	0.4378580	O	-4.6778040	-0.7507220	-0.6594750
C	-1.2025270	-0.0615130	0.3003860	H	-5.3585170	-1.1110100	-1.2311490
C	-1.9110860	-1.0399400	-0.5354630	H	-0.0489320	-1.9940220	0.3781280
N	-3.1951320	-0.9600230	-0.7085840	H	-0.2529790	-0.4365460	1.6746900
N	-5.1777750	0.0214190	-0.1549910	C	3.7876060	-0.2042110	-0.1843020
H	-5.7291480	0.8107840	0.1357020	N	3.1642420	-1.2804720	0.2812720
H	-5.5959890	-0.7431520	-0.6553750	C	1.8403420	-1.1458460	0.4404630
N	-1.2085660	2.2830420	0.6064760	C	1.1898810	0.1588450	0.3039130
H	-1.8117130	3.0978940	0.7122680	C	1.9431080	1.0944830	-0.5054860
N	-1.2443330	-2.0752940	-1.0968140	N	3.2336890	0.9327040	-0.6920310
H	-1.7829510	-2.6566430	-1.7222540	N	5.1299260	-0.2436380	-0.2334620
H	-0.2586780	-1.9910460	-1.2799530	H	5.6043890	-1.0847910	0.0473940
TS10_11				H	5.6281300	0.5171820	-0.6620380
H = -926.2903943 a.u.				N	1.0394530	-2.1598220	0.6716600
G = -926.3516393 a.u.				H	1.4823650	-3.0681180	0.7100570
C	-2.3386360	-0.8277860	-0.0132300	N	1.3671620	2.1894690	-1.0409400
O	-1.1742120	-1.5026250	-0.2773270	H	1.9573060	2.7610390	-1.6269690
C	-0.0207160	0.2932270	0.9059290	H	0.3763070	2.2087850	-1.2117180
C	-1.1151170	1.2786180	0.7498230	Pc			
C	-2.1223730	0.6818250	-0.2792210	H = -926.343990 a.u.			
H	-2.6999640	-0.9324220	1.0276900	G = -926.406101 a.u.			
H	-0.7723380	2.2556320	0.3883490	C	2.4597300	-0.3531090	-0.5718740
H	-1.6830840	0.7664280	-1.2847360	O	1.1457050	-0.6927790	-0.9656160
O	-3.2714160	1.4969720	-0.1571710	C	0.2985540	0.4281250	-0.6683570

C	1.0243540	1.2370570	0.4432640	INT6_{H2O}			
C	2.2518340	0.3751180	0.7556670	H = -1079.158476 a.u.			
H	2.9237850	0.3371640	-1.2906830	G = -1079.235999 a.u.			
H	0.3855570	1.3799790	1.3193770	C	2.5120540	-1.1450350	-0.8782580
H	1.9908350	-0.3642450	1.5250170	O	2.4403760	-0.3436780	-2.0585630
O	3.3199380	1.1917760	1.1643220	C	0.8381330	1.4291420	-0.3769430
H	4.1258150	0.6642890	1.1077450	C	1.4226810	0.5602320	0.7155210
O	1.4000500	2.4886240	-0.0973690	C	2.7067990	-0.1725660	0.2860250
H	2.2035590	2.7733780	0.3560380	H	3.4028930	-1.7819480	-0.9169630
C	3.2832060	-1.6153420	-0.4434680	H	0.6950660	-0.2114530	0.9580660
H	3.4486770	-2.0730270	-1.4233790	H	3.0135680	-0.7449810	1.1626390
H	2.7471720	-2.3227680	0.2011030	O	3.7393370	0.7470790	0.0082660
O	4.5106120	-1.2099530	0.1537710	H	3.6593850	1.0002000	-0.9193670
H	5.0913760	-1.9666410	0.2540700	O	1.6322100	1.3029430	1.8865830
H	-0.7937720	2.6719600	-0.5350290	H	2.1566760	2.0778210	1.6507040
H	0.2829340	1.0767460	-1.5538030	C	1.2496190	-2.0008320	-0.7600910
C	-3.6857060	-0.4295310	0.2626890	H	1.2614500	-2.7721290	-1.5410310
N	-3.3638050	0.8313210	-0.0260120	H	0.3796150	-1.3633580	-0.9587030
C	-2.0759190	1.0465820	-0.3095070	O	1.1817260	-2.5901490	0.5182980
C	-1.1077540	0.0279020	-0.3275830	H	0.2645650	-2.5288780	0.8311280
C	-1.5779430	-1.2453800	0.0265090	O	0.8805630	2.6360170	-0.3143920
N	-2.8668200	-1.4780150	0.3084570	H	2.5719230	-0.8906040	-2.8364260
N	-4.9962900	-0.6641620	0.5839600	H	0.3777460	0.9197170	-1.2388870
H	-5.6559490	0.0432640	0.3060710	C	-2.0856660	-1.7927860	-0.2145740
H	-5.2962560	-1.6244080	0.5570450	N	-2.5462860	-0.8448770	-1.0226260
N	-1.7445070	2.3399130	-0.6143390	C	-2.4925110	0.4127270	-0.5445780
H	-2.4727770	3.0134780	-0.4363500	C	-2.0054380	0.7030470	0.7390330
N	-0.7544080	-2.3352710	0.1418730	C	-1.5573260	-0.3799470	1.4881180
H	-1.2476340	-3.2139740	0.1766750	N	-1.5633530	-1.6409220	1.0104710
H	0.1149240	-2.3015800	-0.3663560	H	-1.9884720	1.7160280	1.1182030

N	-2.0607730	-3.0693910	-0.7162620	O	2.3714230	1.9169420	-0.1637620
H	-2.6369330	-3.2259840	-1.5278980	H	2.5182040	2.7747740	0.2438470
H	-2.0216600	-3.8114920	-0.0355440	O	-0.2022000	0.7258070	-1.1991890
N	-2.9387090	1.3898850	-1.3630610	H	4.8281410	-1.2412550	-0.2773500
H	-3.1669910	1.1229260	-2.3064560	H	0.1337250	-1.1597830	-1.7978940
H	-2.7208790	2.3588050	-1.1580410	C	-2.8967630	-1.1975330	-0.7728130
N	-1.0511160	-0.2191720	2.7484550	N	-3.2660660	0.0615480	-0.9831800
H	-0.5693870	-1.0237980	3.1215400	C	-2.9414490	0.9326770	-0.0177400
H	-0.6225200	0.6701040	2.9638110	C	-2.3173050	0.5397540	1.1677280
O	-1.6333540	3.8806850	-0.6338980	C	-2.0122910	-0.8124710	1.2788400
H	-0.6914630	3.6528650	-0.6314440	N	-2.2635840	-1.6920510	0.2967410
H	-1.6998630	4.7804210	-0.3100350	H	-2.0865810	1.2472650	1.9520170
INT6'				N	-3.1365170	-2.0869660	-1.7944590
H = -1079.157986 a.u.				H	-3.8229330	-1.7856720	-2.4680030
G = -1079.233564 a.u.				H	-3.1673020	-3.0564560	-1.5215090
C	3.3254810	-0.1782960	-0.8524800	N	-3.2789680	2.2408760	-0.2351470
O	4.5793160	-0.7854410	-1.0909490	H	-3.5125880	2.4501330	-1.1943040
C	0.2453800	-0.3765070	-1.0252410	H	-2.6963100	2.9242250	0.2292570
C	0.9979050	-0.8029080	0.2178290	N	-1.4442730	-1.3248260	2.4214010
C	2.4447920	-1.2063600	-0.1213420	H	-1.1225030	-2.2771170	2.3305830
H	2.8857230	0.0462750	-1.8302780	H	-0.8078130	-0.7071260	2.9031490
H	0.5028130	-1.7147210	0.5714060	O	-0.3596610	3.0681350	0.4270820
H	2.4145460	-2.0878950	-0.7697340	H	-0.3693440	2.2122740	-0.0328390
O	3.0940270	-1.6098040	1.0711800	H	-0.0909610	3.6885790	-0.2548510
H	2.7677920	-1.0367840	1.7769940	TS6_7_{H2O}			
O	0.9494790	0.1205470	1.2719610	H = -1079.143235 a.u.			
H	1.1716950	0.9960300	0.9098890	G = -1079.214778 a.u.			
C	3.5650160	1.1423620	-0.1249430	C	2.9982240	-0.5538620	-0.8936110
H	4.3775920	1.6532990	-0.6466990	O	2.3644650	-0.2072730	-2.1084040
H	3.8782950	0.9500910	0.9092170	C	0.1845530	0.6337300	-0.3353620

C	1.1729010	0.2490580	0.7719490	N	-1.1074890	-0.7291540	2.5970820
C	2.6186640	0.3816340	0.2613950	H	-0.9989960	-1.6331350	3.0302930
H	4.0883170	-0.4817440	-1.0015330	H	-0.5347360	0.0420050	2.9164510
H	1.0170320	-0.7786470	1.1031020	O	-1.2421250	3.7203590	0.1944690
H	3.2661760	0.1382460	1.1074400	H	-0.5091300	3.1667760	-0.1589220
O	2.8888290	1.7261700	-0.0993230	H	-0.9822090	4.6371360	0.0931590
H	2.0833110	2.0626810	-0.5349450	INT7_{H2O}			
O	1.0100030	1.0752760	1.9147690	H = -1079.152824 a.u.			
H	1.3604180	1.9467950	1.6949840	G = -1079.222828 a.u.			
C	2.6214130	-2.0034090	-0.6371310	C	2.9520290	-0.5199810	-0.9497300
H	3.0619050	-2.6261510	-1.4221620	O	2.3267200	0.0021100	-2.0999250
H	1.5299790	-2.1055750	-0.6936840	C	0.1268480	0.3779480	-0.1851070
O	3.1095110	-2.3561860	0.6470650	C	1.1649120	-0.0184940	0.8880490
H	2.9863330	-3.2973870	0.7828430	C	2.6051820	0.1752500	0.3745950
O	0.2950530	1.8206730	-0.8005180	H	4.0356500	-0.3958760	-1.0652030
H	2.5214360	0.7280490	-2.2738870	H	1.0331920	-1.0650360	1.1804460
H	0.0033700	-0.1816920	-1.0535260	H	3.2672680	-0.2522270	1.1308570
C	-2.5825590	-1.7288930	-0.4062410	O	2.8990650	1.5617980	0.3342910
N	-2.8764310	-0.6136360	-1.0809390	H	2.2443540	1.9380870	-0.2776640
C	-2.4272640	0.5226000	-0.5419750	O	1.0122310	0.7617260	2.0709490
C	-1.5380510	0.5304430	0.5936880	H	1.5457790	1.5589760	1.9451540
C	-1.5704170	-0.7034790	1.3362730	C	2.6507370	-2.0150720	-0.8945760
N	-1.9982480	-1.8402070	0.8056860	H	3.0403150	-2.4715820	-1.8097960
H	-1.4539330	1.4514700	1.1593740	H	1.5642960	-2.1698480	-0.8744860
N	-2.9351680	-2.8909210	-0.9891180	O	3.2647310	-2.5605730	0.2653100
H	-3.4609760	-2.8626650	-1.8458430	H	3.2681410	-3.5169670	0.2001720
H	-2.8436980	-3.7445700	-0.4662160	O	0.4673600	1.5048640	-0.8574450
N	-2.7603230	1.6684370	-1.1243560	H	1.6532930	0.6698360	-1.8549140
H	-3.2653090	1.6235670	-1.9952450	H	0.0089980	-0.4880560	-0.8650820
H	-2.3963430	2.5541130	-0.7785450	C	-2.9238640	-1.4193890	-0.4181080

N	-3.0036440	-0.2645000	-1.0886060	H	2.2920980	2.0266790	-0.2308960
C	-2.3175280	0.7515220	-0.5771470	O	1.0298180	0.7681850	2.0905520
C	-1.3231150	0.5603730	0.5179990	H	1.5446790	1.5795920	1.9814630
C	-1.6931290	-0.6460440	1.3136140	C	2.6714770	-1.9466590	-0.9259010
N	-2.3927540	-1.6390070	0.8105530	H	3.0550210	-2.3866830	-1.8516220
H	-1.2319980	1.4483400	1.1448910	H	1.5864230	-2.1108320	-0.8978690
N	-3.4898650	-2.4840790	-0.9941840	O	3.3014190	-2.5007440	0.2195830
H	-3.9256890	-2.3815990	-1.8955850	H	3.3137580	-3.4562920	0.1428220
H	-3.4896010	-3.3654280	-0.5091280	O	0.4566860	1.5967270	-0.7965930
N	-2.4755730	1.9512650	-1.0862060	H	1.6983390	0.7827180	-1.8685950
H	-3.0676280	2.0396060	-1.8992620	H	0.0456140	-0.3944890	-0.8857570
H	-1.9116800	2.7441470	-0.7541350	C	-2.8621660	-1.4686720	-0.4462690
N	-1.2590200	-0.7287060	2.5662750	N	-2.9895600	-0.3119380	-1.0837400
H	-1.4226430	-1.5894100	3.0668560	C	-2.3535430	0.7385700	-0.5427490
H	-0.5538760	-0.0716910	2.8895880	C	-1.3109500	0.5390390	0.5317650
O	-0.5950570	3.5803610	0.1197150	C	-1.6457850	-0.7060020	1.3052080
H	-0.0237360	2.8329190	-0.2650880	N	-2.3200480	-1.6995520	0.7868330
H	-0.1412670	4.4120380	-0.0231430	H	-1.2740850	1.4056630	1.1943000
TS7_8_{H2O}				N	-3.3785910	-2.5531030	-1.0371710
H = -1079.148363 a.u.				H	-3.8351090	-2.4548160	-1.9286120
G = -1079.216421 a.u.				H	-3.3586060	-3.4344830	-0.5531760
C	2.9602920	-0.4489490	-0.9621070	N	-2.5776520	1.9481980	-0.9574810
O	2.3159690	0.0717910	-2.1058540	H	-3.2286960	2.0262500	-1.7292270
C	0.1117420	0.4173710	-0.1452290	H	-1.9039580	2.7966110	-0.5604770
C	1.1797180	0.0188910	0.8896970	N	-1.2116580	-0.7922250	2.5595950
C	2.6161630	0.2252270	0.3718980	H	-1.3622800	-1.6591890	3.0533010
H	4.0412190	-0.3113160	-1.0849550	H	-0.5304110	-0.1197830	2.8989530
H	1.0608130	-1.0352500	1.1589370	O	-0.8543260	3.4270480	0.0216240
H	3.2771900	-0.2227320	1.1169400	H	-0.0810870	2.5316520	-0.4056410
O	2.9285400	1.6080710	0.3669780	H	-0.6248970	4.3155240	-0.2543400

TS6'_8_{H2O}

H = -1079.144766 a.u.

G = -1079.212374 a.u.

C 3.0897160 -0.1268000 -0.9873990
O 4.0995830 -0.7309630 -1.7838740
C -0.1326930 0.0430330 -0.5146940
C 0.8319170 -0.9239800 0.1949520
C 2.0938990 -1.2390170 -0.6118790
H 2.5808950 0.6190620 -1.5949490
H 0.3369650 -1.8939330 0.3112530
H 1.7727460 -1.6740040 -1.5639900
O 2.8092510 -2.2722810 0.0677730
H 2.7749390 -2.0586600 1.0078010
O 1.1560750 -0.5095270 1.5174330
H 1.5847960 0.3676050 1.4586660
C 3.8042840 0.5705310 0.1695590
H 4.6141270 1.1544610 -0.2742160
H 4.2461990 -0.1757880 0.8436010
O 2.9072760 1.4220630 0.8769910
H 3.4002130 1.9774190 1.4848900
O 0.4506570 1.1952610 -0.9213150
H 4.3362670 -1.5594360 -1.3503350
H -0.5690220 -0.5067250 -1.3684750
C -3.6389970 -0.6724500 -0.5511400
N -3.4143590 0.6026990 -0.8604270
C -2.3684500 1.1763430 -0.2544750
C -1.3583990 0.3599680 0.4907750
C -2.0102620 -0.8796290 1.0034820
N -3.0615690 -1.4167780 0.4350750
H -0.9219400 0.9429820 1.3033950

N -4.5950370 -1.3049230 -1.2421630
H -5.0954750 -0.8050500 -1.9578060
H -4.8351190 -2.2506410 -0.9978060
N -2.1721890 2.4623000 -0.3368270
H -2.8117740 2.9864940 -0.9179400
H -1.2736930 2.8792970 0.1019040
N -1.4706320 -1.4640490 2.0716850
H -1.8474800 -2.3498250 2.3732950
H -0.5604660 -1.1507250 2.3964440
O 0.1088750 2.8761400 0.7430080
H 0.4200710 2.0394310 -0.0993810
H 0.7243910 3.6097560 0.7370400

INT8_{H2O}

H = -1079.150188 a.u.

H = -1079.223530 a.u.

C -2.8329670 -0.8737450 0.3869230
O -2.1872650 -2.1084890 0.5279600
C -0.1544630 0.5842820 0.3321660
C -0.7884270 -0.0491850 -0.9209430
C -2.3115360 -0.0757810 -0.8223500
H -2.7197720 -0.2433820 1.2815860
H -0.4361630 -1.0760060 -1.0112540
H -2.6938240 -0.5253630 -1.7480360
O -2.7262780 1.2934310 -0.7497790
H -3.6875740 1.2992120 -0.6447870
O -0.3859920 0.6174500 -2.0990870
H -0.8679450 1.4506110 -2.1420050
C -4.3087870 -1.2046830 0.2198990
H -4.6780310 -1.6708060 1.1370710
H -4.4092770 -1.9144770 -0.6082480

O	-5.0122360	0.0066960	-0.0595960	C	1.0276700	-0.5969730	-0.9627100
H	-5.9411160	-0.1839850	-0.2028040	C	2.4888780	-0.3372790	-0.6282930
O	-0.3408100	2.0074990	0.3279050	H	2.4975130	0.9686720	1.0801390
H	-1.2665660	-1.9895810	0.8520180	H	0.6821540	0.1726530	-1.6529490
H	-0.6392280	0.1736690	1.2195720	H	3.0751770	-0.4292300	-1.5513070
C	3.5975480	-1.0486910	-0.2642670	O	2.8683870	-1.3852440	0.2796130
N	2.7687460	-1.7713290	0.4507820	H	3.7886450	-1.2211490	0.5304430
C	1.5393710	-1.2402910	0.7147430	O	0.8806590	-1.8497530	-1.6111020
C	1.3323150	0.2579060	0.5130490	H	1.4735490	-2.4746530	-1.1781680
C	2.3121260	0.8137200	-0.4986720	C	4.1856580	1.4433810	-0.1332520
N	3.4021550	0.1866530	-0.8351880	H	4.3755990	2.3583000	0.4333350
H	1.6401590	0.7305380	1.4592780	H	4.3982750	1.6259500	-1.1920810
N	4.8170620	-1.5632600	-0.5187020	O	4.9712000	0.3557590	0.3634500
H	5.0290610	-2.4934880	-0.2016700	H	5.9038160	0.5525170	0.2581140
H	5.4406620	-1.0627550	-1.1272260	O	0.3215240	-1.7720350	1.0617630
N	0.5630640	-1.9388420	1.1747350	H	1.0622830	2.1130430	-0.1796450
H	0.8914180	-2.8959630	1.3044240	H	0.5925980	0.2755410	0.9434730
H	0.8188450	3.0685360	3.3689920	C	-3.7079600	0.8559000	-0.2826500
N	2.1101360	2.0469250	-0.9601330	N	-2.8326530	1.7306800	0.1753770
H	1.2373800	2.5178400	-0.7739750	C	-1.5357540	1.3106160	0.2952080
H	2.7799460	2.4189560	-1.6146960	C	-1.2708650	-0.1207000	0.1647730
O	1.1950200	2.6648460	2.5852020	C	-2.2664130	-0.8768540	-0.5062660
H	-1.2813130	2.1566890	0.1391820	N	-3.4980090	-0.4191570	-0.6928860
H	0.5045990	2.6860860	1.9080030	H	-1.7256270	-0.7033950	1.7333900
TS8_9_{H2O}				N	-4.9941500	1.2862390	-0.4184850
H = -1079.110982 a.u.				H	-5.2385440	2.1713860	-0.0100780
G = -1079.179539 a.u.				H	-5.7048100	0.6010410	-0.6056000
C	2.7227060	1.0532090	0.0063850	N	-0.5509720	2.1382770	0.5429330
O	1.9654990	2.0516730	-0.6052680	H	-0.9398000	3.0728680	0.6451890
C	0.1679130	-0.4988890	0.3061820	H	-1.2955330	-0.7322560	3.3116000

N -2.0223280 -2.1644800 -0.8939550
H -1.0738920 -2.3889830 -1.1685120
H -2.7584410 -2.5616770 -1.4587270
O -1.4457860 -1.3046030 2.5498320
H 1.2784250 -1.8947640 1.2130460
H -0.4674650 -1.6676050 1.9948890

INT9_{H2O}

H = -1079.144002 a.u.

G = -1079.218854 a.u.

C 2.3918160 -1.4257910 -0.6223940
O 1.5802440 -2.5492730 -0.3261050
C 0.0112780 0.2956680 -0.0109180
C 0.9841380 -0.1464290 1.0645850
C 2.3859970 -0.3692350 0.5023750
H 2.0609030 -0.9317440 -1.5443650
H 0.6561030 -1.1133360 1.4560880
H 3.0104900 -0.7152480 1.3372040
O 2.8796670 0.8610710 0.0004000
H 3.7477380 0.6841670 -0.3844540
O 0.9835470 0.7322670 2.1720070
H 1.1180230 1.6552450 1.8400040
C 3.7845710 -1.9997220 -0.8379040
H 3.7744770 -2.6511390 -1.7160080
H 4.0488220 -2.5939150 0.0440880
O 4.6885010 -0.9139480 -1.0122130
H 5.5855680 -1.2441970 -1.0901220
O 1.4311480 3.0570060 0.9685160
H 0.6708070 -2.3570740 -0.5717980
H 0.4282100 0.7227260 -0.9213550
C -3.7165580 -0.9676930 -0.3146620

N -3.3067080 -0.2404380 -1.3264170
C -2.1749490 0.5082160 -1.1399530
C -1.3238620 0.1806810 0.0458960
C -2.0862980 -0.4085970 1.1729750
N -3.2317660 -1.0033140 0.9723000
H -0.7534660 4.3360950 -1.2732290
N -4.7843000 -1.7712990 -0.5063080
H -5.2834980 -1.7046220 -1.3770860
H -5.2045660 -2.2124670 0.2934300
N -1.7880750 1.4233340 -1.9528980
H -2.4401370 1.4666480 -2.7352920
H -0.7686390 2.7906900 -1.4850190
N -1.5946190 -0.3313320 2.4115950
H -0.7535710 0.2061620 2.6215410
H -2.1549000 -0.7229320 3.1530830
O -0.2259330 3.5457970 -1.1471480
H 2.1715970 2.6687640 0.4856740
H 0.7901240 3.3115750 0.2760520

INT10_{H2O}

H = -1002.722401 a.u.

G = -1002.790933 a.u.

C 2.4114500 0.3723550 -0.4347020
O 1.4350480 0.6917000 -1.4107450
C -0.1405240 0.0047100 0.9627110
C 0.8853230 -1.0992340 1.0501170
C 2.0898030 -1.0453440 0.0506180
H 2.3713320 1.0822480 0.4007550
H 0.3855680 -2.0641530 0.8920450
H 1.8231310 -1.6267920 -0.8382540
O 3.1666630 -1.7074370 0.6885060

H	3.9647100	-1.1637250	0.6240570	C	2.5516480	0.4538380	-0.2923390
O	1.3683600	-1.0132430	2.3727790	O	1.4516950	0.9752330	-0.9498040
H	2.2104060	-1.4868490	2.3791880	C	-0.0519120	0.1162160	0.6823340
C	3.7748350	0.4849970	-1.1075470	C	0.9373880	-0.9680970	1.0186960
H	3.8464900	1.4738530	-1.5681910	C	2.1731060	-0.9829310	0.0872030
H	3.8604440	-0.2785190	-1.8905470	H	2.7983980	1.0075680	0.6296980
O	4.7844140	0.3121180	-0.1134140	H	0.4576160	-1.9533590	0.9774520
H	5.6533720	0.3846820	-0.5143960	H	1.9167000	-1.4988450	-0.8509170
H	1.0094000	1.5306720	-1.1349720	O	3.1609610	-1.7171070	0.7811190
H	0.0086600	0.7756800	1.7160780	H	4.0260340	-1.4103440	0.4733830
C	-3.8236140	-0.4449880	-0.1749450	O	1.3461190	-0.6916980	2.3408150
N	-3.6044680	0.6757240	0.4691640	H	2.2051590	-1.1231170	2.4457070
C	-2.3040650	1.1074780	0.5405600	C	3.7592640	0.4955460	-1.2238360
C	-1.2586330	0.0930100	0.2325930	H	3.9651350	1.5385630	-1.4798390
C	-1.6872430	-0.8659770	-0.7950650	H	3.5131700	-0.0524810	-2.1410500
N	-2.9409440	-1.1690630	-0.9568230	O	4.8829390	-0.0964950	-0.5630800
N	-5.0715710	-0.9554300	-0.1649090	H	5.6546380	-0.0574490	-1.1313170
H	-5.8050790	-0.4298420	0.2792900	H	1.0904960	2.0224640	-0.5120390
H	-5.2849040	-1.7290400	-0.7701300	H	0.1704730	1.0343020	1.2202160
N	-1.9497760	2.2900060	0.8923750	C	-3.9039130	-0.3953680	-0.1886450
H	-2.7741230	2.8368980	1.1360470	N	-3.5670920	0.8407270	0.1647830
N	-0.7316160	-1.4100230	-1.5721650	C	-2.2541080	1.1139030	0.2242980
H	-1.0560670	-1.9748460	-2.3441140	C	-1.2788900	0.0247450	0.1032510
H	0.1098440	-0.8527050	-1.7052270	C	-1.8085490	-1.1491790	-0.5672850
O	0.4863010	2.8788230	-0.1781850	N	-3.0970800	-1.3775080	-0.6716260
H	0.5447830	3.8003210	-0.4363650	N	-5.2075860	-0.7113250	-0.1303580
H	-0.3896130	2.7658950	0.2836700	H	-5.8695400	-0.0079090	0.1497980
TS10_11_{H2O}				H	-5.5110410	-1.6103930	-0.4627110
H = -1002.717118 a.u.				N	-1.8543090	2.3452730	0.4309960
G = -1002.783380 a.u.				H	-2.5989000	3.0166260	0.5612210

N -0.9526390 -2.0407100 -1.0958990
H -1.3535270 -2.8026770 -1.6221050
H -0.0189970 -1.7367020 -1.3274520
O 0.5996390 2.9691830 0.0432980
H 0.8429960 3.7936260 -0.3790310
H -0.8128960 2.6799730 0.2828680

INT11_{H2O}

H = -1002.758353 a.u.

G = -1002.826288 a.u.

C 2.4242470 0.2992740 -0.3818070
O 1.0859190 0.5147010 -0.8002410
C 0.2594940 0.4568820 0.4048580
C 1.0148290 -0.4929410 1.3757340
C 2.2964210 -0.8613310 0.6060160
H 2.8158630 1.1791750 0.1483150
H 0.4217490 -1.3777160 1.6188510
H 2.1319520 -1.7923770 0.0484400
O 3.3743890 -0.9965330 1.4980500
H 4.1853930 -1.0075010 0.9764150
O 1.3209520 0.2425460 2.5380250
H 2.1465520 -0.1094220 2.8921360
C 3.2817030 -0.0222580 -1.5860130
H 3.3970380 0.8558520 -2.2290800
H 2.8020210 -0.8250840 -2.1597950
O 4.5340250 -0.4475610 -1.0614910
H 5.1456840 -0.6279500 -1.7779790
H 0.5607390 2.2609780 -1.2673910
H 0.3038070 1.4385920 0.8831450
C -3.6930190 -0.7028810 -0.1861580
N -3.5087780 0.5509650 0.2221300

C -2.2393520 0.9632300 0.3295830
C -1.1507550 0.1088960 0.0652770
C -1.4986950 -1.1367680 -0.4742970
N -2.7550820 -1.5609050 -0.6013170
N -4.9786870 -1.1616570 -0.1913500
H -5.7071730 -0.4715090 -0.1184530
H -5.1607460 -1.9998680 -0.7170120
N -2.0608360 2.2517090 0.7472530
H -2.9203510 2.7780490 0.7906330
N -0.5114390 -2.0128440 -0.8796960
H -0.8799530 -2.8087530 -1.3811330
H 0.2838750 -1.5706290 -1.3189910
O 0.2217790 3.1400780 -1.0367760
H -0.0277950 3.5568250 -1.8635660
H -1.2606440 2.7519930 0.3766270

INT6_{2H2O}

H = -1155.572908 a.u.

G = -1155.654761 a.u.

C 2.6049790 1.6772350 0.2217800
O 2.5339080 2.4252960 -0.9921010
C -0.1078330 1.3231310 -1.2320550
C 0.1007830 0.9975770 0.2348670
C 1.2388210 1.8098710 0.8848990
H 3.3332730 2.1364520 0.9004130
H 0.3756050 -0.0570180 0.2924870
H 1.3173840 1.4319140 1.9054830
O 0.8570030 3.1678280 0.9784750
H 1.0920660 3.5905870 0.1433190
O -1.0780460 1.1667420 0.9704200
H -1.1985190 2.1119510 1.1351700

C	3.0040210	0.2327620	-0.0688620	TS6_7_{2H2O}
H	4.0280410	0.2230840	-0.4657030	H = -1155.559563 a.u.
H	2.3550200	-0.1701680	-0.8535230	G = -1155.637551 a.u.
O	2.9292810	-0.5348980	1.1108280	C 3.0992600 -0.6105640 -0.8263920
H	2.4324410	-1.3485030	0.9167020	O 2.4731030 -0.5481370 -2.0940740
O	-1.0687780	1.9336260	-1.6363270	C 0.1490600 0.3967920 -0.4801410
H	3.4182910	2.6055400	-1.3191030	C 1.1693400 0.2843450 0.6605090
H	0.6640750	0.9697180	-1.9337480	C 2.5982480 0.4892720 0.1230700
C	0.7208610	-2.3714370	-0.9455800	H 4.1808220 -0.4570620 -0.9325870
N	-0.4027730	-1.9890490	-1.5394990	H 1.1306390 -0.7143350 1.0976830
C	-1.4539350	-1.7668460	-0.7226790	H 3.2490200 0.4976790 1.0003640
C	-1.3758560	-1.9644570	0.6616080	O 2.7436770 1.7482980 -0.5143060
C	-0.1285600	-2.3006390	1.1637790	H 1.9337960 1.8925630 -1.0283240
N	0.9453650	-2.5002120	0.3672590	O 0.9024560 1.1819840 1.7216990
H	-2.2210860	-1.7430360	1.2986360	H 0.9004950 2.0967310 1.3959970
N	1.8091910	-2.5846090	-1.7654720	C 2.8495390 -2.0212200 -0.3213690
H	1.5750320	-2.7423910	-2.7336290	H 3.3798440 -2.7253020 -0.9703510
H	2.5188200	-3.1896550	-1.3812810	H 1.7760030 -2.2417600 -0.3855830
N	-2.5973030	-1.3430290	-1.3030620	O 3.3155790 -2.0903330 1.0163350
H	-2.5345660	-1.0620530	-2.2682530	H 3.2639280 -2.9983690 1.3202860
H	-3.3123040	-0.9283830	-0.7120840	O 0.0689120 1.5113290 -1.0990660
N	0.0933590	-2.4422320	2.5073170	H 2.6617300 0.3145420 -2.4756900
H	1.0591810	-2.4414090	2.7976370	H 0.0779920 -0.5217860 -1.0821430
H	-0.5537200	-1.9861070	3.1300600	C -2.3017930 -2.2769920 -0.3037920
O	-4.1257540	0.0107450	0.7597460	N -2.7315070 -1.2690840 -1.0659670
H	-3.7850920	0.9147450	0.6389040	C -2.4359970 -0.0430720 -0.6208260
H	-5.0478160	0.1119710	1.0023830	C -1.5634360 0.1669970 0.5024880
O	-3.2661640	2.6005740	-0.0006560	C -1.4241840 -0.9924870 1.3390550
H	-2.5267770	2.3636110	-0.5890540	N -1.7060460 -2.2138400 0.9070240
H	-3.7955070	3.2405880	-0.4802360	H -1.5780100 1.1404640 0.9773310

N	-2.5042740	-3.5210370	-0.7846740	C	2.6207420	-2.2030060	-0.7360180
H	-3.0398700	-3.6300940	-1.6287020	H	3.0257730	-2.7553900	-1.5898810
H	-2.3198730	-4.3072050	-0.1860070	H	1.5324100	-2.3402610	-0.7303630
N	-2.9038670	1.0037140	-1.2873740	O	3.1941630	-2.6394390	0.4888410
H	-3.3957050	0.8371450	-2.1506730	H	3.1721660	-3.5972270	0.5243280
H	-2.7068150	1.9503450	-0.9702740	O	0.3677260	1.2610440	-1.0398890
N	-0.9441420	-0.8543390	2.5892970	H	1.6173390	0.3193100	-1.9446060
H	-0.6977600	-1.7021530	3.0765370	H	0.0761030	-0.7495600	-0.8443380
H	-0.4415650	-0.0019160	2.8110670	C	-2.6993460	-1.9172470	-0.2879380
O	-2.4844390	3.4875980	0.1298690	N	-2.8756230	-0.8655050	-1.0926070
H	-1.5746920	3.7831460	0.3150690	C	-2.3236320	0.2749540	-0.6860350
H	-3.0603950	3.9280770	0.7563920	C	-1.3395090	0.3127360	0.4311400
O	0.2161990	3.6289390	0.3796400	C	-1.5986730	-0.8259760	1.3600580
H	0.1747990	2.8809730	-0.2878160	N	-2.1816910	-1.9363390	0.9669800
H	0.8903490	4.2445800	0.0828850	H	-1.3385260	1.2734700	0.9476650
INT7_{2H2O}				N	-3.1384190	-3.0968890	-0.7397130
H = -1155.568647 a.u.				H	-3.5671020	-3.1461750	-1.6488220
G = -1155.644218 a.u.				H	-3.0746870	-3.9064010	-0.1458810
C	2.9643780	-0.7280770	-0.9227440	N	-2.5958160	1.3830200	-1.3291940
O	2.3802680	-0.2663670	-2.1238350	H	-3.1784740	1.3184910	-2.1514550
C	0.1279850	0.1840450	-0.2542650	H	-2.2196950	2.2904970	-1.0328780
C	1.1904280	-0.0247780	0.8491300	N	-1.1785270	-0.7170500	2.6162200
C	2.6308650	0.1210170	0.3129490	H	-1.2493520	-1.5341770	3.2044810
H	4.0505480	-0.6522970	-1.0451980	H	-0.5059060	0.0164290	2.8362280
H	1.1031080	-1.0385280	1.2547850	O	0.6036400	3.2413860	0.4497860
H	3.2846040	-0.2126030	1.1211580	H	0.5477960	2.4494080	-0.2420010
O	2.9715670	1.4743040	0.0763690	H	1.4400870	3.6936970	0.3161390
H	2.5366510	1.7250790	-0.7471170	O	-1.8565040	3.8610770	-0.2370640
O	0.9975520	0.8550170	1.9474970	H	-0.9194730	3.8472780	0.0666840
H	1.1010280	1.7691130	1.6267200	H	-2.3505790	4.4009970	0.3812540

TS7_8₂H₂O

H = -1155.567548 a.u.

G = -1155.639216 a.u.

C 3.0599120 -0.6300420 -0.8717920
O 2.5336770 -0.2327850 -2.1243990
C 0.1031300 0.1522750 -0.2612070
C 1.2012880 0.0768010 0.8224680
C 2.6430430 0.2688120 0.3001760
H 4.1473380 -0.5307630 -0.9502090
H 1.1695390 -0.9283480 1.2583000
H 3.2783450 0.0011880 1.1468140
O 2.9367860 1.6206980 0.0174990
H 2.6271260 1.8191450 -0.8719540
O 0.9554900 0.9773610 1.8837050
H 0.9011310 1.8862700 1.5066500
C 2.7435830 -2.1038070 -0.6353300
H 3.2054260 -2.6826960 -1.4412230
H 1.6601720 -2.2730980 -0.6784010
O 3.2632470 -2.4657540 0.6351810
H 3.2705870 -3.4212460 0.7151060
O 0.3072470 1.1803050 -1.1871880
H 1.7066090 0.2612530 -2.0162010
H 0.1057400 -0.7854250 -0.8287770
C -2.6171970 -1.9695370 -0.3211560
N -2.8408550 -0.9274690 -1.1117530
C -2.3676840 0.2513010 -0.6769420
C -1.3204020 0.2918100 0.4022660
C -1.5519950 -0.8593580 1.3429320
N -2.1109740 -1.9749260 0.9499570
H -1.3459450 1.2476770 0.9280570

N -2.9820970 -3.1746980 -0.7766500
H -3.4194720 -3.2451130 -1.6803120
H -2.9049550 -3.9732670 -0.1699740
N -2.7575820 1.3710150 -1.2017750
H -3.4123310 1.2856720 -1.9700670
H -2.4357650 2.3749260 -0.7833340
N -1.1298080 -0.7245620 2.5958410
H -1.1864850 -1.5297390 3.2018320
H -0.4876870 0.0388110 2.8078950
O 0.3006610 3.1610080 0.4292570
H 0.3684190 2.0492880 -0.6696920
H 0.9053370 3.8987990 0.3286730
O -1.9719070 3.5335210 -0.1842880
H -0.8377450 3.4608040 0.1684100
H -2.5298470 3.9959830 0.4424470

INT8₂H₂O

H = -1155.564666 a.u.

G = -1155.643763 a.u.

C 3.1445060 -0.8305920 -0.4724640
O 2.6429070 -2.1261840 -0.3091870
C 0.3437330 0.4572970 -0.2503370
C 1.1929650 0.0362330 0.9713210
C 2.6860070 0.1058060 0.6577550
H 2.8405240 -0.3872350 -1.4318040
H 0.9371590 -0.9851030 1.2542680
H 3.2248210 -0.1593220 1.5776280
O 2.9382720 1.4778140 0.3327170
H 3.8697350 1.5494710 0.0814540
O 0.9246480 0.8624450 2.0934980
H 1.4844580 1.6431670 2.0090950

C 4.6599000 -0.9756810 -0.4710850
 H 4.9627120 -1.5573660 -1.3454030
 H 4.9510940 -1.5159870 0.4361740
 O 5.2409950 0.3290060 -0.4946350
 H 6.1972970 0.2594510 -0.4745600
 O 0.3070610 1.8831070 -0.3582070
 H 1.6911280 -2.1456670 -0.5624310
 H 0.8088930 0.0489750 -1.1496630
 C -3.2919260 -1.5290160 0.2859550
 N -2.3707850 -2.1851160 -0.3750640
 C -1.1493660 -1.5852510 -0.4985330
 C -1.0866930 -0.0793160 -0.2850920
 C -2.0691390 0.3198580 0.7934600
 N -3.1630960 -0.3567160 0.9992710
 H -1.5646220 0.3413870 -1.1866140
 N -4.5301110 -2.0575770 0.3470750
 H -4.6951310 -2.9552630 -0.0753480
 H -5.2106730 -1.6393030 0.9568570
 N -0.0906040 -2.2193210 -0.8530390
 H -0.3443870 -3.1938870 -1.0180330
 H -4.2191170 1.0881100 -0.7825730
 N -1.8825140 1.4641340 1.4478780
 H -2.5539820 1.7064810 2.1604640
 H -0.9749900 1.9057290 1.4419880
 O -3.7574350 1.2916590 -1.6000300
 H 1.2301140 2.1780420 -0.3661720
 H -3.2667880 2.1095290 -1.4227500
 O -1.9083600 3.3937060 -1.2210480
 H -1.0985270 2.9241960 -0.9630960
 H -1.6945550 3.8583170 -2.0330880

TS8_9₂H₂O

H = -1155.536553 a.u.

G = -1155.610692 a.u.

