Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Nickel-catalyzed hydroalkenylation of styrene with phenylpropanal: theoretical studies on the mechanism, regioselectivity, and role of phenylboronic acid

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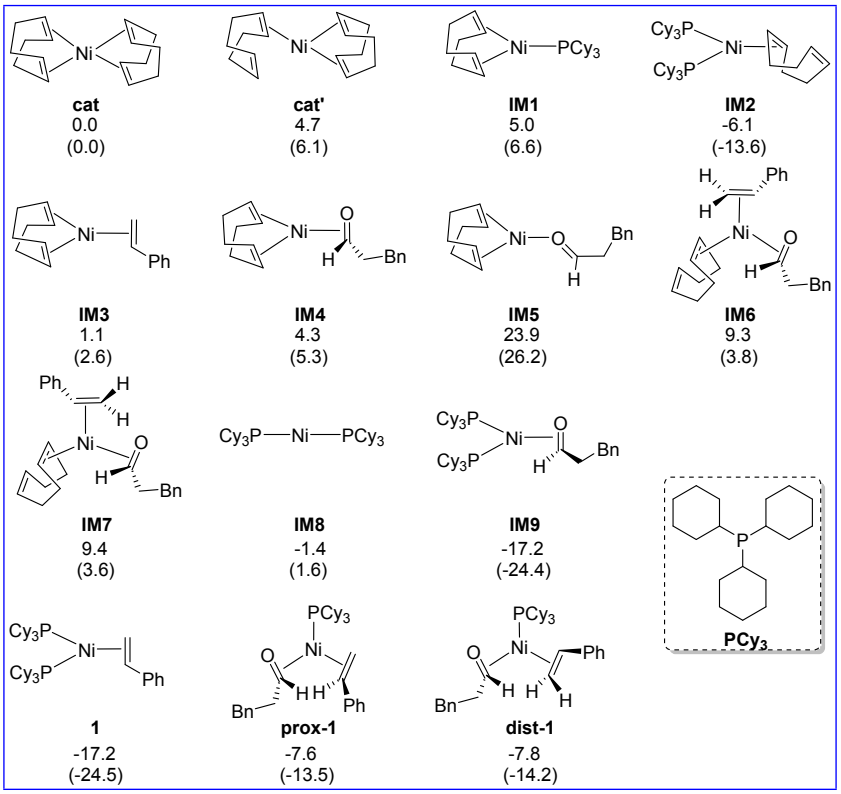
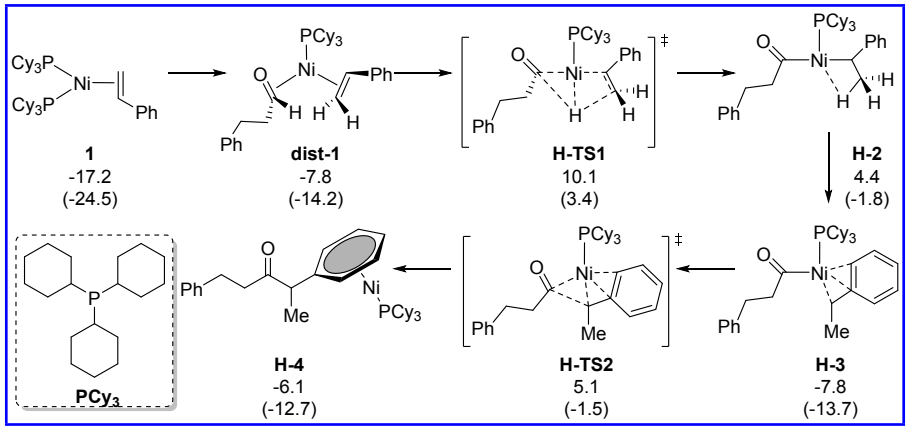
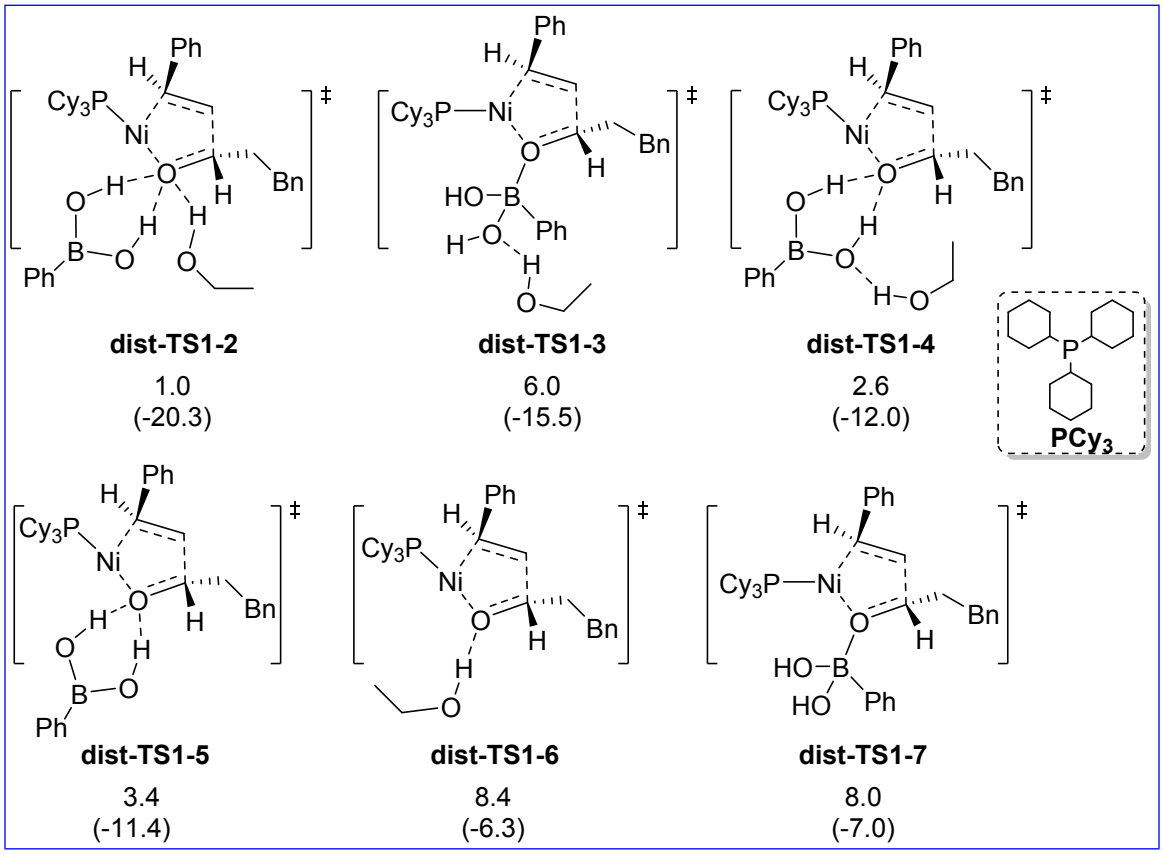


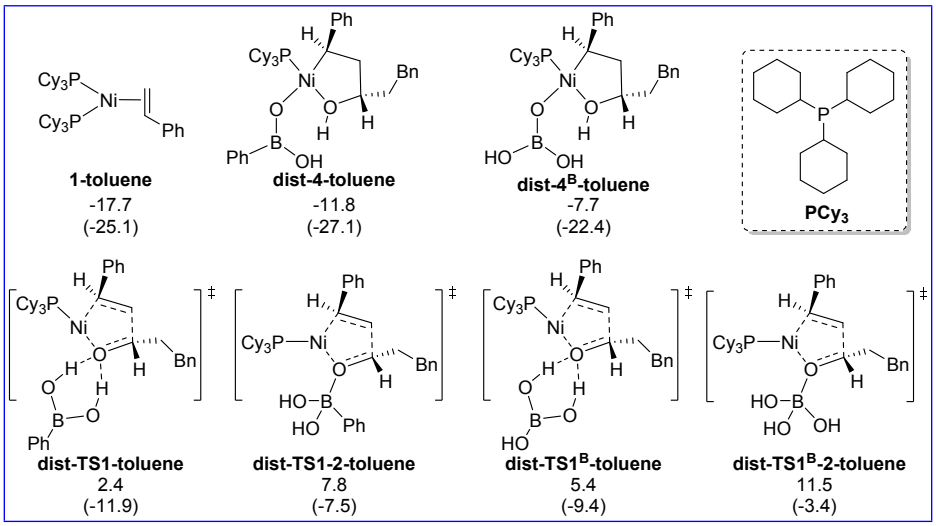
Scheme S1 Relative stabilities of various Ni-adducts in ethanol solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol, where the energy of **cat** is set to be the zero reference energy point.



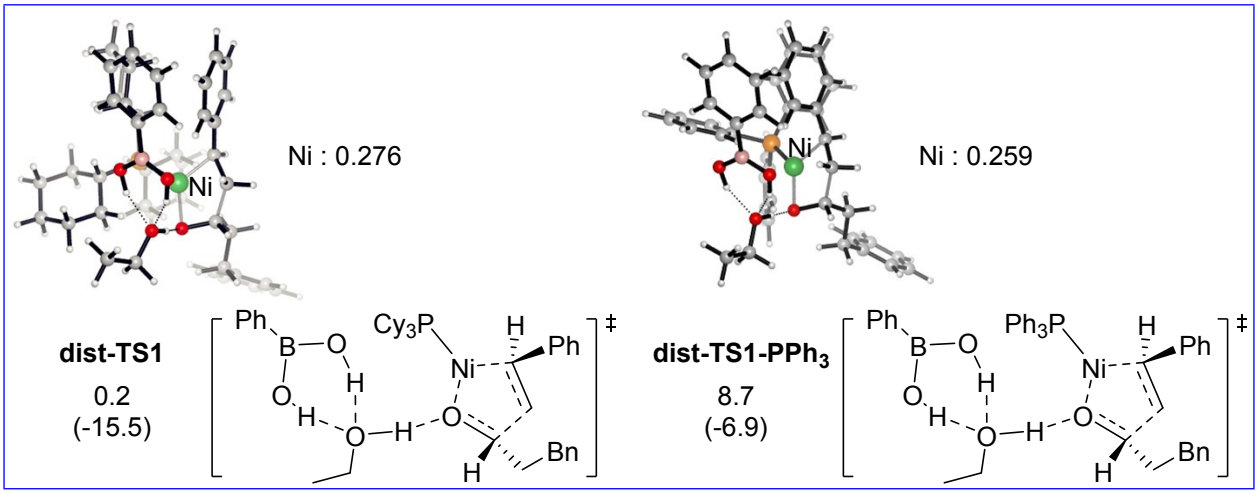
Scheme S2 The mechanism of the nickel-catalyzed intermolecular hydroacylation of alkene to produce branched ketone **P3** in the absence of $PhB(OH)_2$ under this reaction condition. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol, where the energy of **cat** is set to be the zero reference energy point.



Scheme S3 Other unfavorable **dist**-isomers of oxidative cyclization transition state in ethanol solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.



Scheme S4 Other related structures in toluene. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.



Scheme S5 NBO charges (*e*) in the optimized structures of transition states **dist-TS1** and **dist-TS1-PPh$_3$** in ethanol solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

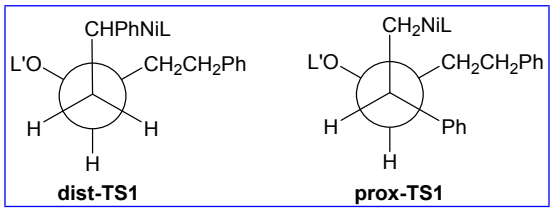


Fig. S1 Newmann projections of the C−C bond that is being formed in **dist-TS1** and **prox-TS1.**

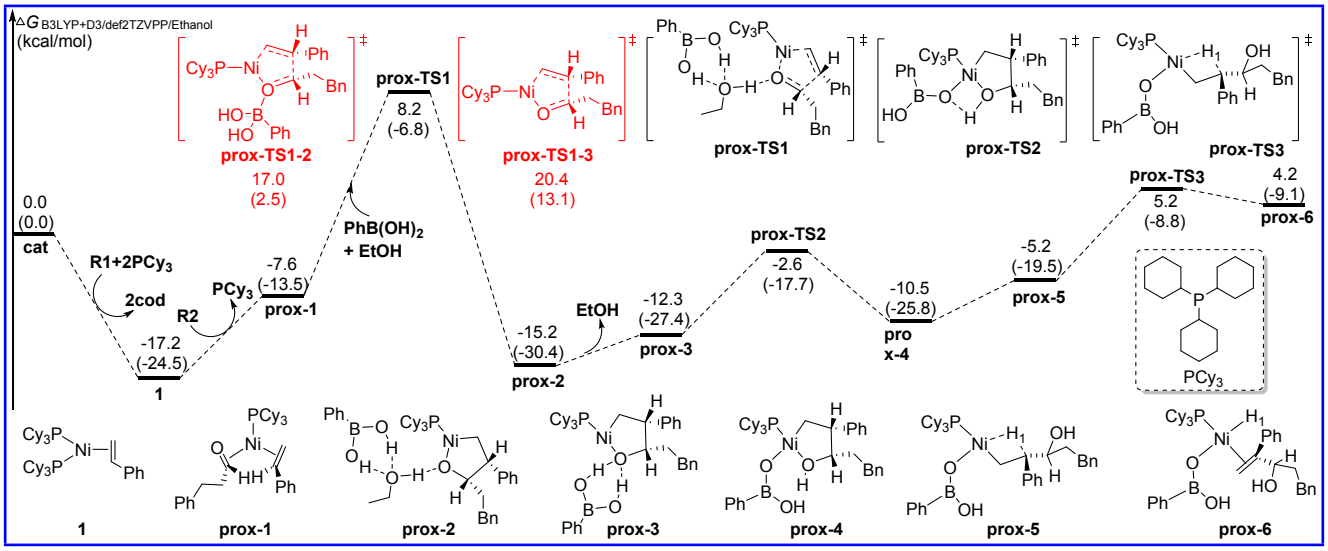


Fig. S2 The unfavorable process for **prox-**isomer to generate branched product in ethanol solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

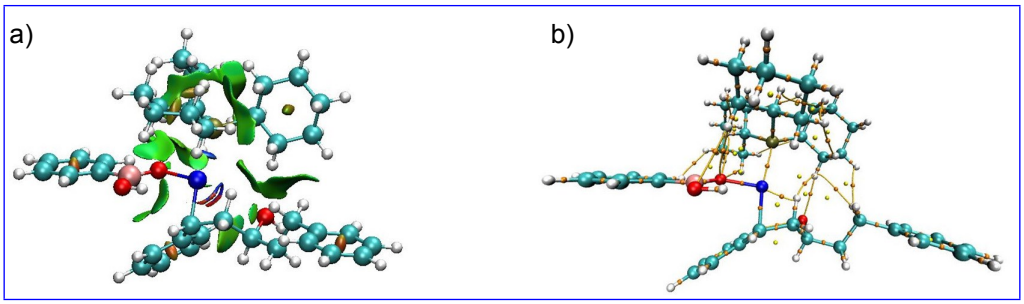


Fig. S3 a) Noncovalent interactions analyses for **dist-5**. Blue, green, and red surfaces represent the strong interaction, weak interaction, and steric effect, respectively. b) Molecular graphs of **dist-5.** Orange and yellow dots represent the bond critical points (BCPs) and ring critical points (RCPs).

