Electronic Supplementary Information

Modeling the cysteamine catalyzed cysteine proteinases by DFT: Mechanistic insights into the hydrolysis of acetyl-p-nitroanilide

Christos E. Kefalidis,[a] *Athanassios C. Tsipis,*[b*] *Dimitrios N. Gkarmpounis,*[b] *Emmanouel M. Papamichael*[c] *and Leonidas G. Theodorou*[c]

[a] LPCNO, CNRS & INSA, Université Paul Sabatier, 135 Avenue de Rangueil, Toulouse 31077, France.

[b] Laboratory of Inorganic and General Chemistry, Department of Chemistry, University of Ioannina, 451 10 Ioannina, Greece. *E-mail: attsipis@uoi.gr*.

[c] Laboratory of Biochemistry, Department of Chemistry, University of Ioannina, 451 10 Ioannina, Greece

New Journal of Chemistry (NJC)

Table of Contents

Table S1. Selected structural parameters for all solvated stationary points in aqueous solution at T = 298 K calculated at the M06-2X/6-311+G(d,p) level.

Stationary point	$d(N_c\text{-}H)$	$d(N_c\cdots H)$	$d(N_a\text{-}H)$	$d(N_a\cdots H)$	$d(C\text{-}N)$	$d(C\text{-}O)$	$d(S\text{-}H)$	$d(S\cdots H_w)$	$d(O_w\cdots H)$	$d(O_a\cdots H)$
R1			1.013		1.369	1.224				
R2	1.016						1.345			
P1			1.007							
P2						1.192				
P3	1.017					1.212				
Im1-A		1.822	1.016		1.398	1.228		3.227	2.464	2.565
TS1_A	1.211	1.020	1.013		1.433	1.261	1.351		1.295	2.535
Im2-A	1.021	1.030	1.012	1.021	3.340	1.223		2.041	2.457	1.021
Im1-B	1.018	1.869			1.366	1.226	1.344			
TS1_B	1.018		1.018		1.312	1.295	2.737			0.978
Im2-B	1.018	1.981	1.012/1.028			1.215				
Im3a	1.017					1.212				
TS2a	1.017					1.248	2.044	2.846	1.022	
Im4a	1.017					1.217	1.346	2.386	1.666	
Im1-C	1.018		1.014		1.368	1.225	1.346			2.248
TS1_C	1.019		1.018		1.312	1.295	2.736			0.978
Im2-C	1.017	1.693	1.012		1.466	1.400	2.626			
Im3-C	1.017	1.944	1.031		1.460	1.410				
TS2_C	1.017	1.836	1.048		1.548	1.380				
Im4-C	1.017	1.980				1.212				
Im1-D	1.017	1.904	1.038		1.363	1.228	1.346			
TS1_D	1.018	2.595	1.019		1.308	1.297	3.082			
Im2-D	1.017	2.864	1.013		1.428	1.410	2.868			
Im3-D	1.016	1.992	1.025		1.452	1.409				
TS2_D	1.016	1.869	1.045		1.553	1.378				
Im4-D	1.018	2.037	1.024/1.011			1.210				

Table S1 Cartesian Coordinates and energies (in au) of all the species participating in the reaction mechanisms

R1

C,0,-0.3745464592,0.8674292386,0.0405808961
C,0,-1.4839844711,0.0088628864,0.0190046036
C,0,-1.3182109794,-1.3619571991,-0.0076440989
C,0,-0.0278991571,-1.8734171906,-0.0126861418
C,0,1.084146102,-1.0473970279,0.0086561076
C,0,0.9186989922,0.3297416016,0.0356269141
C,0,0.2587154352,3.2945387736,0.0706127116
N,0,-0.6387545397,2.2418761299,0.0682052409
H,0,-2.4855868915,0.4248176531,0.0230894319
H,0,-2.1647055238,-2.0346852885,-0.0245667232
N,0,0.1603189335,-3.3318434066,-0.0406423876
H,0,2.0733007485,-1.4853681572,0.0043398268
H,0,1.7761438048,0.9828892302,0.0532245325
O,0,1.2974445928,-3.7523233805,-0.0430962055
H,0,-1.6158547474,2.4933615839,0.0655725598
O,0,-0.8350473898,-4.025488029,-0.0594904288
C,0,-0.3984252372,4.6567566976,0.0321475833
O,0,1.4571593806,3.1476787935,0.0757983131
H,0,0.3024645322,5.3862051067,0.4310670421
H,0,-1.3286403387,4.6881495591,0.6011924216
H,0,-0.6163665769,4.9154575153,-1.0069809793

Sum of electronic and zero-point Energies= -644.529146
Sum of electronic and thermal Energies= -644.517646
Sum of electronic and thermal Enthalpies= -644.516702
Sum of electronic and thermal Free Energies= -644.567911

R2

C,0,-1.187593333,0.5070654021,-0.2954957207
C,0,0.1270029396,0.9482656962,0.3309960955
S,0,1.5145994764,-0.187258678,-0.0234507101
N,0,-1.5840497239,-0.8015919305,0.2192374603
H,0,-1.0906793868,0.5356001652,-1.3889435829
H,0,-1.957047647,1.2306736612,-0.010495664
H,0,0.0214071947,1.0402231949,1.4119121273
H,0,0.4373456642,1.9138670079,-0.0709883839
H,0,1.1288765504,-1.1510411501,0.828237096
H,0,-2.5576460868,-0.9909015519,0.0150870179
H,0,-1.0391035779,-1.5314608269,-0.2276787854

Sum of electronic and zero-point Energies= -533.232206
Sum of electronic and thermal Energies= -533.226634
Sum of electronic and thermal Enthalpies= -533.225690
Sum of electronic and thermal Free Energies= -533.260764

Im1_A

H,0,-3.7862120628,-0.5572980399,-1.5584541608
H,0,-1.7563376227,-0.8004246882,-0.4316837581
N,0,-0.3010503888,1.3458941988,-0.2539998254
C,0,-0.5612590194,2.352841125,-1.1612324473
O,0,0.2394207631,2.7556847644,-1.9747921362
C,0,-1.9609219463,2.9151431628,-1.0372501233
H,0,-2.0953041716,3.36993694,-0.052415496
H,0,-2.0961841571,3.6726165147,-1.8054047953
H,0,-2.7043814338,2.123152554,-1.1545807347
H,0,-1.0670036985,1.1017464377,0.3809936836
C,0,0.8989917195,0.6620878495,-0.051409055
C,0,0.9227415498,-0.2666225442,1.0023332815
C,0,2.0484210189,0.8504594232,-0.8320795874
C,0,2.0625107927,-0.9935305804,1.2819679365
H,0,0.0287530338,-0.4111270137,1.5980675629
C,0,3.1931050368,0.1197387687,-0.5501270465
H,0,2.0379652057,1.560856395,-1.6431801993
C,0,3.1892763466,-0.788839712,0.4967265943
H,0,2.0932955788,-1.7108456962,2.090622005
H,0,4.0917262052,0.2493693127,-1.138219656
N,0,4.408478052,-1.554984584,0.7870766793
O,0,5.3724075991,-1.375108073,0.0725732961
O,0,4.3800981994,-2.3239151261,1.7264361068
S,0,-2.1425081754,-2.0747258848,-0.2526332539
C,0,-3.3847927196,-1.7318186574,1.048734463
H,0,-4.322069637,-1.4215449232,0.5843009835
H,0,-3.5487078923,-2.6896673761,1.54281911
C,0,-2.9523032365,-0.6952907425,2.0726009186
H,0,-3.7379772524,-0.6427247138,2.8368619537
H,0,-2.0318508363,-1.0191935427,2.5663018812
N,0,-2.7163596726,0.6075773638,1.4323408106
H,0,-3.4867767176,0.8196525775,0.7984411136
H,0,-2.6964492017,1.3391991971,2.1361799756
O,0,-4.2142521134,0.2611369284,-1.2763121596
H,0,-4.8474155524,0.4809069081,-1.9639989661

Sum of electronic and zero-point Energies= -1254.185517
Sum of electronic and thermal Energies= -1254.164701
Sum of electronic and thermal Enthalpies= -1254.163757
Sum of electronic and thermal Free Energies= -1254.237071

TS1_A

H,0,-3.3019369186,-0.0051125686,-1.2715502987
H,0,-1.3128837696,-0.6516794603,-0.9830982659
N,0,-0.975452859,0.1458013405,-0.4152914945
C,0,-1.2689759225,1.4689453756,-1.2786962393
O,0,-0.8464502623,1.4377103582,-2.4078892515
C,0,-1.1954920181,2.6650578494,-0.3597369975
H,0,-0.1431690785,2.8793783042,-0.1574946034
H,0,-1.6317185531,3.5175821336,-0.8781791372
H,0,-1.7304538456,2.4933903451,0.5737912757
H,0,-1.6233307228,0.140827136,0.433362159
C,0,0.41352416,0.02591675,-0.0626389803
C,0,0.7947706125,0.2227104778,1.2607482676
C,0,1.3499019984,-0.2500067724,-1.0552194919
C,0,2.1348325427,0.1341867881,1.608366216
H,0,0.0435865733,0.4371357568,2.0121549377
C,0,2.69135875,-0.3381699259,-0.7144702252
H,0,1.0221068183,-0.3745906689,-2.0797306828
C,0,3.0545588602,-0.1461630802,0.610306966
H,0,2.4721177845,0.2751233771,2.6259961329
H,0,3.4515624733,-0.5491120849,-1.4542778233
N,0,4.4851294756,-0.2428116964,0.9749626126
O,0,5.269068144,-0.5033223738,0.0903704635
O,0,4.7780560556,-0.0547558222,2.135264284
S,0,-3.4670105407,-1.6566321009,-1.2214327911
C,0,-4.2231897346,-1.7938367081,0.4390429669
H,0,-5.1330989796,-1.185758262,0.4702264564
H,0,-4.532067338,-2.8326416305,0.5659334313
C,0,-3.3334572391,-1.4209415096,1.6166650996
H,0,-3.8735760617,-1.6363110339,2.5459428826
H,0,-2.4294818829,-2.0377309928,1.6026132228
N,0,-2.9240995596,0.0033296648,1.5691862208
H,0,-3.6673942501,0.5633670741,1.1548428493
H,0,-2.7767531859,0.3586536632,2.5083879743
O,0,-3.0381441689,1.1670330646,-1.2420334437
H,0,-3.3165383573,1.517889232,-2.0972196927

Sum of electronic and zero-point Energies=	-1254.117870
Sum of electronic and thermal Energies=	-1254.098898
Sum of electronic and thermal Enthalpies=	-1254.097954
Sum of electronic and thermal Free Energies=	-1254.166911

Im2_A

H,0,-2.6034781056,-0.3952547664,-0.3769053814
H,0,-0.7588019417,-1.3680914002,-1.4293961773
N,0,-0.4565107128,-1.6167746132,-0.4970995148

C,0,-1.1419546939,1.8010080285,-2.1339721739
O,0,-1.2802303547,0.6204461255,-2.3532752056
C,0,0.0461821686,2.6223395403,-2.5404838573
H,0,0.6784037274,2.0482737535,-3.2131043688
H,0,-0.2849755098,3.5450202567,-3.017112961
H,0,0.608114219,2.8909523341,-1.6431440044
H,0,-1.1911877703,-1.9156795561,0.1370909822
C,0,0.548159938,-0.8551278947,0.0337798209
C,0,0.8033837641,-0.8631685195,1.4191728701
C,0,1.3804092304,-0.0812931112,-0.7997852893
C,0,1.8319502121,-0.1127723561,1.9537639818
H,0,0.1916747692,-1.4828114423,2.064338342
C,0,2.4094607942,0.6684925456,-0.2675341563
H,0,1.1993331388,-0.0866294108,-1.8676581791
C,0,2.6243217735,0.6545758052,1.1072866765
H,0,2.0359925686,-0.1122646367,3.0162011704
H,0,3.0541443017,1.2664357707,-0.8988358507
N,0,3.7061606109,1.4560351265,1.671248705
O,0,4.3690520498,2.1325873092,0.9087688424
O,0,3.8831436944,1.4071344233,2.8732292056
S,0,-3.8924434812,-0.0610755123,-0.5398604627
C,0,-4.3733142369,-0.2615538513,1.2090198027
H,0,-3.8848973071,0.5055224502,1.814173143
H,0,-5.4470159855,-0.0740295473,1.2389983521
C,0,-4.0740840893,-1.6499854013,1.7551996166
H,0,-4.5582554275,-1.7437623443,2.7362647396
H,0,-4.5094623276,-2.4004517766,1.092215367
N,0,-2.6253517746,-1.8822134138,1.8197820747
H,0,-2.2087746847,-1.2438453303,2.4931691013
H,0,-2.4408295319,-2.8202452891,2.1617820197
O,0,-2.0496404455,2.5249269649,-1.4755050608
H,0,-2.7773867361,1.9371613288,-1.1969249453

Sum of electronic and zero-point Energies= -1254.186086
Sum of electronic and thermal Energies= -1254.164997
Sum of electronic and thermal Enthalpies= -1254.164053
Sum of electronic and thermal Free Energies= -1254.240295