C 2.8457950 1.0345210 0.2631420
 O 2.1390090 2.2114780 0.0216010
 C 0.2463860 -0.5058490 0.0185730
 C 1.1232750 -0.1590650 -1.1998300
 C 2.5904860 -0.0360020 -0.8185740
 H 2.5903570 0.5900510 1.2376790
 H 0.7792200 0.8008430 -1.5854270
 H 3.1591470 0.2157350 -1.7234900
 O 2.9791480 -1.3413780 -0.3623900
 H 3.8978850 -1.2781180 -0.0652600
 O 0.9659890 -1.1179320 -2.2358610
 H 1.6116620 -1.8179220 -2.0861150
 C 4.3200430 1.4090340 0.2913720
 H 4.5099330 2.0743220 1.1374260
 H 4.5602990 1.9348610 -0.6388120
 O 5.0810680 0.2027340 0.4053860
 H 6.0171280 0.4035070 0.3489310
 O 0.3954030 -1.9271150 0.3306350
 H 1.1919850 2.1335970 0.3386370
 H 0.6300440 0.0499510 0.8762080
 C -3.6079880 0.9876010 -0.4208500
 N -2.7475990 1.7271140 0.2622770
 C -1.4537000 1.2769070 0.3255810
 C -1.1841690 -0.0856980 -0.1112070
 C -2.1597180 -0.6793720 -0.9391350
 N -3.3883380 -0.1728090 -1.0707990
 H -2.1385190 -0.5651140 1.3386500

N	-4.8817610	1.4711420	-0.5253600	C	4.4710330	-1.5449620	-0.5422700
H	-5.1329070	2.2453230	0.0646690	H	4.6307070	-2.3222220	-1.2946040
H	-5.5935920	0.8382230	-0.8467030	H	4.8251310	-1.9099310	0.4284640
N	-0.4877340	2.0115200	0.8278090	O	5.1272430	-0.3349810	-0.9036280
H	-0.8850890	2.9040270	1.1124320	H	6.0766890	-0.4699640	-0.9198410
H	-2.5589890	0.0035880	2.7513710	O	1.0854650	3.1647670	0.5002680
N	-1.9260870	-1.8657450	-1.5777490	H	1.5032950	-2.5252120	-0.2150500
H	-2.6356610	-2.0981600	-2.2566770	H	0.6688920	0.3299290	-1.0972520
H	-0.9699730	-2.0428090	-1.8549040	C	-3.3855370	-1.4931900	-0.2083310
O	-2.4344900	-0.8300980	2.2811890	N	-2.9822000	-0.9720840	-1.3437270
H	1.3473490	-2.1190290	0.2495850	C	-1.8509550	-0.1889980	-1.3131770
H	-1.4705870	-1.5340140	2.5869560	C	-1.0304880	-0.2001580	-0.0605500
O	-0.5304170	-2.2275400	2.5926930	C	-1.7840260	-0.6009180	1.1483580
H	-0.0943950	-2.1656020	1.6197230	N	-2.9109620	-1.2638160	1.0604800
H	0.1172040	-1.9854820	3.2614220	H	-3.8979170	1.3912700	0.8795460
INT9_{2H2O}				N	-4.4613690	-2.3084290	-0.2374430
H = -1155.556625 a.u.				H	-4.8558270	-2.5639490	-1.1263180
G = -1155.637815 a.u.				H	-4.7731230	-2.7395750	0.6151170
C	2.9811160	-1.2580260	-0.4246550	N	-1.4570260	0.5240200	-2.3032610
O	2.4183870	-2.4609930	0.0711300	H	-2.0872620	0.3746590	-3.0908060
C	0.2852820	0.0547930	-0.1163690	H	-3.9111720	1.2325130	-0.6430380
C	1.2827660	-0.0259080	1.0228840	N	-1.3160660	-0.2821730	2.3550820
C	2.7154050	-0.0498790	0.4964680	H	-1.8673280	-0.5696870	3.1495820
H	2.5830720	-1.0157070	-1.4176020	H	-0.5117900	0.3398980	2.4713980
H	1.1273720	-0.9674980	1.5590570	O	-3.6135770	1.8150120	0.0650460
H	3.3742430	-0.1029060	1.3736570	H	1.7917870	2.8559800	-0.0791670
O	2.9467860	1.1527090	-0.2183230	H	-1.9906330	2.8777500	-0.5096010
H	3.8482920	1.1109770	-0.5629550	O	-1.1850630	3.0707040	-1.0088540
O	1.0966310	0.9947660	1.9821940	H	0.2747300	3.2255800	-0.0484650
H	1.0898870	1.8748320	1.5174950	H	-1.1202270	2.3182380	-1.6243430

INT10₂H₂O

H = -1079.139150 a.u.

G = -1079.214983 a.u.

C	2.3302900	-0.3430270	-0.8525060
O	1.3076890	0.3290660	-1.5391030
C	-0.1275690	0.6955680	0.7900340
C	1.1366990	0.1319860	1.3677920
C	1.8234190	-0.9205600	0.4827260
H	3.1708250	0.3272370	-0.6319160
H	0.9619900	-0.3559820	2.3321250
H	1.1090120	-1.7300020	0.2836820
O	2.8993450	-1.3744310	1.2892490
H	3.4835020	-1.9025520	0.7279500
O	2.0271500	1.2160440	1.6028390
H	2.8591470	0.8180610	1.8899300
C	2.8051210	-1.4489570	-1.7879090
H	3.2250910	-0.9882920	-2.6858740
H	1.9364440	-2.0534210	-2.0720280
O	3.7814180	-2.2450880	-1.1165290
H	4.0720590	-2.9576240	-1.6887950
H	1.4565520	1.2911890	-1.4375350
H	-0.0141350	1.7106910	0.4233980
C	-3.4398620	-1.0951810	-0.5411220
N	-3.3681410	0.1840730	-0.7798210
C	-2.3854060	0.9019020	-0.1409340
C	-1.3386650	0.1418770	0.6181860
C	-1.7364590	-1.2361480	0.9633250
N	-2.7285700	-1.8378090	0.3837030
N	-4.3406820	-1.8298850	-1.2251600
H	-4.9631730	-1.3627320	-1.8620150

H	-4.4838000	-2.7911980	-0.9703080
N	-2.3242040	2.1813840	-0.2187800
H	-3.0849340	2.4972180	-0.8194470
N	-1.0452450	-1.9370550	1.8952020
H	-1.4475260	-2.8271160	2.1498500
H	-0.5135330	-1.4572680	2.6000610
O	-0.3772220	4.1242490	-0.0056710
H	-0.5575980	4.7552760	0.6924730
H	-1.1207360	3.4733160	-0.0087920
O	1.9586990	2.8536910	-0.7571270
H	2.1635380	2.5662670	0.1428580
H	1.2131400	3.4689620	-0.6384220

TS10_11₂H₂O

H = -1079.129560 a.u.

G = -1079.201757 a.u.

C	2.4666630	-0.1613760	-0.6698600
O	1.5114170	0.7322920	-1.1146150
C	-0.0886510	0.4815470	0.7784460
C	1.0430120	-0.2747880	1.3925350
C	1.8123890	-1.1080270	0.3485460
H	3.3073040	0.3430800	-0.1672920
H	0.6566310	-0.9527430	2.1673930
H	1.1156050	-1.7456690	-0.2146690
O	2.7211460	-1.8882890	1.1013780
H	3.3899300	-2.2177700	0.4841570
O	1.9074450	0.6498360	2.0126850
H	2.6880190	0.1521630	2.2851030
C	3.0153450	-0.9447920	-1.8568190
H	3.5438260	-0.2546910	-2.5194540
H	2.1742070	-1.3892680	-2.4007820

O	3.8959800	-1.9623920	-1.3666050	C	1.4393170	-0.3523610	1.3585720
H	4.2868240	-2.4387870	-2.1011940	C	1.5663670	-1.5335110	0.4027530
H	1.8406790	1.7639990	-0.7818490	H	2.6710490	-0.7167830	-1.2606750
H	0.0921310	1.5517520	0.7532960	H	1.0756020	-0.6229380	2.3477570
C	-3.7970640	-0.7397170	-0.4076430	H	0.6797240	-2.1680600	0.4788200
N	-3.5063460	0.5417370	-0.5832990	O	2.7350490	-2.2654830	0.7044550
C	-2.2886150	0.9523190	-0.2037230	H	2.8432620	-2.9297550	0.0148470
C	-1.3067120	0.0149960	0.3817400	O	2.7050760	0.2793730	1.4937770
C	-1.7966880	-1.3653920	0.4773150	H	3.3613940	-0.4289100	1.5350160
N	-3.0099420	-1.7130310	0.1017770	C	0.8664030	-1.6016210	-2.0190250
N	-5.0233700	-1.1387130	-0.7792440	H	0.9453600	-1.1098740	-2.9929890
H	-5.6579460	-0.4676110	-1.1775320	H	-0.1899740	-1.6669990	-1.7317310
H	-5.2833050	-2.1036060	-0.6694670	O	1.4869970	-2.8843170	-2.0293540
N	-2.0168220	2.2239420	-0.3852870	H	1.0269270	-3.4630300	-2.6402700
H	-2.7802970	2.7437690	-0.7962230	H	2.5096700	1.7772570	-0.9558040
N	-1.0682290	-2.3682680	0.9955550	H	0.7265670	1.6178080	0.8807410
H	-1.5152070	-3.2723910	1.0029670	C	-3.5510250	-0.1388730	-0.1068750
H	-0.0914390	-2.3172300	1.2154580	N	-3.0121850	0.9624620	-0.6188480
O	0.0019790	3.7148650	0.3112660	C	-1.7337610	1.2015440	-0.2991230
H	-0.0782020	4.6690790	0.2919510	C	-0.9650010	0.3233010	0.5215530
H	-1.1471130	2.7851960	-0.1168520	C	-1.7086990	-0.7200260	1.0861730
O	2.1873950	2.8883910	-0.2841170	N	-2.9860890	-0.9676890	0.7683580
H	2.6340140	2.7056690	0.5467290	N	-4.8168710	-0.4534030	-0.5204950
H	1.0363200	3.4191540	0.0285940	H	-5.3383940	0.2901410	-0.9550010
INT11₂H₂O				H	-5.3227400	-1.1086610	0.0520910
H = -1079.164560 a.u.				N	-1.2119720	2.3259900	-0.8311850
G = -1079.239098 a.u.				H	-1.8694530	2.9120310	-1.3195750
C	1.6214270	-0.8239520	-0.9605010	N	-1.1920940	-1.6325400	2.0020850
O	1.0653170	0.4724730	-0.7771990	H	-1.9343270	-2.2208540	2.3575930
C	0.5267870	0.5879000	0.5703560	H	-0.6365240	-1.2413970	2.7461290

O	1.0596090	3.9229130	0.1559390	N	3.2449930	1.1048230	0.6315020
H	1.1300730	4.8786440	0.1628700	C	1.9698440	1.1713610	0.2566350
H	-0.3509690	2.7567010	-0.5119220	C	1.2646530	0.0515910	-0.3930130
O	3.1490740	2.3230630	-0.4732500	C	2.0573510	-1.1882470	-0.3724260
H	3.2816030	1.7952880	0.3270880	N	3.3286940	-1.2188960	0.0094430
H	1.9457550	3.5670640	-0.0526460	H	0.9707060	0.5200140	-1.5625940
TS7_12_{H2O}				N	5.1418990	-0.1307740	0.8442260
H = -1079.102067 a.u.				H	5.5906600	0.7009640	1.1871810
G = -1079.170935 a.u.				H	5.6487660	-0.9917440	0.7329720
C	-3.2083610	-0.0498070	0.8185600	N	1.3685850	2.3393700	0.4534030
O	-3.0720470	1.3588440	0.7185690	H	1.9581100	3.0713320	0.8209130
C	-0.2824320	0.1770850	-0.4443630	H	0.4435590	2.6057960	0.0974360
C	-1.1604670	-1.0803310	-0.4714450	N	1.5500630	-2.3486010	-0.7805420
C	-2.6621580	-0.7508900	-0.4453190	H	2.1932940	-3.1247320	-0.8075720
H	-4.2746900	-0.2998340	0.8790530	H	0.6420980	-2.3979600	-1.2463280
H	-0.9375810	-1.7557230	0.3586900	O	-1.1374100	3.1848860	-0.5226880
H	-3.1696810	-1.7147640	-0.5333690	H	-1.7739840	2.8176520	0.1019950
O	-3.0393650	0.0308650	-1.5695340	H	-1.0195110	2.4800830	-1.1944640
H	-2.2510990	0.5210180	-1.8690760	INT12_{H2O}			
O	-0.9158710	-1.8050020	-1.6741330	H = -1079.167379 a.u.			
H	-0.9163710	-1.1431150	-2.3824040	G = -1079.239471 a.u.			
C	-2.5581280	-0.4810750	2.1195120	C	-3.0363380	-0.0418450	0.9725210
H	-3.0715690	0.0151480	2.9489490	O	-2.9575050	1.3505500	0.6886180
H	-1.5049140	-0.1741730	2.1372320	C	-0.2642930	0.1370710	-0.5450170
O	-2.6839730	-1.8918170	2.1926500	C	-1.1141720	-1.1433450	-0.4437370
H	-2.4152730	-2.1901560	3.0636170	C	-2.6147760	-0.8938690	-0.2380380
O	-0.4091120	0.8488390	-1.6926600	H	-4.0782960	-0.2999460	1.1908690
H	-3.4956980	1.5863110	-0.1198090	H	-0.7494330	-1.7535630	0.3863640
H	-0.6201830	0.7979790	0.3951390	H	-3.0665640	-1.8803030	-0.1119810
C	3.8506900	-0.0761000	0.4766240	O	-3.1921770	-0.3505920	-1.4215640

H -2.6253240 0.3766070 -1.7148990
 O -0.9892700 -1.9232530 -1.6299070
 H -1.7041390 -1.6672850 -2.2251300
 C -2.2203190 -0.3057170 2.2264490
 H -2.6497560 0.2712400 3.0514440
 H -1.1814690 0.0178330 2.0862340
 O -2.2997040 -1.7006740 2.4609920
 H -1.8208020 -1.9169830 3.2638120
 O -0.5801760 0.7862270 -1.8047010
 H -3.6957820 1.5643960 0.1090160
 H -0.6550700 0.8380010 0.1953940
 C 3.8197610 -0.0026780 0.4276690
 N 3.1878330 1.1629420 0.5432950
 C 1.8978160 1.1674740 0.1872780
 C 1.2152970 0.0169180 -0.2882640
 C 2.0273910 -1.1380170 -0.3958800
 N 3.3211700 -1.1427810 -0.0400750
 H -0.0233970 0.3935500 -2.4854420
 N 5.1192170 -0.0341460 0.8496090
 H 5.5756800 0.8550070 0.9668050
 H 5.6721640 -0.8181830 0.5460560
 N 1.2677670 2.3588360 0.3665860
 H 1.8792330 3.1101240 0.6454210
 H 0.4255150 2.6288250 -0.1272610
 N 1.5781050 -2.3503460 -0.8204300
 H 2.3039630 -3.0413660 -0.9241240
 H 0.7469140 -2.4382540 -1.3867080
 O -1.3404470 3.2850960 -0.7506740
 H -1.8348430 2.8146980 -0.0681650
 H -1.2252080 2.6292750 -1.4505960

TS12_13_{H2O}

H = -1079.116628 a.u.

G = -1079.186234 a.u.

C -3.0774420 0.2631230 0.9086330
 O -3.2628920 1.3577930 0.0506170
 C -0.1810540 -0.0922330 -0.2399230
 C -1.0827060 -1.2892930 -0.0114540
 C -2.6019900 -1.0098660 0.1604270
 H -4.0823670 0.0060020 1.2562830
 H -0.7350500 -1.7407130 0.9256340
 H -2.9645480 -1.8713700 0.7254410
 O -3.2501770 -1.0618740 -1.0903810
 H -3.2938440 -0.1548750 -1.4245060
 O -0.9547290 -2.2689950 -1.0220660
 H -1.5467740 -1.9728810 -1.7326510
 C -2.2523190 0.6278470 2.1399490
 H -2.8419080 1.3149730 2.7548080
 H -1.3287830 1.1487420 1.8593120
 O -1.9639680 -0.5768410 2.8367860
 H -1.5936180 -0.3655000 3.6958920
 O -0.9510120 0.3026830 -2.1746120
 H -2.4392670 1.8007520 -0.2807370
 H -0.6318090 0.8561450 0.0102030
 C 3.8292740 0.1365970 0.3745630
 N 3.1779480 1.2944410 0.2424670
 C 1.8866730 1.2187430 -0.0872410
 C 1.2036660 -0.0674190 -0.2250900
 C 2.0960440 -1.2167020 -0.2033900
 N 3.3776970 -1.1027580 0.1254370
 N 5.1091200 0.2186000 0.7823950

H	5.5210670	1.1249260	0.9227790	O	-3.3336270	-1.5057710	1.9858600
H	5.6605640	-0.6201020	0.8373650	H	-3.3097210	-1.7146150	2.9218480
N	1.2419730	2.3652140	-0.2594640	O	-1.1527200	2.1354890	-2.2081440
H	1.8049370	3.1881080	-0.1009540	H	-2.1321620	1.8327990	0.7430770
H	0.2647560	2.4848580	-0.6458720	H	-0.5534850	0.7709110	-0.2673580
N	1.6650280	-2.4473180	-0.4779950	C	3.8950350	0.0485100	0.3251950
H	2.3523850	-3.1824230	-0.4189540	N	3.2719570	1.1841680	0.0897120
H	0.7368570	-2.6224560	-0.8613240	C	1.9396580	1.1317800	-0.1674910
H	-0.2079550	0.2476870	-2.7826780	C	1.2382150	-0.2002130	-0.1621040
O	-1.2298830	2.5008440	-1.2162080	C	2.1400030	-1.3686880	-0.0151820
H	-1.1093150	1.3481580	-1.9208600	N	3.4095450	-1.2281870	0.2689640
H	-1.5872840	3.2590700	-1.6809820	N	5.1995570	0.1154640	0.6474410
INT13_{H2O}				H	5.6547150	1.0121640	0.6530710
H = -1079.138669 a.u.				H	5.7195890	-0.7362240	0.7678100
G = -1079.213400 a.u.				N	1.2489570	2.2044530	-0.4032710
C	-3.1791740	0.1942670	0.3318560	H	1.8906510	2.9958640	-0.3808740
O	-2.7762190	1.5261010	0.0790220	H	0.0138720	2.4359820	0.9415190
C	-0.1046150	-0.2129060	-0.2213070	N	1.6603350	-2.6114340	-0.1192730
C	-1.1129700	-1.3398350	-0.2545110	H	2.3446830	-3.3485470	-0.0370680
C	-2.5214040	-0.8321670	-0.6110560	H	0.7821370	-2.7881590	-0.6035550
H	-4.2505410	0.1477770	0.1161110	H	-0.2993630	2.2520180	-1.7558450
H	-1.1376370	-1.8522390	0.7134490	O	-0.6997630	2.4028510	1.6183160
H	-3.1552500	-1.7217520	-0.5888030	H	-1.8076090	2.4796270	-1.5890960
O	-2.5077710	-0.3921590	-1.9513880	H	-0.6429420	3.2191800	2.1191370
H	-2.0663970	0.4759610	-2.0242090	INT7'_{2H2O}			
O	-0.7884220	-2.3269760	-1.2293550	H = -1155.568857 a.u.			
H	-1.0931300	-1.9714320	-2.0777980	G = -1155.645127 a.u.			
C	-2.9556810	-0.1520210	1.7979530	C	2.8588020	-0.9289090	-0.9209180
H	-3.5581730	0.5237740	2.4144950	O	2.3475820	-0.1939000	-2.0202310
H	-1.8979190	0.0070180	2.0544850	C	0.1733610	0.4577130	0.0041870

C	1.1583070	-0.2774710	0.9345140	N	-1.2859890	-1.1065470	2.4540090
C	2.6051580	-0.2168060	0.4195780	H	-1.6024540	-1.9777060	2.8530050
H	3.9484090	-1.0197380	-1.0147430	H	-0.4576710	-0.6222940	2.8093460
H	0.8834800	-1.3348500	0.9961760	O	0.6885830	2.9327830	2.0297250
H	3.2126160	-0.7199660	1.1762180	H	0.6692740	2.6769260	1.0710070
O	3.0678940	1.1157690	0.3164850	H	1.2788890	3.6836090	2.1158210
H	2.2980830	1.6285710	-0.0031130	O	0.1501840	1.5684300	-3.0083890
O	1.0927720	0.2060280	2.2698530	H	0.6136710	0.7628510	-3.2530850
H	1.2203890	1.1733700	2.2930650	H	0.4246530	1.7174950	-2.0821700
C	2.2484400	-2.3152830	-1.0250730	TS7'_12_{H2O}			
H	2.6116510	-2.7904020	-1.9419810	H = -1155.542271 a.u.			
H	1.1562460	-2.2300880	-1.0971810	G = -1155.616484 a.u.			
O	2.6349510	-3.0428290	0.1293120	C	3.0840520	-0.7072120	-0.8959920
H	2.4072680	-3.9666190	0.0108020	O	2.9987540	0.5747760	-1.4984410
O	0.5694720	1.7357580	-0.2984920	C	0.3675200	0.4200170	0.3190980
H	2.7179200	0.6946660	-1.9598750	C	1.1765460	-0.7488270	0.9061820
H	0.0572770	-0.1570970	-0.9052700	C	2.6787190	-0.6540620	0.5927370
C	-3.3440220	-0.9722750	-0.3493660	H	4.1270010	-1.0455470	-0.9226170
N	-3.1799350	0.2338260	-0.9135990	H	0.8140510	-1.7146720	0.5463120
C	-2.2216170	0.9906970	-0.4071780	H	3.1360620	-1.5144070	1.0875840
C	-1.2954770	0.5351160	0.6783180	O	3.2510160	0.5116510	1.1651310
C	-1.8038270	-0.7321930	1.2945970	H	2.5552070	1.1963460	1.1608760
N	-2.7387870	-1.4811140	0.7460880	O	1.0403520	-0.7685540	2.3266450
H	-1.1929640	1.3007330	1.4523500	H	1.3415470	0.0942500	2.6404120
N	-4.2461850	-1.7691220	-0.9284010	C	2.2630300	-1.6619430	-1.7431620
H	-4.7412530	-1.4391890	-1.7403910	H	2.6898630	-1.6943370	-2.7505670
H	-4.4303560	-2.6759160	-0.5331300	H	1.2285380	-1.3045490	-1.8224300
N	-2.0101550	2.1934090	-0.9083970	O	2.3221950	-2.9283510	-1.1076710
H	-2.4520300	2.4015770	-1.7941290	H	1.9184920	-3.5877540	-1.6752020
H	-1.0819970	2.5810460	-0.7186680	O	0.7843920	1.5971090	0.9666220

H	3.5492930	1.1497300	-0.9515970	C	-0.8497300	-1.2348980	0.6858050
H	0.6454570	0.4809360	-0.7409480	C	-2.3296840	-0.9150010	0.9397660
C	-3.6008500	-0.6072640	-0.6840530	H	-3.6286440	0.4787190	1.8840170
N	-3.0572270	0.4430370	-1.3054890	H	-0.2915570	-1.0324000	1.6022800
C	-1.8676280	0.8419090	-0.8606390	H	-2.6015590	-1.5385790	1.7955680
C	-1.2049150	0.2650920	0.3220890	O	-3.1061350	-1.3666330	-0.1529520
C	-1.9294840	-0.9131580	0.8261140	H	-3.2024950	-0.6318170	-0.7785420
N	-3.1025610	-1.3072960	0.3450080	O	-0.7672960	-2.6361900	0.4628410
H	-1.4901900	1.1267950	1.2175420	H	-1.4777570	-2.8420490	-0.1608530
N	-4.7920140	-1.0198240	-1.1510840	C	-1.6538800	1.2334960	2.1564180
H	-5.2279190	-0.5097010	-1.8998630	H	-2.0263500	2.2275980	2.4272110
H	-5.2604450	-1.7845310	-0.6968260	H	-0.7213310	1.3630660	1.5881770
N	-1.3090870	1.8503880	-1.5176100	O	-1.4474310	0.4268610	3.3042590
H	-1.8485900	2.2361270	-2.2779200	H	-0.7810750	0.8357350	3.8605390
H	-0.4039340	2.2787380	-1.3074780	O	-0.3805190	-1.1597970	-1.7286760
N	-1.4845610	-1.5916060	1.8825390	H	-2.2791230	1.7533430	-0.2355130
H	-2.0754940	-2.3350000	2.2204570	H	-0.7221790	0.4764440	-0.6264560
H	-0.6111710	-1.3531190	2.3493450	C	3.8803220	0.4035930	0.1386880
O	-1.2416030	2.1904270	2.0511940	N	3.0617050	1.4492220	0.0460400
H	-0.1825680	2.0409910	1.6582240	C	1.7712230	1.1755530	-0.1804210
H	-1.3076030	1.9819660	2.9866750	C	1.2768870	-0.1375880	-0.2615760
O	1.3065840	2.9777920	-1.3003780	C	2.2597280	-1.1421170	-0.1770580
H	1.8273190	2.3020120	-1.7489740	N	3.5555100	-0.8835820	0.0066500
H	1.2977740	2.6867020	-0.3656090	N	5.1903380	0.6740250	0.4176980
INT12₂H₂O				H	5.4950540	1.6226600	0.2769130
H = -1155.582174 a.u.				H	5.8488870	-0.0676830	0.2474890
G = -1155.658570 a.u.				N	0.9537020	2.2779310	-0.2811300
C	-2.7043200	0.5385190	1.3036010	H	1.4876850	3.1332020	-0.3423570
O	-3.0365380	1.3033610	0.1623410	H	0.1679820	2.2428990	-0.9216250
C	-0.1793180	-0.4589790	-0.4926280	N	1.9378510	-2.4697490	-0.3608460

H 2.7166940 -3.0827870 -0.1655740
H 1.0405660 -2.7903260 -0.0022420
H 0.3197610 -1.8160230 -1.8328880
O -1.5188870 2.3831280 -1.9378610
H -1.7841240 -0.5940690 -2.6164170
H -1.9071430 3.1979580 -2.2638160
O -2.5394580 0.0060720 -2.7718130
H -1.9566930 1.6487040 -2.4121510
H -3.0476080 -0.3494090 -3.5033330

TS12_13_{2H2O}

H = -1155.534069 a.u.

G = -1155.607777 a.u.

C -2.8623840 -0.6149730 1.1584630
O -3.2070120 0.7402390 1.0749510
C -0.0959280 -0.0479060 -0.3566360
C -0.9109330 -1.3332030 -0.4937050
C -2.4180400 -1.2052980 -0.2097880
H -3.7881660 -1.1364160 1.4174690
H -0.4932990 -2.0426690 0.2287280
H -2.7681900 -2.2408390 -0.2453360
O -3.0398350 -0.5250550 -1.2736620
H -3.1969740 0.3962160 -1.0090600
O -0.7732340 -1.9287490 -1.7704550
H -1.2141840 -1.3289870 -2.3900180
C -1.8700830 -0.8712110 2.2861150
H -2.3129270 -0.5061420 3.2179130
H -0.9365190 -0.3142480 2.1171530
O -1.6232380 -2.2690830 2.3379140
H -1.1412200 -2.4765060 3.1408650
O -0.5360990 0.7210810 -2.1171200

H -2.4426550 1.3688380 1.0652090
H -0.6331150 0.7539060 0.1386180
C 3.9377740 0.1473020 0.3636800
N 3.2257400 1.2418680 0.6379950
C 1.9193460 1.1954000 0.3591790
C 1.2975110 0.0054500 -0.2031500
C 2.2322950 -1.0485360 -0.5438570
N 3.5229290 -0.9806040 -0.2274360
N 5.2397620 0.1829950 0.7113530
H 5.6193330 1.0307530 1.0955710
H 5.8339360 -0.5885800 0.4628080
N 1.2271360 2.3014130 0.6203320
H 1.7757800 3.0295260 1.0542460
H 0.1811970 2.4277670 0.6133540
N 1.8529830 -2.1608280 -1.1807050
H 2.5886330 -2.8197570 -1.3824260
H 0.9430960 -2.2474900 -1.6303530
H 0.2658460 1.2024910 -2.3483870
O -1.4156680 2.6470400 0.7054770
H -1.2983660 1.4171230 -1.9862470
H -1.6951460 3.3800490 1.2578720
O -2.3366990 2.3116940 -1.5051090
H -1.9903420 2.6182830 -0.5211170
H -2.6996410 3.0432800 -2.0054060

INT13_{2H2O}

H = -1155.556250 a.u.

G = -1155.636328 a.u.

C -2.7070370 -0.9900280 1.1429600
O -2.8879960 0.3617520 1.5097460
C -0.0458040 -0.0240080 -0.2479060

C	-0.8732600	-1.1963380	-0.7338430	H	2.5286400	-2.5312530	-1.9060440
C	-2.3646740	-1.1592110	-0.3564810	H	0.9246550	-1.8116470	-2.0540230
H	-3.6881750	-1.4497940	1.2846430	H	-0.2398210	1.9352420	-2.5297170
H	-0.4526280	-2.1154040	-0.3125820	O	-1.1783890	2.5633700	1.5410650
H	-2.7383770	-2.1387700	-0.6664170	H	-1.7173180	1.8231390	-2.1346000
O	-3.0510060	-0.2037740	-1.1231520	H	-1.1671630	3.0837740	2.3472350
H	-3.0897570	0.6333910	-0.6363930	O	-2.7026510	2.6185190	-0.7252950
O	-0.7715840	-1.3246380	-2.1449360	H	-2.2873690	2.7785350	0.1435030
H	-1.0516350	-0.4699980	-2.5259950	H	-3.5135740	3.1301460	-0.7557860
C	-1.7222170	-1.6771380	2.0776000	INT7_{3H2O}			
H	-2.1002390	-1.5942550	3.1016940	H = -1231.982932 a.u.			
H	-0.7457100	-1.1713030	2.0310670	G = -1232.064626 a.u.			
O	-1.6121830	-3.0306280	1.6692300	C	-2.9033950	-1.3215960	-0.1140990
H	-1.0896680	-3.5149800	2.3114980	O	-2.5366640	-1.5511610	1.2367250
O	-1.0295360	1.4092720	-2.6807780	C	-0.2063150	0.2114220	0.3839310
H	-2.0614920	0.8522450	1.6320480	C	-1.0823740	0.3856500	-0.8670400
H	-0.5942650	0.8290000	0.1392300	C	-2.5642050	0.1095960	-0.5687840
C	3.9259620	0.0832780	0.4048400	H	-3.9901500	-1.4295120	-0.2215330
N	3.2820000	1.1847600	0.7265250	H	-0.7637770	-0.3119220	-1.6475690
C	1.9651270	1.2734130	0.3889420	H	-3.1010050	0.2923410	-1.5031450
C	1.2956390	0.0811040	-0.2297190	O	-3.0653360	1.0222590	0.3930610
C	2.2429970	-0.9479170	-0.7280640	H	-2.3380260	1.1477010	1.0360180
N	3.4995730	-0.9657910	-0.3586570	O	-0.9341950	1.6796420	-1.4192690
N	5.1953640	-0.0423270	0.8404530	H	-1.3115450	2.3296700	-0.8090940
H	5.6213260	0.7340350	1.3172740	C	-2.2308200	-2.4124760	-0.9280410
H	5.7491000	-0.8122410	0.5069290	H	-2.6251340	-3.3824950	-0.6078650
N	1.2846790	2.3473820	0.6229960	H	-1.1501680	-2.4038290	-0.7353260
H	1.9163970	3.0239220	1.0501030	O	-2.5129000	-2.1577680	-2.2939460
H	-0.2338820	2.5436950	1.1716340	H	-2.1915850	-2.8894930	-2.8237040
N	1.8237130	-1.8907950	-1.5730770	O	-0.6138920	0.9909870	1.4392390

H	-2.9504660	-0.8544110	1.7598600	C	-3.1958430	-1.1625130	0.0814010
H	-0.2177540	-0.8589430	0.6501160	O	-3.1205930	-0.7267480	1.4292690
C	2.8882590	-1.6440860	-0.2428290	C	-0.4183650	0.3744100	0.1214070
N	2.8015230	-1.1776720	1.0188670	C	-1.2122920	0.0533150	-1.1635950
C	2.0917110	-0.0775780	1.1796570	C	-2.7219050	-0.0688660	-0.8964720
C	1.3362670	0.5726060	0.0688350	H	-4.2441700	-1.3663860	-0.1684300
C	1.8413640	0.0893760	-1.2484510	H	-0.8617720	-0.8673080	-1.6374250
N	2.4887070	-1.0568030	-1.3867840	H	-3.1803390	-0.2820880	-1.8655860
H	1.3951460	1.6615490	0.1062710	O	-3.2316280	1.1848730	-0.4616890
N	3.4871000	-2.8321140	-0.3768940	H	-2.5369420	1.5678110	0.1194330
H	3.8394890	-3.2967700	0.4432900	O	-1.0742460	1.0979910	-2.1334760
H	3.6268960	-3.2131290	-1.2975340	H	-1.6926270	1.7947260	-1.8783340
N	1.9462240	0.4420780	2.3890510	C	-2.4333390	-2.4711520	-0.0205050
H	2.1785240	-0.1573220	3.1705750	H	-2.9086750	-3.2059790	0.6369610
H	1.1440240	1.0599600	2.5009110	H	-1.3964940	-2.3363090	0.3123080
N	1.6078150	0.8341610	-2.3084600	O	-2.4900150	-2.8697690	-1.3805530
H	1.9269180	0.5062540	-3.2077070	H	-2.1328420	-3.7557480	-1.4660940
H	1.1169310	1.7241620	-2.2121600	O	-0.8074840	1.6295950	0.5918930
O	-0.5163310	3.4682200	0.7733590	H	-3.6404000	0.0857010	1.4688320
H	-0.5569260	2.5241900	1.1394150	H	-0.7622150	-0.3774520	0.8430690
H	-0.9964070	4.0443180	1.3701650	C	3.4618930	-1.2986910	-0.0310640
O	-0.5365710	-0.9624110	3.3749580	N	2.8584530	-1.2493640	1.1575950
H	-0.9868790	-1.6921740	2.9402540	C	1.7001420	-0.5884780	1.2080550
H	-0.6846630	-0.2088530	2.7695460	C	1.1336770	0.1387930	0.0659540
O	1.3113220	3.5646500	-1.2907800	C	1.8921600	-0.1046750	-1.1616450
H	0.6293860	3.7092650	-0.6088380	N	3.0496970	-0.7599980	-1.1882270
H	1.9011960	4.3190510	-1.2482660	H	1.7142410	1.3189460	0.3253120
TS7' _12_{3H2O}				N	4.6295260	-1.9669020	-0.0787460
H = -1231.954603 a.u.				H	4.9811010	-2.3996450	0.7576600
G = -1232.033360 a.u.				H	5.1159700	-2.0467470	-0.9545260

N	1.0997470	-0.5639610	2.3931800	C	4.2388000	-1.2752360	-0.7009580
H	1.6065040	-1.0038820	3.1466840	H	4.4146220	-2.1287570	-1.3590650
H	0.2702770	-0.0050160	2.6305210	H	4.7613200	-1.4715410	0.2517440
N	1.5245550	0.4505360	-2.3186610	O	4.7607660	-0.1377750	-1.3407000
H	2.1203860	0.2684870	-3.1110750	H	4.4396970	0.6344520	-0.8580450
H	0.6314550	0.9241760	-2.4351280	O	0.5369360	0.8633340	-1.1209330
O	0.2620000	3.5721230	-0.3761810	H	2.8284540	-2.7763100	0.7193240
H	-0.2926710	2.6977250	0.0073240	H	-0.1426600	-1.0041890	-0.6061560
H	0.1535810	3.6323680	-1.3272780	C	-3.5196240	-1.0124500	-0.5843620
O	-1.2480360	0.8127750	3.1009470	N	-3.2236100	0.0104410	-1.3602850
H	-1.9034460	0.1427410	2.8766330	C	-2.2728340	0.8688920	-0.9068430
H	-1.1788760	1.3554430	2.2827640	C	-1.4362470	0.5033420	0.2984650
O	2.2383310	2.4919130	0.5206450	C	-2.1383110	-0.5168510	1.1482110
H	1.4737860	3.1057900	0.0864770	N	-3.0930110	-1.2768290	0.6992580
H	3.0669200	2.6055880	0.0458610	H	-1.2768260	1.4030410	0.8911630
INT14_{H2O}				N	-4.3915910	-1.9199830	-1.0536040
H = -1079.151571 a.u.				H	-4.7979310	-1.7822150	-1.9634780
G = -1079.223254 a.u.				H	-4.6859410	-2.6736640	-0.4570520
C	2.7387910	-1.1883480	-0.4195830	N	-1.9546840	1.9807330	-1.4823360
O	2.2493700	-2.4484150	0.0237270	H	-2.5274740	2.1146090	-2.3149700
C	-0.0309950	-0.0062120	-0.1612780	H	-0.7601130	3.1278810	-0.2783040
C	0.9321650	-0.1137620	1.0391430	N	-1.7357420	-0.6197010	2.4167560
C	2.4107970	-0.1105440	0.6222840	H	-2.1845710	-1.2946750	3.0160630
H	2.2170180	-0.9651010	-1.3538820	H	-0.9861530	-0.0267460	2.7566800
H	0.7353220	-1.0647020	1.5364410	O	-0.1563310	3.3079090	0.4662700
H	2.9880650	-0.3217280	1.5315750	H	-0.1638770	1.4024080	-1.5338910
O	2.8334720	1.1755580	0.1975830	H	-0.0120090	4.2558770	0.4825170
H	2.1927520	1.4636220	-0.4720790	TS14_12_{H2O}			
O	0.7029010	0.8928370	2.0081410	H = -1079.109118 a.u.			
H	0.7986010	1.7645530	1.5896870	G = -1079.178140 a.u.			

C	2.8298910	-1.0304860	-0.5500570	N	-1.9262450	1.7818900	-1.6721790
O	2.2460840	-2.3137960	-0.3837170	H	-2.5554940	1.9513700	-2.4488790
C	0.1025070	0.1842210	-0.1673590	H	-1.6353140	2.6167530	-0.8022260
C	1.0053510	-0.1353580	1.0251350	N	-1.5781330	-0.6483900	2.3629770
C	2.4984500	-0.1507970	0.6597950	H	-2.0837060	-1.2688230	2.9751210
H	2.3771090	-0.5974420	-1.4465720	H	-0.8741180	-0.0170420	2.7242480
H	0.7354390	-1.1265800	1.3896080	O	-1.4046020	3.0065050	0.3821860
H	3.0345130	-0.5403960	1.5344170	H	0.0506040	1.6074430	-1.5155980
O	2.9834670	1.1775510	0.4882650	H	-0.5049930	3.3321870	0.4733350
H	2.4430370	1.5701120	-0.2162260	INT14₂H₂O			
O	0.8118050	0.7702240	2.0998060	H = -1155.568302 a.u.			
H	1.3901030	1.5291630	1.9563060	G = -1155.645463 a.u.			
C	4.3369860	-1.1565890	-0.7755320	C	2.9271940	-0.8549020	0.1153470
H	4.5010160	-1.8793270	-1.5769790	O	2.4354030	-1.7739150	1.0787120
H	4.7964370	-1.5617570	0.1424290	C	0.1062980	0.0102890	-0.3116920
O	4.9538530	0.0450620	-1.1652840	C	0.9601310	0.6650900	0.7759090
H	4.6919730	0.7260790	-0.5346240	C	2.4653970	0.5629930	0.4648910
O	0.6744860	1.3071500	-0.8346410	H	2.4908540	-1.1490980	-0.8445560
H	2.7663840	-2.8134490	0.2536630	H	0.7593200	0.1659020	1.7248940
H	0.1502970	-0.6819420	-0.8429150	H	3.0038650	0.9028890	1.3581630
C	-3.5383270	-1.0840380	-0.4888850	O	2.8247160	1.4859420	-0.5591820
N	-3.2120810	-0.1355080	-1.3720410	H	2.2572490	1.2912370	-1.3228980
C	-2.2158100	0.6680470	-1.0030480	O	0.6333580	2.0342540	0.9394460
C	-1.3856880	0.4452420	0.2056320	H	1.1292800	2.5236010	0.2695800
C	-2.0335510	-0.5048300	1.1117480	C	4.4483440	-0.9566840	0.0049100
N	-3.0841190	-1.2351990	0.7737050	H	4.7093430	-2.0074040	-0.1351430
H	-1.3654690	1.7391440	0.6135270	H	4.8932160	-0.6223110	0.9577160
N	-4.4722520	-1.9693810	-0.8767840	O	4.9833140	-0.2460830	-1.0836510
H	-4.9129730	-1.8510830	-1.7730360	H	4.6198690	0.6469870	-1.0598170
H	-4.8146260	-2.6423250	-0.2128360	O	0.4800570	0.6037010	-1.5442340

H	2.9448910	-1.6797470	1.8899200	C	1.1409820	-0.5420820	0.9444200
H	0.3288060	-1.0642340	-0.3285330	C	2.6391690	-0.3958580	0.6203990
C	-2.2859360	-2.3668070	-0.0777510	H	2.5622530	-0.3011230	-1.5296270
N	-2.3759920	-1.7664960	-1.2506390	H	0.9234690	-1.5966170	1.1127410
C	-2.1188200	-0.4322940	-1.2681430	H	3.1928690	-0.9673260	1.3778170
C	-1.4206180	0.1824440	-0.0736790	O	3.0527190	0.9556690	0.7979600
C	-1.8649090	-0.5257080	1.1746160	H	2.4545210	1.4857030	0.2413420
N	-2.1677700	-1.7933190	1.1664630	O	0.8821910	0.1782400	2.1610080
H	-1.6276530	1.2474280	-0.0116470	H	1.6830100	0.6758960	2.3730250
N	-2.3984650	-3.7051900	-0.0515620	C	4.5424360	-0.9133030	-0.9782690
H	-2.5704390	-4.1968240	-0.9120540	H	4.7519210	-1.4022360	-1.9316260
H	-2.4291070	-4.1774320	0.8354360	H	5.0168380	-1.5115110	-0.1812640
N	-2.3053240	0.3457620	-2.2809540	O	5.0949350	0.3778430	-1.0411000
H	-2.6983600	-0.1890340	-3.0556090	H	4.7689020	0.8730760	-0.2804600
H	-2.5561220	2.1450340	-1.7048160	O	0.6954380	1.3067980	-0.4389950
N	-1.9084020	0.1843400	2.3005720	H	3.0599570	-2.8571680	-0.4445810
H	-2.2656320	-0.2778190	3.1240720	H	0.4442750	-0.6446370	-1.0525420
H	-1.9172930	1.2079850	2.2463670	C	-3.7063590	-1.0789270	-0.5678230
O	-1.9425410	2.9773110	1.6481180	N	-3.2590600	-0.1293760	-1.3776300
H	-0.2877240	0.6500210	-2.1391900	C	-2.0606540	0.4151760	-1.0739250
H	-0.9923630	2.9641100	1.4670660	C	-1.2774840	-0.0657200	0.0714210
O	-2.6093830	2.9607040	-1.1625600	C	-1.9375260	-1.0693500	0.8535050
H	-2.3451620	3.1191490	0.7767050	N	-3.1490790	-1.5305810	0.5739130
H	-3.0970450	3.6020520	-1.6824690	H	-1.3993860	1.1296570	1.0685410
TS14_12_{H2O}				N	-4.8781690	-1.6668790	-0.9070310
H = -1155.531049 a.u.				H	-5.3982130	-1.2916690	-1.6807380
G = -1155.604423 a.u.				H	-5.3052990	-2.3047230	-0.2587850
C	3.0289860	-0.9256540	-0.7626100	N	-1.5793800	1.4191030	-1.8006970
O	2.5129250	-2.2352500	-0.9349080	H	-2.1899190	1.5578190	-2.6021100
C	0.2433700	-0.0228600	-0.1698860	H	-1.4596300	2.7684400	-0.9714200

N -1.3733630 -1.5941040 1.9821400
H -2.0160960 -2.1438870 2.5326110
H -0.6943380 -1.0460410 2.4917880
O -1.2354630 2.0448810 1.6687940
H 0.1484140 1.6078330 -1.1961560
H -0.3197020 1.8925070 1.9559160
O -1.3596100 3.5299430 -0.2732390
H -1.2597750 2.7969840 0.9055820
H -2.1133040 4.1183570 -0.3644920

SINT6

H = -1002.735214 a.u.