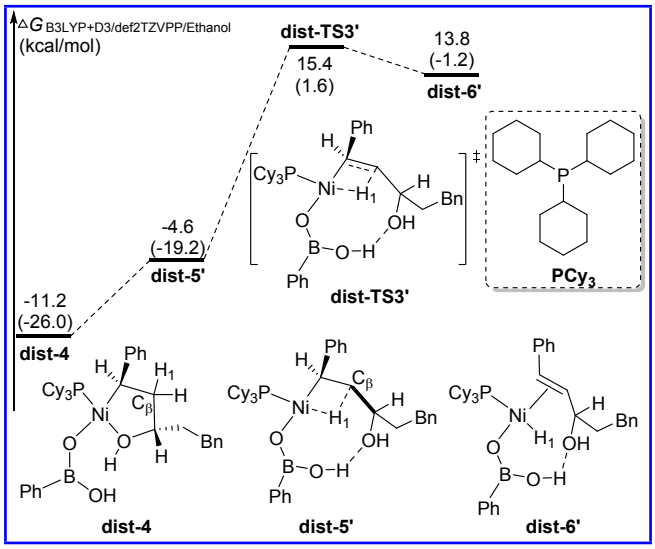


Fig. S4 The unfavorable *β*-hydride elimination process caused by different position of $PhB(OH)_2$ in ethanol solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol. The bond distances are given in Å.

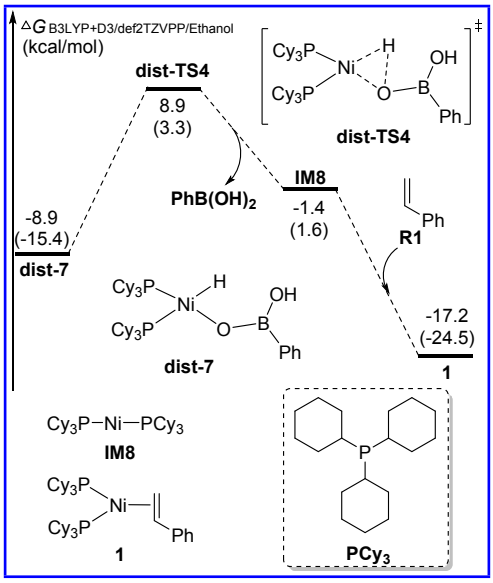


Fig. S5 The reductive elimination process from **dist-7** in ethanol solvent. The relative free energies and relative enthalpic energies (in parentheses) are given in kcal/mol.

Cartesian coordinates and sum of electronic and thermal Gibbs energies for all of the calculated structure

cat

Sum of electronic and thermal Free Energies= -2131.991568

C	1.50816200	0.46273200	-1.47924000
C	1.36554900	1.53460900	-0.61195200
H	0.97655200	0.53052900	-2.42569000
C	2.61442200	-0.58562500	-1.42410200
H	3.52816100	-0.13892000	-1.02288900
H	2.85838300	-0.89841400	-2.44546600
C	2.22501900	1.83758300	0.60197100
H	3.13172000	2.38916700	0.30713100
H	1.65388600	2.51512300	1.24678500
H	0.75730000	2.36863000	-0.95943100
C	2.61438200	0.58563700	1.42420500
H	3.52812400	0.13895200	1.02298000
H	2.85834000	0.89841200	2.44557400
C	2.22508300	-1.83756700	-0.60184700
H	1.65400500	-2.51515200	-1.24666100
H	3.13179800	-2.38910000	-0.30695500
C	1.50813700	-0.46273000	1.47932200
C	1.36555900	-1.53460000	0.61203800
H	0.97644400	-0.53048600	2.42572600
H	0.75725700	-2.36859900	0.95947000
C	-1.50812900	-0.46301400	-1.47921600
C	-1.36551600	-1.53472700	-0.61173300
H	-0.97647500	-0.53095800	-2.42563100
C	-2.61440200	0.58534000	-1.42429500
H	-3.52813600	0.13870900	-1.02299000
H	-2.85836400	0.89791800	-2.44572300
C	-2.22501400	-1.83748800	0.60222300
H	-3.13170300	-2.38913200	0.30745900
H	-1.65389500	-2.51490700	1.24717500
H	-0.75723200	-2.36879400	-0.95903700
C	-2.61441000	-0.58539600	1.42421900
H	-3.52815500	-0.13880000	1.02289900
H	-2.85837900	-0.89798800	2.44564200
C	-2.22506800	1.83744800	-0.60229400
H	-1.65395100	2.51488200	-1.24723200
H	-3.13178000	2.38906500	-0.30755000
C	-1.50818400	0.46300400	1.47916600
C	-1.36559100	1.53471500	0.61168300
H	-0.97653700	0.53096100	2.42558300
H	-0.75732600	2.36879500	0.95898900
Ni	-0.00000100	0.00002100	-0.00003700

cat'

Sum of electronic and thermal Free Energies= -2131.985163

C	2.13611400	1.23363600	-0.79844400
C	1.46713900	1.62708600	0.34315700
H	1.82899100	1.69413700	-1.73772000
C	3.41788200	0.41601200	-0.84377200
H	4.03858300	0.64696000	0.02479200
H	4.00019100	0.71404000	-1.72194000
C	1.82815600	1.29525700	1.77961200
H	2.56072500	2.01682400	2.17042900
H	0.91968900	1.42822900	2.37785000
H	0.70564500	2.39930500	0.23335700
C	2.35615700	-0.14890400	1.99563300
H	3.42823500	-0.19438700	1.79207700
H	2.23611400	-0.40441600	3.05380200
C	3.16373800	-1.11645800	-0.92812400
H	2.95793500	-1.37956900	-1.97147900
H	4.08413700	-1.65198100	-0.65266100
C	1.61981400	-1.17610200	1.15143200
C	1.99197800	-1.61350500	-0.10159600
H	0.82925400	-1.73123300	1.65606400
H	1.50487800	-2.51049200	-0.48457900
C	-3.90607500	0.90942900	0.40937600
C	-4.24380500	-0.39055700	0.33705700
H	-4.74153600	1.61131200	0.39358400
C	-2.54291400	1.57767200	0.42016900
H	-1.85812600	1.13089300	1.14593200
H	-2.68606300	2.61579000	0.73958300
C	-3.40071400	-1.64244900	0.32782200
H	-3.74026300	-2.26855700	1.16730700
H	-3.65351000	-2.21929900	-0.57439400
H	-5.31485600	-0.59972800	0.28640300
C	-1.87225000	-1.48868500	0.41649600
H	-1.62553900	-0.86820900	1.28207200
H	-1.45156000	-2.47593400	0.64222500
C	-1.87208000	1.58798600	-0.97019200
H	-2.64426000	1.81975600	-1.71975900

H	-1.16469900	2.42608800	-1.01443300
C	-1.17903000	-0.99403200	-0.84950400
C	-1.13622500	0.32219100	-1.38966900
H	-1.00002500	-1.79860900	-1.56912300
H	-0.86697600	0.35640700	-2.45123900
Ni	0.52449000	-0.11245700	-0.38803100

R1

Sum of electronic and thermal Free Energies= -309.58862

C	-1.78606300	-1.04921200	0.00004700
C	-0.40698400	-1.28606200	-0.00000100
C	0.51651600	-0.22155100	-0.00004900
C	0.01035000	1.09599000	-0.00006700
C	-1.36507200	1.33387300	-0.00002100
C	-2.27201700	0.26302500	0.00004000
H	-2.47832100	-1.88760000	0.00008800
H	-0.03962200	-2.31037300	0.00000300
H	0.69182700	1.94221200	-0.00013200
H	-1.73438800	2.35660200	-0.00004000
H	-3.34249000	0.45232300	0.00007300
C	1.95980400	-0.53289200	-0.00008200
H	2.19799400	-1.59690800	-0.00026900
C	2.98476000	0.33758900	0.00011300
H	4.01207300	-0.01688100	0.00006600
H	2.84516500	1.41606700	0.00033000

R2

Sum of electronic and thermal Free Energies= -424.137215

C	-2.53545100	1.21000200	0.08368700
C	-1.16271200	1.20682300	-0.19228500
C	-0.45772800	-0.00008300	-0.33432800
C	-1.16282700	-1.20690200	-0.19213300
C	-2.53556800	-1.20991300	0.08384100
C	-3.22760300	0.00008600	0.22356200
H	-3.06446500	2.15466500	0.18589200
H	-0.63354900	2.15179000	-0.30185700
H	-0.63375500	-2.15193300	-0.30158200
H	-3.06467200	-2.15451300	0.18616700
H	-4.29411600	0.00015100	0.43496400
C	1.03548800	-0.00016300	-0.58785600
C	1.83354200	0.00011800	0.72431100
H	1.32085400	0.87801700	-1.17570900
H	1.32082600	-0.87861700	-1.17531200
C	3.32918100	0.00003500	0.55115100
H	1.58083500	0.87141700	1.34549500
H	1.58079500	-0.87088800	1.34588800
H	3.90992600	0.00042300	1.49722700
O	3.90992500	-0.00006600	-0.52510900

P1

Sum of electronic and thermal Free Energies= -733.70725

C	0.99524500	0.73407500	0.94094700
H	0.28075000	1.32742400	1.50803100
C	2.27461800	1.15761200	0.94039200
H	2.48070000	2.08662500	1.47318500
C	-5.51062800	-0.99713100	-0.57482100
C	-4.23238800	-1.12325300	-0.01726900
C	-3.45938400	0.01106300	0.28319400
C	-4.00005700	1.27843800	0.00804900
C	-5.27774200	1.41140100	-0.54932900
C	-6.03872500	0.27246200	-0.84366800
H	-6.09489800	-1.88742500	-0.79593500
H	-3.83085800	-2.11366300	0.19029600
H	-3.41630100	2.16883100	0.23527500
H	-5.68002700	2.40161500	-0.75063500
H	-7.03221900	0.37306200	-1.27390900
C	-2.05909300	-0.13068200	0.84152000
C	-1.00952600	-0.23706100	-0.28328600
H	-1.99345700	-1.02361600	1.47113800
H	-1.83550400	0.72797900	1.48297400
C	0.43783200	-0.45271700	0.19239500
H	-1.28196000	-1.07389000	-0.93998400
H	-1.03927300	0.66512800	-0.90673000
H	1.05507400	-0.62302900	-0.70049300
O	0.54079800	-1.61322100	1.05693300
H	0.16514800	-2.36989100	0.57463800
C	3.45229800	0.55919300	0.27866700
C	4.48924200	1.41316400	-0.15279400
C	3.60782300	-0.82998000	0.08407700
C	5.62289400	0.90596000	-0.79340500
H	4.39794700	2.48561700	0.00760300
C	4.74564400	-1.33681300	-0.55215900
H	2.85269500	-1.51151800	0.46320400
C	5.75398200	-0.47385300	-1.00046300
H	6.40496300	1.58420500	-1.12595800
H	4.85082600	-2.41068100	-0.68791300
H	6.63778800	-0.87227200	-1.49254100

P2

Sum of electronic and thermal Free Energies= -733.705561

C	-2.08223800	1.35671100	-0.69371800
C	-2.79024000	1.87597000	-1.71155400
H	-3.60617400	1.32781800	-2.17686400
C	4.60381000	0.06392300	0.80409900
C	3.25336800	0.37573300	1.00156800
C	2.26104100	-0.13005400	0.14447200
C	2.65783900	-0.95734900	-0.91946700
C	4.00715900	-1.27275300	-1.12298200
C	4.98651500	-0.76226400	-0.26114200
H	5.35604400	0.46149200	1.48162600
H	2.96446000	1.01667600	1.83289100
H	1.90277400	-1.36029500	-1.59225700
H	4.29331600	-1.91818700	-1.95031200
H	6.03446600	-1.00800800	-0.41514600
C	0.80682900	0.24600700	0.33365300
C	0.47045200	1.56666900	-0.38837300
H	0.58190400	0.35700000	1.39939300
H	0.16821100	-0.55627100	-0.04257700
C	-0.92561900	2.16508100	-0.11600500
H	1.20974900	2.32372900	-0.09256000
H	0.58350300	1.43688200	-1.47129300
H	-0.94580300	3.14364000	-0.61477700
O	-1.15213400	2.36439700	1.29555400
H	-0.37754200	2.82891900	1.65497200
H	-2.57674900	2.86623900	-2.10802400
C	-2.38208400	-0.01660700	-0.18985100
C	-2.52994300	-1.07682600	-1.10580400
C	-2.52352600	-0.29700500	1.18308400
C	-2.81200200	-2.37503000	-0.66802900
H	-2.39721300	-0.88485600	-2.16742800
C	-2.80972700	-1.59447900	1.62040000
H	-2.40464400	0.50384200	1.90325600
C	-2.95323700	-2.64044800	0.69965000
H	-2.91167700	-3.17888600	-1.39359700
H	-2.91970300	-1.78933600	2.68471800
H	-3.16822200	-3.64925200	1.04354500

PCy_3

Sum of electronic and thermal Free Energies= -1046.842554

P	0.01624800	-0.12597400	-1.07502600
C	-1.49971200	-1.06250800	-0.46192900
C	-1.76631600	-1.07425500	1.05558900
C	-2.76316500	-0.60586200	-1.22498500
H	-1.30285700	-2.09726900	-0.77681800
C	-2.97640100	-1.95893800	1.40546500
H	-1.97023400	-0.05104000	1.39523500
H	-0.88183800	-1.42049800	1.60195300
C	-3.98003300	-1.47977000	-0.87204400
H	-2.99340000	0.43824500	-0.97152100
H	-2.58248300	-0.63471200	-2.30641900
C	-4.23315200	-1.51221600	0.64304300
H	-3.15749400	-1.93295500	2.48737800
H	-2.74633200	-3.00241900	1.14751900
H	-4.86891800	-1.11121400	-1.39915900
H	-3.80088500	-2.50331400	-1.23028000
H	-5.07582200	-2.17571000	0.87357200
H	-4.51991800	-0.50641900	0.98193300
C	-0.21219800	1.59363800	-0.30601900
C	0.30356900	1.81928100	1.13134900
C	0.34527300	2.68557400	-1.24811500
H	-1.30387500	1.72208800	-0.28415200
C	-0.04662600	3.23094400	1.63597900
H	1.39392300	1.70249300	1.15646200
H	-0.10589000	1.07128900	1.81601100
C	0.01437800	4.09991100	-0.74103200
H	1.43602400	2.57793400	-1.32892000
H	-0.05631400	2.54774200	-2.25891600
C	0.50532300	4.31492400	0.69835200
H	0.34575500	3.36914400	2.65138600
H	-1.13946600	3.32983500	1.70256800
H	0.45420300	4.84943300	-1.41092600
H	-1.07483900	4.24517200	-0.77543400
H	0.21704700	5.31165200	1.05469700
H	1.60399100	4.27799700	0.71417000
C	1.41956200	-0.89086500	-0.07972100
C	1.48004900	-2.42363200	-0.25214700
C	2.76349100	-0.26000600	-0.50841500
H	1.26757200	-0.68169400	0.98630800
C	2.67019300	-3.03142800	0.51191700
H	1.57031700	-2.66950000	-1.32011000
H	0.55415600	-2.88877200	0.10222300
C	3.94816400	-0.86106300	0.26611400
H	2.91241300	-0.43156800	-1.58381300
H	2.74483700	0.82609800	-0.36763400
C	4.00259900	-2.38706200	0.10232700
H	2.70262100	-4.11515700	0.34389700
H	2.51430200	-2.88330200	1.58985500
H	4.88600500	-0.40615900	-0.07623800
H	3.84570600	-0.61282000	1.33198800

