Supporting Information

Cooperative Physisorption and Chemisorption of Hydrogen on Vanadium-decorated Six-membered carbocycle

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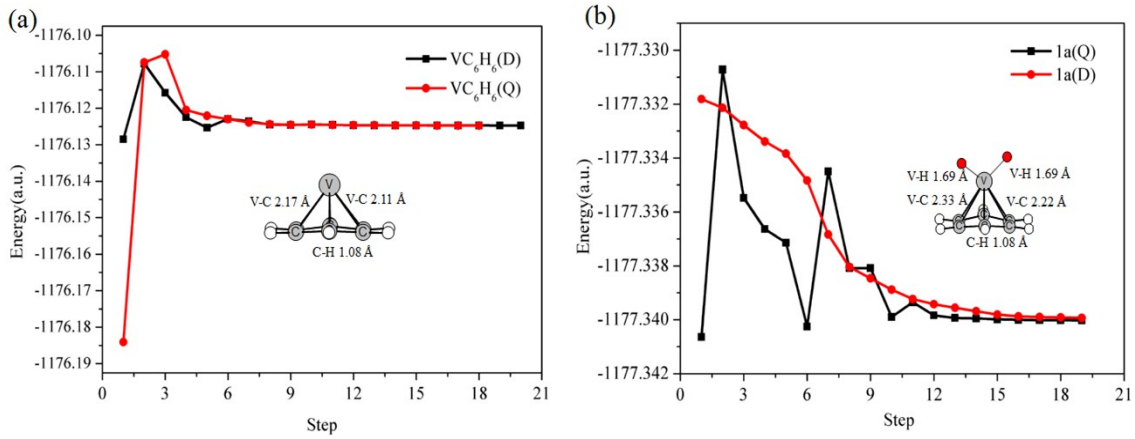
Table S1. Total energies with no zero-point energy correction (in kcal/mol) of points on the VC_6H_6 and structure **1a** at the B3LYP level of theory. The reference points are the energies of the quartet states.

System	E_{tot}(doublet)	E(MECP)	E_{tot}(quartet)
VC_6H_6	37.24	34.89	0.00
1a	5.54	0.39	0.00

Figure S1 The minimum energy crossing points (MECP) between the doublet and quartet potential energy surfaces of the VC_6H_6 and structure **1a** calculated by using the sobMECP program and the geometric structure parameters.



The sobMECP program [1] is used to locating minimum energy crossing points (MECP) between the doublet and quartet potential energy surfaces of the VC_6H_6 and structure **1a** at the B3LYP level of theory. The B3LYP approach was chosen based on the following considerations: (1) the geometry optimization of the MECP using CCSD(T) energies and gradients would be too expensive. (2) Harvey [2] had pointed out that the state splitting of phenyl cation with the B3LYP method is of the right sign and even its magnitude is roughly correct. The data obtained at the B3LYP level should already be quite reliable since as shown in the previous computational studies on the phenyl cation [3,4], this method provides excellent geometries for both states

and quite good energetics. The geometry and relative energy obtained at the CCSD(T) //B3LYP level of theory are indeed similar to those obtained with B3LYP.

As shown in Figure S1 and Table S1, with the basis set we use, the doublet states of VC_6H_6 and **1a** lies 37.24 and 5.54 kcal/mol above their quartet states, respectively. Unlike the relative energies with no zero-point energy correction, the geometries are rather similar.

Related references

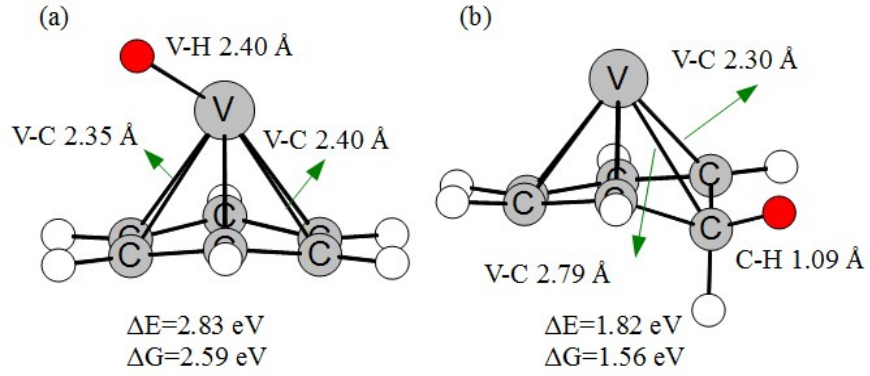
1 Tian Lu, sobMECP program, http://sobereva.com/286

2 J. N. Harvey, M. Aschi, H. Schwarz and W. Koch, *Theoretical Chemistry Accounts*, 1998, **99**, 95-99

3 H. Jan, S. Detlef and S. Iwata, *Journal of Chemical Physics*, 1997, **106**.7541

4 H. Jan, S. Detlef, S. Iwata, A. Nicolaides, D. M. Smith, F. Jensen, C. Amorim and M. A. Keane, *Journal of Chemical Physics*, 1997, **106**, 8083-8088.

Figure S2 Optimized conformations and structural parameters of VC_6H_6-H as well as VC_6H_7. Interatomic distances (Å) and relative energies in eV are also given.



The preferred site of one H atom in VC_6H_6 is determined by comparing the two structures in Figure S2. They are formed by placing an H atom atop a V site (VC_6H_6-H) as well as on top of a C atom (VC_6H_7). The geometries are fully relaxed. We define the binding energy between H and VC_6H_6 as $E_b[H] = E[VC_6H_6] + E[H] - E[VC_6H_6\text{-}H]$. The binding energy of H to the V site is 2.83 eV, which is larger than that of H to the C site (1.82 eV). This indicates that the H atoms prefer to bind at the on-top V site.

Table S2 Energies of **3a** and **3c** at different theoretical levels (in kcal/mol) and symmetry of **3a, 3c,** and corresponding VC_6H_6 units.

Functional	structure	Multi.	E (kcal/mol)	G (kcal/mol)	Total symmetry	Symmetry of the VC_6H_6 unit
B3LYP/6-31G+(d,p)	**3a**	**2**	**-1179.592981**	**-1179.624912**	C_{3V}	C_{6V}
	3c	2	-1179.58825	-1179.620427	C_2	C_2
B3LYP/6-311G++(3df,3pd)	**3a**	**2**	**-1179.712663**	**-1179.744698**	C_{3V}	C_{6V}
	3c	2	-1179.707611	-1179.739929	C_2	C_2
B3LYP/aug-cc-pVTZ	**3a**	**2**	**-1179.758734**	**-1179.790914**	C_{3V}	C_{6V}
	3c	2	-1179.753635	-1179.785923	C_2	C_2
wB97XD/6-311G++(3df,3pd)	**3a**	**2**	**-1179.606611**	**-1179.638449**	C_{3V}	C_{6V}
	3c	2	-1179.601588	-1179.633779	C_2	C_2
wB97XD/aug-cc-pVTZ	**3a**	**2**	**-1179.653447**	**-1179.685417**	C_{3V}	C_{6V}
	3c	2	-1179.648441	-1179.680654	C_2	C_2

Table S3 The original Gibbs free energy in a.u., the energy of deformation (ΔG_R in eV) of VC_6H_6, and hydrogen binding energy between VC_6H_6 unit and $3H_2$ unit in 3a and 3c (ΔG_H in eV)

	G		G
H_2	-1.179853	H_2	-1.179853
V	-943.776769	V	-943.776769
C_6H_6	-232.195439	C_6H_6	-232.195439
VC_6H_6	-1176.059898	VC_6H_6	-1176.059898
$VC_6H_6+3H_2$-3a	-1179.624912	$VC_6H_6+3H_2$-3c	-1179.620427
VC_6H_6 unit in 3a	-1176.051328	VC_6H_6 unit in 3c	-1176.049603
$3H_2$ unit in 3a	-3.49	$3H_2$ unit in 3c	-3.29
ΔG_R	0.23 eV	ΔG_R	0.28 eV
ΔG_H	0.72 eV	ΔG_H	2.52 eV

The energy of deformation (ΔG_R) of VC_6H_6 and hydrogen binding energy between VC_6H_6 unit and $3H_2$ unit in **3a** and **3c** (ΔG_H) are defined to comment on this reversal.

ΔG_R= G (VC_6H_6 unit in **3a**/**3c**) - G (VC_6H_6)

$\Delta G_{H=}$ [G (VC_6H_6 unit in **3a**/**3c**) + G ($3H_2$unit in **3a**/**3c**) - G (**3a**/**3c**)]/3

The values of ΔG_R and ΔG_H are listed in Table S3. The deformation energy of **3c** is 0.28 eV, which is greater than that of 3a (0.23 eV). When deformation energy is not taken into account, the hydrogen binding energy of the VC_6H_6 unit in **3c** and $2H_2$-2H is 2.52 eV, which is greater than that of the VC_6H_6 unit in **3a** and $3H_2$ (0.72 eV).

Figure S3 The Partial orbital density state(PDOS) of V, C_6H_6 and $3H_2$ unit in **3a** ($VC_6H_6(3H_2)$) and **3c** ($VC_6H_6(2H\text{-}2H_2)$), respectively.

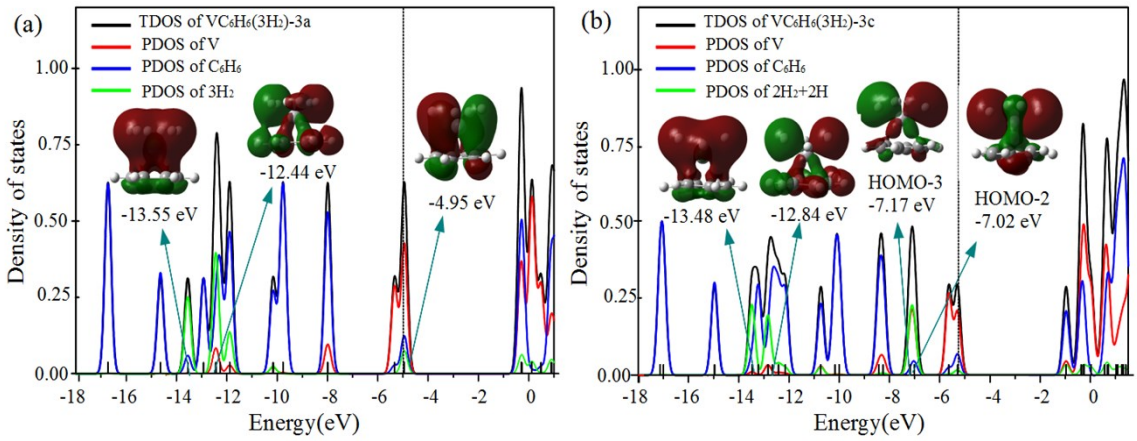


Figure S4 The normal mode analysis of **1a** (Q) and **1b** (Q) at B3LYP/6-31+g(d, p) level

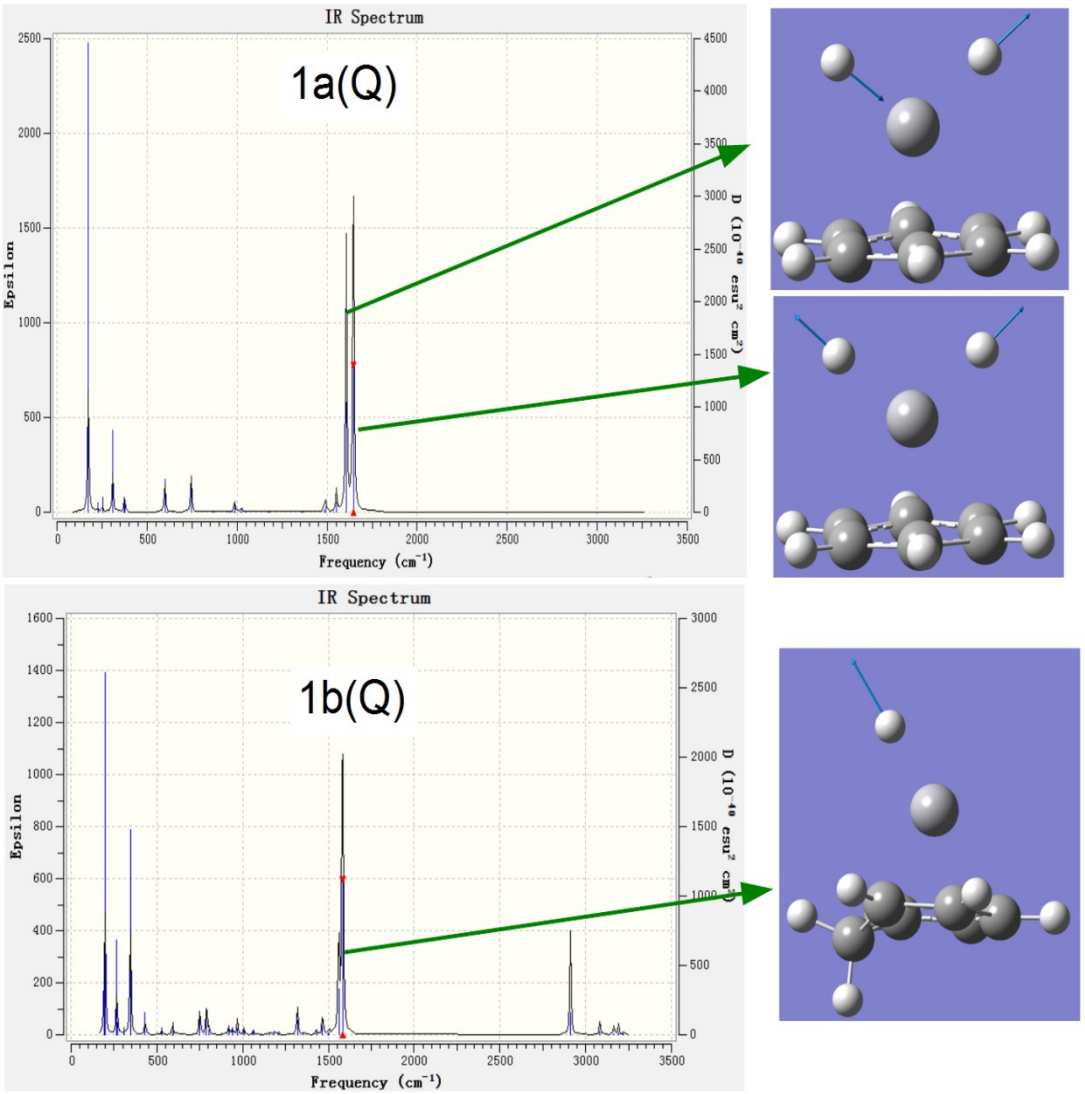
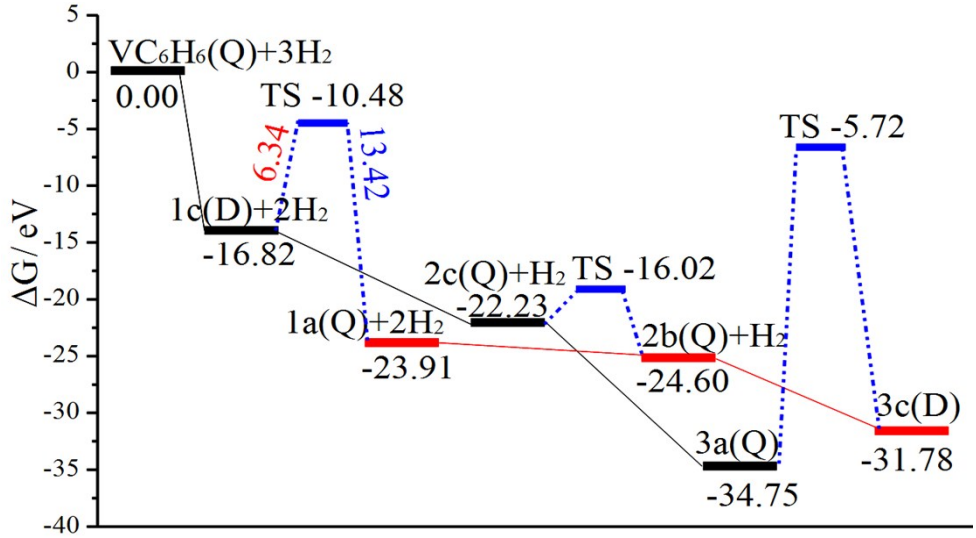


Figure S5 The free energy profiles of hydrogen adsorption on VC_6H_6 complex at 0 K. (Red lines highlight the dissociation adsorption pathway, black lines represent the molecular adsorption pathway, and blue lines represent transition states).



The free energy profiles of the dissociation adsorption pathway and the molecular adsorption pathway are shown in Figure S5. For n=1, H_2 dissociates into two H atoms via the transition state TS. Though the single H_2 dissociation on VC_6H_6 is exothermic, the dissociation barrier is 6.34 kcal/mol. Moreover, **3a** is more stable than **3c.** So, the adsorption pathway along VC_6H_6→**1c**(D) → **2c**(Q) → **3a**(Q) pathway will be more favorable thermodynamically.

All the geometric coordinates and energies at B3LYP/6-31+g(d, p) level (in a.u.):

H_2, E_{ZPE} = -1.168366 , G_{tot} = -1.179853
H 0.0000000000 0.0000000000 0.3713960000
H 0.0000000000 0.0000000000 -0.3713960000

VC_6H_6(D), E_{ZPE} = -1176.0298817 , G_{tot} = -1176.059898
C 0.4867380000 -1.3537650000 -0.5506960000
C 1.4159050000 -0.2554050000 -0.5508400000
C 0.9290530000 1.0985200000 -0.5506240000
C -0.4868050000 1.3537570000 -0.5507290000
C -1.4159020000 0.2553380000 -0.5508070000
C -0.9290540000 -1.0985230000 -0.5505670000
H 0.8531750000 -2.3729980000 -0.4851870000
H 2.4818210000 -0.4477630000 -0.4855320000
H 1.6285280000 1.9254530000 -0.4847480000
H -0.8532680000 2.3729830000 -0.4852350000
H -2.4818200000 0.4476690000 -0.4854860000
H -1.6285230000 -1.9254490000 -0.4846530000
V 0.0000210000 0.0000250000 0.9885400000

VC_6H_6(Q), E_{ZPE} = - 1176.032502 , G_{tot} = - 1176.063855
C -1.2416800000 -0.6959680000 -0.6754240000
C 0.0015840000 -1.4268800000 -0.4622540000
C 1.2474760000 -0.6972380000 -0.6653080000
C 1.2479160000 0.6935680000 -0.6679010000
C 0.0030970000 1.4250780000 -0.4666110000
C -1.2412260000 0.6949460000 -0.6769410000
H 0.0002540000 -2.5104210000 -0.4986330000
H 2.1827350000 -1.2445910000 -0.7406700000
H 2.1838120000 1.2397510000 -0.7443670000
H 0.0045230000 2.5085250000 -0.5055580000
H -2.1760160000 1.2420180000 -0.7596670000
V -0.0052730000 0.0020010000 1.1170540000
H -2.1770350000 -1.2423440000 -0.7567180000

1a(D), E_{ZPE} = -1177.227706 , G_{tot} = -1177.258771
C -0.8866750667 -0.9416794667 -0.6668935333
C 0.4890989333 -0.9193774667 -1.0927325333
C 1.3116409333 0.1408415333 -0.7432325333
C 0.7886359333 1.2211445333 0.0560544667
C -0.6429740667 1.3588385333 0.1330014667
C -1.4667240667 0.3020405333 -0.2240725333
H -1.5206810667 -1.7850064667 -0.9084405333

H 0.9090669333 -1.7888434667 -1.5878305333
H 2.3721059333 0.1023295333 -0.9659765333
H 1.4339939333 2.0320655333 0.3681704667
H -1.0705790667 2.2499415333 0.5808374667
H -2.5363240667 0.3663775333 -0.0582475333
V 0.1886509333 -0.5397074667 1.1775474667
H 1.7378279333 -0.7906994667 1.7866154667
H -1.1070640667 -1.0082654667 2.1451994667

1a(Q), E_{ZPE} = -1177.238994 , G_{tot} = -1177.271959
C -0.7348571333 -1.3092150000 -0.2489999333
C 0.6802398667 -1.3207930000 -0.1876319333
C 1.4208938667 -0.1602010000 -0.5208969333
C 0.7458098667 1.0330140000 -0.8294169333
C -0.6701681333 1.0661930000 -0.8056739333
C -1.4098961333 -0.1160890000 -0.5579689333
H -1.2950761333 -2.2037350000 -0.0022719333
H 1.2003998667 -2.2293000000 0.0959090667
H 2.5039058667 -0.1786480000 -0.4809959333
H 1.3055178667 1.9395780000 -1.0286999333
H -1.1909371333 1.9979570000 -0.9978379333
H -2.4933361333 -0.0857910000 -0.5506279333
V -0.0120211333 0.3403120000 1.3390720667
H -1.1753361333 0.0015490000 2.5328380667
H 1.1248608667 1.2251690000 2.2432030667

1b(D), E_{ZPE} = -1177.221545 , G_{tot} = -1177.25255
C -0.4412525333 -1.3582792000 0.1264113333
C 0.9053154667 -1.1268602000 -0.3147686667
C 1.3332404667 0.1925388000 -0.6276006667
C 0.4798854667 1.3183968000 -0.4674766667
C -0.8748285333 1.1352588000 -0.0292786667
C -1.4642095333 -0.2741082000 -0.3082146667
H -0.8005805333 -2.3627732000 0.3235293333
H 1.6455644667 -1.9197312000 -0.2642876667
H 2.3939504667 0.3679188000 -0.7782686667
H 0.9087754667 2.3141008000 -0.5293286667
H -1.5551125333 1.9764188000 0.0522053333
H -2.4268185333 -0.4103982000 0.1931053333
V 0.2654984667 0.1284048000 1.3174783333
H 1.2537604667 0.3888028000 2.7006533333
H -1.6231885333 -0.3696902000 -1.3941586667