P1

C,0,0.,-0.0724416053,-2.0547325262
C,0,-1.2100995597,-0.0515755671,-1.3423350007
C,0,-1.2120967882,-0.0158975784,0.038763001
C,0,0.,0.0014428489,0.7172146265
C,0,1.2120967882,-0.0158975784,0.038763001
C,0,1.2100995597,-0.0515755671,-1.3423350007
H,0,-2.1488101324,-0.0604879396,-1.8842479157
H,0,-2.1368417129,-0.0014527205,0.5997343197
H,0,2.1368417129,-0.0014527205,0.5997343197

H,0,2.1488101324,-0.0604879396,-1.8842479157
N,0,0.,0.036968588,2.1811627053
O,0,1.0750181194,0.0502477558,2.7460755427
O,0,-1.0750181194,0.0502477558,2.7460755427
N,0,0.,-0.0623748086,-3.4320257785
H,0,0.8465471344,-0.3440359809,-3.8994197156
H,0,-0.8465471344,-0.3440359809,-3.8994197156

Sum of electronic and zero-point Energies=	-491.927124
Sum of electronic and thermal Energies=	-491.918855
Sum of electronic and thermal Enthalpies=	-491.917910
Sum of electronic and thermal Free Energies=	-491.960542

P2

C,0,-0.0041981099,0.1483934664,0.0590029068
O,0,0.1659003346,1.309175966,0.3058937598
O,0,-1.2268103073,-0.3644049274,-0.193105652
H,0,-1.8609701869,0.3625626462,-0.1337815494
C,0,1.061356501,-0.9055486214,-0.0169774778
H,0,0.8308293528,-1.709973118,0.6825144961
H,0,1.075029661,-1.3332562373,-1.0204796492
H,0,2.0251887547,-0.4623441746,0.2169331657

Sum of electronic and zero-point Energies=	-229.002486
Sum of electronic and thermal Energies=	-228.998739
Sum of electronic and thermal Enthalpies=	-228.997794
Sum of electronic and thermal Free Energies=	-229.028495

Im1_B

C,0,-3.1297197959,2.6127300996,0.1582808456
C,0,-3.8884034729,1.761451832,1.164760577
S,0,-2.8562448019,0.5745902886,2.0884063191
N,0,-2.6809914353,1.8025678247,-0.983854997
H,0,-3.4866032165,1.5228410275,-1.5384160953
H,0,-3.7749984291,3.4438245355,-0.1542401186
H,0,-2.2478105381,3.0400848339,0.6402886274
H,0,-4.3208819119,2.404300474,1.9327672658
H,0,-2.100688667,2.3650894436,-1.6000337196
H,0,-4.7151595928,1.2342715036,0.6821571165
C,0,-1.3499499787,-1.7403254022,-1.5261086894
O,0,-0.7013633011,-2.7418976689,-1.7264526541
C,0,-2.7998473467,-1.6155791472,-1.9510725449
H,0,-2.8493505044,-1.0789920444,-2.9021738371
H,0,-3.2056105272,-2.614507248,-2.0922763749
H,0,-3.394464727,-1.0707235491,-1.2150789277
H,0,-2.5442797096,-0.2246612194,1.0563139007

H,0,-1.5035963948,0.1870831772,-0.8420220134
N,0,-0.8615317457,-0.6070202355,-0.9156107276
C,0,0.4327999188,-0.3756304702,-0.4418193321
C,0,0.6338999222,0.8136160245,0.2774863349
C,0,1.5083405337,-1.2485801673,-0.654141686
C,0,1.8845580439,1.1428573936,0.7620306655
H,0,-0.2110967761,1.4659081982,0.4683089955
C,0,2.7626732007,-0.9190291433,-0.1625605081
H,0,1.3564097094,-2.1695561837,-1.1939805021
C,0,2.9379981054,0.2679572744,0.5312467552
H,0,2.0551763711,2.0544002268,1.3183624385
H,0,3.6081575668,-1.5759532697,-0.3164742078
N,0,4.2725690322,0.6113843173,1.0418171429
O,0,5.1743944822,-0.1737562977,0.8379150697
O,0,4.394145986,1.6632815717,1.6357808814

Sum of electronic and zero-point Energies= -1177.775460
Sum of electronic and thermal Energies= -1177.756723
Sum of electronic and thermal Enthalpies= -1177.755779
Sum of electronic and thermal Free Energies= -1177.826961

TS1_B

C,0,-3.4707067717,1.9776706748,0.7767591825
C,0,-4.3498288704,0.7441923412,0.5965262988
S,0,-3.5659533512,-0.8795945074,0.905531594
N,0,-2.4963189179,2.1341376655,-0.3356857399
H,0,-3.0128952914,2.2410385989,-1.2058692326
H,0,-4.1028688509,2.8713254965,0.8510590426
H,0,-2.9040123862,1.8874153379,1.706951234
H,0,-5.1922748223,0.8430018553,1.2851139773
H,0,-1.9832405841,3.0033625006,-0.2134042062
H,0,-4.7811179219,0.7658744629,-0.4139783608
C,0,-1.4925561062,-1.344431353,-0.8810380179
O,0,-1.060334125,-2.4194664529,-0.6261585241
C,0,-2.2002765758,-0.9026680864,-2.1227168172
H,0,-1.4429169193,-0.580056493,-2.8481371236
H,0,-2.7414857759,-1.7557889544,-2.5255128089
H,0,-2.889000297,-0.0879674888,-1.9162923301
H,0,-1.4622988266,-0.3912274943,0.8854962468
H,0,-1.4362126622,0.7398210366,-0.2933105528
N,0,-0.9538684839,-0.1692971626,-0.0153310078
C,0,0.4831170242,-0.0706236619,0.0387642653
C,0,1.1162115182,0.9303936324,-0.690924121
C,0,1.2046501001,-0.9837332982,0.8010119485
C,0,2.4994277603,1.031637796,-0.6567861802
H,0,0.5280749269,1.6251805308,-1.27990602
C,0,2.5880671765,-0.8895616018,0.8373130092
H,0,0.6834727282,-1.7609420464,1.3454820979

C,0,3.2046261978,0.1169417848,0.109108875
H,0,3.030940937,1.7969565428,-1.2056326052
H,0,3.1884606226,-1.5777274264,1.4166138608
N,0,4.6803731124,0.2223678481,0.1518402441
O,0,5.2772958409,-0.5895189208,0.8217343024
O,0,5.1930325949,1.1147308431,-0.4868185308

Sum of electronic and zero-point Energies=	-1177.705612
Sum of electronic and thermal Energies=	-1177.688444
Sum of electronic and thermal Enthalpies=	-1177.687499
Sum of electronic and thermal Free Energies=	-1177.752961

Im2_B

C	-3.92228	1.96007	-0.17819
C	-4.12321	0.56064	-0.74778
S	-3.7461	-0.77293	0.43883
N	-2.50638	2.24656	0.06648
H	-2.00428	2.30645	-0.81555
H	-4.38639	2.67402	-0.87177
H	-4.45085	2.03828	0.7745
H	-5.17299	0.42584	-1.01304
H	-2.41082	3.15684	0.50663
H	-3.54319	0.41983	-1.66063
C	-2.13205	-1.43658	0.00013
O	-1.6797	-2.26531	0.74171
C	-1.43385	-0.9698	-1.25085
H	-0.47233	-1.47888	-1.30542
H	-2.03226	-1.20743	-2.13308
H	-1.26589	0.10763	-1.21273
H	-1.02672	-0.37914	2.32083
H	-1.39969	1.09083	1.56679
N	-0.67022	0.47942	1.92514
C	0.42819	0.34762	1.1126
C	0.83316	1.42317	0.29776
C	1.1813	-0.84082	1.08629
C	1.92142	1.30289	-0.54359
H	0.28446	2.35606	0.34855
C	2.27608	-0.96093	0.25255
H	0.8728	-1.6773	1.70212
C	2.6304	0.10657	-0.56606
H	2.2383	2.12068	-1.17706
H	2.85441	-1.8746	0.2149
N	3.77521	-0.02743	-1.46427
O	4.38931	-1.07568	-1.44998
O	4.04701	0.91662	-2.18112

Sum of electronic and zero-point Energies=	-1177.765733
Sum of electronic and thermal Energies=	-1177.747480

Sum of electronic and thermal Enthalpies= -1177.746535
Sum of electronic and thermal Free Energies= -1177.813617

P1+P3

C	-3.92228	1.96007	-0.17819
C	-4.12321	0.56064	-0.74778
S	-3.7461	-0.77293	0.43883
N	-2.50638	2.24656	0.06648
H	-2.00428	2.30645	-0.81555
H	-4.38639	2.67402	-0.87177
H	-4.45085	2.03828	0.7745
H	-5.17299	0.42584	-1.01304
H	-2.41082	3.15684	0.50663
H	-3.54319	0.41983	-1.66063
C	-2.13205	-1.43658	0.00013
O	-1.6797	-2.26531	0.74171
C	-1.43385	-0.9698	-1.25085
H	-0.47233	-1.47888	-1.30542
H	-2.03226	-1.20743	-2.13308
H	-1.26589	0.10763	-1.21273
H	-1.02672	-0.37914	2.32083
H	-1.39969	1.09083	1.56679
N	-0.67022	0.47942	1.92514
C	0.42819	0.34762	1.1126
C	0.83316	1.42317	0.29776
C	1.1813	-0.84082	1.08629
C	1.92142	1.30289	-0.54359
H	0.28446	2.35606	0.34855
C	2.27608	-0.96093	0.25255
H	0.8728	-1.6773	1.70212
C	2.6304	0.10657	-0.56606
H	2.2383	2.12068	-1.17706
H	2.85441	-1.8746	0.2149
N	3.77521	-0.02743	-1.46427
O	4.38931	-1.07568	-1.44998
O	4.04701	0.91662	-2.18112

Sum of electronic and zero-point Energies= -1177.765733
Sum of electronic and thermal Energies= -1177.747480
Sum of electronic and thermal Enthalpies= -1177.746535
Sum of electronic and thermal Free Energies= -1177.813617

Im1_C

C,0,0.0934501799,-1.2603749044,0.177475422
C,0,0.8020056039,-1.2996892331,-1.0303255372
C,0,1.9403200779,-0.534209447,-1.2006713254

C,0,2.3543995942,0.2782840637,-0.1531742937
C,0,1.6716191475,0.332585817,1.0510237877
C,0,0.5388952965,-0.4490090851,1.2238008796
C,0,-2.1854492758,-1.7637635042,1.006005306
N,0,-1.0452870097,-2.0734152728,0.2989568585
H,0,0.4432025368,-1.9211468972,-1.8430513621
H,0,2.4987938832,-0.5443132056,-2.1266239236
N,0,3.5566427012,1.110119204,-0.3343341008
H,0,2.0213822212,0.9856902604,1.8386440496
H,0,-0.00614907,-0.413279411,2.1545868443
O,0,3.9264460297,1.7767632234,0.6073301066
H,0,-1.1466692935,-2.7876265191,-0.4073372144
O,0,4.1030094746,1.0763598165,-1.4173776404
S,0,-2.8364557041,0.3941060815,-1.5661770945
C,0,-3.3407953737,-2.7052362016,0.763049463
H,0,-3.8803070682,-2.3704895638,-0.1278352818
H,0,-3.0121307814,-3.7329707604,0.6042246093
H,0,-4.0141057233,-2.6575253076,1.6157585324
O,0,-2.2719126213,-0.8007416819,1.7380588374
H,0,-3.2989283048,0.4857926222,-0.3071899146
C,0,-2.0343190584,2.0355815631,-1.6079701471
H,0,-2.8038350969,2.7993175394,-1.4776486853
H,0,-1.6410412043,2.1281429433,-2.6225398408
C,0,-0.9079520059,2.2114539631,-0.5864097893
H,0,-0.1420404827,1.454281422,-0.7724345116
H,0,-0.4440854246,3.186667898,-0.7703589966
N,0,-1.2827595768,2.1446006362,0.8144484467
H,0,-2.005495934,2.8177888215,1.0434972198
H,0,-1.6018866238,1.2200653915,1.0894491243

Sum of electronic and zero-point Energies= -1177.774406
Sum of electronic and thermal Energies= -1177.756541
Sum of electronic and thermal Enthalpies= -1177.755596
Sum of electronic and thermal Free Energies= -1177.822605

Im2_C

C,0,0.388933595,-0.5362317134,-0.2907214458
C,0,1.2871466109,-0.8594585595,-1.325590808
C,0,2.639297247,-0.992240556,-1.0833508709
C,0,3.1097135862,-0.805393853,0.21051593
C,0,2.2499100565,-0.4873418384,1.2519278338
C,0,0.8940103332,-0.3479036137,1.007891862
C,0,-2.0449332902,-0.5540730969,0.3471999734
N,0,-0.9521867259,-0.3740920702,-0.6209712215
H,0,0.9072021742,-1.004785883,-2.3311596456
H,0,3.3324407239,-1.2420132473,-1.8752145763
N,0,4.5421208946,-0.9499060165,0.4781238678
H,0,2.6513099552,-0.3482282727,2.2469229531