H	4.82589000	-2.80652100	0.69366600
H	4.21211000	-2.62846400	-0.94946500

$PhB(OH)_2$

Sum of electronic and thermal Free Energies= -408.254108

C	1.93432600	-1.22305500	-0.00000400
C	0.53603000	-1.20124400	-0.00000600
C	-0.17952400	0.01506100	0.00000100
C	0.56573900	1.21218800	0.00000900
C	1.96510900	1.19992300	0.00001200
C	2.65282600	-0.02012400	0.00000400
H	2.46452100	-2.17250900	-0.00000900
H	-0.01356800	-2.13913800	-0.00001100
H	0.06378900	2.17862600	0.00001700
H	2.51771100	2.13630100	0.00002000
H	3.74016300	-0.03301400	0.00000700
B	-1.74930900	-0.00052800	0.00000200
O	-2.54280000	1.12855600	-0.00001800
H	-2.04246700	1.95803700	-0.00004200
O	-2.39145900	-1.21818900	0.00000700
H	-3.35656800	-1.10510000	-0.00000100

EtOH

Sum of electronic and thermal Free Energies= -155.022738

C	-1.22888600	-0.22468700	0.00000600
C	0.07910900	0.55110100	0.00001300
H	-1.30099500	-0.86062500	0.88868900
H	-2.07810700	0.46675100	0.00003700
H	-1.30101700	-0.86057500	-0.88871000
H	0.13860400	1.19602000	-0.88827700
H	0.13861700	1.19598000	0.88833200
O	1.16307900	-0.39926100	-0.00001500
H	1.99693100	0.09805700	-0.00007000

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Sum of electronic and thermal Free Energies= -3911.416693

Ni	0.02295100	0.66921700	0.71059000
C	2.07726700	2.83323400	1.11224800
C	3.45116100	2.94341900	1.42275300
C	1.58095500	3.68615400	0.09862700
C	4.28254800	3.85626800	0.76506200
H	3.87380700	2.30869500	2.19826000
C	2.40407600	4.60891400	-0.54791200
H	0.53791400	3.60697600	-0.19201900
C	3.76576900	4.70385100	-0.22282600
H	5.33659900	3.90937700	1.03036900
H	1.98719800	5.24626200	-1.32522700
H	4.40908900	5.41456100	-0.73577400
P	1.57213800	-0.80383900	-0.04617800
C	2.85931700	0.14660500	-1.03644200
C	4.18979900	-0.48823800	-1.50052800
C	2.16443500	0.84830900	-2.22389600
H	3.11844300	0.93515800	-0.32084500
C	5.11577100	0.59475500	-2.08175900
H	4.01462700	-1.22630900	-2.28474200
H	4.68894800	-1.02040000	-0.68686100
C	3.08872800	1.87752500	-2.89680800
H	1.85045100	0.09666900	-2.96237800
H	1.25630100	1.34895000	-1.86723300
C	4.44968100	1.28048500	-3.28515600
H	6.07164400	0.14597400	-2.38031500
H	5.34015500	1.34346400	-1.30910200
H	2.59119500	2.29874700	-3.78004900
H	3.24913600	2.70583000	-2.19850300
H	5.10217500	2.06428700	-3.69006100
H	4.31189900	0.53861500	-4.08505500
C	1.04890300	-2.29260100	-1.10038500
C	2.11460400	-3.03605700	-1.92993600
C	0.25383600	-3.30773800	-0.25323400
H	0.35085300	-1.84511600	-1.81331100
C	1.50259200	-4.18111400	-2.76135700
H	2.89778700	-3.43403000	-1.27066000
H	2.59722100	-2.34680300	-2.62237000
C	-0.38324700	-4.41316200	-1.10832600
H	0.92863300	-3.78661900	0.46695500
H	-0.51311600	-2.79467500	0.32744000
C	0.68732900	-5.16291200	-1.91125000
H	2.30217000	-4.70846700	-3.29650800
H	0.84755000	-3.74569900	-3.52904600
H	-0.93751500	-5.10485400	-0.46179300
H	-1.11473600	-3.97202600	-1.79866600
H	0.22768400	-5.92853400	-2.54831000
H	1.35750800	-5.68742400	-1.21543900
C	2.49766000	-1.61800100	1.38955700
C	3.68972200	-0.80960600	1.94656800
C	1.50852600	-1.89601400	2.54911600
H	2.88761800	-2.57789600	1.02263700
C	4.38130400	-1.55198700	3.10307100
H	3.33057500	0.15488400	2.31218800

H	4.42477100	-0.59034400	1.17135500
C	2.18222900	-2.63111900	3.71861500
H	1.10489100	-0.93532700	2.89449600
H	0.64931000	-2.47513000	2.20727800
C	3.40095100	-1.85994700	4.24332100
H	5.22110200	-0.95083600	3.47376400
H	4.80769800	-2.49224300	2.72539300
H	1.45348200	-2.78911400	4.52360900
H	2.50080900	-3.62762200	3.38059100
H	3.90184000	-2.42691600	5.03782400
H	3.06300800	-0.91461600	4.69121500
P	-2.08436000	0.30385300	0.06428200
C	-2.32033400	-0.82862200	-1.42376400
C	-3.76256600	-1.22750100	-1.79462400
C	-1.59611400	-0.25184600	-2.65930200
H	-1.78993800	-1.74211900	-1.13807000
C	-3.77530700	-2.22747800	-2.96519700
H	-4.32868300	-0.33639700	-2.09224300
H	-4.28247300	-1.66268600	-0.93443800
C	-1.61263500	-1.23717200	-3.83992800
H	-2.08810000	0.67542900	-2.98017900
H	-0.57007000	0.02102200	-2.39678900
C	-3.04516600	-1.66406200	-4.19385100
H	-4.81037400	-2.48453400	-3.22260400
H	-3.28824600	-3.16004300	-2.64779800
H	-1.12258700	-0.78219200	-4.70959900
H	-1.02698100	-2.12896600	-3.58115100
H	-3.03243000	-2.40505400	-5.00253700
H	-3.59838800	-0.79214600	-4.57081000
C	-3.17049300	1.77256900	-0.48931400
C	-4.65975100	1.74398400	-0.08046600
C	-2.56336400	3.14360200	-0.14943800
H	-3.14688800	1.69219300	-1.58286000
C	-5.43912700	2.88480400	-0.76061600
H	-4.74961100	1.85302500	1.00710600
H	-5.12479200	0.78932600	-0.34011300
C	-3.33325500	4.28593600	-0.83088700
H	-2.58555400	3.29284000	0.93632200
H	-1.51106700	3.16098000	-0.44776800
C	-4.82216500	4.25742400	-0.45537500
H	-6.48751000	2.85735500	-0.43807500
H	-5.43833600	2.72007900	-1.84748400
H	-2.88799100	5.25049100	-0.55638700
H	-3.23193500	4.18914900	-1.92137900
H	-5.36751300	5.04730800	-0.98657000
H	-4.92593400	4.46731400	0.61870200
C	-3.11341800	-0.53425900	1.39837600
C	-2.69720900	-1.99524100	1.65329200
C	-3.04588600	0.24620300	2.72567900
H	-4.15469900	-0.54240200	1.05873100
C	-3.58914900	-2.64965400	2.72306800
H	-1.65343000	-2.01251600	1.99104400
H	-2.74950500	-2.58678500	0.73375000
C	-3.96194900	-0.38067100	3.78816600
H	-2.01160800	0.22196600	3.08476900
H	-3.29633600	1.30211500	2.57837200
C	-3.58809600	-1.85039400	4.03477600
H	-3.25382200	-3.67860400	2.90345400
H	-4.61682400	-2.71472000	2.33871000
H	-3.89432700	0.19058000	4.72241500
H	-5.00697000	-0.31880100	3.45285200
H	-4.27518700	-2.30592800	4.75842800
H	-2.58388800	-1.89295100	4.48001700
C	1.20979300	1.88446800	1.84091800
C	-0.18730700	2.11666700	2.02702400
H	-0.64421600	1.74512800	2.94415500
H	-0.62180000	3.05325000	1.68777300
H	1.72745700	1.32286200	2.61710900

dist-1

Sum of electronic and thermal Free Energies= -3288.699574

Ni	-0.18021400	-1.10617000	-0.19774000
P	0.97567500	0.81917600	0.06456600
C	2.04262200	1.30874700	-1.38885600
C	2.97951400	2.51760300	-1.19612800
C	1.20078000	1.50669700	-2.66899600
H	2.66818000	0.42159800	-1.54574300
C	3.90002000	2.68658900	-2.41874200
H	2.37992500	3.42819100	-1.07050600
H	3.58563900	2.40886600	-0.29097700
C	2.11007300	1.65791800	-3.89988200
H	0.59193600	2.41480200	-2.57345800
H	0.49785200	0.67851200	-2.80476400
C	3.09494000	2.82441300	-3.72059000
H	4.54794500	3.56060500	-2.27908100
H	4.56026400	1.81076800	-2.48995400
H	1.49979600	1.81078600	-4.79830000
H	2.67079800	0.72506600	-4.05240600
H	3.77246500	2.88601100	-4.58089100
H	2.53018400	3.76702800	-3.69416800
C	-0.10273000	2.34835300	0.32592300

C	0.46263800	3.42511100	1.27658300
C	-1.55278900	1.99421700	0.71178400
H	-0.14513700	2.79725800	-0.67456000
C	-0.43503600	4.67564500	1.28434500
H	0.52066600	3.02653400	2.29652500
H	1.48011700	3.70768700	0.98984400
C	-2.44641900	3.24375000	0.72516200
H	-1.56546000	1.51489700	1.69613100
H	-1.94724300	1.24723900	0.01633500
C	-1.88455200	4.32888300	1.65590700
H	-0.02794000	5.41637400	1.98372900
H	-0.41616500	5.13772800	0.28716000
H	-3.46392100	2.96856800	1.03139100
H	-2.52208200	3.64628500	-0.29526900
H	-2.51201900	5.22798500	1.61965200
H	-1.91210500	3.96361900	2.69232700
C	2.15058500	0.75147100	1.51829300
C	3.35589500	-0.16656400	1.22933400
C	1.40238400	0.25862900	2.77528100
H	2.52725700	1.76369700	1.70816000
C	4.29563000	-0.25600900	2.44257600
H	2.99429600	-1.16925700	0.98267100
H	3.91935700	0.18477000	0.35977100
C	2.34068600	0.17360600	3.98937700
H	0.97312400	-0.72741400	2.56365600
H	0.55346600	0.91254600	3.00197300
C	3.54919000	-0.72873800	3.69820600
H	5.12419700	-0.93689900	2.21150800
H	4.73887200	0.73179700	2.63376100
H	1.78613700	-0.19984700	4.85932700
H	2.69459700	1.18182400	4.24828500
H	4.22699900	-0.75191000	4.56054100
H	3.19898400	-1.75872300	3.54010300
C	-0.42760600	-2.55877600	-1.57631900
C	0.84711500	-1.97851200	-1.70722300
C	-1.75623700	-1.94132600	0.66961900
O	-1.25062900	-0.99082500	1.40524400
H	-0.54845200	-3.55586200	-1.15890800
H	-1.21901000	-2.25431000	-2.25951800
H	1.01169600	-1.28025900	-2.52397700
C	2.08079400	-2.58815800	-1.15764700
C	3.33248600	-2.27757900	-1.72228300
C	2.05595500	-3.45934700	-0.04690400
C	4.51640400	-2.79943800	-1.19140700
H	3.37976500	-1.61461200	-2.58375900
C	3.23640500	-3.98346900	0.48317100
H	1.10576800	-3.69227900	0.42684300
C	4.47659800	-3.65350600	-0.08279100
H	5.47067700	-2.53503500	-1.64118900
H	3.19245400	-4.63868900	1.35014300
H	5.39621500	-4.05242200	0.33792100
C	-3.07041100	-1.69026200	-0.05285600
H	-3.29465300	-2.52433700	-0.72682600
H	-2.97532500	-0.78720100	-0.66537100
C	-4.23002600	-1.49002000	0.95247400
H	-4.38618800	-2.41710900	1.51636700
H	-3.92376900	-0.72072200	1.66945800
C	-5.50856400	-1.07232900	0.26114000
C	-5.72523200	0.27657100	-0.07235700
C	-6.47988500	-2.01561300	-0.11187700
C	-6.87993500	0.67325300	-0.75605400
H	-4.98211500	1.02111900	0.20882400
C	-7.63792600	-1.62482000	-0.79673800
H	-6.32953400	-3.06453400	0.13749600
C	-7.84236600	-0.27788500	-1.12207500
H	-7.03103900	1.72223900	-1.00066200
H	-8.38033000	-2.36998500	-1.07336900
H	-8.74161900	0.02793000	-1.65133200
H	-1.56562900	-2.98384800	0.97465400

dist-TS1

Sum of electronic and thermal Free Energies= -3851.949911

C	0.23299600	-0.31619200	-2.20678100
C	0.60740300	1.15820700	-2.51571100
Ni	0.53656900	0.37835300	-0.50015100
C	1.73451700	1.96696600	-1.60344000
H	1.67522600	2.96475300	-2.06435900
C	3.12852000	1.36579700	-1.84829500
H	3.33257600	1.30953800	-2.92477900
H	3.14197900	0.33734100	-1.46652400
C	4.23830300	2.17287000	-1.15095400
H	4.29055300	3.17202500	-1.60096800
H	3.95465700	2.30259600	-0.10265900
C	5.58005000	1.48150300	-1.25048300
C	6.42505600	1.68488700	-2.35455100
C	5.98425800	0.56705300	-0.26339400
C	7.63810000	0.99473900	-2.47011000
H	6.13029900	2.39024500	-3.12969400
C	7.19350300	-0.12856300	-0.37354000
H	5.34392400	0.39949900	0.59958300
C	8.02659200	0.08239000	-1.47983500