1b(Q), E_{ZPE} = -1177.234975 , G_{tot} = -1177.267278

C -0.6638040000 -1.1713350000 0.1054172667
C 0.6143770000 -1.3091110000 -0.4386547333
C 1.3596400000 -0.1641940000 -0.8439297333
C 0.7767410000 1.1209160000 -0.6423057333
C -0.5030410000 1.2459490000 -0.1003717333
C -1.4761340000 0.0791420000 -0.2038517333
H -1.1651760000 -2.0438560000 0.5143012667
H 1.1136240000 -2.2758900000 -0.4077997333
H 2.3692220000 -0.2635740000 -1.2250287333
H 1.4002560000 2.0045840000 -0.7655217333
H -0.8797440000 2.2324980000 0.1537422667
H -2.2823100000 0.1953010000 0.5268672667
V 0.8011560000 0.0637410000 1.4090912667
H 0.4908910000 0.2593460000 3.1188052667
H -1.9556980000 0.0264830000 -1.2007607333

1c(D), E_{ZPE} = -1177.227685 , G_{tot} = -1177.258748
C -1.0933048000 -0.8435860000 -0.7757864000
C 0.3266302000 -0.9587990000 -0.9664734000
C 1.1695732000 0.1720930000 -0.6736344000
C 0.6068552000 1.3201030000 -0.0737794000
C -0.7948428000 1.3653500000 0.2652356000
C -1.6555668000 0.3013090000 -0.1675324000
H -1.7291588000 -1.6981940000 -0.9913904000
H 0.7515182000 -1.8567600000 -1.3998384000
H 2.2310372000 0.1296150000 -0.8899014000
H 1.2585102000 2.1237870000 0.2568606000
H -1.2083088000 2.2380700000 0.7589026000
H -2.7215238000 0.3474370000 0.0301176000
V 0.0000082000 -0.4305050000 1.0736016000
H 1.6048822000 -1.0243710000 1.3878136000
H 1.2536912000 -1.1855490000 2.1658046000

1c(Q), E_{ZPE} = -1177.219262 , G_{tot} = -1177.251493
C 1.2002410000 -0.5930597333 0.3634236000
C 1.2140210000 0.8342902667 0.5597346000
C 0.0100770000 1.5423592667 0.6069436000
C -1.2641600000 0.8527972667 0.5120176000
C -1.2660330000 -0.5811297333 0.6237196000
C -0.0644460000 -1.2893727333 0.5276096000
H 2.1267190000 -1.1527587333 0.3274956000
H 2.1588950000 1.3683222667 0.5819886000
H 0.0242460000 2.6274322667 0.6491256000
H -2.1896680000 1.4118662667 0.5835486000

H -2.2071250000 -1.1174487333 0.6938756000
H -0.0794420000 -2.3745297333 0.5071386000
V -0.0916150000 0.1684052667 -1.1847684000
H 0.6071490000 -0.7258477333 -2.6838794000
H -0.1788590000 -0.9713257333 -2.6679734000

1d(D), E_{ZPE} = -1177.180215 , G_{tot} = -1177.211678
C -0.9744486667 -0.9817870667 0.1405788667
C 0.4790063333 -1.2876710667 -0.2652011333
C 1.4193033333 -0.0921170667 0.0628808667
C 0.6266123333 1.1864799333 0.3556838667
C -0.6363636667 1.3944629333 -0.2771581333
C -1.5150136667 0.2852909333 -0.3328091333
H 0.8290383333 -2.1983330667 0.2341988667
H 2.1078873333 0.0831859333 -0.7787201333
H 1.2266393333 2.0687049333 0.5735978667
H -1.0117336667 2.4002729333 -0.4613381333
H -2.5456346667 0.3930859333 -0.6631931333
H 2.0538073333 -0.3282870667 0.9276598667
H 0.5102033333 -1.4981690667 -1.3444261333
H -1.6553576667 -1.8332320667 0.1243608667
V -0.9139456667 0.4081129333 1.7038848667

1d(Q), E_{ZPE} = -1177.21351 , G_{tot} = -1177.246103
C -1.0003892000 -0.9839554667 0.0766013333
C 0.4779668000 -1.3138524667 -0.1890496667
C 1.4081928000 -0.0737314667 0.0021533333
C 0.6290788000 1.1835825333 0.4230103333
C -0.6470202000 1.4056535333 -0.2140686667
C -1.4827252000 0.2926665333 -0.3930516667
H 0.7955498000 -2.1340234667 0.4668983333
H 1.9395108000 0.1287545333 -0.9417336667
H 1.2410198000 2.0655335333 0.6114003333
H -1.0277622000 2.4111455333 -0.3851486667
H -2.5171402000 0.4275015333 -0.7045116667
H 2.1860748000 -0.2907064667 0.7447553333
H 0.5859728000 -1.6918454667 -1.2184856667
H -1.6851142000 -1.8272294667 -0.0122496667
V -0.9032152000 0.4005065333 1.7334803333

1e(D), E_{ZPE} = -1177.177149, G_{tot} = -1177.207914
C 0.8009962667 -1.2364146000 -0.1926337333
C 1.4301722667 0.1590114000 -0.1240307333
C 0.4690682667 1.0119234000 0.7379742667

C -1.4585787333 -0.2630366000 -0.0927207333
C -0.5970367333 -1.3388916000 -0.4706647333
H 1.4457712667 -2.0949566000 -0.3582757333
H 2.4303582667 0.1009474000 0.3170502667
H 0.8806782667 1.9218594000 1.1756942667
H -1.5666507333 1.8199494000 0.4991382667
H -2.5348307333 -0.3806156000 -0.1829057333
H -1.0277657333 -2.3165766000 -0.6825967333
V -0.2334587333 -0.7029776000 1.5617922667
H -0.7013237333 1.5672924000 -1.0329217333
H 1.5354672667 0.6014634000 -1.1348977333
C -0.8728667333 1.1510224000 -0.0200017333

1e(Q), E_{ZPE} = -1177.203355 , G_{tot} = -1177.234902
C -0.0915639333 -1.2703868000 -0.4092041333
C 1.2604260667 -0.7067848000 0.0783998667
C 0.9419380667 0.4081842000 1.0801818667
C -1.1509869333 0.9406862000 -0.1042791333
C -0.8835129333 -0.1616338000 -1.1348051333
H -0.0241029333 -2.2149428000 -0.9530941333
H 1.8599940667 -1.4879978000 0.5625328667
H 1.6848330667 0.6932472000 1.8206098667
H -0.2494519333 2.1775212000 1.4199038667
H -1.9815249333 1.6256382000 -0.2540681333
H -1.8327479333 -0.5488448000 -1.5262011333
V -0.9626089333 -0.6826238000 1.3950828667
H 1.8758060667 -0.3160448000 -0.7567971333
H -0.3313389333 0.2449532000 -2.0058201333
C -0.1151579333 1.2990292000 0.7875578667

1f(D), E_{ZPE} = --1177.151227 , G_{tot} = --1177.182478
C -0.3012182667 -1.4117820667 0.1362048667
C 1.0637987333 -0.9789510667 0.1083598667
C 1.3408237333 0.4514259333 -0.3651101333
C -1.0476842667 0.9512839333 0.3173418667
C -1.3666112667 -0.4077320667 -0.3108791333
H -0.5488702667 -2.4719540667 0.1451098667
H 1.8753707333 -1.7047380667 0.0955018667
H 2.3634367333 0.7563939333 -0.1199571333
H 0.5673897333 2.4370409333 0.4127248667
H -1.8556992667 1.6663349333 0.4627678667
H -2.3693762667 -0.7462830667 -0.0316301333
V 0.0666337333 -0.1132740667 1.7487348667
H 1.2487867333 0.5059219333 -1.4698691333

H -1.3537042667 -0.3184230667 -1.4176191333
C 0.3169237333 1.3847359333 0.2883188667

1f(Q), E_{ZPE} = -1177.176224 , G_{tot} = -1177.208323
C -1.2155862667 -0.7640285333 -0.0915780000
C -0.0460052667 -1.2894715333 -0.6364380000
C 1.1507777333 -0.3676915333 -0.8343940000
C 0.0692957333 1.0851764667 0.9632860000
C -1.2520472667 0.7117484667 0.2851740000
H -2.1414452667 -1.3357885333 -0.1139240000
H -0.0435112667 -2.2782315333 -1.0913340000
H 2.0639377333 -0.9473365333 -1.0078770000
H 2.2340277333 1.0652784667 0.5252720000
H 0.1046697333 2.0217084667 1.5177330000
H -2.1071522667 0.9261224667 0.9354050000
V 0.3200107333 -0.8948545333 1.5503970000
H -1.4067202667 1.3016214667 -0.6417550000
H 0.9784077333 0.2293744667 -1.7536210000
C 1.2913407333 0.5363724667 0.3936540000

TS 1c/1a(D), E_{ZPE} = -1177.217582 , G_{tot} = -1177.248334
imaginary frequency(-650.92 cm^{-1})
C -1.0682737333 -0.9153710667 -0.6921874667
C 0.3193082667 -0.9030370667 -1.1039464667
C 1.1560622667 0.1631719333 -0.7618014667
C 0.6446632667 1.2484919333 0.0339235333
C -0.7813707333 1.3502689333 0.2179975333
C -1.6237107333 0.2958919333 -0.1545144667
H -1.7128037333 -1.7422940667 -0.9663184667
H 0.7378802667 -1.7813280667 -1.5851494667
H 2.2104262667 0.1281669333 -1.0100684667
H 1.2970412667 2.0568159333 0.3396265333
H -1.1938647333 2.2092459333 0.7388095333
H -2.6835407333 0.3455139333 0.0769855333
V 0.0777602667 -0.5312840667 1.0711355333
H 1.6630112667 -0.7285380667 1.4428915333
H 0.9574112667 -1.1957150667 2.3526165333

TS 1c/1a(Q), E_{ZPE} = -1177.214351 , G_{tot} = -1177.246513
imaginary frequency(-1110.44 cm^{-1})
C -1.1240458667 -0.8740428667 -0.8085468000
C 0.2386841333 -0.9587868667 -1.1701188000
C 1.1423771333 0.0462731333 -0.7489058000
C 0.6561391333 1.1989311333 -0.0451958000

C -0.7276838667 1.3299491333 0.2252042000
C -1.6104468667 0.2787801333 -0.1069078000
H -1.8110898667 -1.6678628667 -1.0817948000
H 0.6063321333 -1.8245338667 -1.7105948000
H 2.1988671333 -0.0452898667 -0.9694388000
H 1.3469021333 1.9743251333 0.2625812000
H -1.0960218667 2.2069781333 0.7466842000
H -2.6627798667 0.3499921333 0.1470242000
V 0.1049731333 -0.6335758667 1.1142362000
H 1.1657371333 -0.2009828667 2.3696642000
H 1.5720561333 -1.1801538667 1.7761092000

TS 1a/1b(D), E_{ZPE} = -1177.203585 , G_{tot} = -1177.234665
imaginary frequency(-791.89 cm^{-1})
C -0.8590310667 -0.9828034667 -0.6490795333
C 0.4835579333 -0.9195184667 -1.0958875333
C 1.2951829333 0.1942575333 -0.7987265333
C 0.7457059333 1.2978445333 -0.0936075333
C -0.6263420667 1.2992335333 0.2827864667
C -1.4588050667 0.1259465333 0.0988124667
H -1.4437250667 -1.8833264667 -0.7981655333
H 0.9217349333 -1.7922964667 -1.5680065333
H 2.3510699333 0.1769305333 -1.0424645333
H 1.3706239333 2.1447095333 0.1647664667
H -1.0179510667 2.1215645333 0.8726534667
H -2.5416420667 0.2223305333 0.1332234667
V 0.3859019333 -0.4946764667 1.1012704667
H 1.7522089333 -1.0263104667 2.0160264667
H -1.3584900667 -0.4838854667 1.3763984667

TS 1a/1b(Q), E_{ZPE} = -1177.206207 , G_{tot} = -1177.237184
imaginary frequency(-897.81 cm^{-1})
C -0.0719084000 -1.3359105333 0.3234548000
C -1.1016414000 -0.8648475333 -0.4950432000
C -1.3759954000 0.5207574667 -0.6130612000
C -0.6877924000 1.4026254667 0.2654478000
C 0.3281826000 0.9558524667 1.1091718000
C 0.8108356000 -0.4212325333 1.0449558000
H 0.1623156000 -2.3948305333 0.3299818000
H -1.6609564000 -1.5771765333 -1.0931712000
H -2.1690124000 0.8812354667 -1.2563982000
H -0.9406444000 2.4592634667 0.2653648000
H 0.8585586000 1.6669344667 1.7339618000
H 1.3831896000 -0.8101365333 1.8822318000

V 0.9332746000 0.2046154667 -1.0644462000
H 1.4618016000 -0.3427265333 -2.6107142000
H 2.0697926000 -0.3444235333 0.1782638000

TS 1b/1d(D), E_{ZPE} = -1177.182133 , G_{tot} = -1177.212583
imaginary frequency(-912.04 cm^{-1})
C -1.3719570000 -0.1308920000 -0.4815680667
C -0.6311110000 -1.3337970000 -0.3679460667
C 0.7499750000 -1.2663000000 0.0201589333
C 1.4919360000 0.0253940000 -0.3118180667
C 0.6321470000 1.0590010000 0.3837069333
C -0.8019460000 1.1311020000 -0.0036750667
H -2.4325550000 -0.1720620000 -0.7181150667
H -1.1266860000 -2.2817610000 -0.5708250667
H 1.2958060000 -2.2046180000 0.1059149333
H 1.6374760000 0.1749450000 -1.4028120667
H 1.0764090000 1.9976050000 0.7170949333
H -1.2346680000 1.2496050000 1.2750019333
V -0.4968230000 -0.3296760000 1.5302269333
H 2.4876320000 0.0158600000 0.1445849333
H -1.2756350000 2.0655940000 -0.3199300667

TS 1b/1d(Q), E_{ZPE} = -1177.195999, G_{tot} = -1177.227125
imaginary frequency(-998.17 cm^{-1})
C -0.7332708667 -0.9916314667 0.4063936000
C 0.6020961333 -1.2501364667 -0.1648494000
C 1.2877941333 -0.0454554667 -0.6489164000
C 0.7372581333 1.2383965333 -0.4371604000
C -0.5428318667 1.4223315333 0.1157906000
C -1.4989818667 0.2414685333 -0.0570814000
H -1.3015458667 -1.8631894667 0.7286076000
H 0.8891921333 -2.2114244667 -0.5927724000
H 2.3071301333 -0.1353384667 -1.0112914000
H 1.3801071333 2.0999335333 -0.6164284000
H -0.9312998667 2.4310935333 0.2261616000
H -2.3893318667 0.3663415333 0.5687016000
V 0.6947611333 0.0430875333 1.5330216000
H 1.3537971333 -1.5360064667 1.0572146000
H -1.8548738667 0.1905295333 -1.1073914000

TS 1b/1e(D), E_{ZPE} = -1177.145262 , G_{tot} = -1177.175623
imaginary frequency(-733.77 cm^{-1})
C 0.2621890667 -1.1824056000 0.4465831333
C 1.3995130667 -0.3762356000 0.0437671333

C 1.1934120667 0.9167174000 -0.5259558667
C -0.1188179333 1.4367374000 -0.6622198667
C -1.2189019333 0.6532394000 -0.1961768667
C -1.0610429333 -0.8669816000 -0.2727468667
H 0.4622700667 -2.2231626000 0.6942421333
H 2.4125290667 -0.7152236000 0.2396491333
H 2.0559660667 1.5264104000 -0.7774608667
H -0.2527799333 2.4786264000 -0.9453638667
H -2.2187859333 1.0750864000 -0.2486018667
H -1.8894599333 -1.3609336000 0.2438111333
V 0.1896660667 0.7505604000 1.4349681333
H -0.1817989333 -0.8715416000 1.8359111333
H -1.0339579333 -1.2408936000 -1.3104058667

TS 1b/1e(Q), E_{ZPE} = -1177.17678 , G_{tot} = -1177.208091
imaginary frequency(-978.11 cm^{-1})
C 0.2669720000 -1.1921666667 0.4311982667
C 1.3857220000 -0.3698746667 0.0500492667
C 1.1897890000 0.9298303333 -0.5398717333
C -0.1097560000 1.4530713333 -0.6617377333
C -1.2131390000 0.6644773333 -0.1949637333
C -1.0598760000 -0.8582086667 -0.2699107333
H 0.4716880000 -2.2345416667 0.6636292667
H 2.3963740000 -0.7051236667 0.2674002667
H 2.0561770000 1.5217283333 -0.8184657333
H -0.2503320000 2.4808123333 -0.9898137333
H -2.2147280000 1.0805863333 -0.2654397333
H -1.8912960000 -1.3483936667 0.2448182667
V 0.1626620000 0.7314563333 1.4716652667
H -0.1558010000 -0.9115046667 1.9175472667
H -1.0344560000 -1.2421486667 -1.3061047333

TS 1b/1f(D), E_{ZPE} = -1177.155802 , G_{tot} = -1177.186344
imaginary frequency(-396.50 cm^{-1})
C -0.5614665333 -1.3137181333 0.1144644000
C 0.8521074667 -1.0996441333 0.1441864000
C 1.4798264667 0.2570688667 -0.0552376000
C 0.4248294667 1.3324358667 0.0110644000
C -0.9766225333 1.0487108667 -0.0147306000
C -1.4420515333 -0.2852011333 -0.5777516000
H -0.9104175333 -2.3403191333 0.2089824000
H 1.5165374667 -1.9294741333 0.3800734000
H 2.2464174667 0.3491418667 -0.8412336000
H 0.7629674667 2.3589758667 0.1438854000

H -1.6556225333 1.8992878667 -0.0234156000
H -2.4986995333 -0.4582391333 -0.3450236000
V -0.0115145333 0.0879928667 1.6362914000
H 2.1105974667 0.4200358667 0.9008304000
H -1.3368885333 -0.3270541333 -1.6823856000

TS 1b/1f(Q), E_{ZPE} = -1177.174254 , G_{tot} = -1177.206243
imaginary frequency(-780.33 cm^{-1})
C -0.5210372667 -1.2881272667 0.1008630000
C 0.8851667333 -1.0563182667 -0.0751830000
C 1.3829117333 0.2773857333 0.1127320000
C 0.4136177333 1.3766377333 -0.1856490000
C -0.8828262667 1.1351507333 -0.4474070000
C -1.4867912667 -0.2500942667 -0.4699570000
H -0.8515122667 -2.3234992667 0.0208390000
H 1.5913277333 -1.8838872667 -0.1117340000
H 2.4173677333 0.4733457333 -0.1631790000
H 0.7867627333 2.3977637333 -0.1585760000
H -1.5398572667 1.9724417333 -0.6773770000
H -2.4317062667 -0.2440072667 0.0897070000
V 0.3682907333 -0.6149852667 1.9467710000
H 1.6351037333 0.5243927333 1.5300070000
H -1.7668182667 -0.4961992667 -1.5118570000

2a(D), E_{ZPE} = -1178.376825 , G_{tot} = -1178.40911
C -1.2204485294 -0.9182227059 -0.2306354118
C 0.1912634706 -1.2661487059 -0.7538204118
C 1.3073484706 -0.7956457059 0.2060445882
C 1.1016484706 0.6599722941 0.6341495882
C -0.2254435294 1.0748312941 1.0020815882
C -1.3071095294 0.5436712941 0.2168585882
H -1.9645745294 -1.1281897059 -1.0086314118
H 0.3396604706 -0.7936827059 -1.7465194118
H 2.2850644706 -0.9217767059 -0.2749004118
H 1.9397444706 1.1249242941 1.1515465882
H -0.3832535294 1.9106082941 1.6804895882
H -2.3096995294 0.9197622941 0.4160725882
H 0.0295654706 3.3343382941 -1.0964464118
H 0.2767814706 -2.3419967059 -0.9459154118
H -1.4588685294 -1.5832997059 0.6148075882
H 1.3108874706 -1.4497517059 1.0926545882
V 0.0874334706 1.6306062941 -0.9578364118

2a(Q), E_{ZPE} = -1178.409317 , G_{tot} = -1178.442258

C 0.7109969412 -0.1087001176 -1.2698876471
C 1.3281709412 0.7708368824 -0.1858186471
C 0.6026729412 0.5786618824 1.1649793529
C -0.9349100588 0.6633638824 1.0386543529
C -1.4405630588 -0.2086981176 -0.1071986471
C -0.6905260588 -0.2547621176 -1.2995746471
H 1.2681829412 -0.2270291176 -2.1956826471
H 2.3947509412 0.5461848824 -0.0642636471
H 0.8792049412 -0.4124521176 1.5870473529
H -2.5090900588 -0.4025451176 -0.1545956471
H -1.1521520588 -0.6812911176 -2.1903576471
V 0.0682189412 -1.9140351176 -0.0393456471
H -0.1440150588 -3.5510991176 -0.5757956471
H 1.2700789412 1.8310028824 -0.4784426471
H -1.2247850588 1.7130438824 0.8741123529
H 0.9714169412 1.2932088824 1.9092123529
H -1.3976530588 0.3643088824 1.9869573529

2b(D), E_{ZPE} = -1178.407112 , G_{tot} = -1178.438656
C -1.0799335294 0.1257677059 -0.9757054118
C 0.2471124706 -0.0750692941 -1.4774934118
C 1.3427084706 0.3706687059 -0.7484084118
C 1.1470064706 1.0873797059 0.4867345882
C -0.1662785294 1.5618507059 0.7925805882
C -1.2667495294 1.0750897059 0.0942275882
H -1.9337725294 -0.2702492941 -1.5097094118
H 0.3992304706 -0.6876462941 -2.3600744118
H 2.3473524706 0.1115907059 -1.0623974118
H 2.0013474706 1.4144257059 1.0647045882
H -0.3188405294 2.2031117059 1.6549895882
H -2.2700505294 1.3463287059 0.4013155882
V -0.0367455294 -0.7515902941 0.7238385882
H 1.4409344706 -1.4497372941 1.1176045882
H 0.2330574706 -2.4775712941 0.1985245882
H -0.5726865294 -2.4161732941 0.1878245882
H -1.5136925294 -1.1681762941 1.4114435882