H,0,0.2244351285,-0.0809480108,1.8116909552
O,0,4.9249860924,-0.785884872,1.6189285445
H,0,-1.1819157622,-0.7770124484,-1.5202234698
O,0,5.2668249981,-1.2266889828,-0.4570206034
S,0,-3.6216578733,-0.3090524751,-0.5983109161
C,0,-2.0942278834,-1.9695959623,0.9131365123
H,0,-2.9559071525,-2.0706305695,1.5738329454
H,0,-2.1538695035,-2.7082293443,0.1133194001
H,0,-1.1884260527,-2.1431406808,1.497257406
O,0,-1.9206188932,0.3254025678,1.4095742682
H,0,-2.4128780918,1.1623838098,1.2298242337
C,0,-3.2882714269,1.1999968383,-1.578713976
H,0,-4.278795264,1.4675852577,-1.9567621471
H,0,-2.6679592703,0.9544501818,-2.4414934821
C,0,-2.6626598026,2.3833861303,-0.8431708526
H,0,-1.5921211581,2.2012365347,-0.7251088789
H,0,-2.7867169775,3.2677230528,-1.4798013252
N,0,-3.2322688399,2.5617762919,0.4968580239
H,0,-2.9715199126,3.4614981006,0.8847556829
H,0,-4.2461725396,2.5115010889,0.480944618

Sum of electronic and zero-point Energies=	-1177.760857
Sum of electronic and thermal Energies=	-1177.744169
Sum of electronic and thermal Enthalpies=	-1177.743225
Sum of electronic and thermal Free Energies=	-1177.805885

Im3_C

C,0,-0.3702904834,0.609636441,0.336922028
C,0,-0.6560485415,-0.6724285293,0.8217160183
C,0,-1.889710233,-1.2606321946,0.5949378626
C,0,-2.8329040876,-0.5573554781,-0.1389753326
C,0,-2.5838969108,0.7155077278,-0.6332305222
C,0,-1.3533836346,1.2999546989,-0.3819080425
C,0,1.8955923559,1.2760425762,-0.4078496507
N,0,0.8765217068,1.2040743872,0.6318031589
H,0,0.1132502911,-1.2059633419,1.3677843723
H,0,-2.1243058676,-2.2512401666,0.9600047535
N,0,-4.1443897018,-1.1760975657,-0.3929242453
H,0,-3.3566908828,1.2351277868,-1.1834430887
H,0,-1.1565840292,2.3090025086,-0.7187516987
O,0,-4.9426849663,-0.5512132059,-1.0591651417
H,0,1.3157522482,0.6994211173,1.4085786614
O,0,-4.348865571,-2.2746812781,0.0792133879
O,0,2.9922177178,1.9519947402,0.1569199059
H,0,2.6286406637,2.7279563028,0.6000420262
S,0,2.5232385972,-0.3926174915,-0.964445585
C,0,3.8192423546,-0.8022319797,0.2454923486
H,0,4.4317794886,0.0880019622,0.4005738681

H,0,4.4333677187,-1.5399826909,-0.2748141398
C,0,3.3557663237,-1.3856384956,1.5726001111
H,0,4.2293257197,-1.8339641384,2.0658318292
H,0,2.6343950265,-2.1857881494,1.3877727549
N,0,2.7107130972,-0.3641236977,2.4048287319
H,0,2.4691494222,-0.7444228446,3.313817474
H,0,3.3580479791,0.4029790616,2.5664287105
C,0,1.4104614566,1.9735699377,-1.6693122213
H,0,0.6558053173,1.3847788848,-2.1929420463
H,0,0.9845311318,2.9445867215,-1.4040403887
H,0,2.2640843371,2.1223638172,-2.3283012996

Sum of electronic and zero-point Energies=	-1177.754483
Sum of electronic and thermal Energies=	-1177.737659
Sum of electronic and thermal Enthalpies=	-1177.736715
Sum of electronic and thermal Free Energies=	-1177.800273

Im4_C

C,0,-0.6552127036,0.7348114119,0.9513891495
C,0,-0.7799008361,-0.6597816266,0.7902451608
C,0,-1.8520047601,-1.1958639213,0.1067419794
C,0,-2.8216879709,-0.3462786153,-0.4179418906
C,0,-2.7385833201,1.0323755337,-0.2540104288
C,0,-1.6637141387,1.5674180978,0.4273692315
C,0,2.3165370846,0.8653852673,-0.8574904674
N,0,0.4186287056,1.2585052878,1.6090260542
H,0,-0.0106961325,-1.3061636916,1.1947554052
H,0,-1.951382039,-2.2643420921,-0.0315967797
N,0,-3.9505071391,-0.9134992846,-1.1492061093
H,0,-3.5142542265,1.6648636216,-0.6647030412
H,0,-1.5875035206,2.6412548151,0.5587099177
O,0,-4.7854234904,-0.1469736685,-1.5895260826
H,0,1.2483106795,0.6871779241,1.7750436615
O,0,-3.9922802244,-2.1213932824,-1.2814866015
O,0,3.0845106702,1.6299319525,-0.336120817
H,0,0.5840552951,2.2493619722,1.5343069919
S,0,2.4803480693,-0.9123964018,-0.7317392602
C,0,4.021767106,-1.0373879139,0.2210839591
H,0,4.627884338,-0.1664850682,-0.0373459505
H,0,4.5284800407,-1.9317144693,-0.1425019213
C,0,3.8160425004,-1.1279915366,1.7264232438
H,0,4.803419122,-1.2884673063,2.1804696087
H,0,3.200204726,-1.9997387234,1.9632537539
N,0,3.1415763833,0.0656794177,2.2408015253
H,0,3.1414527444,0.0584767167,3.2553758454
H,0,3.6384138083,0.9002566937,1.9388505322
C,0,1.1600247923,1.2905238252,-1.725918598
H,0,0.3601162942,0.5492780813,-1.7333893387

H,0,0.7825055828,2.248773653,-1.3701223075
H,0,1.5355744355,1.4156420542,-2.7448490898

Sum of electronic and zero-point Energies=	-1177.774779
Sum of electronic and thermal Energies=	-1177.756469
Sum of electronic and thermal Enthalpies=	-1177.755525
Sum of electronic and thermal Free Energies=	-1177.823381

TS1_C

C,0,0.4457609101,-1.2391620011,-0.098964737
C,0,1.5389271805,-1.9551564122,-0.5939352296
C,0,2.8058107957,-1.4012046549,-0.5589690331
C,0,2.950263613,-0.1286502637,-0.0258532547
C,0,1.8755063071,0.5960805227,0.4617516989
C,0,0.6030453457,0.0418875391,0.428825075
C,0,-1.9519655468,-1.6009413665,0.424932953
N,0,-0.8196570611,-1.8708294792,-0.2108281849
H,0,1.3981645413,-2.9506511467,-1.0006287353
H,0,3.6706005629,-1.9335651809,-0.9300698409
N,0,4.2991053815,0.4701750396,0.0186787124
H,0,2.0291254936,1.5906549947,0.8594394024
H,0,-0.2315085323,0.6258362908,0.8003440031
O,0,4.4011666743,1.5861469958,0.4771456167
H,0,-0.8814390592,-2.5912084288,-0.9183124123
O,0,5.2187581759,-0.1946100762,-0.4080945987
S,0,-3.6192065158,0.4029974375,-0.4179474082
C,0,-3.1148641773,-2.510900169,0.1882399216
H,0,-4.0351752675,-2.029006279,0.5108910679
H,0,-3.2039788396,-2.7806967021,-0.862571194
H,0,-2.9541790511,-3.408768213,0.7971594194
O,0,-1.9002556548,-0.8421005722,1.4867584352
H,0,-2.6555489749,-0.1761252782,1.3155025844
C,0,-3.0562373917,2.0160315847,-1.0680276742
H,0,-3.7669342784,2.7772739578,-0.7318813244
H,0,-3.1048382963,1.9786238214,-2.1579159539
C,0,-1.6488947889,2.4162061827,-0.6448210672
H,0,-0.9399732411,1.6950449188,-1.0716887372
H,0,-1.41067217,3.3926080911,-1.0810588496
N,0,-1.4758656175,2.4615232645,0.8157616653
H,0,-1.2150846325,3.3878518803,1.1281136662
H,0,-2.349630885,2.2209327024,1.2741760137

Sum of electronic and zero-point Energies=	-1177.707346
Sum of electronic and thermal Energies=	-1177.689921
Sum of electronic and thermal Enthalpies=	-1177.688976
Sum of electronic and thermal Free Energies=	-1177.754638

TS1_C

C,0,-0.9905293315,0.2792871828,0.6150781971
C,0,-1.3609553504,-1.0514454923,0.4182455253
C,0,-2.6754127266,-1.3637684879,0.1057855241
C,0,-3.5930072518,-0.3286670872,-0.0001819312
C,0,-3.2475158957,1.0003902798,0.1919027596
C,0,-1.9295129487,1.3020586998,0.5015641027
C,0,1.4514775908,0.7434829619,-0.2701768883
N,0,0.3715735583,0.5927116666,0.8920899449
H,0,-0.6102034695,-1.8294922576,0.5021992204
H,0,-2.9960461534,-2.3841113069,-0.0546396326
N,0,-4.9960792189,-0.6565021229,-0.3288265574
H,0,-4.0018481488,1.7698321767,0.0987860267
H,0,-1.6211446271,2.3284627112,0.6602737943
O,0,-5.7773692973,0.26419057,-0.4261837205
H,0,0.8117014358,-0.0391778781,1.583134883
O,0,-5.2755797959,-1.8255120184,-0.4797134035
O,0,2.0805893829,1.7769559536,0.2976026139
H,0,0.9610684102,1.6477001348,1.0369055929
S,0,2.4256507556,-0.8303292626,-0.4788130211
C,0,3.7688580106,-0.5663640199,0.7123279658
H,0,3.959411484,0.510344212,0.7232890284
H,0,4.6412615572,-1.0686034348,0.2919728541
C,0,3.4925045974,-1.0869270909,2.1149138279
H,0,4.4225070667,-1.0177416209,2.6952005752
H,0,3.2044532877,-2.1398057613,2.0695505798
N,0,2.3937439047,-0.3360026239,2.7349421525
H,0,2.2406607274,-0.651396919,3.6868637752
H,0,2.6490408356,0.6485956951,2.781495748
C,0,0.7541475076,1.0160074649,-1.59091896
H,0,0.2041295563,0.1463551675,-1.9591800677
H,0,0.06932069,1.8591137521,-1.4753098796
H,0,1.5227378964,1.2879989561,-2.3134865198

Sum of electronic and zero-point Energies= -1177.702193
Sum of electronic and thermal Energies= -1177.685772
Sum of electronic and thermal Enthalpies= -1177.684828
Sum of electronic and thermal Free Energies= -1177.747608

Im1_D

C,0,0.3627089155,-0.6094082397,-0.5791990423
C,0,1.0320648794,-0.590483779,0.657348182
C,0,2.2413418178,0.0606812503,0.7995885584
C,0,2.7893080711,0.6921040036,-0.3093350029
C,0,2.1570439549,0.6792892433,-1.5421507871
C,0,0.9391878052,0.0300536525,-1.6861499342

C,0,-1.7067560116,-1.4422085958,-1.6870973865
N,0,-0.8635669601,-1.2763123553,-0.6101631987
H,0,0.5870592611,-1.1048238852,1.5017072921
H,0,2.7670120055,0.0829754087,1.7445232172
N,0,4.0757634722,1.3886813281,-0.167935759
H,0,2.6209333393,1.1790276308,-2.3820796408
H,0,0.4355660325,0.015923284,-2.6394916586
O,0,4.5467614697,1.9099282185,-1.1563996825
H,0,-1.2052730206,-1.5913903323,0.3011227279
O,0,4.5894852274,1.4019501211,0.9320103148
S,0,-3.8061118847,0.6783119726,0.8830039052
C,0,-2.934479839,-2.2756759878,-1.3923806347
H,0,-3.7910336822,-1.8192169549,-1.8866757323
H,0,-3.1351661669,-2.3790710857,-0.3269987564
H,0,-2.7824700697,-3.2659233943,-1.8275571362
O,0,-1.4905441991,-0.9925726249,-2.7912364084
H,0,-3.3931482619,0.8080536548,-0.3867922812
C,0,-2.163451056,0.878046606,1.6798856489
H,0,-1.3979133152,0.7981583025,0.91018341
H,0,-2.1089643492,1.8711743706,2.1248736076
C,0,-1.9464923692,-0.181183564,2.7536557886
H,0,-2.6723334773,-0.0360749242,3.5632616269
H,0,-0.9507262723,-0.0299288105,3.1799038052
N,0,-2.005388613,-1.5369197179,2.1872955985
H,0,-2.9691345373,-1.7433753563,1.9367668509
H,0,-1.7372725984,-2.2189944616,2.8893811897

Sum of electronic and zero-point Energies= -1177.777279
Sum of electronic and thermal Energies= -1177.758737
Sum of electronic and thermal Enthalpies= -1177.757793
Sum of electronic and thermal Free Energies= -1177.827778

Im2_D

C,0,0.3582366477,-0.6338183585,-0.4233598637
C,0,1.366112502,-1.0613396055,0.4647647204
C,0,2.5778846515,-0.4075320968,0.5394117167
C,0,2.798917626,0.6898284087,-0.2850544259
C,0,1.8276101958,1.133772997,-1.1698381501
C,0,0.6084810406,0.4794200518,-1.2436125733
C,0,-2.0639285878,-1.0162301256,-1.0128018389
N,0,-0.8221838702,-1.3640174354,-0.406708737
H,0,1.1767593703,-1.9215236008,1.0972053353
H,0,3.3531968557,-0.7316196454,1.2204467575
N,0,4.0805397585,1.393801505,-0.2110993772
H,0,2.0329260186,1.9940158948,-1.7931618332
H,0,-0.1465677083,0.8264914581,-1.9301292663
O,0,4.2502762961,2.3418375419,-0.9510156965
H,0,-0.9757783221,-1.8410371708,0.4786419267