H	8.27997700	1.16875100	-3.33079100
H	7.48378100	-0.83405000	0.40173600
H	8.96793500	-0.45465100	-1.56817400
H	1.09256600	1.16826100	-3.49547200
H	-0.28020700	1.79348200	-2.57847000
H	1.04001100	-1.00062900	-2.48768200
C	-1.07508500	-0.81789000	-2.69041600
C	-1.15762600	-2.10058900	-3.27153000
C	-2.26514800	-0.06687700	-2.58777000
C	-2.37139600	-2.60544400	-3.74838800
H	-0.25579500	-2.70431500	-3.35436000
C	-3.47861100	-0.56917100	-3.05881100
H	-2.24232500	0.91451700	-2.12376900
C	-3.53875600	-1.83870000	-3.65081000
H	-2.40529200	-3.59709100	-4.19370500
H	-4.38156500	0.02476500	-2.94698100
H	-4.48571800	-2.22982400	-4.01448800
P	0.14670400	-1.13624900	0.95042800
C	-1.19104200	-2.36185900	0.51325900
C	-0.31802800	-0.37826500	2.59861300
C	1.69494900	-2.15129100	1.18016400
C	-1.18638500	-3.72129000	1.24379300
C	-2.58781200	-1.71244000	0.59283800
H	-0.99069600	-2.55515000	-0.54763200
C	-0.16534100	-1.30143400	3.82495400
C	0.37458900	0.97970600	2.85180100
H	-1.38371200	-0.15674700	2.46303400
C	2.05205600	-2.86874800	-0.14030700
C	2.88460400	-1.28902600	1.65236900
H	1.48424500	-2.90474800	1.94986300
C	-2.25341200	-4.65339600	0.64166200
H	-1.40528500	-3.57643500	2.30756900
H	-0.20592900	-4.20344000	1.18384100
C	-3.65486800	-2.64389600	-0.00120200
H	-2.84003800	-1.51212400	1.64238700
H	-2.59224300	-0.74887500	0.07656200
C	-0.72155000	-0.62209800	5.09000500
H	0.89491600	-1.53811200	3.97928900
H	-0.68054400	-2.25239600	3.66754600
C	-0.19968000	1.65428600	4.10712600
H	1.45257600	0.83718900	2.98522400
H	0.25883000	1.63212400	1.98503600
C	3.32831100	-3.71237600	0.00263800
H	2.20992100	-2.10904300	-0.91565600
H	1.22518300	-3.49924600	-0.48308100
C	4.16898600	-2.12535700	1.78024600
H	3.03807100	-0.47342200	0.93371100
H	2.66318300	-0.82197400	2.61549300
C	-3.65009500	-4.01552500	0.68890600
H	-2.25002500	-5.61033100	1.17774300
H	-1.98875400	-4.87261200	-0.40224100
H	-4.64016100	-2.17263600	0.08465600
H	-3.45966600	-2.77007000	-1.07168800
C	-0.06866700	0.74586300	5.33874200
H	-0.57276000	-1.27941100	5.95531200
H	-1.80631000	-0.49018400	4.97441300
H	0.31145800	2.60938000	4.27923700
H	-1.25946300	1.88902500	3.93580900
C	4.51015500	-2.85288200	0.47288800
H	3.56046400	-4.19019800	-0.95678100
H	3.15069300	-4.52045400	0.72582200
H	4.99933600	-1.47819400	2.08749500
H	4.03544300	-2.86430200	2.58262100
H	-4.38601000	-4.68009900	0.21969000
H	-3.95474200	-3.89591300	1.73850600
H	-0.51768000	1.22505900	6.21715800
H	0.99694300	0.60076500	5.56580000
H	5.40567600	-3.47190300	0.60531200
H	4.74956300	-2.11123500	-0.30070000
O	1.47054300	2.07756100	-0.21983800
B	-3.20252900	2.39723100	-0.08572400
C	-4.60049100	1.78312900	-0.44952900
C	-5.32206300	2.23733300	-1.57141900
C	-5.16003000	0.74348500	0.31761900
C	-6.55282800	1.67085900	-1.92150200
H	-4.90543900	3.03540800	-2.18146700
C	-6.38896600	0.16925400	-0.02531600
H	-4.61741400	0.37425800	1.18372300
C	-7.08786700	0.63109200	-1.14850900
H	-7.09152800	2.03099900	-2.79512000
H	-6.80043700	-0.63855300	0.57577700
H	-8.04126800	0.18368000	-1.42033900
O	-2.67068700	3.36392500	-0.91096800
H	-1.80060700	3.66587100	-0.55376400
O	-2.54265400	1.94059700	1.03347200
H	-1.67787900	2.40632300	1.11253200
C	0.09097200	4.59937600	1.46570500
C	-1.07925100	5.14683900	2.27096700
H	0.58720100	5.40636300	0.90886700
H	0.83541400	4.14702100	2.13469600
H	-0.73869300	5.92803000	2.95898200
H	-1.83569400	5.57709900	1.60582500

H	-1.54861000	4.35010200	2.85732500
O	-0.39107600	3.60565900	0.54913000
H	0.39549300	3.04172300	0.18508900

dist-2

Sum of electronic and thermal Free Energies= -3851.978858

C	-0.31917900	-0.66836800	-1.95907600
C	-0.57819200	-2.16882500	-2.22973400
Ni	-0.45350800	-0.51535400	-0.03392700
C	-1.64216400	-2.66499600	-1.25180500
H	-1.66752400	-3.76673500	-1.24074200
C	-3.04993100	-2.14639000	-1.57671300
H	-3.34357500	-2.47019900	-2.58408500
H	-3.02355800	-1.05041500	-1.58204600
C	-4.10241900	-2.60509800	-0.55160200
H	-4.21738500	-3.69432800	-0.61092500
H	-3.72071000	-2.37181700	0.44778500
C	-5.43504000	-1.92466400	-0.77326600
C	-6.43695900	-2.51464300	-1.56125300
C	-5.67407900	-0.64404500	-0.24401600
C	-7.64205900	-1.84658300	-1.81531100
H	-6.27196300	-3.50581400	-1.98020300
C	-6.87331400	0.03051500	-0.49649400
H	-4.91038200	-0.17445400	0.37189500
C	-7.86438400	-0.56903600	-1.28557300
H	-8.40633500	-2.32253100	-2.42559500
H	-7.03680000	1.02114300	-0.07809300
H	-8.79859500	-0.04849200	-1.48207900
H	-0.85276000	-2.32774400	-3.28403400
H	0.33544000	-2.74048200	-2.04187400
H	-1.16932500	-0.06948600	-2.30636100
C	0.94566700	-0.13896400	-2.54223500
C	0.94205800	0.99935500	-3.37292800
C	2.18457900	-0.76918600	-2.30318900
C	2.12250500	1.48089500	-3.94930400
H	0.00289100	1.50786600	-3.57728500
C	3.36624900	-0.29001100	-2.86834500
H	2.22138300	-1.63334500	-1.64801100
C	3.34102100	0.83761900	-3.70122500
H	2.09058100	2.36089100	-4.58774500
H	4.30720100	-0.78481700	-2.64240700
H	4.26129800	1.21710600	-4.13857800
P	-0.00333300	1.58437400	0.50597200
C	1.48399800	2.51885300	-0.10160800
C	0.14893500	1.51630400	2.38214900
C	-1.48463400	2.65651200	0.12960700
C	1.57239600	3.99132000	0.34727300
C	2.78924000	1.76639800	0.23354600
H	1.37333000	2.49464700	-1.19271100
C	-0.41414100	2.72102500	3.16397900
C	-0.43026000	0.18652200	2.92307700
H	1.23182000	1.48259400	2.55410400
C	-1.55727000	3.00773400	-1.37109800
C	-2.78622200	1.94638000	0.56530300
H	-1.38539300	3.58758700	0.70088000
C	2.78198300	4.68539000	-0.30255000
H	1.68471400	4.03477700	1.43756100
H	0.65573100	4.53608500	0.09805900
C	3.99892600	2.46630000	-0.40628300
H	2.93477600	1.73876100	1.32137500
H	2.72771800	0.72920400	-0.10560800
C	-0.16388600	2.56183500	4.67396900
H	-1.49386900	2.80515500	2.99682300
H	0.03172000	3.65486200	2.80959000
C	-0.20996200	0.04193000	4.43746500
H	-1.50307400	0.12491600	2.70087800
H	0.04790100	-0.66545300	2.42201400
C	-2.79803000	3.85942400	-1.68778700
H	-1.60631100	2.07873700	-1.95080800
H	-0.65515300	3.53690500	-1.69464300
C	-4.02230800	2.80543900	0.25712900
H	-2.85993300	0.99037000	0.02967300
H	-2.76427000	1.70236900	1.63148600
C	4.08829700	3.94113100	0.01167300
H	2.83983100	5.72498400	0.04226900
H	2.63386700	4.71863300	-1.39096700
H	4.91619600	1.93423800	-0.13232900
H	3.91094700	2.39819400	-1.49697200
C	-0.76179600	1.25088000	5.20609200
H	-0.58967600	3.41989500	5.20776100
H	0.91806800	2.57321900	4.86510700
H	-0.67640600	-0.88542100	4.78999900
H	0.86735800	-0.05140200	4.63085100
C	-4.09094500	3.16612900	-1.23286100
H	-2.83360300	4.06706100	-2.76397300
H	-2.70746000	4.82954300	-1.17983400
H	-4.92924900	2.27234500	0.56456200
H	-3.98000100	3.72578800	0.85597300
H	4.93273100	4.42780300	-0.49159400
H	4.28507800	4.00172700	1.09160300
H	-0.55317500	1.14438900	6.27726300

H	-1.85486900	1.28189900	5.09614800
H	-4.95735700	3.80831900	-1.43098000
H	-4.23588400	2.24690500	-1.81755200
O	-1.22861600	-2.19697500	0.03059200
B	3.12485300	-2.63467000	0.66898600
C	4.49410100	-2.21245800	0.02746500
C	5.10160600	-3.00327700	-0.96809600
C	5.13490000	-1.01564100	0.40138300
C	6.30109700	-2.61304400	-1.57420400
H	4.61998400	-3.92788300	-1.27750100
C	6.33724200	-0.62014900	-0.19476900
H	4.67729900	-0.38461900	1.15868600
C	6.92215500	-1.41768100	-1.18715100
H	6.74968000	-3.23269100	-2.34741500
H	6.81659600	0.30869400	0.10572400
H	7.85296700	-1.10881300	-1.65740900
O	2.55938600	-3.83226400	0.28490500
H	1.70836900	-3.97259200	0.75900300
O	2.52045700	-1.79395600	1.57582800
H	1.64453200	-2.17034500	1.82931800
C	-0.47765800	-3.70340900	2.90662500
C	0.48252600	-3.84605600	4.07867000
H	-1.02057300	-4.64302100	2.73572400
H	-1.21946600	-2.92009400	3.11195500
H	-0.06023500	-4.13699300	4.98434200
H	1.23679500	-4.61107400	3.86568000
H	0.99671100	-2.89924900	4.27451000
O	0.26578100	-3.35447500	1.72810900
H	-0.36864000	-2.99049200	1.01017300

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Sum of electronic and thermal Free Energies= -3696.954608

C	0.23299600	-0.31619200	-2.20678100
C	0.60740300	1.15820700	-2.51571100
Ni	0.53656900	0.37835300	-0.50015100
C	1.73451700	1.96696600	-1.60344000
H	1.67522600	2.96475300	-2.06435900
C	3.12852000	1.36579700	-1.84829500
H	3.33257600	1.30953800	-2.92477900
H	3.14197900	0.33734100	-1.46652400
C	4.23830300	2.17287000	-1.15095400
H	4.29055300	3.17202500	-1.60096800
H	3.95465700	2.30259600	-0.10265900
C	5.58005000	1.48150300	-1.25048300
C	6.42505600	1.68488700	-2.35455100
C	5.98425800	0.56705300	-0.26339400
C	7.63810000	0.99473900	-2.47011000
H	6.13029900	2.39024500	-3.12969400
C	7.19350300	-0.12856300	-0.37354000
H	5.34392400	0.39949900	0.59958300
C	8.02659200	0.08239000	-1.47983500
H	8.27997700	1.16875100	-3.33079100
H	7.48378100	-0.83405000	0.40173600
H	8.96793500	-0.45465100	-1.56817400
H	1.09256600	1.16826100	-3.49547200
H	-0.28020700	1.79348200	-2.57847000
H	1.04001100	-1.00062900	-2.48768200
C	-1.07508500	-0.81789000	-2.69041600
C	-1.15762600	-2.10058900	-3.27153000
C	-2.26514800	-0.06687700	-2.58777000
C	-2.37139600	-2.60544400	-3.74838800
H	-0.25579500	-2.70431500	-3.35436000
C	-3.47861100	-0.56917100	-3.05881100
H	-2.24232500	0.91451700	-2.12376900
C	-3.53875600	-1.83870000	-3.65081000
H	-2.40529200	-3.59709100	-4.19370500
H	-4.38156500	0.02476500	-2.94698100
H	-4.48571800	-2.22982400	-4.01448800
P	0.14670400	-1.13624900	0.95042800
C	-1.19104200	-2.36185900	0.51325900
C	-0.31802800	-0.37826500	2.59861300
C	1.69494900	-2.15129100	1.18016400
C	-1.18638500	-3.72129000	1.24379300
C	-2.58781200	-1.71244000	0.59283800
H	-0.99069600	-2.55515000	-0.54763200
C	-0.16534100	-1.30143400	3.82495400
C	0.37458900	0.97970600	2.85180100
H	-1.38371200	-0.15674700	2.46303400
C	2.05205600	-2.86874800	-0.14030700
C	2.88460400	-1.28902600	1.65236900
H	1.48424500	-2.90474800	1.94986300
C	-2.25341200	-4.65339600	0.64166200
H	-1.40528500	-3.57643500	2.30756900
H	-0.20592900	-4.20344000	1.18384100
C	-3.65486800	-2.64389600	-0.00120200
H	-2.84003800	-1.51212400	1.64238700
H	-2.59224300	-0.74887500	0.07656200
C	-0.72155000	-0.62209800	5.09000500
H	0.89491600	-1.53811200	3.97928900
H	-0.68054400	-2.25239600	3.66754600
C	-0.19968000	1.65428600	4.10712600