G = -1002.806913 a.u.

C -3.3591380 -0.7318570 0.0129820
O -3.6620270 -1.4860410 -1.1475770
C -0.3939300 -0.9978300 -0.4155870
C -1.0032850 0.3069020 0.0520450
C -2.4649120 0.4856470 -0.3537600
H -2.8570110 -1.3578320 0.7636490
H 0.5032930 -1.3283570 0.1343270
H -0.4129180 1.1108320 -0.4140260
H -2.5163970 0.6119190 -1.4409690
O -2.8439470 1.6849820 0.3026710
H -3.7602350 1.8735270 0.0590580
O -0.8642180 0.3601910 1.4613330
H -1.4214130 1.0934810 1.7543950
O -0.8372000 -1.6374780 -1.3354680
H -2.8310410 -1.7393030 -1.5687520
C -4.7025820 -0.3000240 0.5690760
H -4.5804160 0.2204230 1.5185850
H -5.3208870 -1.1884690 0.7268010

O -5.3374300 0.6090940 -0.3213380
H -5.4237950 0.1570930 -1.1683490
C 4.0647050 -0.6004460 -0.3331690
N 3.4456720 -1.0117610 0.7771790
C 2.5190600 -0.1810580 1.2681850
C 2.2072230 1.0385890 0.6611640
C 2.9043560 1.3328640 -0.5104520
N 3.8357580 0.5223190 -1.0206770
H 1.4687320 1.7065420 1.0827810
N 5.0547440 -1.4090680 -0.8099190
H 5.0936220 -2.3460900 -0.4460020
H 5.3636410 -1.2441200 -1.7530180
N 1.8774250 -0.5826270 2.4078810
H 2.0486370 -1.5406090 2.6731820
H 0.9363400 -0.2380880 2.5406960
N 2.6284030 2.4664960 -1.2363680
H 3.3264040 2.7047120 -1.9246320
H 2.2190260 3.2441240 -0.7442700

STS6_8

H = -1002.718136 a.u.

G = -1002.783239 a.u.

C -2.8159950 -0.0572480 0.9220660
O -2.5680880 -1.3509210 1.4432110
C -0.0913710 -0.3377090 -0.0343360
C -1.0852200 0.4086050 -0.9341480
C -2.5157150 -0.0271480 -0.5953860
H -2.2139610 0.7003340 1.4437940
H 0.0266160 0.1496800 0.9507630
H -0.8981900 0.1338350 -1.9801940
H -2.6555730 -1.0429590 -0.9758980

O	-3.3437680	0.8864510	-1.3018220	C	2.3698250	-0.8295100	-0.0631810
H	-4.2497400	0.5593520	-1.2399610	O	2.3506290	-1.0192640	1.3395730
O	-0.9638300	1.8139260	-0.7742870	C	0.0046840	1.0432790	0.9821910
H	-1.7694140	2.2047770	-1.1375240	C	0.6827730	1.0814820	-0.4066560
O	-0.2261260	-1.6068770	-0.0730070	C	2.1524980	0.6647020	-0.3822910
H	-1.7423820	-1.6968910	1.0601780	H	1.5772120	-1.4182990	-0.5397730
C	-4.2812970	0.2232820	1.2006430	H	0.6035330	0.4708660	1.6857260
H	-4.5331790	1.2567300	0.9622250	H	0.6561220	2.1255070	-0.7434110
H	-4.4758010	0.0474980	2.2630220	H	2.6723130	1.2489420	0.3894750
O	-5.1095840	-0.5996780	0.3895580	O	2.6395280	1.0044000	-1.6728470
H	-4.8504530	-1.5105840	0.5703240	H	3.5989060	0.9120030	-1.6526610
C	3.9818620	-0.0547990	0.5837860	O	-0.0497000	0.2792900	-1.3146390
N	3.3487530	1.1208850	0.7349150	H	0.4016510	0.3213320	-2.1646570
C	2.2195240	1.2673250	0.0563660	O	-0.1371490	2.3756820	1.4947500
C	1.6179670	0.2013260	-0.7368130	H	1.4499490	-1.3374830	1.5668970
C	2.4421910	-0.9961170	-0.7753390	C	3.7145730	-1.3114870	-0.5804510
N	3.5878280	-1.1250610	-0.1228900	H	3.7281270	-1.3436290	-1.6704060
H	1.2535600	0.5206200	-1.7077200	H	3.8899080	-2.3217330	-0.1988230
N	5.1526990	-0.1754890	1.2300480	O	4.7613380	-0.4302500	-0.1908250
H	5.4815610	0.5854880	1.7989020	H	4.7678790	-0.4057760	0.7718020
H	5.6532300	-1.0461420	1.1792730	C	-3.2528290	-1.0371750	-0.4228200
N	1.5968720	2.4429060	0.1411160	N	-3.2774670	0.3235550	-0.6310270
H	1.9993190	3.1424140	0.7446700	C	-2.3572110	1.0083620	-0.0251010
H	0.6542160	2.5402450	-0.2245240	C	-1.3839130	0.4005790	0.9603080
N	1.9861880	-2.0383120	-1.4837630	C	-1.3252670	-1.1166350	0.8158680
H	2.5067830	-2.8934000	-1.3403290	N	-2.3696700	-1.7621790	0.2180550
H	0.9665140	-2.1338000	-1.4532400	H	-1.8181140	0.5888300	1.9516600
SINT8				N	-4.2968660	-1.6760040	-0.9887860
H = -1002.735127 a.u.				H	-4.9353570	-1.1533640	-1.5623280
G = -1002.800755 a.u.				H	-4.3253220	-2.6805680	-0.9580250

N -2.2996720 2.3311400 -0.2111480
H -1.6331600 2.8964640 0.2950510
H -2.9709380 2.7488100 -0.8361150
N -0.3309850 -1.7406530 1.3366120
H -0.4866170 -2.7408380 1.2102230
H 0.6985600 2.6574640 1.8741150

STS8_9

H = -1002.659002 a.u.

G = -1002.723312 a.u.

C 2.1405990 -0.8281190 -0.3093790
O 2.0436760 -1.7131380 0.7834630
C 0.0624780 0.7135980 1.0573690
C 1.1972110 1.4724350 0.3672250
C 2.4445850 0.5877630 0.2521290
H 1.2057320 -0.8183880 -0.8882260
H 0.4804000 -0.1139900 1.6295220
H 1.4546690 2.3433880 0.9833850
H 2.8653620 0.4387890 1.2532850
O 3.3312360 1.3514740 -0.5478510
H 4.1600340 0.8585790 -0.6078280
O 0.8167160 1.8999900 -0.9229080
H 1.6366660 2.1126430 -1.3891620
O -0.6115260 1.6205280 2.1227900
H 1.0768270 -1.9471740 0.9109910
C 3.2619660 -1.3156890 -1.2105010
H 3.3514170 -0.7020000 -2.1078820
H 3.0517320 -2.3477240 -1.5051830
O 4.5071540 -1.2261460 -0.5262000
H 4.4107740 -1.7399490 0.2841570
C -3.5121140 -0.7863960 -0.4892520

N -3.2551340 0.5079800 -0.8164840
C -2.1046240 0.9984270 -0.3955560
C -1.2102910 0.2241800 0.4292710
C -1.4938630 -1.2196640 0.5077110
N -2.7244940 -1.6556580 0.1058920
H -1.5189000 1.0251670 1.7111200

N -4.7553830 -1.2120750 -0.8387550
H -5.2822850 -0.6355340 -1.4723710
H -4.9292880 -2.2025180 -0.8091150
N -1.8838440 2.3189320 -0.6424190
H -0.9258780 2.5971300 -0.8139470
H -2.5850550 2.7290020 -1.2420040
N -0.5989200 -2.0376740 0.9788270
H -0.9991920 -2.9724290 1.0022960
H -0.3423230 1.3835990 3.0230800

SINT9

H = -1002.722400 a.u.

G = -1002.791188 a.u.

C -2.2676920 0.1817790 -0.6784900
O -2.7825020 1.4147420 -1.1376980
C 0.2067340 0.2233900 1.0456540
C -1.0039290 -0.5502960 1.4467140
C -2.2678990 0.1217700 0.8721050
H -1.2413070 0.0410550 -1.0429710
H 0.1178070 1.2384340 1.4297620
H -1.0790810 -0.4595180 2.5399870
H -2.3097390 1.1519670 1.2415340
O -3.3262100 -0.6499900 1.4195110
H -4.0970500 -0.5828730 0.8363010
O -1.0133610 -1.9215190 1.1038950

H	-1.9120250	-2.2224690	1.3004180	C	-1.3647650	-1.0124810	0.8629700
O	-0.8909820	3.0370480	0.0020800	C	-2.8110990	-0.6766910	0.4671490
H	-2.1687720	2.1161080	-0.8523760	H	-3.8566350	-0.4761890	-1.3930820
C	-3.1549440	-0.8729110	-1.3267930	H	-0.0080980	0.5231570	-0.0409730
H	-2.9405890	-1.8694250	-0.9395020	H	-1.3997270	-1.4082490	1.8856000
H	-2.9827490	-0.8657880	-2.4069630	H	-3.1854850	0.0242300	1.2287110
O	-4.5205920	-0.5955810	-1.0418390	O	-3.5119720	-1.9002650	0.5684430
H	-4.6687410	0.3156200	-1.3246950	H	-4.4220270	-1.7650200	0.2936120
C	3.9407080	-0.2691860	-0.2766170	O	-0.8561790	-1.9649320	-0.0385890
N	3.1335700	-1.3485720	-0.5445760	H	0.0885200	-2.1079470	0.1509840
C	1.8610210	-1.2203820	-0.2838310	O	-0.4745430	0.9506570	1.8814720
C	1.3284350	0.0208970	0.3349390	H	-1.4472580	-1.0474760	-1.6168230
C	2.2534450	1.1965980	0.1674760	C	-3.2332300	1.4773090	-0.8610080
N	3.5898440	0.9593240	0.0105320	H	-4.2099740	1.6586380	-0.3986510
H	0.0860060	2.8429960	0.0287510	H	-3.2557890	1.8637850	-1.8806680
N	5.2564720	-0.5486330	-0.3716330	O	-2.2129640	2.1940330	-0.1780320
H	5.5386870	-1.4518390	-0.7104140	H	-2.4129920	2.2414130	0.7611890
H	5.9181280	0.2045180	-0.2922100	C	2.2143010	-1.3148880	-0.9763130
N	1.0435450	-2.2208580	-0.6294440	N	1.9993500	-1.6093190	0.3177460
H	0.1206040	-2.2876660	-0.2121030	C	2.2641300	-0.6185730	1.1899040
H	1.4984250	-3.0587360	-0.9602930	C	2.6376560	0.6550820	0.7776810
N	1.7586220	2.3835990	0.1943130	C	2.7050150	0.8640300	-0.6042300
H	2.5195550	3.0559160	0.1110370	N	2.5460360	-0.1354040	-1.4865150
H	-0.9796390	3.9901280	0.0648610	H	2.8262650	1.4536580	1.4815290
SINT6_{H2O}				N	1.9822630	-2.3281140	-1.8632070
H	= -1079.150583 a.u.			H	2.0185630	-3.2685180	-1.5059500
G	= -1079.225792 a.u.			H	2.2883810	-2.1699470	-2.8092100
C	-2.9624820	-0.0212910	-0.9352020	N	2.1220040	-0.9329730	2.5144180
O	-1.8528110	-0.1851140	-1.7841440	H	1.6831880	-1.8189210	2.7119450
C	-0.5377890	0.2604850	0.8906850	H	1.9155770	-0.1820700	3.1536130

N 2.9584280 2.1031300 -1.1155190
H 2.5343930 2.8630560 -0.5948080
H 2.8140460 2.1573990 -2.1136890
O 0.5526690 3.2036860 0.3443250
H 0.3875390 2.6214260 1.0974020
H -0.2390620 3.0939170 -0.1968130

STS6_7_{H2O}

H = -1079.136015 a.u.

G = -1079.206165 a.u.

C -2.8263860 -1.0585780 -0.6348190
O -2.1974160 -0.5672030 -1.7971190
C -0.5175050 0.4503270 0.6159050
C -0.4376430 -1.0525870 0.4586150
C -1.8601470 -1.6412020 0.4280670
H -3.4801570 -1.9055870 -0.9111940
H -0.7778870 0.9468120 -0.3272410
H 0.0769860 -1.4926980 1.3210450
H -2.3016920 -1.5043890 1.4221060
O -1.6153980 -3.0277120 0.1875820
H -2.4508630 -3.4940050 0.1073560
O 0.2443620 -1.3686250 -0.7434450
H 0.2913780 -2.3301450 -0.7981110
O -0.9865250 0.8857850 1.7105230
H -1.2947830 -0.9064110 -1.8447390
C -3.8096200 0.0033710 -0.1288850
H -4.3847540 -0.4299500 0.7013020
H -4.5035350 0.2030430 -0.9476880
O -3.2643190 1.2504480 0.2325840
H -2.6952370 1.1469360 1.0136410
C 3.1815450 -0.5274040 -0.4539310

N 2.9147520 -0.6320110 0.8623990
C 2.0535170 0.2563500 1.3399120
C 1.3423480 1.1651390 0.5025170
C 1.7832940 1.1915360 -0.8659010
N 2.6957790 0.3535770 -1.3406110
H 1.0049820 2.1011230 0.9251280
N 4.0501750 -1.4350020 -0.9437460
H 4.5307980 -2.0414570 -0.3019050
H 4.3547940 -1.3458510 -1.8978250
N 1.7745860 0.2520810 2.6603370
H 2.1239230 -0.5330240 3.1892270
H 0.8832430 0.6532150 2.9363170
N 1.2185130 2.0789290 -1.6910250
H 0.4445080 2.6543540 -1.3674860
H 1.4580780 2.0446360 -2.6688920
O -1.2003330 3.2528870 -0.2300340
H -1.1368400 2.9592940 0.6889430
H -2.0189660 2.8247260 -0.5210710

SINT7_{H2O}

H = -1079.148815 a.u.

G = -1079.218343 a.u.

C -2.9358660 -0.7562220 -0.5942370
O -2.4992800 0.0691300 -1.6557830
C -0.3467040 0.1791660 0.6573720
C -0.4114290 -1.1827700 -0.0197130
C -1.8526060 -1.7077710 -0.0385590
H -3.7230880 -1.4308520 -0.9780680
H -0.8935380 0.8682120 0.0052220
H 0.1923570 -1.9131500 0.5360830
H -2.1227150 -1.9783960 0.9864230

O -1.7497370 -2.8834030 -0.8514000
H -2.6204900 -3.2713930 -0.9647230
O 0.0878550 -1.0612900 -1.3507240
H -0.0025180 -1.9286580 -1.7636110
O -0.8420310 0.1221950 1.9209150
H -1.6208150 -0.2117410 -1.9393380
C -3.6843950 0.1036410 0.4374480
H -4.0881890 -0.5730680 1.2042930
H -4.5319480 0.5473760 -0.0918770
O -2.9766160 1.1617740 1.0291380
H -2.2189380 0.7813690 1.5833950
C 3.4592220 -0.1819560 -0.3646780
N 3.1490400 -0.6248300 0.8725140
C 2.0336080 -0.1454050 1.3903120
C 1.1232120 0.7868940 0.6671200
C 1.6609000 1.1575140 -0.6734340
N 2.7955000 0.6832300 -1.1542180
H 0.9813800 1.6983770 1.2552450
N 4.5945740 -0.6707600 -0.8767660
H 5.1393410 -1.3189210 -0.3335650
H 4.8792730 -0.3872120 -1.7990290
N 1.6128540 -0.5105910 2.5884620
H 2.1209790 -1.2427350 3.0634930
H 0.5942670 -0.3164890 2.7543790
N 0.9678990 2.0300530 -1.3823690
H 0.0819920 2.4236020 -1.0485160
H 1.3053830 2.2581360 -2.3054050
O -1.4867420 3.0639920 -0.2737160
H -2.1419000 2.4279590 0.0920570
H -1.7131530 3.9201270 0.0929620

STS7_8_{H2O}

H = -1079.141425 a.u.

G = -1079.210675 a.u

C -2.8608480 -0.9079820 -0.8207730
O -2.0181920 -0.6621160 -1.9248700
C -0.3628900 0.4683640 0.5374630
C -0.6528870 -1.0205590 0.6094940
C -2.1350490 -1.3795340 0.4635740
H -3.5556190 -1.7279020 -1.0778190
H -0.6721540 0.8182340 -0.4568020
H -0.3498500 -1.4128120 1.5866690
H -2.6625110 -0.9815230 1.3379340
O -2.1001430 -2.8109730 0.5346810
H -2.9813340 -3.1585080 0.3788040
O 0.1090670 -1.6599800 -0.4141670
H -0.0548560 -2.6066660 -0.3293870
O -1.0366430 1.1485310 1.5344560
H -1.1808980 -1.1237750 -1.7995260
C -3.7647120 0.3059210 -0.6047370
H -4.5328150 0.0211400 0.1313160
H -4.2691580 0.5061360 -1.5526750
O -3.1161050 1.4918580 -0.2364930
H -2.6080540 1.3561100 0.5821510
C 3.1330510 -0.5345850 -0.7145230
N 2.9710510 -0.8929290 0.5959670
C 2.0498220 -0.2375240 1.2434190
C 1.1943810 0.8177110 0.6318900
C 1.7349520 1.2426510 -0.7007760
N 2.6303400 0.5114970 -1.3679630
H 1.2121030 1.6923500 1.2860910

N	3.9565780	-1.3318630	-1.4024770	C	-3.7933720	0.0264980	-0.4527480
H	4.3836700	-2.1162230	-0.9399360	H	-4.5405410	-0.4175690	0.2191750
H	4.1466670	-1.1233750	-2.3685080	H	-4.2949010	0.3170970	-1.3767900
N	1.8315880	-0.4924490	2.5368310	O	-3.2636490	1.2114160	0.1030360
H	2.3450390	-1.2324780	2.9901790	H	-2.8318780	1.0057720	0.9419860
H	1.0844970	-0.0179080	3.0239780	C	3.2294380	-0.4019290	-0.5966400
N	1.2394790	2.3547460	-1.1641990	N	3.0448170	-0.5675850	0.7703070
H	0.4632470	2.8801220	-0.5190790	C	2.0598840	0.0900190	1.2873180
H	1.5451550	2.6452080	-2.0833970	C	1.1289480	0.9613190	0.4972670
O	-0.4273440	3.2447130	0.5264280	C	1.5995520	1.1663190	-0.9316090
H	-1.1846120	3.7531310	0.2270720	N	2.6303860	0.4107030	-1.4239560
H	-0.8317950	2.2426990	1.1653500	H	1.1179120	1.9498020	0.9653390

SINT8_{H2O}

H = -1079.147639 a.u.

G = -1079.217574 a.u.

C	-2.7526250	-1.0354430	-0.7996610
O	-1.9785000	-0.5448580	-1.8682770
C	-0.3437750	0.4745080	0.5576770
C	-0.4982370	-1.0369390	0.5472550
C	-1.9471460	-1.5263060	0.4350500
H	-3.3334610	-1.9100160	-1.1407200
H	-0.8396940	0.8822560	-0.3226620
H	-0.1029640	-1.4521580	1.4822890
H	-2.4771640	-1.2343750	1.3511580
O	-1.7870560	-2.9456500	0.4161310
H	-2.6432160	-3.3669230	0.3096350
O	0.2630380	-1.5210430	-0.5505720
H	0.2448070	-2.4837910	-0.5080030
O	-0.9646030	0.9654520	1.7402750
H	-1.1058120	-0.9579470	-1.8606300

H	4.1906160	-1.2139990	-1.0859670
H	4.7603130	-1.7321950	-0.4399700
H	4.4766970	-1.0930260	-2.0427490
N	1.8147930	0.0182220	2.6080110
H	2.3639610	-0.6141380	3.1690610
H	0.9667380	0.4215980	2.9796430
N	0.9714250	2.0644340	-1.5932860
H	-0.4098590	3.0457450	-0.5550950
H	1.3444180	2.1197400	-2.5399450
O	-1.0692770	3.2482260	0.1412740
H	-1.9165940	2.9957880	-0.2469750
H	-1.0386490	1.9252960	1.5710920

N	4.1906160	-1.2139990	-1.0859670
H	4.7603130	-1.7321950	-0.4399700
H	4.4766970	-1.0930260	-2.0427490
N	1.8147930	0.0182220	2.6080110
H	2.3639610	-0.6141380	3.1690610
H	0.9667380	0.4215980	2.9796430
N	0.9714250	2.0644340	-1.5932860
H	-0.4098590	3.0457450	-0.5550950
H	1.3444180	2.1197400	-2.5399450
O	-1.0692770	3.2482260	0.1412740
H	-1.9165940	2.9957880	-0.2469750
H	-1.0386490	1.9252960	1.5710920

STS8_9_{H2O}

H = -1002.659002 a.u.

G = -1002.723312 a.u.

C	-2.2826150	0.8389030	0.0059760
O	-2.2935140	1.2594320	1.3504450
C	-0.0524540	-1.0929230	0.7820630

C	-1.1810450	-1.4946880	-0.1956030	N	0.3051330	1.6131430	1.6837530
C	-2.4743410	-0.6985510	-0.0104890	H	3.3371030	-2.0949150	0.9018970
H	-1.3367270	1.1128980	-0.4818170	H	0.5820340	2.5579500	1.9392830
H	-0.4995570	-0.5828060	1.6380630	O	2.8275190	-1.7173850	1.6386560
H	-1.4332400	-2.5442230	0.0155240	H	1.9010980	-2.2253870	1.6483290
H	-2.9077400	-0.9610390	0.9620620	H	-0.1133830	-2.7907360	1.8909990
O	-3.3084010	-1.1689780	-1.0606300	SINT9_{H2O}			
H	-4.1653360	-0.7343330	-0.9598240	H =	-1079.127554	a.u.	
O	-0.7468440	-1.3955940	-1.5362000	G =	-1079.20467	a.u.	
H	-1.5430540	-1.4588160	-2.0803020	C	2.5986850	-0.4974920	-0.7421400
O	0.5249030	-2.3609940	1.3132920	O	2.1826240	-1.8316820	-0.5171560
H	-1.3413610	1.4314400	1.6161960	C	0.1749070	0.1508960	0.5166740
C	-3.4185830	1.5494040	-0.7089130	C	1.2874400	1.0893810	0.8164730
H	-3.4472520	1.2964520	-1.7695910	C	2.5890100	0.2866360	0.6011300
H	-3.2789670	2.6291410	-0.6036480	H	1.9567870	0.0024950	-1.4790380
O	-4.6671530	1.1441920	-0.1556090	H	0.3501490	-0.7934360	1.0240920
H	-4.6121470	1.3222670	0.7908460	H	1.2230290	1.3720220	1.8745310
C	2.9520130	1.4973260	-0.6037520	H	2.6757370	-0.4527080	1.4040600
N	2.8903260	0.2874450	-1.2203090	O	3.6203570	1.2532630	0.6975050
C	1.9407870	-0.5239910	-0.7803890	H	4.4619210	0.7804710	0.6789390
C	1.0700970	-0.2056430	0.2941960	O	1.3231990	2.2423770	-0.0051490
C	1.1517750	1.1697570	0.7991000	H	2.2202270	2.5962500	0.0593540
N	2.1800220	1.9624650	0.3496690	O	-0.6354890	0.1092460	3.2316250
H	2.3689720	-0.8539810	1.2057240	H	1.2133010	-1.9505140	-0.5768430
N	3.9790790	2.2929970	-1.0254150	C	4.0057700	-0.5839960	-1.3067750
H	4.4068120	2.0521570	-1.9037940	H	4.3717650	0.4000060	-1.6009820
H	3.9273390	3.2644330	-0.7666420	H	3.9942410	-1.2361630	-2.1845320
N	2.0082730	-1.8213190	-1.2733200	O	4.9049070	-1.0747830	-0.3192360
H	2.5919030	-1.8490550	-2.1007030	H	4.5703000	-1.9345210	-0.0398790
H	1.0977920	-2.2375020	-1.4360270	C	-3.4984670	-0.1564900	-0.9256640

N	-2.9427330	1.0629210	-1.1953780	O	1.9085030	-1.4809260	-1.5955330
C	-1.6696360	1.2235320	-0.9108210	H	2.7986210	-1.8540310	-1.5372040
C	-0.9054720	0.1275470	-0.2807600	O	-0.2639620	-1.3309470	0.0482030
C	-1.5318040	-1.2154340	-0.4777780	H	0.0468230	-2.0901010	-0.4588730
N	-2.9021850	-1.2841290	-0.6119860	O	0.2961000	2.2044220	-0.4782870
H	-3.2200210	-1.2149890	1.4574550	H	2.8671650	1.2645540	1.0276090
N	-4.8556100	-0.1625720	-0.9914850	C	4.0587030	-0.9292250	0.3446510
H	-5.2972290	0.6304830	-1.4270270	H	4.5656310	-0.9631270	1.3127440
H	-5.3107290	-1.0598800	-1.0374760	H	4.5041590	-0.1214100	-0.2439910
N	-1.1128650	2.4019950	-1.1716080	O	4.2841000	-2.1286240	-0.3950590
H	-1.7205370	3.1272690	-1.5193770	H	4.1406230	-2.8826520	0.1829160
H	-0.1542300	2.5970400	-0.8971430	C	-3.3031050	-1.0707720	-0.0060400
N	-0.7536390	-2.2339880	-0.4983470	N	-3.1391540	-0.1872250	-1.0839520
H	-3.8898380	-0.0834830	2.2362310	C	-2.4367390	0.8586460	-0.8469670
H	-1.3047070	-3.0853640	-0.6020410	C	-1.6956750	1.1088460	0.4336380
O	-3.1931110	-0.7417090	2.3028030	C	-2.1679710	0.1788410	1.5456150
H	-1.5082800	-0.1736550	2.9123000	N	-2.9577940	-0.9116710	1.2295670
H	-0.5851530	-0.2120870	4.1338390	H	-1.8813500	2.1333930	0.7686450
SINT8' _{H₂O}				N	-3.9512160	-2.1998100	-0.3756850
H	-1079.143301	a.u.		H	-4.3883500	-2.2300300	-1.2802970
G	-1079.215471	a.u.		H	-4.2324580	-2.8403830	0.3473420
C	2.5770830	-0.6206820	0.5927330	N	-2.2609060	1.7877690	-1.8395370
O	2.5041320	0.4790740	1.4692540	H	-2.8631320	1.6703050	-2.6433330
C	-0.1580300	1.0401840	0.2214080	H	-2.1031090	2.7409040	-1.5458750
C	0.2983320	-0.1923270	-0.5559430	N	-1.7932270	0.4760420	2.7240930
C	1.8147400	-0.3646650	-0.7179900	H	-2.1514250	-0.2305690	3.3675290
H	2.1053410	-1.4646060	1.1077790	H	0.0546260	2.1032600	-1.4076170
H	0.2907690	1.0716520	1.2131200	O	2.9768490	2.7612960	-0.0637940
H	-0.0908730	-0.0953020	-1.5859510	H	2.0156660	2.7832090	-0.2119770
H	2.2374840	0.5319890	-1.1941790	H	3.2300530	3.6297600	0.2553150

STS8'_9'_H2O

H = -1079.030544 a.u.

G = -1079.103319 a.u.

C 2.5403410 -0.5288170 0.5641280
O 2.2736130 0.6245870 1.2584270
C -0.2209860 0.3218820 0.6012840
C 0.2175150 -0.5446880 -0.5341150
C 1.7496710 -0.5457500 -0.7596450
H 2.2484850 -1.4315620 1.1383070
H 0.3713760 0.2897760 1.5120040
H -0.2898480 -0.2679900 -1.4667840
H 2.0225840 0.3553280 -1.3205940
O 1.9586860 -1.7075740 -1.5455340
H 2.8825840 -1.9799690 -1.4268620
O -0.2153610 -1.8270590 -0.1154320
H 0.4175390 -2.4410920 -0.5220200
O 0.5551810 2.4566660 -0.7564100
H 2.7110360 1.7618720 0.7059250
C 4.0456420 -0.6307360 0.2773390
H 4.5816180 -0.5019800 1.2205860
H 4.3423200 0.1763720 -0.3969010
O 4.4202370 -1.8575760 -0.3644430
H 4.4515690 -2.5526900 0.2976320
C -3.4139310 -0.8116030 -0.2865470
N -3.1302360 0.2891820 -1.0717320
C -2.2974180 1.1594550 -0.5959430
C -1.5197570 0.9453810 0.6815470
C -2.2379460 -0.1824950 1.5850050
N -3.0908330 -1.0265650 0.9620640
H -1.4954290 1.8260920 1.3221210

N -4.1711060 -1.7255910 -0.9129800
H -4.4414660 -1.5688680 -1.8683320
H -4.4059810 -2.5786710 -0.4347010
N -2.1191760 2.3319660 -1.2061200
H -2.6177060 2.4853860 -2.0700970
H -1.2768980 2.8628090 -0.9955600
N -1.8908250 -0.1551480 2.8029120
H -2.3994240 -0.8808730 3.3102110
H 0.7872700 2.3078730 -1.6784820
O 2.8869530 2.6862210 0.1543950
H 1.4524490 2.6965410 -0.3315810
H 3.2598980 3.3468470 0.7397700

SINT9'_H2O

H = -1079.147958 a.u.

G = -1079.220686 a.u.

C 2.2173600 -0.2997850 0.8927560
O 0.9894570 0.3253540 1.2430320
C -0.1186630 -0.4451810 0.7368570
C 0.5029280 -1.6604990 0.0381440
C 1.8814880 -1.1338800 -0.3430040
H 2.5428020 -0.9724770 1.6979290
H -0.7110240 -0.8025740 1.5823500
H -0.0726850 -2.0074680 -0.8221900
H 1.8013800 -0.4713140 -1.2160610
O 2.7640190 -2.2042570 -0.5791680
H 3.6532420 -1.8328220 -0.6200770
O 0.6262090 -2.6882400 1.0002580
H 1.3444990 -3.2618560 0.7072110
O 1.1529260 1.8414170 -2.1667890
H 1.0946650 2.3628980 0.8454290

C	3.2839880	0.7437580	0.6184880	C	-0.7613010	-0.8378170	0.3904740
H	3.4628540	1.3742670	1.4947330	C	-2.2853220	-0.9553210	0.4232160
H	2.9705940	1.3795860	-0.2127240	H	-2.3493300	-0.4309910	-1.6756650
O	4.4746030	0.0754960	0.2032350	H	0.0941980	1.1572820	-0.1234160
H	4.9996490	-0.1398860	0.9776650	H	-0.3768920	-1.4847150	1.1863980
C	-3.4426390	-0.5070860	0.1781540	H	-2.6314670	-0.4793580	1.3490990
N	-2.8567800	-0.7774950	-1.0541970	O	-2.6177230	-2.3271040	0.4216290
C	-1.7080240	-0.2085300	-1.2414950	H	-3.5143560	-2.4046270	0.7625390
C	-0.9833870	0.5090010	-0.1398940	O	-0.2834460	-1.2219020	-0.8734130
C	-2.0214190	1.1912450	0.7251940	H	0.5404000	-1.7117590	-0.7611860
N	-3.1478800	0.4545480	1.0154700	O	-0.4914910	1.0756880	1.8142240
H	-0.3212730	1.2472430	-0.5738710	H	-3.3373830	1.4059530	0.2357460
N	-4.4796510	-1.3194080	0.4608620	C	-4.3631730	-0.6142630	-0.9740120
H	-4.7897780	-1.9742590	-0.2356170	H	-4.4161020	-1.6466280	-1.3312840
H	-5.0300680	-1.1353890	1.2822170	H	-4.8105790	0.0514550	-1.7178930
N	-1.0803820	-0.2529350	-2.4242120	O	-5.0078560	-0.4772000	0.2916390
H	-1.5539630	-0.6797600	-3.2059750	H	-5.9594050	-0.5243730	0.1787400
H	-0.2762250	0.3484400	-2.5789720	C	2.9992440	-1.3990090	-0.9325200
N	-1.7759800	2.3635280	1.1718470	N	2.5485670	-1.8520240	0.2462950
H	-2.5437620	2.6643130	1.7729550	C	2.3877430	-0.9150030	1.1981830
H	1.6262910	2.3422850	-2.8344950	C	2.5874010	0.4372760	0.9562300
O	0.8151750	3.0924900	0.2751690	C	2.9761180	0.7869740	-0.3455540
H	1.0627340	2.4357130	-1.3903430	N	3.2225920	-0.1369260	-1.2874270
H	-0.1241270	3.1730470	0.5443520	H	2.4442580	1.1890390	1.7196900
SINT6_{2H2O}				N	3.1721630	-2.3478890	-1.9062920
H = -1155.572907 a.u.				H	3.2972840	-3.2946020	-1.5868960
G = -1155.657034 a.u.				H	3.6962790	-2.0549210	-2.7148230
C	-2.9169420	-0.2169640	-0.7687360	N	2.0056760	-1.3689880	2.4327850
O	-2.8119980	1.1894630	-0.5448160	H	1.7144270	-2.3327610	2.4798710
C	-0.3472920	0.5910280	0.7165580	H	1.5543960	-0.7215580	3.0596460

N 3.1326720 2.0886980 -0.6891970
H 2.6098890 2.7687420 -0.1436110
H 3.2378320 2.2644580 -1.6761970
O 0.9837450 3.4419900 0.8524440
H 0.5483020 2.8841320 1.5092550
H 0.3142530 3.5399840 0.1573120
O -1.0003260 3.2502130 -1.1691190
H -1.6442930 2.5320740 -1.0638640
H -1.4095000 3.9024990 -1.7403250

STS6_7₂H₂O

H = -1155.554541 a.u.

G = -1155.632473 a.u.

C -2.6460210 -0.3480030 -0.4333280
O -2.9915140 0.7586680 0.3992050
C -0.0898690 0.5053260 0.6067220
C -0.2493640 -0.9666500 0.2651610
C -1.7387090 -1.3393000 0.3259690
H -2.1180790 0.0162440 -1.3253950
H -0.2054400 1.1439820 -0.2859000
H 0.2693360 -1.5970500 0.9980210
H -2.0552470 -1.3451520 1.3744830
O -1.8067090 -2.6425440 -0.2268540
H -2.6890820 -2.9861940 -0.0431300
O 0.2667300 -1.1670890 -1.0295050
H -0.0007440 -2.0498960 -1.3092560
O -0.5163560 0.9088770 1.7276640
H -2.3327340 0.8568110 1.1095140
C -3.9322280 -1.0069360 -0.8954140
H -3.7361980 -1.5981270 -1.7954390
H -4.6528410 -0.2195050 -1.1320560

O -4.4178120 -1.8498650 0.1475900
H -5.3627140 -1.9776350 0.0503200
C 3.3362290 -1.0030900 -0.6153200
N 3.0443020 -1.2409850 0.6794660
C 2.3886730 -0.2705270 1.3000390
C 1.8957300 0.8792440 0.6208570
C 2.3681240 1.0277900 -0.7275730
N 3.0760100 0.0908100 -1.3451950
H 1.7261750 1.7855570 1.1837630
N 3.9875330 -1.9943530 -1.2537260
H 4.2582400 -2.8146680 -0.7402370
H 4.2609350 -1.8609420 -2.2115200
N 2.1019920 -0.4129670 2.6129810
H 2.2600780 -1.3277420 3.0084800
H 1.3195220 0.1256820 2.9683910
N 2.0458340 2.1473780 -1.3819620
H 1.4284940 2.8239320 -0.9369130
H 2.2929620 2.2247440 -2.3549940
O 0.0216370 3.5020380 0.3631970
H -0.1991590 2.9172930 1.1041380
H -0.8177190 3.5750390 -0.1208460
O -2.4816440 3.1423650 -0.8878180
H -2.8074980 2.3353150 -0.4464430
H -3.2180440 3.7564220 -0.9064550

SINT7₂H₂O

H = -1155.567566 a.u.

G = -1155.642612 a.u.