2b(Q), E_{ZPE} = -1178.408435 , G_{tot} = -1178.442037
C -1.0526314118 0.3209106471 -1.2384433529
C 0.2779775882 0.0255996471 -1.5981813529
C 1.3350955882 0.4254526471 -0.7471683529
C 1.0699925882 1.1883616471 0.4159496471
C -0.2625414118 1.4833926471 0.7655536471
C -1.3272494118 1.0558696471 -0.0614133529

H -1.8703354118 -0.0340383529 -1.8544763529
H 0.4847295882 -0.5502153529 -2.4933293529
H 2.3583955882 0.1690146471 -1.0015833529
H 1.8832235882 1.4981026471 1.0625146471
H -0.4753934118 2.0167036471 1.6841836471
H -2.3523284118 1.2504876471 0.2304866471
V -0.1369444118 -0.8733293529 0.5870496471
H 1.1348215882 -2.2763433529 1.0776626471
H 0.5496865882 -2.6434913529 0.7135446471
H -1.1888184118 -2.1558403529 0.2016136471
H -0.4276804118 -0.9006373529 2.2560366471

2c(D), E_{ZPE} = -1178.408454 , G_{tot} = -1178.440032
C -1.2823738235 -0.1009039412 -0.9279840000
C -0.0589298235 -0.5557899412 -1.5362140000
C 1.1652211765 0.0038510588 -1.1384350000
C 1.2170391765 1.0103030588 -0.1162660000
C -0.0160618235 1.5994530588 0.3375940000
C -1.2412668235 1.0529950588 -0.0753030000
H -2.2313568235 -0.5361929412 -1.2177100000
H -0.0810108235 -1.3639639412 -2.2588080000
H 2.0923241765 -0.4210619412 -1.5127740000
H 2.1681031765 1.4171910588 0.2060500000
H 0.0036021765 2.4283200588 1.0364490000
H -2.1643208235 1.4260830588 0.3593380000
V 0.0430151765 -0.5982029412 0.6874970000
H 0.4111491765 0.0645320588 2.2976560000
H 0.3249211765 -0.7499279412 2.4885350000
H -0.2493928235 -2.3012069412 0.2727380000
H -0.1006618235 -2.3754779412 1.0976370000

2c(Q), E_{ZPE} = -1178.404655 , G_{tot} = -1178.437761
C -1.2771368824 -0.0925437647 -0.9625859412
C -0.0306118824 -0.5100297647 -1.5626239412
C 1.1843871176 0.0541102353 -1.1582359412
C 1.2062331176 1.0453872353 -0.1199609412
C -0.0512998824 1.6124732353 0.3102340588
C -1.2673958824 1.0625462353 -0.1102129412
H -2.2134468824 -0.5243317647 -1.2937709412
H -0.0315228824 -1.3239977647 -2.2805569412
H 2.1166361176 -0.3117687647 -1.5762839412
H 2.1416801176 1.4882562353 0.1987840588
H -0.0502318824 2.4273612353 1.0271220588
H -2.2022798824 1.4631372353 0.2681810588

V 0.0450751176 -0.6170817647 0.6992600588
H 0.9442801176 -0.5232477647 2.3531930588
H 0.1761831176 -0.4197997647 2.5756290588
H 0.0421301176 -2.5062827647 0.7507350588
H -0.7326788824 -2.3241877647 0.8810930588

2d(D), E_{ZPE} = -1178.397327 , G_{tot} = -1178.42893
C -0.0484292941 -1.5225474706 -0.4682189412
C 1.1243127059 -0.7282324706 -0.3840669412
C 1.0198017059 0.7199935294 -0.8963039412
C -0.2918712941 1.3170155294 -0.3532899412
C -1.4491952941 0.5006645294 -0.4373759412
C -1.3322342941 -0.9138384706 -0.5158859412
H 0.0129237059 -2.5994884706 -0.3346189412
H 2.0978607059 -1.2069474706 -0.3514349412
H -0.3964862941 2.3957815294 -0.2958769412
H -2.4335532941 0.9339705294 -0.2802669412
H -2.2207512941 -1.5300794706 -0.4491869412
H 1.0201247059 0.7366845294 -2.0009349412
H 1.0016927059 1.1450485294 1.9550970588
H -1.2731182941 -0.9155274706 2.2241990588
H 1.4546187059 0.4898975294 1.9415970588
H 1.8808927059 1.3112545294 -0.5679359412
V -0.1665882941 -0.1336494706 1.2145040588

2d(Q), E_{ZPE} = --1178.404312 , G_{tot} = -1178.437689
C -1.2648069412 0.4619985294 -0.6630018235
C -0.0399769412 0.6903205294 -1.5370278235
C 1.1547700588 0.3022905294 -0.6774298235
C 1.2132900588 0.7389495294 0.6490821765
C 0.0132680588 1.0331585294 1.3589471765
C -1.2302729412 0.8488345294 0.6710881765
H -2.2212109412 0.2355805294 -1.1267508235
H -0.0851799412 0.0608015294 -2.4314358235
H 2.0664780588 -0.0408534706 -1.1591848235
H 2.1477440588 0.6801495294 1.2013031765
H 0.0361890588 1.3308195294 2.4001751765
H -2.1537859412 0.8766235294 1.2474551765
V -0.0480609412 -1.1470124706 0.7090101765
H 0.8281750588 -2.2084414706 1.7726881765
H -0.4220429412 -2.6290114706 -0.5447418235
H -0.0155249412 -2.9713454706 0.0242271765
H 0.0209480588 1.7371375294 -1.8944038235

2e(D), E_{ZPE} = --1178.394062 , G_{tot} = -1178.42546

C -0.3649213529 0.4153301765 -1.2939342353
C 1.0356006471 0.8216761765 -0.8180352353
C 1.3147306471 0.0516361765 0.4930567647
C 0.1294646471 0.0355511765 1.4342607647
C -1.1409373529 0.4956311765 1.0119737647
C -1.4201353529 0.6184891765 -0.3611522353
H -0.5808633529 0.4584871765 -2.3562782353
H 1.7899926471 0.5676021765 -1.5666632353
H 1.5650496471 -1.0189998235 0.1687247647
H 0.3076286471 -0.1839798235 2.4814697647
H -1.9479013529 0.5453561765 1.7349847647
H -2.4523423529 0.7138631765 -0.6857812353
V -0.3816783529 -1.3697328235 -0.1020682353
H 0.4635996471 -2.3060698235 -1.2284602353
H -1.6453753529 -2.0875358235 0.7162697647
H 2.2394536471 0.3387271765 1.0005997647
H 1.0886346471 1.9039681765 -0.6289672353

2e(Q), E_{ZPE} = -1178.392016 , G_{tot} = -1178.425776

C -0.3986664118 0.5659341765 -1.2532982941
C 1.0531135882 0.8141951765 -0.8736722941
C 1.4302935882 0.1935711765 0.4998747059
C 0.2293695882 -0.0279198235 1.4088417059
C -1.0554044118 0.3864751765 1.0843337059
C -1.3954554118 0.6475421765 -0.2898322941
H -0.6665174118 0.6548381765 -2.3028262941
H 1.7228395882 0.4376691765 -1.6520882941
H 1.9645235882 -0.7584088235 0.3577007059
H 0.4368115882 -0.3558818235 2.4242947059
H -1.8445144118 0.3457581765 1.8278367059
H -2.4388844118 0.7511441765 -0.5672722941
V -0.6067724118 -1.5370078235 -0.1747452941
H 0.4129205882 -2.8318408235 -0.6802212941
H -2.1937014118 -2.0352688235 0.0089547059
H 2.1484035882 0.8454701765 1.0167907059
H 1.2016405882 1.9037301765 -0.8346712941

2f(D), E_{ZPE} = -1178.350599 , G_{tot} = -1178.384506

C -1.0754731765 -1.2283558235 -0.6112333529
C 0.3845988235 -1.4152778235 -0.2828583529
C 1.1919368235 -0.1049738235 -0.4113573529
C 0.4561558235 1.0475491765 0.2843446471
C -0.9802091765 1.2459431765 -0.1991563529

C -1.6808801765 -0.0345718235 -0.5689713529
H -1.6418231765 -2.1184638235 -0.8776953529
H 0.8327638235 -2.2002968235 -0.9034833529
H 1.4563768235 0.0855381765 -1.4608023529
H 1.0237958235 1.9852321765 0.2103876471
H -1.0117581765 1.9133141765 -1.0795743529
H -2.7375211765 0.0344671765 -0.8233183529
V 1.1438078235 0.0994171765 1.9713796471
H 1.5484178235 1.0037081765 3.3612116471
H 0.4615738235 -1.8241038235 0.7543096471
H 2.1972448235 -0.2582818235 0.0687116471
H -1.5690071765 1.7691561765 0.5681056471

2f(Q), E_{ZPE} = -1178.384978 , G_{tot} = -1178.384506
C -0.8930438824 -1.1972199412 -0.2615071765
C 0.6226351176 -1.2823249412 -0.2857401765
C 1.2814741176 0.0860500588 -0.5753701765
C 0.5105741176 1.1260560588 0.2490168235
C -0.8773548824 1.3162060588 -0.3717511765
C -1.5769508824 -0.0286079412 -0.3266471765
H -1.4427008824 -2.1361439412 -0.2209441765
H 0.9416481176 -2.0749869412 -0.9738601765
H 1.2449671176 0.2785260588 -1.6628901765
H 1.0558881176 2.0646000588 0.3812248235
H -0.8595538824 1.6759180588 -1.4210321765
H -2.6653848824 -0.0641719412 -0.3547161765
V -0.0429608824 -0.1438739412 1.8705528235
H 0.8352871176 -0.0508949412 3.3658568235
H 0.9998231176 -1.6728599412 0.7005528235
H 2.3389641176 0.0477160588 -0.2924411765
H -1.4733108824 2.0560120588 0.1796958235

2g(D), E_{ZPE} = -1178.372914 , G_{tot} = -1178.406387
C -1.5228071765 0.0068758824 -0.8277488824
C -0.8820931765 -1.2923341176 -0.4110768824
C 0.5176968235 -1.1157241176 0.1685751176
C 1.2333458235 0.1392508824 0.0313071176
C 0.6158498235 1.3244528824 -0.7033608824
C -0.8611201765 1.1632938824 -0.9571818824
H -2.5873671765 -0.0254651176 -1.0516248824
H -1.5414111765 -1.8171031176 0.2970091176
H 1.1190488235 -2.0285461176 0.2209561176
H 2.3258568235 0.0862818824 -0.0072358824
H 1.1303488235 1.4579448824 -1.6695438824

H -1.3995021765 2.0509358824 -1.2837458824
V 0.6631948235 -0.1631251176 1.9723251176
H 1.8585378235 -0.7353241176 3.0034711176
H -0.6374571765 0.6434278824 2.6659641176
H 0.7959548235 2.2651378824 -0.1610468824
H -0.8280761765 -1.9599801176 -1.2870418824

2g(Q), E_{ZPE} = -1178.377822 , G_{tot} = -1178.413202
C -1.5284451765 0.0788939412 -0.8609449412
C -0.9151351765 -1.2043450588 -0.3632409412
C 0.5148808235 -1.0360360588 0.0818280588
C 1.2190818235 0.1161389412 -0.1082999412
C 0.6538578235 1.3139029412 -0.8407729412
C -0.8330001765 1.2023739412 -1.0718329412
H -2.5989281765 0.0667149412 -1.0531929412
H -1.5103641765 -1.6141130588 0.4633270588
H 1.0195678235 -1.9112570588 0.4888330588
H 2.2880458235 0.1257529412 0.1168300588
H 1.1774318235 1.4131769412 -1.8062679412
H -1.3411901765 2.0912979412 -1.4390049412
V 0.7053398235 0.1105929412 2.2068190588
H 2.0636728235 -0.6533970588 2.9257000588
H -0.8546811765 -0.3758800588 2.7214300588
H 0.8891118235 2.2449579412 -0.3037669412
H -0.9492461765 -1.9687750588 -1.1574429412

2h(D), E_{ZPE} = -1178.378072 , G_{tot} = -1178.410964
C 0.9085003529 -0.1253254706 -1.1619327647
C 1.5226273529 0.2051015294 0.2013392353
C 0.4276543529 0.0059215294 1.2708262353
C -0.7914856471 0.9051115294 0.9772052353
C -1.3118586471 0.5445145294 -0.4169727647
C -0.4014166471 0.2850995294 -1.4529887647
H 1.5561843529 -0.4714984706 -1.9587037647
H 2.3903063529 -0.4332704706 0.3926332353
H 0.7579253529 -0.0514814706 2.3076512353
H -1.5787416471 0.7689495294 1.7246342353
H -2.3580666471 0.7095245294 -0.6458017647
H -0.7853436471 0.1312825294 -2.4597197647
V -0.3839936471 -1.3833714706 0.1010862353
H 0.6588373529 -2.5544454706 -0.4831087647
H -1.9863376471 -1.7556064706 0.4084742353
H 1.8839623529 1.2478095294 0.1974982353
H -0.5087536471 1.9716845294 0.9978802353

2h(Q), E_{ZPE} = -1178.378072, G_{tot} = -1178.410964
C 0.9837722941 0.1602915294 -1.2721268824
C 1.5382292941 0.2770985294 0.1279231176
C 0.4161052941 -0.0671234706 1.1175451176
C -0.7897057059 0.8689915294 0.9210741176
C -1.2762637059 0.7323685294 -0.5025988824
C -0.3776757059 0.3790085294 -1.5204118824
H 1.6472962941 -0.0599544706 -2.1040758824
H 2.3951762941 -0.3961124706 0.2483641176
H 0.7455502941 -0.1435064706 2.1561581176
H -1.6016937059 0.6413795294 1.6215141176
H -2.3100357059 0.9548845294 -0.7497448824
H -0.7469547059 0.2896695294 -2.5397558824
V -0.4813407059 -1.6538644706 0.1595071176
H 0.4244422941 -3.0796454706 0.1837451176
H -1.9849237059 -2.1336154706 0.7727531176
H 1.9400172941 1.3007465294 0.2743461176
H -0.5219957059 1.9293835294 1.1057841176

2i(D), E_{ZPE} = -1178.371386, G_{tot} = -1178.402294
C 0.8753407059 -0.2253519412 -1.1063191176
C 1.5073517059 0.2071520588 0.2366688824
C 0.5112577059 -0.3179429412 1.2955238824
C -0.8696632941 0.4010360588 1.1549348824
C -1.5024262941 0.0056300588 -0.2276911176
C -0.4931472941 0.4986990588 -1.3259501176
H 1.5072287059 -0.3175269412 -1.9863391176
H 2.5016027059 -0.2300739412 0.3709468824
H 0.8551677059 -0.4843329412 2.3134678824
H -1.5369932941 0.1685970588 1.9886768824
H -2.5567262941 0.2170520588 -0.3794321176
H -0.8806422941 0.3400400588 -2.3354211176
V -0.2745622941 -1.4768579412 -0.0992361176
H -0.2309782941 -3.1653989412 -0.1613611176
H 1.6095667059 1.3101020588 0.2948208824
H -0.3358942941 1.5794890588 -1.1636151176
H -0.6864822941 1.4896880588 1.1303248824

2i(Q), E_{ZPE} = -1178.336988 , G_{tot} = -1178.369978
C 0.8823856471 -0.1380100000 -1.1349350588
C 1.4931206471 0.1810460000 0.2340909412
C 0.5081526471 -0.2405070000 1.3304529412
C -0.8721043529 0.4091720000 1.1777089412

C -1.4262803529 0.0829940000 -0.2133970588
C -0.4900073529 0.5079760000 -1.3489270588
H 1.5574076471 -0.1712220000 -1.9875350588
H 2.4682056471 -0.3030420000 0.3618229412
H 0.9001186471 -0.3438560000 2.3401309412
H -1.5583253529 0.0855500000 1.9688539412
H -2.4943943529 0.2178150000 -0.3702400588
H -0.9055793529 0.2525260000 -2.3305330588
V -0.1929533529 -1.6174760000 -0.0921500588
H -0.3944733529 -3.3216750000 -0.1889550588
H 1.6787316471 1.2741980000 0.3070739412
H -0.3795253529 1.6137410000 -1.3385440588
H -0.7744793529 1.5107700000 1.2850819412

TS 2b/2d(D), E_{ZPE} = -1178.383846 , G_{tot} = -1178.415216
imaginary frequency(-675.23 cm^{-1})
C -1.2358007059 0.1967155294 -0.9166982941
C 0.1031462941 -0.1230984706 -1.4474112941
C 1.2690162941 0.3138395294 -0.7833152941
C 1.1928542941 1.0085325294 0.4394227059
C -0.0795407059 1.4043335294 0.9467297059
C -1.2595107059 1.0769695294 0.2426527059
H -2.0839677059 0.1974855294 -1.5991692941
H 0.1749642941 -0.7403974706 -2.3348742941
H 2.2356912941 -0.0125224706 -1.1527322941
H 2.0939722941 1.2228315294 1.0008947059
H -0.1467707059 1.9476625294 1.8814377059
H -2.2236367059 1.3300395294 0.6736857059
V -0.1088057059 -0.7837334706 0.6568167059
H 0.4763212941 -1.1697074706 2.2064507059
H 0.7918772941 -2.3857874706 0.6191357059
H 0.3067622941 -2.4210754706 -0.0349002941
H -1.5065727059 -1.0620874706 -0.3981252941

TS 2b/2d(Q), E_{ZPE} = -1178.386153 , G_{tot} = -1178.419046
imaginary frequency(-888.71 cm^{-1})
C -1.2329433529 0.2485017647 -0.8698345294
C 0.0319676471 0.0912437647 -1.5818565294
C 1.2445566471 0.4173107647 -0.9734705294
C 1.2960716471 1.0032157647 0.3214814706
C 0.0688066471 1.3979967647 0.9141904706
C -1.1580083529 1.0736807647 0.3301714706
H -2.1555593529 0.2489377647 -1.4421225294
H 0.0302026471 -0.3981462353 -2.5500515294

H 2.1704376471 0.1898227647 -1.4940795294
H 2.2438376471 1.2571137647 0.7802294706
H 0.0740466471 1.9160397647 1.8675394706
H -2.0775673529 1.3192077647 0.8491164706
V -0.0258373529 -0.9295682353 0.5424204706
H -0.4943323529 -1.4213132353 2.1136914706
H 0.6409786471 -2.5923962353 1.1326024706
H 0.8857266471 -2.6481162353 0.3889064706
H -1.5423843529 -1.1735312353 -0.3289345294

TS 2d/2h(D), E_{ZPE} = -1178.346763 , G_{tot} = -1178.378127
imaginary frequency(-686.46cm^{-1})
C -1.1784448235 0.0754291765 -1.0326775294
C 0.2353281765 0.1026871765 -1.6074235294
C 1.1289571765 -0.1576838235 -0.4114555294
C 0.9499391765 0.6581111765 0.7940534706
C -0.3829338235 1.2525541765 0.9638184706
C -1.4236118235 0.9050361765 0.0847464706
H -2.0190228235 -0.2124188235 -1.6590415294
H 0.3628881765 -0.7096628235 -2.3309745294
H 2.1202711765 -0.5729418235 -0.5776355294
H 1.7866541765 1.1303931765 1.3134894706
H -0.5947928235 1.8309731765 1.8580314706
H -2.4417548235 1.1845821765 0.3527414706
V -0.4165478235 -0.9963628235 0.8000954706
H 0.6474741765 -2.3871068235 0.8860084706
H -0.1312548235 -2.7653178235 0.9909154706
H 0.9197251765 -0.3865938235 1.7274024706
H 0.4371261765 1.0483221765 -2.1520945294

TS 2d/2h(Q), E_{ZPE} = -1178.360366 , G_{tot} = -1178.392924
imaginary frequency(-909.33 cm^{-1})
C -1.1756156471 0.0628640000 -1.0180964118
C 0.2423613529 0.1045110000 -1.5837644118
C 1.1732513529 -0.0809530000 -0.3946414118
C 0.9907023529 0.7618880000 0.7932035882
C -0.3690686471 1.2859870000 0.9591495882
C -1.4108536471 0.8795580000 0.0970785882
H -2.0110146471 -0.2254940000 -1.6497874118
H 0.4006453529 -0.7159440000 -2.2920584118
H 2.1766273529 -0.4625040000 -0.5754804118
H 1.8102603529 1.2984090000 1.2729025882
H -0.6050516471 1.8543090000 1.8534005882
H -2.4331586471 1.1160960000 0.3905475882

V -0.2641296471 -0.9870710000 0.8517025882
H 0.3046533529 -2.8020460000 1.0958475882
H -0.2347926471 -2.8847540000 0.5183695882
H 1.0056213529 -0.2498700000 1.8332415882
H 0.3995623529 1.0450140000 -2.1516154118

TS 2d/2g(D), E_{ZPE} = -1178.361448 , G_{tot} = -1178.393464
imaginary frequency(-691.32 cm^{-1})
C -1.3733258235 0.6899685882 -0.5418526471
C -0.2244988235 0.7025135882 -1.5203326471
C 1.0365941765 0.1846015882 -0.8491806471
C 1.2324121765 0.4379835882 0.5325473529
C 0.1061111765 0.3849515882 1.4378193529
C -1.2248698235 0.5788625882 0.7938873529
H -2.3783268235 0.7977825882 -0.9447486471
H -0.4818268235 0.0826745882 -2.3861846471
H 1.9245331765 0.0914915882 -1.4696466471
H 2.2317281765 0.3638145882 0.9605163529
H 0.2243631765 0.7850845882 2.4429623529
H -2.1000498235 0.5466575882 1.4369563529
V 0.4107611765 -1.5215254118 0.3306673529
H -0.0537468235 -0.9486514118 1.9086503529
H 1.5176451765 -2.7682734118 0.4656713529
H -0.7586678235 -2.1366764118 -0.6892066471
H -0.0888358235 1.7287395882 -1.9085256471