H	1.45257600	0.83718900	2.98522400
H	0.25883000	1.63212400	1.98503600
C	3.32831100	-3.71237600	0.00263800
H	2.20992100	-2.10904300	-0.91565600
H	1.22518300	-3.49924600	-0.48308100
C	4.16898600	-2.12535700	1.78024600
H	3.03807100	-0.47342200	0.93371100
H	2.66318300	-0.82197400	2.61549300
C	-3.65009500	-4.01552500	0.68890600
H	-2.25002500	-5.61033100	1.17774300
H	-1.98875400	-4.87261200	-0.40224100
H	-4.64016100	-2.17263600	0.08465600
H	-3.45966600	-2.77007000	-1.07168800
C	-0.06866700	0.74586300	5.33874200
H	-0.57276000	-1.27941100	5.95531200
H	-1.80631000	-0.49018400	4.97441300
H	0.31145800	2.60938000	4.27923700
H	-1.25946300	1.88902500	3.93580900
C	4.51015500	-2.85288200	0.47288800
H	3.56046400	-4.19019800	-0.95678100
H	3.15069300	-4.52045400	0.72582200
H	4.99933600	-1.47819400	2.08749500
H	4.03544300	-2.86430200	2.58262100
H	-4.38601000	-4.68009900	0.21969000
H	-3.95474200	-3.89591300	1.73850600
H	-0.51768000	1.22505900	6.21715800
H	0.99694300	0.60076500	5.56580000
H	5.40567600	-3.47190300	0.60531200
H	4.74956300	-2.11123500	-0.30070000
O	1.47054300	2.07756100	-0.21983800
B	-3.20252900	2.39723100	-0.08572400
C	-4.60049100	1.78312900	-0.44952900
C	-5.32206300	2.23733300	-1.57141900
C	-5.16003000	0.74348500	0.31761900
C	-6.55282800	1.67085900	-1.92150200
H	-4.90543900	3.03540800	-2.18146700
C	-6.38896600	0.16925400	-0.02531600
H	-4.61741400	0.37425800	1.18372300
C	-7.08786700	0.63109200	-1.14850900
H	-7.09152800	2.03099900	-2.79512000
H	-6.80043700	-0.63855300	0.57577700
H	-8.04126800	0.18368000	-1.42033900
O	-2.67068700	3.36392500	-0.91096800
H	-1.80060700	3.66587100	-0.55376400
O	-2.54265400	1.94059700	1.03347200
H	-1.67787900	2.40632300	1.11253200
C	0.09097200	4.59937600	1.46570500
C	-1.07925100	5.14683900	2.27096700
H	0.58720100	5.40636300	0.90886700
H	0.83541400	4.14702100	2.13469600
H	-0.73869300	5.92803000	2.95898200
H	-1.83569400	5.57709900	1.60582500
H	-1.54861000	4.35010200	2.85732500
O	-0.39107600	3.60565900	0.54913000
H	0.39549300	3.04172300	0.18508900

dist-TS2

Sum of electronic and thermal Free Energies= -3696.937293

Ni	0.25537100	-0.59133100	-0.00971700
C	2.08561400	-2.67082000	0.08113500
H	2.37230100	-3.69817100	-0.18409800
C	0.54519300	-2.50600700	0.05615000
H	0.13994800	-2.96346700	0.95861800
C	7.97499400	0.93906600	0.32383100
C	6.62367800	0.57788200	0.37639000
C	6.23785700	-0.73896100	0.68180100
C	7.24362100	-1.68729300	0.93096300
C	8.59772600	-1.33243900	0.87917100
C	8.96895800	-0.01648900	0.57496700
H	8.25260400	1.96450800	0.09066800
H	5.85758600	1.32647800	0.18083800
H	6.96435300	-2.71195500	1.17022100
H	9.36125100	-2.08084800	1.07882300
H	10.01930400	0.26216200	0.53717600
C	4.77572600	-1.12919500	0.69056700
C	4.27864300	-1.51989500	-0.71635500
H	4.16914900	-0.29272600	1.05324500
H	4.62184000	-1.96248000	1.38367700
C	2.76024000	-1.66008900	-0.83932000
H	4.59688500	-0.75117000	-1.43094700
H	4.75074400	-2.45821800	-1.03248400
H	2.52433400	-1.89431000	-1.88313700
O	2.12579100	-0.40705100	-0.48652300
C	-0.20452200	6.10513400	-0.91969600
C	0.56010900	4.96168300	-0.66136100
C	0.29805000	3.73949100	-1.31205800
C	-0.74930200	3.71321200	-2.25374800
C	-1.52126800	4.84985400	-2.52091000
C	-1.25349200	6.04991100	-1.84797400
H	0.00929200	7.03503700	-0.39685000
H	1.36562700	5.01089400	0.06766800

H	-0.96026900	2.78166300	-2.77150800
H	-2.33090400	4.80233500	-3.24635800
H	-1.85506700	6.93438300	-2.04608600
B	1.09049500	2.41165900	-0.97289800
O	2.14494300	2.54908600	-0.05516000
H	2.50613800	1.66834300	0.15310700
O	0.74509500	1.21845500	-1.50169000
H	1.72529300	0.30773900	-1.22825400
C	-0.14511200	-3.10283500	-1.13817700
C	-0.93703600	-4.25652200	-0.97571800
C	-0.06111000	-2.54837500	-2.43391800
C	-1.62062400	-4.83124300	-2.05273500
H	-1.03046900	-4.70058600	0.01309200
C	-0.74227000	-3.11780700	-3.51225300
H	0.49392700	-1.62791500	-2.59079200
C	-1.52798000	-4.26344300	-3.32891900
H	-2.23331700	-5.71559200	-1.89297200
H	-0.67669800	-2.65465900	-4.49398300
H	-2.06925900	-4.69817500	-4.16553400
H	2.42125500	-2.48834600	1.10675300
P	-1.79670600	-0.21742700	0.74973100
C	-1.58743800	1.58200300	1.23560300
C	-2.54842900	-1.03749700	2.26416900
C	-3.10802500	-0.21405200	-0.57661900
C	-2.87165200	2.36883400	1.55985200
C	-0.55216500	1.74207100	2.37246100
H	-1.14762800	2.02305600	0.33447800
C	-4.08917600	-0.94290000	2.34823500
C	-2.07303600	-2.49025900	2.46405200
H	-2.13850500	-0.45230500	3.09703400
C	-2.68564500	0.71065300	-1.73595700
C	-3.39439500	-1.63750700	-1.09563200
H	-4.02611300	0.18698400	-0.13056600
C	-2.54114800	3.85727000	1.77183000
H	-3.32820500	1.97096300	2.47469500
H	-3.61050700	2.26458800	0.75865200
C	-0.23766100	3.22562900	2.62661900
H	-0.94136100	1.29445200	3.29599600
H	0.37246600	1.20639000	2.12580700
C	-4.60712000	-1.53073400	3.67184100
H	-4.54230900	-1.50066100	1.52159300
H	-4.42290900	0.09341500	2.24898300
C	-2.62501700	-3.09284900	3.76670600
H	-2.38518300	-3.10591500	1.61079800
H	-0.98105600	-2.51280700	2.49159400
C	-3.72608900	0.70590800	-2.86717100
H	-1.70814600	0.39132200	-2.11721500
H	-2.55228400	1.73419600	-1.37650100
C	-4.45406600	-1.62328800	-2.20817600
H	-2.47292500	-2.06166700	-1.49595900
H	-3.71528500	-2.29693000	-0.28308100
C	-1.51000500	4.04303400	2.89543600
H	-3.46039700	4.40940900	2.00291400
H	-2.14235400	4.27353300	0.83689100
H	0.45624100	3.31236800	3.47182700
H	0.27745400	3.62839800	1.74877600
C	-4.15376300	-2.98657500	3.84833700
H	-5.70141900	-1.46348300	3.69625800
H	-4.23247700	-0.92671400	4.50991500
H	-2.30677800	-4.13916900	3.84834400
H	-2.18211200	-2.56004000	4.61979600
C	-4.02070500	-0.71516300	-3.36822700
H	-3.37026600	1.33798200	-3.69036100
H	-4.65759300	1.15981800	-2.50025300
H	-4.61833500	-2.64697900	-2.56561900
H	-5.41181400	-1.26782900	-1.80198200
H	-1.25817400	5.10485700	3.00621400
H	-1.95527900	3.72133200	3.84778100
H	-4.51192100	-3.38515500	4.80511100
H	-4.60460300	-3.60310900	3.05786900
H	-4.79340700	-0.69226400	-4.14649000
H	-3.11450100	-1.13290500	-3.82775200

dist-4

Sum of electronic and thermal Free Energies= -3696.950552

Ni	0.01603600	-0.60718000	-0.36481800
C	1.27175700	-3.01800400	0.19506300
H	1.32825400	-4.11514900	0.24327500
C	-0.17520000	-2.53481600	-0.06612000
H	-0.75736600	-2.82833500	0.80242100
C	7.37422200	0.04241300	0.33508000
C	6.01604200	-0.29615900	0.34286700
C	5.58733900	-1.54539700	0.82438500
C	6.55292100	-2.44844500	1.29764800
C	7.91337900	-2.11503900	1.29087000
C	8.32925400	-0.86740200	0.80860300
H	7.68714800	1.01562800	-0.03616000
H	5.27973500	0.41715500	-0.02440700
H	6.23748300	-3.41886900	1.67683700
H	8.64665300	-2.82610800	1.66437300
H	9.38447900	-0.60520500	0.80543600

C	4.12141100	-1.91783500	0.78331700	H	-1.94553400	0.20173800	3.08949400
C	3.72705900	-2.58287300	-0.55443300	C	-2.91383800	1.20380300	-1.63675100
H	3.51484400	-1.01814400	0.92861500	C	-3.60226900	-1.12502700	-0.93631400
H	3.88412300	-2.59124000	1.61274700	H	-4.05283400	0.70370300	0.12075100
C	2.23398500	-2.52157600	-0.87243900	C	-2.05442500	4.24398000	1.92975500
H	4.26206100	-2.09162600	-1.37617600	H	-2.81535300	2.38351300	2.71750800
H	4.04693800	-3.63124900	-0.56176900	H	-3.38083600	2.74880700	1.08746000
H	2.04233900	-3.04071200	-1.81665300	C	0.33663100	3.47325400	2.28072800
O	1.83786200	-1.11668900	-1.04930600	H	-0.33508200	1.57518000	3.06003600
C	2.22813600	5.74081900	-1.66582100	H	0.70736000	1.42767500	1.64607500
C	2.35012300	4.39959400	-1.27981800	C	-4.34974400	-0.70245100	3.99705800
C	1.29275900	3.48465200	-1.45338200	H	-4.45268700	-1.03931800	1.86648600
C	0.10351000	3.96745000	-2.03524600	H	-4.28227700	0.65182300	2.31553300
C	-0.03187800	5.30543700	-2.42401100	C	-2.35510700	-2.23927900	4.20509100
C	1.03339400	6.19827800	-2.23892500	H	-2.37524100	-2.63478300	2.08135900
H	3.05747000	6.42997500	-1.51894000	H	-0.85127300	-1.96611600	2.66971600
H	3.27771900	4.05567600	-0.82700400	C	-4.10368500	1.24855200	-2.61045400
H	-0.72395700	3.27540100	-2.17266300	H	-2.01239900	0.84895500	-2.14903200
H	-0.96229800	5.65530800	-2.86714500	H	-2.69287700	2.21850100	-1.29163500
H	0.93316500	7.23980800	-2.53687800	C	-4.80765900	-1.07083800	-1.88601600
B	1.37836900	1.97176400	-0.97563800	H	-2.75114300	-1.55117400	-1.47202900
O	2.58602200	1.61177000	-0.33710600	H	-3.80853900	-1.80017600	-0.09874000
H	2.52304300	0.66589500	-0.11906000	C	-0.80937600	4.33984900	2.82515000
O	0.35609900	1.13730500	-1.15709500	H	-2.87635600	4.83325500	2.35468500
H	2.10720600	-0.76462500	-1.91601300	H	-1.82755300	4.67562000	0.94503500
C	-0.83649200	-3.15499600	-1.27143600	H	1.19707600	3.50742300	2.96041900
C	-1.82238300	-4.14650200	-1.08818600	H	0.67498500	3.87768600	1.31863900
C	-0.56431600	-2.76078100	-2.59943800	C	-3.87090800	-2.10285700	4.40340900
C	-2.51467000	-4.70627800	-2.16680400	H	-5.43966600	-0.62670500	4.09310400
H	-2.06674800	-4.46656000	-0.07690600	H	-3.91872300	0.04242400	4.68053300
C	-1.25165000	-3.31582500	-3.68334200	H	-2.02604900	-3.25677500	4.44869400
H	0.15962700	-1.97391900	-2.78857200	H	-1.83591400	-1.56363400	4.89937100
C	-2.23494800	-4.29141000	-3.47521400	C	-4.51517600	-0.15383100	-3.08264500
H	-3.27819100	-5.45987800	-1.98576700	H	-3.84823900	1.88139200	-3.46942000
H	-1.02876800	-2.97477800	-4.69200000	H	-4.95905500	1.72510100	-2.11066900
H	-2.77754400	-4.71583600	-4.31646800	H	-5.04725600	-2.08421200	-2.23054000
H	1.58047200	-2.63317500	1.17245200	H	-5.68929900	-0.69912800	-1.34464400
P	-1.74993700	0.17417400	0.72123800	H	-0.48649400	5.38441000	2.91377600
C	-1.34996800	1.94363200	1.16449600	H	-1.06957100	4.00124900	3.83828900
C	-2.40911900	-0.48455200	2.37011600	H	-4.14033700	-2.31053600	5.44601200
C	-3.21104400	0.27929700	-0.43786600	H	-4.38506900	-2.85321000	3.78639700
C	-2.50417400	2.78287400	1.74394300	H	-5.38937000	-0.09191000	-3.74236700
C	-0.10851000	2.01521800	2.07923300	H	-3.69872900	-0.59073200	-3.67484500
H	-1.06066800	2.37282500	0.20327900				
C	-3.93883500	-0.35795800	2.55460400				
C	-1.93897500	-1.89594100	2.76495400	**dist-TS1'**			