C -2.8128690 -0.1774550 -0.1768560
O -2.7437310 1.1890050 0.1858570
C -0.0352190 0.5319780 0.4257230

C	-0.4424760	-0.9312850	0.5215780	N	1.3706060	0.9221380	-2.2314170
C	-1.9593540	-1.0718000	0.7412060	H	0.5906380	1.5798530	-2.1155650
H	-2.4575150	-0.3078810	-1.2130890	H	1.6604000	0.6494290	-3.1588380
H	-0.4908540	0.9070410	-0.4969980	O	-0.8316440	2.7869680	-1.7613510
H	0.0498250	-1.4149450	1.3776540	H	-1.6652190	2.4166670	-1.4394860
H	-2.1846980	-0.7933470	1.7783660	H	-0.4991470	3.2842960	-0.9875910
O	-2.2132080	-2.4550980	0.5337600	O	0.1580200	3.5621490	0.6752110
H	-3.1266780	-2.5815210	0.2443220	H	-0.1316930	2.7121360	1.1533640
O	-0.0490740	-1.5615490	-0.6824080	H	-0.0310760	4.3060910	1.2489280
H	-0.5079520	-2.4103090	-0.7044000	STS7_8₂H₂O			
O	-0.4283050	1.2355820	1.5366590	H = -1155.564613 a.u.			
H	-2.0489880	1.3217020	0.8739540	G = -1155.638721 a.u.			
C	-4.3004510	-0.5321220	-0.1110020	C	-2.9064340	-0.0268590	-0.2438240
H	-4.8623100	0.2561120	-0.6188460	O	-2.8837770	1.3278780	0.1560190
H	-4.6214790	-0.5555040	0.9330040	C	-0.0345280	0.6007620	0.3821520
O	-4.6067760	-1.8154820	-0.6527580	C	-0.5636070	-0.8200530	0.4964660
H	-4.4974890	-1.7857420	-1.6071020	C	-2.0863600	-0.9133540	0.7051190
C	3.4935210	-1.0966600	-0.3530790	H	-2.4974910	-0.1282470	-1.2621820
N	3.2382590	-0.8754550	0.9578200	H	-0.4432100	1.0552970	-0.5275760
C	2.2952570	0.0039340	1.2156860	H	-0.1054490	-1.3168390	1.3640630
C	1.5124050	0.7133830	0.1623300	H	-2.3213440	-0.6026090	1.7316370
C	1.9562300	0.3244010	-1.2108090	O	-2.3599600	-2.2988530	0.5452690
N	2.9297030	-0.5389090	-1.4376000	H	-3.2399540	-2.4206780	0.1629420
H	1.6605610	1.7949520	0.2705260	O	-0.1840940	-1.4799520	-0.6918890
N	4.4527240	-1.9943290	-0.5976510	H	-0.6555210	-2.3221820	-0.6906890
H	4.9052210	-2.4529130	0.1752690	O	-0.4214170	1.3236710	1.5227460
H	4.6798460	-2.2228650	-1.5509760	H	-2.1833020	1.4770220	0.8101440
N	1.9544940	0.2912930	2.4631950	C	-4.3889090	-0.4041060	-0.2622050
H	2.3747900	-0.2446310	3.2080080	H	-4.9362040	0.3872900	-0.7804380
H	1.0587940	0.7893820	2.5806300	H	-4.7644870	-0.4594430	0.7621280

O	-4.6389210	-1.6786880	-0.8496670	C	-0.4659210	-0.8919880	0.6597060
H	-4.4812330	-1.6251660	-1.7961700	C	-1.9940910	-1.0210740	0.7922720
C	3.1807940	-1.4637380	-0.3588860	H	-2.3050750	-0.4078310	-1.2524790
N	2.9581600	-1.2286120	0.9691240	H	-0.4710060	0.9925390	-0.3325780
C	2.1913160	-0.2104850	1.2482210	H	-0.0342200	-1.3439870	1.5641340
C	1.5237570	0.6439790	0.2124070	H	-2.3001920	-0.6424670	1.7782200
C	1.9938770	0.2872890	-1.1758730	O	-2.2232290	-2.4182720	0.7201580
N	2.7959340	-0.7545140	-1.4125160	H	-3.0921370	-2.5949040	0.3347530
H	1.7886790	1.6928260	0.3946710	O	-0.0150480	-1.5705520	-0.4887050
N	3.9178620	-2.5536790	-0.6030910	H	-0.3987190	-2.4544190	-0.4513160
H	4.2531090	-3.1042730	0.1688580	O	-0.3866500	1.2156480	1.7236210
H	4.1325050	-2.7968940	-1.5555350	H	-2.3128290	1.3325050	0.8328430
N	1.9452320	0.1034610	2.5198420	C	-4.2535860	-0.6271040	-0.3359780
H	2.3003240	-0.5097480	3.2379470	H	-4.7747030	0.0967730	-0.9680040
H	1.1915360	0.7526330	2.7201960	H	-4.6875490	-0.5727030	0.6656830
N	1.6114090	1.0667650	-2.1464570	O	-4.4648150	-1.9593070	-0.7908860
H	1.0242620	2.0211600	-1.9659250	H	-4.2767320	-2.0081430	-1.7322550
H	1.9552100	0.8075410	-3.0624510	C	3.4344840	-1.0893250	-0.6022180
O	0.3741730	3.1966440	-1.5988880	N	3.2536330	-1.0093940	0.7685760
H	-0.5213930	3.3040020	-1.9263330	C	2.3579680	-0.1671930	1.1725560
H	0.4016910	3.4360950	-0.4148410	C	1.5241630	0.6852150	0.2558710
O	0.4711550	3.4931540	0.7755920	C	1.8482110	0.4479950	-1.2138270
H	-0.1302370	2.3104270	1.3354940	N	2.8355490	-0.4318530	-1.5594260
H	0.3156390	4.3764080	1.1108380	H	1.7622620	1.7350510	0.4667080
SINT8_{2H2O}				N	4.3804160	-1.9854500	-0.9465050
H = -1155.567819 a.u.				H	4.8835120	-2.4705550	-0.2246490
G = -1155.644893 a.u.				H	4.6103370	-2.1032100	-1.9180590
C	-2.7752350	-0.2361820	-0.2733700	N	2.1420670	-0.0040920	2.4884250
O	-2.7626250	1.1628180	-0.0061220	H	2.6287180	-0.6133670	3.1274430
C	0.0105230	0.5462340	0.5336500	H	1.3352130	0.5214730	2.7973810

N	1.1859730	1.1278700	-2.0777280	O	-4.1479230	1.3448910	-0.6863080
H	-0.1455320	2.3467800	-1.8841030	H	-5.0337790	1.7041360	-0.7599230
H	1.5147910	0.8809010	-3.0101420	C	1.8451870	2.3349570	-0.4027260
O	-0.8417660	2.9948310	-1.6073680	N	1.8268200	1.4399120	-1.4179190
H	-1.6382580	2.4811130	-1.4238510	C	1.2001930	0.2894760	-1.1474360
H	-0.2401820	3.5768570	-0.1510360	C	0.7050360	-0.0372670	0.1282710
O	0.1213510	3.6658050	0.7665240	C	0.6765690	1.0470310	1.1109970
H	-0.2320390	2.1734130	1.5774850	N	1.3169030	2.2242690	0.7953470
H	0.0540270	4.5873800	1.0206760	H	2.4298970	-0.0999310	0.5245040

STS8_9_{2H2O}

H = -1155.526334 a.u.

G = -1155.598666 a.u.

C	-2.5072580	0.3266260	0.7166080
O	-2.3186360	-0.2131340	1.9948710
C	0.0753010	-1.3614190	0.4934240
C	-1.2848330	-1.8011660	-0.1137410
C	-2.3525270	-0.7359570	-0.3795990
H	-1.7754470	1.1156800	0.5078120
H	-0.0639050	-1.3372150	1.5729780
H	-1.6993600	-2.5270300	0.5882430
H	-3.3031020	-1.2822590	-0.4784390
O	-2.0319140	-0.1497060	-1.6374760
H	-2.7097370	0.5155090	-1.8144780
O	-1.0517880	-2.5014240	-1.3445410
H	-1.4631450	-1.9731870	-2.0429210
O	0.9652410	-2.4896590	0.2480280
H	-1.4303720	0.1319240	2.3033510
C	-3.9016780	0.9330840	0.6606070
H	-3.9535460	1.7814960	1.3482030
H	-4.6273590	0.1731030	0.9729160

N	2.5540960	3.4831270	-0.6692670
H	2.6651430	3.7049520	-1.6457530
H	2.3662160	4.2519300	-0.0453640
N	1.2350510	-0.6371520	-2.1624110
H	1.4578650	-0.2249840	-3.0570940
H	0.4861000	-1.3129030	-2.1794880
N	0.0995150	0.8820520	2.2711350
H	3.8377470	0.1554470	-0.1944370
H	0.2457710	1.7235740	2.8227120
O	3.4611030	-0.2060280	0.6213860
H	3.5900030	-1.2923820	0.7487070
H	0.7133700	-2.8791550	-0.6013100
O	3.4123850	-2.5890140	0.9083850
H	3.5716530	-2.9445500	1.7873220
H	2.4256010	-2.6692250	0.6910640

N	2.5540960	3.4831270	-0.6692670
H	2.6651430	3.7049520	-1.6457530
H	2.3662160	4.2519300	-0.0453640
N	1.2350510	-0.6371520	-2.1624110
H	1.4578650	-0.2249840	-3.0570940
H	0.4861000	-1.3129030	-2.1794880
N	0.0995150	0.8820520	2.2711350
H	3.8377470	0.1554470	-0.1944370
H	0.2457710	1.7235740	2.8227120
O	3.4611030	-0.2060280	0.6213860
H	3.5900030	-1.2923820	0.7487070
H	0.7133700	-2.8791550	-0.6013100
O	3.4123850	-2.5890140	0.9083850
H	3.5716530	-2.9445500	1.7873220
H	2.4256010	-2.6692250	0.6910640

SINT9_{2H2O}

H = -1155.530213 a.u.

G = -1155.612713 a.u.

C	-2.8265570	-0.7503030	-0.5636430
O	-2.4618280	-0.8071610	-1.9211130
C	-0.3937330	0.6101570	-0.6377490

C	-1.5133690	1.5357260	-0.2729190	N	0.2732410	-1.8022500	-1.7297940
C	-2.8034660	0.6834320	0.0143540	H	4.7963050	-0.5050520	-0.2624700
H	-2.1540220	-1.3568010	0.0558910	H	0.7405010	-2.6007600	-2.1564860
H	-0.4629080	0.3805180	-1.6941350	O	4.4753530	-0.1361700	-1.0934730
H	-1.6943360	2.1461800	-1.1577150	H	3.7641070	1.5271530	-0.8773700
H	-3.6559720	1.2448580	-0.3925820	H	0.4012610	3.4533750	-0.2962080
O	-2.9022290	0.6232020	1.4290790	O	3.4030300	2.4219640	-0.7424990
H	-3.6685870	0.0737880	1.6462660	H	4.0119930	3.0116060	-1.1917800
O	-1.2796590	2.4164920	0.8176930	H	1.6299440	2.8686640	-1.0165350
H	-1.9858750	2.2524940	1.4607140	(R)-INT6'			
O	0.7050500	3.1338250	-1.1503720	H = -1079.572137 a.u.			
H	-1.5835410	-1.2358440	-1.9917450	G = -1079.647489 a.u.			
C	-4.2368370	-1.3302600	-0.5025270	C	-2.7665090	0.2905620	-1.0648780
H	-4.1942220	-2.3754660	-0.8193820	O	-2.0238930	-0.5548130	-1.9304970
H	-4.8633340	-0.7713910	-1.2066630	C	-0.4163460	-1.0503540	0.0068900
O	-4.7469090	-1.2198510	0.8262690	C	-1.3934430	-0.4306070	0.9670050
H	-5.6452520	-1.5538070	0.8604000	C	-2.7997340	-0.3399130	0.3236840
C	2.6290100	-1.6193340	0.8066960	H	-3.7991990	0.3882980	-1.4173080
N	2.1119440	-0.7563160	1.7235540	H	-1.0614220	0.5885720	1.1801360
C	1.0924370	-0.0181040	1.3369360	H	-3.4143890	0.2500250	1.0057040
C	0.5047220	-0.1660560	-0.0019220	O	-3.2692460	-1.6748030	0.2075780
C	0.9996440	-1.3524150	-0.7682340	H	-4.1737160	-1.7417900	0.5245940
N	2.1820400	-1.9444980	-0.3811380	O	-1.4275870	-1.1434320	2.1629040
H	3.8006440	-0.7730960	-1.3662840	H	-1.8733200	-1.9841420	1.9961420
N	3.8261680	-2.1689990	1.1898720	C	-2.0898980	1.6537270	-1.0765530
H	4.0341390	-2.1091720	2.1749310	H	-2.3028800	2.1531550	-2.0257590
H	4.0861190	-3.0211220	0.7162280	H	-1.0017190	1.5306950	-0.9971940
N	0.6435210	0.9120020	2.1748170	O	-2.6034780	2.3668450	0.0314890
H	1.1675700	1.0518600	3.0245550	H	-2.3179400	3.2823890	-0.0098620
H	-0.0365050	1.5969660	1.8585840	O	-0.1797990	-2.2643980	0.0853460

H	-2.5307490	-1.3651120	-2.0577230	H	3.8804020	-0.4323570	-1.3590160
H	0.1095740	-0.4476280	-0.7385260	H	0.9099430	-1.0603810	0.8444410
C	1.8205420	1.6582430	-0.6746900	H	3.2477620	-0.8356040	0.9553730
N	1.2318360	1.8823900	0.5045830	O	3.2818120	1.2293180	0.6703360
C	1.5062390	1.0130280	1.4866540	H	4.1871290	1.1428560	0.9811210
C	2.3158270	-0.1211540	1.2721250	O	1.2558710	0.3174470	2.2889330
C	2.8669370	-0.2244760	0.0041220	H	1.7832590	1.1212720	2.3916520
N	2.6245350	0.6294800	-0.9859450	C	2.0795030	-1.5935910	-1.5141030
H	2.5404140	-0.8220680	2.0646740	H	2.3672780	-1.8600680	-2.5343160
N	1.5388580	2.5320190	-1.6743480	H	0.9960230	-1.4069710	-1.5087510
H	1.1683600	3.4306460	-1.4096610	O	2.4285130	-2.5939670	-0.5783330
H	2.1115240	2.4837180	-2.5023250	H	2.1966070	-3.4601230	-0.9209140
N	0.9262980	1.2546360	2.6799600	O	0.4842600	2.1239120	0.3870950
H	0.4547510	2.1347700	2.8161260	H	2.7744240	1.5305820	-1.6647590
H	1.0977950	0.6662990	3.4776170	H	-0.0284340	0.5663560	-0.8145150
N	3.6805050	-1.3182440	-0.3537900	C	-2.5470180	-1.3486910	-0.7261380
H	4.1745360	-1.7339570	0.4283870	N	-1.8856950	-1.9336490	0.2796370
H	4.3285870	-1.0518830	-1.0896970	C	-1.5146480	-1.1398720	1.2851720
H	0.6215010	-2.5911240	-0.5945760	C	-1.6874640	0.2697510	1.2324610
O	1.6831930	-2.8912660	-1.3066150	C	-2.5309000	0.7138410	0.1986040
H	2.5153080	-2.3970500	-1.0550930	N	-2.9219960	-0.0537700	-0.8039160
H	1.6435510	-3.0351870	-2.2566720	H	-1.4602160	0.8876220	2.0914030
(R)-TS6'_8'				N	-2.8769840	-2.1269980	-1.7717490
H = -1079.567218 a.u.				H	-2.7577840	-3.1233830	-1.6880920
G = -1079.641226 a.u.				H	-3.4911670	-1.7546470	-2.4774550
C	2.8194120	-0.3279130	-1.1030060	N	-0.9245470	-1.7203630	2.3419480
O	2.2381520	0.7450890	-1.8225820	H	-0.7928170	-2.7198400	2.3312020
C	0.4205590	0.8893290	0.1250680	H	-0.4882950	-1.1671100	3.0636900
C	1.2826880	-0.0408350	0.9362940	N	-2.9453050	2.0410660	0.1361960
C	2.7324950	-0.0504550	0.3972330	H	-2.9847450	2.5165370	1.0294870

H -3.8130870 2.1315940 -0.3830370
H -0.0083120 2.6861380 -0.3297550
O -0.8694050 3.3181130 -1.3081940
H -1.7762910 3.0205510 -1.1152180
H -0.7413790 3.4243020 -2.2549110

(R)-INT8'

H = -1003.187817 a.u.

G = -1003.253997 a.u.

C -2.9492060 0.2847420 -1.0176170
O -2.2934670 -0.6527290 -1.8615610
C -0.1630310 -0.6685040 -0.0133550
C -1.1828760 0.0592790 0.8759940
C -2.6516060 -0.0742910 0.4393950
H -4.0358500 0.2115940 -1.1413830
H -0.9493520 1.1281870 0.8832040
H -3.2120300 0.6175420 1.0737310
O -3.0339800 -1.4165530 0.7102770
H -3.9809420 -1.4648530 0.8674590
O -1.0718590 -0.4001280 2.2110700
H -1.5581820 -1.2342340 2.2706010
C -2.5049840 1.7018510 -1.3714810
H -2.9055640 1.9671120 -2.3555840
H -1.4094100 1.7324140 -1.4363950
O -2.9873990 2.5579670 -0.3566040
H -2.9587480 3.4708860 -0.6524010
O -0.4822930 -2.0339300 -0.1551010
H -2.8193220 -0.8227160 -2.6465690
H -0.1179080 -0.1768030 -0.9923900
C 3.2737050 0.8201110 -0.5140200
N 2.6549850 1.3728920 0.5537010

C 1.7533660 0.6403470 1.1601840
C 1.2661260 -0.6869120 0.6198390
C 2.2479350 -1.1987590 -0.4124760
N 3.1649720 -0.4459900 -0.9704870
H 1.2076250 -1.3964070 1.4497170
N 4.1210820 1.6033880 -1.1639390
H 4.2797320 2.5440200 -0.8365880
H 4.6469400 1.2301700 -1.9395040
N 1.2517910 1.0624750 2.3085350
H 1.5854010 1.9413360 2.6803730
H 0.5035960 0.5529340 2.7707820
N 2.1464920 -2.4646650 -0.7784760
H 1.3381750 -3.0053490 -0.4986390
H 2.7581310 -2.8020290 -1.5091550
H -1.3321470 -2.0946950 -0.6160350

(R)-

TS8'_9'

H = -1003.117794 a.u.

G = -1003.183943 a.u.

C -3.2425570 0.6779520 0.4185710
O -2.5892860 1.8656260 0.0065190
C -0.2728060 0.2214900 -0.3071210
C -1.2652960 -0.9311610 -0.1844070
C -2.7226440 -0.4955120 -0.4144260
H -4.3192370 0.7458850 0.2175650
H -1.1833540 -1.3449680 0.8254970
H -3.3407410 -1.3666110 -0.1834680
O -2.7900690 -0.2109690 -1.8185930
H -3.6960640 -0.0572460 -2.1044090
O -0.9757890 -1.9673760 -1.1033120
H -1.5158030 -1.8616070 -1.8953590

C	-3.0409280	0.4330260	1.9131640	C	0.0406670	0.4550790	0.1058700
H	-3.5969500	1.1886340	2.4778900	C	1.2047470	-0.2291310	0.7849460
H	-1.9767030	0.5451990	2.1594480	C	2.5505200	0.2743970	0.2616130
O	-3.5012390	-0.8743280	2.1789880	H	3.6716310	0.3532620	-1.5491140
H	-3.6082750	-1.0074230	3.1241400	H	1.1399810	-1.3107890	0.6053030
O	-0.3386950	0.7862280	-1.6965050	H	3.3317780	-0.0609470	0.9544370
H	-3.1480880	2.6273760	0.1814600	O	2.4882100	1.6956960	0.2550010
H	-0.5672070	1.0224310	0.3676980	H	3.3577780	2.0563220	0.0564960
C	3.8454440	0.0579130	0.4426230	O	1.0683650	0.0368670	2.1802870
N	3.2635320	-1.1461120	0.3561560	H	1.9127010	-0.1000820	2.6231410
C	1.9829290	-1.1937320	0.0251770	C	3.4767710	-1.7058660	-1.0170110
C	1.2335950	0.0117830	-0.3264470	H	3.7261000	-2.0498190	-2.0272630
C	1.9916920	1.2408220	-0.0770380	H	2.7274660	-2.3920990	-0.6031270
N	3.2659230	1.2578170	0.2499200	O	4.6218900	-1.6220170	-0.1950630
H	0.7471020	0.2741580	-1.7299380	H	5.1387810	-2.4283110	-0.2624890
N	5.1408390	0.0724670	0.7582080	O	0.2100360	3.4168310	0.5210690
H	5.6233730	-0.7976340	0.9135960	H	1.9428370	-0.3960930	-2.8306940
H	5.6229910	0.9528670	0.8378690	H	0.3107110	1.2391550	-0.5902510
N	1.4326460	-2.4117630	0.0335780	C	-3.6410880	-0.8471680	-0.4446880
H	2.0692280	-3.1695390	0.2346090	N	-2.9853990	-1.5028280	0.5427950
H	0.5656040	-2.6090750	-0.4484290	C	-1.8551280	-0.9788680	0.9556110
N	1.3963750	2.4451550	-0.1900780	C	-1.2639920	0.1806410	0.2539140
H	0.5145080	2.5711660	-0.6599170	C	-2.2660490	0.9460200	-0.5237230
H	1.9977350	3.2485410	-0.0818030	N	-3.3927440	0.3912980	-0.9150290
H	-1.1792860	0.5859740	-2.1682760	H	0.2120520	4.1661880	1.1210780
(R)-INT9'				N	-4.6947740	-1.4716250	-0.9550710
H	-1003.175346	a.u.		H	-4.9598660	-2.3753990	-0.5959410
G	-1003.246787	a.u.		H	-5.2547720	-1.0086040	-1.6539190
C	2.8999260	-0.2956280	-1.1155620	N	-1.2242650	-1.5323840	1.9839610
O	1.7241670	-0.2867170	-1.9012360	H	-1.6710700	-2.3214110	2.4301450

H	-0.4420270	-1.0625550	2.4302200	C	-2.7682520	1.1465620	-0.5250280
N	-1.9999530	2.2002100	-0.8477970	C	-3.1635170	0.8673190	0.7708310
H	-1.2243040	2.7145230	-0.4248680	C	-3.0160710	-0.4699700	1.1778000
H	-2.6836040	2.6911220	-1.4068340	N	-2.5523440	-1.4160720	0.3436150
H	1.0641720	2.9707080	0.6153810	H	-3.5335580	1.6308680	1.4414510
(S)-INT6'				N	-1.8143030	-2.0017020	-1.7608180
H = -1079.574556 a.u.				H	-1.9220430	-1.7622510	-2.7382520
G = -1079.649343 a.u.				H	-2.1430790	-2.9304600	-1.5270500
C	3.2556560	-0.6712770	0.2097460	N	-2.7120980	2.4602210	-1.0100990
O	2.6104840	-0.7941820	1.4827680	H	-2.8037470	2.4881560	-2.0207050
C	0.3350260	-0.4708910	0.8495520	H	-3.3568420	3.0998720	-0.5608190
C	0.8669400	-0.6547150	-0.5381140	N	-3.2875820	-0.8675890	2.4386730
C	2.2441930	0.0431990	-0.6763260	H	-3.3115230	-1.8579770	2.6254780
H	3.4616200	-1.6538580	-0.2236530	H	-3.7570180	-0.2523060	3.0816660
H	0.1676890	-1.3503590	1.4683590	O	-0.0130200	2.5091050	-0.2782150
H	0.1815940	-0.1482530	-1.2324140	H	0.4351030	3.3404060	-0.0892910
H	2.1546020	1.0791850	-0.3334770	H	-0.9276130	2.7040380	-0.5996250
O	2.6958420	-0.0278760	-1.9978050	H	0.0404880	1.4539620	0.6645960
H	2.5008900	0.7893230	-2.4625600	(S)-TS6'_8'			
O	0.9949420	-2.0165830	-0.8035340	H = -1079.564963 a.u.			
H	0.2024680	-2.3014460	-1.2805840	G = -1079.638768 a.u.			
O	-0.0178580	0.6293020	1.3239060	C	2.7771400	-1.0391810	0.3892430
H	2.9275180	-1.5793630	1.9391530	O	2.6966780	-0.4029340	1.6619600
C	4.5308350	0.1488880	0.3492500	C	0.2682810	0.4676050	1.1208760
H	4.9645190	0.3019430	-0.6398840	C	0.5410520	-0.0184410	-0.2690050
H	5.2564540	-0.3976450	0.9615770	C	2.0568920	-0.0753790	-0.5504900
O	4.2546610	1.4233720	0.8912040	H	2.2497070	-1.9999480	0.4055140
H	4.0280040	1.3140460	1.8191910	H	0.0408810	-0.2572730	1.8981020
C	-2.2775360	-1.0238120	-0.8965660	H	0.1207130	0.6896540	-0.9959470
N	-2.3207560	0.2187400	-1.3780310	H	2.4788960	0.9259860	-0.4194250

O	2.1443290	-0.4994820	-1.8887790	H	0.7509630	2.2778290	0.7158190
H	3.0147080	-0.2645050	-2.2307790	(S)-INT8'			
O	-0.0510610	-1.2805070	-0.3784980	H = -1003.192132 a.u.			
H	0.1505110	-1.6258630	-1.2572220	G = -1003.258634 a.u.			
O	0.5301100	1.6472530	1.4927450	C	2.8427260	-0.2281430	0.6186600
H	2.9936600	-1.0050610	2.3506900	O	2.8564870	1.1578940	0.9689760
C	4.2125870	-1.2636540	-0.0701420	C	0.0611550	0.9166150	0.4622920
H	4.2111990	-1.9469940	-0.9210810	C	0.4998520	-0.2253540	-0.4507180
H	4.7891790	-1.7375630	0.7321530	C	2.0128680	-0.3052520	-0.6724430
O	4.8206360	-0.0674980	-0.5167340	H	2.3580660	-0.8085480	1.4145880
H	5.0832300	0.4636200	0.2402160	H	0.4618000	0.7259110	1.4639110
C	-2.8802520	-0.9175760	-1.0231950	H	0.0476760	-0.0958200	-1.4442180
N	-2.5918090	0.3764130	-1.2902580	H	2.3287430	0.5276340	-1.3084110
C	-2.3298590	1.1290350	-0.2402160	O	2.1956810	-1.5414680	-1.3307000
C	-2.2141760	0.6217280	1.0614320	H	3.0602760	-1.5277330	-1.7573630
C	-2.6294190	-0.7306850	1.2134730	O	0.0133880	-1.4005620	0.1612530
N	-2.9735980	-1.4875000	0.1828920	H	0.3759890	-2.1539770	-0.3218460
H	-2.1049850	1.2741140	1.9182440	O	0.4964340	2.1707070	-0.0064040
N	-3.1055350	-1.7056150	-2.0871430	H	3.5590540	1.3428630	1.5982060
H	-3.1910930	-1.2852480	-2.9980070	C	4.2379570	-0.7907260	0.4014870
H	-3.4365960	-2.6438740	-1.9312780	H	4.1823290	-1.8837730	0.4291750
N	-2.0756130	2.4816710	-0.5041630	H	4.8956400	-0.4630890	1.2159440
H	-2.4985780	2.7468170	-1.3892540	O	4.7068820	-0.3379640	-0.8576010
H	-2.3791320	3.0970190	0.2426390	H	5.6439660	-0.5272290	-0.9500760
N	-2.6317160	-1.3090410	2.4375130	C	-3.3916330	-0.7568830	-0.3677390
H	-3.0311410	-2.2342020	2.4994450	N	-3.0171050	0.2216100	-1.2242720
H	-2.6638050	-0.7368730	3.2658380	C	-2.1371520	1.0853220	-0.7892700
O	0.7655400	3.0661980	-0.5640500	C	-1.4855460	1.0005820	0.5728240
H	1.1823820	3.9174250	-0.7291030	C	-2.1056650	-0.1169160	1.3795290
H	-0.1761420	3.1084910	-0.8134560	N	-3.0209460	-0.9247900	0.9215440

H -1.6920070 1.9403820 1.0980470
N -4.2468910 -1.6459090 -0.8446330
H -4.5802260 -1.5576020 -1.7925660
H -4.5737860 -2.3907110 -0.2481320
N -1.7749220 2.0918720 -1.5689770
H -2.1804950 2.1537410 -2.4927620
H -1.0061570 2.6956520 -1.3029620
N -1.7277840 -0.2380830 2.6461260
H -2.1277300 -0.9843830 3.1975370
H -1.0355590 0.3607850 3.0648140
H 1.4376290 2.2486680 0.2156730

(S)-TS8' 9'

H = -1003.120356 a.u.

G = -1003.186652 a.u.

C 3.0077380 0.6554450 -0.3544780
O 2.5443680 0.4321100 -1.6970880
C 0.0484770 0.1433650 -0.3246490
C 0.9136880 -0.2224110 0.8654450
C 2.3841330 -0.4595930 0.5053620
H 2.6607580 1.6356820 -0.0064460
H 0.3332320 1.1491010 -0.6393420
H 0.5454340 -1.1187380 1.3766430
H 2.4757640 -1.3960000 -0.0570100
O 3.0275060 -0.5510510 1.7556170
H 3.8765520 -0.9907330 1.6277720
O 0.7669530 0.9122400 1.6943970
H 1.3090760 0.7820170 2.4824160
O 0.2396230 -0.7297290 -1.5008510
H 3.0588360 0.9507220 -2.3229530
C 4.5242420 0.6201250 -0.2664930

H 4.8299930 1.0871780 0.6751180
H 4.9526070 1.2053290 -1.0893600
O 4.9354570 -0.7345250 -0.3217700
H 5.8849880 -0.7896170 -0.4569450
C -4.1238990 -0.0582180 -0.0136680
N -3.4720030 -1.2302970 0.1002330
C -2.1565180 -1.1888410 0.0101870
C -1.4538130 0.0479220 -0.2867390
C -2.2659030 1.2286540 -0.0721330
N -3.5784510 1.1747630 -0.0335220
H -0.9296520 -0.4007730 -1.6228870
N -5.4535290 -0.1194600 -0.0642880

H -5.9125750 -1.0136330 0.0015840
H -5.9883360 0.7332380 -0.1037010
N -1.5042440 -2.3580240 0.1429990
H -2.0747250 -3.1883840 0.2144490
H -0.5399660 -2.4666490 -0.1232120
N -1.6793170 2.4366170 0.0640880
H -2.3129150 3.1962920 0.2728750
H -0.7662240 2.4892120 0.4940370
H 1.0298340 -0.4204950 -2.0090490

(S)-INT9'

H = -1003.176602 a.u.

G = -1003.24673 a.u.

C -2.7775910 0.7095600 -0.4481850
O -1.9874690 1.5913780 0.3619180
C 0.1837560 0.2897220 -0.8414230
C -0.8156740 -0.7924250 -1.1267510
C -2.1218230 -0.6712190 -0.3240290
H -2.7449870 1.0374220 -1.4934180

H 0.0079330 1.1812940 -1.4391550
H -0.3935440 -1.7776230 -0.9005480
H -1.9282720 -0.8674600 0.7326380
O -2.9566960 -1.6665820 -0.8755890
H -3.6438060 -1.8759700 -0.2334560
O -1.0884840 -0.6678410 -2.5051220
H -1.7648400 -1.3198320 -2.7274310
O -0.6839090 0.2204320 2.4398220
H -2.3931900 2.4638720 0.3677350
C -4.2262420 0.6603980 0.0069650
H -4.8271530 0.2011750 -0.7844380
H -4.5965600 1.6800950 0.1678710
O -4.2801160 -0.1047900 1.2006620
H -5.1620360 -0.0594480 1.5788850
C 3.9142140 -0.2898410 0.0294870
N 3.1053800 -1.2409660 0.5456780
C 1.8255840 -0.9535680 0.5918040
C 1.3051460 0.2377680 -0.1040830
C 2.3234490 1.2998050 -0.2156170
N 3.5991160 1.0084330 -0.2093350
H -0.9675950 0.2774290 3.3558700
N 5.1752620 -0.6335670 -0.1826540
H 5.4781540 -1.5720930 0.0285990
H 5.8316140 0.0578410 -0.5117950
N 0.9766320 -1.7523540 1.2270980
H 1.3735990 -2.5525280 1.7027760
H 0.1276990 -1.3320340 1.6035810
N 1.9354380 2.5616380 -0.3823660
H 2.6411920 3.2734280 -0.5082890
H 0.9760840 2.8350450 -0.2442920

H -1.2486080 0.8251290 1.9333810

INT10'

H = -926.7600897 a.u.

G = -926.8248937 a.u.

C -2.9019890 0.6513220 0.8264340
O -1.7127380 1.1521240 1.4134290
C -0.0643620 0.4639130 -0.5808970
C -1.2075200 -0.5266190 -0.6898960
C -2.5696200 0.1534410 -0.5798080
H -3.6559170 1.4416200 0.7262090
H -1.1025780 -1.2892570 0.0867810
H -3.3256600 -0.5872850 -0.8587330
O -2.5166990 1.1948350 -1.5473100
H -3.4048820 1.5018540 -1.7502160
O -1.1261370 -1.2123770 -1.9341940
H -1.4214620 -0.6105720 -2.6300110
C -3.5009710 -0.4614140 1.6817200
H -3.6737130 -0.0716830 2.6920670
H -2.7963740 -1.2998800 1.7578120
O -4.7056480 -0.8419950 1.0549800
H -5.1844370 -1.4670260 1.6042620
H -1.9197550 1.6340520 2.2191090
H -0.3632380 1.5056020 -0.5496780
C 3.6032030 -0.2659660 0.7198720
N 2.9474690 -1.3694420 0.3089040
C 1.8290020 -1.1850540 -0.3585230
C 1.2439690 0.1680810 -0.4970180
C 2.2443040 1.2390080 -0.2874210
N 3.3601310 1.0178190 0.3592220
N 4.6476630 -0.4590500 1.5116240

H	4.9079770	-1.3978790	1.7725850	C	3.5688690	-0.3170360	-0.4296510
H	5.2021340	0.3305640	1.8052960	N	3.0226960	0.8230820	-0.8605340
N	1.2175470	-2.2370900	-0.8817870	C	1.8015620	1.1166640	-0.4317370
H	1.6599280	-3.1377490	-0.7568440	C	1.0874060	0.2371940	0.4454230
H	0.4312270	-2.1359590	-1.5192070	C	1.8299070	-0.8946780	0.8874310
N	1.9947230	2.4702470	-0.7281430	N	3.0329460	-1.1864040	0.4643090
H	1.2278740	2.6759500	-1.3466780	N	4.7751890	-0.6366280	-0.9040610
H	2.6798210	3.1892680	-0.5435210	H	5.2389380	-0.0120140	-1.5434600

TS10' _11'

H = -926.7358372 a.u.

G = -926.7976322 a.u.

C	-2.4590200	-0.9635830	-0.1201450
O	-1.0103630	-1.1486230	-0.0451450
C	-0.3118860	0.2584830	0.7176290
C	-1.3124500	1.1939500	0.0507270
C	-2.6732800	0.5120610	0.2483410
H	-2.9511220	-1.6124700	0.6058000
H	-1.0783530	1.2686940	-1.0135130
H	-3.4389380	0.9586400	-0.3887590
O	-2.9746910	0.6785080	1.6201660
H	-3.9246290	0.6430280	1.7666620
O	-1.2571740	2.4802160	0.5934200
H	-1.7496610	2.4853650	1.4257220
C	-2.9063320	-1.3009480	-1.5323180
H	-2.6349040	-2.3356100	-1.7657860
H	-2.4036220	-0.6380810	-2.2482650
O	-4.2996090	-1.1027280	-1.5111980
H	-4.6905420	-1.3746700	-2.3456650
H	-0.6909950	-1.9324090	0.4398780
H	-0.6221520	0.0068720	1.7318770

H	5.2339800	-1.4700360	-0.5746220
N	1.2836170	2.2904370	-0.8467700
H	1.9103890	2.8732410	-1.3832850
H	0.5579600	2.7526840	-0.3144520
N	1.2010050	-1.8444580	1.6981910
H	0.7703710	-1.4630300	2.5341240
H	1.8511550	-2.5840300	1.9436640

INT11'

H = -926.7626605 a.u.

G = -926.8262285 a.u.

C	2.4943890	-0.8599230	-0.1849140
O	1.1386780	-0.9470410	-0.6687050
C	0.4851800	0.3379170	-0.6875600
C	1.3543800	1.1986500	0.2607890
C	2.7573180	0.6242480	0.0144130
H	3.1640350	-1.2743590	-0.9410400
H	1.0492750	1.0443710	1.2989190
H	3.4359340	0.8076000	0.8495230
O	3.2053070	1.2504330	-1.1738330
H	4.1602400	1.1751660	-1.2556540
O	1.2993370	2.5708060	-0.0118050
H	1.9404600	2.7584330	-0.7128610

C	2.6168110	-1.6592550	1.1032690	H	2.4540670	1.2738690	1.3969270
H	2.2904230	-2.6893750	0.9188660	H	1.8992790	-2.2831230	0.6597410
H	1.9693450	-1.2235340	1.8763530	H	4.2246830	-1.6068520	-0.6309300
O	3.9782360	-1.5907640	1.4555350	H	3.4165460	0.5577390	-1.3917120
H	4.1473340	-2.1125790	2.2438070	O	4.6524970	1.2132830	0.0560220
H	0.0095300	-2.0738120	-1.1376820	H	4.9119260	0.9299660	0.9410910
H	0.5829670	0.7647900	-1.6945260	O	4.1509150	-1.0487080	1.3749640
C	-3.6013290	-0.2938430	0.3211130	H	4.2876890	-1.9527240	1.6668510
N	-3.1042440	0.9172010	0.5510980	O	1.6967010	-1.5994070	-1.2910750
C	-1.8357060	1.1677300	0.2227400	H	-5.5061110	-1.8594550	1.0887630
C	-0.9790750	0.1437300	-0.3272140	C	1.4140880	1.8943620	-0.3793520
C	-1.6814080	-1.0186270	-0.5565600	H	1.1845350	1.4698030	-1.3673250
N	-2.9295110	-1.3054370	-0.2691770	H	1.9985550	2.8068600	-0.5179660
N	-4.8679490	-0.5351020	0.6922380	O	0.2348980	2.2490110	0.3090270
H	-5.4104970	0.2069660	1.1017940	H	-0.2335000	1.4290660	0.5219580
H	-5.2886080	-1.4275320	0.4976090	C	-4.1224370	-0.5034530	0.4956950
N	-1.4176700	2.4198190	0.4369960	N	-3.9665510	0.8090390	0.3139990
H	-2.0984750	3.0590850	0.8188570	C	-2.8447150	1.1801990	-0.3152020
H	-0.4981870	2.7623650	0.1824220	C	-1.8995410	0.2545880	-0.7664120
N	-1.0257790	-2.1662410	-1.2400070	C	-2.1800230	-1.0899130	-0.5040780
H	-1.2880090	-2.1725550	-2.2294710	N	-3.2894210	-1.4815940	0.1334240
H	-1.3855180	-3.0279390	-0.8209370	H	-1.0366610	0.5473420	-1.3494040
oINT1				N	-5.2497500	-0.8896950	1.1704850
H = -1002.751185 a.u.				H	-5.9896470	-0.2093890	1.2229410
G = -1002.820414 a.u.				H	2.1266330	-2.3740260	-1.6678290
C	2.2316300	0.8872020	0.3976430	N	-2.6776750	2.5246370	-0.5233040
O	1.4548090	-0.3146930	0.5595120	H	-3.3057170	3.1008080	0.0169340
C	2.1389790	-1.4070100	0.0478560	H	-1.7224550	2.8540850	-0.5702590
C	3.6187930	-1.0198040	0.0663620	N	-1.3382580	-2.0784250	-0.9248570
C	3.5302930	0.4641120	-0.3091810	H	-1.5192610	-2.9902470	-0.5365110

H -0.3799300 -1.8390540 -1.1390790

oTS1_2

H = -1002.662664 a.u.

G = -1002.730046 a.u.

C -1.6971540 0.9651600 -0.7102000

O -0.6892700 -0.0927600 -0.4464760

C -1.1865730 -1.0917150 0.1172530

C -2.6930900 -1.0895580 0.1058060

C -3.0127710 0.4060190 -0.1366420

H -1.7203890 1.0586910 -1.7971060

H -0.4978540 -1.9023750 0.3536890

H -3.1330760 -1.5007220 1.0095170

H -3.2230740 0.8843690 0.8176680

O -4.1102670 0.6080710 -0.9744560

H -4.0973780 -0.0726950 -1.6582090

O -3.0518440 -1.8000010 -1.0689750

H -3.2842230 -2.7086660 -0.8610040

O -1.4502290 0.0047580 2.2518850

H 2.8433210 -3.1115720 -1.3932140

C -1.1682970 2.2282730 -0.0590480

H -1.0823300 2.0482400 1.0179840

H -1.9059800 3.0158440 -0.2351540

O 0.0453080 2.6308370 -0.6342760

H 0.7237870 2.0041480 -0.3424000

C 2.6166990 -1.2212730 -0.7253580

N 3.0914600 0.0051080 -0.9515210

C 2.7780670 0.9173920 -0.0159460

C 1.9796550 0.6317720 1.0847110

C 1.5679170 -0.7184380 1.2549130

N 1.8881100 -1.6453620 0.3038910

H 1.7929090 1.3574730 1.8663140

N 2.8810320 -2.1545980 -1.7071740

H 3.6551720 -1.9171580 -2.3078100

H -1.9053490 -0.0122020 3.0976970

N 3.3195850 2.1679010 -0.2135300

H 3.6442020 2.3481630 -1.1507470

H 2.9072260 2.9486670 0.2710250

N 0.8127510 -1.0783620 2.2938320

H 0.7313090 -2.0929550 2.3004110

H -0.4551350 -0.3830820 2.4183060

oINT2

H = -1002.753790 a.u.

G = -1002.825769 a.u.