O,0,4.9013993771,0.9897550866,0.5885534399
S,0,-3.0139879652,0.3726192509,-0.0956183313
C,0,-2.9709716891,-2.240556615,-1.0375166286
H,0,-3.9553581191,-1.9656352706,-1.4203155877
H,0,-3.0957083357,-2.6611820917,-0.0400973208
H,0,-2.520200224,-2.9868408206,-1.6938611799
O,0,-1.8086609467,-0.5887032305,-2.3229164655
H,0,-2.5857739717,-0.1289472068,-2.6542549917
C,0,-1.9536988203,0.8093166786,1.3202182126
H,0,-0.9108670187,0.7406067334,1.02032643
H,0,-2.1649444709,1.8628442285,1.5146458208
C,0,-2.2216415119,-0.0077075069,2.5797757724
H,0,-3.1942914332,0.2786018556,2.9961297846
H,0,-1.4579317364,0.2559816263,3.3167634838
N,0,-2.13458231,-1.4540094389,2.3259242762
H,0,-3.0282812614,-1.7731090993,1.9631716173
H,0,-1.9884982411,-1.9507082542,3.1978082376

Sum of electronic and zero-point Energies= -1177.752970
Sum of electronic and thermal Energies= -1177.735690
Sum of electronic and thermal Enthalpies= -1177.734746
Sum of electronic and thermal Free Energies= -1177.799904

Im3_D

C,0,0.3465807197,-0.0537012126,-0.1984497975
C,0,0.990744956,1.191668461,-0.0491532749
C,0,2.3601921027,1.3033626098,-0.1610815915
C,0,3.1104397086,0.1614921294,-0.4222785939
C,0,2.5060004166,-1.0775885857,-0.5780713385
C,0,1.1301355264,-1.1901549342,-0.4724339973
C,0,-1.8238971308,-1.261073471,0.1391157169
N,0,-1.0307268346,-0.0735033011,-0.1017325535
H,0,0.3896534276,2.0695381512,0.1604145284
H,0,2.8594320489,2.2558831249,-0.0438314936
N,0,4.5641766489,0.2715845952,-0.5394441506
H,0,3.1185207812,-1.9438254474,-0.7906721828
H,0,0.6588711395,-2.1504781803,-0.6243605914
O,0,5.1938090572,-0.7425415416,-0.765318278
H,0,-1.4658558395,0.8131123877,0.1527449859
O,0,5.0607672384,1.3725263229,-0.4039963949
S,0,-3.6001108137,-0.7440956106,0.3447608763
C,0,-1.4707522168,-2.0096754763,1.418572269
H,0,-2.1287231419,-2.8719455515,1.5319378758
H,0,-1.5793846897,-1.3485729789,2.2773880098
H,0,-0.4404146842,-2.3617979792,1.3661021121
O,0,-1.6688912961,-2.1737913121,-0.9135443012
H,0,-1.8223601756,-1.7115122362,-1.7446027985
C,0,-3.8078535335,0.4734517862,-1.0015647249

H,0,-2.932136256,0.4150668211,-1.650767895
H,0,-4.6846740465,0.1835782383,-1.5814215737
C,0,-3.9694839677,1.8998833366,-0.4745153542
H,0,-4.9505175945,2.0009198591,0.0032515842
H,0,-3.9518226576,2.5821496264,-1.3281910245
N,0,-2.869364306,2.2600303522,0.4294321202
H,0,-3.0744893289,1.9260352221,1.3662155579
H,0,-2.7694226866,3.2666655356,0.4870131928

Sum of electronic and zero-point Energies=	-1177.758809
Sum of electronic and thermal Energies=	-1177.741728
Sum of electronic and thermal Enthalpies=	-1177.740784
Sum of electronic and thermal Free Energies=	-1177.804238

Im4_D

C,0,0.2685966176,0.2232202958,-1.3607715894
C,0,0.7433479415,1.2351908129,-0.5023537927
C,0,1.895192449,1.0518443758,0.2376161539
C,0,2.5902205945,-0.1483152684,0.1276609287
C,0,2.1512951004,-1.1635414124,-0.7173582202
C,0,0.9965582975,-0.9803181564,-1.4496522306
C,0,-1.6332424525,-1.3897946522,0.6278260298
N,0,-0.856272222,0.4188906317,-2.1118560912
H,0,0.1992488994,2.1699759967,-0.4386311326
H,0,2.2680809773,1.821759928,0.9000621867
N,0,3.8062695757,-0.3454614393,0.9127078218
H,0,2.7159175287,-2.084460303,-0.7793534882
H,0,0.6315935118,-1.7704955096,-2.0954160393
O,0,4.395608492,-1.4015760574,0.7903967808
H,0,-1.5031367784,1.1458648363,-1.8085752572
O,0,4.1597598175,0.555921322,1.6480840979
S,0,-2.594241807,-0.012507313,1.2831247073
C,0,-0.4756085528,-1.7588088398,1.5171669115
H,0,-0.8182121826,-1.9043106224,2.5430662608
H,0,0.2524722561,-0.9427736241,1.5103457708
H,0,-0.0109614968,-2.6663214508,1.136199247
O,0,-1.9043856307,-1.930450061,-0.4074231042
H,0,-1.2967559426,-0.4144033788,-2.4726822022
C,0,-3.7961536736,0.2328949838,-0.0629583037
H,0,-3.3821539175,-0.2648012573,-0.9403532941
H,0,-4.7315134605,-0.2557028976,0.2103288954
C,0,-4.0269531463,1.7165725288,-0.3264130082
H,0,-4.5064424363,2.1784508547,0.5456170964
H,0,-4.7266575516,1.7996579365,-1.1617187835
N,0,-2.7777934922,2.3843379256,-0.7081054113
H,0,-2.1830354687,2.4804267418,0.1105314163
H,0,-2.968700395,3.3210045727,-1.0467968395

Sum of electronic and zero-point Energies=	-1177.775945
Sum of electronic and thermal Energies=	-1177.757405
Sum of electronic and thermal Enthalpies=	-1177.756460
Sum of electronic and thermal Free Energies=	-1177.824853

TS1_D

C,0,-0.0227958056,-1.1098402023,0.1223120882
C,0,0.7360641022,-1.23267073,1.2902183229
C,0,1.9250482592,-0.5373266835,1.4192771719
C,0,2.3367659225,0.2685020367,0.3679859005
C,0,1.6042859884,0.392397655,-0.8018401182
C,0,0.4140376164,-0.3073820933,-0.9327856028
C,0,-2.3365666004,-1.6107341248,-0.5851947094
N,0,-1.2075153855,-1.8809614042,0.0557273234
H,0,0.3685392446,-1.8552822986,2.0978794188
H,0,2.5292207798,-0.6052754225,2.3136794694
N,0,3.6042314458,1.0130203312,0.4983796065
H,0,1.9711445991,1.0259867456,-1.5978685128
H,0,-0.1694301713,-0.2257750758,-1.8370789791
O,0,3.9401618617,1.712612357,-0.4317061556
H,0,-1.3261866308,-2.5262853531,0.8382632109
O,0,4.2285314757,0.8754046734,1.5279698389
S,0,-3.9469941504,-0.0020925009,0.9332917273
C,0,-3.3603573455,-2.6950585467,-0.6755190129
H,0,-4.335046122,-2.2641340344,-0.8811475479
H,0,-3.399486684,-3.2844459728,0.2397596552
H,0,-3.06533175,-3.3460170544,-1.5082677169
O,0,-2.3965111738,-0.5602216833,-1.3667027877
H,0,-3.1251391436,-0.0126386821,-0.8357531174
C,0,-2.4526849411,0.4445871883,1.8850204904
H,0,-1.5785941863,0.4411642394,1.2300594687
H,0,-2.5588210304,1.4660419776,2.2556042607
C,0,-2.2190832422,-0.4685221926,3.091216672
H,0,-2.9614735623,-0.220716443,3.8591236915
H,0,-1.2268349492,-0.2604263371,3.5067291138
N,0,-2.2820498306,-1.9055972962,2.742318797
H,0,-3.2237548015,-2.0611084815,2.3814718279
H,0,-2.2135292188,-2.4525401013,3.5952420348

Sum of electronic and zero-point Energies=	-1177.719082
Sum of electronic and thermal Energies=	-1177.702257
Sum of electronic and thermal Enthalpies=	-1177.701312
Sum of electronic and thermal Free Energies=	-1177.764525

TS2_D

C,0,0.431716415,-0.1882193587,-0.554418751

C,0,0.8757091449,0.7763882162,0.3508837136
C,0,2.231136218,0.9161587909,0.6060896147
C,0,3.1163528545,0.0768078877,-0.0543735279
C,0,2.6986320924,-0.8940559601,-0.9516852224
C,0,1.3400399687,-1.0230938318,-1.2011501804
C,0,-1.8626177247,-1.2300081942,0.2058229874
N,0,-0.9655500873,-0.3460079758,-0.78652632
H,0,0.1511658827,1.3999168381,0.8624200374
H,0,2.6093420841,1.6535341378,1.3011095572
N,0,4.562805079,0.224589852,0.20935015
H,0,3.4301146241,-1.5247470906,-1.4383947303
H,0,0.9741666768,-1.7680828261,-1.8977163059
O,0,5.3151071839,-0.5356359149,-0.3591902783
H,0,-1.4388892666,0.5693584247,-0.9233027719
O,0,4.9040832519,1.0983683149,0.976234537
S,0,-3.0064159194,-0.1208815478,1.1967168717
C,0,-1.0112777858,-1.9814433846,1.211061249
H,0,-1.6694264907,-2.6772183061,1.7312949281
H,0,-0.5370174599,-1.31848529,1.9381878973
H,0,-0.2472718555,-2.5577896,0.6855166659
O,0,-2.4263486753,-1.9462561367,-0.7619411951
H,0,-1.5133242066,-1.2164783658,-1.4255120732
C,0,-4.1063621825,0.4167634371,-0.1472787999
H,0,-3.9201906242,-0.2842422857,-0.9658478669
H,0,-5.134758473,0.2695319813,0.1840530884
C,0,-3.8982795274,1.868821854,-0.574974856
H,0,-4.3578743454,2.5411405349,0.1568991751
H,0,-4.4129388134,2.0233118933,-1.5265725391
N,0,-2.4701986727,2.1809275091,-0.7696091741
H,0,-2.0693137769,2.4545374754,0.1228277721
H,0,-2.3620895884,2.9722259218,-1.3942326526

Sum of electronic and zero-point Energies= -1177.700577
Sum of electronic and thermal Energies= -1177.683846
Sum of electronic and thermal Enthalpies= -1177.682901
Sum of electronic and thermal Free Energies= -1177.746887

Table S2 Cartesian Coordinates and energies (in au) of all the species participating in the reaction mechanisms in aqeous solution

R1

C,0,0.0079690313,0.9419248045,0.0785866298
C,0,-1.3537613455,0.5976849456,0.044244521
C,0,-1.7471970871,-0.7235025485,0.02680084
C,0,-0.7649999934,-1.7092573778,0.0455529349
C,0,0.5863773837,-1.397276896,0.0829420341
C,0,0.9796270052,-0.0686265207,0.1003587744
C,0,1.5211186224,2.9280883469,0.047412256
N,0,0.302920151,2.3064076459,0.1033179114
H,0,-2.1015037952,1.3822153431,0.0315753812
H,0,-2.7956898273,-0.9868956211,-0.0003728432
N,0,-1.1692608106,-3.1088097437,0.0291420063
H,0,1.3295530415,-2.1828413017,0.1013032901
H,0,2.0283697017,0.1749728794,0.1339032687
O,0,-0.302923011,-3.965324162,0.0547093995
H,0,-0.5028111956,2.9201983082,0.1346751388
O,0,-2.3596523992,-3.368174394,-0.0083278158
C,0,1.4653637168,4.4296435714,0.0554141896
O,0,2.5801094237,2.3186943488,-0.0292185023
H,0,2.2824849015,4.8049498513,0.6703697685
H,0,0.5146515266,4.816548148,0.4193960277
H,0,1.6212589599,4.7774253726,-0.9688852109
Sum of electronic and zero-point Energies= -644.547834
Sum of electronic and thermal Energies= -644.536339
Sum of electronic and thermal Enthalpies= -644.535395
Sum of electronic and thermal Free Energies= -644.587204

R2

C	-1.272	0.6231	-0.3481
C	0.1376	0.918	0.1502
S	1.4059	-0.1837	-0.5741
N	-1.6546	-0.7647	-0.0539
H	-1.3327	0.8503	-1.4193
H	-1.9686	1.2844	0.175
H	0.1963	0.8189	1.2338
H	0.4197	1.935	-0.1243
H	1.3323	-1.1167	0.3912
H	-2.6399	-0.9075	-0.2462
H	-1.1403	-1.3851	-0.6748

Sum of electronic and zero-point Energies= -533.241691
Sum of electronic and thermal Energies= -533.235690
Sum of electronic and thermal Enthalpies= -533.234746
Sum of electronic and thermal Free Energies= -533.271367