Sum of electronic and thermal Free Energies= -3288.661992

C	-0.22372000	1.55872700	1.25032100
C	-1.76261300	1.42572600	1.14936200
Ni	-0.27935000	0.08553500	0.07784800
C	-2.51011000	0.78614800	-0.19667300
O	-1.99289300	-0.39633700	-0.73605500
H	-2.47910700	1.60302700	-0.94236100
C	-3.97501000	0.59792500	0.23574700
H	-4.35876500	1.51873600	0.69513800
H	-4.01596700	-0.19146500	0.99678800
C	-4.87023700	0.20476200	-0.95387500
H	-4.83347000	1.00202500	-1.70655700
H	-4.44809800	-0.69390100	-1.41360900
C	-6.30260500	-0.04181900	-0.53358800
C	-7.26349400	0.98189300	-0.58925400
C	-6.69523000	-1.29448400	-0.02953200
C	-8.57796000	0.76347700	-0.15709600
H	-6.98001300	1.95877700	-0.97729400
C	-8.00680700	-1.51960800	0.40462500
H	-5.96519900	-2.10063300	0.02008900
C	-8.95526700	-0.48958000	0.34270600
H	-9.30700200	1.56877600	-0.21305300
H	-8.29030300	-2.49757300	0.78723200
H	-9.97558700	-0.66264100	0.67646200
H	-2.11260300	0.83681700	2.00200400
H	-2.20926100	2.42331200	1.20679500
H	0.13063000	1.30473100	2.25140900
C	0.42713700	2.78604500	0.72775100
C	1.56707800	3.31681100	1.36677900
C	-0.04390000	3.44851900	-0.42661000
C	2.21237300	4.45459500	0.87419100
H	1.95156000	2.83169700	2.26065900
C	0.59703000	4.58725500	-0.91917100
H	-0.91376900	3.05920600	-0.94745500
C	1.73078000	5.09835700	-0.27279100
H	3.09128200	4.83942900	1.38628400
H	0.21688200	5.07374000	-1.81450400
H	2.23295300	5.98135600	-0.65991100
P	1.70753100	-0.67454700	-0.02068600
C	2.89675000	0.57095500	-0.71708200
C	1.78021000	-2.15053800	-1.19032000
C	2.42157900	-1.25740900	1.59911900
C	4.35141300	0.09464200	-0.89205300
C	2.35422600	1.16677400	-2.03429600
H	2.88264800	1.37783200	0.02595800
C	2.87502900	-3.19522300	-0.88289600
C	0.40565700	-2.83980700	-1.34778000
H	2.02167700	-1.68971200	-2.15738400
C	2.87870000	-0.10488500	2.51501800
C	1.38852500	-2.14738600	2.32438900
H	3.30314200	-1.86504600	1.36369900
C	5.24315900	1.25700800	-1.36329900
H	4.38717300	-0.70562600	-1.64177200
H	4.74398600	-0.32384400	0.04132300
C	3.24750200	2.32194700	-2.51459100
H	2.32374600	0.38981200	-2.80973800
H	1.32672700	1.51600800	-1.88886100
C	2.92306900	-4.27454500	-1.97880800
H	2.66156500	-3.68102400	0.07714500
H	3.85733700	-2.72310200	-0.78747100
C	0.45546300	-3.93232000	-2.42837700
H	0.10964200	-3.28851900	-0.39039700
H	-0.36394500	-2.10208400	-1.59343200
C	3.43943700	-0.64554400	3.84127400
H	2.02709300	0.54771400	2.73129200
H	3.63550100	0.51168300	2.01971500
C	1.94076300	-2.67780900	3.65697300
H	0.48167400	-1.55376200	2.50555000
H	1.08756600	-2.98674600	1.68871800
C	4.71143300	1.87937500	-2.66405700
H	6.27135900	0.90167100	-1.50253600
H	5.27508900	2.02487400	-0.57784800
H	2.86753300	2.71083300	-3.46724800
H	3.18229800	3.14278700	-1.78981100
C	1.56042700	-4.96166300	-2.14959900
H	3.69574200	-5.01265400	-1.73155100
H	3.22013200	-3.80999200	-2.92936300
H	-0.52060700	-4.42797000	-2.49576600
H	0.63851600	-3.46062300	-3.40417100
C	2.41575800	-1.53346600	4.56408700
H	3.73748800	0.19356500	4.48132000
H	4.34839400	-1.22852900	3.63785100
H	1.17159300	-3.27346200	4.16298800
H	2.78284500	-3.35386600	3.45332000
H	5.33675800	2.73082400	-2.95904000
H	4.78468300	1.13758100	-3.47198600
H	1.60619400	-5.70097700	-2.95844500
H	1.31772700	-5.51193800	-1.22954100
H	2.84664200	-1.93490600	5.48913000
H	1.55063400	-0.92142600	4.85561900

dist-2'

Sum of electronic and thermal Free Energies= -3288.687987

C	-0.32525100	1.52623600	0.98693600
C	-1.78962900	1.40261600	1.46552100
Ni	-0.22784700	0.04704200	-0.23902400
C	-2.68476400	1.20992200	0.23934000
O	-1.97738800	0.38511400	-0.67351300
H	-2.86543500	2.19908800	-0.22299700
C	-4.04739400	0.60357300	0.59039800
H	-4.54835000	1.22959800	1.34195800
H	-3.88242900	-0.38179100	1.04660100
C	-4.96178600	0.44788000	-0.63916900
H	-5.14506100	1.43861000	-1.07353400
H	-4.42318000	-0.13855600	-1.39091300
C	-6.27746300	-0.21742400	-0.30024100
C	-7.40397800	0.54241200	0.05867800
C	-6.39063500	-1.61886500	-0.28565400
C	-8.60785600	-0.07567000	0.41998900
H	-7.33773000	1.62910600	0.05279400
C	-7.59061500	-2.24353900	0.07481500
H	-5.52940100	-2.22510700	-0.56156300
C	-8.70613400	-1.47316500	0.43018000
H	-9.46853300	0.53203000	0.69042000
H	-7.65705300	-3.32927100	0.07560300
H	-9.64022200	-1.95561300	0.70793700
H	-1.86381700	0.50794800	2.09804400
H	-2.08857200	2.26755200	2.08010300
H	0.35042800	1.38006700	1.83653700
C	0.01250400	2.83414100	0.31733100
C	0.71032100	3.82054300	1.04280300
C	-0.34526000	3.13677800	-1.01255200
C	1.04787100	5.05143300	0.46857700
H	1.00320100	3.61638900	2.07123800
C	-0.00934800	4.36403400	-1.59169500
H	-0.87034000	2.38285100	-1.59236800
C	0.69243200	5.32929100	-0.85653600
H	1.59729700	5.78673700	1.05232100
H	-0.28712200	4.56469200	-2.62433500
H	0.96420500	6.27871500	-1.31172600
P	1.81586200	-0.76723600	-0.05918900
C	1.84305900	-2.01224100	-1.46441900
C	2.22799800	-1.72169300	1.49623100
C	3.22874100	0.39253900	-0.41740300
C	3.20226100	-2.65414800	-1.80486400
C	0.76459200	-3.10456900	-1.27669500
H	1.52998800	-1.40512000	-2.32547800
C	3.72445200	-1.99519400	1.75829700
C	1.55295500	-1.08865500	2.73321800
H	1.73840700	-2.69088500	1.33280400
C	2.97923600	1.09231900	-1.77261700
C	3.40284300	1.43426500	0.70773200
H	4.14957300	-0.20038500	-0.48628400
C	3.09116300	-3.53514100	-3.06192700
H	3.53210500	-3.27679600	-0.96469700
H	3.97014000	-1.88906400	-1.95842500
C	0.65448100	-3.98914100	-2.53037000
H	1.02413300	-3.73753300	-0.41870500
H	-0.21264500	-2.65943700	-1.05183800
C	3.90901200	-2.87182300	3.00968200
H	4.25601600	-1.04932000	1.91059200
H	4.18975700	-2.47924500	0.89520800
C	1.75406300	-1.96147600	3.98224000
H	1.97462500	-0.09264300	2.91826300
H	0.48491000	-0.94560100	2.53427400
C	4.07604500	2.12043500	-2.09385000
H	2.00476000	1.59729600	-1.73345300
H	2.92542600	0.35598900	-2.58171700
C	4.50331000	2.45379400	0.37266500
H	2.46170600	1.96949200	0.84714200
H	3.63470700	0.94482100	1.65796000
C	2.00875300	-4.61279100	-2.89959100
H	4.06240300	-3.99839100	-3.27370600
H	2.84744400	-2.89975400	-3.92469800
H	-0.09380000	-4.77301700	-2.36289400
H	0.29290300	-3.37838600	-3.36899200
C	3.24205900	-2.24184600	4.24164700
H	4.97882300	-3.02922600	3.19288200
H	3.46954600	-3.86187800	2.82448600
H	1.29950300	-1.47202200	4.85211100
H	1.22523000	-2.91467900	3.84212300
C	4.22988400	3.15126100	-0.96738600
H	3.84026100	2.62010000	-3.04134900
H	5.03066100	1.59565700	-2.24043500
H	4.57123100	3.19230300	1.18087800
H	5.47471300	1.94135600	0.32706200
H	1.91688100	-5.20107800	-3.82048700
H	2.31206100	-5.31059300	-2.10640600
H	3.35917200	-2.89682800	5.11342900
H	3.75061900	-1.29775200	4.48319600
H	5.03819400	3.85448600	-1.20297000
H	3.30601500	3.73900100	-0.88526100

H-TS1

Sum of electronic and thermal Free Energies= -3288.666206

Ni	-0.55845500	0.06592000	-1.85795800
C	1.08042000	-0.81956200	-2.20845800
O	1.22885700	-1.92822500	-2.72990900
C	-1.98813900	2.62776600	-1.25400200
C	-0.80465600	3.39094000	-1.36286200
C	-0.65701200	4.59451700	-0.67132600
C	-1.68135900	5.06703400	0.16153700
C	-2.85188400	4.31048900	0.29850200
C	-3.00193600	3.10828200	-0.40001100
H	0.01218400	3.02301400	-1.97970100
H	0.26741500	5.15938000	-0.76798700
H	-1.56154000	6.00048100	0.70556100
H	-3.65154200	4.65748300	0.94902400
H	-3.92199400	2.53848200	-0.28979400
C	2.31257200	-0.03591300	-1.73480900
H	2.49524700	0.74338100	-2.48721000
H	2.05012800	0.50184900	-0.81976300
C	3.57776300	-0.88746600	-1.51226900
H	3.30492400	-1.77906400	-0.93764100
H	3.95491800	-1.24199200	-2.47576000
C	4.63933000	-0.10451700	-0.77319500
C	5.67214600	0.55647200	-1.45742200
C	4.57755500	0.02396600	0.62636200
C	6.61832600	1.32431700	-0.76585000
H	5.73676900	0.46905500	-2.54051000
C	5.51908700	0.78921400	1.32256900
H	3.78441800	-0.48194100	1.17470300
C	6.54507400	1.44467900	0.62765700
H	7.41251100	1.82605000	-1.31400200
H	5.45508900	0.87267000	2.40511900
H	7.27942300	2.03877400	1.16618200
C	-1.57352300	1.15278800	-3.27029500
H	-2.04771800	0.45432800	-3.95802800
H	-1.04286100	1.96342500	-3.76423400
H	-0.04208300	0.30200500	-3.22630500
P	-0.90792700	-0.72581700	0.21146100
C	-0.84677300	0.64693500	1.48325800
C	-1.21020000	0.35294900	2.95732500
C	0.50370900	1.39062300	1.39348600
H	-1.60643500	1.33662400	1.09505300
C	-1.26790600	1.66495400	3.75883900
H	-0.46003900	-0.29003400	3.41948200
H	-2.16006100	-0.18142200	3.03722000
C	0.50172900	2.66684600	2.25157100
H	1.31803000	0.72952800	1.71928600
H	0.70268300	1.65903600	0.35121600
C	0.08342900	2.39394500	3.70346800
H	-1.54378600	1.44962800	4.79843800
H	-2.05343300	2.31420100	3.34723300
H	1.49552100	3.13060400	2.21906500
H	-0.19665600	3.38360800	1.80539400
H	0.03350700	3.33564000	4.26382900
H	0.84498200	1.77200600	4.19525700
C	0.37364800	-2.02949300	0.68509000
C	0.63896300	-2.30449600	2.17782700
C	0.11729400	-3.35764400	-0.06176300
H	1.29594600	-1.60188200	0.27554000
C	1.78695900	-3.31466600	2.36597200
H	-0.27212200	-2.68292300	2.66000000
H	0.91701700	-1.38211800	2.68926100
C	1.28182300	-4.34317300	0.12086800
H	-0.79557900	-3.82174200	0.33298400
H	-0.03618700	-3.17010000	-1.12584700
C	1.54559600	-4.62420400	1.60548000
H	1.92600400	-3.50999900	3.43631100
H	2.71988900	-2.85752100	2.00604000
H	1.05890900	-5.27488700	-0.41338300
H	2.18520200	-3.92216700	-0.34089200
H	2.40370900	-5.29696900	1.72432300
H	0.67512200	-5.13922100	2.03598100
C	-2.59008000	-1.55146900	0.38597100
C	-3.73718000	-0.58021200	0.75011600
C	-2.96072900	-2.28299600	-0.92867000
H	-2.50107200	-2.29212600	1.19290700
C	-5.07619700	-1.32489300	0.88772400
H	-3.83486400	0.17674900	-0.03346600
H	-3.53275100	-0.04003100	1.67506400
C	-4.30045100	-3.02689800	-0.80894000
H	-3.02142600	-1.53807600	-1.73321500
H	-2.18191600	-2.98547200	-1.22683100
C	-5.43729300	-2.08239600	-0.39702300
H	-5.86576300	-0.60810300	1.14435500
H	-5.00855800	-2.03479900	1.72391200
H	-4.53443400	-3.51489700	-1.76294800
H	-4.20116400	-3.82592600	-0.06081200
H	-6.37088000	-2.64187400	-0.26175500
H	-5.61436500	-1.35761000	-1.20420000
C	-2.18051400	1.37402600	-2.01073700
H	-3.10307600	0.83774600	-1.81022100

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Sum of electronic and thermal Free Energies= -3288.676182