C -2.6690110 0.6811570 -0.1523570

O -1.2572960 0.7191250 -0.4064160

C -0.7878320 -0.5578880 -0.8177690

C -1.9992300 -1.5026560 -0.7669730

C -2.9453140 -0.7810540 0.2022060

H -3.2069680 0.9523190 -1.0700580

H -0.4065100 -0.4621910 -1.8424740

H -1.7366460 -2.5119270 -0.4360110

H -2.6338560 -0.9697230 1.2333050

O -4.2834520 -1.1678870 0.0775480

H -4.4753820 -1.2368350 -0.8650400

O -2.6779370 -1.5369600 -2.0094970

H -2.1980480 -2.0822510 -2.6367440

O -0.8747490 -0.2386920 2.7244790

H 4.4930050 -2.3211380 1.4487240

C -2.9890610 1.6692030 0.9452050

H -2.4424270 1.3853730 1.8504600

H -4.0614130 1.6328540 1.1474020
 O -2.6853920 2.9939860 0.5495030
 H -1.7383030 3.0308030 0.3885870
 C 3.7505530 -0.7688700 0.3704680
 N 4.1176040 0.3956540 -0.1716900
 C 3.1318670 1.1449690 -0.6680290
 C 1.7870750 0.7452170 -0.6401610
 C 1.5486170 -0.4892790 -0.0521190
 N 2.5123760 -1.2600230 0.4627090
 H 0.9877150 1.3792950 -0.9954350
 N 4.7556350 -1.5568620 0.8496920
 H 5.6505470 -1.1192100 0.9906990
 H -0.2393160 -0.2627750 3.4426920
 N 3.4947990 2.3559340 -1.1789800
 H 4.4797490 2.5046590 -1.3280910
 H 2.8523190 2.8538600 -1.7706760
 N 0.2646020 -1.0043230 0.0693770
 H 0.2767720 -1.9891630 0.3047150
 H -0.3517170 -0.2979890 1.9124320
oP_N
 H = -926.343058 a.u.
 G = -926.408055 a.u.
 C -3.1608510 -0.7789010 0.8589310
 N -1.8710810 -0.8816090 0.5235290
 C -1.4774680 -0.1263350 -0.5003800
 C -2.3431610 0.7273770 -1.1842800
 C -3.6625250 0.7506990 -0.7284130
 N -4.0831090 0.0046720 0.2972190
 H -2.0176800 1.3250900 -2.0250220
 N -3.5841210 -1.5825310 1.8758480

H -2.8756710 -2.0073430 2.4498770
 H -4.4787970 -1.3725410 2.2846060
 N -0.1589060 -0.2442290 -0.9053090
 N -4.6153000 1.5245090 -1.3362430
 H -5.4715790 1.6415960 -0.8176350
 H -4.3136250 2.3093380 -1.8887770
 C 2.7647290 0.5041610 0.5094620
 O 1.3940890 0.2615730 0.8093700
 C 0.8505300 -0.7697350 -0.0286140
 C 2.0452490 -1.3365510 -0.7987820
 C 2.9905570 -0.1294440 -0.8599350
 H 3.4010300 0.0007030 1.2467150
 H 0.3908680 -1.5301130 0.5973130
 H 1.7432750 -1.7103060 -1.7822340
 H 2.6801260 0.5618930 -1.6546400
 O 4.3489720 -0.4939430 -1.0079480
 H 4.5747340 -0.5355350 -1.9402790
 O 2.6274410 -2.3559750 -0.0227310
 H 3.5788960 -2.3368580 -0.1804970
 H 0.1468460 0.4950000 -1.5230680
 C 2.9985840 1.9987140 0.5592170
 H 2.3835410 2.4781670 -0.2169030
 H 4.0500310 2.2150650 0.3576220
 O 2.6977210 2.5220340 1.8315140
 H 1.8159680 2.2107440 2.0627270
pINT1
 H = -1002.753600 a.u.
 G = -1002.823036 a.u.
 C -2.2087810 0.8826310 -0.1050390
 O -1.6942770 -0.2673620 -0.7755480

C	-2.6501060	-1.3233250	-0.7587520	H	6.3325220	-0.8905300	0.4373620
C	-3.7989900	-0.8617930	0.1403580	N	2.8394850	2.4988890	-0.6316790
C	-3.1557800	0.2887780	0.9312480	H	1.8930350	2.8575300	-0.5961890
H	-2.7789030	1.4989380	-0.8104200	H	3.5774230	3.1423640	-0.4017460
H	-3.0041320	-1.4968800	-1.7784830	pTS1_2			
H	-4.1475600	-1.6861690	0.7691880	H = -1002.659963 a.u.			
H	-2.5807610	-0.1067830	1.7762910	G = -1002.726351 a.u.			
O	-4.1002530	1.2562230	1.3481490	C	-2.2543910	1.0029890	-0.3673100
H	-4.3904980	1.0623460	2.2422960	O	-1.2770060	-0.0166200	-0.8050190
O	-4.8327640	-0.3666690	-0.6774400	C	-1.6456020	-1.1795920	-0.5452950
H	-5.2303670	0.3836630	-0.2189990	C	-3.0850930	-1.2820220	-0.1135920
O	-2.0646730	-2.4722800	-0.2194590	C	-3.4245680	0.2019400	0.2133720
H	-1.4163130	-2.8074250	-0.8474460	H	-2.5341670	1.5212210	-1.2852200
C	-1.0640380	1.6929900	0.4652000	H	-0.9768920	-1.9882660	-0.8158620
H	-0.4967350	1.0670000	1.1704980	H	-3.2245650	-1.9635860	0.7197270
H	-1.4842430	2.5415730	1.0123760	H	-3.4774970	0.3389360	1.2920960
O	-0.2218230	2.1833000	-0.5474710	O	-4.6145100	0.6030610	-0.4412480
H	0.3923030	1.4502380	-0.7535070	H	-5.3555400	0.5515370	0.1677120
C	2.0651720	-0.8712330	-0.0220560	O	-3.7506600	-1.7359380	-1.2695300
N	3.2051860	-1.4774060	0.3110460	H	-4.3517270	-1.0315130	-1.5522120
C	4.2961470	-0.7030970	0.3192740	O	-1.4263100	-0.8313710	1.9757400
C	4.2626520	0.6586920	0.0150970	H	-1.4596560	-1.1916710	2.8642050
C	3.0115980	1.1834770	-0.3103460	C	-1.5166690	1.9298350	0.5971790
N	1.9092850	0.4181250	-0.3466430	H	-1.3804200	1.4009020	1.5449860
H	5.1503760	1.2753900	0.0461030	H	-2.1637240	2.7992200	0.7578380
N	0.9400530	-1.6396470	-0.0492860	O	-0.3073610	2.3362940	0.0447330
H	0.9851040	-2.5080210	0.4586130	H	0.3461730	1.5779170	0.1735490
H	0.0503250	-1.1593290	-0.1071170	C	1.7716830	-0.8225420	0.4081450
N	5.4598320	-1.3205600	0.6937770	N	2.9114300	-1.5052610	0.1249930
H	5.4346160	-2.3281290	0.6849110	C	3.9696110	-0.8024660	-0.2532520

C	3.9612650	0.5892110	-0.3862400	H	0.0373730	-1.0076920	3.3633950
C	2.7466910	1.2111420	-0.1035870	C	-1.3537040	1.9713090	0.6182700
N	1.6547070	0.5327040	0.2733960	H	-0.7199440	1.3756460	1.2867240
H	4.8454000	1.1520720	-0.6518960	H	-2.0314200	2.5780980	1.2234090
N	0.7065300	-1.5111810	0.8272730	O	-0.5695670	2.8414450	-0.1686050
H	0.9866790	-2.4823740	0.9253730	H	-0.0603320	2.2370990	-0.7297210
H	-0.4471130	-1.0650210	1.5847010	C	1.2577950	-0.6649390	-0.1683510
N	5.1251650	-1.5214980	-0.4773610	N	2.2713150	-1.5278660	-0.1143210
H	4.9775330	-2.5129960	-0.5886960	C	3.4979510	-0.9857770	-0.0707590
H	5.8097690	-1.1120260	-1.0917280	C	3.7093840	0.3926090	-0.0839460
N	2.6366690	2.5797620	-0.1647370	C	2.5645330	1.1880680	-0.1470500
H	1.7088900	2.9794780	-0.1531390	N	1.3316700	0.6567970	-0.1973600
H	3.3245580	3.0701070	-0.7103100	H	4.7020160	0.8183970	-0.0275000

pINT2

H = -1002.746159 a.u.

G = -1002.815602 a.u.

C	-2.1584400	1.0363430	-0.2772170
O	-1.2714120	0.4460190	-1.2373740
C	-1.1232370	-0.9162390	-1.0062480
C	-2.4365530	-1.3679310	-0.3684030
C	-2.8169950	-0.1276300	0.4763060
H	-2.9096950	1.5972300	-0.8386680
H	-0.9569430	-1.3943840	-1.9750830
H	-2.3086340	-2.2651160	0.2489000
H	-2.4112890	-0.2172770	1.4860080
O	-4.2255110	0.0526460	0.5201100
H	-4.5636220	-0.3037120	1.3449160
O	-3.3769270	-1.5881560	-1.3858640
H	-4.2018620	-1.1696380	-1.1092370
O	-0.7223630	-0.9623170	2.7796260

H	0.0373730	-1.0076920	3.3633950
C	-1.3537040	1.9713090	0.6182700
H	-0.7199440	1.3756460	1.2867240
H	-2.0314200	2.5780980	1.2234090
O	-0.5695670	2.8414450	-0.1686050
H	-0.0603320	2.2370990	-0.7297210
C	1.2577950	-0.6649390	-0.1683510
N	2.2713150	-1.5278660	-0.1143210
C	3.4979510	-0.9857770	-0.0707590
C	3.7093840	0.3926090	-0.0839460
C	2.5645330	1.1880680	-0.1470500
N	1.3316700	0.6567970	-0.1973600
H	4.7020160	0.8183970	-0.0275000
N	-0.0152420	-1.2479840	-0.0728620
H	0.1118810	-2.2561490	-0.0594430
H	-0.3686490	-1.0309950	1.8780080
N	4.5355430	-1.8710320	0.0277510
H	4.3099650	-2.8317080	-0.1776900
H	5.4592630	-1.5603430	-0.2222480
N	2.6149130	2.5490180	-0.1711240
H	1.7510020	3.0366840	0.0332260
H	3.4753350	3.0093640	0.0716670

pP_N

H = -926.342559 a.u.

G = -926.406637 a.u.

C	-1.6027430	0.0187670	-0.4500870
N	-2.0215080	-0.9811270	0.3192520
C	-3.3000460	-0.9197250	0.7086000
C	-4.1523400	0.1175510	0.3301340
C	-3.5870870	1.1045370	-0.4785310

N -2.3100470 1.0707190 -0.8704670
H -5.1849360 0.1582180 0.6490180
N -0.3028980 -0.0286250 -0.9050800
H -0.0083710 0.8416870 -1.3269710
N -3.7184770 -1.9256130 1.5372250
H -3.1089790 -2.7266730 1.5888910
H -4.7053940 -2.1008620 1.6214190
N -4.3300110 2.1576040 -0.9459180
H -3.7981020 2.9230390 -1.3291890
H -5.1734980 2.4006700 -0.4540290
C 2.5506760 0.1125190 0.8204610
O 1.1762380 -0.1946190 0.9386160
C 0.6971010 -0.8274690 -0.2639020
C 1.9295870 -1.0112100 -1.1545910
C 2.8306090 0.1290370 -0.6836940
H 3.1668810 -0.6702950 1.2810080
H 0.2553550 -1.7839990 0.0047500
H 1.6703760 -0.9508330 -2.2154320
H 2.4875470 1.0818840 -1.1137220
O 4.1680520 -0.1279480 -1.0320660
H 4.7177410 0.4689040 -0.5096420
O 2.5212350 -2.2511770 -0.8433360
H 3.4625730 -2.1702960 -1.0391400
C 2.8361830 1.4439850 1.4814530
H 2.6852020 1.3785760 2.5628350
H 2.1587480 2.2011270 1.0702370
O 4.1945960 1.7409040 1.1629420
H 4.4628380 2.5529200 1.5965860

oINT1_{H2O}

H = -1079.160996 a.u.

G = -1079.236743 a.u.

C 1.8293900 -0.6282570 -0.2939290
O 0.5295810 -0.0389680 -0.2461350
C 0.6086080 1.3349660 -0.0011530
C 2.0683310 1.7318030 -0.2209770
C 2.7734170 0.4571130 0.2448820
H 2.0857120 -0.8497420 -1.3365160
H -0.0977020 1.8456580 -0.6652260
H 2.3418730 2.6201440 0.3524940
H 2.7826430 0.4328390 1.3381250
O 4.1034510 0.3226490 -0.1828050
H 4.1342320 0.5817860 -1.1121850
O 2.3868700 1.8619270 -1.5935770
H 1.9782890 2.6521310 -1.9543130
O 0.2763160 1.6223100 1.3509740
H -1.8783790 -2.9868220 -2.4466060
C 1.8457640 -1.9076730 0.5194980
H 1.0794830 -2.5913840 0.1522230
H 1.6097390 -1.6662170 1.5662450
O 3.0971520 -2.5548570 0.4015430
H 3.7985370 -1.8964530 0.4598230
C -1.8697000 -1.8424770 -0.7736410
N -1.6601750 -1.9258600 0.5451970
C -1.9548310 -0.8244270 1.2328100
C -2.5041210 0.3129880 0.6593960
C -2.6345540 0.2861840 -0.7338300
N -2.3358310 -0.7968900 -1.4572270
H -2.7458330 1.1985800 1.2303860
N -1.5192460 -2.9426790 -1.5073120
H -1.4138160 -3.8060980 -1.0008170

H -0.1369490 0.8266610 1.7232210
N -1.5668620 -0.8149400 2.5699540
H -1.3617550 -1.7405980 2.9223740
H -2.1586950 -0.2766130 3.1873320
N -3.0840230 1.3876210 -1.4055140
H -2.9520600 1.3589560 -2.4046190
H -2.9398770 2.2797560 -0.9489300
O -1.7747650 3.4057300 0.5217480
H -1.7889550 4.2864150 0.9008570
H -1.0961980 2.9085940 1.0081290

oTS1_2H2O

H = -1079.071102 a.u.

G = -1079.144865 a.u.

C -1.4500370 -1.0292810 -0.5105220
O -0.3981390 -0.5121820 0.3831590
C -0.8324260 0.3040580 1.2193400
C -2.3350720 0.3934770 1.2597620
C -2.7523720 -0.3552700 -0.0381420
H -1.4765720 -2.1046240 -0.3230930
H -0.1049160 0.7423570 1.8993360
H -2.6868350 1.4198830 1.3027250
H -3.0844150 0.3559160 -0.7906200
O -3.7917550 -1.2662020 0.1684220
H -3.7426770 -1.5782000 1.0803930
O -2.7149420 -0.3851060 2.3826700
H -3.0072960 0.1796560 3.1021990
O -1.4328060 2.2425240 -0.5209380
H 2.7283420 -1.9985810 2.8888310
C -1.0080840 -0.7045450 -1.9338190
H -0.0987680 -1.2556880 -2.1862190

H -0.7845760 0.3612860 -1.9890700
O -2.0799620 -0.9695460 -2.8148360
H -2.1148180 -1.9093940 -3.0087300
C 2.3754980 -1.2589990 1.0463340
N 2.4654030 -1.6204140 -0.2366630
C 2.3438440 -0.6079330 -1.1159260
C 2.1010670 0.6974460 -0.7452850
C 1.9990090 0.9716420 0.6499510
N 2.1685130 -0.0480620 1.5480820
H 1.9889020 1.4990660 -1.4643880

N 2.4526880 -2.2928500 1.9645400
H 2.9167110 -3.1173300 1.6155490
H -1.9089360 2.4057100 -1.3395020
N 2.4107490 -0.9892860 -2.4551510
H 2.9167560 -1.8551700 -2.5804920
H 2.7073370 -0.2602320 -3.0873500
N 1.6532000 2.1777890 1.0788010
H 1.7190450 2.2173180 2.0925520
H 1.1696110 3.2286560 0.0754570
O 0.6758570 3.7693640 -0.6682960
H 0.7608430 4.7014840 -0.4625250
H -0.6662060 2.8832640 -0.5539380

oINT2H2O

H = -1079.164993 a.u.

G = -1079.240694 a.u.

C -2.2575570 -1.2949380 -0.4895450
O -0.8308180 -1.1477350 -0.3947010
C -0.4811640 -0.4012180 0.7583670
C -1.7752040 0.2569860 1.2274700
C -2.8292080 -0.7692000 0.8213130

H -2.4891230 -2.3613900 -0.5736060
H -0.0933390 -1.0882110 1.5220160
H -1.9432600 1.1833640 0.6735370
H -3.8158050 -0.3176810 0.6929240
O -2.8586060 -1.8350620 1.7499860
H -2.7430130 -1.4543010 2.6286630
O -1.7261250 0.4990810 2.6195050
H -2.3027460 1.2412640 2.8212400
O -3.8146620 2.1789590 -0.4120700
H 4.5771060 2.8288110 0.4360560
C -2.7046110 -0.5347610 -1.7368500
H -2.2899140 -1.0272320 -2.6220560
H -2.2990600 0.4759820 -1.7080370
O -4.1152760 -0.4029110 -1.8315860
H -4.5150480 -1.2552500 -2.0205520
C 3.9846790 0.9095860 0.1256160
N 4.4522650 -0.2730360 -0.2847860
C 3.5421720 -1.2346800 -0.4472130
C 2.1726200 -1.0302480 -0.2204010
C 1.8258660 0.2465860 0.1925290
N 2.7129940 1.2307650 0.3718820
H 1.4357950 -1.8028680 -0.3846270
N 4.9132950 1.8857950 0.3405760
H 5.8345510 1.7333210 -0.0331630
H -4.2399510 1.5263710 -0.9808830
N 4.0173340 -2.4564240 -0.8250520
H 4.9717770 -2.4880060 -1.1450240
H 3.3779390 -3.1401550 -1.1921870
N 0.4994210 0.6143240 0.4269620
H 0.4692960 1.4047630 1.0657050

H -0.3731730 1.7827480 -0.9746390
O -1.0349250 2.3824600 -1.3618610
H -0.5457290 3.0236120 -1.8817740
H -3.0057190 2.4378590 -0.8725620

pINT_{1H2O}

H = -1079.168993 a.u.

G = -1079.241844 a.u.

C -2.0305080 -0.1371890 -1.1014400
O -1.0120170 -0.6553520 -0.2470370
C -1.4368180 -0.5194400 1.0891700
C -2.9700110 -0.6778960 1.0644630
C -3.3467820 -0.5455200 -0.4468440
H -1.9045750 -0.6233430 -2.0701860
H -0.9550710 -1.3159340 1.6616260
H -3.4226910 0.1088490 1.6666410
H -4.1260310 0.2080180 -0.6024920
O -3.7433120 -1.7878430 -0.9913740
H -4.5582760 -2.0595850 -0.5576790
O -3.4062160 -1.8998550 1.6082070
H -3.0510130 -2.6075070 1.0584820
O -1.1172830 0.7369390 1.6224730
H -0.1606360 0.7796130 1.8093210
C -1.9217680 1.3798980 -1.2449740
H -2.2830750 1.8648750 -0.3279020
H -2.5644000 1.7035750 -2.0679290
O -0.6090880 1.7902950 -1.5456210
H 0.0309590 1.3770850 -0.9239580
C 2.2318050 0.5578560 0.8031480
N 3.1298150 -0.3435800 1.1834450
C 3.5675550 -1.1687180 0.2203190

C	3.1123190	-1.0976320	-1.0948670	O	-3.1071540	-2.2917950	-1.2493920
C	2.1690110	-0.1060310	-1.3700070	H	-3.5321350	-1.7866050	-1.9579290
N	1.7265000	0.7333950	-0.4171680	O	-2.4938530	-0.1607750	2.2352000
H	3.4806820	-1.7620310	-1.8644120	H	-2.7377310	-0.6383520	3.0315930
N	1.7065090	1.3681410	1.7944470	C	-1.6174350	1.9774400	-0.0510740
H	2.2734820	1.3957150	2.6299460	H	-1.8194420	1.7524620	1.0002720
H	1.3554260	2.2699990	1.4714900	H	-2.2861330	2.7873550	-0.3614680
N	4.5226200	-2.0690980	0.6017080	O	-0.3007930	2.3678300	-0.2619730
H	4.6409270	-2.1888220	1.5951580	H	0.3408640	1.6589050	0.0649870
H	4.6908540	-2.8731490	0.0214250	C	1.8081460	-0.6061840	0.7395230
N	1.6683860	0.0866630	-2.6198450	N	2.8343820	-1.4466910	0.4418040
H	0.8611900	0.6904890	-2.7099110	C	3.7975520	-0.9826330	-0.3423940
H	1.7923710	-0.6361180	-3.3074810	C	3.7911100	0.3026940	-0.8955300
O	-0.1820780	3.4381680	0.8267350	C	2.6877210	1.0902130	-0.5715240
H	-0.2100320	3.3210120	-0.1321230	N	1.7036570	0.6616780	0.2261270
H	-0.8557720	2.8278180	1.1510070	H	4.6014550	0.6741310	-1.5072250
pTS1_2_{H2O}				N	0.8340480	-1.0085430	1.5563980
H = -1079.073603 a.u.				H	1.1050780	-1.9050400	1.9498530
G = -1079.145646 a.u.				H	0.2458240	0.1771310	2.3630190
C	-1.9846590	0.7586250	-0.8927310	N	4.8564130	-1.8354720	-0.5685790
O	-0.9343520	-0.2466790	-0.6425370	H	4.6739950	-2.7970730	-0.3256570
C	-1.3737630	-1.2973500	-0.1338940	H	5.4013950	-1.6885650	-1.4020420
C	-2.8781270	-1.4044750	-0.1797350	N	2.5865360	2.3817110	-1.0369520
C	-3.2979220	0.0567540	-0.5257670	H	1.6698570	2.8067510	-1.0052450
H	-1.9170140	0.9682630	-1.9605060	H	3.1453550	2.6167670	-1.8402530
H	-0.6505600	-2.0663490	0.1158780	O	-0.2516560	0.9719350	2.8093980
H	-3.3090540	-1.7810270	0.7415590	H	0.1888750	1.7704620	2.5079760
H	-3.7492770	0.5229680	0.3491180	H	-1.6860300	0.3651250	2.4992370
O	-4.1521090	0.0810650	-1.6540060	pINT2_{H2O}			
H	-5.0669720	0.1507760	-1.3695020	H = -1079.160322 a.u.			

G = -1079.233523 a.u.

C -1.7094600 1.4665770 -0.4616310
O -0.7309160 0.9398650 -1.3740380
C -0.8305930 -0.4460000 -1.4911540
C -2.2261280 -0.8100770 -0.9983700
C -2.4442880 0.2487910 0.0981860
H -2.3942840 2.0920210 -1.0410240
H -0.6957940 -0.7012200 -2.5454770
H -2.2760210 -1.8338690 -0.6096880
H -1.9639890 -0.0731750 1.0259840
O -3.8071840 0.5204790 0.3115480
H -4.1040990 -0.1316390 0.9656440
O -3.1421540 -0.6177340 -2.0453990
H -3.9382240 -0.2391130 -1.6491960
O -3.6350480 -1.6829570 2.0046030
H -4.1404940 -2.4304080 2.3274160
C -0.9940990 2.2880250 0.6059130
H -0.5428190 1.6107510 1.3390260
H -1.7130670 2.9375890 1.1087800
O 0.0045930 3.1077430 0.0292890
H 0.4703600 2.5206690 -0.5830940
C 1.4429010 -0.6542190 -0.3615500
N 2.4709340 -1.4637170 -0.6077770
C 3.6716680 -1.0192020 -0.2040490
C 3.8451310 0.2242020 0.4026920
C 2.6889740 0.9843930 0.5889890
N 1.4765350 0.5326690 0.2237100
H 4.8174220 0.5717020 0.7248920
N 0.1823450 -1.1883210 -0.6804540
H 0.3425040 -2.0943060 -1.1118220

H -0.4786650 -1.8127190 1.0397360
N 4.7188390 -1.8757630 -0.4019380
H 4.5421540 -2.6454990 -1.0280220
H 5.6543480 -1.5059240 -0.3911980
N 2.7007450 2.2068130 1.1870980
H 1.8616190 2.7684680 1.0851940
H 3.5767640 2.6891850 1.2932110
O -0.8860050 -2.1434850 1.8642190
H -0.2582860 -1.9516900 2.5648250
H -2.6961420 -1.9387960 2.0444130

oINT3_{H2O}

H = -1079.151289 a.u.

G = -1079.230671 a.u.

C 3.4645990 -1.5440200 0.3561310
N 2.4956480 -0.9755430 1.0759010
C 2.3406410 0.3450660 0.9002310
C 3.1238410 1.0814080 0.0068230
C 4.0836960 0.3580530 -0.6963350
N 4.2677700 -0.9576230 -0.5331660
H 2.9765030 2.1440690 -0.1266780
N 3.6712010 -2.8811720 0.5701980
H 2.9277840 -3.3780960 1.0321470
H 4.2016660 -3.3682340 -0.1326170
N 1.3555920 0.9373990 1.6265130
H 0.7638920 0.3546590 2.2002010
H 1.0906470 1.8913320 1.4282760
N 4.9340850 0.9727240 -1.5835970
H 5.4196000 0.3466490 -2.2068610
H 4.6393240 1.8502930 -1.9786410
C -3.3872320 -0.9488500 -0.3723130

O	-2.4036270	-1.5634850	-1.1816940	N	4.3914930	0.5304050	-0.7970230
C	-0.5036290	0.0457690	-0.3319950	H	1.5979290	1.6023330	0.8043860
C	-1.5656930	0.5254820	0.6350200	N	4.8887310	-1.6131160	-1.4493770
C	-2.9730040	0.4736600	0.0283770	H	4.5519550	-2.5286380	-1.6941850
H	-3.4534040	-1.5558070	0.5335730	H	5.6718880	-1.2262210	-1.9476540
H	0.0270160	-0.8798190	-0.0594960	N	0.8138120	-0.9661090	0.6327550
H	-1.3549740	1.5831070	0.8433720	H	0.6751680	-1.8720160	0.1780790
H	-2.9798550	1.1204490	-0.8628910	H	0.8479880	-1.0391140	1.8020820
O	-3.8097960	0.9936080	1.0430130	N	3.9386490	2.6621180	-0.0923840
H	-4.7268870	0.7896930	0.8174650	H	4.7594770	2.9383940	-0.6062370
O	-1.4933120	-0.2491050	1.8090210	H	3.2693250	3.3704180	0.1548770
H	-2.2544280	-0.0038660	2.3489190	C	-3.0779130	0.7835710	-0.6121290
O	-0.2588690	0.6600150	-1.3461980	O	-2.4086510	1.9377920	-0.1505330
H	-2.2522900	-1.0310740	-1.9712700	C	-0.4456880	-0.0908660	0.4608890
C	-4.7196860	-0.9884340	-1.1150010	C	-1.6106350	-1.0715270	0.4338090
H	-4.9611160	-2.0312290	-1.3390340	C	-2.9836250	-0.3774740	0.3913600
H	-4.6175010	-0.4389900	-2.0613660	H	-2.6670430	0.4542140	-1.5777240
O	-5.7208350	-0.3915940	-0.2992130	H	-0.3421110	0.3819750	-0.5257690
H	-6.5738820	-0.4364820	-0.7359420	H	-1.5855900	-1.6709500	1.3566410
O	0.4838090	3.1469920	-0.1457860	H	-3.1938620	0.0307870	1.3881100
H	0.2667440	2.5043150	-0.8363510	O	-3.8853060	-1.4363370	0.0981370
H	0.2309360	4.0082910	-0.4825090	H	-4.6082260	-1.1080750	-0.4539690
oTS3_4H₂O				O	-1.4201250	-1.9008960	-0.6935820
H = -1079.134894 a.u.				H	-2.2581650	-2.3599840	-0.8351830
G = -1079.205686 a.u.				O	-0.5310020	0.8096790	1.4726330
C	4.0103200	-0.7469630	-0.8798420	H	-1.8004370	1.7251550	0.5824910
N	2.8548480	-1.2662060	-0.4422350	C	-4.5158680	1.2455860	-0.8315510
C	2.0416390	-0.3968190	0.1422360	H	-4.4786910	2.1743940	-1.4059590
C	2.3034230	0.9426550	0.3178050	H	-4.9781640	1.4494910	0.1418900
C	3.5426690	1.3677390	-0.2018840	O	-5.2392300	0.2370040	-1.5382120

H -6.1292250 0.5464230 -1.7189170
O 0.4622350 -0.6587300 3.0523130
H -0.0875560 0.1748860 2.4977340
H 1.1333170 -0.3166170 3.6469550

oINT4_{H2O}

H = -1079.164097 a.u.

G = -1079.237490 a.u.

C 4.1520360 -0.4953870 -0.8453170
N 2.9671370 -1.0824880 -0.6710340
C 2.0322480 -0.3322830 -0.0784350
C 2.2564010 0.9716180 0.3421730
C 3.5395730 1.4741750 0.0829510
N 4.4911840 0.7536460 -0.5124220
H 1.5037910 1.5483210 0.8590110
N 5.1343160 -1.2608780 -1.4073860
H 4.8381990 -2.0984900 -1.8799990
H 5.9400410 -0.7729360 -1.7611980
N 0.8110140 -0.9740200 0.1171960
H 0.6952790 -1.7387460 -0.5421400
H 0.8952760 -1.9545480 1.9633150
N 3.8903410 2.7379510 0.4658920
H 4.7493690 3.0947410 0.0786590
H 3.1622230 3.4038730 0.6616100
C -3.1576100 0.9258470 -0.3652360
O -2.4604860 1.9328900 0.3449650
C -0.4007040 -0.1876400 0.2804920
C -1.5916970 -1.0978570 0.0115940
C -2.9683070 -0.4591970 0.2723310
H -2.8095710 0.8908190 -1.4061490
H -0.4099310 0.6529780 -0.4228560

H -1.5171010 -1.9668600 0.6837560
H -3.1085160 -0.3484110 1.3565700
O -3.8772640 -1.4268970 -0.2302480
H -4.6496210 -0.9884290 -0.6126630
O -1.4816300 -1.5093070 -1.3327030
H -2.3121180 -1.9538970 -1.5448590
O -0.4875490 0.3891530 1.5667240
H -1.8989590 1.5466540 1.0310460
C -4.6132270 1.3858950 -0.3531100
H -4.6285050 2.4344870 -0.6603720
H -5.0061570 1.3112990 0.6683490
O -5.3725240 0.5783250 -1.2516410
H -6.2728900 0.9064030 -1.2998230
O 0.3821750 -1.9414240 2.7863640
H -0.3255650 -0.3023880 2.2331930
H 0.9827510 -2.1772960 3.4964780

oINT5_{H2O}

H = -1079.16142 a.u.

G = -1079.234039 a.u.

C 4.1520360 -0.4953870 -0.8453170
N 2.9671370 -1.0824880 -0.6710340
C 2.0322480 -0.3322830 -0.0784350
C 2.2564010 0.9716180 0.3421730
C 3.5395730 1.4741750 0.0829510
N 4.4911840 0.7536460 -0.5124220
H 1.5037910 1.5483210 0.8590110
N 5.1343160 -1.2608780 -1.4073860
H 4.8381990 -2.0984900 -1.8799990
H 5.9400410 -0.7729360 -1.7611980
N 0.8110140 -0.9740200 0.1171960

H	0.6952790	-1.7387460	-0.5421400	G = -1079.183923 a.u.			
H	0.8952760	-1.9545480	1.9633150	C	3.8200280	-1.0222970	-0.0871620
N	3.8903410	2.7379510	0.4658920	N	2.4886460	-1.0212260	-0.0373750
H	4.7493690	3.0947410	0.0786590	C	1.8978510	0.1673430	0.1858570
H	3.1622230	3.4038730	0.6616100	C	2.6620930	1.3334890	0.3499420
C	-3.1576100	0.9258470	-0.3652360	C	4.0436890	1.1959350	0.2678910
O	-2.4604860	1.9328900	0.3449650	N	4.6427710	0.0202250	0.0380250
C	-0.4007040	-0.1876400	0.2804920	H	2.1870440	2.2780630	0.5782020
C	-1.5916970	-1.0978570	0.0115940	N	4.4203770	-2.2444040	-0.2647810
C	-2.9683070	-0.4591970	0.2723310	H	3.8336680	-2.9734310	-0.6351070
H	-2.8095710	0.8908190	-1.4061490	H	5.3808690	-2.2219470	-0.5654630
H	-0.4099310	0.6529780	-0.4228560	N	0.5316070	0.2684910	0.2656750
H	-1.5171010	-1.9668600	0.6837560	H	0.0100050	1.3491860	-0.5651330
H	-3.1085160	-0.3484110	1.3565700	H	-0.6615010	0.3422800	-1.7140840
O	-3.8772640	-1.4268970	-0.2302480	N	4.8883590	2.2644820	0.4591520
H	-4.6496210	-0.9884290	-0.6126630	H	5.8364530	2.1149390	0.1510720
O	-1.4816300	-1.5093070	-1.3327030	H	4.5156020	3.1879410	0.3141950
H	-2.3121180	-1.9538970	-1.5448590	C	-3.6317700	-0.2677890	-0.1570720
O	-0.4875490	0.3891530	1.5667240	O	-3.2879540	-1.1237980	-1.2519580
H	-1.8989590	1.5466540	1.0310460	C	-0.2054440	-0.8655760	-0.0293240
C	-4.6132270	1.3858950	-0.3531100	C	-1.4091010	-1.0427460	0.8947350
H	-4.6285050	2.4344870	-0.6603720	C	-2.4608240	0.0637910	0.8016680
H	-5.0061570	1.3112990	0.6683490	H	-4.4042760	-0.7552580	0.4453470
O	-5.3725240	0.5783250	-1.2516410	H	0.3629420	-1.7901520	-0.1080750
H	-6.2728900	0.9064030	-1.2998230	H	-0.9783830	-0.9776520	1.8965180
O	0.3821750	-1.9414240	2.7863640	H	-1.9629150	0.9844780	0.4748180
H	-0.3255650	-0.3023880	2.2331930	O	-2.9881260	0.2417620	2.1045590
H	0.9827510	-2.1772960	3.4964780	H	-3.6013250	0.9851400	2.0590980
oTS5_6_{H2O}				O	-1.9893060	-2.3403300	0.7013320
H = -1079.113015 a.u.				H	-2.2385640	-2.6965630	1.5569400

O -0.7509720 -0.6950240 -1.5205620
H -3.1940130 -2.0108330 -0.8754370
C -4.1898280 1.0056440 -0.7667630
H -5.0756220 0.7760380 -1.3660360
H -3.4207970 1.4545470 -1.4072570
O -4.5087770 1.8616070 0.3231620
H -4.6676480 2.7509470 0.0011650
O -0.5098600 1.7391650 -1.4399390
H -1.7221860 -0.9155340 -1.5813820
H 0.1181220 2.2310220 -1.9756460

oINT6_{H2O}

H = -1079.15336 a.u.

G = -1079.231563 a.u.

C -3.2990890 -1.0341860 0.6811270
N -2.0301310 -1.0930780 0.2719920
C -1.6667520 -0.1565040 -0.5997020
C -2.5239880 0.8107380 -1.0847730
C -3.8392630 0.7630680 -0.5897950
N -4.2255950 -0.1487310 0.2974390
H -2.1978150 1.5453930 -1.8074390
N -3.7049750 -1.9918640 1.5644910
H -2.9754960 -2.4758160 2.0618210
H -4.5647660 -1.8096580 2.0554570
N -0.3147740 -0.1142150 -1.0412400
H 0.2471810 1.7207610 -0.9217140
H -0.0651400 1.8043620 1.2566230
N -4.7934570 1.6389160 -1.0214770
H -5.6431900 1.6676650 -0.4801510
H -4.5029420 2.4951690 -1.4617980
C 2.8790280 -0.3158930 0.7838350

O 1.7480620 -0.8555300 1.4455130
C 0.3678620 -1.1770760 -0.9237520
C 1.8130530 -1.2426070 -1.3267510
C 2.6669230 -0.1286790 -0.7338590
H 3.7429700 -0.9791170 0.9104730
H -0.0720770 -2.1025130 -0.5414550
H 1.8664760 -1.1473440 -2.4192800
H 2.1870660 0.8353460 -0.9302180
O 3.9152410 -0.2092120 -1.4020340
H 4.4828360 0.4637430 -1.0044790
O 2.2999010 -2.5122020 -0.9168930
H 3.2232170 -2.5612290 -1.1887750
O -0.2860240 1.2547680 2.0187900
H 1.7113960 -1.7984610 1.2474340
C 3.1769060 1.0221480 1.4386670
H 3.4221340 0.8757350 2.4942020
H 2.2930350 1.6622540 1.3570940
O 4.2799210 1.5810410 0.7264320
H 4.3234650 2.5235100 0.8980600
O 0.5749970 2.5284810 -0.4828960
H 0.1920180 0.4299460 1.8698760
H 0.1072950 3.2682440 -0.8754230

oINT7_{H2O}

H = -1002.740302 a.u.

G = -1002.813354 a.u.

C -3.2178660 0.4188960 1.2603270
N -1.9836030 -0.0498620 1.0615700
C -1.7387030 -0.5284670 -0.1562590
C -2.6798040 -0.5459070 -1.1694950
C -3.9463460 -0.0280720 -0.8394840

N	-4.2147570	0.4644290	0.3674160	H	-0.0997450	1.6761530	-2.4483860
H	-2.4512640	-0.9647080	-2.1395520	oTS7_8H₂O			
N	-3.5005940	0.8840890	2.5072280	H = -1002.701882 a.u.			
H	-2.7245410	1.0519900	3.1250080	G = -1002.769247 a.u.			
H	-4.3464540	1.4147010	2.6266430	C	3.3122600	0.9483020	0.8563290
N	-0.4474200	-1.0313690	-0.4699930	N	2.0501890	1.0530510	0.4294790
N	-4.9685590	-0.0282000	-1.7382420	C	1.6786190	0.1618600	-0.4858340
H	-5.8004840	0.4818770	-1.4901760	C	2.5224290	-0.8189030	-0.9825270
H	-4.7858250	-0.2012300	-2.7109670	C	3.8192140	-0.8319690	-0.4489230
C	2.8947820	0.5112740	0.3144820	N	4.2182080	0.0428470	0.4744770
O	1.6648320	1.1515670	0.6054320	H	2.1999010	-1.5109510	-1.7479290
C	0.3548260	-1.2399320	0.4955260	N	3.7279700	1.8773380	1.7606900
C	1.7352360	-1.7711160	0.2356790	H	3.0230050	2.4351680	2.2115030
C	2.6677390	-0.7740860	-0.4779230	H	4.5958490	1.7045750	2.2384160
H	3.3397640	0.2613430	1.2815630	N	0.3699990	0.2277050	-0.9981040
H	0.0779730	-1.0723930	1.5378950	N	4.7547120	-1.7289780	-0.8765670
H	1.6283390	-2.6380920	-0.4341000	H	5.5944600	-1.7956310	-0.3239590
H	2.2452600	-0.5280400	-1.4590890	H	4.4552950	-2.5546510	-1.3660100
O	3.9428420	-1.3958930	-0.6159040	C	-2.7771730	-0.2022080	0.6439900
H	3.9367730	-1.9711920	-1.3851080	O	-1.3870410	-0.4300190	0.8155620
O	2.2825650	-2.1662440	1.4711420	C	-0.5463220	0.9241750	-0.3420790
H	3.2184590	-2.3444040	1.3232920	C	-1.8447520	1.3230700	-1.0133010
H	0.1128590	0.2689810	-1.8417640	C	-2.9310640	0.2501460	-0.8033590
C	3.8134170	1.4749870	-0.4254190	H	-3.0778310	0.6070560	1.3167200
H	3.3650510	1.7052300	-1.4040920	H	-0.2126090	1.5890100	0.4489670
H	4.7913910	1.0217160	-0.5846460	H	-1.6479490	1.4660540	-2.0823430
O	4.0056610	2.6509310	0.3307940	H	-2.7505670	-0.5977390	-1.4708310
H	3.1434490	2.8987770	0.6817990	O	-4.2147660	0.8162830	-1.0054490
O	0.5582210	1.1112780	-2.0367140	H	-4.5454250	0.5740600	-1.8728530
H	1.2208830	1.3471060	-0.2367790	O	-2.2485060	2.5317680	-0.4124200

H	-3.1969430	2.6211470	-0.5679020	C	2.0153850	-0.9920170	-1.3064750
H	-0.0671540	-0.8234240	-1.2972550	C	3.0412500	0.0041810	-0.7328400
C	-3.5619420	-1.4587900	0.9744170	H	2.9290710	-0.8806750	1.2285800
H	-3.2380680	-2.2660330	0.3035220	H	0.4444590	-1.7113800	0.0078910
H	-4.6259120	-1.2732720	0.8169260	H	1.7911610	-0.8112470	-2.3628800
O	-3.3965360	-1.8211220	2.3285490	H	2.9022810	0.9952530	-1.1779810
H	-2.4519080	-1.8129750	2.5133500	O	4.3715800	-0.4565830	-0.8771010
O	-0.8113730	-1.9031450	-1.0058790	H	4.8023830	0.0153950	-1.5926470
H	-1.1173510	-1.2524180	0.1218040	O	2.4636590	-2.3120200	-1.1105340
H	-0.3461770	-2.7379460	-0.9271420	H	3.4232120	-2.3077350	-1.2137380

oINT8_{H2O}

H = -1002.754739 a.u.

G = -1002.826183 a.u.

C	-3.0990570	-1.0192560	0.8622030
N	-1.8497900	-1.0362320	0.3879340
C	-1.5910540	-0.1662550	-0.5874310
C	-2.5468490	0.7219840	-1.0822140
C	-3.8102270	0.6462550	-0.4925150
N	-4.0968340	-0.2166360	0.4870580
H	-2.3250980	1.4105130	-1.8862990
N	-3.3901100	-1.9399500	1.8255570
H	-2.6138210	-2.3974220	2.2727870
H	-4.2419460	-1.8087190	2.3438870
N	-0.3208160	-0.1825340	-1.1353290
N	-4.8444490	1.4392060	-0.9122850
H	-5.6474020	1.4673250	-0.3040590
H	-4.6322040	2.2781360	-1.4249550
C	2.6239170	0.0493230	0.7311250
O	1.2025640	0.1164960	0.6425340
C	0.7679670	-0.7687740	-0.4291110

H	-0.0881760	0.6487760	-1.6658010
C	3.1100150	1.2406700	1.5218600
H	2.8143760	2.1623380	1.0025830
H	4.1994250	1.2109380	1.5843180
O	2.6139470	1.2164890	2.8439990
H	1.6677440	1.0466720	2.7942330
O	0.8320870	2.5215860	-0.8088280
H	0.7470740	1.9124260	-0.0593500
H	0.4026700	3.3380210	-0.5452790

oINT3_{2H2O}

H = -1155.569229 a.u.