Im1_A

H,0,-1.2561591372,-0.5832957333,-3.4004814354
H,0,-0.9688370597,-1.1860914969,-1.0163230203
N,0,-1.0350740347,1.7347433627,-0.0173830419
C,0,-1.2677549516,2.6122572305,-1.0435309324
H,0,-1.8530802165,1.5594237211,0.5594792405
C,0,0.1140087676,1.0275570885,0.3495530372
C,0,0.2009972048,0.6084685617,1.684926582
C,0,1.1119678185,0.6636950734,-0.5628352939
C,0,1.26994887,-0.1530348242,2.112572876
H,0,-0.5820375056,0.8845837887,2.3814065611
C,0,2.1939013548,-0.0874494973,-0.1367606112
H,0,1.0321452369,0.9236621734,-1.608150882
C,0,2.2576828935,-0.4853699381,1.1920337741
H,0,1.3415974412,-0.4781626759,3.1414758824
H,0,2.9653982767,-0.3810538604,-0.8355897061
N,0,3.3924331969,-1.2866185333,1.6346147684
O,0,4.2685601024,-1.5481845956,0.8294455269
O,0,3.4201006846,-1.6622460741,2.7932771578
S,0,-1.294805658,-2.2742660976,-0.2993530731
C,0,-2.7335729714,-1.5545492705,0.5673343036
H,0,-3.0226703447,-2.3096686281,1.2995954674
H,0,-2.4104159176,-0.6696802802,1.1206220409
C,0,-3.9196753269,-1.2382354932,-0.3265730295
H,0,-4.1725239476,-2.1174400836,-0.9216965558
H,0,-4.7760263637,-1.0201218176,0.3225298051
N,0,-3.6376904577,-0.1236293493,-1.2426370588
H,0,-4.4323569255,-0.0054112434,-1.8663220073
H,0,-3.5790134909,0.7422485435,-0.7095072269
O,0,-1.4485963902,0.2510688079,-2.9593609138
H,0,-2.2001505907,0.0483160463,-2.3487955164
C,0,-0.1149812004,3.1744595853,-1.8217079227
H,0,0.7990134168,3.2261711948,-1.2315955522
H,0,0.0649572631,2.5590038106,-2.7056389742
H,0,-0.402873499,4.1706610891,-2.1538232741
O,0,-2.4239385382,2.965389415,-1.2592109956
Sum of electronic and zero-point Energies= -1254.214507
Sum of electronic and thermal Energies= -1254.193331
Sum of electronic and thermal Enthalpies= -1254.192387
Sum of electronic and thermal Free Energies= -1254.266650

TS1_A

H,0,-1.2716849325,-0.6063594402,-0.3639219833
H,0,-2.6324344786,0.1902605744,1.6108896875
N,0,-0.0874470216,1.2955071708,0.7526556756
C,0,-1.2087754818,1.686598479,-0.0485554151
H,0,-0.2875525832,1.3639273315,1.7438363978
C,0,1.1214090128,0.7438592358,0.4168515874
C,0,2.077498226,0.6038859515,1.4493709766
C,0,1.4530011361,0.2919319256,-0.8769551131

C,0,3.3175267624,0.0640191668,1.2025089462
H,0,1.8216086981,0.9368372022,2.4486596819
C,0,2.7018804923,-0.2419609379,-1.1280230456
H,0,0.727965901,0.3269924916,-1.6748102766
C,0,3.6279469184,-0.3483974834,-0.0946650968
H,0,4.0442541459,-0.0328078343,1.9979081591
H,0,2.952184808,-0.5898516531,-2.1213406828
N,0,4.9301520203,-0.9069838156,-0.3658406498
O,0,5.2082049345,-1.2266328659,-1.5129849585
O,0,5.7160761272,-1.0410714094,0.5613902303
S,0,-2.9573583821,-1.0588714327,2.0091957299
C,0,-4.6204041025,-1.102656535,1.250523071
H,0,-5.1038003071,-1.9884509616,1.6623744601
H,0,-5.1851216187,-0.2299655252,1.5830878928
C,0,-4.6368087092,-1.2009394895,-0.2616785413
H,0,-4.044737762,-2.0498448623,-0.6056531092
H,0,-5.6683244634,-1.3413440385,-0.5896603262
N,0,-4.0891383798,0.0215512876,-0.8992685753
H,0,-4.388906578,0.0614070941,-1.8729959994
H,0,-4.4535161991,0.8562847993,-0.4372997961
O,0,-1.5859051833,0.1102308894,-0.9302788271
H,0,-2.8793039602,0.0623611274,-0.8865384615
C,0,-0.9101208504,2.5172114401,-1.2765513861
H,0,-0.7129353625,3.5353297609,-0.9310152507
H,0,-0.0571945613,2.1733615682,-1.8547115286
H,0,-1.796242588,2.5288019637,-1.9110574065
O,0,-2.2269786777,1.9847098246,0.6324079333
Sum of electronic and zero-point Energies= -1254.179296
Sum of electronic and thermal Energies= -1254.160002
Sum of electronic and thermal Enthalpies= -1254.159058
Sum of electronic and thermal Free Energies= -1254.228980

Im2_A

H,0,-1.5226832801,-0.2960530719,-1.7925095161
H,0,-1.266800474,-1.6273731853,0.2730929693
N,0,-0.866593914,-1.1643602082,1.0902445401
C,0,-0.8118245409,1.3757320826,-1.0783828387
H,0,-1.523283618,-0.5729355692,1.5837218827
C,0,0.3987396703,-0.6738945889,0.9707197578
C,0,0.8397553386,0.3848352992,1.7936947557
C,0,1.3003035116,-1.2391646887,0.0418803037
C,0,2.1302133281,0.8560942584,1.6994439936
H,0,0.1468484667,0.8281914957,2.4997189435
C,0,2.5897207845,-0.7690902914,-0.0569784502
H,0,0.9614624706,-2.0454349336,-0.5985402857
C,0,3.0007237169,0.2769033096,0.7744336999
H,0,2.4655288095,1.6701661621,2.328065534
H,0,3.2792025615,-1.2000724486,-0.7706473323
N,0,4.3483894163,0.7700163036,0.6710057976
O,0,5.1083682464,0.2490959837,-0.1353935128
O,0,4.6973478954,1.695793037,1.3923981446
S,0,-2.8596517341,-1.8281413343,-1.6175562186
C,0,-4.0321334795,-1.1107600116,-0.4029665986

H,0,-4.6091122661,-1.9062022679,0.0702509933
H,0,-3.489467383,-0.5841069389,0.3874136865
C,0,-5.0211823131,-0.1458302742,-1.0323924606
H,0,-5.6719685813,-0.645020626,-1.7485461235
H,0,-5.6255528723,0.3569783259,-0.2778188376
N,0,-4.2817083234,0.9113134077,-1.7830235844
H,0,-4.9106723165,1.6045747083,-2.1913777149
H,0,-3.5971101731,1.3762894253,-1.1694844403
O,0,-0.7488583603,0.3580739739,-1.919767296
H,0,-3.7411819385,0.4595363391,-2.531062469
C,0,0.391276565,2.2642286611,-1.1281850897
H,0,0.394701016,2.7877526341,-2.0876486905
H,0,0.3590533786,2.9871761173,-0.3166219691
H,0,1.3004224066,1.6624133086,-1.0725615835
O,0,-1.7755180145,1.5704466051,-0.3511459904
Sum of electronic and zero-point Energies= -1254.222478
Sum of electronic and thermal Energies= -1254.201902
Sum of electronic and thermal Enthalpies= -1254.200958
Sum of electronic and thermal Free Energies= -1254.273931

P1

C	-0.00079	-2.07131	0.
C	-0.00325	-1.35861	1.2101
C	-0.00325	0.02295	1.2121
C	-0.00307	0.70162	0.
C	-0.00325	0.02295	-1.2121
C	-0.00325	-1.35861	-1.2101
H	-0.00834	-1.90057	2.14881
H	-0.00321	0.58411	2.13684
H	-0.00321	0.58411	-2.13684
H	-0.00834	-1.90057	-2.14881
N	-0.00078	2.166	0.
O	0.00054	2.73107	-1.07502
O	0.00054	2.73107	1.07502
N	-0.04642	-3.44788	0.
H	0.22307	-3.9224	-0.84655
H	0.22307	-3.9224	0.84655

Sum of electronic and zero-point Energies= -491.942534
Sum of electronic and thermal Energies= -491.934067
Sum of electronic and thermal Enthalpies= -491.933123
Sum of electronic and thermal Free Energies= -491.976172

P2

C,0,0.1281494916,0.1528115035,0.0072837875
O,0,0.6946434669,1.2236242521,0.0092055587
O,0,0.8038036261,-1.0070464114,0.0124509865
C,0,-1.3510269692,-0.0475420788,-0.0003922385
H,0,1.7560808447,-0.8194544407,0.0173993035
H,0,-1.64171168,-0.6160944406,0.8847041324

H,0,-1.8550162481,0.9149892288,-0.010444584
H,0,-1.6315225321,-0.6299876129,-0.8796069461
Sum of electronic and zero-point Energies= -229.014101
Sum of electronic and thermal Energies= -229.010344
Sum of electronic and thermal Enthalpies= -229.009400
Sum of electronic and thermal Free Energies= -229.040108

P3

C	0.1319	0.1399	-0.0001
O	0.6829	1.1965	0.
O	0.859	-1.0042	-0.0001
C	-1.3678	-0.0505	-0.0001
H	1.8003	-0.8107	0.0402
H	-1.6761	-0.6092	0.8868
H	-1.8505	0.9226	-0.0018
H	-1.6763	-0.6131	-0.8843

Sum of electronic and zero-point Energies= -229.012794
Sum of electronic and thermal Energies= -229.008862
Sum of electronic and thermal Enthalpies= -229.007918
Sum of electronic and thermal Free Energies= -229.038916

Im1_B

C,0,-2.9973295739,2.4993571244,0.2238170588
C,0,-3.6846229255,1.6504659935,1.2771647557
S,0,-2.64706612,0.3218820167,1.9862930391
N,0,-2.7140647899,1.7200952207,-0.9895816468
H,0,-3.5912299179,1.367604642,-1.3689344386
H,0,-3.6478697296,3.3567309994,0.0131608946
H,0,-2.0548155518,2.8883452309,0.6162114045
H,0,-3.9607573101,2.2734735399,2.1284356089
H,0,-2.3266115921,2.3391399383,-1.6975617655
H,0,-4.5990816217,1.2079810867,0.8774858089
C,0,-1.3895333325,-1.6661567226,-1.5754222963
O,0,-0.7764794337,-2.7253927859,-1.6519749354
C,0,-2.8245232704,-1.5302994157,-2.0117279428
H,0,-2.9175544468,-0.747240252,-2.7668566585
H,0,-3.1659067004,-2.4789688903,-2.4191918754
H,0,-3.4500325796,-1.2513227493,-1.1595752143
H,0,-2.5663051193,-0.4385884,0.8816344685
H,0,-1.5000795343,0.3001633567,-1.0276113836
N,0,-0.8487211683,-0.5084413237,-1.0921799865
C,0,0.4145836687,-0.3021855609,-0.5484862371
C,0,0.6650534267,0.9841607248,-0.0332459703
C,0,1.4238998662,-1.2766165698,-0.4925782001
C,0,1.8846307065,1.2964491237,0.5275807197
H,0,-0.1153820337,1.7350316526,-0.080011254
C,0,2.6495411913,-0.9650296106,0.0725507335
H,0,1.2551280412,-2.2652158173,-0.8864015661
C,0,2.8668316667,0.3104038925,0.5754685626

H,0,2.0757559484,2.2849820183,0.9227243199
H,0,3.4312480883,-1.7112180748,0.119123871
N,0,4.1581920712,0.6286043922,1.1630555442
O,0,5.0146968934,-0.2388675324,1.1952091693
O,0,4.3369341829,1.7527017522,1.6010294121
Sum of electronic and zero-point Energies= -1177.799780
Sum of electronic and thermal Energies= -1177.781422
Sum of electronic and thermal Enthalpies= -1177.780478
Sum of electronic and thermal Free Energies= -1177.848506

TS1_B

C -0.578831085460 1.243028518338 -0.047914901672
C -1.653645327265 1.835182326246 -0.715868802945
C -2.891412231457 1.220060631782 -0.718847812381
C -3.024197102529 0.009933528222 -0.052062404703
C -1.968208513725 -0.597451687938 0.608378937668
C -0.728119356423 0.023492694013 0.613842465575
C 1.781001778727 1.774103434830 0.508718223811
N 0.653230590563 1.942760734592 -0.139505321789
H -1.515159999208 2.777966151234 -1.232157138254
H -3.732165406249 1.669249881948 -1.228948804619
N -4.333075571044 -0.651404848118 -0.047848501388
H -2.103179422109 -1.545602868590 1.110945792379
H 0.096509931435 -0.459048477653 1.114245061254
O -4.434434244435 -1.724443113287 0.514523740836
H 0.662228635403 2.704266764285 -0.814929040442
O -5.258778212155 -0.096085324200 -0.607416924415
S 3.885499338470 -0.414431013752 -0.599849552308
C 2.921612211563 2.681444345668 0.240286426055
H 3.859795225798 2.190901930872 0.491156890428
H 2.924505152563 3.004723714777 -0.798509762119
H 2.790068584421 3.552751333969 0.891268134405
O 1.812110046282 0.906090923861 1.469335238943
H 2.736062536001 0.641386049001 1.648792518980
C 3.171273368170 -2.030561205767 -1.105414974162
H 3.845083296498 -2.842880370188 -0.812170787861
H 3.088424237250 -2.059366539535 -2.195701385442
C 1.792262757865 -2.303145515844 -0.511789729046
H 1.114250314850 -1.496432638890 -0.808653920297
H 1.391482427987 -3.231526708253 -0.931192360703
N 1.757768918273 -2.422440268517 0.950176545664
H 2.315432950299 -3.232541223042 1.212336454752
H 2.263798169655 -1.621159160107 1.324444694002
Sum of electronic and zero-point Energies= -1177.744442
Sum of electronic and thermal Energies= -1177.726943
Sum of electronic and thermal Enthalpies= -1177.725999
Sum of electronic and thermal Free Energies= -1177.792181