TS 2d/2g(Q), E_{ZPE} = -1178.363074 , G_{tot} = -1178.396277
imaginary frequency(-1214.77 cm^{-1})
C -1.3434637647 0.6217365294 -0.5684566471
C -0.1978457647 0.8693845294 -1.5245406471
C 1.1105042353 0.4356495294 -0.8975526471
C 1.2999982353 0.3648245294 0.4516273529
C 0.1697252353 0.2748975294 1.4010703529
C -1.1619967647 0.4521465294 0.7772593529
H -2.3545017647 0.6662145294 -0.9631916471
H -0.3629527647 0.3358255294 -2.4668206471
H 1.9703592353 0.3236625294 -1.5528436471
H 2.2953982353 0.1629425294 0.8398193529
H 0.3082542353 0.6954935294 2.3975123529
H -2.0325837647 0.3639415294 1.4236563529
V -0.0823467647 -1.5388974706 0.1354273529
H 0.3298442353 -1.0234994706 1.8081733529
H 0.5984422353 -2.2378644706 1.6242003529
H -0.4049117647 -2.7064394706 -1.0913826471

H -0.1419227647 1.9399815294 -1.7939576471

TS 2d/2e(D), E_{ZPE} = -1178.382291 , G_{tot} = -1178.413966
imaginary frequency(-537.87 cm^{-1})
C -1.2792150588 0.2645573529 -0.5698956471
C -0.0997730588 0.5076883529 -1.5053956471
C 1.1498449412 0.1225613529 -0.7153656471
C 1.2378169412 0.5415153529 0.6314003529
C 0.0606429412 0.8504843529 1.3810193529
C -1.2018780588 0.7006003529 0.7565823529
H -2.2472850588 0.0272393529 -0.9967346471
H -0.1906190588 -0.1198426471 -2.3957226471
H 2.0725589412 -0.0672276471 -1.2554306471
H 2.1905089412 0.4883903529 1.1502313529
H 0.1356509412 1.1188583529 2.4265263529
H -2.0979030588 0.7375413529 1.3723283529
V -0.0509210588 -1.2486766471 0.6153443529
H 0.7878679412 -1.6173636471 -0.7417356471
H -0.6932630588 -2.2653466471 -0.5428626471
H 0.2727389412 -1.5981366471 2.2345523529
H -0.0467730588 1.5571573529 -1.8448416471

TS 2d/2e(Q), E_{ZPE} = -1178.413966 , G_{tot} = -1178.406348
imaginary frequency(-1235.92 cm^{-1})
C -1.3894728824 0.4707731176 -0.6015383529
C -0.1629968824 0.4804631176 -1.4999773529
C 0.9997061176 -0.0872708824 -0.6775853529
C 1.1462661176 0.4941241176 0.6670236471
C 0.0204311176 0.9497501176 1.3569476471
C -1.2751868824 0.8177501176 0.7304766471
H -2.3739558824 0.3522111176 -1.0442653529
H -0.3337278824 -0.1428228824 -2.3837653529
H 1.9443571176 -0.2112468824 -1.2083123529
H 2.1169561176 0.4891141176 1.1521756471
H 0.1052851176 1.3294581176 2.3688246471
H -2.1680128824 0.9643351176 1.3335736471
V -0.1491458824 -1.2958538824 0.8042456471
H 0.6483461176 -2.1877968824 2.0219396471
H 0.6977801176 -1.4485168824 -0.6992873529
H 0.1262051176 -2.4758798824 -0.4580453529
H 0.0471661176 1.5014091176 -1.8624303529

TS 2h/2i(D), E_{ZPE} = -1178.325052 , G_{tot} = -1178.356219
imaginary frequency(-780.20 cm^{-1})

C 0.8941526471 -0.1997694118 -0.9262217647
C 1.5304126471 0.3902675882 0.3135682353
C 0.4844316471 -0.0245764118 1.3440722353
C -0.7779893529 0.8612985882 1.1100232353
C -1.3856933529 0.4066165882 -0.2216697647
C -0.4821353529 0.0637555882 -1.3182887647
H 1.5200556471 -0.6830404118 -1.6733667647
H 2.4859496471 -0.1145314118 0.4910032353
H 0.7980366471 -0.1053264118 2.3886932353
H -0.4843873529 1.9293975882 1.0977592353
H -2.4250203529 0.6345735882 -0.4459147647
H -0.7722353529 0.2394605882 -2.3560217647
V -0.5384713529 -1.4302024118 0.1822662353
H -0.2994643529 -2.8624844118 -0.6926267647
H -0.7648873529 -1.3384224118 -1.4774877647
H -1.5226133529 0.7532955882 1.9094272353
H 1.7398586471 1.4796875882 0.2747852353

TS 2h/2i(Q), E_{ZPE} = -1178.315647 , G_{tot} = -1178.34838
imaginary frequency(-826.78 cm^{-1})
C 0.8032545882 -0.2410103529 -1.0764517647
C 1.4195455882 0.2328326471 0.2334932353
C 0.3229585882 -0.1276833529 1.2538042353
C -0.8465204118 0.8572816471 1.0953032353
C -1.2852164118 0.9123946471 -0.3408067647
C -0.5867834118 0.0744416471 -1.3216537647
H 1.4257995882 -0.5170053529 -1.9241887647
H 2.3452375882 -0.3231213529 0.4225802353
H 0.6525325882 -0.2339083529 2.2918812353
H -0.5613884118 1.8768396471 1.4286882353
H -2.1887744118 1.4433406471 -0.6283007647
H -0.9243304118 0.1540546471 -2.3541457647
V -0.1529284118 -1.7708073529 0.0466032353
H 0.9356885882 -3.0829853529 -0.0076127647
H -1.3472754118 -1.1483103529 -1.0992767647
H -1.7005824118 0.5852176471 1.7369832353
H 1.6887825882 1.3084286471 0.2431002353

TS 2g/2f(D), E_{ZPE} = -1178.337699 , G_{tot} = -1178.371122
imaginary frequency(-812.85 cm^{-1})
C -1.4338181176 -0.1247920588 -0.6506077647
C -0.6026641176 -1.3824040588 -0.5528417647
C 0.6749218824 -1.1189190588 0.2383222353
C 1.2957818824 0.1610049412 0.1424812353

C 0.6474698824 1.2435649412 -0.7221347647
C -0.8590781176 1.0888929412 -0.7224897647
H -2.5170791176 -0.2190950588 -0.6800657647
H -0.3339341176 -1.7248100588 -1.5662937647
H 1.3060798824 -1.9888490588 0.4031902353
H 2.3783278824 0.2249009412 0.2634582353
H 1.0144028824 1.1832809412 -1.7624597647
H -1.4739731176 1.9816849412 -0.8104407647
V 0.2310938824 0.3444309412 1.9740602353
H -0.0924021176 1.6034649412 3.1266272353
H -1.1804981176 -2.1927620588 -0.0959587647
H 0.0169558824 -1.3231350588 1.7826882353
H 0.9284128824 2.2435409412 -0.3675347647

TS 2g/2f(Q), E_{ZPE} = -1178.361809 , G_{tot} = -1178.395819
imaginary frequency(-762.92 cm^{-1})
C -1.4361241765 -0.1034410588 -0.7736938235
C -0.6914601765 -1.3666120588 -0.4242288235
C 0.6640738235 -1.0964760588 0.2084551765
C 1.3006728235 0.1479789412 0.0584551765
C 0.6240198235 1.3199409412 -0.6405288235
C -0.8477071765 1.0939199412 -0.8735188235
H -2.5024831765 -0.1976890588 -0.9669368235
H -0.5129441765 -1.9509610588 -1.3422668235
H 1.2945288235 -1.9762500588 0.3199411765
H 2.3932458235 0.1610229412 0.0733771765
H 1.1181938235 1.5029969412 -1.6100958235
H -1.4427581765 1.9643629412 -1.1413708235
V 0.7201958235 0.2244729412 2.1871971765
H -0.3357541765 1.3855119412 2.9228371765
H -1.3005471765 -2.0070180588 0.2234111765
H 0.1920358235 -1.3568050588 1.8545491765
H 0.7628118235 2.2550449412 -0.0755828235

TS 2e/2a(D), E_{ZPE} = -1178.381313 , G_{tot} = -1178.413386
imaginary frequency(-704.94 cm^{-1})
C -0.2481414706 0.4008550588 -1.2839123529
C 1.1614225294 0.6812870588 -0.7480853529
C 1.2943275294 0.3190620588 0.7568086471
C 0.0104825294 -0.3093499412 1.3083846471
C -1.2373194706 0.2687430588 0.9163986471
C -1.3969574706 0.6549390588 -0.4434503529
H -0.3805584706 0.5755010588 -2.3522163529
H 1.8921335294 0.1167460588 -1.3389773529

H 2.1354575294 -0.3636959412 0.9199696471
H 0.0757015294 -0.6441519412 2.3419856471
H -2.0974414706 0.2216930588 1.5828746471
H -2.3334444706 1.0635140588 -0.8137353529
V -0.9352344706 -1.4054079412 -0.4945903529
H -1.0208554706 -2.7868989412 -1.5263743529
H 0.1741845294 -1.7540779412 0.7251526471
H 1.4979355294 1.2193740588 1.3496936471
H 1.4083075294 1.7418680588 -0.8999263529

TS 2e/2a(Q), E_{ZPE} = -1178.386357 , G_{tot} = -1178.419262
imaginary frequency(-444.31 cm^{-1})
C -0.2719244706 0.6159020588 -1.2579352941
C 1.1614095294 0.5976620588 -0.7517012941
C 1.2620785294 0.4337210588 0.7866877059
C 0.0179155294 -0.1833759412 1.4015807059
C -1.2434114706 0.2103330588 0.9543777059
C -1.3693364706 0.6639610588 -0.4094792941
H -0.4183004706 0.8166750588 -2.3158142941
H 1.7240315294 -0.1946339412 -1.2604132941
H 2.1446045294 -0.1559719412 1.0482917059
H 0.1148245294 -0.5844899412 2.4053297059
H -2.1267704706 0.0918450588 1.5749327059
H -2.3550434706 0.8972130588 -0.8059482941
V -0.8695544706 -1.5388309412 -0.4525592941
H -1.1706224706 -2.6394229412 -1.7607882941
H 0.3669135294 -1.9901589412 0.6406767059
H 1.3879065294 1.4208980588 1.2548787059
H 1.6452795294 1.5386740588 -1.0521162941

3a(D), E_{ZPE} = -1179.592981 , G_{tot} = -1179.624912
C -0.5732941053 -0.9507927368 -1.2866112105
C 0.8386908947 -0.9178987368 -1.1583902105
C 1.4907828947 0.2872142632 -0.7629492105
C 0.7272888947 1.4526892632 -0.4985432105
C -0.6928641053 1.4192922632 -0.6269482105
C -1.3414621053 0.2209902632 -1.0203832105
H -1.0667561053 -1.8759917368 -1.5612452105
H 1.4157298947 -1.8182397368 -1.3353342105
H 1.2245348947 2.3589162632 -0.1722532105
H -1.2820421053 2.3000652632 -0.3988742105
H -2.4226931053 0.1927802632 -1.0913562105
H 2.5670758947 0.3089672632 -0.6363042105
H -1.6192391053 -0.8722137368 1.3930067895

H -1.1653661053 -1.5595317368 1.2376417895
H 1.3807238947 -0.7928167368 1.6652967895
H 1.0002908947 -1.5027707368 1.4311327895
H 0.2089038947 0.9907602632 2.0705467895
H -0.6256701053 0.9727312632 1.9936787895
V -0.0646351053 -0.2141507368 0.7578887895

3a(D), E_{ZPE} = -1179.56543 , G_{tot} = -1179.597274
C -0.5564993684 -1.1875263158 -0.8566115789
C 0.8866166316 -0.7915523158 -1.0601605789
C 1.0889046316 0.7341556842 -1.1945665789
C 0.2609356316 1.3911056842 -0.0882725789
C -1.1289913684 1.0725426842 -0.0948605789
C -1.5326063684 -0.2099233158 -0.5376375789
H -0.8664743684 -2.1921553158 -1.1284025789
H 1.4992416316 -1.0698143158 -0.1294615789
H 0.5650066316 2.3741646842 0.2596194211
H -1.8648053684 1.7306726842 0.3609174211
H -2.5787363684 -0.4970773158 -0.5011395789
H 2.1512236316 0.9729436842 -1.0801045789
H -0.9557443684 -0.7154253158 2.6064994211
H -1.5082453684 -0.8291413158 1.9636454211
H 1.4263916316 0.1491716842 1.8773564211
H 0.9816716316 -0.2115613158 2.5428544211
H 0.7740826316 1.0682176842 -2.1955725789
H 1.3844776316 -1.3814943158 -1.8365705789
V -0.0264493684 -0.4073033158 1.0924684211

3b(D), E_{ZPE} = -1179.579492 , G_{tot} = -1179.613091
C -0.4890820000 -1.2101537368 -1.1185010526
C 0.9318520000 -1.1879727368 -0.5367790526
C 1.4893280000 0.2450032632 -0.4810730526
C 0.4950760000 1.2479862632 0.0982269474
C -0.9366820000 0.9937132632 0.0859449474
C -1.4537720000 -0.4136247368 -0.2224710526
H -0.8442020000 -2.2424977368 -1.2210600526
H 0.9111000000 -1.6195727368 0.4740879474
H 2.4338860000 0.2636532632 0.0780389474
H 0.7865350000 2.2966252632 -0.0221870526
H -1.6087360000 1.8291002632 -0.1277540526
H -1.6001120000 -0.9966787368 0.7074259474
H 0.0150270000 -0.3677477368 2.8674069474
H -0.2870870000 2.4824552632 2.8630509474
H -0.4798180000 -0.7700927368 -2.1251670526

H 1.6010730000 -1.8186267368 -1.1334840526
H 1.7402560000 0.5653892632 -1.5047590526
H -2.4480130000 -0.3425957368 -0.6766420526
V -0.2566290000 1.0456372632 1.9956949474

3b(Q), E_{ZPE} = -1179.585089 , G_{tot} = -1179.62055
C -0.4918300526 -1.2476958421 -1.1644010526
C 0.8869299474 -1.2076178421 -0.4897220526
C 1.4360969474 0.2268141579 -0.4292340526
C 0.3866209474 1.2411691579 -0.0493150526
C -0.9502300526 0.9578641579 -0.0083390526
C -1.5138570526 -0.4028298421 -0.3841260526
H -0.8503410526 -2.2795178421 -1.2492200526
H 0.8059369474 -1.5995798421 0.5322989474
H 2.2777359474 0.2875471579 0.2711309474
H 0.7151059474 2.2705741579 0.0867229474
H -1.6577000526 1.7821461579 0.1210729474
H -1.8364430526 -0.9540538421 0.5149139474
H 0.6735109474 -0.2387358421 2.8045959474
H -0.0969780526 2.6024131579 2.7871629474
H -0.4102050526 -0.8537228421 -2.1866130526
H 1.5940669474 -1.8528778421 -1.0225080526
H 1.8380659474 0.5237741579 -1.4112670526
H -2.4269710526 -0.2547628421 -0.9736780526
V -0.3795150526 0.9990921579 2.2505249474

3c(Q), E_{ZPE} = -1179.559008 , G_{tot} = -1179.59548
C -0.8400706842 -1.6966200000 -0.8423717368
C 0.4571253158 -1.2183820000 -1.0780407368
C 0.6734783158 0.1560280000 -1.3363237368
C -0.4268496842 1.0418140000 -1.2511717368
C -1.7166946842 0.5446620000 -1.0137167368
C -1.9363456842 -0.8277210000 -0.8547327368
H -0.9912416842 -2.7565560000 -0.6604657368
H 1.2915503158 -1.9118520000 -1.1252927368
H -0.2781936842 2.1021520000 -1.4328207368
H -2.5527156842 1.2361280000 -0.9656137368
H -2.9366876842 -1.2051420000 -0.6735117368
H 1.6462753158 0.5124530000 -1.6492407368
H 1.3940703158 -0.5903730000 2.5535452632
H 2.3608513158 0.9814550000 0.6942902632
H 2.0653283158 -0.3506610000 2.2298142632
H 1.1555803158 1.9612090000 2.0342402632
H 0.4825453158 1.7272860000 2.3584512632

H -0.6021556842 -0.0797020000 2.0042062632
V 0.7541503158 0.3738220000 1.0087552632

3c(D), E_{ZPE} = -1179.549533 , G_{tot} = -1179.581491
C -0.2754970000 -1.0969387895 -1.2016654211
C 1.0429100000 -0.6642477895 -1.0228484211
C 1.3632520000 0.7914382105 -0.6690954211
C 0.2778510000 1.2467772105 0.3095065789
C -1.1174290000 1.1093312105 -0.3694674211
C -1.3799150000 -0.3851747895 -0.6479234211
H -0.4362090000 -2.1163487895 -1.5546774211
H 1.8533090000 -1.3085447895 -1.3500724211
H 0.4339460000 2.1889932105 0.8367775789
H -1.9165010000 1.5477852105 0.2343885789
H -2.3987440000 -0.7146107895 -0.8202004211
H 2.3572930000 0.8525102105 -0.2117494211
H -0.8932420000 -0.6935677895 2.5723815789
H -1.4936770000 -0.4283297895 2.0285075789
H 0.9188150000 -1.3846107895 2.2607625789
H 1.4187090000 -1.3973907895 1.5332325789
H 1.4034100000 1.4141162105 -1.5844134211
H -1.0924660000 1.6463082105 -1.3335124211
V -0.0658150000 -0.6074947895 0.9900685789

3d(D), E_{ZPE} = -1179.55895 , G_{tot} = -1179.59237
C -0.2031672105 -0.5032041579 -1.6014468947
C 1.1823187895 -0.2087791579 -0.9822488947
C 1.2330547895 1.1698858421 -0.2872588947
C 0.0602827895 1.3105068421 0.6806551053
C -1.2119742105 0.8432488421 0.2925291053
C -1.3013642105 -0.2793981579 -0.5629128947
H -0.2290722105 -1.5358291579 -1.9691228947
H 1.4602617895 -1.0159761579 -0.2588798947
H 0.1197547895 2.1067188421 1.4195931053
H -2.0948822105 1.1764778421 0.8356041053
H -2.2844812105 -0.6880571579 -0.7855968947
H 2.1848237895 1.2776758421 0.2464081053
H 0.8183607895 -2.2291631579 1.8207021053
H -1.4579032105 -0.8585751579 2.5160791053
H -1.0362772105 -1.5025961579 2.6977711053
H 1.2135337895 1.9654618421 -1.0489698947
H -0.3525982105 0.1431488421 -2.4806428947
H 1.9733777895 -0.2982591579 -1.7344248947
V -0.0740492105 -0.8732871579 1.2021631053

3d(Q), E_{ZPE} = -1179.58349 , G_{tot} = -1179.617515
C -0.1951623158 -0.4977872632 -1.6315137368
C 1.1817996842 -0.2099102632 -0.9898967368
C 1.2279926842 1.1614917368 -0.2769747368
C 0.0410046842 1.3081277368 0.6716772632
C -1.2189753158 0.8305577368 0.2585922632
C -1.3131533158 -0.2686722632 -0.6177977368
H -0.2178463158 -1.5287312632 -2.0038227368
H 1.4540106842 -1.0266372632 -0.2757327368
H 0.0845206842 2.1053647368 1.4092542632
H -2.1055073158 1.1373627368 0.8138242632
H -2.2954593158 -0.6685242632 -0.8557187368
H 2.1730316842 1.2586567368 0.2702342632
H 0.8193166842 -2.2397042632 1.8920162632
H -1.4552203158 -0.8528172632 2.6084892632
H -0.9899803158 -1.4295612632 2.8240422632
H 1.2246806842 1.9610997368 -1.0343847368
H -0.3249443158 0.1523977368 -2.5109207368
H 1.9819796842 -0.2894682632 -1.7332407368
V -0.0720883158 -0.9032452632 1.1818732632

3e(D), E_{ZPE} = -1179.574681 , G_{tot} = -1179.606417
C -0.7200025263 -1.1523608421 -1.0565262105
C 0.6298464737 -0.7969908421 -1.2448932105
C 0.9713614737 0.6969221579 -1.3014382105
C 0.1997104737 1.3537731579 -0.1548382105
C -1.1653285263 1.0166781579 0.0031187895
C -1.6365855263 -0.2393158421 -0.4553682105
H -1.0456335263 -2.1745678421 -1.2304762105
H 1.3097884737 -1.5159028421 -1.6920112105
H 0.5573284737 2.2959021579 0.2496057895
H -1.8234695263 1.6378671579 0.6041257895
H -2.6507895263 -0.5537818421 -0.2423052105
H 2.0480184737 0.8481811579 -1.1713252105
H 0.2319214737 0.4295091579 2.4748677895
H -0.4897685263 0.0670341579 2.5163257895
H 0.7054234737 1.1326341579 -2.2827192105
V 0.1191364737 -0.5577718421 0.9023767895
H -1.0125475263 -1.4652198421 1.7463297895
H 1.9263454737 -0.7942478421 0.8736197895
H 1.8452444737 -0.2283418421 1.4615307895

