

Supporting Information

Iodine(I)-based and Iodine(III)-based Halogen Bond Catalysis on the

Friedel-Crafts Reaction: A Theoretical Study

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1. Structural Parameters

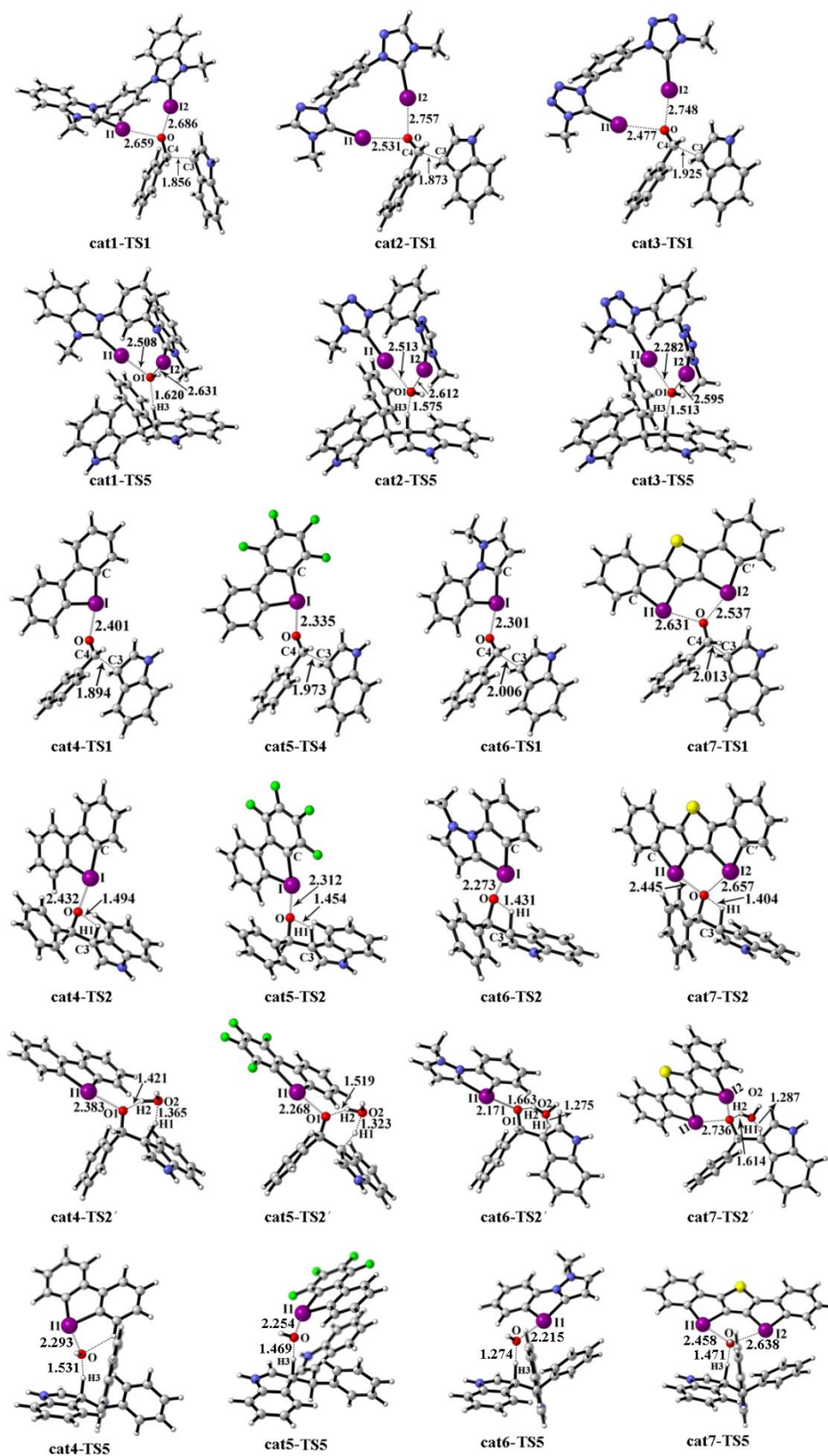


Figure S1. Geometric information of transition states. The bond lengths are in Å.

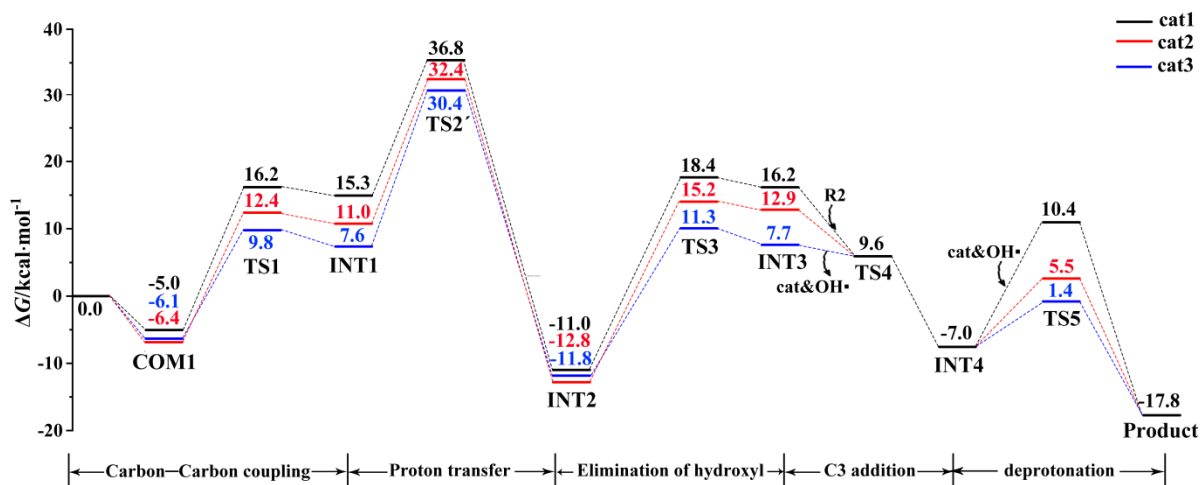
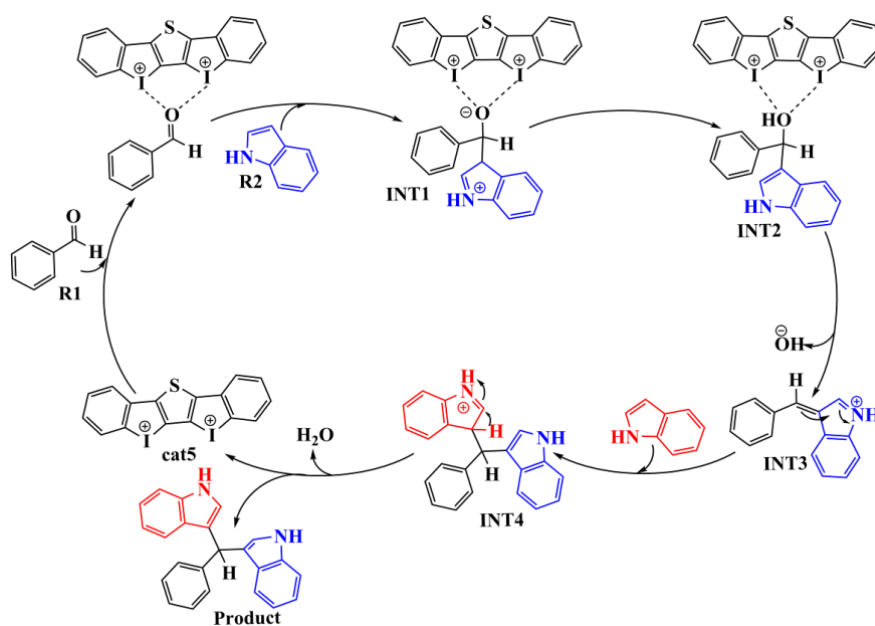


Figure S2. Gibbs free energy curves of water-assisted pathway catalyzed by iodine(I)-based halogen bond donors.



Scheme S1. Catalytic cycle for halogen bond catalyst catalyzed Friedel-Crafts reaction of benzaldehyde and indole.

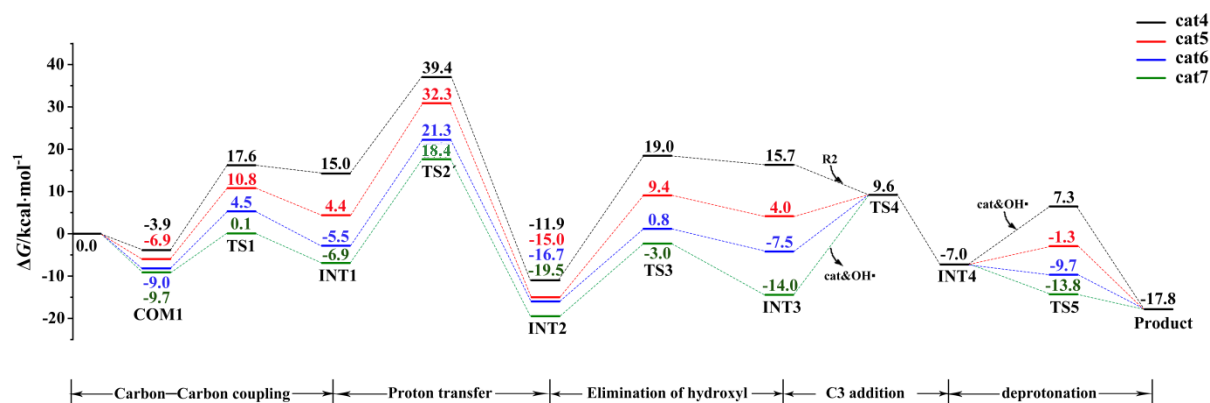


Figure S3. Gibbs free energy curves of water-assisted pathway catalyzed by iodine(III)-based halogen bond catalysts.

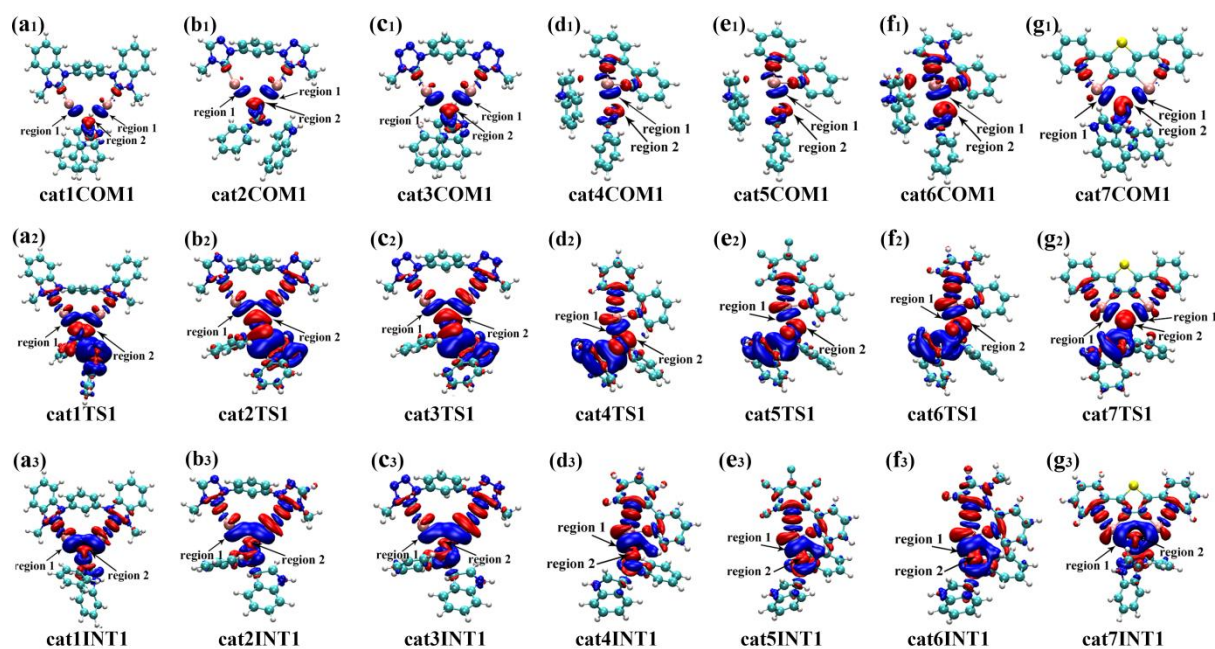


Figure S4. Plots of the computed density differences for COM1, TS1 and INT1. I, C, H, O, and N atoms are shown in pink, light blue, white, red, dark blue, respectively.

2. Energies and Cartesian Coordinates

R1 (benzaldehyde)

Sum of electronic and thermal Free Energies =
-345.44988 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -345.43896 Hartree

C	-0.27411100	2.02232900	0.00000000
O	-1.38220500	2.50755800	0.00000000
H	0.62360400	2.66661900	0.00000000
C	0.00000000	0.56844200	0.00000000
C	1.32583100	0.13423000	0.00000000
C	-1.04662600	-0.35864900	0.00000000
C	1.60994500	-1.22789400	0.00000000
H	2.12815400	0.86573800	0.00000000
C	-0.76126300	-1.71646200	0.00000000
H	-2.07139400	-0.00444600	0.00000000
C	0.56638200	-2.14971500	0.00000000
H	2.63817000	-1.56967500	0.00000000
H	-1.56744400	-2.44084300	0.00000000
H	0.78560000	-3.21153500	0.00000000

R2 (indole)

Sum of electronic and thermal Free Energies =
-363.67484 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -363.66402 Hartree

C	0.00000000	0.71254000	0.00000000
C	0.49662900	-0.61555900	0.00000000
C	-0.41906700	-1.68183200	0.00000000
C	-1.77361800	-1.40212800	0.00000000
C	-2.24411200	-0.07271700	0.00000000
C	-1.36962100	0.99898700	0.00000000
C	2.23689500	0.81181600	0.00000000
C	1.92993700	-0.52143800	0.00000000
H	-0.06592500	-2.70745600	0.00000000
H	-2.48971600	-2.21591100	0.00000000
H	-3.31205400	0.11288800	0.00000000
H	-1.72613400	2.02267700	0.00000000
H	1.03989700	2.56317500	0.00000000
H	3.19759100	1.30369500	0.00000000
H	2.63596800	-1.33739200	0.00000000
N	1.08258800	1.55433100	0.00000000

cat1

Sum of electronic and thermal Free Energies =
-1662.70715 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -1662.69719 Hartree

C	-0.00007400	0.72438800	0.29825500
C	-0.00007700	1.13004500	3.07192100
C	1.18495800	0.82029900	1.01376300
C	-1.18510500	0.82020400	1.01377600
C	-1.20592000	1.02501600	2.38734100
C	1.20576800	1.02514600	2.38732300
H	-2.15463900	1.09745100	2.90627100
H	2.15448600	1.09767400	2.90624100
C	2.99137700	-0.38331500	-0.18787800
N	4.12586600	-0.08889100	-0.81864400
C	-2.99130600	-0.38353100	-0.18804300
N	-4.12586200	-0.08921600	-0.81874300
I	2.22822900	-2.26679700	0.05475700
I	-2.22780200	-2.26688700	0.05441200
C	5.02276200	-1.05307600	-1.46060700
H	5.75084700	-0.49954800	-2.04699000
H	4.44547300	-1.69631100	-2.12285900
H	5.53106800	-1.64132100	-0.69721400
C	-5.02267600	-1.05342800	-1.46077600
H	-5.75030800	-0.49994300	-2.04776500
H	-5.53150300	-1.64126000	-0.69741000
H	-4.44521700	-1.69705600	-2.12249300
H	-0.00007700	1.28764300	4.14279800
C	3.24745400	1.81139700	-0.02214900
C	4.32912900	1.28817000	-0.73164500
C	-3.24777700	1.81111000	-0.02197200
C	-4.32937300	1.28779500	-0.7315210
N	2.42743300	0.73216100	0.30070700
N	-2.42757500	0.73196700	0.30072700
C	5.35058400	2.11014600	-1.20796700
C	5.22635800	3.46237300	-0.94128300
H	5.99671600	4.13905100	-1.29013500
C	4.12942500	3.98525800	-0.22908400
H	4.07972700	5.05175300	-0.04703600
C	3.11576700	3.17176500	0.24469900
C	-3.11632400	3.17146500	0.24506100
C	-4.13013900	3.98484400	-0.22858300
H	-4.08062600	5.05132200	-0.04638600
C	-5.22699900	3.46186500	-0.94082600
H	-5.99748800	4.13845500	-1.28955800
C	-5.35099000	2.10965300	-1.20769900

H	6.19652300	1.71268400	-1.75360700	Sum of electronic and thermal free energies + the entropy			
H	2.26744100	3.55946400	0.79508500	correction at 298.15K =		-1419.60638 Hartree	
H	-2.26805400	3.55923900	0.79548200	C	-0.03566500	1.39856700	-0.27448700
H	-6.19686800	1.71210500	-1.75337000	C	0.02345300	3.08172200	1.97714000
H	-0.00008100	0.58612400	-0.77795400	C	1.15540200	1.83841100	0.28095400
cat2				C	-1.19689000	1.82097400	0.35414300
Sum of electronic and thermal Free Energies =				C	-1.19484000	2.65177000	1.46586600
-1387.61553 Hartree				C	1.21366700	2.67197400	1.38830800
Sum of electronic and thermal free energies + the entropy				H	-2.13269200	2.95194500	1.91793100
correction at 298.15K =				H	2.17450700	2.98744100	1.77734700
-1387.60538 Hartree				C	2.96360000	0.22636600	-0.36250400
C	-0.04208400	1.39304500	-0.27109300	N	4.09990500	0.41137800	-1.02271600
C	0.00650500	3.08241900	1.97092000	C	-2.99164300	0.19624000	-0.31889000
C	1.15044100	1.83315500	0.28351900	N	-4.18479600	0.40282600	-0.86264800
C	-1.21013300	1.81551900	0.34662000	I	2.27541300	-1.50727500	0.45454600
C	-1.20950500	2.65205400	1.45426200	I	-2.19341600	-1.59516400	0.23026700
C	1.19939500	2.67184700	1.38780100	C	5.14402400	-0.56051900	-1.35600500
H	-2.14930500	2.95801200	1.89812100	H	5.91658200	-0.01328600	-1.88941700
H	2.15784400	2.99325100	1.77788700	H	4.71395900	-1.33371600	-1.99044200
C	2.94773800	0.23650900	-0.36886400	H	5.54031700	-0.97819300	-0.43205800
N	4.10471700	0.37409400	-1.02674500	C	-5.21300400	-0.57493100	-1.22751200
C	-2.98302400	0.19453700	-0.32735200	H	-6.01628000	-0.01731000	-1.70130000
N	-4.19658000	0.33999300	-0.87243200	H	-5.56819700	-1.06492600	-0.32240700
I	2.22933700	-1.48797200	0.45449400	H	-4.78132700	-1.29097000	-1.92489600
I	-2.13070000	-1.57129900	0.24215300	H	0.04533100	3.73042000	2.84297500
C	5.08317500	-0.68023700	-1.31471700	N	2.39038500	1.43209300	-0.33252800
H	5.88696200	-0.23014200	-1.89147100	N	-2.46473400	1.41656800	-0.18727700
H	4.60069800	-1.46493000	-1.89517100	H	-0.05243800	0.78836300	-1.17131100
H	5.47157200	-1.07086600	-0.37551900	N	-3.34299400	2.33246400	-0.63976900
C	-5.14633800	-0.72767700	-1.20478300	N	3.18338500	2.31985600	-0.96189100
H	-6.03687100	-0.25491600	-1.61049500	N	-4.37369700	1.71978500	-1.04211000
H	-5.39623600	-1.27757400	-0.29885900	N	4.20765200	1.70304000	-1.37443100
H	-4.69802000	-1.38331100	-1.94951200	cat4			
H	0.02442900	3.73455800	2.83454300	Sum of electronic and thermal Free Energies =			
N	2.38790000	1.44283600	-0.33109300	-759.29800 Hartree			
N	-2.47544000	1.41839400	-0.20137700	Sum of electronic and thermal free energies + the entropy			
H	-0.05731900	0.78108400	-1.16658100	correction at 298.15K =		-759.28745 Hartree	
C	-4.38164100	1.68103500	-1.04859000	C	-0.00753300	3.53398900	-0.90401700
H	-5.28033700	2.09869700	-1.47480400	C	-0.01644800	2.93472400	-2.16347100
C	4.20310100	1.69454700	-1.36005300	C	-0.01538100	1.55353500	-2.30201200
H	5.04243000	2.10179700	-1.90212100	C	-0.00348700	0.73279200	-1.16954400
N	-3.34761000	2.35670100	-0.64556300	C	0.00000000	1.38650000	0.06380600
N	3.16995300	2.36443900	-0.94483700	C	-0.00100300	2.75471500	0.24932400
cat3				C	0.00348700	-0.73279200	-1.16954400
Sum of electronic and thermal Free Energies =				C	0.00000000	-1.38650000	0.06380600
-1419.61656 Hartree							

I	0.00000000	0.00000000	1.63291700	C	-0.61439300	3.41090900	0.00004000
C	0.01538100	-1.55353500	-2.30201200	C	0.48193400	2.55388700	0.00006500
C	0.01644800	-2.93472400	-2.16347100	C	0.25800200	1.18216800	0.00000700
C	0.00753300	-3.53398900	-0.90401700	C	-1.06876400	0.74217200	-0.00003300
C	0.00100300	-2.75471500	0.24932400	C	-2.17063200	1.56648000	-0.00004900
H	-0.00743400	4.61300300	-0.81107600	C	0.84280800	-1.16798500	0.00014000
H	-0.02451100	3.55598100	-3.05066800	I	-1.19398200	-1.35199800	-0.00001100
H	0.02571700	-1.10549400	-3.28843300	C	1.93242100	-1.99611400	0.00002300
H	0.02451100	-3.55598100	-3.05066800	H	-2.75586700	3.62441800	-0.00003800
H	0.00743400	-4.61300300	-0.81107600	H	-0.43002400	4.47768100	0.00009000
H	-0.00282000	-3.20579800	1.23335400	H	1.96131500	-3.07289300	0.00013800
H	-0.02571700	1.10549400	-3.28843300	H	1.47612600	2.97088000	0.00015100
H	0.00282000	3.20579800	1.23335400	H	-3.18067500	1.17686600	-0.00010200
cat5				N	2.56646200	0.15105700	-0.00004200
Sum of electronic and thermal Free Energies =				C	3.39163000	1.36274300	-0.00007700
-1156.25211 Hartree				H	4.42095800	1.01317200	-0.00015600
Sum of electronic and thermal free energies + the entropy				H	3.19216000	1.93437000	-0.90469500
correction at 298.15K =				H	3.19223900	1.93433800	0.90456800
-1156.24163 Hartree				C	3.00824200	-1.10722800	-0.00003700
C	3.88044200	1.63312000	-0.00004900	H	4.07093500	-1.29990000	-0.00012200
C	2.99657600	2.70899500	-0.00002500	N	1.21744900	0.13424800	0.00009900
C	1.62112300	2.51572300	-0.00000400	cat7			
C	1.09630500	1.21829800	0.00000200	Sum of electronic and thermal Free Energies =			
C	2.03195300	0.17820400	-0.00002100	-1607.21999 Hartree			
C	3.40224300	0.32478200	-0.00005700	Sum of electronic and thermal free energies + the entropy			
C	-0.31880000	0.83900700	0.00000200	correction at 298.15K =			
C	-0.61228800	-0.52741500	-0.00003000	-1607.20975 Hartree			
I	1.08554200	-1.69726400	0.00003300	C	0.00686600	2.67728800	1.34221100
C	-1.42174000	1.68802700	0.00003300	C	-0.00875500	3.43622400	0.16685800
C	-2.71508900	1.18939200	0.00001800	C	0.00664800	4.81181600	0.10209800
C	-2.95555200	-0.17694300	-0.00003500	C	0.04001900	5.47833000	1.32599200
C	-1.88388300	-1.05262300	-0.00004700	C	0.05523300	4.77119500	2.52782300
H	4.95008700	1.80213400	-0.00006000	C	0.03809000	3.38371300	2.54728600
H	3.38455100	3.72000200	-0.00003400	C	0.00280800	1.23996500	1.16501200
H	0.95684000	3.36837700	0.00002600	H	-0.00426700	5.35358000	-0.83504500
H	4.07714900	-0.52179900	-0.00007300	H	0.05556200	6.56120100	1.33035100
F	-1.27534100	3.00791900	0.00003600	H	0.08218100	5.31260700	3.46509000
F	-3.73862500	2.02714200	0.00003200	H	0.05180700	2.84674900	3.48930600
F	-4.19602600	-0.63231800	-0.00003500	C	0.00000000	0.70453600	-0.09606300
F	-2.08223900	-2.36331300	-0.00007100	C	0.00875500	-3.43622400	0.16685800
cat6				C	-0.00686600	-2.67728800	1.34221100
Sum of electronic and thermal Free Energies =				C	-0.03809000	-3.38371300	2.54728600
-792.93422 Hartree				C	-0.05523300	-4.77119500	2.52782300
Sum of electronic and thermal free energies + the entropy				C	-0.04001900	-5.47833000	1.32599200
correction at 298.15K =				C	-0.00664800	-4.81181600	0.10209800
-792.92369 Hartree				C	-0.00664800	-4.81181600	0.10209800
C	-1.92016500	2.93626800	-0.00002000	C	0.00000000	-0.70453600	-0.09606300

C	-0.00280800	-1.23996500	1.16501200
H	-0.05180700	-2.84674900	3.48930600
H	-0.08218100	-5.31260700	3.46509000
H	-0.05556200	-6.56120100	1.33035100
H	0.00426700	-5.35358000	-0.83504500
S	0.00000000	0.00000000	2.37007100
I	0.04564300	-2.18352100	-1.52636900
I	-0.04564300	2.18352100	-1.52636900

Pre-complex (cat1)

Sum of electronic and thermal Free Energies =
-2008.15492 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -2008.14514 Hartree

C	2.70290900	-3.39620000	-1.33568100
O	1.84348200	-2.56029600	-1.56759800
C	3.16628400	-3.75201700	0.01150000
C	4.19879000	-4.68476800	0.13556100
C	2.59718800	-3.17035600	1.15123400
C	4.66711900	-5.03484400	1.39681100
H	4.62850400	-5.12690200	-0.75761300
C	3.06417800	-3.52409600	2.40729200
H	1.79068600	-2.45248300	1.04712200
C	4.09960600	-4.45420200	2.52796600
H	5.46926900	-5.75586200	1.49897700
H	2.62759700	-3.08079900	3.29429500
H	4.46263200	-4.72721100	3.51236900
H	3.18724300	-3.93268600	-2.16700600
C	-1.16107900	1.42216700	-0.11763100
C	-2.07158200	2.56371800	-2.50843900
C	-2.32497700	0.97738800	-0.73064000
C	-0.44455900	2.42621400	-0.75520500
C	-0.88421500	3.00772200	-1.93768000
C	-2.79422400	1.53621000	-1.91280700
H	-0.29669700	3.79065800	-2.40317800
H	-3.70874600	1.16239000	-2.35804100
C	-2.70523200	-1.37628600	-0.03699500
N	-3.65506100	-2.08102800	0.57422200
C	1.93525400	2.19452900	-0.08892800
N	2.86546000	2.93073400	0.51497700
I	-0.92952700	-2.12385600	-0.74762300
I	2.19347500	0.28865700	-0.80843300
C	-3.60014500	-3.51829700	0.84989600
H	-4.51272300	-3.79843100	1.36873400
H	-2.74119000	-3.73291300	1.48436000
H	-3.53129700	-4.06623500	-0.08881300

C	4.24835100	2.52264200	0.76802500
H	4.67770900	3.21479300	1.48696300
H	4.81522000	2.55232800	-0.16202800
H	4.25487400	1.51929100	1.19013300
H	-2.42503400	3.00715700	-3.43046100
C	-4.33554100	0.04835900	0.45395500
C	-4.70418600	-1.22206600	0.89845600
C	0.98622500	4.14225800	0.39524600
C	2.31199400	4.17090400	0.82947800
N	-3.07401700	-0.08580400	-0.12318600
N	0.78404400	2.88496300	-0.17200000
C	-5.92538000	-1.44339000	1.53446600
C	-6.74278200	-0.33856100	1.69868500
H	-7.70164200	-0.46307300	2.18667700
C	-6.36441300	0.94194400	1.25148000
H	-7.03976700	1.77445000	1.40587800
C	-5.15298000	1.16331000	0.62021000
C	0.12375600	5.22257800	0.56320800
C	0.65864100	6.33851100	1.18259200
H	0.03176600	7.20818000	1.33670900
C	1.99760700	6.37432100	1.61692500
H	2.37162100	7.27197000	2.09371500
C	2.85030600	5.29653000	1.45215000
H	-6.22033000	-2.42546900	1.88030800
H	-4.85044600	2.14282500	0.27077200
H	-0.90393800	5.18409500	0.22437900
H	3.87938700	5.32860400	1.78597800
H	-0.82629800	1.00584500	0.82664600

Pre-complex (cat2)

Sum of electronic and thermal Free Energies =
-1733.064411 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -1733.05448 Hartree

C	-3.11698600	-1.57992200	-1.53825500
O	-1.95966700	-1.20764800	-1.41408900
C	-4.12161200	-1.50451500	-0.47219600
C	-5.45044800	-1.80139000	-0.78487900
C	-3.76324800	-1.14087600	0.83191600
C	-6.42715500	-1.71563400	0.20072900
H	-5.70954400	-2.09074700	-1.79825000
C	-4.73875900	-1.06421100	1.81329500
H	-2.72379900	-0.94135600	1.06925600
C	-6.06953800	-1.34634100	1.49477600
H	-7.46068600	-1.93755100	-0.03606000
H	-4.47094300	-0.78995600	2.82667600

H	-6.82979800	-1.28233200	2.26506800	H	6.00453600	-0.93851400	1.54962600
H	-3.45959800	-1.99625100	-2.49818000	C	4.46432900	-0.49494200	-1.98142800
C	2.31334800	0.98789800	0.46101300	H	2.56971000	-0.38479300	-0.97614200
C	4.15807400	1.83738800	-1.47324300	C	5.84480200	-0.64841700	-1.82933100
C	2.25552400	2.26196200	-0.08687900	H	7.47804600	-0.92908000	-0.45721400
C	3.30051200	0.14046900	-0.02142700	H	4.03814000	-0.37726200	-2.97057000
C	4.22655400	0.54214300	-0.97443700	H	6.48333000	-0.64615300	-2.70556200
C	3.16203400	2.70448400	-1.04028500	H	3.89856200	-0.84388300	2.56236300
H	4.98263100	-0.15354500	-1.31832300	C	-2.40532500	0.41197400	-0.57185300
H	3.08144100	3.70985400	-1.43609400	C	-4.58989600	0.79714200	1.15309100
C	-0.08887400	3.02470000	0.26730200	C	-2.74389800	1.66799100	-0.09113100
N	-0.62045200	4.14620900	0.76809500	C	-3.17609200	-0.64861700	-0.11953300
C	2.49212100	-2.17864100	0.40396800	C	-4.26207700	-0.48459900	0.72873300
N	3.05076900	-3.24903900	0.98162900	C	-3.82031300	1.88425800	0.75799900
I	-1.10353800	1.41313900	-0.49369200	H	-4.83067700	-1.34799500	1.05351900
I	0.63485000	-2.07540800	-0.45673800	H	-4.04181700	2.88623800	1.10574500
C	-2.04872800	4.45433200	0.89533200	C	-0.65124400	3.03650200	-0.27920100
H	-2.13092200	5.44401900	1.33698800	N	-0.45235600	4.24675700	-0.78687200
H	-2.51603200	3.71502500	1.54417800	C	-1.71982900	-2.67793300	-0.33017400
H	-2.50428200	4.44802600	-0.09355600	N	-1.95636900	-3.85921300	-0.88685800
C	2.44822300	-4.57719300	1.13235400	I	0.70580500	1.79279600	0.61831500
H	3.17459100	-5.20789900	1.63857200	I	-0.02397500	-2.04741500	0.62523700
H	2.22483300	-4.98175100	0.14627300	C	0.78467300	5.02900900	-0.84324000
H	1.54310100	-4.49123900	1.73158800	H	0.55533000	5.93338100	-1.40071500
H	4.87223500	2.16648700	-2.21688300	H	1.54394800	4.44502100	-1.36023700
N	1.23375600	3.16842700	0.35245600	H	1.09288400	5.27162500	0.17233100
N	3.39047800	-1.19726400	0.49080000	C	-1.07996100	-5.03021500	-0.95404200
H	1.64046600	0.68093200	1.25404400	H	-1.62286400	-5.79539400	-1.50210600
C	4.29543800	-2.86638300	1.39176200	H	-0.86603100	-5.36392700	0.06008200
H	4.97962100	-3.53342500	1.89271400	H	-0.16871400	-4.75416400	-1.48197400
C	0.42592300	4.94618700	1.12937900	H	-5.43288700	0.94640500	1.81490100
H	0.29451200	5.92449600	1.56495600	N	-1.95265200	2.80116800	-0.48270100
N	4.52562500	-1.62157600	1.10030300	N	-2.84110700	-1.98008800	-0.54268300
N	1.56491100	4.37209000	0.88260200	H	-1.60359800	0.26876700	-1.28828200
Pre-complex (cat3)				N	-3.72856300	-2.74570100	-1.20669300
Sum of electronic and thermal Free Energies =				N	-2.51309100	3.86507500	-1.08966300
-1765.06511 Hartree				N	-3.19329700	-3.87327400	-1.41115300
Sum of electronic and thermal free energies + the entropy				N	-1.60896200	4.73041300	-1.27057400
correction at 298.15K =				Pre-complex (cat4)			
-1765.05514 Hartree				Sum of electronic and thermal Free Energies =			
C	3.37432900	-0.65437500	1.61339300	-1104.742864 Hartree			
O	2.16505800	-0.45959900	1.61751800	Sum of electronic and thermal free energies + the entropy			
C	4.20580500	-0.65313200	0.40779900	correction at 298.15K =			
C	5.58623900	-0.81341800	0.55605300	-1104.73266 Hartree			
C	3.64302600	-0.49570900	-0.86548500	C	-4.76925400	-1.21737500	1.19903100
C	6.40700800	-0.80795300	-0.56560900	C	-5.03183000	0.15245300	1.23468900