Im2_B

C,0,-3.8654776155,1.7649513407,-0.008439657
C,0,-3.8589338953,0.6310878313,-1.0203303051
S,0,-3.4478373557,-0.9971127372,-0.3000206938
N,0,-2.5214444496,2.0670469049,0.4945270421
H,0,-1.9557447632,2.4325110912,-0.2694254935
H,0,-4.3288164441,2.6282018264,-0.5013102529
H,0,-4.499341016,1.497549141,0.8396993709
H,0,-4.8603867326,0.5097671429,-1.434522115
H,0,-2.5903758494,2.8199841946,1.1741714863
H,0,-3.1855655155,0.838529968,-1.8519641992
C,0,-1.7554399216,-1.3509708633,-0.7218208633
O,0,-1.2985332576,-2.3915597062,-0.2931340367
C,0,-0.9748119892,-0.4202006547,-1.600339088
H,0,0.0553699979,-0.7742010996,-1.6434344451
H,0,-1.4060459546,-0.4245768717,-2.6051178481
H,0,-1.0032404536,0.6020073302,-1.2218960413
H,0,-1.0869621631,-0.8454454148,2.042287878
H,0,-1.3692949885,0.7321890798,1.3983674176
N,0,-0.698132873,0.0476728867,1.7692059615
C,0,0.5515193234,0.0325003676,1.2433609932
C,0,1.0748446484,1.1869209797,0.613342587
C,0,1.3612653479,-1.1237812344,1.3270341891
C,0,2.3385638298,1.1771692882,0.0722213895
H,0,0.4628810329,2.0793784521,0.5504227908
C,0,2.6266913411,-1.1346349209,0.7877797265
H,0,0.964214357,-2.0103727309,1.8078826212
C,0,3.1121528721,0.0151614629,0.1583120695
H,0,2.734785464,2.0576450294,-0.4160821791
H,0,3.2400956578,-2.0242007258,0.8423506779
N,0,4.4277513019,0.0027004328,-0.4127064149
O,0,5.1041069278,-1.0157702193,-0.3246904563
O,0,4.8395141359,1.0106854285,-0.9756861119
Sum of electronic and zero-point Energies= -1177.792537
Sum of electronic and thermal Energies= -1177.774585
Sum of electronic and thermal Enthalpies= -1177.773641
Sum of electronic and thermal Free Energies= -1177.840023

Im1_C

C,0,0.0940459942,-1.2611055382,0.1996109404
C,0,0.7715508088,-1.2795738262,-1.0271121103
C,0,1.9108357541,-0.5204237737,-1.2084638265
C,0,2.3615772774,0.2603189316,-0.1489799932
C,0,1.7181112811,0.2818790413,1.0810781737
C,0,0.58033216,-0.4877756369,1.2591425579
C,0,-2.1685746081,-1.7734578495,1.0411381568
N,0,-1.0428087341,-2.0693082666,0.3230313726
H,0,0.3881716452,-1.8878887661,-1.8379172314
H,0,2.4330813077,-0.5224136752,-2.1553730617
N,0,3.5557536209,1.0775612051,-0.3338847445

H,0,2.1047286187,0.8838076219,1.8921966871
H,0,0.0821808393,-0.494550144,2.2166621168
O,0,3.9125474302,1.7997558994,0.5800575319
H,0,-1.1489374065,-2.779004325,-0.3929544423
O,0,4.1482525837,1.0070330773,-1.3961930549
S,0,-2.7339927105,0.3971071073,-1.6642387674
C,0,-3.330440687,-2.6974864215,0.8133663045
H,0,-4.0361126305,-2.1944051509,0.1460350794
H,0,-3.0337090992,-3.6449575827,0.3657813897
H,0,-3.8318659847,-2.8727150118,1.7644912257
O,0,-2.2415279985,-0.8108736902,1.7960608784
H,0,-3.3094911784,0.4655036956,-0.4496579286
C,0,-1.9899190835,2.0679249848,-1.6541339571
H,0,-2.7887207006,2.8043397637,-1.5501782785
H,0,-1.5504750971,2.1849711057,-2.6464212465
C,0,-0.9255816764,2.2758709043,-0.5832191801
H,0,-0.1133444321,1.5608475781,-0.7319784205
H,0,-0.5073920114,3.2749031379,-0.7371618373
N,0,-1.3901648242,2.1708842752,0.7980782267
H,0,-2.2498116417,2.7050405461,0.9043846809
H,0,-1.6197368168,1.2020017831,1.0116017581
Sum of electronic and zero-point Energies= -1177.800341
Sum of electronic and thermal Energies= -1177.781816
Sum of electronic and thermal Enthalpies= -1177.780872
Sum of electronic and thermal Free Energies= -1177.848700

Im2_C

C,0,0.3933128645,-0.5565989339,-0.2663539044
C,0,1.3008662344,-0.7626340905,-1.3331529852
C,0,2.6489692418,-0.8957901046,-1.103769649
C,0,3.1244207875,-0.8222461477,0.207875767
C,0,2.256409014,-0.6180828028,1.2787771193
C,0,0.9024110037,-0.4849930176,1.0496498211
C,0,-2.0384664356,-0.5444758739,0.3728185215
N,0,-0.9298226794,-0.4038135186,-0.5765223574
H,0,0.9145794924,-0.8219121704,-2.3442297833
H,0,3.3325762737,-1.0585936095,-1.9261205231
N,0,4.534044359,-0.96730032,0.4580785129
H,0,2.6426998808,-0.561944175,2.2877799549
H,0,0.2396306831,-0.3169151743,1.8847393338
O,0,4.9422380797,-0.8796390364,1.6087321701
H,0,-1.1629831005,-0.6077985345,-1.5404576436
O,0,5.2837422138,-1.1749959392,-0.4872502459
S,0,-3.6040824757,-0.3421623806,-0.5872040736
C,0,-2.0912867947,-1.9365681168,0.9916734821
H,0,-2.9802477889,-2.0317199861,1.617348158
H,0,-2.1085480621,-2.7022663921,0.2159595179
H,0,-1.212167978,-2.0875012977,1.6205054928
O,0,-1.9380879656,0.3945415631,1.4061676223
H,0,-2.4350768963,1.2325029374,1.1584986444

C,0,-3.3085411557,1.159329927,-1.5952088265
H,0,-4.3115508627,1.4071806105,-1.9509123171
H,0,-2.7062712047,0.9018938505,-2.4673128619
C,0,-2.6861944718,2.3609716481,-0.8936764216
H,0,-1.6079148529,2.2182030724,-0.8066250707
H,0,-2.8512335298,3.2292652184,-1.5392982575
N,0,-3.2189404027,2.5604058657,0.4606666384
H,0,-2.9232918532,3.468709067,0.8070829311
H,0,-4.2359666182,2.5690348623,0.436833233
Sum of electronic and zero-point Energies= -1177.783928
Sum of electronic and thermal Energies= -1177.767157
Sum of electronic and thermal Enthalpies= -1177.766213
Sum of electronic and thermal Free Energies= -1177.829044

Im3_C

C,0,-0.2839495076,0.6055961615,0.3291991855
C,0,-0.6310674975,-0.5343117332,1.0798290924
C,0,-1.844881211,-1.1673815234,0.9009515653
C,0,-2.7277765298,-0.661725871,-0.0481725669
C,0,-2.4263273742,0.4730646797,-0.7946025234
C,0,-1.2147202793,1.1082879714,-0.5982309244
C,0,1.9449297443,1.4430250447,-0.4360166017
N,0,0.935865085,1.2280796377,0.5976053653
H,0,0.0729574277,-0.9236562251,1.805728321
H,0,-2.0982417972,-2.0488764203,1.4743315207
N,0,-4.0007546215,-1.3270308984,-0.2556196546
H,0,-3.1413420684,0.8670767794,-1.5041837831
H,0,-1.0130960029,2.0198407352,-1.1407713772
O,0,-4.7459256727,-0.9055516595,-1.1256710582
H,0,1.4204859707,0.7330217152,1.3612206057
O,0,-4.279950208,-2.2862572473,0.4456149092
O,0,3.0261695098,2.0870759229,0.1994698109
H,0,2.6934152974,2.9268780995,0.5470571746
S,0,2.6094182842,-0.1481560652,-1.1312089423
C,0,3.6903712739,-0.8199813642,0.177277963
H,0,4.4006587426,-0.0468693611,0.4776332113
H,0,4.2558486398,-1.5872435349,-0.3556758901
C,0,3.0270816114,-1.4488443655,1.3945536406
H,0,3.7451286332,-2.1542658356,1.8295731089
H,0,2.1500257156,-2.0238897767,1.0872960379
N,0,2.6049374166,-0.4333822116,2.368722783
H,0,2.1852292962,-0.8955170248,3.170862857
H,0,3.4294851311,0.0520982767,2.7140766354
C,0,1.4673441874,2.2489130685,-1.6317384949
H,0,0.7838789772,1.6832945042,-2.2650418374
H,0,0.9688878703,3.156747849,-1.2836747478
H,0,2.3380389557,2.5265606724,-2.2252303855
Sum of electronic and zero-point Energies= -1177.776705
Sum of electronic and thermal Energies= -1177.759761

Sum of electronic and thermal Enthalpies= -1177.758817
Sum of electronic and thermal Free Energies= -1177.822396

Im4_C

C,0,-0.5950694386,0.7528240556,0.8659910034
C,0,-0.7254294933,-0.6574866098,0.8506844606
C,0,-1.8148057187,-1.2529208145,0.2616193769
C,0,-2.8035722377,-0.4533799358,-0.3232159773
C,0,-2.7050134324,0.9423777166,-0.3136615087
C,0,-1.6159219274,1.5375317249,0.2763646384
C,0,2.4073253128,1.033609065,-0.9074437357
N,0,0.476388667,1.3322966483,1.4463663463
H,0,0.0515379723,-1.2623027978,1.3031512351
H,0,-1.9096294639,-2.3305829648,0.2468706101
N,0,-3.9348534708,-1.0740999258,-0.9426385355
H,0,-3.4795354277,1.5446419738,-0.769689717
H,0,-1.5214906375,2.617423016,0.2874089685
O,0,-4.7846826165,-0.3672034945,-1.4749781895
H,0,1.3014311745,0.770356359,1.6891016042
O,0,-4.0261881826,-2.2975418027,-0.9265320314
O,0,3.2151622098,1.7521492247,-0.360381671
H,0,0.6192405193,2.3227636856,1.3030837945
S,0,2.4827375331,-0.737964735,-0.8432253268
C,0,3.937083307,-1.0300719713,0.2081558315
H,0,4.6202046957,-0.1899597332,0.0685249849
H,0,4.4120157888,-1.9278879316,-0.1879233662
C,0,3.5977283289,-1.2274394604,1.6754270846
H,0,4.5214955564,-1.5396717082,2.1773384045
H,0,2.8759821538,-2.0404380751,1.7837637239
N,0,3.0256586656,-0.0124998686,2.2676297921
H,0,2.9315539279,-0.1514165093,3.2702936562
H,0,3.6887376678,0.7505331957,2.1475827204
C,0,1.2795521013,1.5535338197,-1.7541301344
H,0,0.4829844981,0.8193028596,-1.8779212901
H,0,0.8862779103,2.4658088669,-1.3036465356
H,0,1.6897970564,1.7989551268,-2.7380712166
Sum of electronic and zero-point Energies= -1177.797137
Sum of electronic and thermal Energies= -1177.778689
Sum of electronic and thermal Enthalpies= -1177.777745
Sum of electronic and thermal Free Energies= -1177.846070

TS1_C

C -0.578833036284 1.242860925718 -0.050321981884
C -1.655390095409 1.836252995912 -0.714182259503
C -2.893273200647 1.221292589487 -0.714636815122
C -3.024064737132 0.009748832586 -0.050121380201