3e(Q), E_{ZPE} = -1179.579685 , G_{tot} = -1179.613626

C -0.7866604211 -1.0626207895 -1.0365261579
C 0.5277425789 -0.7249297895 -1.3506671579
C 0.8979345789 0.7351032105 -1.5690331579
C 0.1976205789 1.5098502105 -0.4613311579
C -1.1127074211 1.1855682105 -0.1265611579
C -1.6523124211 -0.1064487895 -0.4227941579
H -1.1083704211 -2.0991317895 -1.0916501579
H 1.2046755789 -1.5025687895 -1.6937421579
H 0.6114755789 2.4581722105 -0.1292801579
H -1.6919804211 1.8617022105 0.4996108421
H -2.6694894211 -0.3632987895 -0.1531471579
H 1.9825815789 0.8665302105 -1.4993671579
H -0.4275014211 0.2871922105 2.7212428421
H -0.5031664211 -0.4873807895 2.7887298421
H 0.6046365789 1.0958082105 -2.5746911579
V 0.1187035789 -0.4434207895 0.9668578421
H 0.0783655789 -2.0063067895 1.7111818421
H 1.9625785789 -0.2373417895 1.6102318421
H 1.7658735789 -0.9664777895 1.8109358421

3f(Q), E_{ZPE} = -1179.5626 , G_{tot} = -1179.597148
C -0.2948550000 -0.8996781579 -1.3679254737
C 1.0176840000 -0.4958431579 -1.1853774737
C 1.3595650000 0.9419868421 -0.8455884737
C 0.3012010000 1.6376588421 0.0554655263
C -1.0260710000 0.8988688421 0.1129955263
C -1.3564650000 -0.1417051579 -0.7443654737
H -0.5311600000 -1.8340661579 -1.8668114737
H 1.8227120000 -1.1267691579 -1.5526554737
H 0.6939440000 1.7677048421 1.0711455263
H -1.8198700000 1.3726038421 0.6862395263
H -2.3786730000 -0.4954361579 -0.8184474737
H 2.3464400000 0.9935288421 -0.3780864737
H 1.2854510000 -0.8879061579 1.9332055263
H -1.2263450000 -2.3722661579 0.8650175263
H -0.5191520000 -0.9983611579 2.7712015263
H -1.1383930000 -1.3806741579 2.4789415263
H 1.4394010000 1.4870268421 -1.7990874737
H 0.1105460000 2.6545488421 -0.3199354737
V -0.0859600000 -1.1212221579 0.9040685263

3f(D), E_{ZPE} = -1179.58825 , G_{tot} = -1179.620427
C -0.4675866842 -1.5735389474 -0.5619686842
C 0.7676663158 -1.0433419474 -1.0415576842

C 0.8078423158 0.3244470526 -1.4810686842
C -0.2819196842 1.1644260526 -1.2552476842
C -1.4164576842 0.6894010526 -0.5314846842
C -1.5344386842 -0.7209159474 -0.2807046842
H -0.5357216842 -2.6243949474 -0.2998976842
H 1.6199363158 -1.6905979474 -1.2022256842
H -0.2156456842 2.2142680526 -1.5218476842
H -2.2382846842 1.3533210526 -0.2970956842
H -2.4331986842 -1.1088649474 0.1840073158
H 1.7110933158 0.7150480526 -1.9346626842
H 0.5336823158 -1.0454589474 2.0890993158
H 1.9581593158 0.4504190526 0.7562993158
H 1.2705503158 -1.0095149474 1.7500243158
H 0.8668903158 1.8110110526 1.3079503158
H 0.1118273158 1.7650610526 1.6023913158
H -0.8314896842 0.1617800526 1.9733423158
V 0.3070953158 0.1674460526 0.7446473158

3g(Q), E_{ZPE} = -1179.540279 , G_{tot} = -1179.576584
C -0.0470374737 -0.4806994211 -1.4420176842
C 1.3124285263 -0.0112324211 -0.8908616842
C 1.2427695263 1.4119955789 -0.3074626842
C 0.0456865263 1.6157085789 0.5719673158
C -1.0863664737 0.8065985789 0.4688543158
C -1.1600304737 -0.2457044211 -0.4536096842
H -0.0053134737 -1.5391074211 -1.7214966842
H 1.6315035263 -0.6978314211 -0.0967686842
H 0.0476995263 2.4382745789 1.2817813158
H -1.9415674737 1.0078225789 1.1103033158
H -2.1117734737 -0.7560074211 -0.6055406842
H 2.1593165263 1.6425575789 0.2488073158
H -0.8010534737 -3.0957304211 0.7102793158
H -2.1647794737 -1.3479964211 2.4693193158
H 0.6850185263 -1.2843694211 2.2833443158
H 1.2000225263 2.1546315789 -1.1230516842
H -0.2910704737 0.0692695789 -2.3668216842
H 2.0731985263 -0.0595254211 -1.6765486842
V -0.7886514737 -1.6286544211 1.5395233158

3g(D), E_{ZPE} = -1179.521007 , G_{tot} = -1179.554377
C -0.3064090526 -0.5679545263 -1.3821966842
C 1.1474539474 -0.1298585263 -1.3556576842
C 1.4126039474 0.5833704737 -0.0411606842
C 0.4219149474 1.3536614737 0.5684993158

C -0.9507670526 1.5010544737 -0.0650576842
C -1.2976210526 0.2026254737 -0.7724456842
H -0.5937190526 -1.3859345263 -2.0382046842
H 1.8127019474 -0.9983355263 -1.4624376842
H 0.6852399474 2.0017574737 1.4007753158
H -1.7044390526 1.7352014737 0.7000483158
H -2.3436680526 -0.0254565263 -0.9617766842
H 2.4349609474 0.6417944737 0.3241283158
H -0.7406160526 -2.5004345263 1.0165723158
H -1.3293010526 -2.0380295263 1.3819243158
H 0.8240779474 -1.4622665263 2.2475383158
H 0.2303929474 -1.0048435263 2.6089263158
H 1.3833959474 0.5237074737 -2.2181386842
H -0.9751300526 2.3570244737 -0.7673706842
V -0.1110720526 -0.7870835263 0.8160343158

3h(D), E_{ZPE} = -1179.565462 , G_{tot} = -1179.597774
C -0.1674627368 -0.0363751579 -1.5862160000
C 0.7567682632 -0.8661811579 -0.6956100000
C 1.4615332632 0.0258518421 0.3540490000
C 0.2608992632 0.3877548421 1.2601920000
C -0.7069837368 1.3254018421 0.5381810000
C -1.2591137368 0.6822478421 -0.7568320000
H -0.6408587368 -0.6702231579 -2.3446200000
H 1.3936982632 -1.5935181579 -1.2111990000
H 0.5042212632 0.6537398421 2.2948950000
H -1.5396667368 1.5988118421 1.1961530000
H -2.0274347368 -0.0534771579 -0.4805040000
H 2.2532612632 -0.5071851579 0.8969240000
H -1.6290497368 -2.1777391579 0.9832490000
H 0.9998022632 -2.5167241579 1.8678210000
H -0.1851787368 2.2650958421 0.2866920000
H 1.9271902632 0.9152068421 -0.0979410000
H -1.7616877368 1.4395738421 -1.3699570000
H 0.4295242632 0.7133428421 -2.1340250000
V -0.0694617368 -1.5856041579 0.9987480000

3h(Q), E_{ZPE} = -1179.537677 , G_{tot} = -1179.571569
C -0.1397468421 0.0172096842 -1.6342471053
C 0.9009291579 -0.7095943158 -0.8357521053
C 1.4586941579 -0.0051133158 0.3717558947
C 0.2694041579 0.4070046842 1.2829748947
C -0.7024948421 1.3116726842 0.5178498947
C -1.2570838421 0.6224016842 -0.7474141053

H -0.5637708421 -0.6306483158 -2.4089681053
H 1.4664931579 -1.5136203158 -1.3048711053
H 0.6052311579 0.8469076842 2.2279018947
H -1.5404968421 1.5929106842 1.1666808947
H -1.9425338421 -0.1847183158 -0.4509481053
H 2.1892591579 -0.6373683158 0.8943648947
H -1.8002848421 -2.1698763158 1.1835308947
H 0.9356591579 -2.6624533158 1.8221988947
H -0.2097428421 2.2566436842 0.2265688947
H 2.0140261579 0.8924246842 0.0338048947
H -1.8515048421 1.3254226842 -1.3419261053
H 0.3719061579 0.8396896842 -2.1697221053
V -0.2039428421 -1.5988953158 1.1662168947

3i(Q), E_{ZPE} = -1179.597274 , G_{tot} = -1179.59764
C -0.6418894211 -1.1277673158 -0.8370335789
C 0.8323735789 -0.8333793158 -1.0029085789
C 1.1236155789 0.6738906842 -1.1899085789
C 0.2927065789 1.4427866842 -0.1525595789
C -1.1203544211 1.1959376842 -0.1884635789
C -1.5666674211 -0.0825853158 -0.5928465789
H -1.0047754211 -2.1215623158 -1.0787585789
H 1.3924525789 -1.1593423158 -0.0607145789
H 0.6251375789 2.4443176842 0.1077264211
H -1.8395904211 1.9338206842 0.1558464211
H -2.6279914211 -0.3154513158 -0.5693735789
H 2.1927665789 0.8626556842 -1.0455135789
H -0.8190194211 -1.7235323158 2.2153224211
H -1.2368994211 -1.0898673158 2.4635414211
H 1.1505825789 0.6861306842 2.1328404211
H 1.2047935789 -0.0130993158 2.5054124211
H 0.8743095789 0.9757776842 -2.2201395789
H 1.2967285789 -1.4613553158 -1.7727875789
V -0.1282794211 -0.2873753158 1.1303184211

3i(D), E_{ZPE} = -1179.551619 , G_{tot} = -1179.58474
C -0.3234630000 -1.3939398421 -0.7077768421
C 1.1734500000 -1.0020848421 -0.4382838421
C 1.3059270000 0.4275061579 0.1100211579
C 0.4702690000 1.4088641579 -0.7584608421
C -0.9817550000 1.0442371579 -0.4412878421
C -1.3098800000 -0.3139528421 -0.2666008421
H -0.5614350000 -2.3434788421 -0.2142118421
H 1.6255510000 -1.7135378421 0.2636371579

H 2.3374850000 0.7337701579 0.3024351579
H 0.6666290000 2.4575761579 -0.5081018421
H -1.7548260000 1.8088721579 -0.4601198421
H -2.3588320000 -0.5989958421 -0.2237668421
V -0.2124760000 0.5812581579 1.4433941579
H -0.4373350000 2.0242241579 2.2956541579
H -0.4684370000 -1.5745888421 -1.7829738421
H 1.7459520000 -1.1008378421 -1.3739858421
H 0.7016490000 1.2911991579 -1.8323608421
H -1.0552150000 -0.9388938421 1.9722191579
H -0.5632580000 -0.7971968421 2.6205701579

3j(Q), E_{ZPE} = -1179.563048 , G_{tot} = -1179.59726
C -0.4197159474 -1.4293027895 -0.9317026842
C 1.0616520526 -1.0520737895 -0.6664936842
C 1.1232560526 0.1752362105 0.2558973158
C 0.5491360526 1.3823522105 -0.5062236842
C -0.9118169474 1.0626812105 -0.7687686842
C -1.3439799474 -0.2229457895 -0.8913756842
H -0.7632289474 -2.1747437895 -0.1924836842
H 1.5815720526 -1.9112527895 -0.2271736842
H 2.1312380526 0.3584532105 0.6405583158
H 0.6197940526 2.3087682105 0.0763253158
H -1.6337129474 1.8730012105 -0.8460136842
H -2.4018709474 -0.4088737895 -1.0739386842
V -0.6393599474 0.1061132105 1.4470333158
H -1.2476439474 1.4860062105 2.2769763158
H -0.5426939474 -1.9308977895 -1.9027366842
H 1.5562160526 -0.8516247895 -1.6332916842
H 1.0632660526 1.5835172105 -1.4674576842
H -0.1136519474 0.1149262105 3.3257463158
H 0.3315450526 -0.4693397895 3.0851233158

3j(D), E_{ZPE} = -1179.569013, G_{tot} = -1179.6008
C -0.2433501579 -0.9552622105 -1.4403125789
C 1.0516758421 -0.5528692105 -1.0470285789
C 1.2573868421 0.9438217895 -0.7932975789
C 0.2060398421 1.3558587895 0.2544304211
C -1.1711911579 0.8226707895 -0.0372735789
C -1.3568341579 -0.2175792105 -0.9799785789
H -0.4130011579 -1.8983552105 -1.9528685789
H 1.9076048421 -1.1477952105 -1.3447515789
H 0.6042118421 0.8976737895 1.2373834211
H -2.0281281579 1.3241417895 0.3986784211

H -2.3620661579 -0.5535952105 -1.2070135789
H 2.2610288421 1.1319987895 -0.4031365789
H 1.4173398421 -1.0448752105 1.4444074211
H -1.5005641579 -1.7848602105 1.0395144211
H -0.0240601579 -0.6565172105 2.6656564211
H -0.8041021579 -0.7559432105 2.5646694211
H 1.1324868421 1.5286087895 -1.7169805789
H 0.1949498421 2.4182097895 0.5131954211
V -0.1294271579 -0.8553322105 0.8047064211

3k(D), E_{ZPE} = -1179.558268 , G_{tot} = -1179.591779
C -0.2989884737 -0.1613492632 -1.5389323684
C 0.7637315263 -0.8462642632 -0.6566623684
C 1.5521795263 0.1941527368 0.1631576316
C 0.5624595263 0.9978667368 1.0799636316
C -0.8764854737 0.4958157368 0.8464086316
C -1.2838924737 0.6577017368 -0.6312523684
H -0.8462594737 -0.9030082632 -2.1312883684
H 1.3960865263 -1.5587222632 -1.1955143684
H 0.8421685263 0.8939917368 2.1341646316
H -1.6071144737 0.8979877368 1.5551456316
H -2.3168274737 0.3274187368 -0.7862693684
H 2.3268255263 -0.2930722632 0.7652466316
H -1.7322404737 -2.4036942632 0.2512276316
H 0.3473675263 -2.0009022632 2.1696816316
H -1.2594394737 1.7238117368 -0.9039823684
H 0.1967825263 0.5023007368 -2.2636583684
H 0.6179985263 2.0736697368 0.8538866316
H 2.0795665263 0.8761597368 -0.5211243684
V -0.4639184737 -1.4738642632 0.8098016316

3k(Q), E_{ZPE} = -1179.5355 , G_{tot} = -1179. 570306
C -0.3370353684 -0.1930653158 -1.5588832105
C 0.8657676316 -0.6739993158 -0.7957122105
C 1.5509096316 0.2870086842 0.1339177895
C 0.5407526316 0.9504546842 1.1249627895
C -0.8928723684 0.4963146842 0.7968727895
C -1.2156243684 0.7451556842 -0.6852402105
H -0.9152993684 -1.0516343158 -1.9247842105
H 1.4548836316 -1.4822913158 -1.2299072105
H 0.8130766316 0.6668746842 2.1501367895
H -1.6243923684 0.9672556842 1.4645337895
H -2.2737123684 0.5591126842 -0.8968402105
H 2.3716706316 -0.2061763158 0.6639097895

H -1.7207923684 -2.6358483158 0.3159177895
H 0.3306076316 -2.0980563158 2.2990107895
H -1.0295603684 1.7986496842 -0.9544952105
H 0.0186146316 0.3216186842 -2.4716672105
H 0.6304266316 2.0472156842 1.0830387895
H 2.0241416316 1.0635536842 -0.4966912105
V -0.5915623684 -1.5621433158 0.9819197895

3l(D), E_{ZPE} = -1179.557612 , G_{tot} = -1179.589647
C -0.5855150526 -1.1085084737 -0.1951650526
C 0.7985379474 -1.1600984737 -0.8675710526
C 1.4644509474 0.1976545263 -0.6252960526
C 0.6967999474 1.3690105263 -0.7300370526
C -0.6975610526 1.3285795263 -0.5685790526
C -1.4434290526 0.0126345263 -0.8086160526
H -1.0803060526 -2.0632324737 -0.0161970526
H 1.4145179474 -1.9632984737 -0.4528440526
H 2.5461479474 0.2603515263 -0.6289020526
H 1.2021489474 2.3314175263 -0.6659770526
H -1.2619650526 2.2526125263 -0.5281530526
H -2.4365830526 0.0519355263 -0.3517890526
H 0.1509169474 -0.7048944737 2.7920399474
H 1.6275769474 -0.3066454737 1.7338399474
H -0.5481340526 -0.3374024737 2.8107989474
H -1.1044160526 1.1244995263 1.8054959474
H 0.7131449474 -1.3444574737 -1.9531880526
H -1.5913210526 -0.1388584737 -1.8926590526
V 0.1349879474 0.1987005263 1.1427989474

3l(Q), E_{ZPE} = -1179. 527149 , G_{tot} = -1179. 561731
C -0.5576589474 -0.9891635263 -0.1374772105
C 0.7658740526 -1.1844815263 -0.8838482105
C 1.4977390526 0.1337004737 -0.9072332105
C 0.7931370526 1.3444194737 -0.8068622105
C -0.6053879474 1.3935274737 -0.7592122105
C -1.4022819474 0.1048284737 -0.8184412105
H -1.1059649474 -1.9200545263 0.0274657895
H 1.3888410526 -1.9408675263 -0.3912552105
H 2.5796730526 0.1581284737 -0.9997232105
H 1.3538090526 2.2757864737 -0.7826692105
H -1.1111609474 2.3550884737 -0.7554032105
H -2.3737879474 0.2367934737 -0.3276932105
H 0.3262530526 -0.9322495263 2.7988117895
H 1.4564590526 0.4538334737 2.0831087895

H -0.4464599474 -0.9770185263 2.7897947895
H -1.4700269474 0.8148314737 2.2697757895
H 0.6317220526 -1.5451525263 -1.9256022105
H -1.6284889474 -0.1242375263 -1.8800332105
V -0.0922889474 0.3422874737 1.4064967895

3m(Q), E_{ZPE} = -1179.554265 , G_{tot} = -1179.588652
C -0.3245260000 -1.0789846842 -1.3003013158
C 1.0195950000 -0.7531946842 -1.0235323158
C 1.3514930000 0.6834743158 -0.5975073158
C 0.2371150000 1.1201573158 0.3629586842
C -1.1240420000 1.1244753158 -0.3462303158
C -1.3952020000 -0.3243006842 -0.7755463158
H -0.5426850000 -2.0455656842 -1.7570183158
H 1.8058040000 -1.3924266842 -1.4173373158
H 0.4559000000 2.0193923158 0.9436116842
H -1.9135060000 1.4707913158 0.3331316842
H -2.4135400000 -0.6407836842 -0.9866763158
H 2.3280830000 0.7123293158 -0.0970753158
H -1.1637030000 -0.3553156842 2.4913696842
H -1.6763840000 -0.7174576842 2.0314306842
H 1.4396670000 -0.7804816842 2.2107666842
H 1.6904170000 -1.3051656842 1.6937466842
H 1.4455990000 1.3379373158 -1.4872193158
H -1.1593010000 1.7998093158 -1.2245363158
V -0.0607840000 -0.8746896842 0.9459646842

3m(D), E_{ZPE} = -1179.546499 , G_{tot} = -1179.580666
C -0.6766816842 -1.4793018947 -0.2781383158
C 0.5997643158 -0.9271788947 0.3436896842
C 1.2536663158 0.2115641053 -0.2158393158
C 0.6433173158 0.9954601053 -1.3725973158
C -0.7951836842 0.6289051053 -1.6362963158
C -1.3827206842 -0.4724578947 -1.1511953158
H -1.3668066842 -1.8518408947 0.4919086842
H 1.2278383158 -1.6681488947 0.8417536842
H 2.3405243158 0.2825411053 -0.1109423158
H 0.7226043158 2.0814751053 -1.2060533158
H -1.3632556842 1.3021361053 -2.2750313158
H -2.4195696842 -0.6814238947 -1.4070213158
V 0.4865303158 0.8426561053 1.5924016842
H -0.7484326842 1.9701111053 1.6865816842
H -0.4259676842 -2.3646168947 -0.8868743158
H 1.2359453158 0.8128061053 -2.2845003158

H -0.3919766842 -0.6268618947 2.2884906842
H -0.5991796842 -0.0627988947 2.8041676842
H 1.6595843158 1.0069751053 2.7754956842

3n(Q), E_{ZPE} = -1179.554551, G_{tot} = -1179.588517
C -0.6487995789 -1.4986878421 -0.6999911053
C 0.5891524211 -1.2597638421 0.1496248947
C 1.3834804211 -0.1792928421 -0.1133681053
C 1.0115104211 0.7598911579 -1.2493611053
C -0.4981305789 0.9387321579 -1.2029321053
C -1.2924375789 -0.1419158421 -0.9402621053
H -1.3420395789 -2.1708168421 -0.1923301053
H 0.8621794211 -1.9904328421 0.9054518947
H 2.3125784211 -0.0172318421 0.4253148947
H 1.5179884211 1.7196901579 -1.1386851053
H -0.9236635789 1.9061421579 -1.4532221053
H -2.3755995789 -0.0695978421 -0.9737001053
V -0.4703565789 0.6320691579 1.1812528947
H -1.6056565789 -0.4610578421 1.9222328947
H -0.3707275789 -1.9686228421 -1.6614451053
H 1.3182994211 0.3292731579 -2.2203781053
H 0.3246024211 0.9600301579 2.9156498947
H -0.1330605789 0.3423411579 3.0652018947
H 0.3406804211 2.1692511579 1.2809458947

3n(D), E_{ZPE} = -1179.565806 , G_{tot} = -1179.598831
C -0.1283424737 -0.5008313684 -1.5548055789
C 1.2210055263 -0.2011043684 -0.8718745789
C 1.2011535263 1.1113376316 -0.0630655789
C -0.0420034737 1.2060596316 0.8099774211
C -1.2795304737 0.7773386316 0.3000844211
C -1.2913794737 -0.3082753684 -0.5920525789
H -0.1283634737 -1.5227623684 -1.9451325789
H 1.4668175263 -1.0346333684 -0.1905125789
H -0.0310364737 1.9328726316 1.6180044211
H -2.1970124737 1.0544866316 0.8178864211
H -2.2451734737 -0.7519993684 -0.8653455789
H 2.1010855263 1.1804786316 0.5550124211
H -0.5257734737 -2.3236763684 0.5225524211
H -1.5934994737 -1.1079843684 2.6206474211
H 0.9551035263 -0.5307583684 2.1840154211
H 1.2141615263 1.9732336316 -0.7476845789
H -0.2706124737 0.1719396316 -2.4143165789
H 2.0306305263 -0.1859103684 -1.6094955789