C	-4.08966900	1.07368200	0.79862600	C	0.08597500	1.31181800	-0.67873700
C	-2.85399700	0.63503600	0.31255900	I	0.14361300	-0.77623100	-0.89990700
C	-2.63493900	-0.74403100	0.29494200	C	-1.29212800	3.11971400	0.02081900
C	-3.54988100	-1.68949700	0.72362900	C	-0.25092400	3.98172000	-0.29773400
C	-1.77320100	1.49531800	-0.17984900	C	0.95096000	3.50263100	-0.81092400
C	-0.59893000	0.88336400	-0.62585800	C	1.13843400	2.13739000	-1.01386700
I	-0.73576700	-1.19906300	-0.43670100	H	-2.21766200	3.51650400	0.41305800
C	-1.81295200	2.89174600	-0.25149400	H	-0.38328500	5.04575000	-0.14505300
C	-0.72585100	3.59866800	-0.74568000	H	1.75334100	4.18584700	-1.06016600
C	0.42123000	2.93821800	-1.18425400	H	2.06532500	1.75103600	-1.41555900
C	0.50070700	1.54952300	-1.13165700	C	3.81901700	-0.71975900	-1.34624600
H	-5.51355200	-1.92502800	1.54314800	O	2.67226800	-0.48401600	-1.69816600
H	-5.98524900	0.50501700	1.60886600	H	4.53733900	-1.10984700	-2.08305600
H	-2.69914800	3.41978500	0.07984900	C	4.33944200	-0.52720000	0.01015100
H	-0.77299400	4.67975000	-0.79381500	C	5.64864600	-0.94078800	0.27217000
H	1.26191500	3.49964400	-1.57306400	C	3.56468900	0.04917500	1.02448000
H	1.38227000	1.02511900	-1.47440700	C	6.18010400	-0.79265200	1.54765100
H	-4.30926300	2.13404400	0.83502000	H	6.23850400	-1.37954000	-0.52612100
H	-3.33544100	-2.75055200	0.69434100	C	4.09943200	0.19944200	2.29404800
C	3.09058100	-1.26665900	-1.22002400	H	2.55656500	0.39003500	0.81908000
O	1.88257600	-1.32422100	-1.37047400	C	5.40469400	-0.22417700	2.55453800
H	3.75519500	-1.74407100	-1.95756800	H	7.19277400	-1.11581400	1.75621600
C	3.76439400	-0.58545000	-0.10577000	H	3.50710300	0.64744200	3.08274800
C	5.16017100	-0.52723100	-0.11505500	H	5.81754100	-0.10548500	3.54989700
C	3.04053600	-0.00135600	0.94033900	F	-3.88427500	2.09870800	0.94164700
C	5.83365300	0.11993200	0.91472300	F	-5.48901200	0.02317600	1.32906400
H	5.70820400	-0.98802200	-0.93063900	F	-4.70341700	-2.49179700	0.74269500
C	3.71486300	0.63914600	1.96813200	F	-2.20551200	-2.92359000	-0.26519200
H	1.95794100	-0.05915900	0.95122900	Pre-complex (cat6)			
C	5.11017400	0.70155800	1.95227300	Sum of electronic and thermal Free Energies =			
H	6.91583000	0.17006100	0.91013400	-1138.38614 Hartree			
H	3.16110000	1.09024800	2.78278200	Sum of electronic and thermal free energies + the entropy			
H	5.63342300	1.20502200	2.75724400	correction at 298.15K = -1138.37599 Hartree			
Pre-complex (cat5)				C	-2.88257300	-0.92388400	-0.12544700
Sum of electronic and thermal Free Energies =				O	-1.86750500	-0.26102800	0.06020000
-1501.70177 Hartree				H	-2.81065800	-1.99638500	-0.36247700
Sum of electronic and thermal free energies + the entropy				C	-4.22874000	-0.36573900	-0.05129600
correction at 298.15K = -1501.69161 Hartree				C	-5.31284600	-1.21642800	-0.28457500
C	-3.87864500	-1.47807700	0.53593400	C	-4.43281700	0.98830000	0.24493300
C	-4.27755300	-0.18436900	0.83591200	C	-6.60689000	-0.71361000	-0.22367900
C	-3.42789900	0.89021100	0.62647400	H	-5.13328300	-2.26238100	-0.51081900
C	-2.14896300	0.70791300	0.10859500	C	-5.72480100	1.48368900	0.30399800
C	-1.78485100	-0.61070100	-0.17994500	H	-3.57979100	1.63253100	0.42670900
C	-2.61141000	-1.69137200	0.02319600	C	-6.80848000	0.63268200	0.06901400
C	-1.14522100	1.74040800	-0.16727400	H	-7.45340100	-1.36503200	-0.40347000

H	-5.89714300	2.52874000	0.53169700	C	0.67842600	-0.86679200	-0.18111700
H	-7.81756900	1.02619800	0.11623200	C	1.18463000	-2.00266600	0.39631200
C	4.83356500	-1.95963000	0.04770300	S	-0.07728000	-3.04331700	0.95377400
C	5.34020400	-0.66606600	-0.00152400	I	2.19644700	0.32437200	-0.89214000
C	4.50737400	0.44813100	-0.03369300	I	-2.19598000	0.43914200	-0.86381100
C	3.13207800	0.24656500	-0.01548800	C	0.10956200	3.79849000	0.15557300
C	2.64123400	-1.06098900	0.03143400	C	0.15238900	5.19424800	0.25104100
C	3.45876100	-2.17314900	0.06417900	C	0.10186700	3.00680100	1.31405400
C	0.79392500	0.88940200	-0.02392500	C	0.18838900	5.79910700	1.50042800
I	0.55073100	-1.13806600	0.04433900	H	0.15652300	5.79062000	-0.65534900
C	-0.00324500	2.00575800	-0.05629700	C	0.13765900	3.61543000	2.55693800
H	5.50383800	-2.80948300	0.07245400	H	0.06650500	1.92457200	1.24274300
H	6.41105600	-0.50700300	-0.01526900	C	0.18128700	5.00941300	2.64748400
H	-1.07737700	2.06197600	-0.05311100	H	0.22163000	6.87851300	1.58251000
H	4.94906500	1.43073500	-0.07068300	H	0.13175900	3.01355200	3.45742400
H	3.05045200	-3.17566800	0.10152700	H	0.20905300	5.48027600	3.62352800
N	2.15821300	2.58101100	-0.07977500	H	0.08393500	3.89867000	-2.02430600
C	3.38894500	3.37488600	-0.09184000	H	2.71884000	-4.10730300	1.48811300
H	3.06723600	4.41332000	-0.10797100	H	6.48979700	-2.38725800	0.36244700
H	3.95612200	3.17640800	0.81581200	H	5.34685200	-0.43668300	-0.65055900
H	3.95758900	3.14941400	-0.99194800	H	-2.91756700	-3.98882200	1.47178500
C	0.91148500	3.05625400	-0.09077000	H	-6.60677800	-2.09069800	0.36054700
H	0.74732100	4.12300400	-0.12059000	H	-5.37664900	-0.18065000	-0.62842300
N	2.10389600	1.23360400	-0.03965700	H	-5.38301400	-3.97092600	1.40015000
				H	5.18266900	-4.19956400	1.42157700

Pre-complex (cat7)

Sum of electronic and thermal Free Energies =
-1952.67414 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -1952.66413 Hartree

C	0.07477900	3.20423600	-1.17276300
O	0.03727300	1.99042500	-1.38766100
C	-2.72989300	-2.09397000	0.45944300
C	-3.46377700	-1.05106600	-0.11696000
C	-4.84250300	-1.00553700	-0.17349600
C	-5.52405000	-2.08398500	0.38547000
C	-4.83103900	-3.14403300	0.97093400
C	-3.44427500	-3.15898800	1.01340900
C	-1.29002700	-1.94403600	0.40046700
C	-0.73277800	-0.83271200	-0.17755300
C	3.39631400	-1.21655300	-0.13495500
C	2.61624400	-2.21909300	0.45227000
C	3.28244500	-3.30780800	1.02001600
C	4.66852600	-3.35479400	0.98037500
C	5.40837000	-2.33324300	0.38407800
C	4.77578600	-1.23259000	-0.18909500

Cat1-TS1

Sum of electronic and thermal Free Energies =
-2371.78395 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -2371.77428 Hartree

C	3.19392500	0.52153400	-0.58954800
C	6.41516200	-0.67619600	-0.88382900
C	5.54929000	-0.63785000	0.21616500
C	6.04308500	-0.22900900	1.45407800
C	7.38347900	0.12920500	1.54301200
C	8.22475100	0.09693500	0.42053800
C	7.75266500	-0.30787900	-0.82176100
H	9.26288000	0.38928600	0.52457200
H	8.39084200	-0.34035500	-1.69654200
H	5.39618300	-0.18938200	2.32361200
H	7.78876400	0.44442900	2.49744000
C	4.42713900	-1.39274900	-1.62621000
N	5.67092100	-1.14481100	-1.97955500
H	3.70357600	-1.74488600	-2.34800200
H	6.03279900	-1.24346200	-2.92384800

C	4.20905200	-0.99869800	-0.26817700	C	-5.72250600	5.09748700	-0.53087700
H	3.49527300	-1.52778500	0.35208200	H	-6.44491700	5.88005100	-0.72787700
O	2.04299200	0.14007500	-1.07404600	C	-6.08068200	4.03516300	0.32005700
H	3.87231100	1.04862300	-1.27849400	H	-7.07137000	4.02315000	0.75778900
C	3.19236200	1.19037100	0.76401400	C	-5.20182100	3.00452800	0.61241300
C	4.04037800	2.26861300	1.00944800	C	-4.62744800	-3.66871400	1.06978500
C	2.32669500	0.75383800	1.76888300	C	-5.31893900	-4.86097300	0.93052400
C	4.02453500	2.90860300	2.24767300	H	-6.30769700	-4.95068300	1.36353700
H	4.71442100	2.60786500	0.22844300	C	-4.77302600	-5.95935400	0.23972300
C	2.31423500	1.38560400	3.00677600	H	-5.35405900	-6.86961600	0.15645900
H	1.66124200	-0.08197800	1.57647100	C	-3.51464900	-5.90741800	-0.33706700
C	3.16447200	2.46583500	3.24816300	H	-4.19120500	5.98238500	-1.77988100
H	4.68421400	3.74937300	2.42992500	H	-5.46956400	2.18360300	1.26602500
H	1.64198900	1.03968200	3.78405200	H	-5.03991600	-2.81854400	1.59895900
H	3.15276700	2.96021800	4.21287200	H	-3.09204800	-6.74842400	-0.87222200
C	-2.68767900	-0.18871000	0.24075200	H	-2.74090900	-0.26958800	-0.83937100
C	-2.61088500	0.01784200	3.03263000	cat1-INT1			
C	-2.74893500	1.04713700	0.87192500	Sum of electronic and thermal Free Energies =			
C	-2.54056900	-1.31439000	1.04073100	-2371.78536 Hartree			
C	-2.50709200	-1.22953100	2.42740300	Sum of electronic and thermal free energies + the entropy			
C	-2.71885500	1.16604500	2.25589100	correction at 298.15K = -2371.77571 Hartree			
H	-2.39167200	-2.13118700	3.01779400	C	-3.21170900	-0.33952900	0.40770000
H	-2.76824900	2.14835000	2.71116100	C	-5.28413100	-0.70489900	-2.37986800
C	-1.85250500	2.76042800	-0.68670400	C	-5.22903900	0.07775900	-1.22713600
N	-2.28322900	3.89290400	-1.24257800	C	-6.41578600	0.42478300	-0.59447300
C	-1.33856500	-3.05996700	-0.25634900	C	-7.61292200	-0.03951500	-1.13939700
N	-1.55779900	-4.31851200	-0.63590300	C	-7.63297700	-0.83413800	-2.28961300
I	-0.00172800	1.83114800	-0.90404800	C	-6.45371100	-1.18395400	-2.94196000
I	0.32560200	-1.87786700	-0.63410600	H	-8.58084200	-1.17943100	-2.68428200
C	-1.55574100	4.77824200	-2.14810500	H	-6.44802700	-1.79136500	-3.83856200
H	-1.52126200	5.77448800	-1.70880900	H	-6.41516900	1.04159800	0.29680500
H	-2.07575600	4.80644200	-3.10509800	H	-8.54945600	0.22162200	-0.66086600
H	-0.54578000	4.40163600	-2.28612900	C	-3.10248700	-0.27595700	-2.06531500
C	-0.67291900	-5.17475800	-1.42288500	N	-3.94994500	-0.88026200	-2.83285000
H	-1.04179600	-5.22751200	-2.44703100	H	-2.03774800	-0.31520600	-2.25752100
H	-0.66823800	-6.16594600	-0.97255200	H	-3.69295500	-1.42622800	-3.65490100
H	0.33361500	-4.76481300	-1.40603800	C	-3.78759800	0.35454700	-0.92011400
H	-2.58408200	0.09755400	4.11188900	H	-3.53127100	1.41436300	-0.82633400
C	-3.94575500	3.08212100	0.01759200	O	-1.87451300	-0.08140900	0.50228500
C	-3.59009900	4.13229300	-0.82654200	H	-3.42870600	-1.41554900	0.29786200
C	-3.36318400	-3.62158000	0.48886700	C	-4.02040200	0.17457500	1.58576100
C	-2.81910600	-4.70888200	-0.19287100	C	-4.93569700	-0.65192500	2.23352000
N	-2.83627200	2.24004100	0.07797900	C	-3.86563200	1.49253200	2.01847800
N	-2.41115700	-2.60548900	0.42483700	C	-5.69460200	-0.16860700	3.29891400
C	-4.47174200	5.16876900	-1.12280300	H	-5.05922700	-1.67755400	1.89879600

C	-4.62220800	1.97919100	3.07911900	H	5.69566000	6.30971600	-1.86999700
H	-3.15069300	2.13983800	1.51925600	C	3.75212200	5.49846500	-1.52210700
C	-5.54165400	1.14855600	3.72071600	H	3.14226000	-6.57338000	-1.20840900
H	-6.40409200	-0.82042800	3.79633700	H	5.70765100	-2.56327300	0.42464000
H	-4.49776700	3.00535300	3.40663800	H	5.71053500	2.48969400	0.12854900
H	-6.13213400	1.52794800	4.54697700	H	3.20749100	6.31735800	-1.97518200
C	2.86373700	-0.01452500	0.11891400	H	2.47879300	-0.06387800	-0.89321000
C	3.91791600	0.11724500	2.70910800	Cat1-TS2			
C	3.11399000	-1.16984500	0.85044000	Sum of electronic and thermal Free Energies =			
C	3.10883700	1.20732100	0.73348500	-2371.75112 Hartree			
C	3.63771300	1.28900400	2.01615700	Sum of electronic and thermal free energies + the entropy			
C	3.64430300	-1.11860300	2.13402300	correction at 298.15K = -2371.74146 Hartree			
H	3.81847700	2.26025900	2.46232400	C	2.74959100	-2.36688700	-0.19366800
H	3.82882900	-2.03948800	2.67523800	O	1.63770100	-1.56800000	-0.58490500
C	1.58512800	-2.95012000	0.02801600	H	2.57989500	-3.41936800	-0.45939100
N	1.71285200	-4.19729000	-0.42860400	C	3.10920300	-2.28804500	1.27414900
C	1.59993600	2.91955700	-0.26752200	C	2.23712900	-1.72020100	2.19922400
N	1.73947400	4.09989400	-0.87193400	C	4.33162300	-2.80239000	1.71566500
I	-0.17169200	-1.78370400	0.28401700	C	2.58459900	-1.65672800	3.54898200
I	-0.15622200	1.86324600	0.10802700	H	1.28525300	-1.32448400	1.86587900
C	0.64251200	-5.10617300	-0.82589300	C	4.67918000	-2.74003400	3.05983500
H	0.66122900	-5.98103600	-0.17642700	H	5.01829900	-3.24319300	0.99824000
H	0.80030500	-5.40494200	-1.86186500	C	3.80585100	-2.16201300	3.98162300
H	-0.31274600	-4.59655800	-0.73091000	H	1.89849900	-1.20979900	4.25980700
C	0.68471200	4.97185000	-1.38089600	H	5.63322800	-3.13567600	3.38953400
H	-0.28143000	4.59620600	-1.05465500	H	4.07838500	-2.10780600	5.02941500
H	0.73152200	4.98931100	-2.46957200	C	5.67218700	-0.69803200	-1.93501200
H	0.84183400	5.97284100	-0.98124500	C	4.76681300	-0.70593500	-0.86448900
H	4.32842800	0.16723200	3.70956700	C	4.89297700	0.25568000	0.14076400
C	3.77182300	-3.43108600	-0.01065200	C	5.91243200	1.19260100	0.02857700
C	3.06141000	-4.54069800	-0.46526900	C	6.79524800	1.18904900	-1.06287700
C	3.78834500	3.34046500	-0.39243300	C	6.68937600	0.23979200	-2.06932700
C	3.09477800	4.40060400	-0.97254000	C	4.30388200	-2.43281800	-2.30596700
N	2.81870900	-2.45498700	0.28200000	C	3.81288200	-1.79568100	-1.13141000
N	2.82237800	2.42878000	0.03262800	H	4.22095900	0.26744800	0.99151800
C	3.70010300	-5.71413300	-0.85750700	H	6.03228500	1.94224100	0.80208300
C	5.08368600	-5.71863200	-0.77210000	H	7.57630700	1.93792200	-1.11837400
H	5.62826700	-6.60834700	-1.06394400	H	7.36408400	0.22266300	-2.91674800
C	5.80023100	-4.59696300	-0.31644700	H	5.81136100	-1.97769900	-3.65304600
H	6.88124400	-4.64666700	-0.26882700	H	3.90178600	-3.29588200	-2.81939300
C	5.16120000	-3.42992000	0.07328800	H	2.72751400	-1.28060700	-1.54049700
C	5.17861500	3.31686600	-0.32491500	N	5.34126000	-1.76790300	-2.77725300
C	5.83556800	4.40876400	-0.86928100	C	-2.50909500	0.96424400	-0.22161100
H	6.91802200	4.43902100	-0.84284600	C	-3.26720100	1.55806600	-2.85185100
C	5.13606000	5.47939300	-1.45698900	C	-3.28449700	0.08066800	-0.96252300

C	-2.08311400	2.12952800	-0.84731400	-2448.18874 Hartree			
C	-2.45613900	2.44156100	-2.14910300	Sum of electronic and thermal free energies + the entropy			
C	-3.67433200	0.36501500	-2.26567000	correction at 298.15K =			-2448.17907 Hartree
H	-2.10564300	3.36158800	-2.60236200	C	-2.88506900	0.14221200	0.30216600
H	-4.28145100	-0.34853500	-2.81094300	C	-3.03509100	0.04874800	3.09673100
C	-2.89993200	-2.21933600	-0.10132800	C	-2.85421600	1.30465200	1.06213700
N	-3.64882900	-3.21471000	0.37474000	C	-2.94316800	-1.06928700	0.97888000
C	0.05693800	2.84941500	0.19544200	C	-3.02481700	-1.13295000	2.36454900
N	0.53431600	3.94152900	0.79109200	C	-2.93520800	1.27493900	2.44898900
I	-0.81549700	-2.15782500	-0.34929200	H	-3.07088500	-2.09773000	2.85640200
I	1.04850700	1.05795600	-0.12267400	H	-2.91098600	2.20271500	3.00884000
C	-3.20046600	-4.53094800	0.81950600	C	-1.65089300	3.03902300	-0.25059900
H	-3.36655500	-4.61878700	1.89299500	N	-1.89922200	4.27478400	-0.68525600
H	-2.14308100	-4.64451200	0.59591000	C	-1.85334100	-2.80401500	-0.42585000
H	-3.77172100	-5.29064400	0.28746500	N	-2.18314000	-3.98223400	-0.95445100
C	1.87389200	4.12159200	1.34779200	I	0.07906200	1.89602900	-0.52534900
H	1.85636000	3.89727100	2.41430100	I	-0.03466200	-1.82397500	-0.58190600
H	2.17374500	5.15475800	1.18537000	C	-1.00946100	5.15118600	-1.44243900
H	2.56907600	3.46144100	0.83419600	H	-1.50627600	5.43444100	-2.36981300
H	-3.56338600	1.78906700	-3.86713800	H	-0.08713000	4.62196000	-1.66620100
C	-5.01689000	-1.50315100	-0.07607700	H	-0.79430600	6.03641200	-0.84480200
C	-4.98000600	-2.80943400	0.40796900	C	-1.33731600	-4.84951200	-1.77180600
C	-1.60374700	4.33280700	0.25751300	H	-1.53229000	-5.88202600	-1.48754000
C	-0.47761400	4.89627500	0.85647400	H	-0.29272900	-4.61569800	-1.58147900
N	-3.69799500	-1.16442800	-0.37879900	H	-1.57358000	-4.69693200	-2.82481700
N	-1.23460800	3.04788200	-0.13916800	H	-3.09766400	0.01322300	4.17686300
C	-6.13147300	-3.47573800	0.81962000	C	-3.71978200	3.56427200	0.40402600
C	-7.31838800	-2.76731600	0.72045900	C	-3.18344000	4.64393900	-0.29480700
H	-8.24311600	-3.24069400	1.02706900	C	-3.97753900	-3.19160500	0.12446600
C	-7.35460600	-1.44801600	0.23191600	C	-3.51065900	-4.26094600	-0.63854500
H	-8.30649500	-0.93446600	0.17362300	N	-2.73569600	2.57635600	0.40726100
C	-6.20663900	-0.78735700	-0.17638600	N	-2.91535500	-2.29518900	0.23191100
C	-2.80843400	5.02254800	0.15053500	C	-3.90381500	5.81787600	-0.50198600
C	-2.82751800	6.30391700	0.67627400	C	-5.18402400	5.85248400	0.02667400
H	-3.74102500	6.88315600	0.62018900	H	-5.78582400	6.74322600	-0.10587200
C	-1.69291700	6.87364000	1.28432000	C	-5.72522200	4.76012900	0.73033200
H	-1.75856100	7.87871200	1.68263700	H	-6.73222600	4.83409400	1.12237100
C	-0.49631900	6.18375700	1.38866800	C	-5.00680000	3.59286500	0.93369300
H	-6.09489800	-4.49037000	1.19624000	C	-5.27955500	-3.14473400	0.61498900
H	-6.22778100	0.22770200	-0.55335000	C	-6.08959600	-4.22349100	0.30069000
H	-3.67745400	4.57580000	-0.31644400	H	-7.11208900	-4.23644000	0.65767500
H	0.37738500	6.61591200	1.85996200	C	-5.62144600	-5.30293000	-0.47222900
H	-2.24025700	0.74674300	0.80624000	H	-6.29435900	-6.12234900	-0.69322500
Cat1-TS2'				C	-4.32519500	-5.34499900	-0.95871500
Sum of electronic and thermal Free Energies =				H	-3.48248300	6.65404700	-1.04601900

H	-5.41749600	2.74774200	1.47220400	C	2.86473300	-3.07537400	0.62744800
H	-5.63208700	-2.30957800	1.20759000	C	1.90288000	-2.64668800	1.53779800
H	-3.96134900	-6.17076000	-1.55725200	C	3.93095200	-3.85639500	1.08069300
H	-2.85925600	0.17803800	-0.78129300	C	2.00822600	-2.98590200	2.88710000
C	2.92124200	0.07323000	0.22848600	H	1.07590000	-2.02995000	1.21000000
C	6.25768000	1.84291800	0.25736100	C	4.03662000	-4.19537200	2.42377200
C	5.59817800	0.60287300	0.24767300	H	4.68506700	-4.19090100	0.37462700
C	6.34292900	-0.54255400	0.55546300	C	3.07458000	-3.75725800	3.33409500
C	7.68893900	-0.39792700	0.86476000	H	1.25515000	-2.63989400	3.58615400
C	8.31788400	0.85656000	0.85996900	H	4.87013700	-4.80013600	2.76249000
C	7.60767700	2.00502900	0.54799000	H	3.15804000	-4.01824800	4.38282400
H	9.37173000	0.92792000	1.10117800	C	5.58747900	-0.16851000	-1.33116400
H	8.07204800	2.98365400	0.53163600	C	4.64550000	-0.76867100	-0.45899600
H	5.89171000	-1.52651800	0.55369800	C	4.55906900	-0.29181500	0.86395900
H	8.27025600	-1.27848900	1.11258600	C	5.38194300	0.74824100	1.25805500
C	4.13851600	2.27979000	-0.29544100	C	6.30155700	1.33607100	0.36480700
N	5.31944300	2.82298200	-0.08156500	C	6.41892700	0.88530000	-0.93729500
H	3.28808200	2.89298600	-0.56445000	C	4.54558200	-1.78251700	-2.47539000
H	5.52862300	3.81218900	-0.18285700	C	3.98019400	-1.79948000	-1.22413900
C	4.20583100	0.85759700	-0.18843200	H	3.85877300	-0.72639500	1.56799700
H	4.15940800	0.60932200	-1.46138000	H	5.32109300	1.12039200	2.27459600
O	1.95811200	0.13794200	-0.79238800	H	6.92987000	2.15051500	0.70685600
H	2.52866900	0.55254900	1.13512900	H	7.12652500	1.32490000	-1.63099100
C	3.27588700	-1.35805700	0.58965500	H	6.06862200	-0.60536700	-3.35523400
C	3.41330400	-1.72881000	1.92566200	H	4.32966500	-2.40677800	-3.33061900
C	3.48782800	-2.31045600	-0.40936100	H	1.55126500	-1.89926500	-2.07812600
C	3.77002200	-3.03257300	2.26453300	N	5.50010200	-0.80800900	-2.54431700
H	3.24509800	-0.99112300	2.70454500	C	-2.29357800	1.24645000	-0.17201300
C	3.84426200	-3.61283100	-0.07368700	C	-3.10808700	2.12424600	-2.70546700
H	3.37915000	-2.03215400	-1.45280000	C	-3.26514700	0.56470900	-0.89266500
C	3.98903000	-3.97636000	1.26465800	C	-1.71503800	2.35829100	-0.77018400
H	3.87333500	-3.31089000	3.30733600	C	-2.11036200	2.81082400	-2.02240700
H	4.01004900	-4.34534400	-0.85578900	C	-3.68456800	0.98890200	-2.14773700
H	4.26625600	-4.99140800	1.52564600	H	-1.63443800	3.68393900	-2.45349400
O	3.52953200	0.14194000	-2.60545200	H	-4.44890700	0.43084300	-2.67603800
H	3.42419900	0.85714600	-3.24532300	C	-3.29816800	-1.80417400	-0.13677500
H	2.65649300	0.11322800	-1.93468500	N	-4.17421200	-2.65254500	0.39737300
Cat1-INT2				C	0.56871300	2.61325300	0.15863900
Sum of electronic and thermal Free Energies =				N	1.27652100	3.54415100	0.79490000
-2371.82735 Hartree				I	-1.34674200	-2.24889600	-0.60052100
Sum of electronic and thermal free energies + the entropy				I	1.25358300	0.74880800	-0.37177400
correction at 298.15K =			-2371.81765 Hartree	C	-3.90840900	-4.05331500	0.73148900
C	2.83503200	-2.68880400	-0.83514800	H	-3.77142600	-4.62748800	-0.18428100
O	1.57021300	-2.04405100	-1.12034500	H	-4.76306200	-4.43685800	1.28172900
H	2.88310500	-3.60119300	-1.43834900	H	-3.02016700	-4.11173000	1.35880900

C	2.66915800	3.40265200	1.22589400	O	1.42412700	-1.94786500	-0.38962700
H	3.00642000	4.36704200	1.59578600	H	2.70303600	-3.38419000	1.19084100
H	3.28292100	3.10736900	0.37553500	C	2.80066100	-1.39376400	2.00146700
H	2.73068800	2.65951700	2.02089000	C	1.52787200	-1.48033800	2.58682000
H	-3.42464000	2.46479500	-3.68300000	C	3.66166300	-0.35780000	2.38327600
C	-5.19981700	-0.68463300	0.10486600	C	1.09274100	-0.50371500	3.46768300
C	-5.38910300	-1.98963000	0.56130600	H	0.87976500	-2.30575200	2.31454700
C	-0.77643300	4.35968200	0.43018100	C	3.22786600	0.61443500	3.27657400
C	0.46629500	4.66114100	0.99013900	H	4.67737600	-0.32918800	2.01049200
N	-3.87484000	-0.60297200	-0.32140800	C	1.93830300	0.55596700	3.80025700
N	-0.67632400	3.06476800	-0.07665700	H	0.09937900	-0.56355000	3.89692800
C	-6.61827000	-2.41407800	1.06478000	H	3.89790700	1.41464900	3.56846700
C	-7.63205300	-1.47208500	1.08680100	H	1.59894600	1.32327300	4.48704900
H	-8.60534600	-1.75650100	1.46742600	C	6.00019400	-2.09947600	-1.29011600
C	-7.43531700	-0.15513400	0.62893200	C	5.08378500	-1.40596800	-0.47641700
H	-8.26077000	0.54499900	0.66866800	C	5.08168200	-0.00701700	-0.53445500
C	-6.21572100	0.26747100	0.12972400	C	6.00234100	0.63301900	-1.35281400
C	-1.83887400	5.25969800	0.44824500	C	6.92716500	-0.08858100	-2.12161900
C	-1.59501300	6.47910000	1.05600300	C	6.93475700	-1.47532500	-2.10704600
H	-2.38771200	7.21605500	1.09779700	C	4.73236100	-3.66692500	-0.32883200
C	-0.34373100	6.78656300	1.62380200	C	4.26527800	-2.43130000	0.17428500
H	-0.20163600	7.75352400	2.09064500	H	4.37619600	0.57879800	0.03995700
C	0.70984800	5.88868900	1.60471700	H	6.00518500	1.71577400	-1.39845600
H	-6.77338800	-3.42524300	1.41780600	H	7.63660600	0.44315700	-2.74431500
H	-6.05419600	1.27786600	-0.22509500	H	7.62397400	-2.05303800	-2.71114900
H	-2.79709600	5.01192800	0.00848600	H	6.27621700	-4.20253600	-1.61142300
H	1.66880200	6.12650900	2.04628700	H	4.37219800	-4.65964800	-0.09665300
H	-1.99982200	0.92639100	0.82179400	H	1.77224900	-2.29653600	-1.21933600
Cat1-TS3				N	5.75236800	-3.46730500	-1.14694200
Sum of electronic and thermal Free Energies =				C	-2.35795500	1.02624600	-0.38167100
-2371.78056 Hartree				C	-3.12867000	1.59866000	-3.01197800
Sum of electronic and thermal free energies + the entropy				C	-3.25324300	0.20786800	-1.06028000
correction at 298.15K =				C	-1.81874500	2.10742700	-1.06947500
-2371.77084 Hartree				C	-2.19706800	2.40818600	-2.37220500
C	3.18943700	-2.42395100	1.05300000	C	-2.19706800	2.40818600	-2.37220500
C	-3.65004100	0.48528700	-2.36343600	N	1.04076700	3.65111900	0.42683000
H	-1.75675800	3.26112900	-2.87553600	I	-0.99584700	-2.22709700	-0.24883600
H	-4.35272200	-0.17327100	-2.86110900	I	1.15010000	0.65027300	-0.32864300
C	-3.11297900	-2.07068500	-0.06575900	C	-3.67643800	-4.29013900	0.94519100
N	-3.97783200	-2.95741700	0.43210600	H	-2.62703200	-4.51127400	0.76944900
C	0.42176300	2.59673800	-0.10662700				
H	-4.29779800	-5.01557100	0.42118200	H	2.90181600	4.57638600	0.52074000
H	-3.88905900	-4.31791800	2.01377500	H	-3.43009400	1.82176900	-4.02754100
C	2.40389800	3.70703800	0.94817400	C	-5.14985900	-1.14207500	-0.14021000
H	2.93582000	2.80318100	0.66052400	C	-5.26131800	-2.41932500	0.40573900
H	2.36755000	3.79124400	2.03443700	C	-1.03873600	4.28671900	-0.09987200

C	0.16234100	4.73088100	0.45081400	C	1.81532500	-3.83934500	1.22319600
N	-3.79498400	-0.95529900	-0.41600900	C	2.25894300	-2.49011400	1.46749700
N	-0.84309300	2.94566600	-0.42962900	H	4.34053700	-0.36895700	0.89541800
C	-6.48644300	-2.94025400	0.81446200	H	6.31033700	-0.87150000	-0.46416300
C	-7.59072600	-2.11936000	0.64680000	H	6.69099700	-3.12653100	-1.39036200
H	-8.56683500	-2.47861400	0.94918200	H	5.03103600	-4.95257600	-0.97782100
C	-7.47692500	-0.83015700	0.09535300	H	2.62252700	-5.45422700	0.23208000
H	-8.36798100	-0.22417600	-0.01480300	H	0.89221400	-4.29770800	1.55194900
C	-6.25577000	-0.31379700	-0.30963900	H	1.00357200	-3.05960100	-2.16102400
C	-2.14533600	5.12136900	-0.22785900	N	2.71137900	-4.48806000	0.53654400
C	-1.98638700	6.42214200	0.22345800	C	-1.64270600	1.31993500	-0.47482500
H	-2.81800900	7.11192800	0.14656900	C	-2.70235800	2.42342000	-2.81136900
C	-0.77474000	6.87171200	0.78025100	C	-2.87745800	0.90728200	-0.96003200
H	-0.70021100	7.89759000	1.11969100	C	-0.92714900	2.25671100	-1.20891200
C	0.32401100	6.03669800	0.90686100	C	-1.44621800	2.82213100	-2.36754500
H	-6.56740400	-3.93252700	1.24055300	C	-3.41775600	1.45219000	-2.11910900
H	-6.16245000	0.67876500	-0.73279700	H	-0.86549700	3.55524100	-2.91549700
H	-3.07514300	4.76834200	-0.65655100	H	-4.38259300	1.11122900	-2.47644000
H	1.25818500	6.37535800	1.33712300	C	-3.24323200	-1.38612900	-0.06264900
H	-2.08031700	0.82108000	0.64613300	N	-4.21755600	-2.01717700	0.59668000
Cat1-INT3				C	1.51175100	1.90991900	-0.85671200
Sum of electronic and thermal Free Energies =				N	2.54664900	2.65366300	-0.45790900
-2371.784251 Hartree				I	-1.35003300	-2.17491200	-0.68880700
Sum of electronic and thermal free energies + the entropy				I	1.48341200	-0.15168900	-1.29177600
correction at 298.15K =				C	-4.18925600	-3.43060700	0.96935300
-2371.77440 Hartree				H	-5.04171200	-3.63335100	1.61260400
C	1.40826600	-1.65372800	2.12427800	H	-3.26930500	-3.64375900	1.51174100
O	0.91912200	-2.59713900	-1.32009200	H	-4.25109500	-4.04748800	0.07343000
H	0.44537600	-2.09122200	2.38254000	C	3.94923300	2.25410500	-0.40201800
C	1.54034900	-0.24819700	2.45586800	H	4.06635900	1.29286600	-0.89678800
C	0.35702300	0.50745900	2.46736300	H	4.26496300	2.18189800	0.63924000
C	2.76026500	0.38369200	2.73542500	H	4.54228100	3.00689300	-0.92066600
C	0.40134600	1.88324200	2.64364600	H	-3.11572600	2.85367700	-3.71473300
H	-0.59079400	-0.00005100	2.31538400	C	-4.88744800	0.09256800	0.29139300
C	2.79548200	1.75405600	2.95781700	C	-5.26878400	-1.13425800	0.83627300
H	3.66374300	-0.20572500	2.82755100	C	0.71414900	3.92502200	-0.30265900
C	1.62430400	2.50924600	2.88168200	C	2.09329600	3.91865900	-0.09834000
H	-0.51337300	2.46483800	2.61428000	N	-3.61871300	-0.10033500	-0.25605400
H	3.73719700	2.23745800	3.19118000	N	0.38470000	2.65546100	-0.77552100
H	1.66139500	3.58242600	3.03474400	C	-6.49453500	-1.29531700	1.47970800
C	3.79464400	-3.64908700	0.21046300	C	-7.31012500	-0.17712800	1.54892800
C	3.55604700	-2.38669400	0.77792800	H	-8.27285300	-0.25722900	2.03884900
C	4.47856200	-1.37261300	0.52118000	C	-6.92059000	1.05898800	1.00263500
C	5.59445900	-1.65934800	-0.26107700	H	-7.59043600	1.90642300	1.08326100
C	5.80973200	-2.93473400	-0.79023800	C	-5.70129100	1.21993900	0.36431300
C	4.89757100	-3.96043300	-0.56405300				