Ni	-0.55124000	0.12307700	-1.73637700
C	1.13377400	-0.69213000	-2.11439700
O	1.31174500	-1.71417000	-2.79089200
C	-2.02898700	2.59370200	-1.24774900
C	-0.87905300	3.41892000	-1.29290500
C	-0.80739100	4.60753700	-0.56374000
C	-1.87737900	5.01357600	0.24632500
C	-3.01859100	4.20286600	0.31699100
C	-3.09310900	3.01691800	-0.41853700
H	-0.02554800	3.11267200	-1.89460900
H	0.09348600	5.21525000	-0.61651400
H	-1.81825200	5.93637000	0.81787100
H	-3.85693200	4.49844200	0.94440700
H	-3.99297100	2.40851300	-0.35742900
C	2.36323800	0.06418900	-1.58380200
H	2.48187800	0.95156200	-2.22257700
H	2.12424700	0.45671600	-0.59096800
C	3.66759700	-0.75440900	-1.53878100
H	3.46041400	-1.70778900	-1.03982600
H	3.98151900	-0.99711000	-2.55797400
C	4.75891400	-0.01293300	-0.80146800
C	5.72150200	0.74517700	-1.48820000
C	4.79890200	-0.02390900	0.60484000
C	6.69746800	1.47137000	-0.79329700
H	5.70750800	0.76621400	-2.57646700
C	5.77093500	0.69921400	1.30453500
H	4.06121100	-0.60584500	1.15535600
C	6.72592800	1.45198100	0.60698900
H	7.43598300	2.04928900	-1.34430100
H	5.78634600	0.67398600	2.39181900
H	7.48387600	2.01311500	1.14817800
C	-1.42314300	1.23730400	-3.33390700
H	-1.97508300	0.64492800	-4.06571300
H	-1.11439500	2.19176200	-3.76808100
H	-0.37755000	0.69608900	-3.30871900
P	-0.91208000	-0.75140100	0.22535200
C	-0.94728200	0.59679500	1.51902900
C	-1.37502300	0.26283500	2.96680500
C	0.38575900	1.37682400	1.51040600
H	-1.70518300	1.27203200	1.10282600
C	-1.51396100	1.55836400	3.78479000
H	-0.62830100	-0.36582700	3.45451400
H	-2.31090900	-0.30126700	2.98957100
C	0.29743600	2.63996800	2.38309000
H	1.19848300	0.73305400	1.87343600
H	0.63385400	1.66380400	0.48343300
C	-0.18646600	2.33194800	3.80762100
H	-1.83298800	1.31669100	4.80605200
H	-2.29937000	2.18858300	3.34468200
H	1.27597000	3.13541500	2.40981400
H	-0.39924500	3.34035400	1.90891300
H	-0.29675200	3.26307000	4.37689900
H	0.56931100	1.72830800	4.33016700
C	0.39434000	-2.02112700	0.71063300
C	0.57485400	-2.35309200	2.20487200
C	0.23978100	-3.32233400	-0.10793200
H	1.32088300	-1.53712500	0.37975400
C	1.74973500	-3.32590000	2.42244100
H	-0.34869400	-2.78844200	2.60892300
H	0.78030500	-1.44509400	2.77301800
C	1.43283200	-4.26686200	0.10470500
H	-0.67317200	-3.84097100	0.21121400
H	0.13912000	-3.09271900	-1.17046400
C	1.61354900	-4.60636200	1.58970000
H	1.82799000	-3.56643400	3.48966800
H	2.68349700	-2.81571100	2.14560600
H	1.28500100	-5.18046300	-0.48388100
H	2.34527300	-3.78868500	-0.27722900
H	2.49051900	-5.24895800	1.73442300
H	0.74047100	-5.17579800	1.93845800
C	-2.57188200	-1.62891900	0.29051200
C	-3.75882900	-0.68920600	0.60369500
C	-2.85289500	-2.34573200	-1.05407800
H	-2.50217000	-2.38013000	1.08985600
C	-5.08655200	-1.46425700	0.65518800
H	-3.82317700	0.07500700	-0.17587600
H	-3.61912400	-0.15951600	1.54668700
C	-4.17917400	-3.12201500	-1.01911400
H	-2.88893300	-1.58496500	-1.84509700
H	-2.04308800	-3.02494600	-1.32188900
C	-5.35872500	-2.20969800	-0.65808800
H	-5.90456000	-0.76785500	0.87652800
H	-5.05116500	-2.18501600	1.48409500
H	-4.34803400	-3.59980800	-1.99184600
H	-4.10301000	-3.93053600	-0.27850300
H	-6.28523800	-2.79180200	-0.58295800
H	-5.50714100	-1.47678500	-1.46364200
C	-2.11092200	1.33177300	-2.00471500

H	-3.09728500	0.87234400	-1.99093700

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Sum of electronic and thermal Free Energies= -3288.699761

Ni	0.06712000	0.88844100	-0.40061400
H	1.52255600	2.78304800	0.63352600
P	-1.24902200	-0.90188900	-0.01164500
C	-2.64376900	-1.14846800	-1.25406100
C	-3.92160000	-1.88923200	-0.80441200
C	-2.12501500	-1.75779200	-2.57437000
H	-2.94203900	-0.11470500	-1.47446300
C	-4.99864000	-1.82398400	-1.90352200
H	-3.69203200	-2.93876400	-0.58753700
H	-4.32744600	-1.45830800	0.11507700
C	-3.19343600	-1.67879200	-3.67703200
H	-1.87121700	-2.81301200	-2.41027200
H	-1.20668500	-1.25879200	-2.89893200
C	-4.48943300	-2.37951000	-3.24162600
H	-5.89006200	-2.37366500	-1.57739500
H	-5.30498000	-0.77707200	-2.03852000
H	-2.80789600	-2.12901400	-4.59985500
H	-3.40368800	-0.62386400	-3.90187400
H	-5.25973300	-2.27234500	-4.01498100
H	-4.29566600	-3.45611800	-3.13410700
C	-0.29635000	-2.51457000	0.00853300
C	-1.02231300	-3.72549500	0.62889400
C	1.11671700	-2.33561300	0.60704200
H	-0.15002900	-2.72660000	-1.05875200
C	-0.17676000	-5.00545900	0.49994600
H	-1.22432400	-3.53526600	1.68978600
H	-1.99226200	-3.88015000	0.14753200
C	1.94350800	-3.62317600	0.46915700
H	1.04826600	-2.06105200	1.66437800
H	1.61815800	-1.49936700	0.11228100
C	1.22413400	-4.82366400	1.10248900
H	-0.69678500	-5.84095000	0.98451200
H	-0.08140400	-5.26558100	-0.56369300
H	2.92831100	-3.48196900	0.93221000
H	2.12130500	-3.82805100	-0.59618900
H	1.81575500	-5.73772800	0.96972600
H	1.13283600	-4.65860900	2.18546300
C	-2.15057200	-0.73038400	1.61763500
C	-2.92717800	0.60621100	1.60026400
C	-1.22970000	-0.78899300	2.85366700
H	-2.86771000	-1.55738300	1.69227500
C	-3.72288600	0.82121500	2.89680000
H	-2.20640900	1.42446500	1.47257600
H	-3.60589700	0.65562900	0.74125600
C	-2.03306000	-0.58245500	4.14964500
H	-0.45969400	-0.01765400	2.76521000
H	-0.71349200	-1.75213300	2.90125100
C	-2.81119400	0.74126000	4.12961200
H	-4.23259500	1.79190700	2.85875300
H	-4.50611100	0.05370600	2.97241600
H	-1.35322900	-0.61153500	5.01024000
H	-2.73965800	-1.41522400	4.27651700
H	-3.40045300	0.85284100	5.04813600
H	-2.09868100	1.57776900	4.10433400
C	0.11661900	2.44312700	-1.71087000
C	-0.43345400	1.28038900	-2.28418900
H	-1.50237600	1.19553500	-2.46540400
H	0.18360600	0.70241500	-2.97223200
C	7.50162100	0.61864200	-0.74217000
C	7.54887100	-0.76188300	-0.97365200
C	6.46538500	-1.56303500	-0.58709700
C	5.34747900	-0.98468000	0.02391700
C	5.28810100	0.40002000	0.26304400
C	6.37925100	1.19184800	-0.12988200
H	8.33848800	1.24836100	-1.03551100
H	8.41995200	-1.20902700	-1.44646400
H	6.49364900	-2.63666000	-0.75895300
H	4.51030100	-1.61377200	0.32182400
H	6.35134400	2.26564000	0.04656100
C	4.04965700	1.01339800	0.87697800
H	4.29569300	1.96123600	1.36933900
H	3.64113300	0.34504200	1.64250500
C	2.94283600	1.25533400	-0.17849800
H	2.77218800	0.32085900	-0.72529600
H	3.27292500	2.00465700	-0.90697500
C	1.64226400	1.70022000	0.47050400
O	1.02723700	0.89115900	1.28848200
H	1.13403700	2.71803100	-1.98186600
C	-0.67394800	3.52657000	-1.08718100
C	-0.05128700	4.75136100	-0.77103000
C	-2.03632600	3.37320600	-0.74796700
C	-0.75808000	5.78378400	-0.14596000
H	0.99933700	4.89186900	-1.01810300
C	-2.74293400	4.40263500	-0.12371600
H	-2.53844400	2.43277800	-0.95369800
C	-2.10967400	5.61632100	0.18200300
H	-0.25368100	6.71911100	0.08577800

H	-3.78954200	4.25583000	0.13370600
H	-2.66054800	6.41621600	0.67053200

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Sum of electronic and thermal Free Energies= -3851.937369

C	0.25921300	1.20242400	-1.47464500
C	0.86844200	2.25197000	-0.54613500
Ni	0.35060800	0.20284600	0.08202700
C	1.84250500	1.68483200	0.81963700
H	1.96209900	2.66861400	1.29411200
C	3.19831200	1.13902000	0.34890400
H	3.70779300	1.86665700	-0.28706000
H	3.03521300	0.24185700	-0.26168100
C	4.11251700	0.77301300	1.53370300
H	4.35073500	1.68369800	2.09697000
H	3.56038600	0.10934700	2.20466900
C	5.38117000	0.10245500	1.05526200
C	6.51442000	0.85335200	0.70055200
C	5.42799200	-1.29194800	0.88844900
C	7.66176200	0.23002800	0.19415500
H	6.49707900	1.93515600	0.82136500
C	6.56951700	-1.92137700	0.37980200
H	4.56035400	-1.88899100	1.16008400
C	7.69310300	-1.16130800	0.02955800
H	8.53026300	0.82847200	-0.07156900
H	6.58147500	-3.00197400	0.25659000
H	8.58280200	-1.64678300	-0.36423700
H	0.05329000	2.77103800	-0.03296100
H	0.88724700	0.87210000	-2.30476000
P	-0.59265500	-1.62463600	-0.43741600
C	-1.79376200	-1.49105900	-1.85120700
C	-1.52492200	-2.38140600	0.99984900
C	0.71738200	-2.83803800	-0.97452700
C	-2.35932400	-2.80859200	-2.41565900
C	-2.93869700	-0.52033000	-1.50402600
H	-1.19119900	-1.01415200	-2.63517700
C	-1.67217400	-3.91791400	0.97135300
C	-0.96324600	-1.91843200	2.36278800
H	-2.52551500	-1.94016600	0.90644100
C	1.37602500	-2.37699700	-2.29249100
C	1.78624500	-3.00977900	0.12764600
H	0.22828600	-3.80568600	-1.14369900
C	-3.23085200	-2.53028400	-3.65410300
H	-2.97713000	-3.29895700	-1.65411800
H	-1.55493100	-3.50534700	-2.67561500
C	-3.81145100	-0.23584000	-2.73470800
H	-3.56970500	-0.95190600	-0.71876700
H	-2.53715200	0.41233400	-1.09889100
C	-2.57523400	-4.39423700	2.12355900
H	-0.68601200	-4.38583700	1.07744700
H	-2.08048400	-4.25991300	0.01654100
C	-1.86422200	-2.39508900	3.51221200
H	0.04834400	-2.31837400	2.50486800
H	-0.86821800	-0.83016800	2.38282600
C	2.49853700	-3.33338200	-2.72755400
H	1.79201900	-1.37156900	-2.14573700
H	0.63181300	-2.29964600	-3.09181500
C	2.90522600	-3.96551900	-0.31591300
H	2.21353700	-2.02580300	0.36024200
H	1.33424700	-3.37900400	1.05255200
C	-4.36086500	-1.53759400	-3.33752700
H	-3.64498400	-3.47293400	-4.03189900
H	-2.59742300	-2.11907200	-4.45238400
H	-4.63074800	0.43288500	-2.45264300
H	-3.20954000	0.29142500	-3.48836800
C	-2.05018400	-3.91990600	3.48723200
H	-2.65006700	-5.48826000	2.10293400
H	-3.59033900	-4.00337100	1.96777700
H	-1.43704900	-2.07810400	4.47147700
H	-2.84261300	-1.90396200	3.42208100
C	3.55448600	-3.49969200	-1.62596900
H	2.96106800	-2.95760300	-3.64811100
H	2.06450300	-4.31402600	-2.96747400
H	3.65698000	-4.04528300	0.47851800
H	2.48600200	-4.97193000	-0.45350400
H	-4.94125200	-1.32330800	-4.24314300
H	-5.05369100	-1.99855500	-2.61921600
H	-2.73329300	-4.23396000	4.28574600
H	-1.08377700	-4.40369200	3.68776100
H	4.32756200	-4.21038300	-1.94189400
H	4.05781000	-2.53857200	-1.45584500
O	1.22526900	0.79866400	1.71582400
B	-3.41821300	1.76839300	1.17673100
C	-4.71495900	1.76840000	0.29053400
C	-4.95520900	2.79056200	-0.64813300
C	-5.66160900	0.72988400	0.39036600
C	-6.09632100	2.77912300	-1.45894400
H	-4.23419300	3.59868200	-0.74791700
C	-6.80348800	0.70741700	-0.41757900
H	-5.49126700	-0.07486000	1.10173000
C	-7.02370400	1.73497700	-1.34519400

H	-6.26141900	3.57562000	-2.18108000
H	-7.51825800	-0.10791800	-0.33065500
H	-7.90832800	1.71904700	-1.97776700
O	-2.50250900	2.78629200	1.02134000
H	-1.75935900	2.65749900	1.65892200
O	-3.23477700	0.74726300	2.08331600
H	-2.38233400	0.87362900	2.55912300
C	-0.51327900	2.32782100	4.21515200
C	-1.80126000	2.85336400	4.83289700
H	0.22560900	3.13533400	4.12061700
H	-0.07596900	1.54342600	4.84752900
H	-1.60545400	3.27719600	5.82345700
H	-2.23970200	3.63422300	4.20239300
H	-2.53389800	2.04642100	4.94041200
O	-0.80661500	1.78810000	2.91647900
H	0.04375700	1.41273100	2.48163200
H	-0.74358100	1.45705800	-1.82413900
C	1.73187700	3.30489700	-1.21583300
C	1.72138600	4.61083100	-0.69596500
C	2.56383000	3.03705100	-2.31686200
C	2.51722100	5.61905100	-1.25219100
H	1.07961700	4.84306800	0.15185700
C	3.36235700	4.04052100	-2.87446800
H	2.60497900	2.03745000	-2.73887300
C	3.34407600	5.33806700	-2.34602800
H	2.48717500	6.62214800	-0.83328700
H	4.00045600	3.80798400	-3.72383800
H	3.96228300	6.11827900	-2.78308300

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Sum of electronic and thermal Free Energies= -3851.974237