V -0.4572304737 -0.9398113684 1.4261054211

3o(D), E_{ZPE} = -1179. 544925 , G_{tot} = -1179.578509
C -0.3962958947 -0.4600115263 -1.4596419474
C 1.0988491053 -0.3895585263 -1.2730859474
C 1.5260451053 0.4818764737 -0.0629159474
C 0.3928631053 0.6511944737 0.9481510526
C -0.8686268947 1.2498484737 0.3065220526
C -1.2968318947 0.3019634737 -0.7982559474
H -0.7568138947 -1.1532925263 -2.2177729474
H 1.4824141053 -1.4120865263 -1.1693479474
H 0.7041871053 1.1576584737 1.8630130526
H -1.6826048947 1.3640994737 1.0361480526
H -2.3526718947 0.2259874737 -1.0447449474
H 2.4034451053 0.0396934737 0.4205420526
H -0.1100768947 -2.5364375263 0.6364680526
H -2.2654618947 -1.0286395263 1.5267490526
H 0.0535851053 -1.1392735263 2.7440500526
H 1.5433511053 -0.0025305263 -2.2009249474
H -0.6817218947 2.2640904737 -0.0843339474
H 1.8407861053 1.4761254737 -0.4171389474
V -0.6344198947 -1.0907075263 1.2465200526

3o(Q), E_{ZPE} = -1179.5151621 , G_{tot} = -1179.551779
C -0.2245800000 -0.0291464737 -1.9691180000
C 1.0599260000 -0.4492544737 -1.3001830000
C 1.3578850000 0.3796095263 -0.0353570000
C 0.1395790000 0.6581535263 0.7904120000
C -1.1238680000 1.0751795263 0.0973280000
C -1.1934560000 0.6544555263 -1.3489860000
H -0.3648390000 -0.3287464737 -3.0055350000
H 0.9983290000 -1.5152324737 -1.0392460000
H 0.2949560000 1.0394205263 1.8056430000
H -2.0050260000 0.7150385263 0.6509090000
H -2.1017660000 0.9184405263 -1.8855970000
H 2.1495050000 -0.0771384737 0.5684740000
H -0.4745460000 -2.6061594737 0.9393110000
H -1.7227030000 -0.8836734737 2.8564590000
H 1.0821870000 -1.3922494737 2.9936620000
H 1.8981250000 -0.3544054737 -2.0002970000
H -1.2036870000 2.1769845263 0.1772730000
H 1.7494230000 1.3678595263 -0.3467500000
V -0.3154440000 -1.3491354737 2.0515980000

3p(Q), E_{ZPE} = -1179.536414, G_{tot} = -1179.571817
C -0.4638661579 -0.5840807368 -1.3037636842
C 1.0080538421 -0.2053437368 -1.3664236842
C 1.3804068421 0.4503932632 -0.0428916842
C 0.5223828421 1.3548102632 0.5555793158
C -0.8324641579 1.6082172632 -0.0790416842
C -1.3306781579 0.2778992632 -0.6302796842
H -0.8409991579 -1.3594287368 -1.9632046842
H 1.6332808421 -1.0852047368 -1.5507306842
H 0.8568258421 1.9744172632 1.3825123158
H -1.5364611579 2.0067242632 0.6594603158
H -2.4056371579 0.1258752632 -0.7125746842
H 2.3999088421 0.3462432632 0.3221623158
H -0.3449201579 -2.5202637368 0.2845623158
H -0.2391341579 -2.6811257368 1.1171183158
H -0.0243251579 -1.2767687368 2.7467653158
H 0.0039598421 -0.4455997368 2.7191023158
H 1.1993018421 0.4931952632 -2.2064246842
H -0.7586581579 2.3753442632 -0.8772906842
V -0.2269771579 -0.8553037368 0.9453633158

3q(D), E_{ZPE} = -1179.531271 , G_{tot} = -1179.563729
C -0.5642937368 -1.0522183684 -0.7383733684
C 0.8201232632 -0.6701663684 -0.6817433684
C 1.1679462632 0.7982936316 -0.8701333684
C 0.2375852632 1.5127366316 0.0965446316
C -1.1086187368 1.1435696316 0.0971256316
C -1.5812357368 0.0784116316 -0.8965253684
H -0.8389357368 -2.0603033684 -1.0431623684
H 1.5823642632 -1.4178773684 -0.8926893684
H 0.5564472632 2.4228746316 0.5993526316
H -1.8387117368 1.7579316316 0.6245266316
H -2.5929527368 -0.2619363684 -0.6431833684
H 2.2147762632 0.9855406316 -0.6081273684
H 0.2233432632 -2.0916933684 2.1143706316
H -0.4007887368 -2.2614423684 1.6302336316
H 1.4630202632 -0.4040673684 2.1017076316
H 1.3937452632 0.3484986316 1.7131036316
H 1.0270412632 1.1601446316 -1.9097533684
H -1.6451697368 0.4811726316 -1.9271923684
V -0.1156857368 -0.4694693684 1.2339186316

3q(Q), E_{ZPE} = -1179.536307 , G_{tot} = -1179.570841
C -0.4948918421 -1.0811583684 -0.9285584211

C 0.8325431579 -0.6746173684 -1.0451654211
C 1.1938511579 0.8046406316 -1.0899694211
C 0.3403601579 1.5130686316 -0.0544664211
C -0.9611268421 1.0870856316 0.1409855789
C -1.5551688421 -0.0086473684 -0.7346444211
H -0.7999568421 -2.0893383684 -1.1904884211
H 1.5893111579 -1.3979723684 -1.3439074211
H 0.7045091579 2.4221416316 0.4148655789
H -1.6277248421 1.6587456316 0.7832295789
H -2.4563148421 -0.4261083684 -0.2733484211
H 2.2588301579 0.9473226316 -0.8773444211
H -0.1651068421 -1.9463683684 2.1831565789
H -0.4556628421 -2.1212203684 1.3983375789
H 0.9395301579 -0.2395963684 2.8614155789
H 1.1792511579 0.4376096316 2.4332515789
H 1.0234571579 1.2293246316 -2.1006444211
H -1.8726338421 0.4110236316 -1.7109814211
V 0.3269441579 -0.5259353684 1.1342765789

3r(D), E_{ZPE} = -1179.535546 , G_{tot} = -1179.56726
C -0.4642187895 -0.4227090000 -1.4923126316
C 0.8745452105 -0.8047250000 -0.8399386316
C 1.5786442105 0.4459130000 -0.2354766316
C 0.6991292105 1.0117770000 0.9508483684
C -0.7003207895 1.3574590000 0.3230023684
C -1.3142297895 0.0598490000 -0.2965526316
H -0.9251437895 -1.2857990000 -1.9835936316
H 1.5254932105 -1.5306690000 -1.3188216316
H 1.1646862105 1.7483500000 1.5982973684
H -1.3684897895 1.8278350000 1.0492063684
H -2.3968467895 0.0673640000 -0.4030936316
H 2.6013322105 0.2318870000 0.0830443684
H 0.6129512105 -2.2512420000 1.5428613684
H -1.5989007895 -1.4287160000 1.7906663684
H -1.0400177895 -1.9199860000 2.0543173684
H -0.5168337895 2.0679700000 -0.5026366316
H 1.5931872105 1.2322010000 -1.0088186316
H -0.3427907895 0.3742790000 -2.2571486316
V 0.0178242105 -0.7810380000 0.9461493684

3r(Q), E_{ZPE} = -1179.513514 , G_{tot} = -1179.547362
C -0.5963238421 -0.3898020526 -1.2416275789
C 0.8141551579 -0.8410060526 -0.7382465789
C 1.6295601579 0.4142809474 -0.3777725789

C 0.8416561579 1.2253829474 0.6277394211
C -0.5991608421 1.5802759474 0.3307774211
C -1.3498928421 0.2920519474 -0.0530025789
H -1.1674858421 -1.2292610526 -1.6545365789
H 1.3149611579 -1.5647680526 -1.3818315789
H 1.3725521579 1.7656459474 1.4078274211
H -1.0580548421 2.0766249474 1.1923934211
H -2.4259138421 0.3941329474 -0.1965095789
H 2.6156411579 0.1570399474 0.0231224211
H 0.2298451579 -1.1828880526 2.6752334211
H -1.1964548421 -2.7076960526 0.7330134211
H -0.9729538421 -2.7391260526 1.4647304211
H -0.6116048421 2.3203239474 -0.5017935789
H 1.8104951579 1.0504219474 -1.2741875789
H -0.4672658421 0.3476489474 -2.0540775789
V -0.1837548421 -0.9692830526 1.0187484211

TS 3c/3e(Q), E_{ZPE} = -1179.544668 , G_{tot} = -1179.578436
imaginary frequency(-845.31 cm^{-1})
C -0.4862661579 -1.7656353684 -0.9622367895
C 0.6300228421 -1.2012043684 -1.5108237895
C 0.8636298421 0.2229016316 -1.2663297895
C -0.3114861579 1.0503456316 -1.0914747895
C -1.4778811579 0.4518026316 -0.5756847895
C -1.4632451579 -0.9385143684 -0.3006617895
H -0.6547311579 -2.8379123684 -1.0205087895
H 1.3826498421 -1.7913263684 -2.0229567895
H -0.2750711579 2.1118746316 -1.3154267895
H -2.3549081579 1.0513896316 -0.3563567895
H -2.3241551579 -1.3965413684 0.1731832105
H 1.7218968421 0.6810056316 -1.7461927895
H 1.3575898421 1.8719716316 1.5443902105
H 0.7022508421 2.0190926316 1.9398122105
H 1.6806088421 0.2273106316 0.1957892105
H -0.9000511579 0.8544666316 2.3266972105
H 0.5844448421 -0.3905253684 2.7038282105
H 1.1927348421 -0.6292523684 2.2729972105
V 0.1319668421 0.4087506316 1.0119562105

TS 3e/3m(Q), E_{ZPE} = -1179.538574 , G_{tot} = -1179.572163
imaginary frequency(-738.45 cm^{-1})
C -0.7155081053 -1.1676195789 -0.7547483684
C 0.6402798947 -0.7142755789 -1.0862253684
C 0.8667958947 0.7368034211 -1.4824173684

C 0.2030908947 1.5607394211 -0.3827243684
C -1.1159181053 1.2076754211 -0.0650863684
C -1.6100041053 -0.0954535789 -0.2829193684
H -1.1709241053 -2.0492055789 -1.2111963684
H 1.3271618947 -1.4694865789 -1.4645683684
H 0.5456518947 2.5688954211 -0.1667453684
H -1.7469301053 1.9018684211 0.4885206316
H -2.6122671053 -0.3540665789 0.0436536316
H 0.4683588947 1.0165104211 -2.4793413684
H -0.2340791053 0.1612194211 2.8293396316
H -0.5051001053 -0.5708075789 2.7698036316
H 1.9441078947 0.9322284211 -1.5118243684
H -0.4844541053 -1.8467955789 0.4411186316
H 1.8751358947 -1.1255555789 1.6650596316
H 2.0615738947 -0.3613945789 1.6726576316
V 0.2630278947 -0.3312795789 0.9776436316

TS 3m/3d(Q), E_{ZPE} = -1179.542041 , G_{tot} = -1179.57491
imaginary frequency(-1062.25 cm^{-1})
C 1.4411030526 0.5561055263 -0.6833318421
C 0.3629770526 1.0877145263 0.2760961579
C -1.0389969474 1.0189405263 -0.3673008421
C -1.3218269474 -0.4457724737 -0.7202598421
C -0.2605239474 -1.2388914737 -1.2085578421
C 1.0884950526 -0.9047884737 -0.9625308421
H 1.4950200526 1.1505505263 -1.6135568421
H 0.5843140526 2.0798295263 0.6801911579
H -2.3453949474 -0.7513074737 -0.9199758421
H -0.4918239474 -2.2322164737 -1.5962578421
H 1.8675430526 -1.5829434737 -1.2999518421
H -1.1018889474 1.6687325263 -1.2617068421
H 1.1438740526 -0.2672294737 2.2747241579
H 0.8375490526 0.4399005263 1.6238861579
H -1.7959189474 1.3955355263 0.3324231579
H 2.4306650526 0.6180895263 -0.2149808421
H -1.6979899474 -0.8555314737 2.0245511579
H -1.1975509474 -0.7917194737 2.6146261579
V 0.0003750526 -0.9449984737 1.0219131579

TS 3d/3b(Q), E_{ZPE} = -1179.559921 , G_{tot} = -1179.593277
imaginary frequency(-1246.75 cm^{-1})
C -0.1777092632 -0.6839512632 -1.3506758947
C 1.2164147368 -0.2253312632 -0.8778558947
C 1.2191227368 1.2328327368 -0.3783528947

C 0.0482317368 1.5195907368 0.5442971053
C -1.1260822632 0.7971837368 0.4628601053
C -1.1934472632 -0.5065622632 -0.2137418947
H -0.1348282632 -1.7344452632 -1.6611198947
H 1.5627577368 -0.9000072632 -0.0682118947
H 0.0561937368 2.4537557368 1.0995051053
H -1.9950822632 1.1340387368 1.0242571053
H -2.2105312632 -0.8215102632 -0.4512738947
H 2.1708767368 1.4610877368 0.1162791053
H -0.3733842632 -2.3584052632 1.3242321053
H -0.7638982632 -0.5027242632 3.2602651053
H -0.8981202632 -1.6638142632 0.5889171053
H 1.1615497368 1.9121667368 -1.2438088947
H -0.4838542632 -0.1010732632 -2.2299318947
H 1.9587877368 -0.3555722632 -1.6727258947
V -0.0369972632 -0.6572592632 1.7270861053

4a(D), E_{ZPE} = -1180. 7532 , G_{tot} = -1180. 787387
C 0.0237214762 -1.6492836190 -0.2450140000
C 1.3793924762 -1.1463976190 -0.7721180000
C 1.6540894762 0.2847223810 -0.2864250000
C 0.5819624762 1.2602003810 -0.8004960000
C -0.8343515238 0.7447563810 -0.5747710000
C -1.1073375238 -0.6551446190 -0.4945630000
H 0.1451994762 -1.8444346190 0.8431960000
H 2.1794704762 -1.8217076190 -0.4468740000
H 2.6456624762 0.6172343810 -0.6146710000
H 0.7177174762 2.2491213810 -0.3444370000
H -1.6204625238 1.3628113810 -1.0137010000
H -2.0444555238 -1.0401176190 -0.9054170000
H -3.0810525238 0.4180853810 1.7550430000
H -1.0085865238 1.8277733810 1.3248490000
H -1.1388795238 1.7183163810 2.1025990000
H 1.3684644762 -1.1635326190 -1.8704480000
H 1.6693404762 0.2937703810 0.8134700000
H 0.7261124762 1.4034083810 -1.8834460000
H -0.2382245238 -2.6203816190 -0.6779100000
H -0.5291885238 -0.3019276190 2.7095670000
V -1.4885945238 0.0627273810 1.3815670000

4a(Q), E_{ZPE} = -1180.756931 , G_{tot} = -1180.79313
C 0.0937343810 -1.7020755238 -0.3177599524
C 1.4771183810 -1.2714065238 -0.8360119524
C 1.7933013810 0.1802604762 -0.4452129524

C 0.7577923810 1.1484214762 -1.0425839524
C -0.6616436190 0.6517764762 -0.8543889524
C -0.9588406190 -0.6418745238 -0.5421709524
H 0.1415463810 -1.9350775238 0.7546880476
H 2.2465483810 -1.9480475238 -0.4483649524
H 2.7980083810 0.4599444762 -0.7814799524
H 0.8737263810 2.1524944762 -0.6126759524
H -1.4751616190 1.3187694762 -1.1574899524
H -2.0025486190 -0.9540945238 -0.5250919524
H -3.1451696190 0.7599024762 1.1651590476
H -2.3508006190 1.7838924762 2.8286820476
H -1.6721446190 1.6136234762 3.1603010476
H 1.4996123810 -1.3613405238 -1.9309079524
H 1.7872413810 0.2675194762 0.6494210476
H 0.9350093810 1.2700834762 -2.1224029524
H -0.2306146190 -2.6262735238 -0.8132079524
H -0.4676176190 -0.0123865238 2.5028790476
V -1.4390976190 0.8458884762 1.3686200476

4b(D), E_{ZPE} = -1180.738268, G_{tot} = -1180.771827
C -0.2034981905 -1.4769133810 0.0019722381
C 1.2924108095 -1.2534153810 -0.2217807619
C 1.6177628095 0.2508086190 -0.3952207619
C 0.6677548095 0.9449636190 -1.4013827619
C -0.7929991905 0.6042966190 -1.1071047619
C -1.1298001905 -0.7151123810 -0.7409207619
H -0.5010311905 -2.4591313810 0.3581952381
H 1.6199828095 -1.7983803810 -1.1201377619
H 2.6612338095 0.3826626190 -0.6999677619
H 0.8235358095 2.0293896190 -1.3683937619
H -1.5442391905 1.2181946190 -1.5959927619
H -2.1715301905 -1.0285133810 -0.7754797619
H -0.9902051905 -0.8204333810 2.2350542381
H -1.6743241905 1.7319326190 0.8803492381
H -2.0777451905 1.2332866190 1.4274042381
H 0.2038758095 1.3049466190 2.3904812381
H 1.8707488095 -1.6621193810 0.6148532381
H 1.5869528095 0.7706796190 0.5888422381
H 0.9270498095 0.6254976190 -2.4222747619
H -1.6651111905 -0.3171053810 2.2448662381
V -0.5208241905 0.4344656190 1.1066382381

4b(Q), E_{ZPE} = -1180.754551 , G_{tot} = -1180.789239
C -0.3854702381 -1.4779092857 -0.2172537619

C 1.1374177619 -1.4022182857 -0.3013377619
C 1.5989927619 0.0720077143 -0.3171177619
C 0.8650547619 0.9110917143 -1.3877067619
C -0.6442602381 0.7293817143 -1.2624547619
C -1.1468222381 -0.5522282857 -0.9582907619
H -0.8286302381 -2.4368242857 0.0369752381
H 1.5058147619 -1.9037552857 -1.2103197619
H 2.6846017619 0.1413937143 -0.4454857619
H 1.1350897619 1.9663377143 -1.2739447619
H -1.2822002381 1.4364367143 -1.7849227619
H -2.2133882381 -0.7397352857 -1.0862277619
H -0.3212892381 0.2085677143 2.9066662381
H -2.2895642381 1.2835357143 1.5939452381
H -2.5746372381 0.5781387143 1.4214822381
H -0.3904162381 2.0210057143 1.7492052381
H 1.5997337619 -1.9244262857 0.5448102381
H 1.4540537619 0.5397227143 0.6882162381
H 1.2155597619 0.6006387143 -2.3851137619
H -0.4587022381 -0.5273592857 2.6916352381
V -0.6609382381 0.4761977143 0.9972402381

4c(D), E_{ZPE} = -1180.746726, G_{tot} = -1180.778948
C -0.4295951905 -1.4164793810 -0.8996620952
C 0.9617038095 -1.2079343810 -0.6768850952
C 1.4598638095 0.1070706190 -0.6557530952
C 0.7086808095 1.1725626190 -1.4424560952
C -0.7406931905 1.0002586190 -1.0090160952
C -1.2934281905 -0.2929323810 -1.0403230952
H -0.8432311905 -2.4182603810 -0.8529760952
H 1.5859338095 -2.0530383810 -0.4011410952
H 2.5000038095 0.2725346190 -0.3913710952
H 1.0670488095 2.1658056190 -1.1632180952
H -1.4066451905 1.8579176190 -1.0196450952
H -2.3684561905 -0.4482483810 -1.0396150952
H -1.2444821905 -1.2918043810 1.6105919048
H -1.1789441905 1.2525106190 1.6584839048
H -1.6930241905 0.6207736190 1.7266519048
H 0.4058788095 1.5039726190 1.2721149048
H 1.2114318095 0.2745466190 2.0397929048
H 1.1036098095 -0.5231593810 2.1774869048
H 0.8403418095 1.0639366190 -2.5360430952
H -0.4844761905 -1.6026693810 1.7375749048
V -0.1615211905 -0.0373633810 0.9054079048

4c(Q), E_{ZPE} = -1180.754486, G_{tot} = -1180.789144

C 0.0002688095 -1.5928181905 -0.0296329048
C 1.4424478095 -1.1607321905 -0.2739259048
C 1.5206148095 0.3710598095 -0.4630179048
C 0.5157828095 0.8913928095 -1.5144729048
C -0.8869481905 0.3718508095 -1.2070019048
C -1.0276731905 -0.9549411905 -0.7535249048
H -0.1676071905 -2.5951981905 0.3536960952
H 1.8515648095 -1.6515711905 -1.1715389048
H 2.5417448095 0.6806248095 -0.7107069048
H 0.5301558095 1.9877958095 -1.5271279048
H -1.7219331905 0.8421738095 -1.7189509048
H -2.0222661905 -1.4021201905 -0.7532289048
H -1.8779191905 -0.2999611905 2.4089940952
H -0.8459881905 2.0381488095 1.9345750952
H -1.2145691905 2.1666508095 1.2604390952
H 0.0730318095 0.2507208095 2.6894940952
H 2.0794858095 -1.4584531905 0.5656520952
H 1.3572448095 0.8775348095 0.5202370952
H 0.8434208095 0.5683008095 -2.5154369048
H -2.3726441905 -0.2166301905 1.8116690952
V -0.6182141905 0.2861718095 1.0938100952