C	-0.06736400	5.04070700	-0.01722300	H	3.15276700	2.96021800	4.21287200
C	0.60196100	6.14661900	0.48438700	C	-2.68767900	-0.18871000	0.24075200
H	0.03794200	7.03959700	0.72501600	C	-2.61088500	0.01784200	3.03263000
C	1.99389500	6.14109500	0.69053600	C	-2.74893500	1.04713700	0.87192500
H	2.47089900	7.02940500	1.08633400	C	-2.54056900	-1.31439000	1.04073100
C	2.76878100	5.02776100	0.40418600	C	-2.50709200	-1.22953100	2.42740300
H	-6.79580000	-2.24382500	1.90502200	C	-2.71885500	1.16604500	2.25589100
H	-5.39426200	2.16954500	-0.05600500	H	-2.39167200	-2.13118700	3.01779400
H	-1.13848500	5.03782300	-0.17845100	H	-2.76824900	2.14835000	2.71116100
H	3.83938000	5.01402100	0.56740300	C	-1.85250500	2.76042800	-0.68670400
H	-1.24077300	0.91042400	0.44161900	N	-2.28322900	3.89290400	-1.24257800
TS4				C	-1.33856500	-3.05996700	-0.25634900
Sum of electronic and thermal Free Energies=				N	-1.55779900	-4.31851200	-0.63590300
-996.77109 Hartree				I	-0.00172800	1.83114800	-0.90404800
Sum of electronic and thermal free energies + the entropy				I	0.32560200	-1.87786700	-0.63410600
correction at 298.15K=				C	-1.55574100	4.77824200	-2.14810500
-996.76079 Hartree				H	-1.52126200	5.77448800	-1.70880900
C	3.19392500	0.52153400	-0.58954800	H	-2.07575600	4.80644200	-3.10509800
C	6.41516200	-0.67619600	-0.88382900	H	-0.54578000	4.40163600	-2.28612900
C	5.54929000	-0.63785000	0.21616500	C	-0.67291900	-5.17475800	-1.42288500
C	6.04308500	-0.22900900	1.45407800	H	-1.04179600	-5.22751200	-2.44703100
C	7.38347900	0.12920500	1.54301200	H	-0.66823800	-6.16594600	-0.97255200
C	8.22475100	0.09693500	0.42053800	H	0.33361500	-4.76481300	-1.40603800
C	7.75266500	-0.30787900	-0.82176100	H	-2.58408200	0.09755400	4.11188900
H	9.26288000	0.38928600	0.52457200	C	-3.94575500	3.08212100	0.01759200
H	8.39084200	-0.34035500	-1.69654200	C	-3.59009900	4.13229300	-0.82654200
H	5.39618300	-0.18938200	2.32361200	C	-3.36318400	-3.62158000	0.48886700
H	7.78876400	0.44442900	2.49744000	C	-2.81910600	-4.70888200	-0.19287100
C	4.42713900	-1.39274900	-1.62621000	N	-2.83627200	2.24004100	0.07797900
N	5.67092100	-1.14481100	-1.97955500	N	-2.41115700	-2.60548900	0.42483700
H	3.70357600	-1.74488600	-2.34800200	C	-4.47174200	5.16876900	-1.12280300
H	6.03279900	-1.24346200	-2.92384800	C	-5.72250600	5.09748700	-0.53087700
C	4.20905200	-0.99869800	-0.26817700	H	-6.44491700	5.88005100	-0.72787700
H	3.49527300	-1.52778500	0.35208200	C	-6.08068200	4.03516300	0.32005700
O	2.04299200	0.14007500	-1.07404600	H	-7.07137000	4.02315000	0.75778900
H	3.87231100	1.04862300	-1.27849400	C	-5.20182100	3.00452800	0.61241300
C	3.19236200	1.19037100	0.76401400	C	-4.62744800	-3.66871400	1.06978500
C	4.04037800	2.26861300	1.00944800	C	-5.31893900	-4.86097300	0.93052400
C	2.32669500	0.75383800	1.76888300	H	-6.30769700	-4.95068300	1.36353700
C	4.02453500	2.90860300	2.24767300	C	-4.77302600	-5.95935400	0.23972300
H	4.71442100	2.60786500	0.22844300	H	-5.35405900	-6.86961600	0.15645900
C	2.31423500	1.38560400	3.00677600	C	-3.51464900	-5.90741800	-0.33706700
H	1.66124200	-0.08197800	1.57647100	H	-4.19120500	5.98238500	-1.77988100
C	3.16447200	2.46583500	3.24816300	H	-5.46956400	2.18360300	1.26602500
H	4.68421400	3.74937300	2.42992500	H	-5.03991600	-2.81854400	1.59895900
H	1.64198900	1.03968200	3.78405200				

H	-3.09204800	-6.74842400	-0.87222200
H	-2.74090900	-0.26958800	-0.83937100

INT4

Sum of electronic and thermal Free Energies =
-996.797456 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -996.78726 Hartree

C	-2.67661100	-2.12193000	0.02926800
C	-2.21756800	-0.85937800	-0.33968200
C	-3.14375100	0.11984800	-0.67070300
C	-4.49938300	-0.20663600	-0.60168000
C	-4.92678600	-1.47970100	-0.21760700
C	-4.00996700	-2.47727000	0.10553500
C	-0.43568200	-2.28519400	0.09896300
C	-0.71016400	-0.87515100	-0.29436900
H	-2.82994100	1.10951900	-0.98056500
H	-5.23745000	0.54498000	-0.85528700
H	-5.98677600	-1.69887800	-0.17587800
H	-4.31769600	-3.47437800	0.39530900
H	-1.58209400	-3.91065600	0.56684500
H	0.53069500	-2.75126400	0.24880000
H	-0.27768700	-0.70145400	-1.28675700
N	-1.53437300	-2.93166200	0.28141900
C	-0.06920200	0.11980000	0.72448200
H	-0.53955500	-0.08251400	1.69116900
C	-0.42585200	1.54763200	0.34560800
C	-1.21941300	2.30814800	1.20396300
C	0.00524700	2.11267400	-0.85677400
C	-1.58070500	3.61165200	0.86860500
H	-1.56455800	1.87412800	2.13702600
C	-0.35583800	3.41290500	-1.19479900
H	0.62211300	1.53497200	-1.53707500
C	-1.15244100	4.16596200	-0.33350000
H	-2.20048100	4.18954300	1.54491200
H	-0.01633500	3.83853200	-2.13234000
H	-1.43527400	5.17816000	-0.59903700
C	3.66843200	-0.45351200	0.65553800
C	2.45668600	-0.33646900	-0.07556000
C	2.51404200	-0.47948000	-1.47676200
C	3.73349200	-0.71907100	-2.08489700
C	4.92073200	-0.82188400	-1.33223400
C	4.90356000	-0.69212200	0.04401600
C	2.02394700	-0.10146000	2.12543800
C	1.41213500	-0.10613800	0.89837800
H	1.62327000	-0.40647000	-2.08907400

H	3.77822700	-0.82900900	-3.16227900
H	5.85995800	-1.00704000	-1.84060400
H	5.80882700	-0.77179600	0.63514000
H	4.03675000	-0.34306000	2.74384200
H	1.58465800	0.03417300	3.10307800
N	3.37064400	-0.30074400	1.98506900

Cat1-TS5

Sum of electronic and thermal Free Energies =
-2735.45735 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -2735.44764 Hartree

C	4.87362800	1.88828200	1.86606500
C	4.00247600	1.93219600	0.77380500
C	3.41532000	3.15090100	0.44709200
C	3.71646700	4.26700200	1.22372900
C	4.57788100	4.18293300	2.32339700
C	5.17856600	2.97751600	2.66693700
C	4.87857300	-0.18200900	1.01091400
C	3.87719600	0.54049700	0.23282000
H	2.74312500	3.23587500	-0.39533600
H	3.27177800	5.22287500	0.97128600
H	4.78597700	5.06911800	2.91071100
H	5.85411200	2.88890500	3.50902100
H	6.00963500	0.24397900	2.67360000
H	5.16479000	-1.22244000	0.92955200
H	2.89958700	0.14093200	0.78850200
N	5.36520800	0.56987800	1.95584000
C	3.77499200	0.28773100	-1.29228500
H	4.45864200	0.99917600	-1.76459300
C	2.37798300	0.59739700	-1.82889500
C	2.11777000	1.82192400	-2.44801400
C	1.34078600	-0.33366700	-1.73812500
C	0.84601800	2.12358500	-2.93336100
H	2.92029700	2.54484200	-2.55809800
C	0.07474700	-0.04421900	-2.23631100
H	1.51907500	-1.29810000	-1.27910900
C	-0.18275900	1.19107600	-2.82635100
H	0.66524100	3.08112600	-3.40965100
H	-0.71338800	-0.78640100	-2.15703200
H	-1.17101300	1.42002900	-3.21148300
C	4.60590600	-3.35101400	-1.90687100
C	3.93290100	-2.38123200	-1.12226000
C	3.16974600	-2.81613000	-0.02225400
C	3.08662400	-4.17068300	0.24710600
C	3.75624800	-5.11685300	-0.55675800

C	4.52400400	-4.72188100	-1.63792500	H	-6.23578100	4.70615300	-2.22846900
C	5.07867300	-1.33583600	-2.75247400	C	-4.82800900	3.53548000	-1.13195500
C	4.24954400	-1.09090700	-1.68837600	C	-5.46571600	-3.13820600	-0.28088900
H	2.65339600	-2.09821300	0.60817900	C	-6.04826400	-4.28495900	-0.79634400
H	2.49903800	-4.51214900	1.09230600	H	-7.09861200	-4.27019700	-1.06053200
H	3.67106600	-6.17142200	-0.32069000	C	-5.31025500	-5.46717600	-0.98897200
H	5.04617400	-5.44273500	-2.25684600	H	-5.80767800	-6.33764700	-1.39899000
H	5.87142100	-3.11202500	-3.59706700	C	-3.96350100	-5.54707800	-0.67248800
H	5.53667400	-0.63472400	-3.43494500	H	-2.21512400	6.25643600	-2.30267700
N	5.29001500	-2.68353100	-2.89044100	H	-5.53788300	2.78516600	-0.80641600
O	1.58958400	-0.18417000	1.68349000	H	-6.02571400	-2.22282300	-0.13328700
H	1.87844300	-0.15469100	2.60402700	H	-3.39315900	-6.45398400	-0.82793300
C	-3.02030900	0.13145700	0.22629900	H	-2.34793600	-0.02455700	-0.60993100
C	-4.79687000	0.54571100	2.34920100	Product			
C	-3.34636000	1.41373000	0.64925400	Sum of electronic and thermal Free Energies =			
C	-3.56884300	-0.93996700	0.92115600	-996.387958 Hartree			
C	-4.45710900	-0.74893000	1.97291700	Sum of electronic and thermal free energies + the entropy			
C	-4.23210800	1.63571600	1.69687600	correction at 298.15K =			
H	-4.86811900	-1.60775200	2.49108300	C	-2.92897400	-1.83059500	-0.30326200
H	-4.46570100	2.65079000	1.99667900	C	-2.43474200	-0.65369700	0.31008500
C	-1.47251600	2.93498900	0.03897400	C	-3.34009300	0.34985000	0.69379000
N	-1.32800800	4.05795900	-0.66853900	C	-4.69123900	0.15515400	0.46161700
C	-2.00452100	-2.85674200	0.68109700	C	-5.16160100	-1.02465400	-0.15166300
N	-2.07910400	-4.12397100	0.26964100	C	-4.29290500	-2.03026800	-0.54138900
I	0.01992700	1.79374500	0.94518000	C	-0.69986300	-2.00647800	-0.15060300
I	-0.28255300	-1.80614700	1.28758500	C	-1.00234700	-0.78792100	0.39619200
C	-0.10823200	4.83680300	-0.85886900	H	-2.98488500	1.26150100	1.16358700
H	0.02225800	5.02711700	-1.92330300	H	-5.40261400	0.91963300	0.75245700
H	0.73953600	4.27168600	-0.48077500	H	-6.22541000	-1.14614300	-0.32161100
H	-0.20024100	5.77860000	-0.31743600	H	-4.65170800	-2.93822000	-1.01285500
C	-0.96379300	-5.06621800	0.20101500	H	-1.88843100	-3.54617500	-1.00418100
H	-1.36174700	-6.07515900	0.28546800	H	0.25816200	-2.48901000	-0.27410800
H	-0.28640900	-4.87877000	1.03110600	N	-1.84987200	-2.63384700	-0.57248700
H	-0.44000200	-4.94760300	-0.74807700	C	-0.06900200	0.22665000	1.00423000
H	-5.48736600	0.70539100	3.16755400	H	-0.40240300	0.40173900	2.03453400
C	-3.48422100	3.47141200	-0.77453200	C	-0.12517500	1.58966500	0.30685300
C	-2.56279700	4.43065800	-1.19106700	C	0.29664500	2.72059900	1.01204300
C	-4.11299500	-3.22338000	0.03711500	C	-0.55504800	1.74609200	-1.01037500
C	-3.37952500	-4.39543000	-0.14926800	C	0.29383400	3.97703300	0.41607000
N	-2.76715100	2.54879400	-0.01280300	H	0.63090000	2.60972900	2.03983900
N	-3.22012800	-2.28204200	0.54937600	C	-0.55473000	3.00359800	-1.61368400
C	-2.93484100	5.51276000	-1.98455100	H	-0.89537500	0.88230300	-1.57177600
C	-4.27240800	5.58191300	-2.34092600	C	-0.13187700	4.12264500	-0.90363600
H	-4.61290100	6.40474600	-2.95758900	H	0.62033800	4.84309600	0.98107400
C	-5.20090300	4.61076900	-1.92311600	H	-0.89067100	3.10594000	-2.63967200

H	-0.13631200	5.10074100	-1.37111500	C	3.03903400	-3.82234100	-0.25644300
C	3.50290100	-0.92113700	0.61448200	H	2.38178400	-2.35666300	-1.69173700
C	2.27621800	-0.53444200	0.01830600	C	3.42462100	-4.05170600	1.06513800
C	2.18584400	-0.50430300	-1.38515000	H	3.74984200	-3.17351900	3.00177800
C	3.29637300	-0.84666500	-2.13710100	H	3.02094800	-4.64200000	-0.96586400
C	4.50697500	-1.22556300	-1.52020100	H	3.70399300	-5.05002400	1.38227200
C	4.62701000	-1.26965800	-0.14230200	C	-3.46615200	0.39608200	0.33607700
C	2.04881700	-0.47622000	2.25617500	C	-4.13066200	0.36244900	3.05864500
C	1.35688200	-0.25640400	1.09507100	C	-3.46915400	1.56005200	1.09411300
H	1.25795600	-0.22322900	-1.87052900	C	-3.76061600	-0.79030000	0.99461500
H	3.23808700	-0.82677900	-3.21939900	C	-4.09833500	-0.82674900	2.34102400
H	5.35834100	-1.48874800	-2.13758400	C	-3.80212300	1.56359800	2.44206600
H	5.55369300	-1.56291300	0.33808300	H	-4.32648500	-1.77397500	2.81485800
H	4.03799000	-1.10027300	2.66304100	H	-3.79759200	2.49444400	2.99605600
H	1.71744200	-0.37121800	3.27906200	C	-2.01156100	3.14020700	-0.17020800
N	3.33294000	-0.87638900	1.97503900	N	-2.15318700	4.43221700	-0.49788900
Cat2-TS1				C	-2.71438500	-2.60173500	-0.36909700
Sum of electronic and thermal Free Energies =				N	-3.16831700	-3.78560300	-0.80213400
-2096.69834 Hartree				I	-0.39875800	1.86523000	-0.57047800
Sum of electronic and thermal free energies + the entropy				I	-0.82699200	-1.80300400	-0.64060000
correction at 298.15K =				C	-1.18558900	5.25428400	-1.22812300
-2096.68853 Hartree				H	-0.25088500	5.28785000	-0.67098300
C	2.29732900	-0.10120900	-0.18493600	H	-1.60326800	6.25435300	-1.31307800
C	5.18779500	1.74547700	0.14702800	H	-1.03040000	4.82970000	-2.21858600
C	4.98134100	0.43352100	-0.29910100	C	-2.41077000	-4.78258500	-1.56331500
C	5.81313400	-0.58157500	0.17324200	H	-3.05104800	-5.65157300	-1.69096100
C	6.81822800	-0.24532500	1.07236300	H	-1.51887100	-5.05662300	-1.00209400
C	6.99372800	1.07556500	1.51289600	H	-2.14420200	-4.36682200	-2.53369300
C	6.17552500	2.10087700	1.05690200	H	-4.39164000	0.35039100	4.10902600
H	7.78448800	1.30069000	2.21855100	N	-3.13300300	2.81127200	0.47786500
H	6.30043600	3.12538800	1.38597800	N	-3.73711700	-2.03209100	0.27408400
H	5.67727500	-1.60686300	-0.15312200	H	-3.26998000	0.41768200	-0.72929400
H	7.48039100	-1.01816300	1.44500300	N	-4.83247500	-2.83512800	0.27517400
C	3.48281000	1.83472800	-1.30129200	N	-3.98029000	3.86814900	0.58648100
N	4.24125800	2.55603500	-0.49953600	C	-4.46476200	-3.88991200	-0.38675300
H	2.69920000	2.29357200	-1.88814200	H	-5.08209300	-4.74944500	-0.59657900
H	4.13839800	3.55619300	-0.35245000	C	-3.36445700	4.83894200	-0.01626900
C	3.79544400	0.44833200	-1.16653600	H	-3.73925300	5.84331600	-0.13703500
H	3.66790000	-0.22704700	-2.00303000	Cat2-INT1			
O	1.24921000	-0.01640200	-0.95721800	Sum of electronic and thermal Free Energies =			
H	2.36737800	0.61004200	0.65329700	-2096.70070 Hartree			
C	2.70928900	-1.48395000	0.24522600	Sum of electronic and thermal free energies + the entropy			
C	3.09881500	-1.71439200	1.56276100	correction at 298.15K =			
C	2.67978300	-2.54306800	-0.66420600	-2096.69089 Hartree			
C	3.45184900	-2.99834400	1.97431200	C	2.31652700	-0.20470000	-0.13287200
H	3.12573900	-0.88713700	2.26561600	C	5.38416600	1.47634400	0.00044600

C	4.90051500	0.17229800	-0.09754300	H	0.16645500	5.25542500	-0.54861700
C	5.59105900	-0.84831400	0.54303400	C	-2.60118800	-4.60640100	-1.66563200
C	6.73999100	-0.51667100	1.26172100	H	-3.27911000	-5.44398400	-1.80810800
C	7.19414000	0.80245500	1.34646000	H	-1.72668600	-4.92715600	-1.10167400
C	6.51654000	1.83742000	0.70741000	H	-2.30782400	-4.19264300	-2.62916600
H	8.08951300	1.02487000	1.91424300	H	-4.45674700	0.56070400	4.02896100
H	6.85437100	2.86523300	0.75552500	N	-2.90962900	2.98039900	0.48222100
H	5.25317300	-1.87631900	0.48395900	N	-3.80905900	-1.81612000	0.18943200
H	7.29405000	-1.29998100	1.76532600	H	-3.15087800	0.61259100	-0.76146800
C	3.55507700	1.62723900	-1.29407100	N	-4.94528000	-2.56115400	0.16612400
N	4.51294800	2.30640700	-0.75423100	N	-3.69112900	4.08972700	0.58802100
H	2.80309700	2.10269300	-1.91046500	C	-4.62335800	-3.62563900	-0.50365100
H	4.63276600	3.31402600	-0.85823800	H	-5.28192400	-4.44873600	-0.73263100
C	3.64111700	0.20126300	-0.91503000	C	-2.99416500	5.02644200	0.02154900
H	3.66535600	-0.42837600	-1.81022400	H	-3.29868200	6.05518700	-0.09149300
O	1.22570900	-0.02794500	-0.95085100	Cat2-TS2			
H	2.28564700	0.43602900	0.76500400	Sum of electronic and thermal Free Energies =			
C	2.45885000	-1.64332200	0.33328400	-2096.66685 Hartree			
C	2.43494400	-1.95570000	1.69030500	Sum of electronic and thermal free energies + the entropy			
C	2.57238700	-2.67310500	-0.60392400	correction at 298.15K = -2096.65704 Hartree			
C	2.52163700	-3.28253500	2.11091900	C	2.16065500	-2.01366700	-0.31639700
H	2.34665600	-1.15809800	2.42165900	O	1.00605800	-1.22017900	-0.59233500
C	2.66342100	-3.99650300	-0.18760500	H	1.98873500	-3.05468000	-0.62097000
H	2.58341600	-2.43719600	-1.66395400	C	2.61550200	-1.99366500	1.12595900
C	2.63730800	-4.30403300	1.17301100	C	1.76976800	-1.54980000	2.13944400
H	2.49952400	-3.51603200	3.16946600	C	3.89756300	-2.44209300	1.45469200
H	2.75392100	-4.78960800	-0.92146900	C	2.20243100	-1.54251200	3.46555900
H	2.70766200	-5.33582700	1.49818000	H	0.77056800	-1.20942200	1.89463300
C	-3.38973200	0.59111300	0.29471100	C	4.32982300	-2.43606500	2.77560900
C	-4.15594800	0.56827900	2.98922100	H	4.56310600	-2.78579500	0.66790900
C	-3.34772300	1.74583000	1.06653800	C	3.48275200	-1.98103700	3.78612900
C	-3.78089300	-0.58302100	0.92496200	H	1.53652100	-1.19162600	4.24601400
C	-4.16983000	-0.61289600	2.25781000	H	5.32941100	-2.77906200	3.01763200
C	-3.73087700	1.75354700	2.40124000	H	3.82126600	-1.96997700	4.81579900
H	-4.47310900	-1.54941700	2.71017300	C	4.90148800	-0.18461800	-2.18414500
H	-3.68915400	2.67635900	2.96720000	C	4.07466400	-0.26413200	-1.05456600
C	-1.74664800	3.23979800	-0.12603700	C	4.23913000	0.66438500	-0.02409300
N	-1.79833100	4.54556800	-0.43073400	C	5.21552600	1.64145800	-0.17033900
C	-2.80665400	-2.43037200	-0.44651100	C	6.01952800	1.70884000	-1.31919400
N	-3.31720900	-3.58375000	-0.89945800	C	5.87530100	0.79321400	-2.35154300
I	-0.19882300	1.81712800	-0.53065900	C	3.56590900	-1.94996500	-2.52873600
I	-0.87299600	-1.71595900	-0.68219700	C	3.13970200	-1.37530100	-1.29870600
C	-0.75740000	5.30778700	-1.12199900	H	3.62963000	0.62093100	0.87153600
H	-1.09308700	6.33947700	-1.19070100	H	5.36372400	2.36677600	0.62117400
H	-0.61345500	4.89523600	-2.11943300	H	6.76914200	2.48703200	-1.39937600

H	6.48934300	0.83020000	-3.24325700	C	5.56369300	-0.70595200	0.59785600
H	4.96077000	-1.39335500	-3.95680700	C	6.91301900	-0.63430700	0.91709000
H	3.15638000	-2.80657800	-3.04697900	C	7.61677000	0.57962100	0.88581800
H	2.00916300	-0.87319800	-1.60585800	C	6.97985800	1.76003000	0.53778000
N	4.54640600	-1.23256700	-3.04333300	H	8.67089600	0.59385600	1.13569600
C	-3.16580700	1.15503500	0.16217300	H	7.50261000	2.70820500	0.50164600
C	-4.51662400	2.21217600	-2.05387200	H	5.05405100	-1.66068300	0.61896800
C	-4.07402500	0.39270900	-0.56168900	H	7.43802000	-1.54117200	1.19405400
C	-2.92268900	2.44732200	-0.28462300	C	3.53848300	2.22138900	-0.33943600
C	-3.58614800	2.99068600	-1.37678300	N	4.75013400	2.69778700	-0.13140500
C	-4.75717100	0.90203700	-1.65800600	H	2.72889400	2.87779900	-0.63114400
H	-3.37037700	4.00549400	-1.68862900	H	5.01846300	3.66985400	-0.25496400
H	-5.46193600	0.27564000	-2.19159900	C	3.52121100	0.80183600	-0.19997600
C	-3.47980000	-1.97779800	-0.05859600	H	3.46771100	0.54384000	-1.48349600
N	-4.22434100	-3.04218100	0.27329400	O	1.23558600	0.20983600	-0.80888200
C	-0.67242800	3.04472600	0.61965400	H	1.82813800	0.60170500	1.11867100
N	-0.20581900	4.13729300	1.23900600	C	2.45610900	-1.35241200	0.58258000
I	-1.40297000	-1.87024500	-0.34065700	C	2.51620700	-1.73396100	1.92118700
I	0.37064900	1.32996600	0.11707700	C	2.65051100	-2.31377800	-0.41197900
C	-3.73405100	-4.40115100	0.51508000	C	2.77761400	-3.05812200	2.26769800
H	-4.59388600	-5.02448400	0.74767300	H	2.36165700	-0.98920300	2.69598200
H	-3.04454900	-4.38874000	1.35777800	C	2.91141900	-3.63647000	-0.06841500
H	-3.23926000	-4.76905300	-0.38217300	H	2.60354700	-2.02834400	-1.45814700
C	1.17044600	4.36051500	1.69132000	C	2.97812400	-4.01131800	1.27287700
H	1.21993800	5.36356300	2.10727700	H	2.82138700	-3.34468000	3.31241800
H	1.84459300	4.27811600	0.84010300	H	3.06393000	-4.37582800	-0.84672100
H	1.42012800	3.62643300	2.45580500	H	3.18148100	-5.04214900	1.53984200
H	-5.04176400	2.62180100	-2.90713900	O	2.82395700	0.11496800	-2.61510800
N	-4.34130000	-0.96159600	-0.16945600	H	2.77210000	0.82736200	-3.26534800
N	-1.97046800	3.27346700	0.40368400	H	1.94736700	0.14172500	-1.97223300
H	-2.68642700	0.76672100	1.05295400	C	-3.58949700	0.29299000	0.29652500
N	-2.34071800	4.49937700	0.85602300	C	-4.36050300	0.14273700	2.98542800
N	-5.62069900	-1.35673500	0.06615700	C	-3.68151700	1.43179900	1.08570000
C	-1.25555300	5.00233000	1.36127300	C	-3.85270200	-0.92572700	0.90659400
H	-1.16769300	5.97201200	1.82566400	C	-4.24167600	-1.02145600	2.23583600
C	-5.52269900	-2.62254400	0.33578700	C	-4.06833200	1.37746900	2.41804600
H	-6.34254200	-3.27841700	0.58327900	H	-4.44352000	-1.99326800	2.67036800
Cat2-TS2'				H	-4.13305500	2.29008100	2.99804200
Sum of electronic and thermal Free Energies =				C	-2.26481300	3.10690500	-0.09694200
-2173.10208 Hartree				N	-2.46190600	4.39550100	-0.41005900
Sum of electronic and thermal free energies + the entropy				C	-2.68237800	-2.62362100	-0.49820600
correction at 298.15K =				N	-3.07449800	-3.79134700	-1.02521100
C	2.19423800	0.09642400	0.21514800	I	-0.56904000	1.92812800	-0.46112800
C	5.62484000	1.67222000	0.23747900	I	-0.81362500	-1.75809700	-0.62945300
C	4.89200700	0.47368800	0.25153400	C	-1.51471400	5.27367000	-1.10111800

H	-1.99399500	6.24121800	-1.22742300	H	4.91166800	1.44362300	2.16012200
H	-1.27714100	4.84680000	-2.07412400	H	6.46083900	2.55898300	0.59145600
H	-0.61561300	5.37931600	-0.49621000	H	6.54857400	1.88288600	-1.79995900
C	-2.25542400	-4.70016900	-1.83194200	H	5.39450800	0.07492300	-3.59592700
H	-1.39068300	-5.01439400	-1.24961400	H	3.63932900	-1.71148700	-3.60751200
H	-1.94436800	-4.18740300	-2.74080400	H	0.91469800	-1.19195000	-2.12116900
H	-2.86972200	-5.56202600	-2.08068000	N	4.85927400	-0.17384200	-2.77522400
H	-4.66295600	0.08577300	4.02313500	C	-2.91765100	1.49428400	0.33837600
N	-3.38615000	2.71340800	0.51394100	C	-4.21665500	2.89621700	-1.71435900
N	-3.74759600	-2.13502100	0.14110500	C	-3.98675900	0.94275700	-0.35344400
H	-3.35142900	0.35540500	-0.75866900	C	-2.49851400	2.75793700	-0.05497000
C	-4.37912200	-3.97011100	-0.66449100	C	-3.13112000	3.47090300	-1.06392800
H	-4.95532400	-4.83576900	-0.95200000	C	-4.64657000	1.62060400	-1.36942800
C	-3.70441200	4.73476300	0.04376600	H	-2.77229100	4.45734700	-1.33242000
H	-4.12514200	5.72121400	-0.07347600	H	-5.48068700	1.15127500	-1.87708100
N	-4.81031300	-2.97525400	0.05005700	C	-3.80408400	-1.52112600	-0.00311500
N	-4.28774000	3.72518900	0.61447600	N	-4.67654100	-2.45054600	0.40602700
Cat2-INT2				C	-0.13128000	2.93137600	0.70086200
Sum of electronic and thermal Free Energies =				N	0.54221600	3.85983700	1.39085800
-2096.73867 Hartree				I	-1.85158800	-1.83133400	-0.55538400
Sum of electronic and thermal free energies + the entropy				I	0.63687400	1.19773300	-0.08622100
correction at 298.15K =				C	-4.41930400	-3.88592100	0.55903800
-2096.72883 Hartree				H	-5.33089800	-4.34196000	0.93651200
C	2.25770700	-2.13897800	-1.06588800	H	-3.60893200	-4.02727700	1.27221600
O	0.99005600	-1.44653500	-1.18875000	H	-4.16412800	-4.31003900	-0.41082300
H	2.23726900	-2.98631700	-1.75872500	C	1.96400500	3.81586800	1.74707200
C	2.38811300	-2.67393700	0.34386000	H	2.18524800	4.71389700	2.31810800
C	1.49659200	-2.34699800	1.36169200	H	2.56016300	3.79427200	0.83587000
C	3.47628600	-3.50184800	0.63260400	H	2.15091100	2.93099000	2.35383600
C	1.69262700	-2.83356100	2.65465700	H	-4.71974600	3.43875600	-2.50425000
H	0.65340600	-1.69718600	1.16537000	N	-4.46118800	-0.36138300	0.01236100
C	3.67179200	-3.98790300	1.91906200	N	-1.38676100	3.37031500	0.61386300
H	4.17559900	-3.75835300	-0.15741000	H	-2.45664300	0.97621700	1.17225500
C	2.77970100	-3.65185600	2.93755700	N	-1.53058900	4.57601000	1.21971200
H	0.99325000	-2.56606700	3.43868000	N	-5.74784900	-0.52970300	0.40812400
H	4.52091400	-4.62813800	2.12936100	C	-0.34913400	4.85162000	1.68505500
H	2.93288100	-4.02830700	3.94236000	H	-0.08098200	5.73782200	2.23906400
C	5.00501100	0.38858700	-1.52984900	C	-5.85478200	-1.80274900	0.64309900
C	4.09489700	-0.25739000	-0.65658900	H	-6.74402900	-2.30858200	0.98584000
C	4.07214500	0.13192900	0.69690000	Cat2-TS3			
C	4.92212700	1.13855400	1.11987300	Sum of electronic and thermal Free Energies =			
C	5.80837500	1.77430600	0.22600700	-2096.69404 Hartree			
C	5.86500500	1.40699800	-1.10616500	Sum of electronic and thermal free energies + the entropy			
C	3.89808800	-1.14291500	-2.72577200	correction at 298.15K =			
C	3.38781200	-1.23366000	-1.45444900	-2096.68417 Hartree			
H	3.40196200	-0.34562900	1.40271400	C	2.63365100	-2.21950300	0.69023000

O	0.82937700	-1.58223700	-0.56123200	H	-3.61463700	-4.02498200	1.42816000
H	2.18836500	-3.20808100	0.65094500	H	-3.90739900	-4.46979400	-0.28195700
C	2.25411000	-1.41574100	1.84313900	C	1.93490300	3.86596000	1.14219300
C	0.99569200	-1.63882300	2.42240900	H	2.16258900	4.83548700	1.57840400
C	3.11800300	-0.47851900	2.42120600	H	2.55077200	3.70044300	0.25945700
C	0.57726200	-0.88320400	3.50524400	H	2.09615000	3.07908700	1.87827100
H	0.34734400	-2.39356800	1.99247700	H	-4.68799600	3.01477000	-3.11867700
C	2.70239200	0.26857400	3.51755800	N	-4.42503400	-0.53504200	-0.26154500
H	4.12401200	-0.35820500	2.04000300	N	-1.39376000	3.29101900	0.02745400
C	1.42704600	0.08379300	4.04551900	H	-2.47260700	0.95797000	0.81945900
H	-0.40488700	-1.04584300	3.93367100	C	-0.35238200	4.91696500	0.85649300
H	3.37682000	0.99022500	3.96333900	H	-0.07916400	5.87906400	1.26071800
H	1.10224900	0.67608600	4.89349300	C	-5.83203500	-1.97136900	0.34584300
C	5.36327600	-1.32157600	-1.60133400	H	-6.73590100	-2.48252500	0.63859600
C	4.45964600	-0.84476400	-0.63190900	N	-1.52873700	4.58715700	0.41752100
C	4.43482800	0.53323700	-0.37981200	N	-5.74465200	-0.72043900	0.01167900
C	5.31827100	1.35735000	-1.06321400	Cat2-INT3			
C	6.22871600	0.84352700	-1.99840000	Sum of electronic and thermal Free Energies =			
C	6.26009900	-0.51202000	-2.28784900	-2096.69768 Hartree			
C	4.16499300	-3.09478700	-0.96298600	Sum of electronic and thermal free energies + the entropy			
C	3.68639200	-2.00994900	-0.19463900	correction at 298.15K = -2096.68778 Hartree			
H	3.74139700	0.96467700	0.32995800	C	2.71520300	-2.39270600	0.80464500
H	5.30417600	2.42337600	-0.86856000	O	0.52642500	-1.71953100	-0.97644100
H	6.90878300	1.51532200	-2.50828800	H	2.28265900	-3.37504500	0.62990200
H	6.94025500	-0.92819700	-3.02131300	C	2.07297400	-1.61545500	1.83972100
H	5.67180300	-3.29638800	-2.37901600	C	0.72639400	-1.89735300	2.12030900
H	3.83587300	-4.12430700	-0.93913400	C	2.73425200	-0.61487900	2.56808300
H	1.15732900	-1.79784200	-1.44332400	C	0.02784700	-1.13018300	3.03961100
N	5.15119100	-2.69434100	-1.74887800	H	0.23438600	-2.69579200	1.57774900
C	-2.92506200	1.38589700	-0.06656500	C	2.03876300	0.13362000	3.50636300
C	-4.19416100	2.55893300	-2.27014200	H	3.79624000	-0.45714000	2.42924200
C	-3.97032900	0.74659500	-0.72170000	C	0.68090400	-0.10524700	3.72346900
C	-2.50127800	2.60660000	-0.57789200	H	-1.02042100	-1.33128800	3.22868700
C	-3.12348200	3.20592900	-1.66505000	H	2.55300600	0.89945500	4.07503900
C	-4.61536200	1.31667000	-1.81152700	H	0.13842100	0.49294100	4.44694500
H	-2.76692700	4.16102400	-2.03120000	C	5.52957600	-1.26088400	-1.24516200
H	-5.43079000	0.78962600	-2.29190900	C	4.57632800	-0.87336100	-0.28769500
C	-3.72214200	-1.66338500	-0.11049500	C	4.52420400	0.47535800	0.07247800
N	-4.61272400	-2.58387900	0.28736600	C	5.43215600	1.35972000	-0.49917300
C	-0.14668500	2.84553400	0.21184800	C	6.39083000	0.93061800	-1.42432000
N	0.52360700	3.87394000	0.75086300	C	6.44897600	-0.39915900	-1.82167500
I	-1.63965300	-1.87687300	-0.38902300	C	4.33218700	-3.10147000	-0.82923300
I	0.55081200	0.90986900	-0.19815200	C	3.78861800	-2.07930700	0.01257400
C	-4.32102900	-3.98437800	0.60028600	H	3.78980500	0.84316700	0.77413000
H	-5.25531500	-4.46253900	0.88463800	H	5.39396300	2.40622800	-0.21961300