G = -1155.653698 a.u.

C	3.7531500	0.6788390	-0.5199010
N	2.8183210	0.9347500	0.4000740
C	2.3678230	-0.1243570	1.0954120
C	2.8385070	-1.4191970	0.8575460
C	3.7988340	-1.5498170	-0.1451670
N	4.2638150	-0.5086110	-0.8453200
H	2.4953720	-2.2642600	1.4390270
N	4.2563760	1.7561830	-1.1887840

H	3.7700510	2.6321680	-1.1062300	H	-0.8084540	3.2528440	-2.1525260
H	4.7967350	1.5725120	-2.0165940	O	0.7051950	2.8030720	0.9991890
N	1.4240130	0.1300080	2.0387580	H	1.5096080	2.4158260	0.6141440
H	0.8742210	-0.6241260	2.4186620	H	0.1235290	3.0069580	0.2541500
H	1.0135730	1.0573860	2.0518300	oTS3_4₂H₂O			
N	4.3551340	-2.7643700	-0.4467980	H = -1155.554205 a.u.			
H	4.8730040	-2.8008110	-1.3104760	G = -1155.630026 a.u.			
H	3.8595610	-3.5982230	-0.1801560	C	-4.0287350	0.2451760	0.4616660
C	-3.4183740	-1.1039150	-0.3269890	N	-2.8856990	0.7834920	0.0111040
O	-2.5000800	-1.8138630	-1.1378530	C	-2.0488650	-0.0766880	-0.5557560
C	-0.4318000	-0.4776720	-0.2335310	C	-2.2991250	-1.4217830	-0.7143880
C	-1.4331740	0.0841370	0.7491220	C	-3.5349290	-1.8667880	-0.2077730
C	-2.8379790	0.2339450	0.1540510	N	-4.3921020	-1.0365130	0.3834980
H	-3.5947570	-1.7339750	0.5476050	H	-1.5891570	-2.0883150	-1.1850210
H	0.0208240	-1.4444050	0.0384310	N	-4.9221370	1.0986060	1.0318880
H	-1.0936760	1.0945030	1.0157490	H	-4.5806960	1.9990980	1.3226960
H	-2.7769120	0.9452110	-0.6833900	H	-5.6836250	0.6870650	1.5452300
O	-3.6048180	0.7653980	1.2171220	N	-0.8027100	0.4880190	-1.0109860
H	-4.5356440	0.7379460	0.9618210	H	-0.5654520	0.1340170	-1.9403890
O	-1.4554070	-0.7630900	1.8788880	H	-0.9048250	1.7170570	-0.9987970
H	-2.1787970	-0.4517400	2.4364970	N	-3.9212780	-3.1645930	-0.3205110
O	-0.1274360	0.0940030	-1.2554970	H	-4.7376990	-3.4443320	0.1991250
H	-2.2892110	-1.2918650	-1.9207030	H	-3.2425100	-3.8704510	-0.5480550
C	-4.7188800	-0.9264200	-1.1047310	C	3.0718500	-0.9754060	0.6290390
H	-5.1012670	-1.9135350	-1.3803320	O	2.2669170	-1.0503860	1.7856510
H	-4.5067620	-0.3602810	-2.0226590	C	0.3842120	0.1223500	-0.0995200
O	-5.6482940	-0.2226980	-0.2908550	C	1.6210810	0.5450960	-0.8843390
H	-6.4721590	-0.0953710	-0.7656680	C	2.9325230	0.3720120	-0.1003640
O	-0.9556670	2.7384410	-1.3565280	H	2.8244210	-1.7847720	-0.0739340
H	-0.6190530	1.8441450	-1.5352890	H	0.3742150	-0.9761470	-0.0395780

H	1.5484850	1.6107240	-1.1424960	H	2.5467930	2.0439990	-2.2943130
H	2.9896270	1.1724120	0.6489730	H	4.2174020	1.7140520	-2.4425150
O	3.9330570	0.5581690	-1.0938940	N	0.6490040	-0.9474530	0.7247840
H	4.7033470	0.0101750	-0.8909380	H	0.4720990	-1.8664940	1.1046120
O	1.6225250	-0.2445370	-2.0605880	H	2.6394800	2.9545030	0.1850530
H	2.4982170	-0.1344750	-2.4537400	N	5.2565030	-2.0970360	-0.0419480
O	0.2638320	0.6823750	1.1215290	H	6.0234490	-1.9156450	-0.6696350
H	1.5474390	-0.3906970	1.7644270	H	5.1455060	-3.0425830	0.2824800
C	4.4873050	-1.2074240	1.1521140	C	-3.2833530	0.2170310	-0.8799110
H	4.4565380	-2.0854930	1.8017930	O	-2.5511280	1.3918250	-1.1690010
H	4.7940770	-0.3381840	1.7460810	C	-0.5243190	-0.2261890	0.2911230
O	5.3778810	-1.4163480	0.0551220	C	-1.7475830	-0.9438250	0.8464590
H	6.2577860	-1.6048160	0.3877640	C	-3.0884250	-0.2350970	0.5760710
O	0.7039600	3.0213260	0.8712690	H	-2.9805610	-0.5984450	-1.5511780
H	0.5094990	1.8675940	1.0972490	H	-0.5680760	-0.1978790	-0.8019520
H	0.6873180	3.5698090	1.6567090	H	-1.6405320	-1.0029460	1.9416110
O	-1.0144840	2.9695680	-0.8263770	H	-3.1512820	0.6588040	1.2105630
H	-1.8884590	3.0278680	-0.4230660	O	-4.0556600	-1.1873900	0.9966850
H	-0.2724690	3.1581670	-0.0447620	H	-4.8279670	-1.1537410	0.4153030
oINT4₂H₂O				O	-1.7485520	-2.2399650	0.2909370
H = -1155.579426 a.u.				H	-2.6144940	-2.6139840	0.4989110
G = -1155.659066 a.u.				O	-0.5155040	1.1203360	0.7074990
C	3.2257500	0.5153510	-1.1546710	H	-1.9036020	1.5813170	-0.4748220
N	2.0060070	0.3161520	-0.6488890	C	-4.7299720	0.5901600	-1.1919730
C	1.8706710	-0.7605260	0.1357100	H	-4.7415330	1.0615220	-2.1778150
C	2.9269650	-1.6413140	0.3805800	H	-5.0837300	1.3154890	-0.4491730
C	4.1402940	-1.3299880	-0.2285580	O	-5.5363620	-0.5877410	-1.1783830
N	4.3024880	-0.2454850	-1.0024870	H	-6.4301350	-0.3701340	-1.4511010
H	2.8130380	-2.5019150	1.0251710	O	0.7997780	1.9595580	2.9311430
N	3.3884470	1.6841880	-1.8684490	H	-0.2261750	1.2111400	1.6380070

H 0.5259610 2.5885210 3.6009290
O 1.7579010 2.9649090 0.5712610
H 1.3096790 2.2131620 0.1477260
H 1.3135920 2.4628100 2.2709490

oINT5_{2H2O}

H = -1155.583999 a.u.

G = -1155.664672 a.u.

C -3.4464050 -1.7259580 0.1553290
N -2.2195740 -1.2060200 0.0790530
C -2.1595660 0.0938340 -0.2305240
C -3.3049280 0.8645630 -0.4547740
C -4.5211370 0.1975760 -0.3464460
N -4.6081390 -1.1024560 -0.0390950
H -3.2398850 1.9116330 -0.7174610
N -3.5220160 -3.0486270 0.5102820
H -2.6782980 -3.5840850 0.3909380
H -4.3955700 -3.5068870 0.3089690
N -0.9212870 0.6636170 -0.3502220
H -0.8752850 1.6716620 -0.4632060
H 0.9368110 -0.6350330 1.7841280
N -5.7148470 0.8324770 -0.5898610
H -6.5299870 0.3436780 -0.2536440
H -5.7366860 1.8353800 -0.5087150
C 3.1444830 -1.2207710 0.0031010
O 2.3765370 -1.7822070 1.0723550
C 0.2622650 0.0018170 0.0726140
C 1.4726730 0.6346450 -0.6173050
C 2.8218030 0.2738390 0.0174240
H 2.8407680 -1.6513080 -0.9577090
H 0.1924650 -1.0537680 -0.1905010

H 1.3714090 1.7287750 -0.5486300
H 2.8542580 0.6177600 1.0564290
O 3.8419830 0.9379100 -0.7382480
H 3.8345880 1.8711990 -0.5059860

O 1.4416490 0.2233500 -1.9653930

H 2.2091280 0.6045210 -2.4041440

O 0.3975250 0.1160240 1.4991810

H 2.3648000 -2.7388000 0.9838470

C 4.6310770 -1.5016200 0.2300680

H 4.7441060 -2.5513350 0.5142430

H 4.9923600 -0.8891080 1.0673400

O 5.4026150 -1.3142210 -0.9308130

H 5.2967420 -0.3920620 -1.1878630

O 1.1947650 2.6598910 2.0159860

H 0.8633050 1.7376610 1.9858190

H 1.1242780 2.9424550 2.9301740

O -0.2018280 3.5523280 -0.1964500

H 0.2608180 3.4710680 0.6560630

H -0.5566500 4.4414980 -0.2410540

oTS5_6_{2H2O}

H = -1155.539576 a.u.

G = -1155.615893 a.u.

C -3.4193680 -1.7021010 0.1409520

N -2.1978720 -1.1727620 0.0834250

C -2.1319180 0.1335600 -0.2280150

C -3.2889840 0.8840300 -0.4724230

C -4.5024300 0.2107930 -0.3774970

N -4.5850190 -1.0883110 -0.0654160

H -3.2282440 1.9235150 -0.7644130

N -3.4926200 -3.0292070 0.4935180

H	-2.6458320	-3.5579740	0.3645200	H	0.8248520	2.8205020	2.7954180
H	-4.3583540	-3.4892570	0.2630440	O	-0.4113220	3.1555990	0.0721680
N	-0.9120450	0.7539290	-0.3211470	H	0.3808210	2.8646810	1.2178710
H	-0.7627060	2.0983000	-0.1893390	H	-1.1475090	3.7670980	0.1278610
H	1.1805310	-0.6032860	1.7373000	oINT6₂H₂O			
N	-5.6983890	0.8357120	-0.6450750	H = -1155.573617 a.u.			
H	-6.5137790	0.3421780	-0.3162310	G = -1155.655190 a.u.			
H	-5.7282960	1.8381880	-0.5605550	C	-3.9536070	-1.1782910	-0.0088310
C	3.2187440	-1.1047000	0.0421540	N	-2.6863890	-1.2924150	-0.4198310
O	2.4954320	-1.6310960	1.1638560	C	-1.9856170	-0.1591690	-0.4118090
C	0.2062440	0.0246330	-0.0582690	C	-2.4946550	1.0629590	-0.0207860
C	1.4574350	0.6297090	-0.7034720	C	-3.8349980	1.0483360	0.4038190
C	2.8181410	0.3693580	-0.0371690	N	-4.5681360	-0.0646620	0.4016840
H	2.9218200	-1.6160600	-0.8792850	H	-1.8770680	1.9505940	0.0115330
H	0.1268250	-1.0499400	-0.2229960	N	-4.6900600	-2.3256490	0.0238370
H	1.3211230	1.7194340	-0.7331030	H	-4.3262910	-3.1174300	-0.4791030
H	2.8387100	0.7875650	0.9757270	H	-5.6872230	-2.2279080	0.1146230
O	3.8064840	1.0298790	-0.8343910	N	-0.6339560	-0.2068980	-0.8398830
H	3.7532140	1.9758250	-0.6691820	H	0.0728780	1.1215190	-1.7202230
O	1.4656880	0.0989120	-2.0121240	H	0.4649290	1.6644710	1.1606900
H	2.1830320	0.5204670	-2.4961450	N	-4.4576990	2.1912870	0.8079330
O	0.4567190	0.0283530	1.5475880	H	-5.3440120	2.0787740	1.2736370
H	2.4898520	-2.5913450	1.1283130	H	-3.8949270	2.9848100	1.0656430
C	4.7194750	-1.2978500	0.2649450	C	2.3616150	-0.4976580	1.4129450
H	4.8860560	-2.3179740	0.6208460	O	1.0289000	-0.1841460	1.8175420
H	5.0631070	-0.6102590	1.0495070	C	0.0593910	-1.2135830	-0.4983720
O	5.4610920	-1.1575070	-0.9206570	C	1.5085060	-1.2962170	-0.8755460
H	5.3175470	-0.2578850	-1.2338410	C	2.3818590	-0.2913920	-0.0973110
O	0.9944870	2.4060300	1.9464330	H	2.5993120	-1.5425060	1.6429830
H	0.6861680	1.0147630	1.8373340	H	-0.3577150	-2.0363810	0.0859310

H	1.6043910	-1.0330970	-1.9390810	H	-2.8391240	3.1513240	-0.5376740
H	2.0253700	0.7249680	-0.3055270	H	-4.3953800	2.8816980	0.1740400
O	3.7191990	-0.4451090	-0.5390510	N	-0.5182550	-0.8878080	-0.7776200
H	3.7825510	0.0373640	-1.3834070	N	-4.8544630	-1.5995820	1.2481120
O	1.9451300	-2.6151650	-0.6446240	H	-5.7574360	-1.1895460	1.4197370
H	2.9003930	-2.6205610	-0.7768520	H	-4.7486200	-2.5963410	1.3100240
O	0.3916080	2.5683400	0.8264000	C	2.7743240	0.1873330	0.8967140
H	0.9112370	-0.4279850	2.7396790	O	1.5151960	0.7110980	1.2776940
C	3.3711000	0.4098740	2.1193420	C	0.3081560	-1.3656690	0.0583840
H	3.1185130	0.4509270	3.1827410	C	1.6898690	-1.7563820	-0.3782140
H	3.2837350	1.4290380	1.7177330	C	2.6580390	-0.5548200	-0.4315920
O	4.6855320	-0.0846730	2.0342860	H	3.0682320	-0.5122390	1.6849770
H	4.8775820	-0.1951120	1.0957370	H	0.0749190	-1.4949200	1.1182070
O	3.1440090	1.0420970	-2.7613430	H	1.6212760	-2.1576030	-1.3995240
H	0.5886160	2.5079330	-0.1159920	H	2.3117890	0.1364920	-1.2069430
H	3.6527790	1.6845570	-3.2593320	O	3.9472750	-1.0693160	-0.7513740
O	0.5980760	1.8874330	-2.0801150	H	4.0331460	-1.1317220	-1.7063060
H	2.2611270	1.4320420	-2.6145230	O	2.1605230	-2.7361390	0.5167360
H	0.0162930	2.3629710	-2.6785320	H	3.1126530	-2.8070050	0.3774100
oINT7_{2H2O}				H	0.1888330	-0.2050280	-2.4171970
H = -1079.160500 a.u.				C	3.7984560	1.3138870	0.8261400
G = -1079.237060 a.u.				H	3.5178600	1.9958480	0.0082210
C	-3.2746120	1.2123720	-0.0968730	H	4.7920710	0.9152040	0.6238830
N	-2.0648230	0.8110390	-0.5093010	O	3.8558860	2.0019270	2.0556810
C	-1.7836150	-0.4806140	-0.3099200	H	2.9446520	2.1453490	2.3341710
C	-2.6662060	-1.3714670	0.2656090	O	0.7856350	0.2880620	-3.0139120
C	-3.9093610	-0.8324840	0.6516450	H	1.1917990	1.2987550	0.5635090
N	-4.2142500	0.4523760	0.4701670	H	0.3710560	0.2901250	-3.8790230
H	-2.4185690	-2.4152550	0.3953970	O	0.4536900	2.1608670	-0.8551220
N	-3.5860680	2.5194820	-0.3011160	H	-0.4601880	1.8254310	-0.7832220

H 0.7401120 1.8359560 -1.7203490

oTS7_8₂H₂O

H = -1079.127718 a.u.

G = -1079.198213 a.u.

C -3.0585430 -0.5711360 1.2115830

N -1.7928300 -0.7781280 0.8359580

C -1.5058800 -0.5088040 -0.4465590

C -2.4665820 -0.0112760 -1.3290190

C -3.7512520 0.1671300 -0.8113100

N -4.0590670 -0.1062410 0.4618380

H -2.2295290 0.1752030 -2.3670990

N -3.3482490 -0.8180760 2.5246080

H -2.6876430 -1.3814750 3.0335030

H -4.3225970 -0.8950140 2.7644160

N -0.2122700 -0.6884910 -0.9046600

N -4.7869080 0.5970670 -1.5956000

H -5.6172280 0.8899880 -1.1056300

H -4.5767040 1.0654280 -2.4604010

C 2.6871810 0.2683500 0.6020680

O 1.3038220 -0.0030750 0.9347160

C 0.6990620 -1.2067920 -0.0255960

C 2.0050740 -1.6959740 -0.6211740

C 2.9145820 -0.4668360 -0.7182170

H 3.2895220 -0.1833600 1.3921670

H 0.2985510 -1.8639500 0.7406000

H 1.8090600 -2.1404650 -1.6019770

H 2.6032260 0.1674720 -1.5540690

O 4.2788150 -0.8376150 -0.8114260

H 4.5703730 -0.7684580 -1.7228740

O 2.5647410 -2.6333900 0.2684450

H 3.5155290 -2.6502390 0.1060000

H 0.1668030 0.2990070 -1.5753620

C 2.9658360 1.7607910 0.4945420

H 2.4357890 2.1689100 -0.3727190

H 4.0400500 1.8632570 0.3178350

O 2.6502430 2.4605220 1.6736300

H 1.7177760 2.7001470 1.6225680

O 0.5654420 1.4327910 -1.8681020

H 0.6994830 0.8536060 0.8148610

H 0.2191920 1.7938550 -2.6856950

O 0.0444320 2.0818310 0.4521480

H -0.8963760 2.0587080 0.6548520

H 0.1631680 1.9832270 -0.5891810

oINT8₂H₂O

H = -1079.175877 a.u.

G = -1079.249876 a.u.

C -2.9694310 -0.6573780 1.1817450

N -1.7135450 -0.9269640 0.8096400

C -1.4212880 -0.6778800 -0.4706360

C -2.3575270 -0.1664720 -1.3705340

C -3.6306860 0.0733620 -0.8552000

N -3.9481100 -0.1608220 0.4251750

H -2.1039560 0.0266020 -2.4034600

N -3.2633620 -0.8653760 2.5002120

H -2.6228240 -1.4443020 3.0177570

H -4.2390120 -0.8996660 2.7450780

N -0.1347550 -0.9440970 -0.8904360

N -4.6482950 0.5363760 -1.6440390

H -5.4623300 0.8762110 -1.1571760

H -4.4205690 0.9767700 -2.5190260

C	2.5944750	0.3372880	0.6085020	C	-0.7065000	0.4396540	0.1880900
O	1.2410240	-0.0619120	0.8387640	C	-1.6473040	0.4412000	-1.0047200
C	0.8932270	-1.2335660	0.0674800	C	-3.0500220	0.0481310	-0.4988700
C	2.1909450	-1.6624300	-0.6146050	H	-2.5500710	-1.1405500	1.2286390
C	2.9635500	-0.3395900	-0.7080190	H	-1.3045790	-0.2891050	-1.7358900
H	3.2252500	-0.0532990	1.4144940	H	-3.7022660	-0.0289440	-1.3737000
H	0.5356420	-1.9924580	0.7586360	O	-3.5899820	1.1060840	0.2873050
H	1.9944970	-2.1209940	-1.5894820	H	-2.9830380	1.2911270	1.0179290
H	2.5925620	0.2628560	-1.5462920	O	-1.7032700	1.7028630	-1.6185300
O	4.3635190	-0.5367500	-0.7837240	H	-2.3256530	2.2438140	-1.1186890
H	4.6474320	-0.4946350	-1.6993830	C	-4.5103940	-1.7156820	0.5830190
O	2.8689770	-2.5545100	0.2366610	H	-4.4839820	-2.7331440	0.9840180
H	3.8146970	-2.4143000	0.1050820	H	-5.0858990	-1.7403590	-0.3521070
H	0.1489570	-0.3851610	-1.6889870	O	-5.1283560	-0.9165240	1.5628080
C	2.7082020	1.8497650	0.5464340	H	-5.1043790	-0.0035960	1.2550660
H	2.1160290	2.2160600	-0.2999300	O	-0.6815510	1.3691330	0.9660600
H	3.7591420	2.0914710	0.3629000	H	-2.4036350	-3.0664780	-0.1199540
O	2.3293340	2.4809770	1.7469890	H	-0.1306610	-0.4804660	0.3812450
H	1.3699460	2.5744850	1.7361240	C	3.5732190	-1.5319210	-0.4353630
O	0.3465960	1.6893180	-2.0082570	N	4.0820010	-1.1121260	0.7251310
H	-0.0243420	1.1786210	0.9043960	C	3.6662740	0.0902020	1.1393160
H	0.2509050	2.4603450	-2.5705940	C	2.7489860	0.8614960	0.4228860
O	-0.4118020	2.0536520	0.6982080	C	2.2804430	0.2952200	-0.7605900
H	-1.3125110	2.0294180	1.0340810	N	2.6790090	-0.9045730	-1.2028430
H	-0.0430400	1.9333790	-1.1482070	H	2.4235600	1.8409800	0.7464680
oRINT3_{H2O}				N	4.0375720	-2.7310030	-0.9017090
H	-1079.151289	a.u.		H	4.5228120	-3.3163180	-0.2431040
G	-1079.230671	a.u.		H	3.5054000	-3.1695440	-1.6340580
C	-3.0800780	-1.2712240	0.2717640	N	4.2219990	0.5473820	2.3037060
O	-2.4168750	-2.2097020	-0.5547620	H	4.7049910	-0.1404210	2.8590940

H	3.7551780	1.2892780	2.7976110	C	3.9852660	-0.3095330	-0.9792300
N	1.3082270	0.9215560	-1.5047290	N	4.3148310	-0.9757140	0.1293960
H	1.1881640	1.9202660	-1.3647370	C	3.4244980	-0.9628540	1.1219730
H	1.2322990	0.5905890	-2.4556010	C	2.1956940	-0.2823800	1.0207250
O	0.8027400	3.5127150	-0.1530970	C	1.9949080	0.3552170	-0.1816730
H	0.4649660	4.3626020	-0.4422580	N	2.8461440	0.3642640	-1.1984770
H	0.0657430	3.0626230	0.2816720	H	1.4596470	-0.2492600	1.8129340

oRTS3_4H₂O

H = -1079.134894 a.u.

G = -1079.205686 a.u.

C	-3.0067560	-1.2156630	-0.4212350
O	-2.4788870	-1.7390080	-1.6315720
C	-0.5183070	0.3665000	0.0011220
C	-1.5947510	0.8416260	-0.9839030
C	-2.9695920	0.3046460	-0.5695010
H	-2.3881600	-1.5018150	0.4410380
H	-1.3614590	0.4901250	-1.9919780
H	-3.6891160	0.6003280	-1.3405620
O	-3.3835680	0.9320670	0.6374620
H	-2.6193090	0.8291880	1.2450590
O	-1.6275500	2.2576530	-1.0179690
H	-2.2308810	2.5374930	-0.3180660
C	-4.4316090	-1.7167200	-0.1824500
H	-4.4403220	-2.8092460	-0.2519180
H	-5.0806610	-1.3281060	-0.9798810
O	-4.9186690	-1.3898390	1.0961430
H	-4.7551900	-0.4480040	1.2322110
O	-0.8163710	0.6446520	1.2982780
H	-2.5084740	-2.6987130	-1.5973050
H	-0.3087120	-0.6993000	-0.1662950

H	5.6806740	-0.9278260	-1.9163350
H	4.6166320	0.0522360	-2.8796160
N	3.7475150	-1.6634020	2.2394320
H	4.6964330	-1.9904320	2.3207260
H	3.2151970	-1.5322470	3.0822290
N	0.7873220	1.1036850	-0.3982340
H	0.7607000	2.0277780	0.3390720
H	0.7685860	1.4193620	-1.3678720
O	0.4501830	2.6587980	1.4799210
H	-0.0282130	3.4818630	1.3542820
H	-0.2581490	1.7981440	1.5841740

oRINT4H₂O

H = -1079.164097 a.u.

G = -1079.237490 a.u.

C	-3.1514610	-1.0650170	-0.5475460
O	-2.6539460	-1.4654780	-1.8142690
C	-0.4922800	0.2520520	-0.0657920
C	-1.5917610	0.9438660	-0.8780080
C	-2.9957360	0.4544250	-0.5015960
H	-2.5642980	-1.5091060	0.2695950
H	-1.4198570	0.7250040	-1.9341670
H	-3.6953350	0.8988400	-1.2162610

O	-3.3739020	0.9568870	0.7763960	H	-0.3852230	1.1102660	1.6995580
H	-2.6872500	0.6554570	1.3936720	oRINT5_{H2O}			
O	-1.5214250	2.3478220	-0.7210580	H = -1079.16142 a.u.			
H	-2.0373150	2.5735900	0.0629320	G = -1079.234039 a.u.			
C	-4.6118970	-1.4852000	-0.3734580	C	3.0302740	-0.6787380	1.0451200
H	-4.6989050	-2.5566100	-0.5794430	O	2.6145720	-0.0096000	2.2203420
H	-5.2236960	-0.9528820	-1.1148770	C	0.4281840	0.1232590	-0.5599880
O	-5.0856950	-1.2902010	0.9370100	C	1.6544450	1.0189900	-0.2977920
H	-4.9104520	-0.3717960	1.1743210	C	2.9458480	0.2101700	-0.2123650
O	-0.7709750	0.2951110	1.3295700	H	2.4336220	-1.5819730	0.8654660
H	-2.7640250	-2.4150510	-1.9119150	H	1.5211470	1.5622780	0.6398080
H	-0.4725660	-0.8103560	-0.3317010	H	3.7719880	0.9332430	-0.1976560
C	4.1727780	0.0964050	-0.7237320	O	3.0242600	-0.5987920	-1.3793190
N	4.4129230	-0.9854210	0.0221630	H	3.8435700	-1.1071960	-1.3256550
C	3.3649280	-1.4797240	0.6839690	O	1.7544960	1.9990770	-1.3171550
C	2.0853000	-0.9149460	0.6093380	H	1.4775170	1.5735360	-2.1405220
C	1.9722550	0.1957190	-0.2190110	C	4.4687010	-1.0879470	1.3301350
N	3.0038710	0.7174510	-0.8917880	H	4.4819610	-1.8040050	2.1563250
H	1.2530340	-1.2930980	1.1854250	H	5.0251920	-0.1915430	1.6255430
N	5.2493820	0.6413550	-1.3638910	O	5.0130990	-1.6585070	0.1443760
H	6.0671000	0.0606460	-1.4452860	H	5.9335540	-1.8879190	0.2862150
H	5.0529780	1.2948280	-2.1033060	O	0.3809290	-0.2108750	-1.9447530
N	3.5984190	-2.6031850	1.4273630	H	1.6555620	-0.0156140	2.2821600
H	4.5669320	-2.8162940	1.6067520	H	0.5161970	-0.8092980	0.0167860
H	2.9375940	-2.8501870	2.1446270	C	-4.1426690	0.3185800	0.5663990
N	0.7739980	0.8659630	-0.3777240	N	-4.4342470	-0.9609630	0.3107580
H	0.9330030	2.5767910	1.0495980	C	-3.4301040	-1.6910690	-0.1787610
H	0.7782520	1.5458630	-1.1277530	C	-2.1522210	-1.1739250	-0.4026590
O	0.5500290	2.6682490	1.9318630	C	-1.9730090	0.1686220	-0.0617030
H	0.3344370	3.5963610	2.0442780	N	-2.9683780	0.9272420	0.4197860

H -1.3749740 -1.7604490 -0.8691130
N -5.1814890 1.0970380 1.0043020
H -5.9821680 0.6064330 1.3663480
H -4.9285070 1.9694320 1.4378030
N -3.7154490 -3.0116910 -0.4290880
H -4.6990450 -3.2262220 -0.4873320
H -3.1209230 -3.4999260 -1.0784590
N -0.7637610 0.7952230 -0.1748310
H 1.1763280 -0.7324700 -2.1257370
H -0.7448160 1.7977890 -0.0038360
O 0.0999280 3.6184170 0.1406520
H 0.7241100 3.4380750 -0.5779660
H -0.3420180 4.4424620 -0.0701290

oRTS5_6H₂O

H = -1079.113015 a.u.

G = -1079.183923 a.u.

C -2.9126430 -1.1942000 -0.5438910
O -2.3459220 -1.5581340 -1.7850500
C -0.4018780 0.4768290 0.0050100
C -1.6401810 1.0413800 -0.7124070
C -2.9463780 0.3309280 -0.3580890
H -2.3670840 -1.6364320 0.2993190
H -1.4474310 0.9143960 -1.7790100
H -3.7282010 0.7502940 -1.0055780
O -3.2267260 0.6721520 1.0021540
H -4.0439260 0.2230490 1.2586480
O -1.7968980 2.4304420 -0.4809810
H -2.4284950 2.5315730 0.2405600
C -4.3198030 -1.7734420 -0.5764540
H -4.2594310 -2.8646110 -0.5925070

H -4.8114760 -1.4285860 -1.4927160
O -5.0125560 -1.3107300 0.5797690
H -5.9059310 -1.6599900 0.5878480
O -0.5874860 0.9276620 1.5595010
H -1.3856550 -1.5299430 -1.7371510
H -0.4477280 -0.6130070 0.1133280
C 4.1255660 -0.0234730 -0.7005560
N 4.3038470 -1.1014430 0.0742060
C 3.2279420 -1.4886680 0.7578490
C 1.9953560 -0.8401670 0.6635060
C 1.9179050 0.2488190 -0.2214210
N 3.0055860 0.6640560 -0.8941500
H 1.1722550 -1.1352640 1.2992490
N 5.2434770 0.4375210 -1.3492920

H 6.0061290 -0.2135300 -1.4350870
H 5.0735720 1.0643700 -2.1183920
N 3.3904910 -2.6012530 1.5571250
H 4.3532250 -2.8163280 1.7694780
H 2.7506110 -2.7030470 2.3283380
N 0.7733130 0.9795970 -0.4636210
H -1.5326780 0.9044010 1.7925970
H 0.8593280 2.3518250 0.2533030
O 0.5877240 2.9541610 1.0808650
H 0.0289960 3.6421370 0.7029470
H -0.1234770 1.9768870 1.5136120

oRINT6H₂O

H = -1079.15336 a.u.

G = -1079.231563 a.u.

C 2.8501260 -1.3214960 -0.5582760
O 2.9384910 -2.5268850 0.1856790

C	0.4024160	-0.5046100	0.9926600	H	-4.0100720	2.0765390	-2.1056230
C	1.7837640	-0.2151840	1.5230580	N	-0.5144260	0.3661020	0.9590540
C	2.7696210	-0.0828160	0.3490500	H	0.7296940	2.1007610	-1.0229000
H	1.9726890	-1.3182280	-1.2166020	H	-0.3332010	2.1850810	1.5119510
H	2.0993820	-1.0708510	2.1273530	O	0.0798160	3.0667080	1.5996360
H	3.7545270	0.1038670	0.7975510	H	-0.1903400	3.4202780	2.4495250
O	2.3448520	1.0463800	-0.3920790	H	0.1415130	3.3276460	-0.3761260
H	2.9955090	1.1985730	-1.0895720	oRINT3_{2H2O}			
O	1.8511240	0.9080320	2.3459280	H = -1155.564496 a.u.			
H	1.5853690	1.6970340	1.8490570	G = -1155.648393 a.u.			
C	4.1196110	-1.3024160	-1.4001440	C	-3.1887570	-1.5289890	0.4045030
H	4.0799200	-2.1146680	-2.1315090	O	-2.4330890	-2.6132760	-0.1019190
H	4.9677810	-1.4716220	-0.7267650	C	-0.6668350	-0.0562040	0.2805570
O	4.2193760	-0.0359870	-2.0389370	C	-1.5979810	-0.0327660	-0.9288200
H	5.0392860	0.0156120	-2.5340350	C	-3.0471220	-0.2688950	-0.4626140
O	0.1308550	2.8356690	-1.2066990	H	-2.7729430	-1.3074960	1.3923950
H	2.0592720	-2.8635230	0.3708600	H	-1.2985610	-0.8554510	-1.5792380
H	0.2162150	-1.5114670	0.5970820	H	-3.6597190	-0.3709250	-1.3726770
C	-3.4463030	-1.5081110	0.2289090	O	-3.4441490	0.8850440	0.2566900
N	-4.1494270	-0.7679800	-0.6312630	H	-4.3124670	0.7028910	0.6377120
C	-3.6095210	0.3998390	-0.9857850	O	-1.5120900	1.1402190	-1.6837210
C	-2.3843210	0.8504650	-0.4615160	H	-1.6762020	1.9048860	-1.1121790
C	-1.7626580	-0.0232680	0.4050100	C	-4.6409160	-1.9659550	0.5628110
N	-2.2565920	-1.2103870	0.7628530	H	-4.6834160	-2.8125050	1.2539320
H	-1.9091180	1.7773100	-0.7582030	H	-5.0228550	-2.2888860	-0.4160680
N	-4.0172330	-2.6826140	0.6264130	O	-5.3929640	-0.8616850	1.0488350
H	-4.7874820	-3.0282940	0.0796960	H	-6.3043430	-1.1217400	1.1976150
H	-3.4298420	-3.3405010	1.1093800	O	-0.4681150	0.9047410	0.9830510
N	-4.2924310	1.1338580	-1.9017200	H	-2.7569680	-2.8484800	-0.9774090
H	-5.2228520	0.8378400	-2.1444870	H	-0.2239610	-1.0364040	0.5274380

C	4.1129150	-1.4667040	-0.2769290	H	-2.3301620	-1.2794420	1.1279020
N	4.5052840	-0.8314660	0.8288080	H	-1.2906980	-0.5051660	-1.9529660
C	3.8097260	0.2688180	1.1407700	H	-3.5757800	-0.3945640	-1.5102210
C	2.7446150	0.7335400	0.3727790	O	-3.4607170	0.8623610	0.1205180
C	2.4337120	-0.0273910	-0.7538670	H	-4.2253930	0.5410120	0.6116050
N	3.1144330	-1.1313770	-1.0945610	O	-1.6044570	1.4704940	-1.7729810
H	2.1837340	1.6255990	0.6158910	H	-1.7622150	2.1405250	-1.0665870
N	4.7948880	-2.6171870	-0.5892180	C	-4.2316080	-2.0895010	0.5209960
H	5.7013880	-2.7153610	-0.1620260	H	-4.0877630	-2.9975140	1.1146180
H	4.6951310	-2.9377240	-1.5384020	H	-4.7315890	-2.3599250	-0.4207000
N	4.2347410	0.9496810	2.2563140	O	-4.9992390	-1.1268410	1.2305340
H	4.8289920	0.4182720	2.8736390	H	-5.8567940	-1.4929660	1.4553350
H	3.5702990	1.5609220	2.7022600	O	-0.6381280	0.7549380	1.0638050
N	1.3600930	0.2987970	-1.5417460	H	-2.5320160	-2.7014800	-1.3120990
H	1.0268670	1.2588920	-1.5043280	H	-0.1937440	-0.9401710	0.0619140
H	1.3590060	-0.1366850	-2.4520040	C	3.9165260	-1.0514840	-0.7748560
O	-1.7449840	3.2673820	0.3203420	N	4.3664100	-0.9947620	0.4806480
H	-2.6961160	3.1265990	0.3445190	C	3.6059460	-0.3432130	1.3606370
H	-1.3788830	2.5207590	0.8264210	C	2.3912110	0.2701270	0.9954930
O	0.7977540	3.1846690	-0.8827130	C	2.0605480	0.1278760	-0.3311340
H	1.2572790	3.9523320	-1.2280120	N	2.7789140	-0.5150590	-1.2408290
H	-0.0773630	3.4918930	-0.6063070	H	1.7395270	0.7828530	1.6889260
oRTS3_4₂H₂O				N	4.6712800	-1.7460710	-1.6664760
H = -1155.554192 a.u.				H	5.6073060	-1.9925160	-1.3931980
G = -1155.630908 a.u.				H	4.4562040	-1.6404650	-2.6432720
C	-2.8616640	-1.5016090	0.1987620	N	4.0730530	-0.2689890	2.6337350
O	-2.1042430	-2.4991700	-0.4737130	H	4.8592730	-0.8521000	2.8704780
C	-0.4522490	0.1141230	-0.0963280	H	3.4579210	0.0236450	3.3734040
C	-1.5602410	0.2104540	-1.1671790	N	0.8312410	0.7019860	-0.8203770
C	-2.9390050	-0.2092540	-0.6261590	H	0.8514290	1.7735210	-0.6494400

H	0.7810220	0.5516860	-1.8296750	C	4.2127950	-0.1794230	-0.8250430
O	-1.3771630	2.9601770	0.4562170	N	4.4942040	-1.0246160	0.1717220
H	-2.1362680	3.3740690	0.8660570	C	3.4690410	-1.3506370	0.9611110
H	-1.0783580	1.7859210	0.8829600	C	2.1743410	-0.8554030	0.7686450
O	0.9238220	3.3006110	-0.3514390	C	2.0174330	0.0053960	-0.3153820
H	1.5333150	3.5977730	0.3271180	N	3.0288460	0.3592410	-1.1171470
H	-0.0272830	3.3999030	0.0260140	H	1.3627340	-1.0798360	1.4462880

oRINT4_{2H2O}

H = -1155.583289 a.u.

G = -1155.662974 a.u.

C	-3.0612290	-1.4069770	-0.1816680	N	5.2481440	0.1373570	-1.6593810
O	-2.4072580	-2.3353760	-1.0332270	H	6.1748250	-0.0564460	-1.3184030
C	-0.4483360	-0.0011240	-0.1495510	H	5.1173950	0.9412440	-2.2505240
C	-1.5331780	0.3817140	-1.1745460	N	3.7606810	-2.1730820	2.0174280
C	-2.9579020	0.0220280	-0.7305480	H	4.6483750	-2.6474380	1.9624770
H	-2.5386020	-1.4429540	0.7771130	H	3.0044720	-2.6815750	2.4443630
H	-1.3045540	-0.1888200	-2.0788280	N	0.8029430	0.5990230	-0.5941280
H	-3.5956150	0.1025860	-1.6280640	H	1.2136740	2.1795730	0.6163290
O	-3.3573390	0.9863410	0.2210070	H	0.7751030	1.1041100	-1.4725790
H	-4.1745970	0.6811060	0.6327360	O	-1.3720050	3.1012880	0.9452330
O	-1.4653260	1.7359660	-1.5473790	H	-1.9871080	3.6803010	1.3979910
H	-1.6785600	2.2861500	-0.7751790	H	-1.1836540	1.1953730	1.2160180
C	-4.5040570	-1.8655270	0.0045350	O	1.2959060	2.8669090	1.2992070
H	-4.4972540	-2.8757470	0.4244260	H	1.6073050	2.3904360	2.0733410
H	-4.9970120	-1.8953100	-0.9780090	H	-0.4627160	3.3335300	1.2106790
O	-5.1736070	-0.9541930	0.8666520				
H	-6.0769290	-1.2428190	1.0114200				
O	-0.7448630	0.3289000	1.1829430				
H	-2.8270340	-2.3174360	-1.8994130				
H	-0.3414870	-1.0904520	-0.1624500				

oRINT5_{2H2O}

H = -1155.583445 a.u.

G = -1155.663799 a.u.