4d(D), E_{ZPE} = -1180.746518, G_{tot} = -1180.778764

C -0.4683122381 -1.3604408095 -0.9522839524
C 0.9323277619 -1.1992958095 -0.7350259524
C 1.4735067619 0.0928521905 -0.6528149524
C 0.7497457619 1.2389261905 -1.3466949524
C -0.7112072381 1.0739081905 -0.9421049524
C -1.2897822381 -0.2027148095 -1.0393409524
H -0.9129762381 -2.3492588095 -0.9720839524
H 1.5360847619 -2.0704658095 -0.4986389524
H 2.5215477619 0.2019981905 -0.3914159524
H 1.1336017619 2.1984781905 -0.9865389524
H -1.3626592381 1.9430361905 -0.9336379524
H -2.3696802381 -0.3251008095 -1.0391709524
H -0.8394342381 -1.6486898095 1.6252190476
H -0.0419542381 -1.6273108095 1.8890420476
H -1.5206672381 0.7919181905 1.7509000476
H -1.8358242381 0.0578581905 1.6602090476
H 0.9334147619 1.0962901905 1.5914940476
H 0.2532717619 1.5451831905 1.4254760476
H 1.0608087619 -0.5443378095 2.0643430476
H 0.8910777619 1.2319901905 -2.4443379524

V -0.1328902381 -0.1448238095 0.9274070476

4d(Q), E_{ZPE} = -1180.747111, G_{tot} = -1180.787932
C -0.7727422857 -0.9808118571 -1.1002588095
C 0.6107277143 -1.1205828571 -0.7734478095
C 1.4565237143 -0.0139538571 -0.7960588095
C 1.1016127143 1.1858801429 -1.6623778095
C -0.3884952857 1.4192061429 -1.4566138095
C -1.2510172857 0.3287871429 -1.4238448095
H -1.4448562857 -1.8295768571 -1.0656238095
H 0.9534687143 -2.0564828571 -0.3404218095
H 2.4701027143 -0.1167968571 -0.4183298095
H 1.6728387143 2.0647151429 -1.3465448095
H -0.7978182857 2.4155621429 -1.6000988095
H -2.3251342857 0.4889521429 -1.4972008095
H 0.5402257143 -3.7300638571 3.1860361905
H 0.4079347143 -3.0331318571 2.9579411905
H -2.1155202857 0.7613961429 1.4740421905
H -1.8229612857 0.2026051429 1.9342091905
H 0.4289337143 1.3354831429 2.1575431905
H 0.3152477143 1.9226921429 1.6553731905
H -0.0459532857 -0.5970378571 2.1373941905
H 1.3497697143 1.0200431429 -2.7292508095
V -0.3428872857 0.3331161429 0.7075331905

4e(D), E_{ZPE} = -1180.745007 , G_{tot} = -1180.777218
C -0.6063589048 -1.3745912857 -0.8014015714
C 0.8107530952 -1.2716302857 -0.7759605714
C 1.4105570952 0.0061657143 -0.6671535714
C 0.5950080952 1.2571397143 -0.8146815714
C -0.7715069048 1.0282377143 -1.4891555714
C -1.3888439048 -0.2043402857 -0.8299315714
H -1.0656759048 -2.3499962857 -0.6593445714
H 1.4289260952 -2.1620222857 -0.7451235714
H 2.4900690952 0.0892567143 -0.5951095714
H 0.3267010952 1.6711157143 0.2338784286
H -1.4065159048 1.9070187143 -1.3354375714
H -2.4703289048 -0.2964942857 -0.8174935714
H 0.3099160952 -1.7225432857 1.7711154286
H -0.2606599048 -1.3739602857 2.2817204286
H -1.3758449048 0.8015077143 1.4876854286
H -1.0611539048 0.5267897143 2.2398914286
H 1.5467780952 0.1571447143 1.9303944286
H 0.9827450952 0.4813877143 2.4162594286

H 1.1671700952 2.0952727143 -1.2253305714
H -0.6484119048 0.8924277143 -2.5750935714
V -0.0133229048 -0.1578862857 0.9702724286

4e(Q), E_{ZPE} = -1180.740312 , G_{tot} = -1180.775266
C -0.7147429524 -1.1782583333 -0.9058944762
C 0.6772430476 -1.2793713333 -0.6626884762
C 1.3627300476 -0.0466433333 -0.3720294762
C 0.9729240476 1.1671746667 -1.2268984762
C -0.5663329524 1.3541456667 -1.2672074762
C -1.3042389524 0.1095846667 -0.7650824762
H -1.3211029524 -2.0741423333 -1.0255624762
H 1.1692400476 -2.2488223333 -0.6277874762
H 2.4256550476 -0.1306163333 -0.1447894762
H 1.4588690476 2.0732196667 -0.8445294762
H -0.8646089524 2.2224396667 -0.6654464762
H -2.3916749524 0.1616986667 -0.8183684762
H 0.9110080476 -1.2864653333 2.5549245238
H 0.6537390476 -1.8947823333 2.1471345238
H -1.8820039524 -0.9731913333 2.0028135238
H -1.6472849524 -0.3805323333 2.4605435238
H 0.6955560476 1.0946546667 1.5035325238
H 0.1219470476 1.1458916667 2.0732775238
H 1.3530890476 1.0265866667 -2.2506024762
H -0.8840399524 1.5847136667 -2.2973744762
V -0.2259699524 -0.4472843333 1.1320355238

4f(D), E_{ZPE} = -1180.745789 , G_{tot} = -1180.777954
C -0.3392221905 -1.4054460476 -0.9359377619
C 1.0243858095 -1.1938200476 -0.6216857619
C 1.4868958095 0.1329699524 -0.4778147619
C 0.7840278095 1.2067189524 -1.3099257619
C -0.7096561905 1.0975039524 -0.9543487619
C -1.2288091905 -0.3075850476 -0.9846767619
H -0.7356631905 -2.4126430476 -0.9914677619
H 1.6472368095 -2.0463890476 -0.3670137619
H 2.5147788095 0.3040999524 -0.1774987619
H 1.1543458095 2.2002299524 -1.0424867619
H -0.7513951905 1.5188619524 0.1306282381
H -2.2915931905 -0.4746760476 -1.1197327619
H 0.5652428095 -1.2810310476 2.1945942381
H -1.2861391905 0.7773509524 2.1668432381
H -1.7073931905 0.1144209524 2.0407572381
H 0.9702178095 -0.6033670476 2.2938042381

H 0.5537978095 1.1632119524 1.6567002381
H 0.9422058095 1.0608679524 -2.3893257619
H -1.3702261905 1.8024569524 -1.4664377619
H -1.0081901905 -1.5156450476 1.4281602381
V -0.2148471905 -0.1380910476 0.9268652381

4f(Q), E_{ZPE} = -1180.735627 , G_{tot} = -1180.77081
C -0.6630912857 -1.2136831429 -0.9016888095
C 0.7801317143 -1.2385291429 -0.7584458095
C 1.4608237143 -0.0361211429 -0.6604948095
C 0.9194267143 1.2623818571 -1.2247858095
C -0.6294262857 1.2939688571 -1.3619368095
C -1.3109302857 0.0099998571 -0.9342208095
H -1.2207492857 -2.1427191429 -0.8529168095
H 1.2856017143 -2.1854391429 -0.6025938095
H 2.5214287143 -0.0561041429 -0.4196468095
H 1.2625457143 2.0995548571 -0.6106048095
H -1.0437402857 2.1330098571 -0.7958718095
H -2.3982612857 0.0238838571 -0.9046328095
H 1.0328607143 -0.8347681429 2.6492451905
H -1.5274282857 0.0130318571 2.4091011905
H -1.5388132857 -0.7700511429 2.4110931905
H 1.0610547143 -0.0530211429 2.6481781905
H -0.1302252857 1.2371898571 1.6621851905
H 1.3774577143 1.4030288571 -2.2167278095
H -0.9000482857 1.4729498571 -2.4146488095
H -0.2194692857 -2.0134441429 1.7194701905
V -0.1191482857 -0.4051191429 1.1599431905

4g(D), E_{ZPE} = -1180.724537 , G_{tot} = - 1180.757845
C -0.9866897619 -1.4937857619 -0.6242245238
C 0.5270502381 -1.3875697619 -0.5545465238
C 1.2535802381 -0.2649247619 -0.8968845238
C 0.5128802381 1.0586542381 -1.0583185238
C -0.7326797619 0.9706632381 -0.1380185238
C -1.6809507619 -0.1055497619 -0.6664765238
H -1.2535097619 -2.0928367619 -1.5083845238
H 1.0615672381 -2.3277467619 -0.4312945238
H 2.3127462381 -0.3301947619 -1.1295985238
H 0.2155932381 1.2178162381 -2.1088605238
H -1.2179477619 1.9355602381 0.0340554762
H -1.9923157619 0.1268012381 -1.6988135238
V 0.5827612381 0.1374002381 1.2087584762
H 0.1905702381 1.2994142381 2.5917254762

H -0.4239277619 0.7843862381 2.5932304762
H 2.2728902381 0.7204642381 1.0989054762
H 1.9559332381 1.2003612381 1.7198704762
H 0.1702452381 -1.1556667619 2.2048414762
H -1.3369857619 -2.0670357619 0.2424034762
H -2.5985427619 -0.1327757619 -0.0690375238
H 1.1677322381 1.9065652381 -0.8093325238

4g(Q), E_{ZPE} = -1180.733452 , G_{tot} = - 1180.768632
C -0.9165376190 -1.5185449048 -0.6932245714
C 0.5774773810 -1.3000229048 -0.7538445714
C 1.1763933810 -0.1138649048 -1.0484285714
C 0.3483853810 1.1573790952 -1.1769665714
C -0.8868516190 0.9715050952 -0.2563885714
C -1.7190136190 -0.1981869048 -0.7894445714
H -1.1876716190 -2.2112809048 -1.5055505714
H 1.2039693810 -2.1839549048 -0.6397865714
H 2.2536263810 -0.0809559048 -1.2061955714
H 0.0805763810 1.3314610952 -2.2355685714
H -1.4773396190 1.8912140952 -0.1810545714
H -2.0197386190 -0.0331179048 -1.8405265714
V 0.5459033810 0.3803820952 1.1906164286
H 0.0561993810 1.7749080952 2.5125274286
H 0.0005163810 1.1062660952 2.9003934286
H 2.1006053810 -0.2015109048 2.3052334286
H 2.4569973810 0.3605180952 1.9049414286
H 0.2476893810 -0.8160689048 2.3856864286
H -1.1527506190 -2.0479589048 0.2385114286
H -2.6477136190 -0.2991619048 -0.2170185714
H 0.9592773810 2.0309960952 -0.8939115714

4h(D), E_{ZPE} = -1180.718048 , G_{tot} = -1180.751824
C -0.0460838571 -1.3354431905 0.0035697619
C 1.4278751429 -1.1240341905 -0.3428802381
C 1.7220371429 0.2974308095 -0.9137052381
C 0.5553391429 1.2319838095 -0.5777552381
C -0.7218488571 0.6715088095 -1.2963692381
C -1.1056498571 -0.6083971905 -0.5551292381
H -0.2780758571 -2.2795521905 0.4964447619
H 2.0264881429 -1.2940351905 0.5632437619
H 2.6605321429 0.6769248095 -0.4952972381
H 0.7413951429 2.2835328095 -0.8118682381
H -1.5516618571 1.3868698095 -1.3201832381
H -2.1115138571 -1.0106231905 -0.6230382381

H -1.0903768571 -0.5760511905 2.7542377619
H -1.6465088571 -0.7384581905 2.2498107619
H -1.7606748571 1.5940218095 1.4038387619
H -2.0813838571 0.9314808095 1.0526997619
H 0.4177101429 0.6033348095 2.6793117619
H 1.7473591429 -1.9054581905 -1.0489462381
H -0.4741778571 0.4403328095 -2.3475422381
H 1.8703561429 0.2355378095 -2.0048342381
V -0.3011358571 0.5190938095 1.1343917619

4h(Q), E_{ZPE} = -1180.728976 , G_{tot} = -1180.763773
C -0.1426009524 -1.5295093333 -0.4315231905
C 1.2745890476 -1.0677363333 -0.1304731905
C 1.6089100476 0.2758066667 -0.8185791905
C 0.3702480476 1.1659346667 -0.6376181905
C -0.7355539524 0.6399056667 -1.5613881905
C -1.0497129524 -0.7722843333 -1.1032681905
H -0.4130519524 -2.5386873333 -0.1244541905
H 1.4145570476 -0.9468063333 0.9801628095
H 2.4928390476 0.7135676667 -0.3430741905
H 0.5806780476 2.2286206667 -0.7864631905
H -1.6448059524 1.2522666667 -1.5023361905
H -2.0233159524 -1.2067633333 -1.3279601905
H -0.7316299524 -0.5518523333 2.9767268095
H -1.2325649524 -0.9742113333 2.5668268095
H -1.3619909524 1.7192606667 1.9489228095
H -1.9130319524 1.4396136667 1.4749558095
H 0.4650410476 1.0370956667 2.5071418095
H 1.9828260476 -1.8737553333 -0.3590301905
H -0.4636859524 0.6146476667 -2.6379271905
H 1.8672210476 0.0866866667 -1.8771121905
V -0.3449639524 0.2881996667 1.1864708095

4i(D), E_{ZPE} = -1180.715994 , G_{tot} = -1180.74965
C -0.4326858571 -1.4355397143 -0.5155787619
C 0.9332641429 -1.2200047143 -0.7000377619
C 1.4552341429 0.0833512857 -1.3102427619
C 0.5522641429 1.1929652857 -0.7660047619
C -0.9128508571 0.9327192857 -1.1995377619
C -1.3545918571 -0.3500587143 -0.4767047619
H -0.7575228571 -2.4137337143 -0.1626417619
H 1.6160551429 -2.0558537143 -0.5915377619
H 2.4965101429 0.2375712857 -1.0109787619
H 0.8959881429 2.2208492857 -0.8851547619

H -1.5642918571 1.7721712857 -0.9368977619
H -2.4120058571 -0.5461937143 -0.3317907619
H -0.4462068571 -1.0530327143 2.7974152381
H -0.6788438571 1.3984962857 2.0466002381
H -1.2802008571 1.2282852857 1.5303212381
H 1.5591281429 -0.5133447143 1.4627082381
H 0.7436251429 0.7755922857 2.4155652381
H -0.9823618571 0.7923792857 -2.2932257619
H 1.4470821429 0.0165742857 -2.4144497619
H -1.0422878571 -1.2573197143 2.3860532381
V 0.1646991429 0.1941262857 0.9561202381

4i(Q), E_{ZPE} = -1180.728962 , G_{tot} = -1180.763745
C -0.4681039048 -1.4433567619 -0.4952497619
C 1.0352400952 -1.2187497619 -0.4635567619
C 1.4386080952 0.1254972381 -1.1134657619
C 0.4150180952 1.1609782381 -0.6226737619
C -0.9183479048 0.8878122381 -1.3304117619
C -1.3567009048 -0.5033597619 -0.9123327619
H -0.8303129048 -2.4290207619 -0.2068867619
H 1.5486240952 -2.0897897619 -0.8891977619
H 2.4556270952 0.3848842381 -0.8014727619
H 0.7579050952 2.1923992381 -0.7421667619
H -1.6904069048 1.6140532381 -1.0444867619
H -2.4116849048 -0.7717167619 -0.9594747619
H -0.2018169048 -0.7320187619 3.0179202381
H -0.6561209048 1.6905022381 2.3078882381
H -1.3302649048 1.5395962381 1.9478522381
H 1.4065320952 -1.2307157619 0.5992052381
H 1.1092610952 0.7095012381 2.4156842381
H -0.8683429048 0.9286792381 -2.4391147619
H 1.4546110952 0.0059252381 -2.2127387619
H -0.8353839048 -1.0382557619 2.6980262381
V -0.0539399048 0.2171552381 1.2466532381

4j(D), E_{ZPE} = -1180.751776 , G_{tot} = -1180.787781
C -0.4957369524 -1.5184024762 -0.6162798095
C 0.9494120476 -1.0007904762 -0.5017858095
C 1.0036810476 0.3680595238 0.1868391905
C 0.0443950476 1.4112015238 -0.3979298095
C -1.3875889524 0.8583495238 -0.5138628095
C -1.4198429524 -0.4790804762 -1.2693458095
H -0.8744629524 -1.7612064762 0.3869571905
H 1.5730200476 -1.7348074762 0.0270891905

H 0.0462500476 2.3313845238 0.2027191905
H -2.0281669524 1.5946755238 -1.0137618095
H -2.4463019524 -0.8624074762 -1.3135728095
H 1.3823480476 -0.9129944762 -1.5120608095
H 2.0509280476 0.7606435238 0.2001351905
H 0.3998270476 1.7070375238 -1.3989138095
H -0.5082699524 -2.4535744762 -1.1887678095
H -1.1021229524 -0.3149314762 -2.3096198095
H 2.5896210476 0.8728675238 2.5213121905
H -1.8032129524 0.7157225238 0.4940091905
H 0.9325800476 -1.1645304762 2.8764411905
H 0.0101700476 1.2669505238 2.9792571905
V 1.0834740476 0.3158335238 2.1611411905

4j(Q), E_{ZPE} =-1180.72453 , G_{tot} = -1180.761282
C -0.6640640952 -1.4642475238 -0.5413858095
C 0.8383799048 -1.1307375238 -0.4816748095
C 1.1245979048 0.2714674762 -0.0284288095
C 0.2300959048 1.3886034762 -0.4814728095
C -1.2593550952 0.9999664762 -0.5416448095
C -1.4639210952 -0.3535885238 -1.2390448095
H -1.0417350952 -1.5941275238 0.4805011905
H 1.3909729048 -1.8566785238 0.1267911905
H 0.3905369048 2.2867794762 0.1268441905
H -1.8178030952 1.7890704762 -1.0571638095
H -2.5292070952 -0.6108545238 -1.2479198095
H 1.2682249048 -1.2197585238 -1.4994628095
H 2.1749889048 0.5247914762 0.1582831905
H 0.5718629048 1.6633604762 -1.4993738095
H -0.8015240952 -2.4215965238 -1.0560598095
H -1.1512680952 -0.2782925238 -2.2912348095
H 1.5654959048 1.8469464762 2.7004721905
H -1.6559220952 0.9435884762 0.4798901905
H 2.2429289048 -0.9217705238 2.6981691905
H -0.4990880952 -0.1255005238 2.8141351905
V 1.0858029048 0.2625784762 2.3797801905

4k(D), E_{ZPE} = -1180.717899 , G_{tot} = -1180.750769
C -0.6635718571 -1.0638735714 -1.2367561429
C 0.8353111429 -1.1548095714 -0.8959761429
C 1.5418071429 0.0587764286 -0.7566541429
C 0.8795741429 1.2780774286 -0.5064521429
C -0.5684878571 1.4477964286 -0.9575051429
C -1.2540758571 0.1628604286 -0.5021071429

H -1.1831518571 -1.9940045714 -0.9784351429
H 1.3636871429 -2.0827605714 -1.0864721429
H 2.6198441429 0.0095624286 -0.6004591429
H 1.4801461429 2.1607644286 -0.3061981429
H -1.0163788571 2.3162894286 -0.4631501429
H -2.3435118571 0.1765944286 -0.4502691429
V 0.1188731429 -0.3004435714 0.9577128571
H -1.2881758571 0.5939934286 1.8124888571
H -1.0855358571 0.0394224286 2.3634738571
H 0.9098991429 0.9895524286 1.9518948571
H 0.9158341429 0.3510514286 2.4788038571
H 0.1517401429 -2.0265695714 1.4014338571
H 0.0058291429 -1.6553675714 2.1507338571
H -0.6402768571 1.6287924286 -2.0487411429
H -0.7793788571 -0.9357045714 -2.3273661429

4k(Q), E_{ZPE} = -1180.725464 , G_{tot} = -1180.760677
C -0.5005638095 -1.1469434762 -1.2869659524
C 0.9536971905 -1.0003884762 -0.8205839524
C 1.4800691905 0.3036075238 -0.6905159524
C 0.6519481905 1.4249415238 -0.5068759524
C -0.8103578095 1.3379115238 -0.9551209524
C -1.2942918095 -0.0610514762 -0.5401509524
H -0.8789438095 -2.1456594762 -1.0336239524
H 1.6439711905 -1.8327334762 -0.9337869524
H 2.5514761905 0.4155625238 -0.5181489524
H 1.1137991905 2.3970415238 -0.3521029524
H -1.4017418095 2.1176035238 -0.4575589524
H -2.3784378095 -0.1939044762 -0.5781489524
V 0.0880941905 -0.1226854762 1.0644800476
H -0.8377298095 1.1359395238 2.2634390476
H -1.3986888095 0.8226695238 1.8207610476
H 1.7847451905 -0.4436284762 2.1603020476
H 1.5746441905 0.2492155238 2.4231960476
H -0.1073238095 -2.0024954762 1.5357090476
H -0.7664208095 -1.7255484762 1.8391270476
H -0.8993858095 1.5344895238 -2.0426489524
H -0.5685588095 -1.0639434762 -2.3907809524

4l(D), E_{ZPE} = -1180.721111 , G_{tot} = - 1180.754956
C -0.2027978095 -1.5353115238 -0.6944474762
C 1.2637141905 -0.9877135238 -0.5554344762
C 1.2401611905 0.4461644762 0.0213735238
C 0.4258781905 1.3605174762 -0.9223444762