H	7.08823600	1.64481600	-1.84510400	C	5.54929000	-0.63785000	0.21616500
H	7.16534900	-0.75135200	-2.55380900	C	6.04308500	-0.22900900	1.45407800
H	5.89633900	-3.16397700	-2.17845200	C	7.38347900	0.12920500	1.54301200
H	4.01380400	-4.13221900	-0.90784000	C	8.22475100	0.09693500	0.42053800
H	0.80041900	-1.96630400	-1.86692900	C	7.75266500	-0.30787900	-0.82176100
N	5.33820500	-2.62629500	-1.51967900	H	9.26288000	0.38928600	0.52457200
C	-2.74711500	1.51987700	0.09791100	H	8.39084200	-0.34035500	-1.69654200
C	-4.10601000	2.98608200	-1.86476500	H	5.39618300	-0.18938200	2.32361200
C	-3.91874400	1.04152700	-0.47749400	H	7.78876400	0.44442900	2.49744000
C	-2.24852600	2.72786100	-0.37582100	C	4.42713900	-1.39274900	-1.62621000
C	-2.91333200	3.47121900	-1.34245300	N	5.67092100	-1.14481100	-1.97955500
C	-4.60766500	1.75978200	-1.44677700	H	3.70357600	-1.74488600	-2.34800200
H	-2.49501200	4.41108800	-1.68158200	H	6.03279900	-1.24346200	-2.92384800
H	-5.51954800	1.35484300	-1.86865700	C	4.20905200	-0.99869800	-0.26817700
C	-3.87871700	-1.42913300	-0.10798200	H	3.49527300	-1.52778500	0.35208200
N	-4.83106400	-2.28649000	0.29106800	O	2.04299200	0.14007500	-1.07404600
C	0.19597600	2.67935700	0.13685100	H	3.87231100	1.04862300	-1.27849400
N	1.02135500	3.60264300	0.65303000	C	3.19236200	1.19037100	0.76401400
I	-1.83280900	-1.80198800	-0.61960300	C	4.04037800	2.26861300	1.00944800
I	0.62068400	0.70098800	-0.47485500	C	2.32669500	0.75383800	1.76888300
C	-4.67483400	-3.73535500	0.43105800	C	4.02453500	2.90860300	2.24767300
H	-5.64268200	-4.15041200	0.70260400	H	4.71442100	2.60786500	0.22844300
H	-3.94675300	-3.94396000	1.21342500	C	2.31423500	1.38560400	3.00677600
H	-4.34587000	-4.15296100	-0.51885900	H	1.66124200	-0.08197800	1.57647100
C	2.45925500	3.44193300	0.87647500	C	3.16447200	2.46583500	3.24816300
H	2.85829300	4.40625400	1.18237900	H	4.68421400	3.74937300	2.42992500
H	2.93172700	3.12158200	-0.05104300	H	1.64198900	1.03968200	3.78405200
H	2.61816100	2.70415400	1.66299000	H	3.15276700	2.96021800	4.21287200
H	-4.63371100	3.55476100	-2.61973000	C	-2.68767900	-0.18871000	0.24075200
N	-4.46160600	-0.22413500	-0.07080900	C	-2.61088500	0.01784200	3.03263000
N	-1.01476100	3.25026500	0.14170500	C	-2.74893500	1.04713700	0.87192500
H	-2.24979800	0.98142400	0.89554700	C	-2.54056900	-1.31439000	1.04073100
C	0.27069700	4.70749800	0.93926100	C	-2.50709200	-1.22953100	2.42740300
H	0.68405900	5.60697000	1.36759600	C	-2.71885500	1.16604500	2.25589100
C	-5.96116300	-1.56067600	0.54101800	H	-2.39167200	-2.13118700	3.01779400
H	-6.88550800	-2.00305700	0.87789700	H	-2.76824900	2.14835000	2.71116100
N	-0.97562900	4.51970300	0.63101100	C	-1.85250500	2.76042800	-0.68670400
N	-5.76343900	-0.29721100	0.32247500	N	-2.28322900	3.89290400	-1.24257800
TS4				C	-1.33856500	-3.05996700	-0.25634900
Sum of electronic and thermal Free Energies =				N	-1.55779900	-4.31851200	-0.63590300
-996.77109 Hartree				I	-0.00172800	1.83114800	-0.90404800
Sum of electronic and thermal free energies + the entropy				I	0.32560200	-1.87786700	-0.63410600
correction at 298.15K =				C	-1.55574100	4.77824200	-2.14810500
				H	-1.52126200	5.77448800	-1.70880900
C	3.19392500	0.52153400	-0.58954800	H	-1.52126200	5.77448800	-1.70880900
C	6.41516200	-0.67619600	-0.88382900	H	-2.07575600	4.80644200	-3.10509800

H	-0.54578000	4.40163600	-2.28612900	H	-4.31769600	-3.47437800	0.39530900
C	-0.67291900	-5.17475800	-1.42288500	H	-1.58209400	-3.91065600	0.56684500
H	-1.04179600	-5.22751200	-2.44703100	H	0.53069500	-2.75126400	0.24880000
H	-0.66823800	-6.16594600	-0.97255200	H	-0.27768700	-0.70145400	-1.28675700
H	0.33361500	-4.76481300	-1.40603800	N	-1.53437300	-2.93166200	0.28141900
H	-2.58408200	0.09755400	4.11188900	C	-0.06920200	0.11980000	0.72448200
C	-3.94575500	3.08212100	0.01759200	H	-0.53955500	-0.08251400	1.69116900
C	-3.59009900	4.13229300	-0.82654200	C	-0.42585200	1.54763200	0.34560800
C	-3.36318400	-3.62158000	0.48886700	C	-1.21941300	2.30814800	1.20396300
C	-2.81910600	-4.70888200	-0.19287100	C	0.00524700	2.11267400	-0.85677400
N	-2.83627200	2.24004100	0.07797900	C	-1.58070500	3.61165200	0.86860500
N	-2.41115700	-2.60548900	0.42483700	H	-1.56455800	1.87412800	2.13702600
C	-4.47174200	5.16876900	-1.12280300	C	-0.35583800	3.41290500	-1.19479900
C	-5.72250600	5.09748700	-0.53087700	H	0.62211300	1.53497200	-1.53707500
H	-6.44491700	5.88005100	-0.72787700	C	-1.15244100	4.16596200	-0.33350000
C	-6.08068200	4.03516300	0.32005700	H	-2.20048100	4.18954300	1.54491200
H	-7.07137000	4.02315000	0.75778900	H	-0.01633500	3.83853200	-2.13234000
C	-5.20182100	3.00452800	0.61241300	H	-1.43527400	5.17816000	-0.59903700
C	-4.62744800	-3.66871400	1.06978500	C	3.66843200	-0.45351200	0.65553800
C	-5.31893900	-4.86097300	0.93052400	C	2.45668600	-0.33646900	-0.07556000
H	-6.30769700	-4.95068300	1.36353700	C	2.51404200	-0.47948000	-1.47676200
C	-4.77302600	-5.95935400	0.23972300	C	3.73349200	-0.71907100	-2.08489700
H	-5.35405900	-6.86961600	0.15645900	C	4.92073200	-0.82188400	-1.33223400
C	-3.51464900	-5.90741800	-0.33706700	C	4.90356000	-0.69212200	0.04401600
H	-4.19120500	5.98238500	-1.77988100	C	2.02394700	-0.10146000	2.12543800
H	-5.46956400	2.18360300	1.26602500	C	1.41213500	-0.10613800	0.89837800
H	-5.03991600	-2.81854400	1.59895900	H	1.62327000	-0.40647000	-2.08907400
H	-3.09204800	-6.74842400	-0.87222200	H	3.77822700	-0.82900900	-3.16227900
H	-2.74090900	-0.26958800	-0.83937100	H	5.85995800	-1.00704000	-1.84060400

INT4

Sum of electronic and thermal Free Energies =
-996.797456 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -996.78726 Hartree

C	-2.67661100	-2.12193000	0.02926800
C	-2.21756800	-0.85937800	-0.33968200
C	-3.14375100	0.11984800	-0.67070300
C	-4.49938300	-0.20663600	-0.60168000
C	-4.92678600	-1.47970100	-0.21760700
C	-4.00996700	-2.47727000	0.10553500
C	-0.43568200	-2.28519400	0.09896300
C	-0.71016400	-0.87515100	-0.29436900
H	-2.82994100	1.10951900	-0.98056500
H	-5.23745000	0.54498000	-0.85528700
H	-5.98677600	-1.69887800	-0.17587800

H	-4.31769600	-3.47437800	0.39530900
H	-1.58209400	-3.91065600	0.56684500
H	0.53069500	-2.75126400	0.24880000
H	-0.27768700	-0.70145400	-1.28675700
N	-1.53437300	-2.93166200	0.28141900
C	-0.06920200	0.11980000	0.72448200
H	-0.53955500	-0.08251400	1.69116900
C	-0.42585200	1.54763200	0.34560800
C	-1.21941300	2.30814800	1.20396300
C	0.00524700	2.11267400	-0.85677400
C	-1.58070500	3.61165200	0.86860500
H	-1.56455800	1.87412800	2.13702600
C	-0.35583800	3.41290500	-1.19479900
H	0.62211300	1.53497200	-1.53707500
C	-1.15244100	4.16596200	-0.33350000
H	-2.20048100	4.18954300	1.54491200
H	-0.01633500	3.83853200	-2.13234000
H	-1.43527400	5.17816000	-0.59903700
C	3.66843200	-0.45351200	0.65553800
C	2.45668600	-0.33646900	-0.07556000
C	2.51404200	-0.47948000	-1.47676200
C	3.73349200	-0.71907100	-2.08489700
C	4.92073200	-0.82188400	-1.33223400
C	4.90356000	-0.69212200	0.04401600
C	2.02394700	-0.10146000	2.12543800
C	1.41213500	-0.10613800	0.89837800
H	1.62327000	-0.40647000	-2.08907400
H	3.77822700	-0.82900900	-3.16227900
H	5.85995800	-1.00704000	-1.84060400
H	5.80882700	-0.77179600	0.63514000
H	4.03675000	-0.34306000	2.74384200
H	1.58465800	0.03417300	3.10307800
N	3.37064400	-0.30074400	1.98506900

Cat2-TS5

Sum of electronic and thermal Free Energies=
-2460.37344 Hartree

Sum of electronic and thermal free energies + the entropy
correction) at 298.15K= -2460.36360 Hartree

C	2.71520300	-2.39270600	0.80464500
O	0.52642500	-1.71953100	-0.97644100
H	2.28265900	-3.37504500	0.62990200
C	2.07297400	-1.61545500	1.83972100
C	0.72639400	-1.89735300	2.12030900
C	2.73425200	-0.61487900	2.56808300
C	0.02784700	-1.13018300	3.03961100

H	0.23438600	-2.69579200	1.57774900	H	-4.63371100	3.55476100	-2.61973000
C	2.03876300	0.13362000	3.50636300	N	-4.46160600	-0.22413500	-0.07080900
H	3.79624000	-0.45714000	2.42924200	N	-1.01476100	3.25026500	0.14170500
C	0.68090400	-0.10524700	3.72346900	H	-2.24979800	0.98142400	0.89554700
H	-1.02042100	-1.33128800	3.22868700	C	0.27069700	4.70749800	0.93926100
H	2.55300600	0.89945500	4.07503900	H	0.68405900	5.60697000	1.36759600
H	0.13842100	0.49294100	4.44694500	C	-5.96116300	-1.56067600	0.54101800
C	5.52957600	-1.26088400	-1.24516200	H	-6.88550800	-2.00305700	0.87789700
C	4.57632800	-0.87336100	-0.28769500	N	-0.97562900	4.51970300	0.63101100
C	4.52420400	0.47535800	0.07247800	N	-5.76343900	-0.29721100	0.32247500
C	5.43215600	1.35972000	-0.49917300	Cat3-TS1			
C	6.39083000	0.93061800	-1.42432000	Sum of electronic and thermal Free Energies=			
C	6.44897600	-0.39915900	-1.82167500	-2128.70354 Hartree			
C	4.33218700	-3.10147000	-0.82923300	Sum of electronic and thermal free energies + the entropy			
C	3.78861800	-2.07930700	0.01257400	correction at 298.15K= -2128.69371 Hartree			
H	3.78980500	0.84316700	0.77413000	C	2.28380500	-0.09757900	-0.15901400
H	5.39396300	2.40622800	-0.21961300	C	5.18024000	1.74441300	0.14553700
H	7.08823600	1.64481600	-1.84510400	C	4.98484400	0.43795400	-0.32461500
H	7.16534900	-0.75135200	-2.55380900	C	5.81953400	-0.58128800	0.13587200
H	5.89633900	-3.16397700	-2.17845200	C	6.81651600	-0.25555400	1.04675100
H	4.01380400	-4.13221900	-0.90784000	C	6.98196000	1.05920400	1.51115800
H	0.80041900	-1.96630400	-1.86692900	C	6.16141200	2.08772100	1.06834400
N	5.33820500	-2.62629500	-1.51967900	H	7.76693000	1.27601000	2.22586200
C	-2.74711500	1.51987700	0.09791100	H	6.27866700	3.10668300	1.41697400
C	-4.10601000	2.98608200	-1.86476500	H	5.69028800	-1.60155600	-0.20861700
C	-3.91874400	1.04152700	-0.47749400	H	7.48027400	-1.03108200	1.41087400
C	-2.24852600	2.72786100	-0.37582100	C	3.48010500	1.84189100	-1.30719300
C	-2.91333200	3.47121900	-1.34245300	N	4.23210900	2.55848400	-0.48903100
C	-4.60766500	1.75978200	-1.44677700	H	2.69908000	2.30524900	-1.89369900
H	-2.49501200	4.41108800	-1.68158200	H	4.12216700	3.55515500	-0.32695600
H	-5.51954800	1.35484300	-1.86865700	C	3.80630200	0.46258600	-1.19498800
C	-3.87871700	-1.42913300	-0.10798200	H	3.64944400	-0.22164000	-2.01816600
N	-4.83106400	-2.28649000	0.29106800	O	1.22893700	-0.01060500	-0.91591800
C	0.19597600	2.67935700	0.13685100	H	2.38337000	0.62498900	0.66401700
N	1.02135500	3.60264300	0.65303000	C	2.71341300	-1.47532800	0.25073400
I	-1.83280900	-1.80198800	-0.61960300	C	3.13791200	-1.70490500	1.55784000
I	0.62068400	0.70098800	-0.47485500	C	2.66550800	-2.53205300	-0.66118100
C	-4.67483400	-3.73535500	0.43105800	C	3.50446700	-2.98837500	1.95766200
H	-5.64268200	-4.15041200	0.70260400	H	3.18039200	-0.87822200	2.26042000
H	-3.94675300	-3.94396000	1.21342500	C	3.03893100	-3.81039700	-0.26422500
H	-4.34587000	-4.15296100	-0.51885900	H	2.34785400	-2.34470100	-1.68268200
C	2.45925500	3.44193300	0.87647500	C	3.45716200	-4.03999700	1.04730600
H	2.85829300	4.40625400	1.18237900	H	3.82935100	-3.16433900	2.97670100
H	2.93172700	3.12158200	-0.05104300	H	3.00760200	-4.62862000	-0.97464900
H	2.61816100	2.70415400	1.66299000	H	3.74767400	-5.03784700	1.35564400

C	-3.48327400	0.40927000	0.32816900	H	7.24422400	-1.36606300	1.80551900
C	-4.17592500	0.38754900	3.04735600	C	3.57926400	1.63745900	-1.27235700
C	-3.48980200	1.57172800	1.08640100	N	4.55067400	2.29372800	-0.73147900
C	-3.78748200	-0.76981100	0.99264900	H	2.84426600	2.12937300	-1.89643300
C	-4.13752400	-0.80490000	2.33552200	H	4.69596300	3.29789500	-0.83967400
C	-3.83388700	1.58514100	2.43096700	C	3.63573200	0.20586100	-0.89641300
H	-4.36708600	-1.75043200	2.81237000	H	3.66959600	-0.41084500	-1.80119500
H	-3.82469600	2.51694300	2.98351700	O	1.21820400	-0.00161800	-0.95288200
C	-1.98734800	3.13478000	-0.17196800	H	2.27484500	0.43436000	0.77484900
C	-2.71689100	-2.59319600	-0.36459900	C	2.42047500	-1.64162800	0.31878500
I	-0.37020500	1.84651000	-0.55483800	C	2.33603600	-1.97229500	1.66932900
I	-0.82248300	-1.81677900	-0.63425200	C	2.54895000	-2.65958400	-0.62967000
H	-4.44735300	0.38006800	4.09487400	C	2.37672000	-3.30644000	2.07198000
N	-3.12259200	2.81290100	0.46448700	H	2.23463500	-1.18375900	2.40857300
N	-3.74320500	-2.01351700	0.27340800	C	2.59317400	-3.99060000	-0.23007800
H	-3.27654600	0.42631000	-0.73552300	H	2.60659500	-2.41061700	-1.68514300
N	-4.81682900	-2.82735400	0.23947100	C	2.50604400	-4.31654400	1.12337500
N	-3.94084000	3.88350600	0.52000500	H	2.30775800	-3.55479200	3.12505300
N	-4.49371900	-3.87098900	-0.39648200	H	2.69438800	-4.77480500	-0.97191000
N	-3.21157100	-3.75307300	-0.78228300	H	2.54003000	-5.35421900	1.43519200
N	-3.35891000	4.84351800	-0.06041700	C	-3.38750900	0.61811600	0.28127200
N	-2.16198700	4.41083300	-0.49694200	C	-4.18198200	0.61209600	2.97179200
C	-2.54262500	-4.81143800	-1.54056900	C	-3.34911200	1.77243800	1.05181800
H	-2.23826600	-4.41199300	-2.50626000	C	-3.79006000	-0.54698600	0.91846100
H	-1.68403900	-5.16196200	-0.97022300	C	-4.19146100	-0.57314700	2.24729500
H	-3.26735700	-5.61102400	-1.66892500	C	-3.74264200	1.79168400	2.38294200
C	-1.25040300	5.29650600	-1.22186000	H	-4.49674000	-1.50731100	2.70345200
H	-0.30301900	5.33667100	-0.68773700	H	-3.69496400	2.71549500	2.94715600
H	-1.11707800	4.91231300	-2.23173900	C	-1.70838400	3.25442300	-0.13240900
H	-1.71559800	6.27843500	-1.24483900	C	-2.79455700	-2.41421700	-0.43936300
Cat3-INT1				I	-0.14933700	1.79482500	-0.54454900
Sum of electronic and thermal Free Energies=				I	-0.85732900	-1.72071500	-0.68553000
-2128.70706 Hartree				H	-4.49245000	0.61107200	4.00845000
Sum of electronic and thermal free energies + the entropy				N	-2.88279700	2.99696600	0.46557300
correction at 298.15K=				N	-3.79916300	-1.78578900	0.18898800
			-2128.69722 Hartree	H	-3.13756300	0.63335900	-0.77257500
C	2.31387600	-0.19549900	-0.12834800	H	-3.13756300	0.63335900	-0.77257500
C	5.40141700	1.44587200	0.02748600	N	-4.91077800	-2.54744600	0.14632300
C	4.89055100	0.15252900	-0.06985900	N	-3.63140800	4.11882200	0.54152700
C	5.55608200	-0.88111700	0.57549600	N	-4.63261000	-3.60588500	-0.48617500
C	6.70919000	-0.57219900	1.29796400	N	-3.34243400	-3.54913900	-0.86005000
C	7.19146000	0.73675500	1.38117400	N	-2.97184500	5.05447100	0.00810400
C	6.53870700	1.78464500	0.73716200	N	-1.79518100	4.55130700	-0.41320400
H	8.08930000	0.94118300	1.95177100	C	-2.71640000	-4.64064900	-1.60706600
H	6.89798800	2.80518800	0.78385200	H	-2.38367300	-4.26103300	-2.57141000
H	5.19716800	-1.90193800	0.51747000	H	-1.88035200	-5.02765900	-1.02674500

H	-3.47578600	-5.40680300	-1.73935500	C	4.77603000	0.81526600	1.66141400
C	-0.81192900	5.39666100	-1.08851400	H	3.45215600	3.94595100	1.70491300
H	0.14128500	5.30590400	-0.57160600	H	5.45857800	0.16835900	2.19954800
H	-0.72465600	5.07719900	-2.12558900	C	3.41049200	-2.03498500	0.06492400
H	-1.17726400	6.41887600	-1.03326300	C	0.72543800	3.04734500	-0.60697800
Cat3-TS2				I	1.32032700	-1.86984600	0.33497700
Sum of electronic and thermal Free Energies=				I	-0.36866300	1.36095800	-0.13403300
-2128.67072 Hartree				H	5.09764200	2.52502100	2.91501100
Sum of electronic and thermal free energies + the entropy				N	4.30040600	-1.03681400	0.17295300
correction at 298.15K=				N	2.03347800	3.24271200	-0.39044500
-2128.66089 Hartree				H	2.71558300	0.73546200	-1.06377700
C	-2.16153900	-1.99604100	0.27868400	N	2.39141000	4.45949300	-0.84677900
O	-1.00733100	-1.18998200	0.55984100	N	5.54491700	-1.49545800	-0.07550300
H	-1.96952400	-3.03676600	0.56855400	N	5.45489800	-2.72775500	-0.33938300
C	-2.62280000	-1.95447900	-1.15969000	N	1.36400300	5.00853800	-1.33824000
C	-1.78305300	-1.50136800	-2.17416900	C	3.73355400	-4.45836600	-0.52262600
C	-3.90908900	-2.39433000	-1.48260700	H	3.02678900	-4.45714600	-1.35066800
C	-2.22684600	-1.47613100	-3.49627000	H	4.62638500	-5.01993600	-0.78504400
H	-0.77895500	-1.16877500	-1.93804800	H	3.27959900	-4.86282600	0.38012300
C	-4.35167100	-2.37076000	-2.79975900	C	-1.01130000	4.51399800	-1.68331700
H	-4.56927200	-2.74498400	-0.69456000	H	-1.30447000	3.80991700	-2.46014100
C	-3.51123000	-1.90626300	-3.81132000	H	-1.70001000	4.48188700	-0.84056900
H	-1.56589800	-1.11825200	-4.27763100	H	-0.94623100	5.52187300	-2.08447700
H	-5.35433000	-2.70743000	-3.03761400	N	4.15855800	-3.08244800	-0.26504000
H	-3.85799400	-1.88139500	-4.83795300	N	0.32797300	4.16197100	-1.20902800
C	-4.85889400	-0.17889800	2.21239100	Cat3- TS2'			
C	-4.05556000	-0.25360100	1.06532800	Sum of electronic and thermal Free Energies=			
C	-4.23086700	0.68780400	0.04804300	-2205.10553 Hartree			
C	-5.19342500	1.67315900	0.22455500	Sum of electronic and thermal free energies + the entropy			
C	-5.97315800	1.73627800	1.39044300	correction at 298.15K=			
C	-5.81836800	0.80783700	2.40946800	-2205.09569 Hartree			
C	-3.53235900	-1.95952600	2.51084400	C	2.19573800	0.11207200	0.26401100
C	-3.12806200	-1.37541300	1.27990400	C	5.65880700	1.61604000	0.20315500
H	-3.64181600	0.64694400	-0.86136400	C	4.89635900	0.43638500	0.25502000
H	-5.34993400	2.40843700	-0.55602700	C	5.54634600	-0.75460900	0.60612200
H	-6.71256700	2.52138900	1.49419200	C	6.90468100	-0.71293500	0.88815800
H	-6.41420200	0.84141500	3.31356100	C	7.63900000	0.48153000	0.81582900
H	-4.89509100	-1.40636600	3.97190200	C	7.02389700	1.67216800	0.46543100
H	-3.12001400	-2.82510800	3.01147400	H	8.69955200	0.47181500	1.03711700
H	-1.97898600	-0.87484300	1.57786500	H	7.56949000	2.60585200	0.40043900
N	-4.49737600	-1.23906000	3.05230200	H	5.01285700	-1.69473900	0.66030900
C	3.19775300	1.11014800	-0.16839300	H	7.41321700	-1.62813100	1.16831100
C	4.56631700	2.13026400	2.05884600	C	3.57095600	2.20938800	-0.32037000
C	4.08479800	0.32950900	0.56022800	N	4.80164800	2.65798100	-0.15388000
C	2.98384700	2.40305700	0.28809100	H	2.77082400	2.88359300	-0.59690100
C	3.65251700	2.93046800	1.38464800	H	5.09043500	3.62078100	-0.30017600

C	3.52450600	0.79516800	-0.16268300	N	-4.21484800	3.79792600	0.48848700
H	3.45277700	0.54843400	-1.47203300	N	-4.40963000	-3.92956700	-0.73236300
O	1.21879600	0.24738700	-0.74833300	N	-3.62362800	4.79624200	-0.01208400
H	1.84914400	0.61653000	1.17500800	Cat3-INT2			
C	2.41730100	-1.34752200	0.61081600	Sum of electronic and thermal Free Energies=			
C	2.41136700	-1.75773400	1.94230300	-2128.737935 Hartree			
C	2.62184400	-2.29465000	-0.39624000	Sum of electronic and thermal free energies + the entropy			
C	2.61500100	-3.09684200	2.26949100	correction at 298.15K= -2128.72808 Hartree			
H	2.24770000	-1.02488300	2.72627500	C	-2.23383900	-2.13655800	1.04495100
C	2.82497400	-3.63197100	-0.07130900	O	-0.97502100	-1.42203100	1.17672800
H	2.62874800	-1.98954700	-1.43782700	H	-2.19798700	-2.98669000	1.73316300
C	2.82345500	-4.03581300	1.26297500	C	-2.35353400	-2.66376900	-0.36834400
H	2.60686600	-3.40598200	3.30852600	C	-1.46938500	-2.31540900	-1.38535800
H	2.98522500	-4.35963200	-0.85888200	C	-3.42755000	-3.50877200	-0.66086800
H	2.98134900	-5.07811700	1.51558200	C	-1.65826400	-2.79733900	-2.68110400
O	2.81538700	0.14571200	-2.57914000	H	-0.63661400	-1.65251900	-1.18869800
H	2.78168500	0.85239100	-3.23850800	C	-3.61589900	-3.99031100	-1.94994900
H	1.94226200	0.17578500	-1.98126400	H	-4.12125300	-3.78217700	0.12834000
C	-3.61288000	0.34490300	0.21730800	C	-2.73107400	-3.63272200	-2.96747000
C	-4.52745700	0.21434000	2.86704900	H	-0.96450000	-2.51272700	-3.46399600
C	-3.72963500	1.48277400	1.00296600	H	-4.45392700	-4.64403800	-2.16304900
C	-3.92515700	-0.86410300	0.82134000	H	-2.87895500	-4.00570100	-3.97432600
C	-4.38346500	-0.95377800	2.12861500	C	-5.00064800	0.36267100	1.53027100
C	-4.18358400	1.44212400	2.31407700	C	-4.08689300	-0.26927200	0.65058300
H	-4.61364800	-1.92179500	2.55764200	C	-4.06681500	0.13326800	-0.69908300
H	-4.25562600	2.35678200	2.89051200	C	-4.92027500	1.14139300	-1.11112800
C	-2.19355300	3.12983600	-0.09311800	C	-5.80918100	1.76379600	-0.21065800
N	-2.38669100	4.41323000	-0.37907100	C	-5.86516600	1.38145800	1.11727100
C	-2.68587000	-2.60138600	-0.50368400	C	-3.88492800	-1.17347900	2.71190400
N	-3.10540100	-3.75745600	-1.00599500	C	-3.37382200	-1.24845100	1.43967000
I	-0.49193600	1.89924900	-0.41603700	H	-3.39657100	-0.33539900	-1.41081400
I	-0.80032500	-1.77625000	-0.58495200	H	-4.91089000	1.45749000	-2.14803600
C	-1.45299800	5.35448200	-0.99697100	H	-6.46458800	2.54982700	-0.56773900
H	-0.54416400	5.38978500	-0.39926900	H	-6.55124200	1.84651000	1.81588400
H	-1.94117700	6.32538400	-1.00503500	H	-5.38921800	0.02554000	3.59288800
H	-1.24162900	5.02423700	-2.01259800	H	-3.62208800	-1.74852500	3.58820600
C	-2.34709800	-4.75788200	-1.75873600	H	-0.90907900	-1.17463300	2.11265500
H	-3.01028100	-5.60592300	-1.90688700	N	-4.85215100	-0.21178600	2.76990500
H	-1.47738000	-5.05039600	-1.17295800	C	2.92366600	1.49343400	-0.35487600
H	-2.05198400	-4.32847300	-2.71468700	C	4.24552400	2.89524100	1.68838700
H	-4.88343000	0.16474100	3.88776500	C	3.99305700	0.94261600	0.33509100
N	-3.36138900	2.75371000	0.44814200	C	2.51748300	2.75872300	0.04285700
N	-3.77856000	-2.08011300	0.06998000	C	3.15637700	3.47277500	1.04664500
H	-3.31576400	0.40251000	-0.82341900	C	4.66500200	1.61552700	1.34584900
N	-4.81805300	-2.92432800	-0.08381100	H	2.79911500	4.45826100	1.32106700

H	5.49579300	1.13972600	1.85311700	C	5.33704900	1.26772600	-1.41836200
C	3.77204300	-1.53600600	0.01658400	C	6.25633500	0.61946700	-2.25722100
N	4.65801500	-2.43691300	-0.39052600	C	6.29579800	-0.76419700	-2.33415400
C	0.12555700	2.93475900	-0.68334100	C	4.19273600	-3.11671400	-0.63948300
N	-0.50366600	3.88241900	-1.36715000	C	3.71721700	-1.92927300	-0.04680300
I	1.82065200	-1.83699800	0.57006200	H	3.75375300	1.08470700	0.01188900
I	-0.65843900	1.20600700	0.09404600	H	5.31473900	2.35093300	-1.39352500
C	4.48874000	-3.88201000	-0.55546000	H	6.93553300	1.20801700	-2.86228900
H	4.23676400	-4.31751500	0.41000200	H	6.98105100	-1.28355400	-2.99336200
H	5.43998800	-4.26732200	-0.91199700	H	5.71229300	-3.53363700	-1.99730600
H	3.70470400	-4.06081600	-1.28907300	H	3.86273200	-4.13076700	-0.46149900
C	-1.91399700	3.94072800	-1.75800900	H	1.29781800	-1.65964200	-1.28677200
H	-2.05434700	4.87974600	-2.28686900	N	5.18605900	-2.84182000	-1.47330000
H	-2.52795200	3.91181300	-0.85916300	C	-3.07137400	1.19757300	-0.13202900
H	-2.12967800	3.09685300	-2.41150000	C	-4.36424300	2.07003000	-2.46226300
H	4.75619700	3.43675500	2.47381600	C	-4.01967700	0.41193100	-0.77255500
N	4.43851500	-0.37668300	-0.01857100	C	-2.75491300	2.41140500	-0.72735700
N	1.39057400	3.36327900	-0.61117700	C	-3.38545700	2.86479700	-1.87788500
H	2.45384800	0.97532300	-1.18409300	C	-4.67501400	0.82716200	-1.92391100
N	1.49972300	4.55354800	-1.23303700	H	-3.10414800	3.81734200	-2.31088200
N	5.70304400	-0.59615700	-0.42770200	H	-5.40738400	0.18071300	-2.39272600
N	5.83071700	-1.83467600	-0.64924300	C	-3.52759500	-1.93384100	-0.02707000
N	0.35927100	4.86201200	-1.68504000	N	-4.35733800	-2.87878900	0.40246100
Cat3-TS3				C	-0.43994500	2.93924400	0.08688600
Sum of electronic and thermal Free Energies=				N	0.05704500	4.07044000	0.57470600
-2128.70125 Hartree				I	-1.41133700	-1.93815100	-0.26354700
Sum of electronic and thermal free energies + the entropy				I	0.46910600	1.07304800	-0.18723000
correction at 298.15K=				C	-4.03734900	-4.24761400	0.80606500
-2128.69138 Hartree				H	-4.97958100	-4.74314200	1.02569000
C	2.66257400	-1.99395300	0.86428600	H	-3.40660400	-4.21484800	1.69281300
O	0.94419700	-1.41920800	-0.41999400	H	-3.52846500	-4.74540900	-0.01713100
H	2.20211200	-2.97252800	0.96137300	C	1.42235500	4.33930200	1.02574100
C	2.33384000	-1.05378800	1.92809000	H	1.47412000	5.39845300	1.26372600
C	1.10836300	-1.20970100	2.59434000	H	2.11108000	4.09573200	0.21873700
C	3.21480600	-0.04812100	2.34201600	H	1.62574700	3.73660300	1.90983500
C	0.73678000	-0.32896800	3.59718600	H	-4.86658100	2.40823100	-3.35924200
H	0.44837600	-2.01912300	2.30209900	N	-4.33755200	-0.88484800	-0.24069700
C	2.84565400	0.82711200	3.35702000	N	-1.72802300	3.23362600	-0.14604500
H	4.19903900	0.03075000	1.89890200	H	-2.61216700	0.88532600	0.79833500
C	1.60134200	0.70161200	3.96962600	N	-1.97456500	4.51700300	0.18784500
H	-0.21906200	-0.44481400	4.09447700	N	-5.61443800	-1.21586100	0.04546500
H	3.53282500	1.60238300	3.67481400	N	-0.89813900	5.01682200	0.62289300
H	1.31327200	1.39168000	4.75454600	N	-5.62190100	-2.41791200	0.43435000
C	5.39898600	-1.46412800	-1.53520500	Cat3-INT3			
C	4.49130500	-0.84607300	-0.65301400	Sum of electronic and thermal Free Energies=			
C	4.45478300	0.55402900	-0.61978900				