C	-1.966282154791	-0.598879204562	0.606316923188
C	-0.726247746824	0.022168624753	0.609675337310
C	1.780308225552	1.776761441993	0.506310744394
N	0.653208811098	1.942585962276	-0.143789159352
H	-1.518351319420	2.780022388397	-1.228994569185
H	-3.735523798609	1.671533346635	-1.221336856135
N	-4.332486529548	-0.652521350348	-0.045042220178
H	-2.099766792825	-1.548171273615	1.107116705087
H	0.099677680061	-0.461182665807	1.107192004896
O	-4.431459045545	-1.727901135991	0.513229142206
H	0.661909614385	2.703198109973	-0.820219324938
O	-5.260001237810	-0.095870632329	-0.600237206745
S	3.897616634596	-0.426362773379	-0.580962772052
C	2.919795460170	2.685466760827	0.237274960259
H	3.859230715401	2.195343816306	0.484014233621
H	2.919830696886	3.011896664631	-0.800521904536
H	2.789182296889	3.554650014185	0.891255672721
O	1.811000209315	0.911027887118	1.468908938324
H	2.734735776378	0.647081752768	1.650985064322
C	3.175680026868	-2.034703520643	-1.100413591425
H	3.843442127988	-2.853021296761	-0.809765228717
H	3.097193984819	-2.055797126537	-2.191230733246
C	1.792755457822	-2.302564159982	-0.513965222173
H	1.119570321151	-1.492271731793	-0.812125921539
H	1.389835103002	-3.228330535111	-0.937111844355
N	1.751866763109	-2.424220487771	0.947629209139
H	2.306425834861	-3.236289746579	1.210398144340
H	2.259607954504	-1.624982472566	1.324340911252

Sum of electronic and zero-point Energies= -1177.744554
Sum of electronic and thermal Energies= -1177.726990
Sum of electronic and thermal Enthalpies= -1177.726046
Sum of electronic and thermal Free Energies= -1177.792750

TS2_C

C,0,-0.3585804169,0.2211318848,0.5416961656
C,0,-0.7787032361,-0.9444080761,-0.0982632865
C,0,-2.1328578241,-1.1857223499,-0.2727331434
C,0,-3.0341803898,-0.2434322245,0.2030874846
C,0,-2.6386850293,0.9204844494,0.8490607685
C,0,-1.2828879173,1.148404124,1.0192283376
C,0,1.7928729814,1.304291445,-0.370439417
N,0,1.0393078219,0.4740300335,0.6968860434
H,0,-0.046367333,-1.65566887,-0.461569868
H,0,-2.4805153738,-2.0820109132,-0.7679513043
N,0,-4.4690520075,-0.4876781121,0.0169867064
H,0,-3.371933896,1.6275034744,1.2115343195
H,0,-0.9347783243,2.0430310205,1.5214055671
O,0,-5.2536622363,0.3366214389,0.4458287476
H,0,1.5717961695,-0.4124632378,0.8678317479
O,0,-4.8120793021,-1.5025575067,-0.5586325623

O,0,2.3947324795,2.1523411257,0.5360447012
H,0,1.5813421974,1.4336852606,1.2672009052
S,0,2.9400695007,0.2568644545,-1.374100178
C,0,4.1877741851,-0.2782996622,-0.1576146593
H,0,4.2217012867,0.4757393172,0.6328915026
H,0,5.1433510952,-0.246277183,-0.6825539898
C,0,3.9609003269,-1.6704781419,0.4110492918
H,0,4.8813187773,-1.9823087281,0.9173310793
H,0,3.7811542426,-2.3744899211,-0.4027311377
N,0,2.8028304598,-1.6995455267,1.3151785783
H,0,2.5410027509,-2.6621851085,1.5048610945
H,0,3.0738351135,-1.2970508807,2.2102067759
C,0,0.8600630219,1.9874288124,-1.351008561
H,0,0.3349484136,1.2727551634,-1.9885694214
H,0,0.1292528922,2.585845491,-0.803697469
H,0,1.4543915704,2.6562849473,-1.9745188191
Sum of electronic and zero-point Energies= -1177.729004
Sum of electronic and thermal Energies= -1177.712562
Sum of electronic and thermal Enthalpies= -1177.711618
Sum of electronic and thermal Free Energies= -1177.774273

Im1_D

C,0,0.357533152,-0.5653414047,-0.5937195262
C,0,1.0139392541,-0.548873772,0.6496390715
C,0,2.2365229582,0.0739281552,0.7942065663
C,0,2.8075610718,0.6825865784,-0.3191059692
C,0,2.1794468172,0.687070199,-1.5570732912
C,0,0.9497041067,0.0655258674,-1.6974420279
C,0,-1.5722531124,-1.6175184875,-1.7342505365
N,0,-0.8866661478,-1.1974598295,-0.633205377
H,0,0.556398717,-1.0407051983,1.4999410544
H,0,2.744573848,0.0813365029,1.7489400906
N,0,4.1018623212,1.3358418295,-0.1801628752
H,0,2.6402304011,1.1782700078,-2.4033235675
H,0,0.4526329548,0.0807938573,-2.6535166886
O,0,4.6070277642,1.8430533363,-1.1666756245
H,0,-1.3171811732,-1.3781876895,0.2935127611
O,0,4.630617302,1.3502398293,0.918060636
S,0,-3.8632203831,0.9893036635,1.0077477333
C,0,-2.9060369521,-2.2546027858,-1.4562746287
H,0,-3.6839667574,-1.6166005176,-1.8823651193
H,0,-3.0993849574,-2.3992187454,-0.3941982788
H,0,-2.9419465608,-3.2157624652,-1.9707703194
O,0,-1.1521945191,-1.4999673836,-2.8820179056
H,0,-3.6512392005,-0.0571371035,0.1883382958
C,0,-2.2023541388,1.0073339021,1.7755494104
H,0,-1.4534080221,1.0395669208,0.9831337511
H,0,-2.1521146176,1.9500225876,2.3216658162
C,0,-1.9542750754,-0.1516290592,2.726336509

H,0,-2.633455948,-0.0752711693,3.5818694837
H,0,-0.9332571642,-0.0586435462,3.1059749307
N,0,-2.0698755526,-1.4479681191,2.0408298334
H,0,-3.0530844773,-1.6867348945,1.931799633
H,0,-1.6681269086,-2.1724570663,2.6294251591
Sum of electronic and zero-point Energies= -1177.800977
Sum of electronic and thermal Energies= -1177.782600
Sum of electronic and thermal Enthalpies= -1177.781656
Sum of electronic and thermal Free Energies= -1177.849629

Im2_D

C,0,0.4159261154,-0.6618163716,-0.4506751778
C,0,1.4973601682,-1.1728689313,0.3007557507
C,0,2.6931324493,-0.4972744001,0.366815515
C,0,2.8256750731,0.7095274659,-0.3224893471
C,0,1.7737266348,1.2400053085,-1.0646105801
C,0,0.5731725155,0.5612397635,-1.1330447529
C,0,-1.9971732459,-1.0107104244,-1.0316299792
N,0,-0.7405986387,-1.3986047494,-0.4752750597
H,0,1.372142345,-2.1099814536,0.8308588579
H,0,3.5176674394,-0.8929609641,0.9445353546
N,0,4.0779781445,1.423555487,-0.2622900236
H,0,1.8952130303,2.1810386243,-1.5841372596
H,0,-0.2429875384,0.9774515525,-1.7036928739
O,0,4.1839260105,2.4806244776,-0.8679992954
H,0,-0.8011839127,-2.1373635507,0.2151027504
O,0,4.9951621119,0.9485336573,0.3927107599
S,0,-2.7808264251,0.4922717467,-0.1610496678
C,0,-2.9591234774,-2.1847440702,-0.9767767346
H,0,-3.9232882542,-1.8814265019,-1.3874413514
H,0,-3.1124042072,-2.5341381961,0.0432859606
H,0,-2.5545998366,-3.0012874331,-1.579106362
O,0,-1.7800034693,-0.6370316832,-2.3735166121
H,0,-2.6338517149,-0.5714935539,-2.8207459433
C,0,-1.8780778253,0.7731942125,1.4050958115
H,0,-0.8232304726,0.5361423196,1.2702289839
H,0,-1.9525025831,1.8538678098,1.5448835903
C,0,-2.4377950668,0.0729545344,2.6290464456
H,0,-3.5016448381,0.3174107992,2.729317195
H,0,-1.9264388018,0.4902977088,3.5002068289
N,0,-2.1823641875,-1.370041483,2.6041907548
H,0,-2.755059057,-1.7884572913,1.8760183882
H,0,-2.5194434855,-1.7735374099,3.4738530731
Sum of electronic and zero-point Energies= -1177.777183
Sum of electronic and thermal Energies= -1177.759920
Sum of electronic and thermal Enthalpies= -1177.758976
Sum of electronic and thermal Free Energies= -1177.822878

Im3_D

C,0,0.3523475244,-0.0533229972,-0.0745462705
C,0,0.9895271822,1.2132918271,-0.0312016378
C,0,2.3451952503,1.335751496,-0.2078350247
C,0,3.1081891991,0.186825054,-0.4385667352
C,0,2.5110459596,-1.0709259653,-0.4980545953
C,0,1.1488017015,-1.1960201505,-0.3219555323
C,0,-1.8267628923,-1.2707783734,0.1725229175
N,0,-0.994871771,-0.0822032759,0.1250515759
H,0,0.3871086882,2.0948899533,0.1527709464
H,0,2.8178938822,2.3079691607,-0.1678027307
N,0,4.5272464459,0.3062839153,-0.6272067742
H,0,3.1138322746,-1.9493052561,-0.6870402559
H,0,0.7026535665,-2.1757439326,-0.3951234919
O,0,5.1818423867,-0.7025131155,-0.860553514
H,0,-1.4685701011,0.8234231355,0.2071118871
O,0,5.0425704728,1.415009262,-0.5496567943
S,0,-3.5919777664,-0.7408424701,0.3595767656
C,0,-1.5454154117,-2.1591753454,1.3770154634
H,0,-2.2010277377,-3.030772589,1.3531104345
H,0,-1.7160740125,-1.6036445242,2.2985425802
H,0,-0.5115033095,-2.503907943,1.3624068105
O,0,-1.6418166477,-2.0640710662,-0.9775619947
H,0,-1.7491595955,-1.5145456869,-1.7654215333
C,0,-3.7955553734,0.4738766321,-0.9942310326
H,0,-2.9334435904,0.3983708009,-1.6600589312
H,0,-4.6799186532,0.1816186812,-1.560800609
C,0,-3.9445515307,1.9006400736,-0.4804784483
H,0,-4.8987583711,2.0025138743,0.0455843703
H,0,-3.9799474633,2.5624917991,-1.3482452861
N,0,-2.8040293644,2.2939493011,0.3599717843
H,0,-2.9994311731,2.0509021389,1.3274582182
H,0,-2.6969977687,3.3026565863,0.336735438
Sum of electronic and zero-point Energies= -1177.781357
Sum of electronic and thermal Energies= -1177.764322
Sum of electronic and thermal Enthalpies= -1177.763378
Sum of electronic and thermal Free Energies= -1177.826198

Im4_D

C,0,0.2400484664,0.2415706256,-1.3467762286
C,0,0.7058058909,1.2335889099,-0.4507538014
C,0,1.8521476907,1.033297107,0.2817602805
C,0,2.5591362746,-0.1650862026,0.1353267691
C,0,2.1233741891,-1.1610758373,-0.7431227976
C,0,0.976063909,-0.9593228959,-1.4743484982
C,0,-1.5886329434,-1.4167452561,0.6842285352
N,0,-0.8753547054,0.453132289,-2.0858746321
H,0,0.1459046337,2.1557318647,-0.3462597154

H,0,2.2048352244,1.7915433479,0.9683593871
N,0,3.7495105288,-0.3789957215,0.9063117049
H,0,2.6801794931,-2.0837522548,-0.8390119408
H,0,0.617979149,-1.7255955609,-2.1524369924
O,0,4.3576065465,-1.4358368057,0.7792491076
H,0,-1.5286047539,1.1826713263,-1.787588471
O,0,4.1269119943,0.5003391041,1.6725319167
S,0,-2.4192108793,0.0707733335,1.2007818001
C,0,-0.4315233741,-1.7908394714,1.5657557319
H,0,-0.7975826784,-1.9946729829,2.5749950929
H,0,0.2798446668,-0.9632552162,1.6243748406
H,0,0.0562765844,-2.6773303826,1.1633358181
O,0,-1.9447681567,-2.058761883,-0.2781797451
H,0,-1.2845766703,-0.3490382661,-2.5463921276
C,0,-3.6957145694,0.2481022581,-0.0907320327
H,0,-3.3061246917,-0.2181369545,-0.9955755781
H,0,-4.591754735,-0.2829462928,0.2295008826
C,0,-4.0031207948,1.7190734023,-0.3290956013
H,0,-4.4052023748,2.170511853,0.5846886696
H,0,-4.7909193499,1.763831945,-1.0830526296
N,0,-2.8298934251,2.4362149965,-0.8467746807
H,0,-2.1783982242,2.613011776,-0.0848348509
H,0,-3.1222989155,3.3499718453,-1.1800732137
Sum of electronic and zero-point Energies= -1177.797620
Sum of electronic and thermal Energies= -1177.779393
Sum of electronic and thermal Enthalpies= -1177.778449
Sum of electronic and thermal Free Energies= -1177.844780