C -1.0405258095 0.8130574762 -1.0660844762
C -1.2119498095 -0.4670485238 -0.2165144762
H -0.3194828095 -2.4660465238 -0.1261564762
H 1.8628221905 -1.6541225238 0.0768885238
H 0.4145441905 2.3934894762 -0.5536864762
H -1.7660958095 1.5801014762 -0.7691254762
H -2.2442328095 -0.8339565238 -0.2091364762
H 0.1798461905 -1.1583775238 2.5809695238
H -0.1085018095 -0.5202575238 3.0983315238
H -0.8329848095 1.6683914762 2.1454125238
H -0.7091738095 1.1571344762 2.8402485238
H 1.7570391905 -0.9818245238 -1.5420274762
H 2.2436291905 0.8357424762 0.2252135238
H 0.9113351905 1.3977764762 -1.9120774762
H -0.4086268095 -1.7951095238 -1.7465684762
H -1.2548778095 0.5874154762 -2.1242924762
V -0.1997198095 0.1599774762 1.4494585238

4l(Q), E_{ZPE} = -1180.721777 , G_{tot} = -1180.756149
C -0.1036328095 -1.4204454762 -0.7856754286
C 1.3140431905 -0.8941224762 -0.4365084286
C 1.2780251905 0.6342235238 -0.2429264286
C 0.2486561905 1.3178305238 -1.1533244286
C -1.1816088095 0.8308885238 -0.7652114286
C -1.0640108095 -0.5041894762 -0.0033374286
H -0.2023518095 -2.4753714762 -0.5014854286
H 1.5955741905 -1.3844034762 0.5581845714
H 0.3294161905 2.4071135238 -1.0511144286
H -1.6816288095 1.5869345238 -0.1419474286
H -2.0438328095 -0.9624104762 0.1761785714
H -0.2471818095 -1.2591454762 2.9946925714
H -0.8015688095 -1.3067674762 2.4515165714
H -0.0878228095 1.7804605238 1.9834835714
H -0.4835598095 1.4189305238 2.5459775714
H 2.1119311905 -1.2757104762 -1.0876774286
H 2.2768841905 1.0829015238 -0.2933024286
H 0.4401051905 1.1059985238 -2.2194744286
H -0.2653498095 -1.3706194762 -1.8764044286
H -1.8082768095 0.7270115238 -1.6688914286
V 0.3761901905 -0.0391074762 1.5172475714

4m(D), E_{ZPE} = -1180.716258 , G_{tot} = -1180.750856
C 0.1151030476 -1.5378312857 -1.1593164286
C 1.0549390476 -0.5121002857 -0.5339494286

C 0.7280860476 0.8666707143 -0.4755664286
C -0.5306409524 1.4087937143 -1.1407894286
C -1.5269079524 0.3332387143 -1.4901414286
C -1.2402449524 -0.9739372857 -1.4983044286
H -0.0078029524 -2.4207432857 -0.5110964286
H -1.0158929524 2.1743547143 -0.5190174286
H 2.1114720476 -0.7909422857 -0.5004094286
H 1.5540340476 1.5745287143 -0.4017994286
H -0.2417949524 1.9373237143 -2.0650674286
H -2.0108099524 -1.6896342857 -1.7782124286
H 2.0602950476 0.0568247143 2.2121255714
H -2.5262039524 0.6622007143 -1.7689344286
H -0.9133229524 -0.7644152857 1.9913705714
H 0.1718520476 -0.7348312857 3.1984345714
H 0.1382610476 1.6198847143 1.5184235714
H 0.9527390476 -0.5169902857 3.2606745714
H -0.0208179524 1.4004247143 2.2688455714
H 0.5808950476 -1.9345642857 -2.0765904286
V 0.5667630476 -0.1582552857 1.4693205714

4m(Q), E_{ZPE} = -1180.719387 , G_{tot} = -1180.75422

C 0.2127070476 -1.4583422857 -1.3749903810
C 1.3134110476 -0.5328432857 -0.8933093810
C 1.0781720476 0.8044687143 -0.8184373810
C -0.2896549524 1.3409337143 -1.2170103810
C -1.3323779524 0.3650797143 -0.6859643810
C -1.0932059524 -0.9719642857 -0.7760823810
H 0.4155160476 -2.4875932857 -1.0789243810
H -0.4497499524 2.3472447143 -0.8208503810
H 2.2918020476 -0.9454822857 -0.6693373810
H 1.8706040476 1.4974927143 -0.5496043810
H -0.3661249524 1.4221347143 -2.3157383810
H -1.8413949524 -1.7009762857 -0.4807073810
H 1.3687900476 0.2490847143 2.4229876190
H -2.2953919524 0.7417717143 -0.3511773810
H 0.4352450476 -1.7906462857 1.3117696190
H -1.1109319524 -0.4163872857 2.7495276190
H 0.2838600476 1.6607987143 2.0370086190
H -0.4075589524 -0.3749332857 3.0762306190
H -0.3894169524 1.7946857143 1.6591966190
H 0.1537540476 -1.4284352857 -2.4786033810
V 0.1519470476 -0.1160912857 1.2540166190

4n(D), E_{ZPE} = -1180.716307 , G_{tot} = -1180.750968

C -0.2656340000 -1.2315553810 -0.2703131905
C 1.1629010000 -1.3202503810 -0.7978101905
C 1.6464510000 -0.0383763810 -1.4245071905
C 0.8486600000 0.9952546190 -1.7182091905
C -0.6361410000 1.0093076190 -1.4604771905
C -1.0950780000 -0.1126203810 -0.5380091905
H -0.7490520000 -2.1848443810 -0.0405451905
H 1.2165030000 -2.1296893810 -1.5446481905
H 2.7078520000 0.0211526190 -1.6573951905
H 1.2728940000 1.8792626190 -2.1905351905
H -0.9354480000 1.9941696190 -1.0748951905
H -2.1736160000 -0.2682713810 -0.5009501905
H -0.4533370000 -0.2621243810 3.3977068095
H -1.2014630000 1.4197936190 1.9092518095
H -1.4163360000 1.2615766190 1.1574138095
H 0.2249730000 0.1688096190 3.2742898095
H 1.0351200000 0.6725286190 1.9606798095
H 1.8669400000 -1.6299733810 -0.0083741905
H -1.1634870000 0.9120756190 -2.4246001905
H -1.5405790000 -0.9778343810 2.4169808095
V -0.3521230000 -0.1783913810 1.5349468095

4n(Q), E_{ZPE} = -1180.71768 , G_{tot} = -1180.753531
C -0.5307540000 -1.4552352857 -0.3954640952
C 0.9420500000 -1.4464282857 -0.7721680952
C 1.4420850000 -0.0179702857 -0.6288090952
C 0.6475440000 1.0116007143 -1.0184960952
C -0.7306120000 0.7200837143 -1.5894480952
C -1.3270370000 -0.4231582857 -0.7841900952
H -0.9480280000 -2.3154192857 0.1193289048
H 1.0749120000 -1.7956532857 -1.8121470952
H 2.4518970000 0.1631167143 -0.2723130952
H 1.0058880000 2.0361357143 -0.9801210952
H -1.3698640000 1.6062117143 -1.5515360952
H -2.3947130000 -0.4405982857 -0.5867280952
H 0.7464580000 -1.0611552857 2.2932269048
H -0.8471890000 2.1390097143 1.4577629048
H -1.4934380000 1.7969647143 1.1946179048
H 1.1709210000 -0.4235362857 2.4226109048
H 0.8697270000 1.4746657143 2.0814959048
H 1.5155010000 -2.1316342857 -0.1421540952
H -0.6521340000 0.4387437143 -2.6552420952
H -1.4013030000 -0.2286222857 2.3263599048
V -0.1719110000 0.3528787143 1.2934139048

4o(D), E_{ZPE} = -1180.740396 , G_{tot} = -1180.773462

C 0.0529038571 -1.5117775714 -0.3208552381
C 1.4764958571 -0.9678825714 -0.3047492381
C 1.4802548571 0.5696684286 -0.1882882381
C 0.5163578571 1.2381344286 -1.1889152381
C -0.8541291429 0.5725924286 -1.1567422381
C -0.9339691429 -0.8284235714 -1.0551812381
H -0.0743451429 -2.5738925714 -0.1338952381
H 1.9848298571 -1.2689085714 -1.2331552381
H 1.1870998571 0.8549544286 0.8407647619
H 0.4243138571 2.3046164286 -0.9626562381
H -1.6790581429 1.1132924286 -1.6109442381
H -1.8796441429 -1.3246475714 -1.2668142381
H -0.8983671429 0.2684324286 2.8156287619
H -1.2011421429 0.9584394286 2.5396167619
H -1.2809051429 1.5899984286 0.9104847619
H -2.5935181429 -0.6005205714 1.3194607619
H -0.1269601429 -1.0525645714 1.9701637619
H 2.0392028571 -1.4062935714 0.5248367619
H 2.4953948571 0.9647094286 -0.3043332381
H 0.9279578571 1.1594854286 -2.2064582381
V -1.0627731429 -0.0594125714 1.0120317619

4o(Q), E_{ZPE} = -1180.71187 , G_{tot} = -1180.749734

C 0.4194798095 -1.7148474762 -0.6736901905
C 1.7753118095 -1.0783614762 -0.7458451905
C 1.7337898095 0.4313165238 -0.4436331905
C 0.5911628095 1.1419055238 -1.1925001905
C -0.7198951905 0.4220835238 -1.0131871905
C -0.7502551905 -0.9617204762 -0.8041601905
H 0.3480448095 -2.7916074762 -0.5480991905
H 2.1856088095 -1.2499404762 -1.7561721905
H 1.5885438095 0.5678445238 0.6352368095
H 0.5001928095 2.1812505238 -0.8602551905
H -1.6460961905 0.9487835238 -1.2442731905
H -1.7124561905 -1.4691564762 -0.7699811905
H -1.7681231905 0.5030195238 3.2640138095
H -2.4768661905 0.6218235238 2.9814578095
H -1.3324561905 2.0957595238 1.3818878095
H -3.0001191905 -0.1820914762 1.1581078095
H -0.2771871905 -0.3699924762 2.3050808095
H 2.4649318095 -1.5863874762 -0.0606931905
H 2.6940638095 0.8926905238 -0.6961211905
H 0.8156218095 1.1819315238 -2.2719631905

V -1.4332971905 0.4156965238 1.3547898095

4p(D), E_{ZPE} = -1180.751319 , G_{tot} = -1180.783387
C -0.7394309524 -1.1279086667 -0.8566457619
C 0.7264150476 -1.3533106667 -1.2141747619
C 1.4629350476 -0.1558976667 -0.6208727619
C 0.9349570476 1.1298533333 -0.8356807619
C -0.4566299524 1.2956173333 -1.0840047619
C -1.2950459524 0.1455273333 -1.0734247619
H -1.4069079524 -1.9818016667 -0.7851567619
H 1.0867360476 -2.2811496667 -0.7579367619
H 2.5148450476 -0.2512126667 -0.3677227619
H 1.5465400476 2.0130333333 -0.6720017619
H -0.8835309524 1.6756933333 1.3706372381
H -2.3728469524 0.2832463333 -1.0884027619
V -0.1948819524 0.2318103333 0.8747562381
H -1.8337119524 0.3224603333 1.6857652381
H -1.6772619524 -0.4707226667 1.7552582381
H 0.6730260476 1.4291543333 1.9543962381
H 1.1386160476 0.7726013333 2.0575042381
H 0.0052200476 -1.4219956667 1.5363812381
H 0.7665510476 -1.0876336667 1.6155482381
H -0.8822559524 2.2855823333 -1.1896377619
H 0.8866630476 -1.4529466667 -2.3045847619

4p(Q), E_{ZPE} = -1180.712219 , G_{tot} = -1180.746419
C -0.7069589524 -1.1020705238 -0.7923108095
C 0.7253140476 -1.1159205238 -1.3203388095
C 1.4485110476 0.0476194762 -0.6556378095
C 0.8154320476 1.2679224762 -0.5679148095
C -0.5927159524 1.3985714762 -1.1244008095
C -1.3370979524 0.1472594762 -0.6695708095
H -1.2898009524 -2.0179465238 -0.8280148095
H 1.2225340476 -2.0628545238 -1.0888678095
H 2.4961400476 -0.0540345238 -0.3845128095
H 1.3534710476 2.1500354762 -0.2317898095
H -1.0781269524 2.3017084762 -0.7428818095
H -2.4166839524 0.1990784762 -0.5451878095
V -0.1089339524 -0.1162695238 1.1408441905
H -1.4963049524 0.7713904762 2.1358091905
H -1.6133599524 0.0255344762 2.3707921905
H 0.7552550476 0.9842384762 2.3671221905
H 1.0325860476 0.2472044762 2.5782061905
H 0.0614710476 -1.8947615238 1.1832611905

H 0.5547480476 -1.6618115238 1.8278151905
H -0.5736899524 1.4925464762 -2.2296778095
H 0.7482110476 -1.0074405238 -2.4227438095

4q(D), E_{ZPE} = -1180.731744 , G_{tot} = -1180.765514
C -1.1638615238 -0.2763754762 -0.6921135714
C -0.0028975238 -1.2630754762 -0.4894705714
C 1.1646124762 -0.6718784762 0.3170264286
C 1.5671254762 0.7435035238 -0.1159385714
C 0.3603874762 1.6883775238 -0.1717765714
C -0.7197615238 1.1318255238 -1.1074075714
H -1.8664125238 -0.6912814762 -1.4239475714
H 0.3473904762 -1.6610894762 -1.4536305714
H 2.0224774762 -1.3517314762 0.2612874286
H 2.0323094762 0.6885045238 -1.1105025714
H 0.6746314762 2.6833605238 -0.5062465714
H -0.3264255238 1.0885405238 -2.1331045714
V -0.9047385238 -1.0397774762 1.6853614286
H -1.2852315238 -2.6590214762 1.9499274286
H -1.3427095238 -0.1158824762 3.0451344286
H -1.8440715238 -0.1842254762 0.2147614286
H -1.5894965238 1.7983605238 -1.1326265714
H 2.3309514762 1.1326525238 0.5670454286
H -0.0560545238 1.8190745238 0.8387374286
H 0.9833864762 -0.6633544762 1.4405374286
H -0.3816115238 -2.1965064762 0.0169464286

4r(D), E_{ZPE} = -1180.730224 , G_{tot} = -1180.763066
C 0.2549739524 -1.6664736667 -0.5779321429
C 1.4919899524 -0.9163256667 -0.0305921429
C 1.1373719524 0.4721483333 0.4983108571
C 0.4904119524 1.3211983333 -0.6295171429
C -0.8815640476 0.6043623333 -0.8174871429
C -0.6748380476 -0.7771436667 -1.4384981429
H -0.3192840476 -2.0424406667 0.2785908571
H 1.9554419524 -1.5137666667 0.7625878571
H 1.9303069524 0.9710403333 1.0629128571
H 0.3969719524 2.3868973333 -0.3862621429
H -1.6651970476 1.2142143333 -1.2817731429
H -1.6394000476 -1.2805116667 -1.5758841429
H -1.8459030476 0.2974193333 2.6614088571
H -0.4766830476 -0.5562056667 2.1000548571
H -1.0343490476 2.3927143333 1.6215658571
H -2.0433430476 1.0564903333 2.5659028571

H 2.2444919524 -0.8211576667 -0.8333171429
H 1.0881349524 1.2612533333 -1.5487281429
H -0.2408910476 -0.6610016667 -2.4470441429
H 0.5716169524 -2.5429866667 -1.1566311429
V -0.7402600476 0.8002753333 1.1723318571

4r(Q), E_{ZPE} = -1180.703041 , G_{tot} = -1180.738029
C 0.2692182857 -1.6421206667 -0.5317011429
C 1.4751082857 -0.8755316667 0.0702668571
C 1.1514732857 0.5504043333 0.4083238571
C 0.4281972857 1.3498973333 -0.6392331429
C -0.8791467143 0.5859083333 -1.0150211429
C -0.5231977143 -0.8034486667 -1.5574041429
H -0.4030267143 -1.9332116667 0.2871018571
H 1.8784962857 -1.4045286667 0.9407268571
H 1.7381552857 1.0570733333 1.1738328571
H 0.2400972857 2.3764353333 -0.3016121429
H -1.5020747143 1.1606823333 -1.7077721429
H -1.4378947143 -1.3450366667 -1.8259291429
H -0.9386847143 0.3450543333 3.0878128571
H -2.0209767143 -0.6813016667 1.7057688571
H -1.5211617143 2.2331483333 1.5228688571
H -0.8122267143 1.0993403333 3.0347348571
H 2.2908982857 -0.8539246667 -0.6773601429
H 1.0837722857 1.4281463333 -1.5306761429
H 0.0685642857 -0.7191946667 -2.4870581429
H 0.6254872857 -2.5738266667 -0.9860361429
V -1.2110777143 0.6460353333 1.0283658571

4s(Q), E_{ZPE} = -1180.678195 , G_{tot} =- 1180.712856
C 0.1578569524 -1.2012352857 -0.4660349524
C 1.4920029524 -0.8112202857 0.1920450476
C 1.3861389524 0.6122177143 0.6903870476
C 0.8873029524 1.6827237143 -0.2531249524
C -0.4414920476 1.2051087143 -0.8702989524
C -0.1918890476 -0.1731342857 -1.5715049524
H 0.0770439524 -2.2471792857 -0.7626829524
H 1.7566339524 -1.4886512857 1.0120190476
H 0.7752139524 2.6371857143 0.2715320476
H -0.9533160476 1.9373747143 -1.4956899524
H -1.0692340476 -0.4913922857 -2.1471529524
H -1.2229300476 -1.3702502857 2.2340850476
H -2.9584060476 -0.2447372857 0.7252690476
H -2.7993150476 -0.5993492857 0.0648840476

H -1.4620910476 0.5264677143 2.2898300476
H 2.3309799524 -0.8631472857 -0.5392379524
H 1.9152339524 0.9012487143 1.5958460476
H 1.6657349524 1.8411147143 -1.0357849524
H -0.9961340476 -1.8193232857 1.6489400476
H 0.6475819524 -0.0800452857 -2.2888909524
V -0.9969170476 0.0462237143 0.7055660476

TS 4j/4q(D), E_{ZPE} = -1180.733442 , G_{tot} = -1180.767065
imaginary frequency(-862.82 cm^{-1})
C 0.1124772857 1.4649768095 -0.6806863333
C -1.3593087143 1.0254608095 -0.7117773333
C -1.4948707143 -0.4422171905 -1.1450703333
C -0.6919357143 -1.3719411905 -0.2227313333
C 0.7877992857 -0.9550921905 -0.1494653333
C 0.9617992857 0.5321178095 0.1858156667
H 0.2039272857 2.4946818095 -0.3150893333
H -1.7953387143 1.1528148095 0.2889826667
H -1.1366077143 -0.5526681905 -2.1790563333
H -1.1247037143 -1.3414961905 0.7867116667
H 1.3267442857 -1.2110951905 -1.0700053333
H 2.0372982857 0.8192998095 0.1339666667
H 2.9924352857 0.1961148095 2.6046466667
H 1.3061122857 -1.6156931905 0.6101376667
H 0.5631572857 1.0998568095 1.4552596667
H -1.9252267143 1.6771718095 -1.3872523333
H -2.5489547143 -0.7430371905 -1.1460123333
H -0.7635727143 -2.4123171905 -0.5594033333
H 0.5139442857 1.4524008095 -1.7047083333
H 0.5780172857 -1.0879901905 3.1605536667
V 1.4568072857 -0.1813481905 2.0451836667

TS 4a/4j(Q), E_{ZPE} = -1180.711711 , G_{tot} = -1180.746724
imaginary frequency(-1129.76 cm^{-1})
C 0.1713512857 -1.5662200952 -0.0932890476
C 1.4453482857 -1.0615630952 -0.8011610476
C 1.7219152857 0.4060809048 -0.4521040476
C 0.5643972857 1.3060479048 -0.9019120476
C -0.8064917143 0.8099349048 -0.3929860476
C -0.9954697143 -0.6156500952 -0.2543840476
H 0.4117332857 -1.7098480952 0.9755139524
H 2.2946502857 -1.6946070952 -0.5211000476
H 2.6515732857 0.7426979048 -0.9251800476
H 0.7314272857 2.3409549048 -0.5823360476

H -1.6583197143 1.3258069048 -0.8406270476
H -1.9684607143 -1.0338380952 -0.5144530476
H -3.1666597143 0.7916769048 1.3518779524
H -0.7194357143 1.3349219048 0.7951199524
H -0.5733767143 1.4345849048 1.9777659524
H 1.3182762857 -1.1596740952 -1.8877120476
H 1.8709402857 0.5051389048 0.6324549524
H 0.5191472857 1.3183539048 -1.9998710476
H -0.1172767143 -2.5601010952 -0.4529880476
H -1.9795197143 -1.0116580952 3.0760439524
V -1.7157497143 0.0969599048 1.8113269524

TS 4a/4j(D), E_{ZPE} = -1180.743685 , G_{tot} = -1180.777174
imaginary frequency(-1039.68 cm^{-1})
C 0.0010782857 -1.5608641429 -0.1441289524
C 1.3672802857 -1.1148241429 -0.6981809524
C 1.6642112857 0.3345028571 -0.2868239524
C 0.5893172857 1.2991308571 -0.8112169524
C -0.8359487143 0.8245488571 -0.4930439524
C -1.1302007143 -0.6017711429 -0.4798239524
H 0.1270972857 -1.6364171429 0.9675140476
H 2.1559042857 -1.7836051429 -0.3338409524
H 2.6480252857 0.6442968571 -0.6573369524
H 0.7579292857 2.3086158571 -0.4157739524
H -1.6064377143 1.4266128571 -0.9819469524
H -1.9836127143 -0.9757641429 -1.0444179524
H -3.0795047143 0.4598428571 1.7760410476
H -0.9275877143 1.4134218571 0.8243840476
H -1.0762697143 1.4684748571 1.9479830476
H 1.3540002857 -1.1944871429 -1.7935899524
H 1.7101832857 0.3941578571 0.8099550476
H 0.6729632857 1.3716348571 -1.9049919524
H -0.2583897143 -2.5745441429 -0.4643899524
H -0.6204067143 -0.4663161429 2.7564360476
V -1.5296317143 -0.0366471429 1.4271940476