-2128.70703 Hartree				I	-1.82782200	-1.80691500	-0.81498300
Sum of electronic and thermal free energies + the entropy				I	0.61895200	0.68248700	-0.75470300
correction at 298.15K=				C	-4.64871800	-3.79724900	0.46965200
		-2128.69708 Hartree		H	-5.60423000	-4.14809500	0.85053100
C	2.73903700	-2.36263700	1.07488200	H	-3.84123900	-4.07808400	1.14366700
O	0.47175500	-1.62958400	-1.34195000	H	-4.47249000	-4.18450400	-0.53194300
H	2.39004200	-3.39070300	0.99878100	C	2.53722600	3.55391000	0.56748800
C	1.90969000	-1.49378700	1.87818400	H	2.87861000	4.58296200	0.64921500
C	0.55156400	-1.82890900	1.99547900	H	2.93244700	3.09444200	-0.33623800
C	2.39917500	-0.35617200	2.54013500	H	2.82022100	2.98413800	1.45232600
C	-0.31930800	-0.99261000	2.67875200	H	-4.85278600	3.62415800	-2.16435800
H	0.18782200	-2.73236600	1.51886900	N	-4.38150500	-0.29139900	0.12992600
C	1.53031900	0.46209600	3.24525200	N	-0.95761600	3.19685700	0.17298800
H	3.46110700	-0.14487400	2.53654000	H	-2.09762600	0.88591200	0.93833300
C	0.16770900	0.15882000	3.29419400	N	-0.84650500	4.42087900	0.73215900
H	-1.37286900	-1.24115300	2.74150900	N	-5.60320100	-0.43722200	0.68703100
H	1.91105000	1.33259100	3.76659700	N	0.38204400	4.65069100	0.91271700
H	-0.50929300	0.80965400	3.83637100	N	-5.80445500	-1.67332900	0.85252700
C	5.72139400	-1.33189600	-0.77654900				
C	4.63889800	-0.88337900	-0.00153700	TS4			
C	4.47818100	0.49318000	0.16192700	Sum of electronic and thermal Free Energies=			
C	5.40730500	1.35202500	-0.41585300	-996.77109 Hartree			
C	6.49133800	0.86748700	-1.15564400	Sum of electronic and thermal free energies + the entropy			
C	6.66210600	-0.49725100	-1.35618700	correction at 298.15K=			
C	4.57807600	-3.17855000	-0.24575500			-996.76079 Hartree	
C	3.87974200	-2.08713700	0.37329400	C	3.19392500	0.52153400	-0.58954800
H	3.64847400	0.90090100	0.71994800	C	6.41516200	-0.67619600	-0.88382900
H	5.28562300	2.42152800	-0.28705300	C	5.54929000	-0.63785000	0.21616500
H	7.20081100	1.56330000	-1.58683800	C	6.04308500	-0.22900900	1.45407800
H	7.48040500	-0.89569900	-1.94346700	C	7.38347900	0.12920500	1.54301200
H	6.29870000	-3.31712400	-1.37692100	C	8.22475100	0.09693500	0.42053800
H	4.32442300	-4.22959700	-0.21177200	C	7.75266500	-0.30787900	-0.82176100
H	0.71492900	-1.84703300	-2.24936700	H	9.26288000	0.38928600	0.52457200
N	5.63368300	-2.73334600	-0.87463300	H	8.39084200	-0.34035500	-1.69654200
C	-2.68127700	1.46369200	0.23075400	H	5.39618300	-0.18938200	2.32361200
C	-4.24691200	3.02145300	-1.50034900	H	7.78876400	0.44442900	2.49744000
C	-3.90440000	1.01120600	-0.24822300	C	4.42713900	-1.39274900	-1.62621000
C	-2.24541600	2.69956700	-0.22930000	N	5.67092100	-1.14481100	-1.97955500
C	-3.00688300	3.48776900	-1.08215100	H	3.70357600	-1.74488600	-2.34800200
C	-4.69613900	1.76890100	-1.10091200	H	6.03279900	-1.24346200	-2.92384800
H	-2.62634300	4.44473300	-1.41839300	C	4.20905200	-0.99869800	-0.26817700
H	-5.64249300	1.37548500	-1.45202400	H	3.49527300	-1.52778500	0.35208200
C	-3.81257700	-1.49228600	-0.06700200	O	2.04299200	0.14007500	-1.07404600
N	-4.72330900	-2.33890800	0.40313400	H	3.87231100	1.04862300	-1.27849400
C	0.25901800	2.65453800	-0.00839000	C	3.19236200	1.19037100	0.76401400
N	1.07885400	3.58635500	0.47012600	C	4.04037800	2.26861300	1.00944800
				C	2.32669500	0.75383800	1.76888300

C	4.02453500	2.90860300	2.24767300	H	-6.30769700	-4.95068300	1.36353700
H	4.71442100	2.60786500	0.22844300	C	-4.77302600	-5.95935400	0.23972300
C	2.31423500	1.38560400	3.00677600	H	-5.35405900	-6.86961600	0.15645900
H	1.66124200	-0.08197800	1.57647100	C	-3.51464900	-5.90741800	-0.33706700
C	3.16447200	2.46583500	3.24816300	H	-4.19120500	5.98238500	-1.77988100
H	4.68421400	3.74937300	2.42992500	H	-5.46956400	2.18360300	1.26602500
H	1.64198900	1.03968200	3.78405200	H	-5.03991600	-2.81854400	1.59895900
H	3.15276700	2.96021800	4.21287200	H	-3.09204800	-6.74842400	-0.87222200
C	-2.68767900	-0.18871000	0.24075200	H	-2.74090900	-0.26958800	-0.83937100
C	-2.61088500	0.01784200	3.03263000	INT4			
C	-2.74893500	1.04713700	0.87192500	Sum of electronic and thermal Free Energies =			
C	-2.54056900	-1.31439000	1.04073100	-996.797456 Hartree			
C	-2.50709200	-1.22953100	2.42740300	Sum of electronic and thermal free energies + the entropy			
C	-2.71885500	1.16604500	2.25589100	correction at 298.15K =			
H	-2.39167200	-2.13118700	3.01779400	C	-2.67661100	-2.12193000	0.02926800
H	-2.76824900	2.14835000	2.71116100	C	-2.21756800	-0.85937800	-0.33968200
C	-1.85250500	2.76042800	-0.68670400	C	-3.14375100	0.11984800	-0.67070300
N	-2.28322900	3.89290400	-1.24257800	C	-4.49938300	-0.20663600	-0.60168000
C	-1.33856500	-3.05996700	-0.25634900	C	-4.92678600	-1.47970100	-0.21760700
N	-1.55779900	-4.31851200	-0.63590300	C	-4.00996700	-2.47727000	0.10553500
I	-0.00172800	1.83114800	-0.90404800	C	-0.43568200	-2.28519400	0.09896300
I	0.32560200	-1.87786700	-0.63410600	C	-0.71016400	-0.87515100	-0.29436900
C	-1.55574100	4.77824200	-2.14810500	H	-2.82994100	1.10951900	-0.98056500
H	-1.52126200	5.77448800	-1.70880900	H	-5.23745000	0.54498000	-0.85528700
H	-2.07575600	4.80644200	-3.10509800	H	-5.98677600	-1.69887800	-0.17587800
H	-0.54578000	4.40163600	-2.28612900	H	-4.31769600	-3.47437800	0.39530900
C	-0.67291900	-5.17475800	-1.42288500	H	-1.58209400	-3.91065600	0.56684500
H	-1.04179600	-5.22751200	-2.44703100	H	0.53069500	-2.75126400	0.24880000
H	-0.66823800	-6.16594600	-0.97255200	H	-0.27768700	-0.70145400	-1.28675700
H	0.33361500	-4.76481300	-1.40603800	N	-1.53437300	-2.93166200	0.28141900
H	-2.58408200	0.09755400	4.11188900	C	-0.06920200	0.11980000	0.72448200
C	-3.94575500	3.08212100	0.01759200	H	-0.53955500	-0.08251400	1.69116900
C	-3.59009900	4.13229300	-0.82654200	C	-0.42585200	1.54763200	0.34560800
C	-3.36318400	-3.62158000	0.48886700	C	-1.21941300	2.30814800	1.20396300
C	-2.81910600	-4.70888200	-0.19287100	C	0.00524700	2.11267400	-0.85677400
N	-2.83627200	2.24004100	0.07797900	C	-1.58070500	3.61165200	0.86860500
N	-2.41115700	-2.60548900	0.42483700	H	-1.56455800	1.87412800	2.13702600
C	-4.47174200	5.16876900	-1.12280300	C	-0.35583800	3.41290500	-1.19479900
C	-5.72250600	5.09748700	-0.53087700	H	0.62211300	1.53497200	-1.53707500
H	-6.44491700	5.88005100	-0.72787700	C	-1.15244100	4.16596200	-0.33350000
C	-6.08068200	4.03516300	0.32005700	H	-2.20048100	4.18954300	1.54491200
H	-7.07137000	4.02315000	0.75778900	H	-0.01633500	3.83853200	-2.13234000
C	-5.20182100	3.00452800	0.61241300	H	-1.43527400	5.17816000	-0.59903700
C	-4.62744800	-3.66871400	1.06978500	C	3.66843200	-0.45351200	0.65553800
C	-5.31893900	-4.86097300	0.93052400	C	2.45668600	-0.33646900	-0.07556000

C	2.51404200	-0.47948000	-1.47676200	H	0.82410000	1.14790700	-2.46168700
C	3.73349200	-0.71907100	-2.08489700	H	1.49911200	-0.91776000	-3.66957000
C	4.92073200	-0.82188400	-1.33223400	C	-4.77146300	2.73618300	-1.37957400
C	4.90356000	-0.69212200	0.04401600	C	-3.83670400	1.88144600	-0.74312500
C	2.02394700	-0.10146000	2.12543800	C	-3.00608700	2.42197700	0.25663400
C	1.41213500	-0.10613800	0.89837800	C	-3.11298700	3.76442300	0.57272500
H	1.62327000	-0.40647000	-2.08907400	C	-4.04356100	4.59574300	-0.08484700
H	3.77822700	-0.82900900	-3.16227900	C	-4.88421800	4.09450100	-1.06256000
H	5.85995800	-1.00704000	-1.84060400	C	-5.01425100	0.68956500	-2.24509300
H	5.80882700	-0.77179600	0.63514000	C	-4.00924200	0.56847600	-1.32011200
H	4.03675000	-0.34306000	2.74384200	H	-2.29328000	1.79121100	0.77814600
H	1.58465800	0.03417300	3.10307800	H	-2.47314600	4.18560700	1.34049300
N	3.37064400	-0.30074400	1.98506900	H	-4.10385100	5.64413900	0.18377500
Cat3-TS5				H	-5.60667000	4.72535900	-1.56794700
Sum of electronic and thermal Free Energies=				H	-6.20994300	2.31944600	-2.88617200
-2492.38107 Hartree				H	-5.44085900	-0.06522700	-2.88965200
Sum of electronic and thermal free energies + the entropy				N	-5.46917100	1.98183800	-2.28762000
correction at 298.15K=				O	-0.84295900	-0.03083500	1.58376300
-2492.37121 Hartree				H	-1.00878800	-0.13139900	2.53088400
C	-3.56558300	-2.56122400	2.15510100	C	3.55879200	0.38203900	-0.43628700
C	-2.91413400	-2.44551300	0.92129600	C	5.97389900	0.15830600	0.97095400
C	-2.20912000	-3.54837200	0.44074800	C	4.19385900	-0.84128000	-0.27264900
C	-2.17890500	-4.70743700	1.20996800	C	4.14742300	1.48125700	0.17325600
C	-2.82174600	-4.78085100	2.45219000	C	5.34479600	1.39315900	0.87087700
C	-3.53327800	-3.69747000	2.95065400	C	5.39218300	-0.97472200	0.41473700
C	-4.06278700	-0.51546000	1.39510500	C	5.76754400	2.27714200	1.33293800
C	-3.11888200	-1.04800400	0.43599700	H	5.85140800	-1.95050800	0.51960000
H	-1.69382700	-3.51399600	-0.50984700	C	2.38584400	-2.55648800	-0.55333000
H	-1.64288200	-5.57393800	0.83991400	N	2.36501400	-3.66934600	-1.27948200
H	-2.77060800	-5.69668200	3.02859300	C	2.25921600	3.11619300	0.44704300
H	-4.04562500	-3.73282600	3.90440000	N	2.23099500	4.42523600	0.22015800
H	-4.78436000	-1.14373200	3.22105600	I	0.86819300	-1.70402900	0.57952500
H	-4.52703500	0.46166600	1.40488500	I	0.72555500	1.83446600	1.11385300
H	-2.11749900	-0.49319200	0.91174800	C	1.31093300	-4.68034300	-1.35746600
N	-4.24014500	-1.35018300	2.38660600	H	1.55694300	-5.33318700	-2.19096800
C	-3.25735600	-0.71762500	-1.06696800	H	0.36040300	-4.17808600	-1.53375700
H	-3.86745900	-1.51916200	-1.49393700	H	1.29019600	-5.23812500	-0.42220400
C	-1.91446900	-0.76058900	-1.79583200	C	1.11604400	5.35299600	0.40991700
C	-1.54032000	-1.90274500	-2.50722400	H	0.31665100	5.08870000	-0.28065700
C	-1.04634300	0.33397300	-1.79531300	H	1.49366500	6.34919200	0.19464100
C	-0.31471300	-1.96660900	-3.16866500	H	0.77818800	5.28769600	1.44253500
H	-2.21897900	-2.74905500	-2.55178800	H	6.90800900	0.07317300	1.51070300
C	0.17014400	0.28137400	-2.46838300	N	3.58856700	-2.02488300	-0.81969700
H	-1.32403800	1.24329300	-1.27662500	N	3.50421500	2.76345100	0.09112600
C	0.54947400	-0.87480700	-3.14677700	H	2.65503900	0.47498700	-1.02665200
H	-0.04304000	-2.86499300	-3.71270100				

N	3.52426200	-3.80995700	-1.94742000	C	-3.26986500	1.26979300	-0.60870700
N	4.26336900	-2.82129600	-1.67432600	C	-2.02949200	1.18807900	0.03012600
N	4.19250000	3.84874200	-0.32108700	I	-1.68643400	-0.72930300	0.81432600
N	3.42138100	4.84689100	-0.24357300	C	-3.60332300	2.50104600	-1.18426900
Cat4-TS1				C	-2.72848700	3.57518900	-1.10080700
Sum of electronic and thermal Free Energies=				C	-1.50949600	3.45217400	-0.43537600
-1468.37245 Hartree				C	-1.14298900	2.24237600	0.14778100
Sum of electronic and thermal free energies + the entropy				H	-6.13200500	-3.24349600	-0.40557300
correction at 298.15K=				H	-7.08385200	-1.27514300	-1.56691700
-1468.36243 Hartree				H	-4.55202700	2.61455500	-1.69518200
C	1.43623200	0.03765600	0.54791300	H	-3.00172000	4.52105300	-1.55297400
C	3.60174700	-2.42773700	-0.60493700	H	-0.83684500	4.29850600	-0.36218400
C	3.83779300	-1.29988300	0.19265400	H	-0.20936100	2.13425200	0.68137900
C	4.94362700	-0.49521700	-0.08073600	H	-5.82382400	0.83447100	-1.70257000
C	5.76762200	-0.84628600	-1.14333000	H	-3.88588400	-3.11150600	0.63361800
C	5.49820500	-1.97245400	-1.93657300	Cat4-INT1			
C	4.40334500	-2.78805600	-1.68104700	Sum of electronic and thermal Free Energies=			
H	6.15858900	-2.21291500	-2.76123200	-1468.37650 Hartree			
H	4.18512900	-3.66235200	-2.28229000	Sum of electronic and thermal free energies + the entropy			
H	5.15177800	0.38387600	0.51941000	correction at 298.15K=			
H	6.63550300	-0.23760800	-1.36904800	-1468.36645 Hartree			
C	1.98982700	-2.40364700	0.94800100	C	-1.57935900	-0.09408600	-0.45177400
N	2.45889100	-3.06197400	-0.09477800	C	-4.64989400	-1.71476300	-0.05082100
H	1.10887100	-2.74858000	1.47180300	C	-4.13562000	-0.42032100	-0.11156900
H	2.03174600	-3.89349000	-0.49304900	C	-4.70705000	0.56475900	0.68211100
C	2.73208900	-1.20385900	1.15267400	C	-5.77424700	0.20906000	1.50828600
H	2.84256100	-0.78050600	2.14272400	C	-6.26418400	-1.09874300	1.54746800
O	0.48798000	0.07438800	1.43983200	C	-5.70402400	-2.09913300	0.75661300
H	1.20164800	-0.41040300	-0.43195800	H	-7.09425200	-1.34000700	2.20031100
C	2.27365500	1.27655800	0.38630100	H	-6.06967400	-3.11840600	0.76924700
C	2.71367300	1.65487000	-0.88053700	H	-4.34071300	1.58416700	0.66126500
C	2.58744500	2.06434100	1.49472200	H	-6.23429100	0.96501500	2.13364200
C	3.46651500	2.81617000	-1.04208100	C	-2.97920100	-1.82495100	-1.54947800
H	2.46585900	1.03891700	-1.74001400	N	-3.89540800	-2.51174600	-0.95415400
C	3.34723100	3.21746500	1.33511300	H	-2.30031000	-2.27497600	-2.26152400
H	2.23335400	1.76642500	2.47607800	H	-4.05595300	-3.50794600	-1.10505800
C	3.78777400	3.59514900	0.06574700	C	-2.98410100	-0.42018000	-1.07895500
H	3.80269400	3.10941500	-2.03010900	H	-3.12454800	0.24933800	-1.93455700
H	3.59518800	3.82539600	2.19784800	O	-0.60575400	-0.30254200	-1.40958000
H	4.37734200	4.49659800	-0.05699000	H	-1.47222000	-0.77969000	0.40871800
C	-5.56649500	-2.32092900	-0.46050600	C	-1.55885500	1.32360000	0.09889000
C	-6.10146700	-1.20975700	-1.11466200	C	-1.09063200	1.55265400	1.39094500
C	-5.39195600	-0.01887700	-1.19310100	C	-1.90458000	2.41445000	-0.70254800
C	-4.12348600	0.07369200	-0.61086600	C	-0.95888500	2.85306700	1.87833800
C	-3.61352400	-1.05250100	0.03714500	H	-0.81961700	0.70829900	2.01824800
C	-4.30616600	-2.25131000	0.12481700	C	-1.78095600	3.71175200	-0.21808800

H	-2.25864400	2.25519800	-1.71676000	C	-4.24513300	1.30191600	1.11129800
C	-1.30397200	3.93437000	1.07434100	C	-3.20020200	0.67622900	0.41580700
H	-0.58803500	3.01800900	2.88371100	C	-2.67921200	1.29076700	-0.72547600
H	-2.05156500	4.55168700	-0.84821900	C	-3.20679700	2.51677800	-1.11131900
H	-1.20399800	4.94646200	1.44976500	C	-4.23644900	3.13261500	-0.38371200
C	4.91765500	-2.79960600	1.37966700	C	-4.77783200	2.53185800	0.74389800
C	5.69163700	-1.64738000	1.53100300	C	-3.85492400	-0.61953400	2.19545100
C	5.22735300	-0.41607200	1.08693700	C	-2.87737700	-0.55093900	1.16290000
C	3.96939200	-0.32730300	0.48000000	H	-1.90701200	0.81492200	-1.31947200
C	3.21207500	-1.49091600	0.33455800	H	-2.82158000	3.00472100	-1.99889400
C	3.66445900	-2.72671300	0.77858800	H	-4.62226700	4.08971900	-0.71356100
C	3.35800100	0.90500300	-0.04379400	H	-5.57863600	2.99111600	1.31070800
C	2.09344400	0.80396000	-0.62833500	H	-5.30684900	0.69332400	2.87521200
I	1.31026400	-1.14186300	-0.54955100	H	-3.97877200	-1.38277800	2.95194100
C	3.94630100	2.17577000	-0.02076800	H	-1.82713500	-0.30284100	1.82459200
C	3.28805700	3.26506800	-0.57470800	N	-4.60143300	0.46854800	2.17907300
C	2.03894500	3.11259100	-1.17691400	C	3.57459500	3.46619300	-1.27384900
C	1.42534700	1.86385800	-1.21397900	C	4.79464600	2.80697900	-1.11319400
H	5.29149500	-3.75440600	1.73068500	C	4.84989400	1.53454100	-0.56046500
H	6.66619200	-1.71255400	2.00034000	C	3.67023200	0.90009500	-0.15641800
H	4.92252600	2.30959400	0.42999100	C	2.46484100	1.58344500	-0.32805800
H	3.75676100	4.24159100	-0.54642400	C	2.38890400	2.85398500	-0.88001800
H	1.53904900	3.96384000	-1.62432500	C	3.58057900	-0.43815500	0.44458300
H	0.46171200	1.71063600	-1.67811000	C	2.31395200	-0.91517900	0.79375100
H	5.84266400	0.46736300	1.21222500	I	0.80916900	0.46741200	0.33124400
H	3.06067200	-3.62069000	0.66265700	C	4.66478700	-1.28473600	0.70299200

Cat4-TS2

Sum of electronic and thermal Free Energies=
-1468.33772 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K= -1468.32769 Hartree

C	-1.91232600	-1.66504000	0.76617200
O	-0.70292600	-1.15427200	1.33100200
H	-2.20361200	-2.57475600	1.30841400
C	-1.86151500	-1.99286900	-0.71099600
C	-0.65742300	-2.36559100	-1.30790700
C	-3.02665200	-1.98568900	-1.48126400
C	-0.61294000	-2.70453700	-2.65863300
H	0.24824400	-2.40428000	-0.71295900
C	-2.98481700	-2.32756600	-2.82926400
H	-3.97149800	-1.70445800	-1.02626200
C	-1.77526500	-2.68147100	-3.42385900
H	0.33092800	-2.98796300	-3.11059900
H	-3.89558200	-2.31130100	-3.41714000
H	-1.74056100	-2.94016600	-4.47594000

C	4.46097100	-2.53019900	1.28068200
C	3.17800700	-2.96084200	1.61688900
C	2.07466600	-2.14678300	1.37586900
H	3.54637300	4.45926700	-1.70624400
H	5.71183700	3.29353500	-1.42302000
H	5.66871700	-0.96461500	0.45059600
H	5.31177400	-3.17261900	1.47376600
H	3.02934400	-3.93287000	2.07165300
H	1.06578300	-2.44409300	1.63090800
H	5.80571000	1.03786600	-0.44297800
H	1.43899900	3.36214400	-1.00333000

Cat4-TS2'

Sum of electronic and thermal Free Energies=
-1544.78153 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K= -1544.77152 Hartree

C	1.53694100	-0.94216000	0.64631400
C	5.11910000	0.12218700	0.64728400
C	3.77900200	0.45313600	0.40670300

C	3.47857400	1.59686000	-0.33514200	H	-4.70020000	2.94245400	-1.14287800
C	4.53349500	2.36296700	-0.81363200	H	-3.00194600	4.69530900	-1.45226100
C	5.86881400	2.01582200	-0.55036400	H	-0.63574200	4.27997800	-0.83788700
C	6.18733000	0.88739900	0.19171500	H	0.03935800	2.06998500	0.09106800
H	6.66603100	2.64156400	-0.93369600	H	-6.08236400	1.28328700	-0.80365100
H	7.21294700	0.61119800	0.40463500	H	-3.99072700	-2.80820300	1.10975300
H	2.44882800	1.87431600	-0.53003300	Cat4-INT2			
H	4.32507700	3.25013500	-1.40021200	Sum of electronic and thermal Free Energies=			
C	3.89350700	-1.47562800	1.62750900	-1468.41947 Hartree			
N	5.12718400	-1.06123400	1.39598200	Sum of electronic and thermal free energies + the entropy			
H	3.70088500	-2.38166000	2.18683300	correction at 298.15K= -1468.40942 Hartree			
H	5.96305000	-1.51401500	1.75393000	C	2.38481400	-1.57052100	-1.06018900
C	2.95263300	-0.54694800	1.10432200	O	1.02151000	-1.80750300	-1.47751600
H	2.63648200	0.09432200	2.19869000	H	3.03159700	-2.20501600	-1.67538700
O	0.64886000	0.11482300	0.89266600	C	2.51648700	-2.00009800	0.38674200
H	1.26572800	-1.83753800	1.23195400	C	1.45920400	-2.57477100	1.08886800
C	1.56598400	-1.34710100	-0.82232900	C	3.73695500	-1.79708400	1.03697200
C	2.14032800	-2.56729600	-1.18498600	C	1.61223500	-2.91686200	2.43333800
C	1.05379700	-0.51463000	-1.81490200	H	0.51433900	-2.76466300	0.59299600
C	2.20499900	-2.94887600	-2.52057900	C	3.89165800	-2.14661600	2.37219800
H	2.53629500	-3.22234600	-0.41334300	H	4.56430700	-1.35032800	0.49429700
C	1.11759800	-0.89585600	-3.15498100	C	2.82385800	-2.70066300	3.07884200
H	0.60606300	0.43322400	-1.53839700	H	0.77943700	-3.35572400	2.97117100
C	1.69354600	-2.11102600	-3.51132600	H	4.84275100	-1.98097000	2.86541500
H	2.65032100	-3.90015200	-2.78947900	H	2.94054100	-2.96501900	4.12358600
H	0.71569300	-0.24020700	-3.91945400	C	2.99815900	2.14470000	-1.19111600
H	1.74178200	-2.40731200	-4.55294700	C	2.60855200	1.01426400	-0.42871800
O	1.78934000	0.91424700	2.88702700	C	2.16957400	1.22181800	0.89638200
H	1.48785400	0.51100200	3.71175300	C	2.10371800	2.51456000	1.38925300
H	1.09863400	0.68329100	2.11538400	C	2.48358300	3.61981200	0.60130400
C	-5.80587200	-1.87832600	0.41656400	C	2.94227200	3.44964100	-0.69231800
C	-6.38458100	-0.72681900	-0.12024200	C	3.26343100	0.33919500	-2.48058500
C	-5.61614100	0.39819200	-0.38727300	C	2.77325200	-0.13594600	-1.28869700
C	-4.24339700	0.38241300	-0.11700900	H	1.89652100	0.38657400	1.53267500
C	-3.69037400	-0.78150200	0.41955800	H	1.76428600	2.67919400	2.40549900
C	-4.44275300	-1.91523300	0.69267100	H	2.42227400	4.61784700	1.01938100
C	-3.31435300	1.49843500	-0.34899300	H	3.24435400	4.29187900	-1.30425300
C	-1.96839100	1.30918800	-0.02292900	H	3.74608900	2.27854900	-3.17553200
I	-1.61701100	-0.60765500	0.74191100	H	3.52571900	-0.20655900	-3.37571000
C	-3.66938800	2.74706900	-0.87252600	H	0.99699500	-1.70884300	-2.43886000
C	-2.70992900	3.73434400	-1.04595400	N	3.39661400	1.69653900	-2.42634900
C	-1.37857900	3.50311800	-0.70189500	C	-3.09161700	3.33004500	1.41334900
C	-0.98756600	2.27383200	-0.17916700	C	-4.35474700	2.73893000	1.36698000
H	-6.41723700	-2.74932500	0.62086100	C	-4.53080500	1.46286800	0.84896800
H	-7.44709300	-0.70884100	-0.33176100	C	-3.43247800	0.74642500	0.36259200

C	-2.18743100	1.37682500	0.42936000	H	4.27276000	2.31875200	-2.52477700
C	-1.97689600	2.64680000	0.93746500	H	6.24010200	0.99508500	-3.20988600
C	-3.47023000	-0.60672200	-0.20460100	H	6.76892400	-1.16093600	-2.06731200
C	-2.26389400	-1.16060300	-0.64203400	H	5.84369300	-2.84943700	-0.08498300
I	-0.67519600	0.16411500	-0.34181500	H	3.97638600	-3.01537200	1.53412600
C	-4.61053700	-1.40554000	-0.34072800	H	1.03026900	-1.99109200	-0.50866300
C	-4.51022500	-2.67985700	-0.88209800	N	5.13559200	-2.12942700	0.01636100
C	-3.28047500	-3.19085300	-1.29685300	C	-0.04679200	2.43444100	-1.16612500
C	-2.12296800	-2.42674700	-1.17881300	C	-1.21871000	3.16335800	-1.37011900
H	-2.97008600	4.32675400	1.81968100	C	-2.46109900	2.56214700	-1.22312500
H	-5.21393700	3.28289700	1.74034400	C	-2.55761800	1.21384900	-0.85746200
H	-5.57353200	-1.02768600	-0.01846400	C	-1.36035700	0.52742000	-0.64227100
H	-5.40239400	-3.28643500	-0.97955100	C	-0.10876600	1.09417700	-0.79670400
H	-3.21537700	-4.18903400	-1.71230900	C	-3.81405000	0.46526400	-0.69439000
H	-1.15931500	-2.81123700	-1.48758300	C	-3.67975700	-0.87516300	-0.32918800
H	-5.51983900	1.02123300	0.82233400	I	-1.65316400	-1.46129900	-0.04319100
H	-0.99039100	3.09475600	0.96588000	C	-5.09901000	0.98599200	-0.88429200
Cat4-TS3				C	-6.20594500	0.16655300	-0.70549300
Sum of electronic and thermal Free Energies=				C	-6.05175300	-1.17166800	-0.33799400
-1468.37025 Hartree				C	-4.77966100	-1.70290700	-0.14492300
Sum of electronic and thermal free energies + the entropy				H	0.92070000	2.90773700	-1.29134300
correction at 298.15K=				H	-1.16139500	4.20807400	-1.65183900
-1468.36016 Hartree				H	-5.23658100	2.02237800	-1.17029900
C	2.22863100	-0.85042400	1.57862000	H	-7.19998700	0.57191400	-0.85354800
O	0.58526500	-1.58145300	0.24464100	H	-6.92378700	-1.80068100	-0.20177300
H	1.97566300	-1.71992300	2.17528500	H	-4.65921900	-2.74216300	0.14255300
C	1.55260800	0.38266000	1.96231500	H	-3.36271600	3.13832000	-1.39411100
C	0.26875800	0.29170700	2.52033700	H	0.77989900	0.50325300	-0.62448800
C	2.16132900	1.63733100	1.84504400	Cat4-INT3			
C	-0.42903900	1.43801100	2.86611700	Sum of electronic and thermal Free Energies=			
H	-0.17812200	-0.68737600	2.65411900	-1468.37550 Hartree			
C	1.46884400	2.78496600	2.21406000	Sum of electronic and thermal free energies + the entropy			
H	3.18314300	1.71520300	1.49569800	correction at 298.15K=			
C	0.16678000	2.68942000	2.69854200	-1468.36540 Hartree			
H	-1.43203800	1.36158800	3.26980300	C	2.37653900	-1.02067700	1.64320800
H	1.94564900	3.75368000	2.12145600	O	0.45205900	-1.84494100	-0.26265300
H	-0.37753000	3.58764100	2.96743100	H	2.12096300	-1.99325000	2.05640100
C	5.08509900	-0.95223100	-0.73309100	C	1.51551000	0.06671300	2.05056800
C	3.97622700	-0.20468400	-0.29108800	C	0.20056400	-0.25135100	2.42534600
C	3.67783000	0.98769100	-0.96278400	C	1.94836500	1.39984100	2.11826600
C	4.49992700	1.39611500	-2.00361300	C	-0.69431800	0.75384600	2.75977300
C	5.61631200	0.64309200	-2.39695700	H	-0.10944600	-1.29039200	2.41810400
C	5.92369600	-0.55322400	-1.76713400	C	1.05974100	2.39916900	2.48715800
C	4.12374200	-2.17576400	0.86913400	H	2.98543800	1.64249900	1.92193900
C	3.35582900	-0.99498900	0.77404800	C	-0.26731000	2.08153600	2.77888600
H	2.82229600	1.59098100	-0.68875600	H	-1.71984500	0.50687200	3.01064100

H	1.39765600	3.42702300	2.54617900	C	6.41516200	-0.67619600	-0.88382900
H	-0.96361500	2.86872400	3.04532300	C	5.54929000	-0.63785000	0.21616500
C	5.17881600	-0.70905500	-0.68715500	C	6.04308500	-0.22900900	1.45407800
C	4.07602900	-0.05003800	-0.11721400	C	7.38347900	0.12920500	1.54301200
C	3.75211300	1.22077900	-0.59695100	C	8.22475100	0.09693500	0.42053800
C	4.55019700	1.78877800	-1.58386900	C	7.75266500	-0.30787900	-0.82176100
C	5.66311400	1.11730000	-2.10324300	H	9.26288000	0.38928600	0.52457200
C	5.99317800	-0.15851100	-1.66367800	H	8.39084200	-0.34035500	-1.69654200
C	4.26785700	-2.19018800	0.71745100	H	5.39618300	-0.18938200	2.32361200
C	3.47449900	-1.00490300	0.82450200	H	7.78876400	0.44442900	2.49744000
H	2.89559100	1.76289300	-0.22226500	C	4.42713900	-1.39274900	-1.62621000
H	4.30268100	2.77512600	-1.95829500	N	5.67092100	-1.14481100	-1.97955500
H	6.26798800	1.59216900	-2.86624500	H	3.70357600	-1.74488600	-2.34800200
H	6.83443400	-0.70770200	-2.06859900	H	6.03279900	-1.24346200	-2.92384800
H	5.96010300	-2.68659200	-0.36098600	C	4.20905200	-0.99869800	-0.26817700
H	4.13558200	-3.12517000	1.24491400	H	3.49527300	-1.52778500	0.35208200
H	0.80353800	-2.07767800	-1.13027800	O	2.04299200	0.14007500	-1.07404600
N	5.25040400	-1.99639100	-0.12768800	H	3.87231100	1.04862300	-1.27849400
C	0.14598500	2.37423200	-1.05516700	C	3.19236200	1.19037100	0.76401400
C	-0.97081800	3.20838800	-1.09875000	C	4.04037800	2.26861300	1.00944800
C	-2.24691600	2.68748600	-0.93821700	C	2.32669500	0.75383800	1.76888300
C	-2.43078800	1.31462100	-0.73422800	C	4.02453500	2.90860300	2.24767300
C	-1.28698400	0.51298300	-0.68603700	H	4.71442100	2.60786500	0.22844300
C	-0.00201200	1.00639400	-0.83933500	C	2.31423500	1.38560400	3.00677600
C	-3.73778100	0.65613200	-0.57053800	H	1.66124200	-0.08197800	1.57647100
C	-3.69629600	-0.72604000	-0.38733600	C	3.16447200	2.46583500	3.24816300
I	-1.70167200	-1.52034900	-0.34989400	H	4.68421400	3.74937300	2.42992500
C	-4.97744100	1.30548000	-0.59271500	H	1.64198900	1.03968200	3.78405200
C	-6.14185400	0.56571800	-0.43103500	H	3.15276700	2.96021800	4.21287200
C	-6.08689300	-0.81768900	-0.24760700	C	-2.68767900	-0.18871000	0.24075200
C	-4.85797800	-1.47182600	-0.22389000	C	-2.61088500	0.01784200	3.03263000
H	1.13807800	2.79071300	-1.18665800	C	-2.74893500	1.04713700	0.87192500
H	-0.84326400	4.27223900	-1.26093100	C	-2.54056900	-1.31439000	1.04073100
H	-5.03681900	2.37836400	-0.73565800	C	-2.50709200	-1.22953100	2.42740300
H	-7.10177500	1.06850400	-0.44855700	C	-2.71885500	1.16604500	2.25589100
H	-7.00269700	-1.38422100	-0.12312700	H	-2.39167200	-2.13118700	3.01779400
H	-4.81742400	-2.54695000	-0.07944300	H	-2.76824900	2.14835000	2.71116100
H	-3.10729100	3.34544700	-0.97497300	C	-1.85250500	2.76042800	-0.68670400
H	0.84877100	0.33941800	-0.77720600	N	-2.28322900	3.89290400	-1.24257800
TS4				C	-1.33856500	-3.05996700	-0.25634900
Sum of electronic and thermal Free Energies=				N	-1.55779900	-4.31851200	-0.63590300
-996.77109 Hartree				I	-0.00172800	1.83114800	-0.90404800
Sum of electronic and thermal free energies + the entropy				I	0.32560200	-1.87786700	-0.63410600
correction at 298.15K=				C	-1.55574100	4.77824200	-2.14810500
-996.76079 Hartree				C	-1.55574100	4.77824200	-2.14810500
C	3.19392500	0.52153400	-0.58954800	H	-1.52126200	5.77448800	-1.70880900