C	-3.1724740	-1.2248130	-0.6967420				
O	-2.7447990	-1.3427940	-2.0405250				
C	-0.4800450	0.1373550	0.1422320				
C	-1.6751170	0.8571390	-0.5059400				
C	-3.0129990	0.2062660	-0.1504200				

H	-2.6199400	-1.9072900	-0.0382310	H	0.8304680	1.5003650	-0.8121390
H	-1.5544150	0.8084690	-1.5899150	O	0.4161080	3.0109610	1.8424960
H	-3.7936020	0.8462680	-0.5816690	H	0.8605020	3.3117330	2.6375070
O	-3.1202280	0.1995230	1.2688810	H	0.3655130	2.0423960	1.9013640
H	-3.9714110	-0.1952780	1.4977770	O	0.7409510	3.4954820	-0.9807710
O	-1.6951200	2.2281450	-0.1764740	H	0.9086990	3.5532730	-0.0297960
H	-1.5554850	2.3373280	0.7738770	H	-0.2218970	3.4632860	-1.0162750
C	-4.6369110	-1.6415750	-0.7242580	oRTS5_6₂H₂O			
H	-4.7064770	-2.6974110	-0.9995690	H = -1155.538163 a.u.			
H	-5.1457040	-1.0400030	-1.4856680	G = -1155.613502 a.u.			
O	-5.1915920	-1.4075130	0.5662000	C	-3.0457570	-1.3082320	-0.5509400
H	-6.1297850	-1.6074530	0.5581770	O	-2.5166750	-1.7046130	-1.7990190
O	-0.4488190	0.3920510	1.5528060	C	-0.4393020	0.2326600	-0.0436630
H	-1.7930090	-1.4696670	-2.0748700	C	-1.6587670	0.8487490	-0.7474250
H	-0.5895010	-0.9467410	-0.0033500	C	-2.9987210	0.2173640	-0.3686060
C	4.1387380	-0.2490220	-0.6667890	H	-2.5082460	-1.7744250	0.2847190
N	4.3350030	-1.3821910	0.0169440	H	-1.4949680	0.6936820	-1.8150340
C	3.2562000	-1.8792240	0.6226170	H	-3.7642850	0.6793840	-1.0053070
C	1.9969250	-1.2767220	0.5502370	O	-3.2450430	0.5704650	0.9959890
C	1.9217120	-0.1201720	-0.2302470	H	-4.0828820	0.1637530	1.2581970
N	2.9920080	0.4054220	-0.8363090	O	-1.7327420	2.2484570	-0.5530540
H	1.1573790	-1.6595170	1.1109870	H	-2.1880430	2.4059940	0.2817250
N	5.2475800	0.3136550	-1.2340130	C	-4.4802450	-1.8167150	-0.5612880
H	6.0549190	-0.2782420	-1.3333550	H	-4.4755490	-2.9095510	-0.5725130
H	5.0839490	1.0224930	-1.9297200	H	-4.9665750	-1.4512620	-1.4723790
N	3.4419720	-3.0525940	1.3124500	O	-5.1336320	-1.3147490	0.6017800
H	4.4034310	-3.2724050	1.5226440	H	-6.0422780	-1.6214410	0.6249970
H	2.7701390	-3.2881390	2.0239840	O	-0.6115220	0.5885390	1.5081240
N	0.7416560	0.5477650	-0.4509240	H	-1.5556460	-1.7241420	-1.7630870
H	-1.3294770	0.1899070	1.9061590	H	-0.5171380	-0.8626070	0.0143090

C	4.0823610	-0.3324890	-0.7178520	H	-2.3846890	-1.9810740	-0.0606520
N	4.2470720	-1.3913770	0.0867500	H	-1.7915720	0.6293720	-2.1088490
C	3.1622280	-1.7508190	0.7725620	H	-3.7520770	0.6486360	-0.7196600
C	1.9375420	-1.0934250	0.6586820	O	-2.7330880	0.2629430	1.0356090
C	1.8738990	-0.0246550	-0.2552360	H	-3.5331900	-0.0849320	1.4504890
N	2.9713720	0.3589190	-0.9367020	O	-1.6466100	2.1272320	-0.7798390
H	1.1068200	-1.3661830	1.2942290	H	-1.4807790	2.2803540	0.1667740
N	5.2099670	0.0995890	-1.3726720	C	-4.4926470	-1.8395660	-0.4480560
H	5.9599340	-0.5677650	-1.4449990	H	-4.5633520	-2.9250410	-0.5600260
H	5.0482140	0.7070680	-2.1590330	H	-5.1299560	-1.3614440	-1.2007650
N	3.3096700	-2.8493060	1.5970200	O	-4.8584480	-1.4296770	0.8644650
H	4.2699770	-3.0636850	1.8211160	H	-5.7671560	-1.6798180	1.0424680
H	2.6674540	-2.9219300	2.3697370	O	-0.3703320	0.3471800	2.6670060
N	0.7439660	0.7003910	-0.5252740	H	-1.9073770	-1.8737840	-2.2252650
H	-1.5584120	0.5662930	1.7385950	H	-0.3760650	-1.0162210	-0.5063310
H	0.9897020	2.2626670	-0.7149630	C	4.0044140	-0.5774710	-0.9295560
O	0.5133660	2.6902470	1.7953480	N	4.2563180	-1.2864370	0.1768750
H	0.2469070	3.3699110	2.4163800	C	3.2729090	-1.3462610	1.0729450
H	-0.1055090	1.6120360	1.7094050	C	2.0312340	-0.7153700	0.8739570
O	0.9872380	3.2829960	-0.5231880	C	1.9154650	-0.0189350	-0.3136940
H	0.7375570	3.0764170	0.8098600	N	2.8776680	0.0748590	-1.2301530
H	0.1712800	3.5729120	-0.9450530	H	1.2427260	-0.7056270	1.6163600
oRINT6_{2H2O}				N	5.0202270	-0.4860610	-1.8336480
H = -1155.565553 a.u.				H	5.7938770	-1.1200550	-1.7326180
G = -1155.649361 a.u.				H	4.8004190	-0.1155430	-2.7421640
C	-3.0570650	-1.3987040	-0.7020570	N	3.5091330	-2.0833240	2.1967870
O	-2.8344240	-1.6741760	-2.0753020	H	4.4694970	-2.3315270	2.3738640
C	-0.3563190	0.0704590	-0.6688850	H	2.9136440	-1.9399200	2.9955850
C	-1.6626760	0.7505070	-1.0268950	N	0.7349640	0.7044290	-0.6128670
C	-2.8744750	0.0924740	-0.3643170	H	-1.2150450	0.2074770	2.2211980

H 1.0573500 2.6487380 -0.8465880
O -0.3819120 3.0184920 1.5984190
H -0.5907710 3.7490530 2.1845620
H -0.1613540 1.2636440 2.4365730
O 0.8988490 3.6019320 -0.7212140
H 0.2126770 3.3693930 0.8999870
H 0.0977060 3.7398550 -1.2377090

pINT3_{H2O}

H = -1079.154689 a.u.

G = -1079.233179 a.u.

C -2.3357570 -0.1681310 0.9561440
N -2.9370850 -1.0785720 0.1756170
C -3.9008750 -0.6198960 -0.6319830
C -4.2633540 0.7256060 -0.6740320
C -3.5451080 1.5769570 0.1676230
N -2.5804690 1.1439460 0.9862670
H -5.0436010 1.0883640 -1.3285470
N -1.3745420 -0.6320230 1.7961670
H -1.0385650 -1.5738580 1.6505520
H -0.7638790 0.0367090 2.2417470
N -4.5402820 -1.5585240 -1.3956480
H -4.0936820 -2.4604440 -1.4536550
H -5.0339070 -1.2497410 -2.2161080
N -3.7671470 2.9277760 0.1748560
H -3.3720080 3.4251960 0.9574950
H -4.6429330 3.2710560 -0.1822170
C 3.4738760 0.8794060 -0.3545040
O 2.5486710 1.5863800 -1.1575030
C 0.5116260 0.1252090 -0.3366520
C 1.5238070 -0.4375140 0.6393830

C 2.9369400 -0.5010890 0.0505410
H 3.6047370 1.4761750 0.5511920
H 0.0228940 1.0688470 -0.0418350
H 1.2250250 -1.4750890 0.8449630
H 2.9041590 -1.1558080 -0.8339120
O 3.7176880 -1.0733640 1.0817960
H 4.6499110 -0.9700080 0.8514070
O 1.5011040 0.3423270 1.8138810
H 2.2375850 0.0395170 2.3587740
O 0.2529890 -0.4423480 -1.3705680
H 2.3320860 1.0650510 -1.9395460
C 4.7992310 0.7920770 -1.1063150
H 5.1390560 1.8070820 -1.3307270
H 4.6366040 0.2567580 -2.0520170
O 5.7438010 0.0998750 -0.2985380
H 6.5907850 0.0535600 -0.7467720
O -0.7895840 -2.9570650 -0.1620620
H -1.6523990 -2.5068490 -0.1528210
H -0.3048620 -2.4969360 -0.8560510

pTS3_4_{H2O}

H = -1079.133491 a.u.

G = -1079.204851 a.u.

C 2.0445610 -0.3488160 0.1777230
N 2.1731630 0.9557800 0.1809710
C 3.2928990 1.4213560 -0.4023280
C 4.2377920 0.5644770 -0.9696910
C 3.9626170 -0.8003980 -0.9004450
N 2.8463930 -1.2735770 -0.3154240
H 5.1366820 0.9395190 -1.4403500
N 0.8644350 -0.8653460 0.8273020

H 0.9977450 -0.8037260 1.9751830
 H 0.7268820 -1.8231070 0.4984350
 N 3.4477430 2.7686380 -0.3787570
 H 2.6618180 3.3130060 -0.0603410
 H 4.1489560 3.2150480 -0.9427310
 N 4.7871550 -1.7354490 -1.4495470
 H 4.6062810 -2.6951790 -1.2027820
 H 5.7312650 -1.4855250 -1.6885130
 C -3.0150730 0.7368560 -0.5779100
 O -2.4847840 1.9083880 -0.0006910
 C -0.4449780 -0.0458030 0.6311800
 C -1.5466600 -1.0904430 0.5096060
 C -2.9476040 -0.4616030 0.3855880
 H -2.4862120 0.4769500 -1.5072530
 H -0.3105010 0.4593850 -0.3355480
 H -1.5516130 -1.7028420 1.4257030
 H -3.2536550 -0.1008360 1.3747860
 O -3.7758730 -1.5481130 -0.0119350
 H -4.4470370 -1.2381600 -0.6355660
 O -1.2466330 -1.8962800 -0.6105220
 H -2.0621890 -2.3667780 -0.8272900
 O -0.6540880 0.8037290 1.6565380
 H -1.8604390 1.6994630 0.7244050
 C -4.4492240 1.1183300 -0.9326200
 H -4.4124010 2.0715530 -1.4654270
 H -5.0231290 1.2515750 -0.0076180
 O -5.0280330 0.0987530 -1.7496390
 H -5.9087500 0.3660150 -2.0203380
 O 0.8357000 -0.2128150 3.2120760
 H 0.4326410 -0.7123570 3.9253540

H 0.0651450 0.3926370 2.6648400
pINT₄H₂O
 H = -1079.162469 a.u.
 G = -1079.236754 a.u.
 C 2.0578410 -0.2919130 -0.1169040
 N 2.0981810 0.9618240 0.3070400
 C 3.2739280 1.5892570 0.1562230
 C 4.3818230 0.9704100 -0.4204490
 C 4.1979890 -0.3490410 -0.8374540
 N 3.0377360 -0.9964280 -0.6837650
 H 5.3269600 1.4821010 -0.5416820
 N 0.8642850 -0.9888300 0.0619650
 H 0.9818770 -2.2153930 1.7507790
 H 0.7545140 -1.7064420 -0.6477240
 N 3.3259900 2.8675140 0.6335670
 H 2.4387620 3.2859060 0.8650320
 H 4.0577350 3.4800150 0.3165970
 N 5.1956640 -1.0465560 -1.4649620
 H 5.0507800 -2.0413240 -1.5361140
 H 6.1452260 -0.7362570 -1.3459050
 C -3.0941470 0.9361080 -0.1890950
 O -2.4984090 1.7984210 0.7594320
 C -0.3640210 -0.2558590 0.3280980
 C -1.5324350 -1.1240360 -0.1228260
 C -2.9238050 -0.5428900 0.1944410
 H -2.6636910 1.0996770 -1.1869710
 H -0.3606640 0.6904250 -0.2199530
 H -1.4666200 -2.0886530 0.4058340
 H -3.1063030 -0.6247290 1.2738560
 O -3.8132720 -1.4060060 -0.5023520

H -4.5387440 -0.8939580 -0.8854790
O -1.3813440 -1.3209220 -1.5111630
H -2.2104370 -1.7122480 -1.8146750
O -0.5043790 0.0909670 1.6858760
H -1.8589420 1.3257020 1.3120310
C -4.5563120 1.3718580 -0.2148040
H -4.5729150 2.4605200 -0.3063620
H -5.0331890 1.0884610 0.7313830
O -5.2142220 0.7552490 -1.3217130
H -6.1158950 1.0777240 -1.3813150
O 0.5082770 -2.3421650 2.5868810
H 0.4708410 -3.2845450 2.7584880
H -0.3706650 -0.6973540 2.2361950

pINT5_{H2O}

H = -1079.161593 a.u.

G = -1079.235786 a.u.

C 1.9016810 0.2925690 -0.3733620
N 2.3251580 -0.9720960 -0.2594170
C 3.5920520 -1.1244420 0.1484140
C 4.4169600 -0.0488580 0.4649010
C 3.8433310 1.2195220 0.3278240
N 2.5933360 1.4038170 -0.0963270
H 5.4338550 -0.1854480 0.8059940
N 0.6310720 0.4848730 -0.8217680
H 0.2567560 1.4241870 -0.7609260
N 4.0482210 -2.4174550 0.2093070
H 3.3326170 -3.1265290 0.1929300
H 4.8468340 -2.6083990 0.7913400
N 4.5386660 2.3527320 0.6582890
H 4.1368030 3.2162110 0.3282070

H 5.5432370 2.3056460 0.6865460
C -3.4000870 -0.5077700 0.3475470
O -3.5348940 -1.0352050 -0.9703220
C -0.2722770 -0.5985730 -1.1199860
C -0.9073510 -1.1552810 0.1687340
C -1.9424070 -0.2109540 0.7761880
H -3.8015970 -1.2217230 1.0738070
H 0.3069420 -1.4016810 -1.5839590
H -0.0990170 -1.2514670 0.8977480
H -1.6846570 0.8116130 0.4692070
O -1.8460420 -0.3194710 2.1844370
H -2.4647530 0.3245910 2.5502550
O -1.4982130 -2.4385870 -0.0651740

H -0.8220740 -3.1142440 0.0170280
O -1.2187210 -0.0885150 -2.0390070
H -3.2437380 -1.9549140 -0.9230100
C -4.2162780 0.7734850 0.3656030
H -5.2672210 0.5490740 0.1618080
H -3.8252510 1.4401850 -0.4110080
O -4.0603010 1.3569240 1.6560900
H -4.2332230 2.2983990 1.6009470
O -1.6345650 2.5479670 -1.3499670
H -2.0912890 -0.4867040 -1.8642280
H -1.4864800 3.2686490 -1.9655120
H -1.5447820 1.7263650 -1.8614030

pTS5_6_{H2O}

H = -1079.110626 a.u.

G = -1079.182398 a.u.

C -1.9139220 0.1901040 -0.0158340
N -2.4509230 -1.0489290 0.0059730

C	-3.7764520	-1.1311770	-0.1109360	H	3.7837100	1.6424730	0.8083800
C	-4.5931390	-0.0167490	-0.2813660	O	4.4548610	1.5838600	-1.1621770
C	-3.9287370	1.2134840	-0.3045090	H	4.9057430	2.4286290	-1.1079230
N	-2.6128050	1.3324030	-0.1662390	O	0.3745250	2.1485890	1.6243120
H	-5.6657220	-0.0972270	-0.3948220	H	1.9221060	-0.4738220	1.7930800
N	-0.5670060	0.3439780	0.0840470	H	0.8521750	2.9171930	1.3069110
H	-0.1319960	1.7188120	0.8435740	H	0.8341060	0.7485920	1.9068340
N	-4.3126140	-2.4007090	-0.0241720	pINT6_{H2O}			
H	-3.6442770	-3.1396950	-0.1799950	H = -1079.153542 a.u.			
H	-5.2128020	-2.5432810	-0.4534200	G = -1079.231221 a.u.			
N	-4.6228060	2.3865400	-0.5112560	C	-1.6527840	-0.3872460	-0.6257760
H	-4.1036840	3.2168540	-0.2686040	N	-2.3486960	-1.4103680	-0.1595300
H	-5.5962050	2.3951600	-0.2530180	C	-3.6025660	-1.1342640	0.2344950
C	3.6235220	-0.3189460	-0.0236320	C	-4.1362370	0.1522250	0.1713260
O	3.4561210	-0.8162180	1.3087760	C	-3.3036980	1.1433600	-0.3434860
C	0.1679790	-0.7347230	0.5055120	N	-2.0670590	0.8646970	-0.7810860
C	1.2450820	-1.1939580	-0.4779970	H	-5.1396040	0.3713790	0.5107040
C	2.2972930	-0.1300600	-0.7973740	N	-0.3134560	-0.5870360	-1.0289350
H	4.2289210	-1.0221930	-0.6019200	H	-0.6259940	2.0032120	-0.9726270
H	-0.4013080	-1.5877690	0.8799940	N	-4.3128820	-2.1849800	0.7368310
H	0.7021540	-1.3775970	-1.4094060	H	-3.9253540	-3.1011760	0.5781480
H	1.8566780	0.8467120	-0.5548480	H	-5.3124320	-2.1119360	0.8173340
O	2.5689590	-0.2032990	-2.1821970	N	-3.7081050	2.4423920	-0.4735370
H	3.1786470	0.5142960	-2.3910570	H	-2.9672000	3.1127320	-0.6184890
O	1.8958880	-2.3960450	-0.0475170	H	-4.4722720	2.7552410	0.1024080
H	1.3299690	-3.1476220	-0.2373670	C	2.9379850	-0.0792900	0.8217210
O	0.9479410	-0.2743900	1.8432180	O	1.9230420	-0.4851450	1.7225330
H	3.3013830	-1.7671160	1.2189250	C	0.3600030	-1.4591690	-0.4074220
C	4.3599190	1.0007140	0.1290570	C	1.7987070	-1.6859480	-0.7876560
H	5.3478570	0.8225160	0.5633730	C	2.6224520	-0.4081060	-0.6542140

H	3.8810420	-0.5827560	1.0666290	H	-0.5429540	1.9540690	-0.6723000
H	-0.0558660	-2.0689910	0.4008860	N	-4.6167710	-1.9824700	0.7077110
H	1.8315190	-1.9852500	-1.8416220	H	-4.2964090	-2.9172060	0.5113830
H	2.0479940	0.4050110	-1.1115360	H	-5.6071890	-1.8330440	0.7927190
O	3.8311030	-0.6303010	-1.3591010	N	-3.5908040	2.6442720	-0.1584380
H	4.3621540	0.1694740	-1.2573740	H	-2.8049240	3.2684610	-0.2584740
O	2.3180340	-2.7192900	0.0401270	H	-4.3713420	2.9868770	0.3758750
H	3.2162010	-2.9012860	-0.2555820	C	2.7086700	0.2517430	0.7914840
O	-0.3927240	1.2758860	1.8420700	O	1.4553460	0.6496490	1.2912250
H	1.9442020	-1.4491370	1.7641170	C	0.2480480	-1.3295030	-0.1332100
C	3.1111570	1.4180540	1.0032550	C	1.6535910	-1.6738820	-0.5311120
H	3.4559440	1.6343150	2.0183290	C	2.5777090	-0.4490840	-0.5681400
H	2.1477160	1.9113230	0.8328620	H	3.1204540	-0.4694200	1.5060730
O	4.0716650	1.8270190	0.0312690	H	-0.0849790	-1.6776370	0.8483710
H	4.1305230	2.7843290	0.0227430	H	1.6292220	-2.0706520	-1.5544580
O	0.1275590	2.6018630	-0.7836790	H	2.1629760	0.2588150	-1.3000630
H	0.3126670	0.6231730	1.9269460	O	3.8220950	-0.9670890	-1.0097180
H	0.7391480	2.4627720	-1.5098890	H	4.5062300	-0.3072740	-0.8338390
H	-0.1585290	1.7766820	1.0505910	O	2.1431560	-2.6424870	0.3691740
pINT7_{H2O}				H	3.0690160	-2.7803880	0.1392000
H = -1002.743056 a.u.				H	1.0698800	1.3059260	0.6808670
G = -1002.813284 a.u.				C	3.6222150	1.4787160	0.7186980
C	-1.7770990	-0.3411980	-0.4729570	H	3.5965810	1.9897830	1.6848310
N	-2.5737600	-1.3261890	-0.0926000	H	3.2418180	2.1718930	-0.0371090
C	-3.8112680	-0.9664990	0.2911980	O	4.9612400	1.1629670	0.3372040
C	-4.2356090	0.3623030	0.2978410	H	5.4311000	0.8265850	1.1044590
C	-3.2995800	1.3109900	-0.1091670	O	0.3243690	2.4138030	-0.6129220
N	-2.0686290	0.9604280	-0.5115350	H	0.6815010	2.3726650	-1.5034200
H	-5.2331980	0.6435110	0.6070170	pTS7_8_{H2O}			
N	-0.4839640	-0.6559310	-0.9163720	H = -1002.699716 a.u.			

G = -1002.766728 a.u.

C 1.7967120 -0.0118450 -0.3962690
N 2.1691580 1.0888980 0.2492070
C 3.4446720 1.1327120 0.6501470
C 4.3388540 0.0915180 0.4045940
C 3.8235410 -1.0038620 -0.2884040
N 2.5506620 -1.0619580 -0.6975040
H 5.3695520 0.1325020 0.7305570
N 0.4746950 -0.1007810 -0.8612050
H 0.0465790 -1.2475690 -0.8362930
N 3.8152250 2.2501940 1.3509790
H 3.1788230 3.0293900 1.2880360
H 4.7942520 2.4750550 1.4089040
N 4.6067320 -2.0749840 -0.6276550
H 4.1011070 -2.8954350 -0.9243210
H 5.4523040 -2.2330830 -0.1057370
C -2.6756220 -0.0113680 0.8132370
O -1.3027720 -0.2430230 1.0256350
C -0.4311320 0.7445470 -0.3830230
C -1.7102160 1.0386440 -1.1509500
C -2.8430840 0.1075310 -0.7045870
H -2.9597290 0.9403400 1.2746260
H -0.0822830 1.5755590 0.2233990
H -1.5103930 0.9137280 -2.2203700
H -2.7039430 -0.8797360 -1.1636880
O -4.0611340 0.6871040 -1.1127130
H -4.7660100 0.2606620 -0.6089910
O -2.0493640 2.3758450 -0.8568540
H -2.9845690 2.4761560 -1.0740210
H -1.0484430 -1.2510940 0.5785270

C -3.5006510 -1.1389240 1.4140410
H -3.3969170 -1.1337710 2.5026740
H -3.1391110 -2.0989650 1.0268120
O -4.8526930 -0.9122270 1.0216500
H -5.4253040 -1.5663330 1.4269740
O -0.5601890 -2.1694760 -0.1908240
H -1.0904320 -2.8064880 -0.6717030

pINT8_{H2O}

H = -1002.75627 a.u.

G = -1002.825536 a.u.

C -1.6365090 -0.2182410 -0.4875870
N -2.0702780 -1.1935760 0.3009980
C -3.3371800 -1.0838820 0.7214280
C -4.1668830 -0.0272680 0.3426080
C -3.5885130 0.9396970 -0.4781170
N -2.3130630 0.8652180 -0.8857380
H -5.1930260 0.0444190 0.6758810
N -0.3500450 -0.3164760 -0.9806970
H -0.0608630 0.5299270 -1.4572390
N -3.7668190 -2.0617740 1.5712950
H -3.1828110 -2.8804130 1.6348920
H -4.7542310 -2.1879200 1.7138500
N -4.2996510 2.0130350 -0.9343990
H -3.7676850 2.7506490 -1.3679350
H -5.1436660 2.2779550 -0.4559150
C 2.5327150 0.0530290 0.7685620
O 1.1274240 -0.1264570 0.8527360
C 0.6743450 -0.9793800 -0.2327780
C 1.9173140 -1.2672280 -1.0830650
C 2.8357260 -0.1020960 -0.7212640

H	3.0537300	-0.7430860	1.3182950	H	5.5301820	1.0497440	2.1872100
H	0.2668860	-1.8943640	0.1905020	H	6.1318930	-0.4459160	1.5895870
H	1.6678100	-1.3078560	-2.1468940	N	2.5281360	-2.0129260	-1.4701910
H	2.5138090	0.8079660	-1.2481020	H	1.5578600	-2.0947540	-1.7423520
O	4.1711200	-0.4239470	-1.0198730	H	3.0259550	-2.8819920	-1.3706370
H	4.7245360	0.2345460	-0.5821440	C	-3.3513510	-0.6205230	0.9960270
O	2.4820480	-2.4827000	-0.6462220	O	-2.9001620	-1.9556830	1.1526120
H	3.4236160	-2.4448030	-0.8540400	C	-0.5019020	-1.4350240	-0.0393300
H	0.2481280	1.6981700	0.5730440	C	-1.0300830	-0.0438470	0.2262760
C	2.9377200	1.4108970	1.3118690	C	-2.5223230	0.0796950	-0.0836720
H	2.6647180	1.5128090	2.3658240	H	-3.1679760	-0.1197750	1.9485610
H	2.4434720	2.2047790	0.7478840	H	0.0353360	-1.8997570	0.8059110
O	4.3449280	1.5676920	1.1180870	H	-0.5234480	0.5963850	-0.4982050
H	4.8076590	1.2267090	1.8866030	H	-2.7035090	-0.4155940	-1.0518950
O	0.0841060	2.5034120	0.0639980	O	-2.8007030	1.4636310	-0.1851820
H	-0.8025080	2.3683520	-0.2944500	H	-3.7462550	1.6033880	-0.0445530
pINT3_{2H2O}				O	-0.7370900	0.3439180	1.5408950
H = -1155.575945 a.u.				H	-0.0896400	1.0616300	1.4942370
G = -1155.656446 a.u.				O	-0.6147440	-1.9908250	-1.1101570
C	2.3226300	1.0411950	0.2587030	H	-3.0149860	-2.4275200	0.3197550
N	3.4069540	1.1159860	1.0267950	C	-4.8457260	-0.6396560	0.6950130
C	4.2502340	0.0785580	0.9613300	H	-5.3579680	-1.1631140	1.5072680
C	4.0188440	-1.0285630	0.1442070	H	-5.0186340	-1.1861970	-0.2430230
C	2.8532370	-0.9969780	-0.6177280	O	-5.3032640	0.7025930	0.5795660
N	1.9983290	0.0429400	-0.5774600	H	-6.2476820	0.7169200	0.4111070
H	4.6968180	-1.8702990	0.1131570	O	0.1664860	0.2528010	-2.8906150
N	1.4195600	2.0705150	0.3815710	H	-0.3566900	-0.5405410	-2.7292590
H	0.8185190	2.2911650	-0.4173590	H	0.8692930	0.2106990	-2.2167760
H	1.8026910	2.8760720	0.8549500	O	-0.6000910	2.6806150	-1.6563350
N	5.3429530	0.1492170	1.7758140	H	-1.4516540	2.5028540	-1.2320280

H -0.5064500 1.9909490 -2.3325870

pTS3_4₂H₂O

H = -1155.555866 a.u.

G = -1155.632223 a.u.

C -2.0888530 -0.0728470 -0.5404560

N -2.3244360 -1.3302460 -0.8638030

C -3.4670680 -1.8386940 -0.3668150

C -4.3259150 -1.0770670 0.4253910

C -3.9439100 0.2407270 0.6749520

N -2.8038710 0.7577500 0.1783920

H -5.2424280 -1.4892000 0.8264900

N -0.8389400 0.4560120 -1.0368390

H -0.8727960 1.6001030 -1.1581570

H -0.6183420 0.0091080 -1.9307540

N -3.7154190 -3.1440190 -0.6603320

H -3.1282130 -3.5742180 -1.3562260

H -4.6341190 -3.5254560 -0.5164490

N -4.7093980 1.0973240 1.4028580

H -4.2729680 1.9657290 1.6699040

H -5.4362390 0.7362120 1.9961760

C 3.0112860 -1.0095700 0.6492650

O 2.1893030 -1.1349240 1.7901710

C 0.3374180 0.0988270 -0.1013970

C 1.5891970 0.5734670 -0.8287980

C 2.8805800 0.3701060 -0.0176200

H 2.7729730 -1.7872110 -0.0913600

H 0.3329080 -0.9984160 -0.0713680

H 1.5129990 1.6507100 -1.0245360

H 2.9108080 1.1326880 0.7718160

O 3.9058610 0.6145430 -0.9728470

H 4.6702280 0.0526330 -0.7858370

O 1.6319170 -0.1465850 -2.0463650

H 2.5254800 -0.0270500 -2.3936050

O 0.1709730 0.6199630 1.1352550

H 1.4778870 -0.4702110 1.7927590

C 4.4188670 -1.2649780 1.1821200

H 4.3791110 -2.1701230 1.7929420

H 4.7180500 -0.4220550 1.8165590

O 5.3236720 -1.4268200 0.0887570

H 6.1978660 -1.6353950 0.4243220

O 0.4603280 3.0009150 0.8992250

H 0.3026100 1.7462980 1.1166080

H 0.1539470 3.5444020 1.6266290

O -0.7964870 2.9894220 -1.1498590

H -0.3253120 3.4161460 -1.8689830

H -0.2341360 3.1356140 -0.1933940

pINT4₂H₂O

H = -1155.579048 a.u.

G = -1155.659954 a.u.

C 2.0550090 -0.0154290 0.2834520

N 3.0644640 0.4657010 1.0112640

C 4.2209460 -0.1984140 0.9014910

C 4.3727510 -1.3062190 0.0661520

C 3.2379530 -1.6988950 -0.6422110

N 2.0646270 -1.0577220 -0.5312740

H 5.3151710 -1.8291360 -0.0243360

N 0.8689040 0.7122840 0.3856090

H 1.4622160 2.3673200 -0.4895390

H 0.7691960 1.1133470 1.3137020

N 5.2484830 0.2517080 1.6859190

H 5.1205430 1.1642340 2.0936530
 H 6.1894430 -0.0090730 1.4438030
 N 3.2572740 -2.7453770 -1.5174320
 H 2.3589510 -3.0618930 -1.8470460
 H 3.9967170 -3.4240760 -1.4589870
 C -3.1209400 -1.1210040 -0.0749040
 O -2.5444170 -1.5611090 -1.2879990
 C -0.3730890 0.1416760 -0.1216430
 C -1.5236530 0.7839470 0.6437420
 C -2.9254500 0.3891850 0.1424940
 H -2.6939650 -1.6630880 0.7809930
 H -0.3717980 -0.9398020 0.0384740
 H -1.4504870 1.8765950 0.5321070
 H -3.1117680 0.8903790 -0.8165960
 O -3.7953680 0.9230180 1.1327410
 H -4.5288330 0.3135120 1.2916870
 O -1.3574390 0.4196570 1.9978360
 H -2.1744190 0.6807680 2.4413380
 O -0.5172920 0.3303560 -1.5058870
 H -1.8622120 -0.9445550 -1.5957660
 C -4.5901600 -1.5103490 -0.2104050
 H -4.6234880 -2.5485720 -0.5495900
 H -5.0619390 -0.8742490 -0.9692390
 O -5.2396440 -1.3644280 1.0525370
 H -6.1487160 -1.6631510 0.9827940
 O -0.9780130 3.0567810 -1.7860730
 H -0.6757190 1.2761910 -1.6909890
 H -1.2161880 3.4658700 -2.6203130
 O 1.5600990 3.2557790 -0.8780830
 H 2.1464220 3.7367660 -0.2911360

H -0.1089980 3.4190430 -1.5331930

pINT5_{2H2O}

H = -1155.578772 a.u.

G = -1155.656980 a.u.

C -2.1603250 -0.0745020 0.3163210
 N -2.5213350 1.1771650 0.0321100
 C -3.8106770 1.3546000 -0.2735090
 C -4.7332210 0.3095490 -0.2902820
 C -4.2260670 -0.9526340 0.0268810
 N -2.9403540 -1.1597180 0.3197460
 H -5.7749990 0.4663770 -0.5344950
 N -0.8545310 -0.2906030 0.6725590
 H 0.9261730 -2.6747320 -0.1799980
 H -0.5731890 -1.2599900 0.7948000
 N -4.1738380 2.6349320 -0.6095050
 H -3.5090920 3.3470340 -0.3505490
 H -5.1453970 2.8854370 -0.5310620
 N -5.0379900 -2.0552380 0.0856310
 H -4.5603380 -2.9420830 0.1209980
 H -5.9158070 -2.0325830 -0.4050810
 C 3.4895490 0.9309580 -0.1121930
 O 2.7639010 2.0897510 -0.4958660
 C 0.1642370 0.6753850 0.4221620
 C 1.4180760 0.3278710 1.2624440
 C 2.5956880 -0.2006740 0.4428200
 H 4.2165510 1.1840260 0.6685960
 H -0.1971180 1.6585420 0.7313460
 H 1.1404930 -0.4550830 1.9699870
 H 2.2163670 -0.8011590 -0.3889350
 O 3.3558800 -1.0295820 1.3165410

H	4.1418290	-1.3025100	0.8246620	H	-3.5764770	-3.2169550	0.6508450
O	1.7935950	1.5020560	1.9921380	H	-5.1991350	-2.7050360	0.6274270
H	2.3635840	1.2298350	2.7174050	N	-4.8954920	2.1230500	-0.5248150
O	0.4181040	0.7048900	-0.9874710	H	-4.3761490	2.9851140	-0.5933690
H	2.4654370	2.5034580	0.3257510	H	-5.7863210	2.1835340	-0.0597660
C	4.2323750	0.4596620	-1.3491000	C	3.5514270	-0.6708980	0.1394080
H	4.9221240	1.2368210	-1.6903680	O	3.0017140	-1.7335730	0.9181020
H	3.5006000	0.2526110	-2.1390370	C	0.1290650	-0.8195340	-0.3005620
O	4.9306400	-0.7244990	-0.9780230	C	1.3645430	-0.7936340	-1.2153890
H	5.2536980	-1.1716120	-1.7625390	C	2.5220000	0.0854220	-0.7397420
O	0.6319960	-1.8960670	-1.9110840	H	4.3084120	-1.0761780	-0.5400800
H	1.0788030	1.3917360	-1.1641930	H	-0.3560510	-1.7934290	-0.3587680
H	-0.1537610	-2.2390560	-2.3429500	H	1.0066410	-0.3697980	-2.1554010
O	0.8877290	-2.7526040	0.7865260	H	2.1146450	0.9347910	-0.1805970
H	1.7852900	-2.5981000	1.1024970	O	3.1813150	0.5595270	-1.9020180
H	0.4425060	-0.9575770	-1.7259730	H	3.9004830	1.1291680	-1.6022370
pTS5_6₂H₂O				O	1.8077700	-2.1400780	-1.4416000
H = -1155.535340 a.u.				H	2.2517880	-2.1688490	-2.2935590
G = -1155.610573 a.u.				O	0.5820450	-0.7727750	1.1823180
C	-2.0462630	0.0746510	-0.2825450	H	2.7723050	-2.4324970	0.2879400
N	-2.4920310	-1.1275680	0.1271080	C	4.2102290	0.2827670	1.1193650
C	-3.8032670	-1.2406450	0.3390620	H	5.0044520	-0.2338530	1.6657650
C	-4.6939940	-0.1850870	0.1579150	H	3.4527040	0.6426590	1.8258770
C	-4.1177040	1.0159370	-0.2666720	O	4.7300420	1.3566010	0.3430610
N	-2.8144710	1.1596120	-0.4847270	H	4.9829420	2.0798260	0.9200340
H	-5.7559530	-0.2877060	0.3351630	O	0.8941950	1.5245160	1.9195910
N	-0.7154840	0.2547210	-0.5324330	H	1.4461050	-1.2366990	1.3061410
H	0.6596990	2.1069360	1.0417780	H	0.3006220	1.8057390	2.6215960
H	-0.2583950	1.5792320	-0.4767190	O	0.1895580	2.5518410	-0.1581470
N	-4.2353950	-2.4678210	0.7991210	H	0.7168340	2.9466360	-0.8548360

H 0.6716280 0.2710560 1.5474940

pINT6_{2H2O}

H = -1155.569625 a.u.

G = -1155.650160 a.u.

C -1.8185130 -0.3740680 -0.6403740

N -2.4210820 -1.4300130 -0.1228090

C -3.6244100 -1.2096980 0.4296920

C -4.2118170 0.0546210 0.4496940

C -3.4875770 1.0828060 -0.1476600

N -2.2897340 0.8671250 -0.7121560

H -5.1803600 0.2270930 0.8996220

N -0.5286030 -0.5162410 -1.2049750

H 0.9326590 2.7611480 -0.3113220

H -0.9217540 1.9813670 -1.2566390

N -4.2269160 -2.2927750 0.9968190

H -3.8255760 -3.1917940 0.7846890

H -5.2076150 -2.2592900 1.2152940

N -3.9748160 2.3563670 -0.2325450

H -3.3132100 3.0700080 -0.4948870

H -4.7058980 2.6338650 0.4004190

C 2.9614660 -0.7148390 0.8096870

O 1.9657010 -1.3498500 1.6003610

C 0.2104190 -1.4335290 -0.7418960

C 1.6334960 -1.5205910 -1.2147490

C 2.4769070 -0.3883860 -0.6136100

H 3.8269420 -1.3782010 0.7002430

H -0.1309060 -2.1377500 0.0218710

H 1.6448710 -1.3796040 -2.3007070

H 1.8589430 0.5189950 -0.6100210

O 3.6018250 -0.2313790 -1.4584490

H 4.1449080 0.4610640 -1.0554090

O 2.1436830 -2.7999970 -0.8643480

H 3.0259340 -2.8757990 -1.2420200

O -0.2059020 0.6448910 1.7059020

H 1.8908950 -2.2602660 1.2900840

C 3.3702740 0.5563080 1.5633170

H 4.0869630 0.3102840 2.3489500

H 2.4754740 0.9709160 2.0362600

O 3.9550080 1.5125010 0.6955100

H 3.2586890 2.1583580 0.4966110

O 1.4975740 2.8355970 0.4986820

H 0.4171160 -0.0828260 1.8291770

H 1.3874730 3.7319960 0.8246110

O -0.1115660 2.4351710 -1.5809350

H 0.2587090 1.7752290 -2.1767750

H 0.3317410 1.3827630 1.3912030

pINT7_{2H2O}

H = -1079.157456 a.u.

G = -1079.232927 a.u.

C -1.8174030 0.3180080 0.3935160

N -2.5699470 1.3615570 0.0909830

C -3.8089080 1.0829750 -0.3520570

C -4.2759980 -0.2248750 -0.4836930

C -3.3823060 -1.2378710 -0.1419000

N -2.1460040 -0.9701830 0.3094790

H -5.2758560 -0.4423960 -0.8343450

N -0.5170280 0.5542570 0.8858400

H 0.6995460 -2.3296510 0.9107150

H 0.1918690 -0.6331610 2.1933610

N -4.5691660 2.1590010 -0.6906540

H	-4.2193880	3.0641980	-0.4209840	G = -1079.199853 a.u.			
H	-5.5589600	2.0545470	-0.8298850	C	-1.8531020	-0.0942770	-0.4655900
N	-3.7217230	-2.5579090	-0.2120660	N	-2.1705830	-1.2718320	0.0377890
H	-2.9640420	-3.2192410	-0.1387300	C	-3.4115380	-1.3688800	0.5400690
H	-4.5033770	-2.8277070	-0.7851110	C	-4.3035940	-0.2956180	0.5158980
C	2.6394670	0.0124830	-1.0782040	C	-3.8369270	0.8855760	-0.0585920
O	1.3502540	-0.2722050	-1.5687720	N	-2.5938590	0.9956740	-0.5577100
C	0.2201190	1.3420860	0.2156820	H	-5.3038140	-0.3775740	0.9195700
C	1.6294400	1.6275780	0.6397060	N	-0.5494130	0.0557250	-0.9970090
C	2.5966090	0.4568190	0.3917620	H	0.5698380	2.3091320	-0.1259110
H	3.0392360	0.8374970	-1.6750300	H	-0.2463390	1.0778710	-1.2798760
H	-0.1291050	1.8448710	-0.6885010	N	-3.7364950	-2.5658370	1.0981770
H	1.6335760	1.8003180	1.7247010	H	-3.0977180	-3.3292950	0.9459850
H	2.2854100	-0.3861180	1.0235720	H	-4.6966500	-2.7846840	1.2988480
O	3.8489620	0.9718740	0.8158410	N	-4.6243100	1.9920340	-0.1786760
H	4.5403390	0.3792410	0.4926370	H	-4.1566660	2.8469550	-0.4342790
O	2.0571990	2.7782620	-0.0518070	H	-5.4573160	2.0692230	0.3792630
H	3.0064940	2.8458320	0.1077520	C	2.5782830	-0.4920860	0.8563550
H	1.0042870	-1.0484880	-1.0847760	O	1.2145000	-0.4623940	1.1848570
C	3.5073040	-1.2288230	-1.2764490	C	0.3678360	-0.8451470	-0.8367690
H	3.5112610	-1.4788790	-2.3412040	C	1.7209140	-0.7137910	-1.4745220
H	3.0599820	-2.0616240	-0.7192790	C	2.7219940	0.0351780	-0.5747880
O	4.8306260	-0.9636470	-0.8115190	H	2.9289050	-1.5304780	0.8851310
H	5.3642880	-1.7569610	-0.8878270	H	0.0824710	-1.8154290	-0.4481780
O	0.3663380	-2.3830360	0.0018550	H	1.6177100	-0.1519780	-2.4109680
H	-0.5417740	-2.0426180	0.0994400	H	2.4791500	1.1042300	-0.5993530
O	0.7167570	-1.3521700	2.5985480	O	3.9911640	-0.2179750	-1.1471540
H	0.3122770	-1.5496280	3.4450640	H	4.6515040	-0.0079320	-0.4728340
pTS7_8₂H₂O				O	2.1671180	-2.0274960	-1.7201080
H = -1079.127690 a.u.				H	3.1273560	-1.9636390	-1.8127720

H 0.9259030 0.5622600 1.2441870
C 3.3811050 0.3392850 1.8509740
H 3.2661700 -0.0905620 2.8504790
H 2.9931820 1.3624870 1.8464410
O 4.7522970 0.3029850 1.4398260
H 5.2573340 0.9294580 1.9614770
O 0.7094920 1.9482750 1.1249810
H 0.0244140 2.2986950 1.6962850
O 0.4812470 2.3552760 -1.2403050
H 0.0408220 3.1601090 -1.5164760

pINT8_{2H2O}

H = -1079.170086 a.u.