TS1_D

C,0,-0.3369811115,-0.6180070156,-0.8165636567
C,0,-0.9009971389,0.622571062,-1.1105120093
C,0,-2.1940041606,0.897404107,-0.7012070648
C,0,-2.887553079,-0.0877463358,-0.0113356421
C,0,-2.3461913119,-1.3326120828,0.2716925204
C,0,-1.050809441,-1.6040729762,-0.1414656183
C,0,1.9711757417,-1.3968757849,-0.6000876209
N,0,0.9952729694,-0.8325103705,-1.263026044
H,0,-0.3181881112,1.3661320968,-1.6408598393
H,0,-2.650470983,1.855413363,-0.9078597893
N,0,-4.2589719011,0.1971462723,0.4283937825
H,0,-2.9253632844,-2.080602692,0.7951111301
H,0,-0.6152251585,-2.5744230519,0.0489200793
O,0,-4.8552196258,-0.6620652724,1.0479453164
H,0,1.2964035415,-0.2545589004,-2.0459037332
O,0,-4.7366812526,1.280277753,0.1524757302
S,0,3.3780632639,0.7021095012,1.8000889647
C,0,3.3419191704,-1.4409281602,-1.1542069061
H,0,4.0075391154,-0.9658993067,-0.4290673371

H,0,3.3982617044,-0.9401749533,-2.1179485741
H,0,3.623347486,-2.4921650636,-1.2590077137
O,0,1.6889240487,-1.9460474181,0.5400718004
H,0,2.4992971421,-2.1521349822,1.0384952437
C,0,1.7679926499,1.4487348856,1.3122865105
H,0,1.0632649839,0.6574117591,1.03717693
H,0,1.3309310675,1.9654335826,2.1709150963
C,0,1.8688667087,2.4588043751,0.1739617679
H,0,2.4714257858,3.3086749075,0.5215321143
H,0,0.8671722902,2.8414569755,-0.0542042347
N,0,2.4255900955,1.857382124,-1.0475509819
H,0,3.2921004777,1.3948066791,-0.772084552
H,0,2.6909583169,2.5973099226,-1.6906396689
Sum of electronic and zero-point Energies= -1177.745973
Sum of electronic and thermal Energies= -1177.728430
Sum of electronic and thermal Enthalpies= -1177.727486
Sum of electronic and thermal Free Energies= -1177.793634

TS2_D

C,0,0.389012112,-0.1550612144,-0.5309676263
C,0,0.8250621441,0.8774022596,0.2985379244
C,0,2.1811670176,1.0517408219,0.5267012169
C,0,3.0677575606,0.1765473061,-0.0859371346
C,0,2.6559123763,-0.8572703427,-0.9158323664
C,0,1.2976730771,-1.0180857336,-1.1390353415
C,0,-1.7991428142,-1.2694630941,0.2214296281
N,0,-1.0127142799,-0.3465090203,-0.7493606872
H,0,0.1035840232,1.535372085,0.7690447786
H,0,2.5415771232,1.8453233815,1.1667448007
N,0,4.5050243818,0.3512526531,0.1543189603
H,0,3.3781394942,-1.5160410899,-1.3777236787
H,0,0.93615011,-1.8105988537,-1.7832232181
O,0,5.2762436711,-0.4207055677,-0.382276585
H,0,-1.5022143594,0.5708778583,-0.8560503875
O,0,4.8625983169,1.2595414167,0.879533986
S,0,-3.1221566027,-0.3331197134,1.1194543329
C,0,-0.9272821082,-1.9193073031,1.2763189406
H,0,-1.5400383616,-2.6274232713,1.8358007288
H,0,-0.5022082118,-1.1892891743,1.9680765183
H,0,-0.1190346289,-2.4716866703,0.7933308745
O,0,-2.251023882,-2.1229962874,-0.7621733567
H,0,-1.4873686892,-1.2817579782,-1.4086779773
C,0,-4.1004419898,0.3232264165,-0.2743597073
H,0,-3.8212553627,-0.256681813,-1.1567694951
H,0,-5.14891941,0.1139702815,-0.0602317001
C,0,-3.9029316412,1.8152977715,-0.5087856074
H,0,-4.3576056024,2.3808371724,0.3095769612
H,0,-4.4358671956,2.080980777,-1.4240566422

N,0,-2.4813895233,2.153735638,-0.6824980993
H,0,-2.07679593,2.3741660552,0.2242976819
H,0,-2.3947318152,2.9942872331,-1.2445957225

Sum of electronic and zero-point Energies=	-1177.728352
Sum of electronic and thermal Energies=	-1177.711871
Sum of electronic and thermal Enthalpies=	-1177.710926
Sum of electronic and thermal Free Energies=	-1177.773685

Im3a

C	1.136635687619	-0.790967334758	-0.597174167368
H	0.752727092960	1.833539277967	-1.407349256730
O	0.936475692300	1.639759011431	1.805925523982
H	0.492102546837	0.788250205741	1.908368183168
S	0.097747909613	-1.592871143033	0.606288313367
H	0.876561178895	2.253674240045	0.053277923460
O	0.889871713131	2.610812291623	-0.852358095474
H	1.861204843714	1.452753447101	2.008582822346
C	2.597116720607	-0.802579048824	-0.261092925572
H	2.858533328426	-1.618520210247	0.412533019977
H	3.176813896591	-0.864762042963	-1.182360232165
H	2.824817468768	0.147980067475	0.233106297139
O	0.680278231373	-0.258029342693	-1.584939070705
C	-1.541793730241	-1.155519705401	-0.041942856347
H	-2.240216122651	-1.855219980568	0.418650031671
H	-1.531710940709	-1.333090198131	-1.118866103996
C	-1.917160791032	0.283441647030	0.278049761841
H	-1.126936147569	0.953164643402	-0.079233224539
H	-1.987730502876	0.404627755001	1.360945071890
N	-3.226293960810	0.579609816849	-0.309622237017
H	-3.504125844586	1.517681828681	-0.035939389692
H	-3.130005270363	0.601867774269	-1.321722389229

Sum of electronic and zero-point Energies=	-838.677039
Sum of electronic and thermal Energies=	-838.661967
Sum of electronic and thermal Enthalpies=	-838.661023
Sum of electronic and thermal Free Energies=	-838.718734

TS2a

C,0,0.4812178373,4.1375391866,4.1431427814
H,0,1.5381039423,2.4986352066,3.8755551983
O,0,-0.4971909866,2.0666784375,1.8279599494
H,0,-1.2244606379,2.3800001058,2.4728468351
S,0,-1.6235902358,3.4329002347,4.1787338526
H,0,0.3310196263,2.5154830235,2.3245019441
O,0,1.1382054229,3.1587625561,3.28826358
H,0,-0.6423654888,2.4915166799,0.9658370315
C,0,0.2987419281,5.3980883567,3.3316971357
H,0,-0.3089795076,6.1053053291,3.8932593018
H,0,1.2883108035,5.8310521691,3.1571033173
H,0,-0.1723691813,5.1911024859,2.3698233823

O,0,0.9123272778,4.1524906238,5.3141618733
C,0,-1.4299246897,2.2140111868,5.5112037055
H,0,-2.3792920965,2.141124732,6.0445425565
H,0,-0.6867637432,2.6230035167,6.2044714971
C,0,-0.9952864371,0.8390732103,5.0290860507
H,0,-0.0571098908,0.9313746797,4.4677118869
H,0,-1.7456428157,0.4397616772,4.3430156838
N,0,-0.8803272726,-0.0759928044,6.1717771362
H,0,-0.6005247834,-0.9929026972,5.8357302453
H,0,-0.1216440712,0.2444541038,6.7685240554
Sum of electronic and zero-point Energies= -838.624614
Sum of electronic and thermal Energies= -838.612522
Sum of electronic and thermal Enthalpies= -838.611578
Sum of electronic and thermal Free Energies= -838.662632

Im4a

C,0,1.4406117139,1.5418876587,-0.217733427
H,0,1.2411814021,0.4922994107,-1.8090843248
O,0,0.3921525752,-0.7685822038,-2.4897612603
H,0,-2.6944442298,-2.5959439327,-1.0538444375
S,0,-2.6004619743,-1.2534686065,-1.0457880279
H,0,-0.480475322,-0.9113267581,-2.084637946
O,0,1.7999392143,1.2412630624,-1.4623745404
H,0,0.2122526458,-0.6172809143,-3.4255222298
C,0,2.2327753448,2.6672838383,0.3672985155
H,0,1.9323057886,2.8422992216,1.3969818717
H,0,3.2959627983,2.4271657361,0.3173554651
H,0,2.065631801,3.5661661499,-0.2294085419
O,0,0.5508403797,0.9478817142,0.3620639655
C,0,-1.9715881397,-1.0858365328,0.6616087059
H,0,-2.7566501607,-1.3732438997,1.3604902306
H,0,-1.7757878181,-0.0191274125,0.7827813528
C,0,-0.7045181284,-1.8882148388,0.9052681696
H,0,0.0155699998,-1.6846944804,0.1052024059
H,0,-0.9414221074,-2.9539996191,0.8705597407
N,0,-0.1812316784,-1.5664690544,2.2359930242
H,0,0.597176769,-2.1851305997,2.4433497379
H,0,0.2068771262,-0.6268839392,2.1997195499
Sum of electronic and zero-point Energies= -838.681040
Sum of electronic and thermal Energies= -838.666099
Sum of electronic and thermal Enthalpies= -838.665155
Sum of electronic and thermal Free Energies= -838.724786

Im3b

C,0,-2.3657383825,0.4059258652,-0.1431370007
C,0,-0.966011443,1.0030627711,-0.1315652346
S,0,-0.0155053427,0.2766080822,1.2541748886
N,0,-2.3316924004,-1.0385644258,-0.4179257953
H,0,-3.2716475198,-1.3550725535,-0.6374886986

H,0,-2.913644591,0.8920596741,-0.9517216386
H,0,-2.8850380392,0.6429611695,0.7914370242
H,0,-1.0206048102,2.0825284417,0.006372937
H,0,-2.0584648666,-1.5413779253,0.4229466486
H,0,-0.4602987892,0.7754698771,-1.069102939
C,0,1.6781905471,0.703814632,0.9199778266
O,0,2.5110536707,0.3424531187,1.7254238688
C,0,2.0099349071,1.4718194288,-0.3228416895
H,0,3.0673375191,1.730081198,-0.2987506586
H,0,1.4019716835,2.3750060677,-0.3965084011
H,0,1.8020531561,0.8527405823,-1.1996428771
H,0,-0.9981698991,-1.4225649575,-1.6215507361
O,0,-0.2399935579,-1.5767426845,-2.2341695472
H,0,-0.0648808419,-2.5217113618,-2.1781849773
Sum of electronic and zero-point Energies= -762.257455
Sum of electronic and thermal Energies= -762.245748
Sum of electronic and thermal Enthalpies= -762.244804
Sum of electronic and thermal Free Energies= -762.296396

TS2b

C	-2.821881943342	0.555879272905	-0.004913219483
C	-1.335844159104	0.817166143847	-0.187402359962
S	-0.302585052707	-0.280160181793	0.862323889760
N	-3.180062967891	-0.794088994701	-0.454611356564
H	-4.159773862372	-0.964059564733	-0.248203131021
H	-3.375368691259	1.277651622340	-0.611236194741
H	-3.088781288038	0.736618458705	1.043526974865
H	-1.118444437771	1.854656816362	0.073547782105
H	-2.652715828930	-1.459428555536	0.106045050427
H	-1.073550323542	0.668179314081	-1.238339176513
C	2.048686437361	-0.006134893676	-0.001751491978
O	2.804945389943	-0.376905541091	0.833835566750
C	1.930997177793	1.302884669940	-0.692604328124
H	2.827935030787	1.409754679517	-1.311790355575
H	1.916023296671	2.086794263539	0.062924556482
H	1.049134902139	1.357072972912	-1.323588660127
H	0.641950834210	-1.249190983785	-0.583465935439
O	1.576669241680	-1.140819842066	-1.006625553430
H	2.088172245293	-1.955387656834	-0.834331058553

Sum of electronic and zero-point Energies= -762.188061
Sum of electronic and thermal Energies= -762.177601
Sum of electronic and thermal Enthalpies= -762.176656
Sum of electronic and thermal Free Energies= -762.224841

Im4b

C,0,-2.9197482121,0.5829621448,0.0807370212
C,0,-1.422072997,0.548077995,-0.1573862981
S,0,-0.592525812,-0.9212901825,0.5541305583
N,0,-3.5957500663,-0.5356259457,-0.5823061882
H,0,-4.599650341,-0.4047375757,-0.501692946
H,0,-3.2992747597,1.5120781832,-0.3507964594
H,0,-3.1121421209,0.6188030673,1.1591705267

H,0,-0.9469589143,1.4015354431,0.3279461059
H,0,-3.3907845852,-1.3932907463,-0.0758813343
H,0,-1.1953354711,0.590655277,-1.2232345329
C,0,2.6173761145,0.0173566911,-0.2268222616
O,0,3.012991847,-0.1156347721,0.9110321811
C,0,1.9410399216,1.2328635499,-0.7685107443
H,0,2.700658542,1.8415580615,-1.2671717824
H,0,1.5045972048,1.8058440331,0.0464589223
H,0,1.1845466656,0.9605328565,-1.5030560969
H,0,-1.0798525313,-1.8221586627,-0.3158122173
O,0,2.8017233815,-0.931653989,-1.1570416054
H,0,3.2766721337,-1.6773824287,-0.7564458488
Sum of electronic and zero-point Energies= -762.258782
Sum of electronic and thermal Energies= -762.247128
Sum of electronic and thermal Enthalpies= -762.246184
Sum of electronic and thermal Free Energies= -762.298728