H	-2.07575600	4.80644200	-3.10509800	H	-5.98677600	-1.69887800	-0.17587800
H	-0.54578000	4.40163600	-2.28612900	H	-4.31769600	-3.47437800	0.39530900
C	-0.67291900	-5.17475800	-1.42288500	H	-1.58209400	-3.91065600	0.56684500
H	-1.04179600	-5.22751200	-2.44703100	H	0.53069500	-2.75126400	0.24880000
H	-0.66823800	-6.16594600	-0.97255200	H	-0.27768700	-0.70145400	-1.28675700
H	0.33361500	-4.76481300	-1.40603800	N	-1.53437300	-2.93166200	0.28141900
H	-2.58408200	0.09755400	4.11188900	C	-0.06920200	0.11980000	0.72448200
C	-3.94575500	3.08212100	0.01759200	H	-0.53955500	-0.08251400	1.69116900
C	-3.59009900	4.13229300	-0.82654200	C	-0.42585200	1.54763200	0.34560800
C	-3.36318400	-3.62158000	0.48886700	C	-1.21941300	2.30814800	1.20396300
C	-2.81910600	-4.70888200	-0.19287100	C	0.00524700	2.11267400	-0.85677400
N	-2.83627200	2.24004100	0.07797900	C	-1.58070500	3.61165200	0.86860500
N	-2.41115700	-2.60548900	0.42483700	H	-1.56455800	1.87412800	2.13702600
C	-4.47174200	5.16876900	-1.12280300	C	-0.35583800	3.41290500	-1.19479900
C	-5.72250600	5.09748700	-0.53087700	H	0.62211300	1.53497200	-1.53707500
H	-6.44491700	5.88005100	-0.72787700	C	-1.15244100	4.16596200	-0.33350000
C	-6.08068200	4.03516300	0.32005700	H	-2.20048100	4.18954300	1.54491200
H	-7.07137000	4.02315000	0.75778900	H	-0.01633500	3.83853200	-2.13234000
C	-5.20182100	3.00452800	0.61241300	H	-1.43527400	5.17816000	-0.59903700
C	-4.62744800	-3.66871400	1.06978500	C	3.66843200	-0.45351200	0.65553800
C	-5.31893900	-4.86097300	0.93052400	C	2.45668600	-0.33646900	-0.07556000
H	-6.30769700	-4.95068300	1.36353700	C	2.51404200	-0.47948000	-1.47676200
C	-4.77302600	-5.95935400	0.23972300	C	3.73349200	-0.71907100	-2.08489700
H	-5.35405900	-6.86961600	0.15645900	C	4.92073200	-0.82188400	-1.33223400
C	-3.51464900	-5.90741800	-0.33706700	C	4.90356000	-0.69212200	0.04401600
H	-4.19120500	5.98238500	-1.77988100	C	2.02394700	-0.10146000	2.12543800
H	-5.46956400	2.18360300	1.26602500	C	1.41213500	-0.10613800	0.89837800
H	-5.03991600	-2.81854400	1.59895900	H	1.62327000	-0.40647000	-2.08907400
H	-3.09204800	-6.74842400	-0.87222200	H	3.77822700	-0.82900900	-3.16227900
H	-2.74090900	-0.26958800	-0.83937100	H	5.85995800	-1.00704000	-1.84060400

INT4

Sum of electronic and thermal Free Energies =
-996.797456 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -996.78726 Hartree

C	-2.67661100	-2.12193000	0.02926800
C	-2.21756800	-0.85937800	-0.33968200
C	-3.14375100	0.11984800	-0.67070300
C	-4.49938300	-0.20663600	-0.60168000
C	-4.92678600	-1.47970100	-0.21760700
C	-4.00996700	-2.47727000	0.10553500
C	-0.43568200	-2.28519400	0.09896300
C	-0.71016400	-0.87515100	-0.29436900
H	-2.82994100	1.10951900	-0.98056500
H	-5.23745000	0.54498000	-0.85528700

H	-5.98677600	-1.69887800	-0.17587800
H	-4.31769600	-3.47437800	0.39530900
H	-1.58209400	-3.91065600	0.56684500
H	0.53069500	-2.75126400	0.24880000
H	-0.27768700	-0.70145400	-1.28675700
N	-1.53437300	-2.93166200	0.28141900
C	-0.06920200	0.11980000	0.72448200
H	-0.53955500	-0.08251400	1.69116900
C	-0.42585200	1.54763200	0.34560800
C	-1.21941300	2.30814800	1.20396300
C	0.00524700	2.11267400	-0.85677400
C	-1.58070500	3.61165200	0.86860500
H	-1.56455800	1.87412800	2.13702600
C	-0.35583800	3.41290500	-1.19479900
H	0.62211300	1.53497200	-1.53707500
C	-1.15244100	4.16596200	-0.33350000
H	-2.20048100	4.18954300	1.54491200
H	-0.01633500	3.83853200	-2.13234000
H	-1.43527400	5.17816000	-0.59903700
C	3.66843200	-0.45351200	0.65553800
C	2.45668600	-0.33646900	-0.07556000
C	2.51404200	-0.47948000	-1.47676200
C	3.73349200	-0.71907100	-2.08489700
C	4.92073200	-0.82188400	-1.33223400
C	4.90356000	-0.69212200	0.04401600
C	2.02394700	-0.10146000	2.12543800
C	1.41213500	-0.10613800	0.89837800
H	1.62327000	-0.40647000	-2.08907400
H	3.77822700	-0.82900900	-3.16227900
H	5.85995800	-1.00704000	-1.84060400
H	5.80882700	-0.77179600	0.63514000
H	4.03675000	-0.34306000	2.74384200
H	1.58465800	0.03417300	3.10307800
N	3.37064400	-0.30074400	1.98506900

Cat4-TS5

Sum of electronic and thermal Free Energies =
-1832.052638 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -1832.04276 Hartree

C	-3.07910300	3.00983000	-0.79839600
C	-3.39842200	1.83119000	-0.11485500
C	-4.26487000	1.89923200	0.97458000
C	-4.77661800	3.14282000	1.33269200
C	-4.42532500	4.30855100	0.63900300
C	-3.56109100	4.26271300	-0.44754900

C	-2.00919500	1.37005400	-1.88469400	C	1.31408700	-0.46107300	2.41426000
C	-2.60816400	0.73183100	-0.73439100	C	4.44953000	0.20924200	0.44705900
H	-4.54175600	1.00963000	1.52704400	C	3.84332800	1.12596400	-0.41305000
H	-5.46182300	3.21270100	2.16940500	I	1.78299300	1.39972400	-0.00419400
H	-4.83728200	5.26044300	0.95186800	C	5.80865100	-0.07497400	0.27533900
H	-3.27971800	5.15211700	-0.99821900	C	6.51981200	0.55358100	-0.73810100
H	-1.81176700	3.32540500	-2.50966900	C	5.89428900	1.46749700	-1.58868100
H	-1.37421300	0.91963600	-2.63715700	C	4.54301000	1.76068000	-1.43094700
H	-1.58107900	0.82785200	-0.07699700	H	1.04015700	-1.81393900	4.05199800
N	-2.22422700	2.65993900	-1.86016600	H	3.39549000	-2.59186100	4.04784300
C	-3.14208700	-0.70130800	-0.84540500	H	5.00751200	-1.68486300	2.42265900
H	-4.12700800	-0.62814500	-1.31800800	H	0.29037000	-0.11332600	2.39063400
C	-3.35217600	-1.38829300	0.50100000	H	6.46057100	1.95172700	-2.37565000
C	-2.64408800	-1.05117300	1.65455100	H	4.05592900	2.47001800	-2.09140700
C	-4.27675600	-2.43506600	0.56446700	H	7.57242600	0.33180100	-0.86875100
C	-2.85130900	-1.75026400	2.84363600	H	6.30718300	-0.78157000	0.92865100
H	-1.92664800	-0.23762200	1.63840500	Cat5-TS1			
C	-4.48707600	-3.13221200	1.74882700	Sum of electronic and thermal Free Energies=			
H	-4.83513200	-2.70350500	-0.32779800	-1865.33735 Hartree			
C	-3.77068100	-2.79246300	2.89555300	Sum of electronic and thermal free energies + the entropy			
H	-2.29158500	-1.47362600	3.73058700	correction at 298.15K= -1865.32738 Hartree			
H	-5.21099900	-3.93889200	1.77832900	C	2.11597100	0.06215300	0.44977700
H	-3.93243900	-3.33352000	3.82087600	C	4.18741900	-2.57308900	-0.49652900
C	-0.59711000	-2.78267300	-2.69158600	C	4.50104100	-1.40068200	0.20766800
C	-0.94009200	-2.00445000	-1.55688700	C	5.62570800	-0.66348200	-0.16671900
C	0.01117600	-1.83916400	-0.53517700	C	6.39051900	-1.12260100	-1.23144100
C	1.24707500	-2.45068600	-0.66410000	C	6.04496000	-2.29113200	-1.92974300
C	1.56507800	-3.21920200	-1.80271900	C	4.93160000	-3.04009000	-1.57388700
C	0.65336200	-3.39388200	-2.82964100	H	6.66117400	-2.61667800	-2.75945800
C	-2.69636300	-2.05693100	-2.96453900	H	4.65575100	-3.94475800	-2.10225300
C	-2.29434200	-1.55103300	-1.75694100	H	5.89146100	0.24661700	0.36005000
H	-0.22300000	-1.24043700	0.33838900	H	7.27108500	-0.56786800	-1.53405700
H	1.98554500	-2.34237500	0.12350200	C	2.64148100	-2.36037500	1.10691000
H	2.54232100	-3.68297700	-1.87375600	N	3.04318300	-3.11836000	0.09702000
H	0.89268800	-3.98342500	-3.70738500	H	1.77041600	-2.62751900	1.68892700
H	-1.73817000	-3.27401700	-4.41571400	H	2.56620200	-3.95585500	-0.22213900
H	-3.64504100	-1.94726200	-3.46960500	C	3.44236200	-1.19452900	1.19406600
N	-1.68410200	-2.79278700	-3.52887000	H	3.56620300	-0.64980700	2.11993800
O	-0.37794600	1.28431200	0.75293200	O	1.19260500	0.20031500	1.35188800
H	-0.60526300	2.01184500	1.34597800	H	1.87149600	-0.50279200	-0.46186200
C	1.74555600	-1.41286900	3.33386500	C	2.99525400	1.23929700	0.17247600
C	3.07054400	-1.84813900	3.33006300	C	3.46170400	1.45933100	-1.12255200
C	3.98074500	-1.33834500	2.41470500	C	3.32083600	2.13433300	1.19365900
C	3.57938100	-0.38232100	1.47431800	C	4.24854300	2.57504400	-1.39968300
C	2.24190700	0.02137300	1.50807900	H	3.20671600	0.75807600	-1.91138800

C	4.11436100	3.24088600	0.91787700	H	-2.88228600	-2.14271600	-2.39211700
H	2.94924900	1.95645100	2.19748600	H	-4.52384400	-3.58655700	-1.32083900
C	4.57830200	3.46276300	-0.37994900	C	-3.61694200	-0.46137100	-0.99377700
H	4.60546100	2.74700500	-2.40859400	H	-3.85312100	0.26896700	-1.77675000
H	4.37102500	3.93330000	1.71137500	O	-1.27897500	-0.15441500	-1.42063200
H	5.19460400	4.32864900	-0.59349900	H	-2.01951000	-0.84803100	0.38715900
C	-4.98390500	-1.82319500	-0.30964400	C	-2.24669400	1.26599800	0.27968500
C	-5.54732100	-0.64143100	-0.76515800	C	-1.64780000	1.41838900	1.52898800
C	-4.82382000	0.53939600	-0.75165500	C	-2.76028900	2.39075500	-0.37045900
C	-3.51416100	0.57216800	-0.28177200	C	-1.54977400	2.67781100	2.11971900
C	-2.97299200	-0.63254800	0.17359700	H	-1.24975800	0.54756900	2.04167700
C	-3.68301700	-1.80967100	0.16083800	C	-2.67240500	3.64642600	0.21988300
C	-2.63029400	1.74238600	-0.20450100	H	-3.21999100	2.29440500	-1.34920300
C	-1.34290800	1.53653100	0.30632500	C	-2.06211300	3.79344000	1.46570700
I	-0.98021600	-0.47155000	0.82347500	H	-1.07618700	2.78416100	3.08909800
C	-2.95584400	3.05057100	-0.58472000	H	-3.07488400	4.51291900	-0.29271900
C	-2.02677600	4.07256000	-0.44116300	H	-1.98940700	4.77372600	1.92280000
C	-0.76366100	3.82261100	0.08679100	C	4.65591300	-2.09234400	0.74119400
C	-0.40353700	2.53429200	0.47404800	C	5.31411700	-0.88025700	0.87512100
H	-3.93336200	3.26923700	-0.99040100	C	4.68448300	0.30534800	0.53434800
H	-2.29682800	5.07786800	-0.74073600	C	3.38019000	0.30836400	0.04861400
H	-0.04803700	4.62733900	0.20531000	C	2.73551700	-0.92402400	-0.08281400
H	0.56855900	2.32598300	0.89773800	C	3.35777600	-2.09919900	0.26195300
F	-5.43605900	1.63252500	-1.20715300	C	2.59548500	1.48126200	-0.36659000
F	-6.79496100	-0.64726200	-1.21851000	C	1.30015000	1.24200400	-0.83808900
F	-5.69064100	-2.94536900	-0.33133200	I	0.70879900	-0.77688800	-0.77276600
F	-3.13098000	-2.94389900	0.59873500	C	3.03156500	2.81301100	-0.35312700
Cat5-INT1				C	2.19965700	3.82726800	-0.80903300
Sum of electronic and thermal Free Energies=				C	0.92936600	3.54126100	-1.30245200
-1865.34762 Hartree				C	0.46587300	2.22860500	-1.32693100
Sum of electronic and thermal free energies + the entropy				H	4.02024100	3.05641600	0.00919900
correction at 298.15K=				H	2.55357000	4.85093800	-0.78838400
-1865.33761 Hartree				H	0.29328000	4.33549400	-1.67533500
C	-2.22165000	-0.09584600	-0.39369000	H	-0.51122200	1.97686700	-1.71249100
C	-5.16590400	-1.95439700	-0.05308900	H	5.38713200	1.43070900	0.69285000
C	-4.72310800	-0.63429500	0.01339700	F	6.56221300	-0.86065500	1.33421200
C	-5.31137100	0.22306100	0.93261100	F	5.27425000	-3.22160000	1.07124900
C	-6.32297200	-0.28200600	1.75134500	F	2.72102000	-3.27201500	0.13749200
C	-6.74209900	-1.61123000	1.66050500	Cat5-TS2			
C	-6.16360600	-2.48465800	0.74250700	Sum of electronic and thermal Free Energies=			
H	-7.53017000	-1.97009200	2.31132300	-1865.30310 Hartree			
H	-6.47402100	-3.51835500	0.65297300	Sum of electronic and thermal free energies + the entropy			
H	-5.00126900	1.25778900	1.01473900	correction at 298.15K=			
H	-6.79460700	0.37330800	2.47397700	-1865.29311 Hartree			
C	-3.55174100	-1.81075900	-1.60992000	C	-2.67542000	-1.65055200	0.24215400
N	-4.40751800	-2.60572300	-1.06418900	O	-1.49201700	-1.41021000	1.03847500

H	-3.06596300	-2.63734900	0.51762600	F	5.60018800	-0.34750400	0.14027400
C	-2.46866800	-1.61903400	-1.25512400	F	5.94894700	2.19040700	-0.54464400
C	-1.31507200	-2.18863700	-1.79969300	F	3.85551500	3.87480900	-0.81766200
C	-3.44103900	-1.10409000	-2.11242100	F	1.32452700	2.96616100	-0.37568300
C	-1.12390800	-2.21677800	-3.17726100	Cat5-TS2'			
H	-0.56784900	-2.62618000	-1.14540000	Sum of electronic and thermal Free Energies=			
C	-3.25284200	-1.13673000	-3.49220500	-1941.74705 Hartree			
H	-4.35040000	-0.67435700	-1.70565600	Sum of electronic and thermal free energies + the entropy			
C	-2.09131700	-1.68556900	-4.02739900	correction at 298.15K= -1941.73708 Hartree			
H	-0.22198600	-2.65782400	-3.58605100	C	-2.11498200	-1.06621500	-0.48929400
H	-4.01421500	-0.72889100	-4.14725300	C	-5.73384200	-0.13009200	-0.57554400
H	-1.94226500	-1.70485000	-5.10084900	C	-4.40360700	0.27797400	-0.40220400
C	-4.74539500	1.34781800	1.26691000	C	-4.13980600	1.53071300	0.15654400
C	-3.68737800	0.83315000	0.50246000	C	-5.21738100	2.32306600	0.52803800
C	-2.96630700	1.69625100	-0.32700200	C	-6.54169800	1.89505400	0.33642900
C	-3.31837100	3.03954300	-0.34491400	C	-6.82488800	0.65893700	-0.22529900
C	-4.36971700	3.53196400	0.44385300	H	-7.35776900	2.54334600	0.63266900
C	-5.10565800	2.69056100	1.26507800	H	-7.84138800	0.31861600	-0.38180400
C	-4.67483400	-0.84394600	1.72325600	H	-3.12093600	1.87281500	0.29723100
C	-3.58220100	-0.59353400	0.85054700	H	-5.03643600	3.29448000	0.97318400
H	-2.17559000	1.33202100	-0.97320400	C	-4.45942100	-1.81332500	-1.32075100
H	-2.77606300	3.72143300	-0.98924800	N	-5.70735100	-1.40976200	-1.13879700
H	-4.61591500	4.58622200	0.40428600	H	-4.23817200	-2.78592300	-1.73994200
H	-5.92367900	3.05432600	1.87506400	H	-6.52903100	-1.93838000	-1.41536800
H	-6.07001800	0.37804300	2.64797900	C	-3.55139800	-0.78829100	-0.95152200
H	-4.96104500	-1.77717300	2.18916000	H	-3.29432200	-0.30232500	-2.17041300
H	-2.57436000	-0.65295200	1.64670200	O	-1.27002300	-0.02383400	-0.92717800
N	-5.30864200	0.28510100	1.98182300	H	-1.82446300	-2.02580000	-0.94710000
C	3.64442500	2.61145900	-0.47023100	C	-2.08461100	-1.24584300	1.02286900
C	4.71656100	1.74402500	-0.33014200	C	-2.54735900	-2.44222700	1.57412600
C	4.51572600	0.42133100	0.02784700	C	-1.63578100	-0.23438700	1.86930000
C	3.23465100	-0.07178500	0.25755800	C	-2.56385100	-2.62459600	2.95253100
C	2.17282600	0.82445300	0.11524000	H	-2.89477100	-3.23461000	0.91661100
C	2.36483500	2.13745200	-0.24293800	C	-1.65003500	-0.41655500	3.25165900
C	2.86640100	-1.44312600	0.63430100	H	-1.27678600	0.69828500	1.44893100
C	1.50300500	-1.71315400	0.80543700	C	-2.11459200	-1.60943500	3.79631300
I	0.27938900	-0.03716800	0.47017000	H	-2.92210000	-3.55931000	3.36886900
C	3.75211800	-2.50877600	0.83816600	H	-1.29735400	0.37687400	3.90105000
C	3.26954800	-3.76127800	1.19370500	H	-2.12408200	-1.75112000	4.87094500
C	1.90510100	-3.98271600	1.35693200	O	-2.54765800	0.40357400	-3.00390800
C	0.99482000	-2.94644200	1.16448200	H	-2.27750300	-0.10844000	-3.78118900
H	4.81580200	-2.35925900	0.71905600	H	-1.79936500	0.35921300	-2.29886700
H	3.97008200	-4.57329800	1.34629100	C	0.38936800	3.72158500	0.15811100
H	1.53853700	-4.96250000	1.63814800	C	1.68754100	4.10603800	0.48015600
H	-0.07000200	-3.08755600	1.29163100	C	2.72791200	3.18706000	0.46083700

C	2.48481300	1.85069900	0.11789700	H	2.11464200	0.66094900	1.57434000
C	1.16357600	1.50502300	-0.19169800	H	1.53593800	2.92131000	2.34376300
C	0.11075700	2.40197700	-0.18733500	H	1.93734900	4.90093500	0.92113200
C	3.49250600	0.78312400	0.04370900	H	2.94454400	4.65420800	-1.33894700
C	3.01899300	-0.47198300	-0.34512500	H	3.92795700	2.70431000	-3.08550900
I	0.93015200	-0.52120000	-0.69233700	H	4.18960100	0.21858400	-3.17970200
C	4.85387900	0.89539900	0.31137400	H	1.96468300	-1.79712200	-2.31889400
C	5.69594200	-0.19719000	0.19076400	N	3.63427400	2.09360300	-2.33508800
C	5.20222200	-1.43174700	-0.20057200	C	-3.40958400	2.38708600	0.59340300
C	3.85058600	-1.55948800	-0.46574600	C	-4.46451400	1.48994200	0.66102300
H	-0.41701200	4.44499500	0.17122100	C	-4.27858300	0.14833500	0.36913700
H	1.89563400	5.13497400	0.74740000	C	-3.03002700	-0.34120400	-0.00265600
H	3.72875700	3.50890100	0.71065800	C	-1.99047200	0.59258900	-0.05082400
H	-0.89077900	2.08351600	-0.43937500	C	-2.15540500	1.92901300	0.23126500
F	5.40818100	2.04747900	0.69345700	C	-2.68389200	-1.72303900	-0.35140100
F	6.99239200	-0.06475500	0.44935900	C	-1.35089800	-1.97352000	-0.70154000
F	6.02434000	-2.46771900	-0.31522400	I	-0.17577300	-0.23682700	-0.59818900
F	3.36883000	-2.74919700	-0.84136600	C	-3.55228800	-2.82072300	-0.37202200

Cat5-INT2

Sum of electronic and thermal Free Energies=
-1865.37858 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K= -1865.36855 Hartree

C	3.17543700	-1.25154400	-0.86589300
O	1.91351200	-1.77844200	-1.35183900
H	3.96900000	-1.77385400	-1.40946600
C	3.29062700	-1.58194300	0.60801700
C	2.32410200	-2.32399800	1.28286500
C	4.40126300	-1.10754900	1.31181200
C	2.45146400	-2.56421600	2.65182600
H	1.47192800	-2.72865000	0.74970900
C	4.53308900	-1.35655700	2.67152300
H	5.15811800	-0.52991600	0.79026700
C	3.55085600	-2.07925600	3.34956200
H	1.68758900	-3.13532600	3.16724100
H	5.39846000	-0.98122500	3.20577200
H	3.64807700	-2.26557300	4.41292100
C	3.07366800	2.50219100	-1.14923900
C	2.84343800	1.34604800	-0.36166700
C	2.28471000	1.51221400	0.92369100
C	1.96767300	2.78728700	1.35858400
C	2.19845000	3.91716600	0.54867100
C	2.75682600	3.79127900	-0.71034500
C	3.76240500	0.73555400	-2.33238800
C	3.28473200	0.21882700	-1.15240500

C	-3.07856800	-4.07755100	-0.72478700
C	-1.74247400	-4.27552000	-1.06137900
C	-0.84637700	-3.20937800	-1.05252800
H	-4.59359400	-2.69337100	-0.11193500
H	-3.76481000	-4.91544700	-0.73489800
H	-1.38513600	-5.26125600	-1.33273300
H	0.19624200	-3.35190700	-1.30393600
F	-5.34176100	-0.64672700	0.45702600
F	-5.66590000	1.92564300	1.01083400
F	-3.60836600	3.66614300	0.87119100
F	-1.13137200	2.77364000	0.15888200

Cat5-TS3

Sum of electronic and thermal Free Energies=
-1865.33967 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K= -1865.32963 Hartree

C	2.85354700	-0.94922600	1.47342900
O	1.26166600	-1.48381400	0.15558200
H	2.59303400	-1.83276200	2.04665600
C	2.25778700	0.29549400	1.95641100
C	0.99237000	0.23703400	2.55823200
C	2.92749100	1.52150000	1.88832800
C	0.36792200	1.39457100	2.99539000
H	0.50101100	-0.72450100	2.66277900
C	2.30958800	2.67907000	2.34875700
H	3.93840600	1.56872300	1.50395300
C	1.02228000	2.62184500	2.87629400

H	-0.62128100	1.34442400	3.43538200	C	3.01365700	-1.02941600	1.71291100
H	2.83365000	3.62595900	2.29361100	O	1.17062200	-1.77522000	-0.53299300
H	0.53609600	3.52886900	3.21710300	H	2.78110100	-2.00372500	2.13812900
C	5.70487100	-1.02547700	-0.85412400	C	2.09193000	0.02635700	2.06596500
C	4.61288100	-0.27317800	-0.37764500	C	0.78019400	-0.34484000	2.40404100
C	4.33917900	0.95415700	-0.99642800	C	2.45963600	1.37989300	2.11852200
C	5.16747000	1.38955200	-2.02048100	C	-0.17168500	0.62467600	2.68360000
C	6.26661800	0.62942600	-2.44966800	H	0.51735700	-1.39722900	2.41943300
C	6.54963000	-0.59874600	-1.87311300	C	1.51390600	2.34349100	2.43526800
C	4.71882500	-2.29005200	0.70021100	H	3.49101100	1.66596400	1.95423100
C	3.98004600	-1.09259300	0.65562400	C	0.19280200	1.97070700	2.68736200
H	3.49809200	1.56397600	-0.69207500	H	-1.19284700	0.33510300	2.90578400
H	4.96023200	2.33890700	-2.50031000	H	1.80171400	3.38712800	2.48274600
H	6.89610100	1.00287600	-3.24854400	H	-0.54793700	2.73000000	2.91208400
H	7.38134800	-1.21021300	-2.20212000	C	5.85634500	-0.68054500	-0.56084000
H	6.42477400	-2.96136900	-0.28582100	C	4.73030000	-0.03634700	-0.02049700
H	4.55490000	-3.15306500	1.33035500	C	4.39564300	1.22421100	-0.51871700
H	1.69276900	-1.86766300	-0.62073000	C	5.20329800	1.79559100	-1.49648400
N	5.73192800	-2.23171300	-0.15526100	C	6.33664000	1.13809900	-1.98737200
C	0.63938500	2.60718400	-0.97250400	C	6.68006800	-0.12715100	-1.52693200
C	-0.52603500	3.36253800	-1.07529400	C	4.94981900	-2.16408000	0.84393200
C	-1.77382600	2.77085400	-0.92740500	C	4.12767000	-0.99301000	0.92009900
C	-1.87907100	1.39947400	-0.65887800	H	3.52450000	1.75720600	-0.16612400
C	-0.68283300	0.68426600	-0.53647300	H	4.94694400	2.77405200	-1.88535500
C	0.56824900	1.24429300	-0.69908500	H	6.94818300	1.61516300	-2.74363700
C	-3.12781700	0.63754500	-0.50796100	H	7.53901100	-0.66565700	-1.90836800
C	-2.97403700	-0.72798300	-0.25544700	H	6.67041500	-2.63902900	-0.19561700
I	-0.93815700	-1.34808600	-0.06305500	H	4.82564000	-3.09506400	1.38042900
C	-4.42574600	1.13160000	-0.59911700	H	1.49210200	-1.93595600	-1.42885600
C	-5.51789300	0.29503800	-0.44012200	N	5.94230700	-1.96059300	0.01555400
C	-5.34233800	-1.05605500	-0.18743700	C	0.83804900	2.46480700	-1.06131400
C	-4.05656800	-1.55875000	-0.09497300	C	-0.27316300	3.29927600	-0.99164900
H	1.61026000	3.07188600	-1.10310900	C	-1.54230300	2.77418600	-0.78569100
H	-0.46534600	4.42433700	-1.28139500	C	-1.72265900	1.39121800	-0.65165200
H	-2.66517200	3.37436800	-1.02384200	C	-0.57980300	0.58520300	-0.72203500
H	1.45533100	0.63449000	-0.60934800	C	0.69373700	1.08652300	-0.91953900
F	-4.67966800	2.42009800	-0.84213800	C	-3.01051100	0.70800500	-0.44703000
F	-6.74913200	0.78805300	-0.53031300	C	-2.94375300	-0.68533800	-0.37829200
F	-6.40157700	-1.84365100	-0.03716400	I	-0.92671200	-1.48086800	-0.50737200
F	-3.88635200	-2.86322300	0.15432400	C	-4.26037400	1.30721500	-0.31770300
Cat5-INT3				C	-5.39916000	0.54183200	-0.13049500
Sum of electronic and thermal Free Energies=				C	-5.31572200	-0.83957500	-0.06580500
-1865.348370 Hartree				C	-4.07534600	-1.44024000	-0.19053100
Sum of electronic and thermal free energies + the entropy				H	1.82525800	2.88305100	-1.22061900
correction at 298.15K=			-1865.33829 Hartree	H	-0.15291300	4.37074000	-1.09846300

H	-2.39240700	3.43976800	-0.73700800	C	-2.50709200	-1.22953100	2.42740300
H	1.54658700	0.42072600	-0.94633100	C	-2.71885500	1.16604500	2.25589100
F	-4.42616400	2.63387800	-0.36538400	H	-2.39167200	-2.13118700	3.01779400
F	-6.58570500	1.13331300	-0.01100800	H	-2.76824900	2.14835000	2.71116100
F	-6.41870700	-1.56071300	0.11688400	C	-1.85250500	2.76042800	-0.68670400
F	-4.00102700	-2.77923700	-0.11953600	N	-2.28322900	3.89290400	-1.24257800
TS4				C	-1.33856500	-3.05996700	-0.25634900
Sum of electronic and thermal Free Energies=				N	-1.55779900	-4.31851200	-0.63590300
-996.77109 Hartree				I	-0.00172800	1.83114800	-0.90404800
Sum of electronic and thermal free energies + the entropy				I	0.32560200	-1.87786700	-0.63410600
correction at 298.15K=				C	-1.55574100	4.77824200	-2.14810500
-996.76079 Hartree				H	-1.52126200	5.77448800	-1.70880900
C	3.19392500	0.52153400	-0.58954800	H	-2.07575600	4.80644200	-3.10509800
C	6.41516200	-0.67619600	-0.88382900	H	-0.54578000	4.40163600	-2.28612900
C	5.54929000	-0.63785000	0.21616500	C	-0.67291900	-5.17475800	-1.42288500
C	6.04308500	-0.22900900	1.45407800	H	-1.04179600	-5.22751200	-2.44703100
C	7.38347900	0.12920500	1.54301200	H	-0.66823800	-6.16594600	-0.97255200
C	8.22475100	0.09693500	0.42053800	H	0.33361500	-4.76481300	-1.40603800
C	7.75266500	-0.30787900	-0.82176100	H	-2.58408200	0.09755400	4.11188900
H	9.26288000	0.38928600	0.52457200	C	-3.94575500	3.08212100	0.01759200
H	8.39084200	-0.34035500	-1.69654200	C	-3.59009900	4.13229300	-0.82654200
H	5.39618300	-0.18938200	2.32361200	C	-3.36318400	-3.62158000	0.48886700
H	7.78876400	0.44442900	2.49744000	C	-2.81910600	-4.70888200	-0.19287100
C	4.42713900	-1.39274900	-1.62621000	N	-2.83627200	2.24004100	0.07797900
N	5.67092100	-1.14481100	-1.97955500	N	-2.41115700	-2.60548900	0.42483700
H	3.70357600	-1.74488600	-2.34800200	C	-4.47174200	5.16876900	-1.12280300
H	6.03279900	-1.24346200	-2.92384800	C	-5.72250600	5.09748700	-0.53087700
C	4.20905200	-0.99869800	-0.26817700	H	-6.44491700	5.88005100	-0.72787700
H	3.49527300	-1.52778500	0.35208200	C	-6.08068200	4.03516300	0.32005700
O	2.04299200	0.14007500	-1.07404600	H	-7.07137000	4.02315000	0.75778900
H	3.87231100	1.04862300	-1.27849400	C	-5.20182100	3.00452800	0.61241300
C	3.19236200	1.19037100	0.76401400	C	-4.62744800	-3.66871400	1.06978500
C	4.04037800	2.26861300	1.00944800	C	-5.31893900	-4.86097300	0.93052400
C	2.32669500	0.75383800	1.76888300	H	-6.30769700	-4.95068300	1.36353700
C	4.02453500	2.90860300	2.24767300	C	-4.77302600	-5.95935400	0.23972300
H	4.71442100	2.60786500	0.22844300	H	-5.35405900	-6.86961600	0.15645900
C	2.31423500	1.38560400	3.00677600	C	-3.51464900	-5.90741800	-0.33706700
H	1.66124200	-0.08197800	1.57647100	H	-4.19120500	5.98238500	-1.77988100
C	3.16447200	2.46583500	3.24816300	H	-5.46956400	2.18360300	1.26602500
H	4.68421400	3.74937300	2.42992500	H	-5.03991600	-2.81854400	1.59895900
H	1.64198900	1.03968200	3.78405200	H	-3.09204800	-6.74842400	-0.87222200
H	3.15276700	2.96021800	4.21287200	H	-2.74090900	-0.26958800	-0.83937100
C	-2.68767900	-0.18871000	0.24075200				
C	-2.61088500	0.01784200	3.03263000	INT4			
C	-2.74893500	1.04713700	0.87192500	Sum of electronic and thermal Free Energies =			
C	-2.54056900	-1.31439000	1.04073100	-996.797456 Hartree			

Sum of electronic and thermal free energies + the entropy correction at 298.15K =	-996.78726 Hartree	N	3.37064400	-0.30074400	1.98506900		
C	-2.67661100	-2.12193000	0.02926800	Cat5-TS5			
C	-2.21756800	-0.85937800	-0.33968200	Sum of electronic and thermal Free Energies=			
C	-3.14375100	0.11984800	-0.67070300	-2229.020759 Hartree			
C	-4.49938300	-0.20663600	-0.60168000	Sum of electronic and thermal free energies + the entropy correction at 298.15K=			
C	-4.92678600	-1.47970100	-0.21760700	-2229.01077 Hartree			
C	-4.00996700	-2.47727000	0.10553500	C	4.98981500	-1.62319000	1.07708300
C	-0.43568200	-2.28519400	0.09896300	C	4.51470800	-0.60807100	0.23664100
C	-0.71016400	-0.87515100	-0.29436900	C	5.33024800	0.50238600	0.00891800
H	-2.82994100	1.10951900	-0.98056500	C	6.57035500	0.55342100	0.63593100
H	-5.23745000	0.54498000	-0.85528700	C	7.00526500	-0.46795900	1.49181800
H	-5.98677600	-1.69887800	-0.17587800	C	6.21525100	-1.58391500	1.72858000
H	-4.31769600	-3.47437800	0.39530900	C	3.00515500	-2.33105300	0.32537800
H	-1.58209400	-3.91065600	0.56684500	C	3.14234100	-0.99377800	-0.19203600
H	0.53069500	-2.75126400	0.24880000	H	5.01726700	1.30576300	-0.64515000
H	-0.27768700	-0.70145400	-1.28675700	H	7.21696800	1.40490100	0.45901700
N	-1.53437300	-2.93166200	0.28141900	H	7.97452100	-0.38907000	1.96930400
C	-0.06920200	0.11980000	0.72448200	H	6.53456100	-2.38955500	2.37860100
H	-0.53955500	-0.08251400	1.69116900	H	4.08079600	-3.48293800	1.65888600
C	-0.42585200	1.54763200	0.34560800	H	2.15986700	-2.99995200	0.23427600
C	-1.21941300	2.30814800	1.20396300	H	2.44598900	-0.53911500	0.74722600
C	0.00524700	2.11267400	-0.85677400	N	4.02014000	-2.63693400	1.09767500
C	-1.58070500	3.61165200	0.86860500	C	2.56966700	-0.59566200	-1.56511300
H	-1.56455800	1.87412800	2.13702600	H	3.27630100	-0.99246900	-2.30208100
C	-0.35583800	3.41290500	-1.19479900	C	2.52283000	0.90868300	-1.77925500
H	0.62211300	1.53497200	-1.53707500	C	2.39141600	1.82182600	-0.73439000
C	-1.15244100	4.16596200	-0.33350000	C	2.53251300	1.38563000	-3.09238400
H	-2.20048100	4.18954300	1.54491200	C	2.25437800	3.18423700	-0.99761200
H	-0.01633500	3.83853200	-2.13234000	H	2.38419500	1.48044600	0.29436800
H	-1.43527400	5.17816000	-0.59903700	C	2.39144500	2.74302000	-3.35874200
C	3.66843200	-0.45351200	0.65553800	H	2.63509800	0.68074600	-3.91227800
C	2.45668600	-0.33646900	-0.07556000	C	2.24666900	3.64898000	-2.30880800
C	2.51404200	-0.47948000	-1.47676200	H	2.14846800	3.88030400	-0.17263200
C	3.73349200	-0.71907100	-2.08489700	H	2.39441500	3.09464200	-4.38433300
C	4.92073200	-0.82188400	-1.33223400	H	2.13556600	4.70780600	-2.51304600
C	4.90356000	-0.69212200	0.04401600	C	-0.98651400	-1.67329400	-2.33919500
C	2.02394700	-0.10146000	2.12543800	C	-0.08809100	-0.62004800	-2.02218400
C	1.41213500	-0.10613800	0.89837800	C	-0.61880600	0.68693500	-1.93861500
H	1.62327000	-0.40647000	-2.08907400	C	-1.96680700	0.88820900	-2.17801300
H	3.77822700	-0.82900900	-3.16227900	C	-2.83078400	-0.17990900	-2.49381000
H	5.85995800	-1.00704000	-1.84060400	C	-2.35230700	-1.47374000	-2.57175700
H	5.80882700	-0.77179600	0.63514000	C	1.04655200	-2.56723300	-2.11410000
H	4.03675000	-0.34306000	2.74384200	C	1.21975100	-1.22717800	-1.86643700
H	1.58465800	0.03417300	3.10307800	H	0.00824900	1.53480500	-1.69211900
				H	-2.37067600	1.89317500	-2.11276200