G = -1079.243984 a.u.

C -1.6943360 -0.2192870 -0.4086730
N -2.1837500 -1.3168020 0.1606640
C -3.4791030 -1.2801180 0.4932290
C -4.2922340 -0.1733200 0.2387930
C -3.6596820 0.9243340 -0.3407570
N -2.3523830 0.9266130 -0.6432940
H -5.3446290 -0.1635380 0.4872860
N -0.3814700 -0.2357150 -0.8131840
H 0.6549780 2.5900320 -0.4624990
H -0.0492340 0.6425690 -1.2058210
N -3.9618400 -2.3917010 1.1214490
H -3.3771510 -3.2113970 1.0789430
H -4.9559870 -2.5373840 1.1629020
N -4.3450140 2.0655580 -0.6523510
H -3.7865520 2.8663850 -0.9009470
H -5.2246890 2.2443620 -0.1986500
C 2.5740480 -0.2032330 0.8380470

O 1.1601770 -0.2707850 0.9610580
C 0.5980380 -1.0326970 -0.1419000
C 1.7882800 -1.4217700 -1.0252770
C 2.8418920 -0.3799180 -0.6574810
H 3.0474970 -1.0268650 1.3866900
H 0.1149100 -1.9218830 0.2562180
H 1.5145260 -1.4034910 -2.0834900
H 2.6378540 0.5628500 -1.1784800
O 4.1282620 -0.8744550 -0.9533820
H 4.7600620 -0.3102520 -0.4920540
O 2.2183410 -2.7067520 -0.6318690
H 3.1657570 -2.7500020 -0.8111830
H 0.1454830 1.3954690 1.2705200
C 3.0714000 1.1256870 1.3666030
H 2.8771780 1.2153610 2.4402980
H 2.5647100 1.9367750 0.8331690
O 4.4720390 1.1339400 1.0945100
H 4.8401810 1.9863880 1.3339600
O -0.2452530 2.2629350 1.0749640
H -1.1008230 2.0483520 0.6748580
O 1.1008030 2.3753190 -1.3045790
H 0.9223690 3.1009130 -1.9058380

pRINT3_{H2O}

H = -1079.151248 a.u.

G = -1079.231621 a.u.

C 2.6100860 -0.9822740 -0.5289750
O 1.7193750 -2.0176220 -0.1476050
C 0.5364460 1.1403750 -0.2916250
C 1.2249310 0.6013420 0.9509200
C 2.6295000 0.1135210 0.5436230

H	2.2176020	-0.5748580	-1.4675430	H	-4.2578680	0.6510720	-2.3007850
H	0.6417040	-0.2303670	1.3485680	O	-2.0822860	3.3431140	-0.7944540
H	3.1033810	-0.2762180	1.4522030	H	-2.4520950	2.4549700	-0.9277110
O	3.4393910	1.2130170	0.1467650	H	-1.1875840	3.3014600	-1.1472370
H	2.9807460	1.7203350	-0.5367520	pRTS3_4_{H2O}			
O	1.3221390	1.5782480	1.9539870	H = -1079.140185 a.u.			
H	1.8183330	2.3257740	1.6004580	G = -1079.212567 a.u.			
C	4.0041800	-1.5463710	-0.8056820	C	2.7584460	1.2358610	0.0416980
H	3.8963270	-2.4007780	-1.4761020	O	1.8358670	2.2940360	-0.1774400
H	4.4300780	-1.9130090	0.1432990	C	0.5769230	-0.7614130	0.4313600
O	4.8665170	-0.6327650	-1.4359000	C	1.0320820	-0.3576270	-0.9758760
H	4.8887070	0.1701230	-0.9027420	C	2.4969230	0.0976890	-0.9507460
O	0.7674570	2.2556850	-0.6966780	H	2.5809010	0.8737120	1.0587890
H	2.1052580	-2.5025980	0.5892400	H	0.3966530	0.4482990	-1.3500400
H	-0.1278780	0.4551910	-0.8489520	H	2.7570190	0.4407810	-1.9607840
C	-2.1690560	0.3686140	0.8185450	O	3.3374430	-1.0172230	-0.6830120
N	-1.8489040	-0.8194570	1.3432740	H	2.9386320	-1.4526890	0.1023170
C	-2.2724380	-1.8926820	0.6654410	O	0.8891030	-1.4507290	-1.8646190
C	-2.9909340	-1.7994980	-0.5288240	H	1.6626550	-2.0146260	-1.7357730
C	-3.2471000	-0.5082670	-0.9867280	C	4.1929090	1.7560910	-0.0493660
N	-2.8387150	0.5834760	-0.3269020	H	4.2809180	2.6291630	0.6006760
H	-3.3287580	-2.6755840	-1.0645520	H	4.3768180	2.0887600	-1.0861170
N	-1.7341390	1.4662870	1.4774860	O	5.1601190	0.8234460	0.3627430
H	-1.1476950	1.3549570	2.2884560	H	4.9355010	-0.0234120	-0.0438930
H	-1.8603640	2.3805690	1.0592600	O	1.4093710	-1.6769620	0.9908900
N	-1.9905260	-3.1039460	1.2314730	H	2.0781600	2.7485950	-0.9905750
H	-1.3187110	-3.0893540	1.9820360	H	0.3906970	0.1244920	1.0515640
H	-2.0032820	-3.9236670	0.6482480	C	-1.9299570	-0.5049480	0.1410580
N	-3.8973360	-0.2813390	-2.1692490	N	-2.6913020	-0.7140050	-0.9156270
H	-4.4449870	-1.0291410	-2.5610500	C	-3.7359130	0.1267570	-1.0414490

C	-3.9761310	1.1463970	-0.1221250	H	1.6549470	-1.9144590	-2.0058580
C	-3.0820590	1.2493040	0.9447800	C	4.3203750	1.5095430	0.1425680
N	-2.0420250	0.4064990	1.0836460	H	4.4367810	2.2909190	0.8957450
H	-4.8125370	1.8238010	-0.2302810	H	4.5247170	1.9598420	-0.8437700
N	-0.8240930	-1.4097840	0.2840300	O	5.2507770	0.4983860	0.4433810
H	-0.7824660	-2.0088090	-0.5456860	H	5.0424900	-0.2623540	-0.1124910
H	-0.8472890	-2.0623830	1.2568980	O	1.3209940	-1.8557710	0.7354420
N	-4.5533330	-0.1022120	-2.1053460	H	2.1939820	2.6619710	-0.6829620
H	-4.2083200	-0.7353930	-2.8092070	H	0.4500160	0.0195900	0.9718450
H	-5.2047270	0.6069930	-2.3944430	C	-1.9250470	-0.4161820	0.0090950
N	-3.1903630	2.2147090	1.8925300	N	-3.0454360	-0.9153900	-0.5124730
H	-4.0337600	2.7546620	1.9751110	C	-4.0888760	-0.0787980	-0.5494310
H	-2.5916700	2.1348580	2.6986500	C	-4.0182520	1.2341990	-0.0786640
O	-0.2807950	-2.6246160	2.3578180	C	-2.7833630	1.6346200	0.4286750
H	-0.3067920	-3.5786210	2.4548610	N	-1.7266240	0.8102660	0.4774510
H	0.6892050	-2.2768930	1.8662470	H	-4.8677170	1.9025070	-0.1165690
pRINT4_{H2O}				N	-0.8648360	-1.3112290	0.0982370
H = -1079.167944 a.u.				H	-0.9285920	-2.0360830	-0.6104010
G = -1079.242569 a.u.				H	-1.0765510	-2.1422400	2.0136890
C	2.8664680	1.0362970	0.1687710	N	-5.2531400	-0.5985400	-1.0467080
O	1.9860290	2.1472890	0.1037110	H	-5.1584780	-1.4640650	-1.5546010
C	0.4933330	-0.8105030	0.2645240	H	-5.9644800	0.0368880	-1.3668830
C	1.0762640	-0.3279320	-1.0671910	N	-2.5583680	2.9060730	0.8719540
C	2.5596940	0.0512870	-0.9641650	H	-3.3420370	3.4890180	1.1111530
H	2.6775720	0.5506160	1.1313380	H	-1.6994930	3.0497660	1.3797590
H	0.4983450	0.5487640	-1.3662290	O	-0.4828100	-2.3168570	2.7595920
H	2.8473960	0.5102700	-1.9187110	H	-0.9018850	-2.9820610	3.3084720
O	3.3658290	-1.1197160	-0.8553530	H	0.9638890	-2.1746320	1.5810950
H	3.0142180	-1.6234610	-0.1028510	pRINT5_{H2O}			
O	0.9054480	-1.3101120	-2.0687820	H = -1079.161664 a.u.			

G = -1079.233796 a.u.	H 0.2385980 3.8980740 -0.2266160
C 2.1756040 -1.3417510 0.1522340	N -5.2443170 -0.2104600 -0.0347160
O 1.4066290 -2.0293740 1.1287980	H -5.4976620 0.7547090 0.1085930
C 0.4408040 1.2438490 -0.6458470	H -5.8324350 -0.8972340 0.4066260
C 1.0606620 0.8799300 0.7300100	N -1.3636770 -3.0906010 0.0221160
C 2.3783190 0.1348540 0.5333210	H -1.8763300 -3.8341920 0.4685830
H 1.6077160 -1.4096120 -0.7796330	H -0.3960520 -2.9998210 0.3112200
H 0.3558490 0.2184930 1.2400290	H 1.9450360 2.3272450 -1.1048940
H 2.9205840 0.1703850 1.4931620	O -0.3684320 4.1100010 0.5024910
O 3.1129420 0.8406360 -0.4565340	H -0.3703250 5.0619360 0.6149430
H 3.8056100 0.2708470 -0.8145820	pRTS5_6H₂O
O 1.3501570 2.0155860 1.5159530	H = -1079.117464 a.u.
H 0.6286800 2.6575770 1.4516420	G = -1079.189008 a.u.
C 3.4925610 -2.1042310 0.0059930	C -3.1070540 1.1125260 0.0475870
H 3.2562670 -3.1499500 -0.2098970	O -2.5185750 2.0880100 0.8831770
H 4.0397700 -2.0556680 0.9575920	C -0.3571300 -0.3840850 -0.0322260
O 4.2634980 -1.5292310 -1.0434730	C -1.4508300 -0.5718890 1.0223310
H 5.0711600 -2.0315380 -1.1695340	C -2.8865620 -0.3196700 0.5634000
O 0.9849690 2.4457980 -1.1531090	H -2.6132380 1.2088360 -0.9242550
H 1.7120300 -1.7849680 2.0084800	H -1.2117340 0.1800170 1.7854810
H 0.6328110 0.4262360 -1.3437570	H -3.5335300 -0.5011560 1.4348110
C -1.8103520 0.3588070 -0.3947050	O -3.2084020 -1.2642980 -0.4543450
N -3.1185320 0.6128240 -0.2798600	H -4.0675170 -1.0286970 -0.8313930
C -3.8953820 -0.4550210 -0.0923300	O -1.4084470 -1.8670580 1.5640890
C -3.3915250 -1.7561380 0.0171940	H -0.4698220 -2.0613870 1.7007470
C -2.0082810 -1.8832760 -0.0917150	C -4.5885950 1.4464340 -0.1117020
N -1.2118010 -0.8345540 -0.3267270	H -4.6770140 2.4512780 -0.5335600
H -4.0368720 -2.6069510 0.1884680	H -5.0616470 1.4352290 0.8801230
N -0.9894060 1.4291920 -0.5868130	O -5.1936530 0.4769950 -0.9599590
H -1.3628680 2.3501470 -0.3963630	H -6.1220580 0.6817180 -1.0893550

O	-0.7766440	-1.2268280	-1.2880600	H	2.2779680	-0.1893490	-1.3748980
H	-2.8595760	1.9892310	1.7781640	H	2.1606820	-2.0295820	1.3474290
H	-0.3194390	0.6374810	-0.4110650	H	3.8001660	-0.2145900	1.2704240
C	1.9827380	-0.1585240	0.1914740	O	2.4049290	1.2190520	0.7516560
N	3.1383680	-0.8449030	0.2948810	H	3.0873510	1.7779630	0.3581540
C	4.2614130	-0.1534480	0.1163040	O	1.7363610	-0.6319540	2.7560490
C	4.2788720	1.2129420	-0.1740410	H	0.9547750	-0.0709300	2.8503400
C	3.0262020	1.8174760	-0.2726760	C	4.4180480	0.0525430	-1.3070770
N	1.8852870	1.1547540	-0.0871330	H	4.4764340	-0.1365820	-2.3826860
H	5.1986570	1.7562250	-0.3425300	H	5.2623150	-0.4518410	-0.8137060
N	0.8571050	-0.8954650	0.4108520	O	4.4488860	1.4440940	-1.0220120
H	1.0313010	-2.3050620	-0.1634090	H	5.2065130	1.8502820	-1.4470730
H	-0.1488020	-2.1216320	-1.2790280	O	0.4250060	1.3320860	-1.3238760
N	5.4309130	-0.8793290	0.1870510	H	3.9163580	-2.2937060	-0.4353070
H	5.3337380	-1.7715280	0.6478110	H	0.4391390	-1.2858110	-0.3213790
H	6.2754660	-0.3731360	0.3979640	C	-1.7333470	-0.4429290	0.6296430
N	2.9007240	3.1488530	-0.6060350	N	-2.4696260	0.6572380	0.7737170
H	3.6889700	3.7466190	-0.4181290	C	-3.6521730	0.6572670	0.1436790
H	1.9966910	3.5439660	-0.3965750	C	-4.1054130	-0.4250350	-0.6005180
H	-1.7357960	-1.4531310	-1.2095050	C	-3.2444200	-1.5233730	-0.6683340
O	0.7698600	-3.0371160	-0.8807890	N	-2.0568470	-1.5366960	-0.0472980
H	1.5411310	-3.1704430	-1.4392250	H	-5.0628450	-0.4147560	-1.1039090
pRINT6_{H2O}				N	-0.5053760	-0.4374260	1.3148160
H = -1079.151956 a.u.				H	-1.6780440	2.4630730	0.2583780
G = -1079.229249 a.u.				H	-0.2463530	2.0278280	-1.3107520
C	3.1178160	-0.5374530	-0.7674580	N	-4.3716360	1.8312720	0.2381600
O	3.1625320	-1.9470210	-0.9234700	H	-4.1508860	2.3840740	1.0553870
C	0.4953440	-0.9192530	0.7064080	H	-5.3555980	1.7781790	0.0249520
C	1.8236970	-0.9889230	1.4075620	N	-3.5524050	-2.6363270	-1.3892590
C	2.8686530	-0.1170380	0.6915820	H	-4.4959930	-2.7910570	-1.6985520

H -2.9601880 -3.4396660 -1.2542740
H 0.9487440 1.4915090 -0.5267320
O -1.5958080 3.1659870 -0.4062470
H -2.4737790 3.2057610 -0.7964710

pRINT3_{2H2O}

H = -1155.569731 a.u.

G = -1155.65265 a.u.

C 2.5414050 0.4228780 0.6051360
O 1.5100430 1.3557480 0.3609120
C 0.2992720 -1.4261790 0.3206800
C 1.1462770 -1.1357920 -0.9009640
C 2.5542560 -0.7096870 -0.4345820
H 2.3060900 -0.0181410 1.5826030
H 0.6887870 -0.3068160 -1.4439430
H 3.1035100 -0.4015130 -1.3309980
O 3.2758440 -1.8322600 0.0598300
H 2.8566960 -2.1500970 0.8692600
O 1.2228800 -2.2296770 -1.7680510
H 1.5789640 -2.9783150 -1.2761930
C 3.9010380 1.1094590 0.7128200
H 3.8211800 1.9291560 1.4284350
H 4.1559770 1.5390250 -0.2695920
O 4.9178620 0.2510690 1.1744410
H 4.8625500 -0.5829730 0.6942230
O 0.1817850 -2.5395580 0.7757460
H 1.6586750 1.8628650 -0.4479250
H -0.1545610 -0.5508480 0.8193890
C -1.9001910 0.3473200 -0.9136680
N -1.1113660 1.2105890 -1.5656050
C -0.9018050 2.3816470 -0.9602520

C -1.5082800 2.7440260 0.2356580
C -2.3030730 1.7601480 0.8315410
N -2.4919940 0.5565480 0.2736090
H -1.3176890 3.6938460 0.7151770
N -2.0414120 -0.8830670 -1.4572300
H -1.6629270 -1.0209750 -2.3806880
H -2.7768720 -1.5098230 -1.1330980
N 0.0350950 3.1963720 -1.5761330
H 0.1234960 3.0175760 -2.5675030
H -0.0091280 4.1770350 -1.3412420
N -2.8892140 1.9497340 2.0447000
H -2.9332350 2.8723760 2.4404600
H -3.5782600 1.2758490 2.3383810
O -2.5685670 -1.8802810 1.8382960
H -2.5358430 -1.0139060 1.3905020
H -1.6805580 -2.2524080 1.7659260
O -4.0464510 -2.6907580 -0.3157820
H -4.2786770 -3.6113320 -0.4451550
H -3.6564900 -2.6189950 0.5752430

pRT3_4_{2H2O}

H = -1155.562610 a.u.

G = -1155.639137 a.u.

C 2.7950900 -1.1347310 -0.4886290
O 1.9264760 -2.0494090 -1.1422860
C 0.5665560 0.7659300 0.0769550
C 0.8210740 -0.4422190 0.9889160
C 2.2974090 -0.8567300 0.9338070
H 2.7610120 -0.2075640 -1.0682690
H 0.1945840 -1.2780100 0.6741390
H 2.4078350 -1.7715320 1.5310540

O	3.0985730	0.1298660	1.5711400	H	1.4903100	2.5894290	-0.5627280
H	2.8003750	0.9815940	1.1844820	O	-1.0420860	3.1765380	-1.2562650
O	0.4643120	-0.1252370	2.3218300	H	-1.4590030	3.9953610	-0.9783880
H	1.2152030	0.3434790	2.7080820	H	0.0327330	3.3555710	-1.4539220
C	4.2300030	-1.6614760	-0.4999270	pRINT4_{2H2O}			
H	4.4790930	-1.9520430	-1.5226740	H = -1155.584146 a.u.			
H	4.2738650	-2.5685820	0.1275120	G = -1155.66547 a.u.			
O	5.1815340	-0.7119370	-0.0890200	C	2.9374620	-0.9693660	-0.5204240
H	4.8482850	-0.3021230	0.7198510	O	2.0977860	-1.9842990	-1.0491780
O	1.4325670	1.7790960	0.3519180	C	0.5275920	0.6826690	0.1889430
H	2.0363680	-2.9172930	-0.7402970	C	1.0626860	-0.3972110	1.1375700
H	0.5513550	0.4535440	-0.9747810	C	2.5580680	-0.6725370	0.9343610
C	-1.9297150	0.3380630	0.1178780	H	2.7613110	-0.0772650	-1.1296960
N	-2.9135240	0.3958640	0.9933360	H	0.4967100	-1.3087950	0.9389530
C	-3.9362700	-0.4470860	0.7573500	H	2.8182220	-1.5432130	1.5498040
C	-3.9386090	-1.3185000	-0.3312480	O	3.3366830	0.4014140	1.4563700
C	-2.8266680	-1.2691590	-1.1722740	H	2.9855350	1.2104950	1.0475070
N	-1.8054740	-0.4210400	-0.9497740	O	0.8248560	-0.0364030	2.4836530
H	-4.7577920	-2.0018680	-0.5106380	H	1.5627840	0.5165070	2.7676290
N	-0.8541990	1.2647790	0.3528220	C	4.4073790	-1.3659830	-0.6643260
H	-0.8810190	1.5414180	1.3368740	H	4.5737160	-1.6852200	-1.6949320
H	-1.0067890	2.2131440	-0.3464650	H	4.6052080	-2.2304760	-0.0080720
N	-4.9767890	-0.3749160	1.6318380	O	5.3029710	-0.3132620	-0.4031830
H	-4.8119960	0.1367890	2.4840150	H	5.0533170	0.0725390	0.4453870
H	-5.6543370	-1.1173700	1.6590900	O	1.3422840	1.8205440	0.3295010
N	-2.6868750	-2.0901470	-2.2449930	H	2.2892220	-2.8113880	-0.5952420
H	-3.4768240	-2.5992320	-2.6008550	H	0.5258570	0.3019550	-0.8349140
H	-1.9203450	-1.8970800	-2.8698300	C	-1.8761460	0.1386140	0.2570480
O	1.3444620	3.3742750	-1.4255810	N	-3.0215420	0.3837410	0.8924240
H	1.8151830	3.1504930	-2.2296950	C	-4.0340390	-0.4400250	0.5961520

C	-3.9080390	-1.4861930	-0.3201010	O	3.2443940	-0.9794030	1.0261650
C	-2.6545180	-1.6337040	-0.9112120	H	4.1160150	-0.7315030	1.3590850
N	-1.6267280	-0.8203160	-0.6249360	O	1.5863420	-2.3176270	-0.8148820
H	-4.7323590	-2.1473320	-0.5504150	H	1.5146520	-2.6024820	0.1041300
N	-0.8499920	1.0425030	0.5237050	C	4.9367420	1.2556240	-0.2863560
H	-0.9209190	1.4092060	1.4689850	H	5.0858420	2.3390130	-0.2733980
H	-1.6517170	2.4404200	-0.5818780	H	5.4577390	0.8371970	-1.1590230
N	-5.2224230	-0.1742270	1.2204980	O	5.4139000	0.6530660	0.9101570
H	-5.1641600	0.4374400	2.0196710	H	6.3459540	0.8474190	1.0286820
H	-5.9147210	-0.9032260	1.2623330	O	0.5767330	-0.6786470	1.2903840
N	-2.3781940	-2.6433420	-1.7877350	H	3.3952960	1.0966530	-2.3740570
H	-3.1386880	-3.1144930	-2.2473660	H	0.7255810	0.8542560	-0.1031900
H	-1.5114610	-2.5573080	-2.2956740	C	-1.7702570	0.1444800	-0.4438470
O	0.7187340	3.4510130	-1.7601380	N	-2.9089740	-0.4246030	-0.8624260
H	0.9820820	3.3065350	-2.6706490	C	-4.0322430	0.2609160	-0.6284080
H	1.1672660	2.4449210	-0.4041800	C	-4.0333870	1.5061810	0.0050380
O	-1.9080270	3.0982450	-1.2535650	C	-2.7827630	2.0002790	0.3736890
H	-2.6882470	3.5422670	-0.9167210	N	-1.6459290	1.3265330	0.1614000
H	-0.2517830	3.5423050	-1.7539660	H	-4.9481460	2.0454460	0.2089740
pRINT5_{2H2O}				N	-0.6280450	-0.5705030	-0.6900330
H = -1155.587064 a.u.				H	-0.7765920	-1.5633390	-0.8588060
G = -1155.667959 a.u.				H	-2.1250560	-2.7795940	0.8636980
C	3.4452760	0.9616310	-0.4212440	N	-5.1945200	-0.3471510	-1.0099630
O	2.9755890	1.5340480	-1.6260240	H	-5.1024970	-1.1377640	-1.6278670
C	0.6112470	-0.2311110	-0.0675240	H	-6.0290770	0.2070070	-1.0966160
C	1.7487940	-0.9199520	-0.8300920	N	-2.6507170	3.1960050	1.0278800
C	3.1451640	-0.5423410	-0.3233940	H	-3.4002320	3.8640030	0.9631460
H	2.9070580	1.4703020	0.3838810	H	-1.7148080	3.5678890	1.0653450
H	1.6649880	-0.6105050	-1.8725500	O	-1.9520130	-1.3937630	2.2756600
H	3.8637380	-1.1018060	-0.9420260	H	-1.0695590	-1.0551180	2.0530530

H 1.4737250 -0.6564290 1.6536580
O -2.1663910 -3.1486010 -0.0313490
H -2.6926450 -2.4880010 -0.4992280
H -2.5345520 -0.6314430 2.2270470

pRT5_6_{2H2O}

H = -1155.539423 a.u.

G = -1155.615400 a.u.

C -3.2107450 -1.1652610 -0.4412210
O -2.6876180 -1.7416250 -1.6196950
C -0.4246350 0.1474360 -0.1069290
C -1.5952060 0.7987000 -0.8499990
C -2.9855840 0.3521100 -0.3830280
H -2.6671580 -1.6272460 0.3878670
H -1.4686610 0.5017140 -1.8923410
H -3.7141540 0.8564060 -1.0353850
O -3.1560970 0.8295760 0.9524460
H -4.0198520 0.5355430 1.2713490
O -1.5216290 2.2044670 -0.8311550
H -1.7144160 2.5216000 0.0586150
C -4.6898220 -1.5253970 -0.3296760
H -4.7876040 -2.6135040 -0.2831850
H -5.2112430 -1.1609490 -1.2256130
O -5.2220830 -0.9080430 0.8374230
H -6.1405920 -1.1589660 0.9547880
O -0.5624700 0.6001380 1.4008190
H -3.0831750 -1.3188210 -2.3888980
H -0.5275710 -0.9363480 -0.0200380
C 1.8856470 -0.1467700 -0.2892040
N 3.0648160 0.4441120 -0.6036170
C 4.1699370 -0.2527670 -0.3568330

C 4.1576930 -1.5302700 0.2059270
C 2.8925920 -2.0381410 0.5032080
N 1.7667640 -1.3695670 0.2675320
H 5.0662350 -2.0734530 0.4274070
N 0.7860920 0.5921220 -0.5762870
H 1.1550740 2.0958320 -0.7679530
H 0.9604550 3.0137060 0.6979740
N 5.3620290 0.3810140 -0.6481900
H 5.2700930 1.1428040 -1.3033440
H 6.1633770 -0.2106630 -0.7981540
N 2.7477410 -3.2699290 1.1075090
H 3.4940840 -3.9334060 0.9768890
H 1.8161920 -3.6512860 1.0434430
O 0.3798570 2.8199920 1.5922980
H -0.0878410 1.6162610 1.5243410
H -1.5090240 0.6385300 1.6410150
O 1.5566080 3.0325310 -0.5395550
H 2.4949340 2.8053350 -0.5169000
H 0.9269250 2.9784980 2.3653730

pPRINT6_{2H2O}

H = -1155.567965 a.u.

G = -1155.652378 a.u.

C -3.3976410 -1.0528070 -0.3316890
O -3.5221580 -1.4649770 -1.6809480
C -0.4859540 -0.0417250 -0.7917040
C -1.7302430 0.7349850 -1.1549020
C -2.8820340 0.3902530 -0.2016960
H -2.6717680 -1.7289440 0.1268000
H -2.0246650 0.4208460 -2.1622500
H -3.7008060 1.0841100 -0.4498550

O	-2.4172510	0.6418460	1.1123870	H	-0.6131190	0.3093790	1.9555960
H	-3.1303670	0.4309430	1.7285900	O	1.9946490	3.1036190	-1.0057180
O	-1.5176340	2.1153620	-1.1989500	H	2.4336760	2.2847860	-0.7039260
H	-1.0804380	2.3920370	-0.3726410	H	-0.0408530	3.8279740	1.4336240
C	-4.7505470	-1.2362680	0.3520810	mTS1			
H	-5.0282190	-2.2933970	0.3078490	H =	-735.654445	a.u.	
H	-5.5022190	-0.6514780	-0.1973590	G =	-735.708417	a.u.	
O	-4.6566340	-0.7817230	1.6952230	C	-1.1730960	-0.2299320	0.8663000
H	-5.4839380	-0.9379800	2.1550390	C	-1.3358800	-1.7345030	1.1046640
O	0.3141810	0.4054080	2.2017130	H	-0.3923370	-2.2815620	1.1535300
H	-4.1339480	-0.8757760	-2.1344470	O	-2.1117910	-2.2722360	0.0445200
H	-0.6023310	-1.0565630	-0.4011140	H	-2.8161860	-1.6104600	-0.0630680
C	1.7750570	-0.2759380	-0.5063760	O	-2.4198160	0.2572290	0.6381860
N	2.8231790	0.4754090	-0.1774720	H	-0.6639380	0.2171370	1.7376550
C	3.9110020	-0.1777870	0.2603900	C	2.4685180	0.1829000	0.1764400
C	3.9514290	-1.5682710	0.3347480	N	1.8304390	1.3464890	0.2421080
C	2.8015160	-2.2427720	-0.0747860	C	0.5508350	1.3538060	-0.1565510
N	1.7072220	-1.5969650	-0.5028170	C	-0.1975860	0.0747230	-0.4102650
H	4.8243310	-2.0944550	0.6971240	C	0.7732400	-1.0260670	-0.7094940
N	0.6576760	0.4824940	-0.9276550	N	2.0354170	-0.9913290	-0.3621460
H	1.3329480	2.7502960	-1.6141670	H	-0.8854460	0.1930170	-1.2483740
H	0.8676030	3.2147960	0.3177570	N	3.7172790	0.1487410	0.6561670
N	4.9632270	0.5987590	0.6480520	H	4.1204940	0.9893780	1.0348060
H	4.9254870	1.5736500	0.3968080	H	4.2514630	-0.6999230	0.5770480
H	5.8730760	0.1827850	0.7472650	N	-0.0853300	2.4863680	-0.2608610
N	2.7149690	-3.6039750	-0.0375590	H	0.4489860	3.3047210	0.0031010
H	3.5546860	-4.1521990	0.0326530	H	-1.1841310	2.5345620	-0.4780610
H	1.9287010	-4.0139100	-0.5151020	N	0.3133720	-2.0997820	-1.3536980
O	0.1226210	3.0268730	0.9315700	H	0.9510400	-2.8769820	-1.4491340
H	0.5105510	1.2937740	1.8753020	H	-0.6866010	-2.2909470	-1.3248740

O -2.5705080 2.3591510 -0.4912790
H -2.5579040 1.3397920 0.0768830
H -3.1035170 2.3259630 -1.2865130
H -1.8594250 -1.8568330 2.0580350

mTS1_O

H = -755.531585 a.u.

G = -755.585909 a.u.

C -1.2279010 -0.2396340 0.9820000
C -1.3158800 -1.7608310 1.0982490
H -0.3493000 -2.2657930 1.0773270
O -2.1086600 -2.2491140 0.0319340
H -2.8325030 -1.6052170 -0.0271590
O -2.3962700 0.2791820 0.7616060
H -0.6055540 0.2056660 1.7763470
C 2.4453620 0.1730100 0.1896700
N 1.7962260 1.3466760 0.2538830
C 0.5466870 1.3466950 -0.1653380
C -0.1627710 0.1038720 -0.4902860
C 0.7659710 -0.9915810 -0.7641310
N 2.0215400 -0.9866050 -0.3546390
H -0.9469160 0.2090410 -1.2334830
N 3.6831300 0.1607020 0.6965940
H 4.0633130 1.0136790 1.0723420
H 4.2369210 -0.6764200 0.6291360
H -1.0460160 2.4557350 -0.4718290
N 0.3242240 -2.0690430 -1.4253180
H 0.9573470 -2.8535920 -1.4771790
H -0.6738190 -2.2582150 -1.4248790
O -2.5037860 2.3585650 -0.5775830
H -2.6029770 1.5207840 0.0125750

H -3.0124370 2.2524620 -1.3825520
H -1.7951090 -1.9718480 2.0619030
O -0.0509830 2.4891690 -0.2043530

mTS1_S

H = -1078.473137 a.u.

G = -1078.529031 a.u.

C 1.0390510 0.5702830 0.9909880
C 0.9731010 2.0986590 1.1065500
H -0.0326590 2.5144750 1.0280600
O 1.7771900 2.6567040 0.0813620
H 2.5635560 2.0854260 0.0900360
O 2.3004250 0.2036620 0.8651140
H 0.4712100 0.0930330 1.8086610
C -2.4865900 -0.1668520 0.1550060
N -1.7534280 -1.2926270 0.2750110
C -0.4933010 -1.2242240 -0.0998350
C 0.1445010 0.0746690 -0.4187930
C -0.8724410 1.0727680 -0.8084160
N -2.1405880 0.9834830 -0.4544430
H 0.9348880 -0.0051070 -1.1604640
N -3.7220170 -0.2221110 0.6561930
H -4.0379920 -1.0794240 1.0795010
H -4.3335760 0.5709010 0.5565640
H 1.6776560 -2.1987810 -0.5050660
N -0.4897000 2.1365300 -1.5170530
H -1.1808210 2.8614740 -1.6486170
H 0.4886040 2.4114660 -1.4773520
O 3.0206410 -1.6207510 -0.5930010
H 2.7956640 -0.8216180 0.0580290
H 3.4180630 -1.2874920 -1.4001840

H 1.3779280 2.3555790 2.0918800
S 0.3741010 -2.7003500 -0.1012380

mTS2

H = -795.311124 a.u.

G = -795.366615 a.u.

C 1.4397800 -0.1324210 -0.8612780
C 2.2348720 -1.4006460 -0.6936630
H 1.5953490 -2.2529040 -0.4639870
O 3.1974920 -1.2748540 0.3123350
H 3.5562220 -0.3814280 0.2640870
O 2.0492880 0.9443640 -0.6363870
H 0.5762920 -0.1460170 -1.5374340
C -0.5269270 0.7950460 0.8952820
C 0.0274100 -0.4928820 0.9025090
O 0.9099890 3.0421500 -0.4546730
H 1.4903340 2.1022020 -0.6731780
H 1.4874950 3.7923840 -0.2827380
H 2.6963430 -1.5752620 -1.6812710
N -1.7024780 0.9884410 0.1927800
H -2.1081620 1.9152890 0.1878620
C -2.4898550 -0.0135470 -0.3675550
O -3.5429490 0.2174680 -0.9056280
N -1.9366580 -1.2673900 -0.2535550
H -2.4903260 -2.0331160 -0.6164430
C -0.7465270 -1.6140940 0.4151580
H 0.8577200 -0.6956770 1.5650950
O -0.4212920 -2.7824800 0.4703990
O 0.0250940 1.8181290 1.3956070
H 0.4391830 2.6602330 0.4674950

mTS3

H = -795.296028 a.u.

G = -795.350469 a.u.

C -1.2576940 -0.1631240 -0.9012580
C -2.5314530 0.6409440 -0.8132000
H -2.3182410 1.6917930 -0.6162740
O -3.3601850 0.1469740 0.2082540
H -3.4755760 -0.7966630 0.0517710
O -1.3617630 -1.4141780 -0.7360620
H -0.4439800 0.2279590 -1.5258000
C 0.3931970 -0.4150230 1.1156660
C -0.3260000 0.7599690 0.8836640
O 0.7162530 -2.6580810 -0.7911200
H -0.2885530 -2.1412310 -0.8245170
H 0.6606340 -3.5262380 -0.3784660
H -3.0160270 0.5649000 -1.7989440
N 1.5444940 -0.7345840 0.5482830
H 1.2929630 -1.9763100 -0.1681370
C 2.2384700 0.2431920 -0.1596620
O 3.2853060 0.0252120 -0.7157470
N 1.6412910 1.5063920 -0.2240690
H 2.1587630 2.2145790 -0.7298570
C 0.3735320 1.8541880 0.2310420
H -1.2074240 1.0005640 1.4643040
O -0.0977170 2.9531360 0.0193950
O -0.1722640 -1.4265860 1.7790110
H -1.0804060 -1.1947060 2.0090700

mTS4

H = -717.147647 a.u.

G = -717.200611 a.u.

C 1.7232880 -0.0656580 -0.6485530

C	2.5279190	-1.3352220	-0.7167100	H	1.0397510	1.8610030	-0.7075680
H	1.8940520	-2.1958720	-0.5219090	O	3.2170010	0.3321810	-0.1878240
O	3.5809390	-1.3411990	0.2039380	H	2.4310810	-0.4601690	1.5124980
H	4.0903150	-0.5319510	0.0923380	N	-0.3564750	-1.4357080	0.6712420
O	2.4398820	0.9891530	-0.4609290	C	0.6425220	-0.9149100	-0.1522400
H	0.7960180	0.0148570	-1.2230550	N	0.1280580	0.0426910	-0.9205790
N	-0.1640470	0.8530750	0.9794940	C	-1.2157320	0.1197640	-0.6164080
C	0.5676880	-0.3096960	1.1003220	C	-2.2708890	0.9086120	-1.0665370
N	-0.0793520	-1.4471450	0.7359670	N	-3.4885850	0.7437540	-0.5580460
C	-1.2619100	-0.9893170	0.3027230	C	-3.6587440	-0.1926140	0.3877510
C	-2.3946300	-1.6119720	-0.2711990	N	-2.7413430	-1.0034930	0.9086340
N	-3.4239920	-0.8862460	-0.6291440	C	-1.5377860	-0.8105110	0.3854780
C	-3.3563700	0.4699880	-0.4389440	H	1.9847470	-1.6785630	-0.5558020
N	-2.3790990	1.1761700	0.0688960	H	-4.6668050	-0.2987590	0.7738710
C	-1.3172870	0.4282520	0.4549790	H	-0.2582290	-2.2093160	1.3097040
H	1.4690930	-0.3518530	1.7025120	O	3.0103330	-1.9092020	-0.8472110
H	-4.2400700	1.0135950	-0.7575960	H	3.4022090	-0.7389780	-0.4859020
H	0.3549250	2.4211620	0.3971170	H	3.3245860	-2.7064350	-0.4147150
O	0.9227620	2.9340040	-0.2411720	H	-2.1405280	1.6656730	-1.8341790
H	1.8909140	1.8724820	-0.4527840	H	2.2162790	2.1144420	1.8336050
H	1.1438300	3.7857400	0.1422760				
H	-2.4453140	-2.6880100	-0.4180280				
H	2.8908140	-1.3850470	-1.7577680				

mTS5

H = -717.124707 a.u.

G = -717.178000 a.u.

C	2.3909550	0.3300250	0.7565280
C	1.6218420	1.5755100	1.0825620
H	0.6820480	1.2752650	1.5668870
O	1.4427000	2.4082550	-0.0112110

mTS6

H = -720.054381 a.u.

G = -720.107534 a.u.

C	1.2707920	0.4959650	-0.6368720
C	2.4972410	-0.3576880	-0.7200200
H	2.2344620	-1.4130740	-0.6303900
O	3.4400370	-0.0350310	0.2585210
H	3.5609040	0.9200640	0.2702300
O	1.4043110	1.6906870	-0.2586380
H	0.3803840	0.2158160	-1.2099110

C	-0.4866300	0.2882570	1.4045610	H	-2.7040650	-1.1238850	0.1992350
C	0.2514740	-0.8432150	1.1132300	H	-2.7197810	-2.6664000	-0.5044750
H	-0.0757570	1.0016560	2.1181020	H	-2.0275450	2.4391550	-1.2265270
O	-0.7323740	2.7884710	-0.2644770	N	1.9532790	-0.4786910	-1.2200540
H	0.4253720	2.3029790	-0.2790380	H	2.5978770	-0.5432470	-1.9966730
H	-0.8900250	3.6923330	0.0187320	C	2.5481480	-0.0923530	0.0018580
H	2.8856820	-0.1976560	-1.7420450	O	3.7265370	0.1310370	0.0719660
N	-1.5976190	0.6860710	0.7906710	N	1.6527720	-0.0184460	1.0296960
H	-1.3334490	2.0822680	0.2386540	H	2.0335210	0.2435960	1.9316810
C	-2.1869220	-0.1728550	-0.1302520	C	0.2664250	-0.3035130	0.9959440
O	-3.1914340	0.0995040	-0.7438850	H	-1.1595910	-1.5534200	-0.2321110
N	-1.5259410	-1.3896610	-0.3541580	O	-0.3630940	-0.2995020	2.0183810
H	-1.9626740	-2.0089390	-1.0265750				
C	-0.3027930	-1.7982120	0.1731080				
H	1.1321760	-1.1145550	1.6782440				
O	0.2355680	-2.8222900	-0.2057860				

mTS7

H = -720.028635 a.u.

G = -720.080912 a.u.

C	-1.7282060	0.3901890	-0.8176990
C	-1.2069680	1.8215150	-0.8346290
H	-0.3435550	1.9275550	-1.4969070
O	-0.8205130	2.2365000	0.4481900
H	-1.4790820	1.8827280	1.0634280
O	-2.6808140	0.1936770	0.0386760
H	-1.8721410	-0.0120780	-1.8393940
C	0.6378110	-0.7120280	-1.3653070
C	-0.2749500	-0.6179710	-0.3461180
H	0.3252090	-0.9514240	-2.3794040
O	-2.2804610	-2.1464200	0.1739560