H	-3.88196100	0.01666200	-2.67431000	N	2.63208800	-2.97536100	-0.23714900
H	-3.00132100	-2.31000700	-2.80889200	H	1.31387600	-2.80785600	1.38789400
H	-0.64005400	-3.75198400	-2.60258100	H	2.22283300	-3.79254400	-0.67850200
H	1.78106200	-3.36014700	-2.12964400	C	2.88569500	-1.21193400	1.13408000
N	-0.26681500	-2.83975500	-2.37917500	H	2.92710700	-0.75999700	2.11484600
O	1.64745000	-0.03396300	1.87179300	O	0.51573800	0.06918800	1.38746600
H	1.98138000	-0.26550100	2.74832900	H	1.25753300	-0.39584000	-0.48020600
C	-0.28214500	3.78224000	1.78744900	C	2.27384300	1.32244500	0.37635900
C	-1.57913600	4.15258900	1.44430300	C	2.76673600	1.70113400	-0.87220700
C	-2.53784500	3.19352000	1.14459100	C	2.52173900	2.11479500	1.49991700
C	-2.20993400	1.83231600	1.17816000	C	3.50187600	2.87660000	-1.00097700
C	-0.89002800	1.50446400	1.51364800	H	2.57048200	1.07669000	-1.73847400
C	0.07951700	2.43781400	1.82711300	C	3.26758500	3.27893600	1.37042100
C	-3.12027300	0.71848600	0.88146600	H	2.13174900	1.81142700	2.46547100
C	-2.56840300	-0.55927500	0.99769500	C	3.75609600	3.66158400	0.11968800
I	-0.51491700	-0.56151300	1.51705800	H	3.87854700	3.17476600	-1.97244500
C	-4.44080600	0.80639000	0.45259000	H	3.46771600	3.89238100	2.24123200
C	-5.17025700	-0.33232700	0.15405700	H	4.33412600	4.57341200	0.02198500
C	-4.59870900	-1.58919500	0.27011900	C	-1.74343100	3.29630800	-0.38118100
C	-3.28573100	-1.69043800	0.69262900	C	-2.99253600	3.31655000	-0.98668800
H	0.45829000	4.53633800	2.02585100	C	-3.79114200	2.17904300	-1.03919100
H	-1.85121100	5.20069400	1.41318700	C	-3.31532000	0.99648600	-0.48466600
H	-3.54147400	3.50223900	0.88906300	C	-2.04662400	0.99322200	0.10731300
H	1.08100100	2.12529300	2.08703900	C	-1.25589300	2.12087600	0.18403200
F	-5.05731700	1.98028100	0.28933100	C	-3.43411400	-1.30122200	0.21372000
F	-6.42694300	-0.22210000	-0.26616700	I	-1.49563200	-0.86913500	0.90926000
F	-5.30580300	-2.67078000	-0.03993100	C	-4.29317200	-2.37759700	0.15296800
F	-2.72075800	-2.90113800	0.77926100	H	-1.13937000	4.19369800	-0.33483200
Cat6-TS1				H	-3.36958500	4.23337500	-1.42202000
Sum of electronic and thermal Free Energies=				H	-4.14818100	-3.36550700	0.55621400
-1502.02948 Hartree				H	-4.76202400	2.23952800	-1.50253100
Sum of electronic and thermal free energies + the entropy				H	-0.29617900	2.09986800	0.68028000
correction at 298.15K=				N	-5.20475500	-0.62842000	-0.89127900
-1502.01948 Hartree				C	-6.11739800	0.20864700	-1.67148600
C	1.44743500	0.09162000	0.48545100	H	-6.95266100	-0.43477600	-1.93752800
C	3.74301400	-2.27782600	-0.71679100	H	-6.47143900	1.03686000	-1.06054800
C	3.96491000	-1.19923600	0.15500800	H	-5.61446000	0.55151700	-2.57374100
C	5.04031200	-0.34046900	-0.08410100	C	-5.39620900	-1.90584800	-0.55161300
C	5.84971500	-0.58838300	-1.18448300	H	-6.31120300	-2.40064400	-0.84071700
C	5.59692700	-1.66587000	-2.05033000	N	-3.99435000	-0.24927000	-0.42111300
C	4.53481700	-2.53203100	-1.83202900	Cat6-INT1			
H	6.24634400	-1.82618300	-2.90277600	Sum of electronic and thermal Free Energies=			
H	4.33135300	-3.36757100	-2.49096100	-1502.04542 Hartree			
H	5.23322100	0.50090000	0.57274100	Sum of electronic and thermal free energies + the entropy			
H	6.69240400	0.06297900	-1.38514200	correction at 298.15K=			
C	2.16339300	-2.39357300	0.86279000	-1502.03539 Hartree			

C	-1.66768600	-0.16833600	-0.34001900	C	6.03006900	0.14077600	1.30678700
C	-4.91480500	-1.42527300	0.02962700	H	6.78482500	-0.39675600	1.87613400
C	-4.23993900	-0.20961600	-0.06833800	H	6.45588900	0.48305400	0.36533500
C	-4.71695200	0.88013700	0.64601700	H	5.64367100	0.96666400	1.90105100
C	-5.85613900	0.70378400	1.43354500	C	4.95518000	-2.11132500	1.41071500
C	-6.50858100	-0.52862600	1.51052200	H	5.80954100	-2.51889400	1.92993200
C	-6.04427600	-1.63203400	0.79832100	N	3.78770700	-0.56614100	0.42468100
H	-7.39089300	-0.62954100	2.13071500	Cat6-TS2			
H	-6.53595600	-2.59596800	0.84019300	Sum of electronic and thermal Free Energies=			
H	-4.22645400	1.84458900	0.59477300	-1502.00268 Hartree			
H	-6.24387600	1.54373400	1.99759400	Sum of electronic and thermal free energies + the entropy			
C	-3.20749400	-1.83113400	-1.37456700	correction at 298.15K= -1501.99269 Hartree			
N	-4.22786600	-2.36020000	-0.79244700	C	-1.51234500	-0.13877600	-0.59845600
H	-2.56549500	-2.40088900	-2.03319300	O	-0.68307700	-0.31257300	0.57653200
H	-4.51000500	-3.33482200	-0.90393900	H	-1.01702900	-0.56174900	-1.47861500
C	-3.06251300	-0.40240900	-0.98907100	C	-1.89369100	1.29763200	-0.86145400
H	-3.12619000	0.20631700	-1.89938800	C	-1.77154700	2.27820600	0.12129700
O	-0.69349700	-0.54940000	-1.27959000	C	-2.42025400	1.63544900	-2.10885800
H	-1.62863900	-0.80792900	0.55574200	C	-2.16904600	3.58732700	-0.14284700
C	-1.48382500	1.26920500	0.10972600	H	-1.39861800	2.01869300	1.10641100
C	-0.91469800	1.52155000	1.35692500	C	-2.82657600	2.93962900	-2.36866800
C	-1.77582400	2.34192700	-0.73627700	H	-2.51541300	0.87124400	-2.87439000
C	-0.62601800	2.82694000	1.75291700	C	-2.69912300	3.91989500	-1.38569000
H	-0.69209400	0.69245000	2.02231500	H	-2.07077600	4.34382500	0.62729200
C	-1.49717600	3.64504100	-0.34009400	H	-3.23755500	3.19288200	-3.33919800
H	-2.21067700	2.16698500	-1.71547000	H	-3.01096600	4.93774900	-1.58944800
C	-0.91659500	3.89015400	0.90435300	C	-4.74227800	-1.90759300	0.30836300
H	-0.17906700	3.01015100	2.72342700	C	-4.03995100	-0.69222100	0.25415700
H	-1.72807000	4.47101000	-1.00328900	C	-4.71433800	0.48700400	0.58723600
H	-0.69608900	4.90665000	1.20973000	C	-6.04709400	0.40123100	0.96651600
C	2.08442700	2.74853100	-1.51680400	C	-6.71727900	-0.83003300	1.03089800
C	3.34550500	2.89314500	-0.95240600	C	-6.07123700	-2.01187200	0.70271900
C	3.96715400	1.83903900	-0.29105100	C	-2.68853600	-2.42815900	-0.40666600
C	3.29813500	0.62442200	-0.17800800	C	-2.66562600	-1.02929600	-0.14927400
C	2.01458600	0.50667500	-0.72104800	H	-4.21841900	1.44816800	0.55207100
C	1.40719100	1.53694200	-1.40937400	H	-6.58324800	1.30808100	1.22063500
C	3.04665100	-1.69325900	0.39332000	H	-7.75593500	-0.85732400	1.33776500
I	1.08940300	-1.35869500	-0.45299300	H	-6.57148700	-2.97188200	0.74213200
C	3.75975100	-2.70082500	1.01805400	H	-4.10954900	-3.91105200	-0.12416600
H	1.62119100	3.57113700	-2.04772900	H	-1.88242700	-3.05972700	-0.75709600
H	3.87221200	3.83582000	-1.03351500	H	-1.79752400	-1.05721300	0.86551000
H	3.45886500	-3.72360500	1.17014100	N	-3.87219700	-2.92361200	-0.09865100
H	4.95419000	1.98539600	0.11558700	C	1.97335700	-3.39666400	-0.88335400
H	0.43112000	1.39149800	-1.84908300	C	3.34482400	-3.39459000	-1.10014000
N	4.96228000	-0.82417500	1.04999900	C	4.12409000	-2.28337400	-0.79684700

C	3.51041300	-1.15185900	-0.27040300	C	1.71053900	2.23631400	0.57871000
C	2.12469500	-1.16695200	-0.07349000	C	2.16420100	2.97561000	-2.06714300
C	1.34676800	-2.26861600	-0.36167600	H	1.77231100	0.91241100	-2.54277900
C	3.40887100	1.07839300	0.61597800	C	2.02624400	3.55657800	0.26813100
I	1.33799200	0.62249000	0.69387200	H	1.53873100	1.95470500	1.61287900
C	4.24692900	2.13511700	0.90758700	C	2.26008800	3.92713900	-1.05423000
H	1.38111000	-4.27268500	-1.11623700	H	2.33445800	3.26069300	-3.09909600
H	3.83104500	-4.27119400	-1.50947700	H	2.09355300	4.29451100	1.05944100
H	3.98309000	3.09459000	1.31927800	H	2.50784900	4.95460000	-1.29486700
H	5.18625500	-2.32412500	-0.97584600	O	2.31102500	-0.53208500	2.71458000
H	0.28319400	-2.25272600	-0.17506100	H	2.34657900	-1.27578500	3.33824700
N	4.14163800	0.06220500	0.11346100	H	1.36905900	-0.41461900	2.39858400
N	5.44063600	0.44250400	0.07798300	C	-1.94540800	-3.51076200	-0.54483800
C	5.51547600	1.68879500	0.55414200	C	-3.27047100	-3.52317600	-0.96053300
H	6.47645400	2.17707100	0.61037600	C	-4.06469000	-2.38424300	-0.87998900
C	6.56326100	-0.37607200	-0.38007700	C	-3.51011100	-1.20905800	-0.38409800
H	6.64274500	-1.26877900	0.23778600	C	-2.17262200	-1.21263900	0.02750100
H	6.43759100	-0.61869600	-1.43345800	C	-1.38385700	-2.34319400	-0.03602500
H	7.44941900	0.24016200	-0.24921800	C	-3.52583600	1.07099600	0.36747300

Cat6-TS2'

Sum of electronic and thermal Free Energies=
-1578.43860 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K= -1578.42859 Hartree

C	1.34897000	-0.17751200	-0.10721900
C	4.79108000	-1.73606800	-0.24574100
C	4.04389800	-0.54804700	-0.15347700
C	4.72176400	0.67259200	-0.29047800
C	6.08801100	0.65082400	-0.52714700
C	6.80558100	-0.55390600	-0.61308700
C	6.16543800	-1.77231200	-0.46587800
H	7.87358100	-0.52846400	-0.79356700
H	6.69856700	-2.71394200	-0.51896800
H	4.20343000	1.61944500	-0.21283600
H	6.61710200	1.58942800	-0.64432900
C	2.68232800	-2.36362600	0.13525500
N	3.91493300	-2.80369300	-0.06314300
H	1.86352100	-3.05442300	0.28667200
H	4.18956500	-3.78115800	-0.04511000
C	2.65896000	-0.94610900	0.16980000
H	2.69009700	-0.86268000	1.54269600
O	0.46953400	-0.32121700	1.00347700
H	0.88399800	-0.63561700	-0.98980800
C	1.62710800	1.27874300	-0.43209700
C	1.84448600	1.65713300	-1.75579700

C	1.71053900	2.23631400	0.57871000
C	2.16420100	2.97561000	-2.06714300
H	1.77231100	0.91241100	-2.54277900
C	2.02624400	3.55657800	0.26813100
H	1.53873100	1.95470500	1.61287900
C	2.26008800	3.92713900	-1.05423000
H	2.33445800	3.26069300	-3.09909600
H	2.09355300	4.29451100	1.05944100
H	2.50784900	4.95460000	-1.29486700
O	2.31102500	-0.53208500	2.71458000
H	2.34657900	-1.27578500	3.33824700
H	1.36905900	-0.41461900	2.39858400
C	-1.94540800	-3.51076200	-0.54483800
C	-3.27047100	-3.52317600	-0.96053300
C	-4.06469000	-2.38424300	-0.87998900
C	-3.51011100	-1.20905800	-0.38409800
C	-2.17262200	-1.21263900	0.02750100
C	-1.38385700	-2.34319400	-0.03602500
C	-3.52583600	1.07099600	0.36747300
I	-1.47774800	0.61506900	0.78976600
C	-4.38558300	2.15161600	0.42095300
H	-1.34252100	-4.40826400	-0.60384000
H	-3.70915900	-4.43371800	-1.34903000
H	-4.18801300	3.13319700	0.81742300
H	-5.09375000	-2.43981800	-1.19512600
H	-0.36387300	-2.31138300	0.31791100
N	-5.42628400	0.42708600	-0.53599100
C	-6.42856900	-0.39129200	-1.21757000
H	-7.27966500	0.26364700	-1.38842000
H	-6.03204700	-0.73451300	-2.17131700
H	-6.72471300	-1.22152300	-0.57943900
C	-5.56707000	1.70057000	-0.15594500
H	-6.50616300	2.20399600	-0.33006700
N	-4.17053300	0.03661000	-0.21179700

Cat6-INT2

Sum of electronic and thermal Free Energies=
-1502.06333 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K= -1502.05335 Hartree

C	-1.64193800	-0.01610800	0.52896800
O	-0.84027300	0.08918300	-0.67683400
H	-0.97030100	0.31519200	1.32762100
C	-2.03461100	-1.46039500	0.79730000
C	-1.84476100	-2.47802800	-0.13400700
C	-2.61154600	-1.76416700	2.03308600

C	-2.23049600	-3.78551400	0.16479300	H	7.47835500	0.26055700	0.29915500
H	-1.41797600	-2.26533300	-1.10815500	Cat6-TS3			
C	-2.99310600	-3.06594200	2.33132200	Sum of electronic and thermal Free Energies=			
H	-2.76125700	-0.97228500	2.76083100	-1502.03543 Hartree			
C	-2.80352000	-4.08273000	1.39526200	Sum of electronic and thermal free energies + the entropy			
H	-2.08287800	-4.56775200	-0.57097000	correction at 298.15K= -1502.02536 Hartree			
H	-3.43833700	-3.28908400	3.29417600	C	-2.20120900	-0.84560800	-1.48584300
H	-3.10203400	-5.09859100	1.62679600	O	-0.77816500	-1.51893500	-0.17707800
C	-4.78941500	1.94746000	-0.00957300	H	-2.02887800	-1.72874000	-2.09316000
C	-4.01867400	0.79326000	-0.28981800	C	-1.49600500	0.35550800	-1.94438900
C	-4.53384900	-0.16915400	-1.17685800	C	-0.24210500	0.19641400	-2.55086200
C	-5.77795400	0.04453200	-1.74377600	C	-2.04883800	1.63550600	-1.84338500
C	-6.52742700	1.20145500	-1.44809100	C	0.48901700	1.30225100	-2.95692200
C	-6.04657300	2.16653400	-0.58095800	H	0.15414300	-0.80355000	-2.69427100
C	-2.88825800	2.10636200	1.16047300	C	-1.32432800	2.74276800	-2.27142600
C	-2.80105400	0.92144200	0.47485800	H	-3.05179700	1.76800100	-1.45888500
H	-3.96761600	-1.06305100	-1.41471400	C	-0.04702700	2.58139600	-2.80116000
H	-6.18739300	-0.68984000	-2.42779400	H	1.46768000	1.17095700	-3.40365400
H	-7.49872500	1.33695500	-1.90971700	H	-1.75825600	3.73238000	-2.18965600
H	-6.61724000	3.05841000	-0.34884700	H	0.52139400	3.44866100	-3.11724700
H	-4.38531800	3.59700000	1.27137800	C	-5.12832800	-0.70286900	0.75321900
H	-2.18326500	2.55216100	1.84723900	C	-3.95255900	-0.04784000	0.33312300
H	-1.40510700	0.13710500	-1.46485900	C	-3.58608600	1.13307200	0.99548300
N	-4.07372400	2.72107100	0.87405400	C	-4.40212200	1.61792700	2.00662100
C	1.67154500	3.41571700	0.57834500	C	-5.58153900	0.95450100	2.38145100
C	3.02764600	3.55491200	0.84266100	C	-5.96122100	-0.22377000	1.75955100
C	3.91750700	2.50191300	0.65991300	C	-4.22164500	-2.00815600	-0.81446100
C	3.43137300	1.28349700	0.20107300	C	-3.37208400	-0.89545900	-0.70758400
C	2.05804500	1.16706700	-0.04366100	H	-2.68519000	1.67296100	0.73246800
C	1.16247100	2.20047100	0.12755700	H	-4.12276100	2.53116800	2.51887700
C	3.55799300	-1.03158300	-0.46282500	H	-6.19806000	1.36507500	3.17217300
I	1.52260900	-0.76701200	-0.66611900	H	-6.85856700	-0.76045800	2.04365300
C	4.47763200	-2.03621800	-0.63990600	H	-6.01655800	-2.53816000	0.10235100
H	0.99439500	4.24828100	0.72121000	H	-4.12456200	-2.86292700	-1.46905600
H	3.41462000	4.50101200	1.19927300	H	-1.27313500	-1.87722700	0.57607300
H	4.30573100	-3.05078100	-0.95748500	N	-5.25229200	-1.87700100	0.01541200
H	4.96308000	2.65020000	0.87760800	C	0.28374000	2.44439300	1.07207700
H	0.10907500	2.07833200	-0.08430200	C	1.52820000	3.05084900	1.18959000
N	4.17564000	0.10110000	-0.05518100	C	2.70578500	2.32653000	1.03148500
N	5.49806600	-0.16255000	0.02630100	C	2.62839600	0.96898200	0.73656200
C	5.69340300	-1.43662300	-0.31899700	C	1.36683100	0.38365200	0.58899100
H	6.69519900	-1.83891200	-0.31994300	C	0.19632300	1.08948000	0.76697100
C	6.53937400	0.79989300	0.39551100	C	3.47198900	-1.23767500	0.30084300
H	6.52087400	1.63813200	-0.29907700	I	1.38942900	-1.64493700	0.06142500
H	6.39731500	1.11482200	1.42740500	C	4.68048800	-1.89955200	0.20396400

H	-0.62572000	3.01637500	1.21355700	H	4.44929200	-2.88656200	1.36263900
H	1.59816200	4.10706200	1.41794700	H	0.93683300	-2.00244300	-1.51865800
H	4.84672900	-2.94279800	-0.00504400	N	5.46339000	-1.63257900	0.02430900
H	3.64940000	2.83473000	1.14346300	C	0.00845700	2.34386600	-1.04693200
H	-0.75581800	0.58950500	0.66687300	C	-1.15950800	3.08859800	-0.95812900
N	5.04917200	0.25278300	0.65642200	C	-2.39068900	2.47577200	-0.74836400
C	5.71757900	1.51947000	0.95101700	C	-2.44415100	1.09098000	-0.63230600
H	6.78271400	1.30170800	0.93233500	C	-1.25890500	0.35173700	-0.72409300
H	5.47878100	2.25011800	0.18089000	C	-0.03363600	0.95687600	-0.92381500
H	5.43038600	1.86510000	1.94235200	C	-3.52021900	-1.03961800	-0.38771000
C	5.64316000	-0.92393700	0.43637500	I	-1.45601100	-1.73119800	-0.55302000
H	6.72050800	-0.98715600	0.46335800	C	-4.79453500	-1.54905000	-0.19506200
N	3.71119000	0.06327300	0.57073000	H	0.95908500	2.83715200	-1.21046000
Cat6-INT3				H	-1.12576600	4.16685000	-1.05304100
Sum of electronic and thermal Free Energies=				H	-5.08274100	-2.58349500	-0.11292300
-1502.04872 Hartree				H	-3.27476700	3.08839200	-0.68862100
Sum of electronic and thermal free energies + the entropy				H	0.86545800	0.35566700	-0.96926400
correction at 298.15K=				N	-4.90637300	0.67495500	-0.26959700
-1502.03862 Hartree				C	-5.41354000	2.04478700	-0.22432800
C	2.44554000	-1.00267900	1.70425800	H	-6.48072500	1.95665600	-0.03678300
O	0.61612200	-1.88221900	-0.61539600	H	-4.94183700	2.58575400	0.59400000
H	2.30426500	-1.99807000	2.12127100	H	-5.25071200	2.53534900	-1.18205100
C	1.42324000	-0.04336700	2.05654700	C	-5.62931800	-0.44100900	-0.12665500
C	0.15227900	-0.54269700	2.38516700	H	-6.69635200	-0.36251500	0.01875400
C	1.65712300	1.33896200	2.12066100	N	-3.61100500	0.30494500	-0.42889200
C	-0.89014200	0.32763300	2.66881700	TS4			
H	-0.00736700	-1.61581200	2.39344700	Sum of electronic and thermal Free Energies=			
C	0.62061200	2.20380000	2.43856400	-996.77109 Hartree			
H	2.65698300	1.72492500	1.96649500	Sum of electronic and thermal free energies + the entropy			
C	-0.65853000	1.70276100	2.68385300	correction at 298.15K=			
H	-1.87834000	-0.06206500	2.88736700	-996.76079 Hartree			
H	0.80610900	3.26997800	2.49481800	C	3.19392500	0.52153400	-0.58954800
H	-1.46987500	2.38449500	2.91345300	C	6.41516200	-0.67619600	-0.88382900
C	5.26061200	-0.35910900	-0.53939700	C	5.54929000	-0.63785000	0.21616500
C	4.07236200	0.16689900	-0.00507500	C	6.04308500	-0.22900900	1.45407800
C	3.62673200	1.39868700	-0.48761100	C	7.38347900	0.12920500	1.54301200
C	4.38784700	2.05894700	-1.44673300	C	8.22475100	0.09693500	0.42053800
C	5.58228600	1.51818900	-1.93434700	C	7.75266500	-0.30787900	-0.82176100
C	6.03842300	0.28354100	-1.48802300	H	9.26288000	0.38928600	0.52457200
C	4.48693700	-1.94189300	0.83729000	H	8.39084200	-0.34035500	-1.69654200
C	3.55330400	-0.85535800	0.91662200	H	5.39618300	-0.18938200	2.32361200
H	2.70748300	1.84415300	-0.13628100	H	7.78876400	0.44442900	2.49744000
H	4.04565300	3.01600800	-1.82256500	C	4.42713900	-1.39274900	-1.62621000
H	6.15424700	2.06206800	-2.67632800	N	5.67092100	-1.14481100	-1.97955500
H	6.94842700	-0.16631700	-1.86591600	H	3.70357600	-1.74488600	-2.34800200
H	6.25670100	-2.23371700	-0.18605800	H	6.03279900	-1.24346200	-2.92384800

C	4.20905200	-0.99869800	-0.26817700	C	-5.72250600	5.09748700	-0.53087700
H	3.49527300	-1.52778500	0.35208200	H	-6.44491700	5.88005100	-0.72787700
O	2.04299200	0.14007500	-1.07404600	C	-6.08068200	4.03516300	0.32005700
H	3.87231100	1.04862300	-1.27849400	H	-7.07137000	4.02315000	0.75778900
C	3.19236200	1.19037100	0.76401400	C	-5.20182100	3.00452800	0.61241300
C	4.04037800	2.26861300	1.00944800	C	-4.62744800	-3.66871400	1.06978500
C	2.32669500	0.75383800	1.76888300	C	-5.31893900	-4.86097300	0.93052400
C	4.02453500	2.90860300	2.24767300	H	-6.30769700	-4.95068300	1.36353700
H	4.71442100	2.60786500	0.22844300	C	-4.77302600	-5.95935400	0.23972300
C	2.31423500	1.38560400	3.00677600	H	-5.35405900	-6.86961600	0.15645900
H	1.66124200	-0.08197800	1.57647100	C	-3.51464900	-5.90741800	-0.33706700
C	3.16447200	2.46583500	3.24816300	H	-4.19120500	5.98238500	-1.77988100
H	4.68421400	3.74937300	2.42992500	H	-5.46956400	2.18360300	1.26602500
H	1.64198900	1.03968200	3.78405200	H	-5.03991600	-2.81854400	1.59895900
H	3.15276700	2.96021800	4.21287200	H	-3.09204800	-6.74842400	-0.87222200
C	-2.68767900	-0.18871000	0.24075200	H	-2.74090900	-0.26958800	-0.83937100
C	-2.61088500	0.01784200	3.03263000	INT4			
C	-2.74893500	1.04713700	0.87192500	Sum of electronic and thermal Free Energies =			
C	-2.54056900	-1.31439000	1.04073100	-996.797456 Hartree			
C	-2.50709200	-1.22953100	2.42740300	Sum of electronic and thermal free energies + the entropy			
C	-2.71885500	1.16604500	2.25589100	correction at 298.15K =			
H	-2.39167200	-2.13118700	3.01779400	-996.78726 Hartree			
H	-2.76824900	2.14835000	2.71116100	C	-2.67661100	-2.12193000	0.02926800
C	-1.85250500	2.76042800	-0.68670400	C	-2.21756800	-0.85937800	-0.33968200
N	-2.28322900	3.89290400	-1.24257800	C	-3.14375100	0.11984800	-0.67070300
C	-1.33856500	-3.05996700	-0.25634900	C	-4.49938300	-0.20663600	-0.60168000
N	-1.55779900	-4.31851200	-0.63590300	C	-4.92678600	-1.47970100	-0.21760700
I	-0.00172800	1.83114800	-0.90404800	C	-4.00996700	-2.47727000	0.10553500
I	0.32560200	-1.87786700	-0.63410600	C	-0.43568200	-2.28519400	0.09896300
C	-1.55574100	4.77824200	-2.14810500	C	-0.71016400	-0.87515100	-0.29436900
H	-1.52126200	5.77448800	-1.70880900	H	-2.82994100	1.10951900	-0.98056500
H	-2.07575600	4.80644200	-3.10509800	H	-5.23745000	0.54498000	-0.85528700
H	-0.54578000	4.40163600	-2.28612900	H	-5.98677600	-1.69887800	-0.17587800
C	-0.67291900	-5.17475800	-1.42288500	H	-4.31769600	-3.47437800	0.39530900
H	-1.04179600	-5.22751200	-2.44703100	H	-1.58209400	-3.91065600	0.56684500
H	-0.66823800	-6.16594600	-0.97255200	H	0.53069500	-2.75126400	0.24880000
H	0.33361500	-4.76481300	-1.40603800	H	-0.27768700	-0.70145400	-1.28675700
H	-2.58408200	0.09755400	4.11188900	N	-1.53437300	-2.93166200	0.28141900
C	-3.94575500	3.08212100	0.01759200	C	-0.06920200	0.11980000	0.72448200
C	-3.59009900	4.13229300	-0.82654200	H	-0.53955500	-0.08251400	1.69116900
C	-3.36318400	-3.62158000	0.48886700	C	-0.42585200	1.54763200	0.34560800
C	-2.81910600	-4.70888200	-0.19287100	C	-1.21941300	2.30814800	1.20396300
N	-2.83627200	2.24004100	0.07797900	C	0.00524700	2.11267400	-0.85677400
N	-2.41115700	-2.60548900	0.42483700	C	-1.58070500	3.61165200	0.86860500
C	-4.47174200	5.16876900	-1.12280300	H	-1.56455800	1.87412800	2.13702600
				C	-0.35583800	3.41290500	-1.19479900

H	0.62211300	1.53497200	-1.53707500	C	0.55834000	0.05518600	2.77908200
C	-1.15244100	4.16596200	-0.33350000	C	0.73444300	-2.68585200	2.37494300
H	-2.20048100	4.18954300	1.54491200	H	2.36455800	-2.24586600	1.07372600
H	-0.01633500	3.83853200	-2.13234000	C	-0.34730500	-0.80335700	3.40217300
H	-1.43527400	5.17816000	-0.59903700	H	0.47819400	1.12060600	2.95762200
C	3.66843200	-0.45351200	0.65553800	C	-0.26479400	-2.17811500	3.20518500
C	2.45668600	-0.33646900	-0.07556000	H	0.81569600	-3.75442300	2.20891600
C	2.51404200	-0.47948000	-1.47676200	H	-1.11641400	-0.39073600	4.04559100
C	3.73349200	-0.71907100	-2.08489700	H	-0.96313600	-2.84747800	3.69459600
C	4.92073200	-0.82188400	-1.33223400	C	1.06821300	3.94751800	1.26351100
C	4.90356000	-0.69212200	0.04401600	C	1.04229400	2.60480300	0.81854700
C	2.02394700	-0.10146000	2.12543800	C	-0.00903700	2.18239600	-0.00917500
C	1.41213500	-0.10613800	0.89837800	C	-1.00177000	3.08024400	-0.35793800
H	1.62327000	-0.40647000	-2.08907400	C	-0.96009500	4.41251300	0.10510500
H	3.77822700	-0.82900900	-3.16227900	C	0.07143400	4.86453400	0.91128500
H	5.85995800	-1.00704000	-1.84060400	C	2.85445400	2.89790900	2.11271100
H	5.80882700	-0.77179600	0.63514000	C	2.19655600	1.94884400	1.37593300
H	4.03675000	-0.34306000	2.74384200	H	-0.01553800	1.16771100	-0.38983700
H	1.58465800	0.03417300	3.10307800	H	-1.81648200	2.76023400	-1.00031200
N	3.37064400	-0.30074400	1.98506900	H	-1.74880700	5.09839600	-0.18179900
Cat6-TS5				H	0.10761400	5.88995200	1.26103700
Sum of electronic and thermal Free Energies=				H	2.47521500	4.94839100	2.50503000
-1865.716088 Hartree				H	3.75755400	2.80469800	2.69809700
Sum of electronic and thermal free energies + the entropy				N	2.18667700	4.09591600	2.04553200
correction at 298.15K=				O	0.74839100	-1.18563000	-1.20306400
-1865.70615 Hartree				H	0.99058700	-1.91831400	-1.78665900
C	4.47620300	-0.48009500	-1.81936600	C	-2.03642100	1.13814600	-3.50607500
C	4.06063000	-0.80306900	-0.52130400	C	-3.37820000	1.42732200	-3.29363000
C	4.74639800	-1.80308700	0.16951500	C	-4.07658200	0.87526100	-2.22507500
C	5.78468000	-2.46356700	-0.47726600	C	-3.41109700	0.01631200	-1.35628400
C	6.14582700	-2.14918600	-1.79504100	C	-2.05639300	-0.25944200	-1.57872000
C	5.49646200	-1.13962200	-2.49173700	C	-1.35825900	0.28626300	-2.63895700
C	2.88193000	0.99869200	-1.29506700	C	-3.17898600	-1.43450700	0.54341200
C	2.91571700	0.08197900	-0.18707000	I	-1.17002700	-1.50835500	-0.14328800
H	4.49459400	-2.05210000	1.19372300	C	-3.94037600	-1.94608300	1.57607600
H	6.33076100	-3.23670700	0.05034200	H	-1.50634700	1.57650200	-4.34235700
H	6.95489300	-2.69023700	-2.27073700	H	-3.90280500	2.09471300	-3.96600100
H	5.77550000	-0.86509000	-3.50181500	H	-3.62534000	-2.61113400	2.36226800
H	3.77328800	1.04842100	-3.15798200	H	-5.11782700	1.12177800	-2.09673000
H	2.21782800	1.83819400	-1.45217100	H	-0.30971500	0.05881000	-2.77487300
H	1.91140800	-0.54226000	-0.66156200	N	-5.21220400	-0.63678700	0.29433600
N	3.71239600	0.61764000	-2.23919100	C	-6.36290800	0.08484300	-0.24743200
C	2.57672700	0.49684600	1.26379800	H	-7.20021800	-0.16946300	0.39780700
H	3.51041300	0.37553800	1.82489500	H	-6.17904200	1.15680200	-0.20571000
C	1.55382500	-0.43737900	1.93083600	H	-6.56583000	-0.25340600	-1.26182100
C	1.62370500	-1.82292600	1.74057000				

C	-5.21128000	-1.41900800	1.37764200	H	1.82360100	-5.17027500	0.32811400
H	-6.12522900	-1.55130200	1.93664500	H	4.09334500	-6.14502400	0.16664200
N	-3.95930900	-0.64109400	-0.22100100	H	6.07497600	-4.68414400	-0.06428300
Cat7-TS1				H	5.82947900	-2.22938400	-0.14177700
Sum of electronic and thermal Free Energies= -2316.32252 Hartree				C	2.04673500	-0.48643400	0.11632700
Sum of electronic and thermal free energies + the entropy correction at 298.15K= -2316.31265 Hartree				C	1.80247600	3.61270400	-0.23812000
C	-2.07986200	-0.10260200	-0.05512600	C	3.07132900	3.02028800	-0.28120400
C	-4.97971900	1.72220100	0.44703900	C	4.18277800	3.84742800	-0.45888400
C	-4.69383500	0.38140500	0.75003600	C	3.99730800	5.21675900	-0.58709400
C	-5.58696700	-0.61207400	0.34070800	C	2.71985500	5.77691700	-0.54254800
C	-6.72821800	-0.22847000	-0.35008800	C	1.59579100	4.97428700	-0.36436600
C	-6.98506500	1.12028900	-0.64915000	C	1.88671800	0.90989400	0.03072300
C	-6.11103200	2.12322000	-0.25647700	C	3.07005800	1.57609700	-0.14176000
H	-7.88397900	1.38211200	-1.19459000	H	5.18010100	3.42320000	-0.49534300
H	-6.29677600	3.16689900	-0.47973400	H	4.85869600	5.85855500	-0.72511400
H	-5.39170900	-1.65670600	0.55752200	H	2.59344200	6.84755300	-0.64728400
H	-7.43717800	-0.98355600	-0.66911700	H	0.60374000	5.40780300	-0.33089200
C	-3.05427400	1.72137000	1.58520000	S	4.40651900	0.47644900	-0.19181500
N	-3.94595000	2.49715400	0.98039700	I	0.28663100	2.18672100	0.05587200
H	-2.20339600	2.14842700	2.09775100	I	0.77645700	-2.08315600	0.30323700
H	-3.87914600	3.50753700	0.90679200	Cat7-INT1			
C	-3.38713100	0.35978600	1.40463100	Sum of electronic and thermal Free Energies= -2316.33353 Hartree			
H	-3.04648600	-0.40324000	2.08995800	Sum of electronic and thermal free energies + the entropy correction at 298.15K= -2316.32368 Hartree			
O	-0.87559400	-0.03875100	0.42104400	C	2.17552300	0.00795200	0.21557100
H	-2.39739400	0.69040100	-0.74680100	C	5.02272600	1.18848900	-1.47558800
C	-2.61425300	-1.44765000	-0.43168700	C	4.59177100	0.09485200	-0.72524500
C	-3.18292900	-1.60831100	-1.69338000	C	5.50055000	-0.54051900	0.10911900
C	-2.52737600	-2.53960000	0.43706600	C	6.80812700	-0.05309900	0.15321600
C	-3.64070400	-2.86105900	-2.09710000	C	7.20716000	1.04366700	-0.61328600
H	-3.26413700	-0.75448300	-2.35831900	C	6.30831700	1.69461500	-1.45477700
C	-2.98827800	-3.78661300	0.03464300	H	8.23003000	1.39504300	-0.55415100
H	-2.13081800	-2.40786500	1.44011500	H	6.59377500	2.54741500	-2.05818400
C	-3.54288000	-3.94863400	-1.23586200	H	5.21370300	-1.39324400	0.71134100
H	-4.07751100	-2.98314500	-3.08136400	H	7.53064600	-0.53841800	0.79852400
H	-2.92670100	-4.62948700	0.71305500	C	2.85036100	0.95681600	-1.99896200
H	-3.90477900	-4.92156900	-1.54755900	N	3.90973500	1.65342000	-2.22697800
C	3.68280300	-2.29410300	0.04868000	H	1.91111100	1.17079000	-2.49336100
C	2.58195000	-3.15101400	0.18106700	H	3.94935500	2.44344300	-2.87231800
C	2.69071700	-4.52889200	0.22691200	C	3.12758700	-0.12062700	-1.01303600
C	3.97101500	-5.06934800	0.13513500	H	2.92688900	-1.07410900	-1.52083900
C	5.08815000	-4.24332000	0.00448900	O	0.84640400	0.08321700	-0.21575500
C	4.95529000	-2.86283800	-0.03980000	H	2.46151500	0.94009500	0.73066900
C	3.35306500	-0.88264800	0.01121300	C	2.33644400	-1.13034600	1.21165800

C	1.93628000	-0.89059400	2.52858500	C	1.75116700	-1.92369100	1.59585800
C	2.71936800	-2.42048700	0.84364500	C	0.92490700	-1.13377600	2.39225800
C	1.90744400	-1.92292300	3.45963900	C	2.87339200	-2.53160400	2.16421600
H	1.63832300	0.11236500	2.82032500	C	1.22486100	-0.93914600	3.74003000
C	2.69157300	-3.45668900	1.77621300	H	0.03887900	-0.66668600	1.97594200
H	3.04067300	-2.63829200	-0.16981100	C	3.17036200	-2.34027600	3.50785200
C	2.28247500	-3.21135800	3.08302200	H	3.52056900	-3.14759000	1.54718500
H	1.59445400	-1.72299500	4.47800900	C	2.34836500	-1.53783100	4.29865500
H	2.99035400	-4.45487500	1.47734700	H	0.57719600	-0.31907400	4.34897800
H	2.26031800	-4.01813400	3.80656700	H	4.04674500	-2.81138200	3.93780700
C	-3.44487500	-2.33434900	-0.55386200	H	2.58381300	-1.38292900	5.34519600
C	-2.28645000	-3.12630200	-0.58238800	C	4.59973800	-1.39284100	-1.79234900
C	-2.32407500	-4.50077600	-0.74069600	C	3.75751200	-1.09286400	-0.70982500
C	-3.57273900	-5.10321800	-0.87400600	C	4.12458800	-0.07333100	0.17504100
C	-4.73961200	-4.33802300	-0.84790500	C	5.29810100	0.62530500	-0.07705700
C	-4.68643200	-2.96016900	-0.68883900	C	6.10722500	0.32398700	-1.18361100
C	-3.19445400	-0.91476900	-0.37763000	C	5.77302000	-0.69686600	-2.06096000
H	-1.41839000	-5.09548200	-0.76072400	C	2.90667400	-2.85399500	-1.91356200
H	-3.63248400	-6.17752900	-0.99946200	C	2.60487400	-1.99579000	-0.82531100
H	-5.70157500	-4.82450500	-0.95363200	H	3.53706700	0.15001700	1.05895800
H	-5.59865400	-2.37373100	-0.67016000	H	5.60240900	1.41262800	0.60229800
C	-1.90462700	-0.47362900	-0.28059900	H	7.01549600	0.89091300	-1.34862700
C	-1.79512400	3.56112100	0.41748500	H	6.39342000	-0.94859200	-2.91255600
C	-3.05607200	2.96932300	0.24710800	H	4.42008100	-2.87463200	-3.33198300
C	-4.19487800	3.77286800	0.33886900	H	2.32060400	-3.67396400	-2.30605100
C	-4.04988600	5.12946900	0.59479800	H	1.60132200	-1.32734400	-1.35250300
C	-2.78557300	5.69674100	0.76066500	N	4.03518700	-2.46804200	-2.48402100
C	-1.63741800	4.91293500	0.67143000	C	-4.37405200	-0.50392200	-0.16099200
C	-1.80293800	0.91143800	-0.07098200	C	-3.90822800	-1.81516500	-0.32525700
C	-3.01438200	1.53870800	-0.00534300	C	-4.75250500	-2.90933500	-0.39565900
H	-5.18170400	3.34124300	0.21066100	C	-6.12162800	-2.67353400	-0.29842000
H	-4.93160600	5.75459200	0.66602100	C	-6.61233300	-1.37716800	-0.13508500
H	-2.69046800	6.75711400	0.96117300	C	-5.75131100	-0.29106200	-0.06505400
H	-0.65614500	5.35526000	0.79946500	C	-3.32863900	0.50260000	-0.10991500
S	-4.31122400	0.40457100	-0.21722200	H	-4.37173600	-3.91612500	-0.52169400
I	-0.21809400	2.16353600	0.21364800	H	-6.80834400	-3.50970600	-0.35023100
I	-0.52807500	-1.97684900	-0.36957800	H	-7.68048100	-1.21378300	-0.06094200
Cat7-TS2				H	-6.14349200	0.71186200	0.06304300
Sum of electronic and thermal Free Energies=				C	-2.01751200	0.12244100	-0.20774600
-2316.29335 Hartree				C	0.41480300	3.45388800	-0.05184400
Sum of electronic and thermal free energies + the entropy				C	-0.97162900	3.64018900	0.03796300
correction at 298.15K=				C	-1.45096500	4.94618100	0.16512700
-2316.28348 Hartree				C	-0.55073700	6.00177600	0.20045000
C	1.44196300	-2.16602600	0.13854700	C	0.82390000	5.77965700	0.10980200
O	0.53526100	-1.19997000	-0.44771600	C	1.33067400	4.48880000	-0.01859700
H	1.02727700	-3.17489400	0.01380900				

C	-1.12748500	1.21300000	-0.15393200	C	-2.39884900	-3.14147000	-0.41386500
C	-1.75676700	2.42129600	-0.01997800	C	-2.42394300	-4.51824300	-0.53713600
H	-2.51712700	5.13229300	0.23497300	C	-3.67427400	-5.13024100	-0.57573500
H	-0.92345000	7.01379700	0.29955800	C	-4.84298500	-4.37229000	-0.49000300
H	1.51149400	6.61608800	0.13827900	C	-4.79335900	-2.99107500	-0.36471300
H	2.39758200	4.31391800	-0.08970800	C	-3.30385000	-0.92680000	-0.19977300
S	-3.47564000	2.22163900	0.04941200	H	-1.51491300	-5.10396200	-0.60142000
I	0.90911600	1.42041300	-0.21967000	H	-3.73226700	-6.20738800	-0.67310900
I	-1.80688000	-1.90287300	-0.44516700	H	-5.80535500	-4.86804500	-0.52097200

Cat7-TS2'

Sum of electronic and thermal Free Energies=
-2392.72546 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K=-2392.71556 Hartree

C	2.08892200	0.20383100	0.43014100
C	5.47541800	1.42261700	-0.68331500
C	4.72701800	0.39084900	-0.08852300
C	5.41853200	-0.61552000	0.60099900
C	6.80357500	-0.56204800	0.64212600
C	7.52287200	0.46527600	0.00897700
C	6.86650200	1.47991400	-0.66603400
H	8.60527400	0.46777300	0.05717500
H	7.39924800	2.28804700	-1.15260700
H	4.89504800	-1.41898500	1.10119000
H	7.34553600	-1.33341600	1.17663100
C	3.33086800	1.92562300	-1.03899500
N	4.57818400	2.32251400	-1.25026300
H	2.50266600	2.49929000	-1.43470700
H	4.83957700	3.13542600	-1.79945400
C	3.31102500	0.66933500	-0.38232800
H	2.97529400	0.10424800	-1.61034600
O	0.89735000	0.27338300	-0.35379700
H	1.99436700	0.88116600	1.28939700
C	2.21972200	-1.20344100	0.97984500
C	1.75916400	-1.46219800	2.27044300
C	2.61753000	-2.27144200	0.16985200
C	1.66837400	-2.77054900	2.74117700
H	1.44755600	-0.63457900	2.90019500
C	2.52114000	-3.57924500	0.63572900
H	2.99312100	-2.09378000	-0.83256000
C	2.03664400	-3.83176300	1.91973800
H	1.30126200	-2.95931300	3.74334700
H	2.82386600	-4.40149400	-0.00235900
H	1.95743500	-4.85130100	2.27887900
C	-3.55259300	-2.35007500	-0.32529700

C	-2.01591400	-0.46320000	-0.19369800
C	-1.97998900	3.60969500	0.33608500
C	-3.22553000	2.97122800	0.27314800
C	-4.38387500	3.73940300	0.41408600
C	-4.26867500	5.10848800	0.61055300
C	-3.01652100	5.72275100	0.66872700
C	-1.85007300	4.97457700	0.52897500
C	-1.92481600	0.93258000	-0.04417900
C	-3.14822200	1.53503600	0.07320500
H	-5.36211300	3.27289200	0.37151100
H	-5.16479500	5.70685100	0.72068000
H	-2.94558600	6.79241400	0.82463400
H	-0.87825700	5.45271300	0.57316000
S	-4.43206100	0.37469700	-0.01646400
I	-0.37351100	2.26609600	0.06451200
I	-0.65025100	-1.98245400	-0.31906900
O	2.14134400	-0.43102800	-2.43230400
H	2.09115200	0.04058500	-3.28023200
H	1.37251400	-0.15087700	-1.83658800

Cat7-INT2

Sum of electronic and thermal Free Energies=
-2316.35367 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K=-2316.34379 Hartree

C	1.49042600	-2.49615000	-0.48253800
O	0.43516700	-1.56822300	-0.90618500
H	1.23440200	-3.47131600	-0.90728600
C	1.48835600	-2.59378700	1.02688700
C	0.63044100	-1.86569000	1.84648500
C	2.42756700	-3.44597900	1.61563900
C	0.72016000	-1.96999000	3.23539200
H	-0.11536700	-1.19845900	1.43249000
C	2.51429100	-3.55458700	2.99648200
H	3.09962000	-4.01648800	0.98236300
C	1.66285500	-2.80980100	3.81326600

H	0.04956600	-1.38914600	3.85792400	I	-2.31695000	-1.68075100	-0.60096900
H	3.24992400	-4.21688000	3.43808400	Cat7-TS3			
H	1.73515600	-2.88857900	4.89169200	Sum of electronic and thermal Free Energies=			
C	4.73706500	-0.91337700	-1.51941700	-2316.32733 Hartree			
C	3.75985400	-1.10444100	-0.51060500	Sum of electronic and thermal free energies + the entropy			
C	3.90911100	-0.40616100	0.70640600	correction at 298.15K=		-2316.31744 Hartree	
C	4.97543600	0.46543500	0.85381000	C	1.99371900	-1.52860000	1.24677700
C	5.92051800	0.64882100	-0.17516000	O	0.80277300	-1.04755300	-0.41331300
C	5.82015200	-0.04317700	-1.36821300	H	1.32206100	-2.33813200	1.52143600
C	3.24578000	-2.38009200	-2.30534600	C	1.75092100	-0.28143000	1.97262100
C	2.80053100	-2.04278600	-1.04841600	C	0.44625100	-0.02803400	2.42261500
H	3.21683800	-0.55542400	1.52835300	C	2.75757300	0.65312400	2.23662200
H	5.09471400	1.00564600	1.78581900	C	0.13163900	1.17621200	3.03335100
H	6.74451900	1.33623000	-0.02407500	H	-0.32486000	-0.77789100	2.27562800
H	6.54760000	0.08118400	-2.16206800	C	2.44395400	1.85559500	2.86130300
H	4.92419500	-1.79408400	-3.44552900	H	3.78566300	0.43613300	1.97843800
H	2.80999700	-3.06088400	-3.02260200	C	1.13044800	2.13004500	3.23465700
H	0.50201700	-1.53071800	-1.87583200	H	-0.88452900	1.37135800	3.35583900
N	4.39600900	-1.70840200	-2.58707900	H	3.22713800	2.57781900	3.05833400
C	-4.46711800	0.20603300	-0.07204300	H	0.88813200	3.07543600	3.70637800
C	-4.32783500	-1.16081400	-0.33730500	C	5.17465900	-2.29790900	-0.45068500
C	-5.38191200	-2.05096200	-0.40684500	C	4.28827000	-1.28127300	-0.04100300
C	-6.65573400	-1.52819000	-0.19784400	C	4.57224300	0.03570500	-0.42784800
C	-6.83779000	-0.17063000	0.06775800	C	5.72472600	0.28988800	-1.15584700
C	-5.75847300	0.69864500	0.13289200	C	6.60669600	-0.74173900	-1.51501900
C	-3.22831300	0.95769500	-0.03415900	C	6.33989400	-2.05746400	-1.17174900
H	-5.23877700	-3.10479600	-0.61218400	C	3.47406700	-3.32971000	0.56389800
H	-7.51019400	-2.19216000	-0.24278900	C	3.19013600	-1.95718200	0.64396300
H	-7.83772500	0.21345400	0.22699700	H	3.91655700	0.85571500	-0.16276300
H	-5.91569400	1.75105600	0.34113900	H	5.94991000	1.30753700	-1.45208500
C	-2.02624300	0.33259200	-0.24923100	H	7.50247100	-0.50676100	-2.07738300
C	1.02451100	3.11491100	0.13189400	H	6.99646700	-2.87012300	-1.45866300
C	-0.30127700	3.54076100	0.27329700	H	5.08219400	-4.42041500	-0.18915800
C	-0.52329800	4.89012500	0.55936900	H	2.89249500	-4.15682500	0.94634700
C	0.56140600	5.74557800	0.69041200	H	1.34462700	-1.41657300	-1.12816200
C	1.86917600	5.28115100	0.54333400	N	4.64304300	-3.51803200	-0.04263300
C	2.12348000	3.94200000	0.25768000	C	-4.14216700	-1.32382300	-0.03357600
C	-0.92468900	1.21702500	-0.17470200	C	-3.44410300	-2.53165800	-0.17564500
C	-1.30154200	2.50448400	0.11049900	C	-4.06789500	-3.76635700	-0.13672100
H	-1.53446500	5.26443500	0.67724600	C	-5.44853300	-3.78692600	0.04637800
H	0.38762600	6.79139600	0.91144700	C	-6.16659500	-2.59895000	0.19053200
H	2.70271100	5.96423800	0.65080500	C	-5.52564500	-1.36847300	0.15263300
H	3.13647500	3.57533000	0.14300200	C	-3.30939500	-0.13681700	-0.10880400
S	-3.01607300	2.64568200	0.26929000	H	-3.51122500	-4.68953100	-0.24596300
I	1.12901100	1.06863400	-0.29342100	H	-5.96468700	-4.73872700	0.07727800

H	-7.23945200	-2.63547900	0.33459300	H	-0.07861200	-3.56674400	0.28627300
H	-6.09153300	-0.45035300	0.26706000	H	-0.72004000	-5.25555700	-1.36232500
C	-1.95992600	-0.27334700	-0.28304900	H	-3.08673800	-5.69214900	-1.90323300
C	-0.18944400	3.41522700	-0.65583800	H	-4.89679800	-4.36577100	-0.79901800
C	-1.57028200	3.37470400	-0.41238000	H	-5.29979500	-2.32060700	0.98843500
C	-2.26330500	4.58364500	-0.31567300	H	-4.01057100	-0.75251600	2.39218000
C	-1.57095200	5.77787300	-0.45930700	H	-1.26740500	-1.70715600	-1.52084400
C	-0.19585100	5.78753900	-0.69799900	N	-4.28488900	-2.34646900	1.05972900
C	0.51796100	4.59577700	-0.79760100	C	-1.10611700	3.60727700	0.17661100
C	-1.28899800	0.95712200	-0.38741100	C	-2.30626800	2.98581600	-0.20604100
C	-2.12168800	2.03755400	-0.28982500	C	-3.53283300	3.61794100	-0.08384000
H	-3.33133200	4.58768100	-0.12735300	C	-3.55629300	4.91131000	0.43349500
H	-2.10790800	6.71541400	-0.38344500	C	-2.37391900	5.54612000	0.81662800
H	0.32826800	6.72914000	-0.80726600	C	-1.14913600	4.90449500	0.69312100
H	1.58598700	4.60217800	-0.98095300	C	0.07577900	2.78354300	-0.01672500
S	-3.76533000	1.53544500	-0.05830500	H	-4.45384300	3.12934700	-0.38096700
I	0.65544900	1.48951600	-0.70612700	H	-4.50415200	5.42572800	0.53670900
I	-1.36705200	-2.22725200	-0.39777000	H	-2.40997400	6.55257000	1.21555900

Cat7-INT3

Sum of electronic and thermal Free Energies=
-2316.34601 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K=-2316.33602 Hartree

C	-1.26076400	-1.06292000	2.29039100
O	-0.78250900	-0.87644200	-1.61103300
H	-1.67577400	-0.18227500	2.77912500
C	0.17595900	-1.19021100	2.37978400
C	0.92549600	-0.01014100	2.53513200
C	0.83551400	-2.43042900	2.36955100
C	2.30981700	-0.06591900	2.59564500
H	0.40745000	0.94303800	2.58986300
C	2.21899100	-2.48067100	2.44936900
H	0.26011500	-3.34752700	2.35246000
C	2.95750300	-1.29961200	2.53971100
H	2.88656600	0.84671300	2.69498500
H	2.72476700	-3.43878300	2.45145000
H	4.04007700	-1.34198400	2.59116600
C	-3.46234100	-3.24884600	0.35780200
C	-2.12776500	-2.98757600	0.71218800
C	-1.12680900	-3.72370000	0.07310100
C	-1.49443900	-4.68465600	-0.86425900
C	-2.83575200	-4.93162000	-1.17404900
C	-3.85167700	-4.20602300	-0.56344000
C	-3.56840400	-1.53453200	1.78897100
C	-2.17346100	-1.85911700	1.65682800

H	-0.07861200	-3.56674400	0.28627300
H	-0.72004000	-5.25555700	-1.36232500
H	-3.08673800	-5.69214900	-1.90323300
H	-4.89679800	-4.36577100	-0.79901800
H	-5.29979500	-2.32060700	0.98843500
H	-4.01057100	-0.75251600	2.39218000
H	-1.26740500	-1.70715600	-1.52084400
N	-4.28488900	-2.34646900	1.05972900
C	-1.10611700	3.60727700	0.17661100
C	-2.30626800	2.98581600	-0.20604100
C	-3.53283300	3.61794100	-0.08384000
C	-3.55629300	4.91131000	0.43349500
C	-2.37391900	5.54612000	0.81662800
C	-1.14913600	4.90449500	0.69312100
C	0.07577900	2.78354300	-0.01672500
H	-4.45384300	3.12934700	-0.38096700
H	-4.50415200	5.42572800	0.53670900
H	-2.40997400	6.55257000	1.21555900
H	-0.23520200	5.40548300	0.99392700
C	-0.07301200	1.52967800	-0.53615000
C	3.51691200	-0.40927100	-0.75810900
C	3.53358400	0.91981500	-0.30504200
C	4.74533900	1.47750200	0.10857600
C	5.90004900	0.70803500	0.05739500
C	5.86313000	-0.60874500	-0.40381800
C	4.66359500	-1.18331900	-0.81895400
C	1.13952000	0.84251100	-0.69102400
C	2.22826400	1.55699400	-0.28306600
H	4.78224700	2.49973200	0.47004100
H	6.84080700	1.13707400	0.38034200
H	6.77298900	-1.19593200	-0.43713600
H	4.63852300	-2.20880200	-1.16973500
S	1.75118400	3.12384100	0.29686700
I	1.56608000	-1.06262000	-1.26705600
I	-2.00045800	1.02581100	-0.96705000

TS4

Sum of electronic and thermal Free Energies=
-996.77109 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K=-996.76079 Hartree

C	3.19392500	0.52153400	-0.58954800
C	6.41516200	-0.67619600	-0.88382900
C	5.54929000	-0.63785000	0.21616500
C	6.04308500	-0.22900900	1.45407800
C	7.38347900	0.12920500	1.54301200

C	8.22475100	0.09693500	0.42053800	H	-0.66823800	-6.16594600	-0.97255200
C	7.75266500	-0.30787900	-0.82176100	H	0.33361500	-4.76481300	-1.40603800
H	9.26288000	0.38928600	0.52457200	H	-2.58408200	0.09755400	4.11188900
H	8.39084200	-0.34035500	-1.69654200	C	-3.94575500	3.08212100	0.01759200
H	5.39618300	-0.18938200	2.32361200	C	-3.59009900	4.13229300	-0.82654200
H	7.78876400	0.44442900	2.49744000	C	-3.36318400	-3.62158000	0.48886700
C	4.42713900	-1.39274900	-1.62621000	C	-2.81910600	-4.70888200	-0.19287100
N	5.67092100	-1.14481100	-1.97955500	N	-2.83627200	2.24004100	0.07797900
H	3.70357600	-1.74488600	-2.34800200	N	-2.41115700	-2.60548900	0.42483700
H	6.03279900	-1.24346200	-2.92384800	C	-4.47174200	5.16876900	-1.12280300
C	4.20905200	-0.99869800	-0.26817700	C	-5.72250600	5.09748700	-0.53087700
H	3.49527300	-1.52778500	0.35208200	H	-6.44491700	5.88005100	-0.72787700
O	2.04299200	0.14007500	-1.07404600	C	-6.08068200	4.03516300	0.32005700
H	3.87231100	1.04862300	-1.27849400	H	-7.07137000	4.02315000	0.75778900
C	3.19236200	1.19037100	0.76401400	C	-5.20182100	3.00452800	0.61241300
C	4.04037800	2.26861300	1.00944800	C	-4.62744800	-3.66871400	1.06978500
C	2.32669500	0.75383800	1.76888300	C	-5.31893900	-4.86097300	0.93052400
C	4.02453500	2.90860300	2.24767300	H	-6.30769700	-4.95068300	1.36353700
H	4.71442100	2.60786500	0.22844300	C	-4.77302600	-5.95935400	0.23972300
C	2.31423500	1.38560400	3.00677600	H	-5.35405900	-6.86961600	0.15645900
H	1.66124200	-0.08197800	1.57647100	C	-3.51464900	-5.90741800	-0.33706700
C	3.16447200	2.46583500	3.24816300	H	-4.19120500	5.98238500	-1.77988100
H	4.68421400	3.74937300	2.42992500	H	-5.46956400	2.18360300	1.26602500
H	1.64198900	1.03968200	3.78405200	H	-5.03991600	-2.81854400	1.59895900
H	3.15276700	2.96021800	4.21287200	H	-3.09204800	-6.74842400	-0.87222200
C	-2.68767900	-0.18871000	0.24075200	H	-2.74090900	-0.26958800	-0.83937100
C	-2.61088500	0.01784200	3.03263000	INT4			
C	-2.74893500	1.04713700	0.87192500	Sum of electronic and thermal Free Energies =			
C	-2.54056900	-1.31439000	1.04073100	-996.797456 Hartree			
C	-2.50709200	-1.22953100	2.42740300	Sum of electronic and thermal free energies + the entropy			
C	-2.71885500	1.16604500	2.25589100	correction at 298.15K =			
H	-2.39167200	-2.13118700	3.01779400	-996.78726 Hartree			
H	-2.76824900	2.14835000	2.71116100	C	-2.67661100	-2.12193000	0.02926800
C	-1.85250500	2.76042800	-0.68670400	C	-2.21756800	-0.85937800	-0.33968200
N	-2.28322900	3.89290400	-1.24257800	C	-3.14375100	0.11984800	-0.67070300
C	-1.33856500	-3.05996700	-0.25634900	C	-4.49938300	-0.20663600	-0.60168000
N	-1.55779900	-4.31851200	-0.63590300	C	-4.92678600	-1.47970100	-0.21760700
I	-0.00172800	1.83114800	-0.90404800	C	-4.00996700	-2.47727000	0.10553500
I	0.32560200	-1.87786700	-0.63410600	C	-0.43568200	-2.28519400	0.09896300
C	-1.55574100	4.77824200	-2.14810500	C	-0.71016400	-0.87515100	-0.29436900
H	-1.52126200	5.77448800	-1.70880900	H	-2.82994100	1.10951900	-0.98056500
H	-2.07575600	4.80644200	-3.10509800	H	-5.23745000	0.54498000	-0.85528700
H	-0.54578000	4.40163600	-2.28612900	H	-5.98677600	-1.69887800	-0.17587800
C	-0.67291900	-5.17475800	-1.42288500	H	-4.31769600	-3.47437800	0.39530900
H	-1.04179600	-5.22751200	-2.44703100	H	-1.58209400	-3.91065600	0.56684500
				H	0.53069500	-2.75126400	0.24880000

H	-0.27768700	-0.70145400	-1.28675700	H	6.27147700	3.40008500	-2.83980300
N	-1.53437300	-2.93166200	0.28141900	H	4.64012400	4.39126600	-1.22701900
C	-0.06920200	0.11980000	0.72448200	H	2.84756000	3.65818900	0.76929800
H	-0.53955500	-0.08251400	1.69116900	H	1.95928900	1.65301200	1.84589600
C	-0.42585200	1.54763200	0.34560800	H	2.05433300	0.44404400	-0.42550000
C	-1.21941300	2.30814800	1.20396300	N	3.10857200	2.72043800	0.47284500
C	0.00524700	2.11267400	-0.85677400	C	3.27040600	-0.92216000	0.95104100
C	-1.58070500	3.61165200	0.86860500	H	4.35122100	-1.09037600	1.02699400
H	-1.56455800	1.87412800	2.13702600	C	2.71562200	-2.07558100	0.10000900
C	-0.35583800	3.41290500	-1.19479900	C	2.79980200	-2.05637900	-1.29780700
H	0.62211300	1.53497200	-1.53707500	C	2.15016400	-3.20311200	0.70428600
C	-1.15244100	4.16596200	-0.33350000	C	2.34787900	-3.12722800	-2.06482000
H	-2.20048100	4.18954300	1.54491200	H	3.20237300	-1.19504000	-1.81383800
H	-0.01633500	3.83853200	-2.13234000	C	1.66859000	-4.26485800	-0.05962200
H	-1.43527400	5.17816000	-0.59903700	H	2.06926700	-3.25373100	1.78347800
C	3.66843200	-0.45351200	0.65553800	C	1.76544200	-4.23503900	-1.44968400
C	2.45668600	-0.33646900	-0.07556000	H	2.43038300	-3.08337600	-3.14510200
C	2.51404200	-0.47948000	-1.47676200	H	1.21837100	-5.11792100	0.43562300
C	3.73349200	-0.71907100	-2.08489700	H	1.40113100	-5.06471000	-2.04488800
C	4.92073200	-0.82188400	-1.33223400	C	1.33331100	-0.94444600	4.18069300
C	4.90356000	-0.69212200	0.04401600	C	1.36945300	-0.73277400	2.78181200
C	2.02394700	-0.10146000	2.12543800	C	0.18446200	-0.37002000	2.12171400
C	1.41213500	-0.10613800	0.89837800	C	-0.98794400	-0.24653700	2.84505500
H	1.62327000	-0.40647000	-2.08907400	C	-1.00117500	-0.47585800	4.23672900
H	3.77822700	-0.82900900	-3.16227900	C	0.15257000	-0.81912800	4.92107100
H	5.85995800	-1.00704000	-1.84060400	C	3.43667300	-1.26344100	3.48428100
H	5.80882700	-0.77179600	0.63514000	C	2.72942700	-0.94262800	2.35606300
H	4.03675000	-0.34306000	2.74384200	H	0.20725900	-0.16510800	1.05711200
H	1.58465800	0.03417300	3.10307800	H	-1.90650400	0.03657400	2.34124500
N	3.37064400	-0.30074400	1.98506900	H	-1.93221800	-0.37336800	4.78188600
Cat7-TS5				H	0.14592000	-0.98638900	5.99207900
Sum of electronic and thermal Free Energies=				H	2.89504300	-1.46197000	5.52649900
-2316.346007 Hartree				H	4.48385900	-1.50790600	3.58779500
Sum of electronic and thermal free energies + the entropy				N	2.60719600	-1.26522700	4.57791900
correction at 298.15K=				O	0.84852500	0.47623800	-1.26764800
-2316.33602 Hartree				H	1.19220200	0.55322400	-2.17114100
C	4.01656600	2.43484900	-0.55695800	C	-3.28284800	2.92514500	0.10625000
C	4.10869500	1.04047000	-0.65577200	C	-2.12800900	3.67425200	-0.15820600
C	5.04707400	0.49804100	-1.53516200	C	-2.07772600	5.04932400	-0.00757700
C	5.81538300	1.36496800	-2.30385700	C	-3.23430900	5.69510900	0.42295900
C	5.66159000	2.75569800	-2.21823700	C	-4.39715600	4.97163400	0.69173100
C	4.75664800	3.31923500	-1.33012500	C	-4.43170000	3.59285900	0.53689700
C	2.65561700	1.61440600	1.01796500	C	-3.13243900	1.49772000	-0.10992500
C	3.10919500	0.46156300	0.28295200	H	-1.17630900	5.61347100	-0.21688900
H	5.20005900	-0.57202400	-1.60557200	H	-3.22513200	6.77093300	0.54906600
H	6.55512400	0.95587200	-2.98185500				

H	-5.28659700	5.49180000	1.02572700	C	-0.55473000	3.00359800	-1.61368400
H	-5.34022800	3.03917300	0.74830700	H	-0.89537500	0.88230300	-1.57177600
C	-1.92916600	1.00099600	-0.53161000	C	-0.13187700	4.12264500	-0.90363600
C	-2.15208700	-3.07715800	-0.98301300	H	0.62033800	4.84309600	0.98107400
C	-3.30244600	-2.40160500	-0.54862600	H	-0.89067100	3.10594000	-2.63967200
C	-4.45076000	-3.15182600	-0.28384400	H	-0.13631200	5.10074100	-1.37111500
C	-4.41972700	-4.52836800	-0.45848900	C	3.50290100	-0.92113700	0.61448200
C	-3.26002000	-5.17243300	-0.89226400	C	2.27621800	-0.53444200	0.01830600
C	-2.10080000	-4.44818300	-1.15965300	C	2.18584400	-0.50430300	-1.38515000
C	-1.93749600	-0.39363600	-0.71368900	C	3.29637300	-0.84666500	-2.13710100
C	-3.14628300	-0.96472500	-0.42072500	C	4.50697500	-1.22556300	-1.52020100
H	-5.35683700	-2.66221300	0.05631000	C	4.62701000	-1.26965800	-0.14230200
H	-5.31011500	-5.10986200	-0.25297100	C	2.04881700	-0.47622000	2.25617500
H	-3.25394800	-6.24763100	-1.02319300	C	1.35688200	-0.25640400	1.09507100
H	-1.19753500	-4.94618500	-1.49248800	H	1.25795600	-0.22322900	-1.87052900
S	-4.30068500	0.23048400	0.07392600	H	3.23808700	-0.82677900	-3.21939900
I	-0.53487100	-1.77007200	-1.28314400	H	5.35834100	-1.48874800	-2.13758400
I	-0.51158300	2.46198000	-0.76770700	H	5.55369300	-1.56291300	0.33808300

Product

Sum of electronic and thermal Free Energies =
-996.387958 Hartree

Sum of electronic and thermal free energies + the entropy
correction at 298.15K = -996.37777 Hartree

C	-2.92897400	-1.83059500	-0.30326200
C	-2.43474200	-0.65369700	0.31008500
C	-3.34009300	0.34985000	0.69379000
C	-4.69123900	0.15515400	0.46161700
C	-5.16160100	-1.02465400	-0.15166300
C	-4.29290500	-2.03026800	-0.54138900
C	-0.69986300	-2.00647800	-0.15060300
C	-1.00234700	-0.78792100	0.39619200
H	-2.98488500	1.26150100	1.16358700
H	-5.40261400	0.91963300	0.75245700
H	-6.22541000	-1.14614300	-0.32161100
H	-4.65170800	-2.93822000	-1.01285500
H	-1.88843100	-3.54617500	-1.00418100
H	0.25816200	-2.48901000	-0.27410800
N	-1.84987200	-2.63384700	-0.57248700
C	-0.06900200	0.22665000	1.00423000
H	-0.40240300	0.40173900	2.03453400
C	-0.12517500	1.58966500	0.30685300
C	0.29664500	2.72059900	1.01204300
C	-0.55504800	1.74609200	-1.01037500
C	0.29383400	3.97703300	0.41607000
H	0.63090000	2.60972900	2.03983900