C	-0.63160100	1.21512600	0.99965500
C	-1.49440400	2.39705700	0.50431100
Ni	-0.14678700	0.22579600	-0.56043700
C	-2.27365300	1.89989400	-0.73526200
H	-2.71769600	2.76140600	-1.26074800
C	-3.38575100	0.88555000	-0.44317000
H	-4.14071100	1.33113100	0.21395500
H	-2.95165400	0.03062200	0.08965200
C	-4.05474200	0.37963500	-1.73429200
H	-4.57712700	1.21741800	-2.21433600
H	-3.26950000	0.05252800	-2.42154400
C	-5.02349500	-0.75315200	-1.47452800
C	-6.27976200	-0.50710300	-0.89197800
C	-4.67595700	-2.08231400	-1.76413800
C	-7.16038800	-1.55614900	-0.60622700
H	-6.56890400	0.51686300	-0.66128900
C	-5.55278300	-3.13712300	-1.48173100
H	-3.70693200	-2.29487500	-2.21107300
C	-6.79906800	-2.87882100	-0.89990400
H	-8.12806500	-1.34397900	-0.15707400
H	-5.25980200	-4.15936000	-1.70971000
H	-7.48138100	-3.69591600	-0.67813200
H	-0.80230900	3.14489400	0.10123900
H	-1.18778400	0.54012000	1.65712300
P	0.93122400	-1.39166800	0.47231400
C	1.76193700	-0.96133300	2.07723500
C	2.23332900	-2.17668100	-0.62927100
C	-0.30074600	-2.73792600	0.88569600
C	2.39553800	-2.13604500	2.84787300
C	2.78853800	0.17180700	1.88735600
H	0.94101200	-0.55709200	2.68401400
C	2.44910000	-3.69183100	-0.42826400
C	1.95526900	-1.84197500	-2.11468700
H	3.16121300	-1.66070300	-0.34951900
C	-1.22991000	-2.34350000	2.05297600
C	-1.14464300	-3.09379000	-0.35935600
H	0.26643700	-3.62566900	1.18991400
C	2.93458100	-1.66050400	4.20907000
H	3.22650900	-2.54768400	2.26191400
H	1.67459700	-2.94732100	2.99619800
C	3.31447200	0.65628200	3.24687800
H	3.63377700	-0.18555400	1.28826100
H	2.34682100	1.00175600	1.32968700
C	3.55997500	-4.21999300	-1.35131200
H	1.52495900	-4.23424400	-0.65938000
H	2.69244100	-3.91499900	0.61452400
C	3.03305400	-2.42347500	-3.04580600
H	0.97602200	-2.24302200	-2.40745100
H	1.90948600	-0.75454000	-2.24531200
C	-2.23299500	-3.46629300	2.36575700
H	-1.78595600	-1.43861100	1.78113000
H	-0.65264200	-2.10800700	2.95255800
C	-2.15885900	-4.20720000	-0.05178400
H	-1.68027800	-2.19347400	-0.69120800
H	-0.50437700	-3.40134300	-1.19192600
C	3.93001200	-0.50057400	4.04840900
H	3.40768700	-2.50041500	4.73207800
H	2.09114400	-1.33269800	4.83256300
H	4.05487000	1.44787500	3.08998300
H	2.48601900	1.09829900	3.81825200

C	3.23835800	-3.92818500	-2.82378500
H	3.68657600	-5.29757100	-1.19171000
H	4.51363700	-3.74366100	-1.08391000
H	2.76337700	-2.21942600	-4.08887500
H	3.98507400	-1.90987700	-2.86092000
C	-3.06475700	-3.83286500	1.12903700
H	-2.88802500	-3.15177200	3.18718000
H	-1.68510000	-4.35179100	2.71699400
H	-2.76172900	-4.41019200	-0.94439900
H	-1.61537300	-5.13343200	0.18174000
H	4.26340500	-0.14898000	5.03235300
H	4.82378600	-0.86340900	3.52127100
H	4.04160600	-4.29959900	-3.47144100
H	2.32447800	-4.46901800	-3.10746400
H	-3.74958200	-4.65805700	1.35888500
H	-3.68803900	-2.97592600	0.84281200
O	-1.27760000	1.30984100	-1.57600700
B	2.92943900	2.26139400	-1.46183900
C	4.25204000	1.72960700	-0.80465100
C	4.83215300	2.36443300	0.30982000
C	4.85944200	0.55315900	-1.28261500
C	5.96795700	1.83734800	0.93381100
H	4.37314700	3.26739800	0.70557300
C	5.98650500	0.00910500	-0.65798800
H	4.42723900	0.05392700	-2.14424800
C	6.54275600	0.65162600	0.45650200
H	6.39639200	2.33707400	1.79971500
H	6.42687400	-0.91259500	-1.03223500
H	7.41599900	0.23137000	0.95033000
O	2.24838100	3.29377300	-0.85429200
H	1.42483700	3.49041400	-1.35994300
O	2.48904900	1.66738500	-2.62451700
H	1.63752500	2.08104900	-2.90591400
C	-0.51174800	3.93609600	-3.57370900
C	0.47466700	4.93295900	-4.16514300
H	-1.32872700	4.46288100	-3.06106200
H	-0.95723500	3.31963800	-4.36680400
H	-0.02667300	5.58911500	-4.88470000
H	0.91187800	5.55380700	-3.37573000
H	1.28673700	4.40886400	-4.68054600
O	0.17861500	3.09543600	-2.63901100
H	-0.46017000	2.39483900	-2.22931500
H	0.25141500	1.56629500	1.54536600
C	-2.32781200	3.08235300	1.57305800
C	-2.40081700	4.48635300	1.60466600
C	-3.06894300	2.36479700	2.53026700
C	-3.18640800	5.15447500	2.55164800
H	-1.83314800	5.06394400	0.87712900
C	-3.85515900	3.02554100	3.48053200
H	-3.03858300	1.27887400	2.53591100
C	-3.91890100	4.42506500	3.49637000
H	-3.22363000	6.24151600	2.55385300
H	-4.41894700	2.44748800	4.20933000
H	-4.52827000	4.93909700	4.23582300

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Sum of electronic and thermal Free Energies= -3696.9335

Ni	-0.30231700	-0.54335200	0.23681400
C	1.34056500	-1.93468100	0.36034100
H	1.87332200	-1.93244900	1.31325900
C	-0.04996000	-2.43031100	0.57715400
H	-0.24824200	-2.68036400	1.62064600
C	8.17893800	-1.42864600	-0.34406100
C	6.82826800	-1.26288600	-0.67536600
C	5.82723500	-1.35694700	0.30549000
C	6.21305300	-1.62179400	1.63051000
C	7.56136100	-1.78793900	1.96822400
C	8.55080200	-1.69258500	0.98039500
H	8.93954100	-1.34835500	-1.11728400
H	6.54807500	-1.05512200	-1.70658600
H	5.45051400	-1.69550400	2.40411700
H	7.84038500	-1.98824000	3.00014300
H	9.59891400	-1.81881800	1.24067300
C	4.36619800	-1.22181700	-0.06292900
C	3.71427500	-2.58844000	-0.34601600
H	4.26177100	-0.59492700	-0.95135300
H	3.83012000	-0.71543100	0.74717500
C	2.23725000	-2.51264700	-0.75767100
H	4.27003400	-3.09007800	-1.14880800
H	3.79704500	-3.23466000	0.53648500
H	1.88814700	-3.53147400	-0.96966600
O	2.06001900	-1.69937900	-1.93313400
C	-6.79409900	-1.62159800	1.84082700
C	-5.42333800	-1.46689700	2.08706700
C	-4.52132300	-1.15039100	1.05193300
C	-5.04779100	-0.99557700	-0.24649500
C	-6.41485900	-1.14783200	-0.50512100
C	-7.29408000	-1.46182000	0.54132700
H	-7.47190300	-1.86562100	2.65647300
H	-5.04461000	-1.59359800	3.09915100
H	-4.36530000	-0.75610000	-1.05849200

H	-6.79722900	-1.02477300	-1.51655900
H	-8.35756000	-1.58155000	0.34570200
B	-2.96477300	-0.97446200	1.29859200
O	-2.52041300	-1.25132500	2.60644400
H	-1.56054600	-1.10002000	2.63330500
O	-2.17196200	-0.56712800	0.30866800
H	2.54564300	-2.11835500	-2.66313000
C	-0.84001800	-3.26277200	-0.35004400
C	-1.80689200	-4.13968800	0.18806900
C	-0.75611000	-3.16469200	-1.75721200
C	-2.64900700	-4.88981600	-0.63608300
H	-1.90669900	-4.21952300	1.26858600
C	-1.59408900	-3.91975000	-2.58129200
H	-0.04672200	-2.47282500	-2.19929500
C	-2.54655300	-4.78798300	-2.02997000
H	-3.38830900	-5.55199000	-0.19090800
H	-1.51170700	-3.82171300	-3.66179700
H	-3.20146500	-5.36916800	-2.67459200
H	1.34274200	-0.77490900	0.11848700
P	-0.23005800	1.69498200	-0.14718200
C	-1.74482900	2.14232200	-1.12551500
C	-1.97069700	3.64046700	-1.39407700
C	-1.79157200	1.32682500	-2.43522300
H	-2.55749500	1.76234100	-0.49688400
C	-3.30442500	3.86489600	-2.12881000
H	-1.15529900	4.03219600	-2.01567100
H	-1.95918800	4.20964800	-0.45723800
C	-3.11971400	1.56033200	-3.17416700
H	-0.96086200	1.61872500	-3.09267300
H	-1.66727600	0.26369100	-2.20398600
C	-3.36817200	3.05455600	-3.43310100
H	-3.43961000	4.93346100	-2.33665200
H	-4.13118100	3.56129600	-1.47155800
H	-3.12371400	1.00313700	-4.11903600
H	-3.94046900	1.15765400	-2.56474200
H	-4.33929900	3.19916800	-3.92215000
H	-2.60413000	3.43192500	-4.12770100
C	1.19677500	2.51042300	-1.05994100
C	1.52141900	3.96070800	-0.64149600
C	2.46850400	1.63994100	-1.02968300
H	0.85028600	2.53676000	-2.10230600
C	2.62708000	4.55625900	-1.53042500
H	1.86653300	3.97508400	0.39968700
H	0.62937000	4.59246400	-0.68738000
C	3.58644200	2.24388300	-1.89518200
H	2.82459300	1.54402600	0.00489700
H	2.23703500	0.63113700	-1.37896700
C	3.89719600	3.69385500	-1.49726500
H	2.85029000	5.57896000	-1.20273100
H	2.26075800	4.62696700	-2.56418500
H	4.48947400	1.62583200	-1.81850200
H	3.27412000	2.21702600	-2.94874900
H	4.66216500	4.11593000	-2.16031300
H	4.31504900	3.70776400	-0.48064900
C	-0.37321400	2.57782500	1.49214600
C	-1.75131000	2.36237000	2.15021600
C	0.75203700	2.07623400	2.42514800
H	-0.24072800	3.65322200	1.32603600
C	-1.81761200	3.02386300	3.53653500
H	-1.94086900	1.28911600	2.24802800
H	-2.54693800	2.76641200	1.51577600
C	0.68079400	2.73707300	3.81027500
H	0.65279100	0.98649400	2.53500900
H	1.73612000	2.25526800	1.97788800
C	-0.69525500	2.52390200	4.45760900
H	-2.79769800	2.82743900	3.98808700
H	-1.73360200	4.11390200	3.42268400
H	1.47386400	2.33503000	4.45247700
H	0.87176400	3.81436200	3.70654500
H	-0.74312700	3.03219800	5.42827800
H	-0.83988700	1.45169000	4.65238600

dist-TS3

Sum of electronic and thermal Free Energies= -3696.923523

Ni	-0.16490000	-0.48703200	0.25419900
C	1.20573900	-2.07855000	0.34645300
H	1.78746300	-1.96823300	1.25992200
C	-0.12211800	-2.50426600	0.56646300
H	-0.40475600	-2.63277600	1.61063000
C	8.05033800	-1.73648800	-0.29099600
C	6.72186900	-1.49071300	-0.66033200
C	5.68499400	-1.55841000	0.28483100
C	6.01227100	-1.87972700	1.61317900
C	7.33810800	-2.12560600	1.98900800
C	8.36368800	-2.05527900	1.03655000
H	8.83959700	-1.67521800	-1.03676900
H	6.48737600	-1.23966000	-1.69336400
H	5.22134200	-1.93387800	2.35945300
H	7.57175800	-2.36801500	3.02318300
H	9.39465200	-2.24306600	1.32653600
C	4.24617300	-1.33223600	-0.12422900

C	3.53708700	-2.65064000	-0.48924300
H	4.20513500	-0.66194800	-0.98570500
H	3.70791600	-0.83265800	0.68804400
C	2.05464700	-2.49443500	-0.86220500
H	4.06132000	-3.11498300	-1.33423900
H	3.61103000	-3.35897400	0.34515100
H	1.68247500	-3.47825200	-1.18081900
O	1.87810500	-1.56750900	-1.95131800
C	-6.68785100	-1.60310800	1.90699100
C	-5.32428100	-1.39602200	2.15560400
C	-4.42053800	-1.11143400	1.11285200
C	-4.93875400	-1.04316200	-0.19638100
C	-6.29800500	-1.24963800	-0.45807400
C	-7.17894700	-1.53063500	0.59639600
H	-7.36667500	-1.82106600	2.72921100
H	-4.95239100	-1.45725300	3.17636200
H	-4.25520200	-0.83185900	-1.01532500
H	-6.67304100	-1.19503100	-1.47830000
H	-8.23645600	-1.69234000	0.39840400
B	-2.86889500	-0.88620600	1.35792400
O	-2.42549700	-1.12385900	2.67938900
H	-1.47355100	-0.93024200	2.71027100
O	-2.07318700	-0.49209400	0.37133700
H	2.33835400	-1.93707200	-2.72388500
C	-1.02720100	-3.18754100	-0.37978100
C	-2.01734900	-4.04358400	0.14124400
C	-0.99345300	-2.98257300	-1.77508500
C	-2.93075600	-4.68816800	-0.69719200
H	-2.07845800	-4.19495400	1.21679100
C	-1.90649500	-3.62672400	-2.61292800
H	-0.27160400	-2.28783300	-2.19221800
C	-2.87920500	-4.48520800	-2.08205000
H	-3.68862800	-5.34009600	-0.26910000
H	-1.86883700	-3.44719900	-3.68522100
H	-3.59351500	-4.97854200	-2.73671000
H	1.28046000	-0.35741000	0.12222700
P	-0.13049500	1.69467600	-0.12290000
C	-1.64717000	2.10870700	-1.11207600
C	-1.87896600	3.60027200	-1.41226300
C	-1.68902800	1.26531800	-2.40458600
H	-2.45564200	1.73719100	-0.47435700
C	-3.21710100	3.79953700	-2.14644900
H	-1.06906200	3.98323700	-2.04609200
H	-1.86817700	4.19052800	-0.48854600
C	-3.02085300	1.47452300	-3.14375600
H	-0.86207800	1.54998400	-3.06984600
H	-1.55709000	0.20831200	-2.15237700
C	-3.28036700	2.96126100	-3.43303000
H	-3.35963300	4.86253800	-2.37645600
H	-4.03916200	3.50478500	-1.47949300
H	-3.02351300	0.89769800	-4.07678700
H	-3.83646800	1.07853400	-2.52331600
H	-4.25432600	3.08926300	-3.92101700
H	-2.52155100	3.32901800	-4.13840600
C	1.28450400	2.50777800	-1.05958100
C	1.58243700	3.97050000	-0.66074300
C	2.57843100	1.67328500	-1.04073100
H	0.92387900	2.51619300	-2.09724900
C	2.65281300	4.58342000	-1.58064700
H	1.95171300	4.00092400	0.37187100
H	0.67678600	4.58310200	-0.69177000
C	3.66285800	2.29295100	-1.93673800
H	2.95610800	1.60162900	-0.01192900
H	2.36375000	0.65530100	-1.36895400
C	3.94585100	3.75550600	-1.56593100
H	2.85523600	5.61538300	-1.26904600
H	2.26179600	4.63259300	-2.60657900
H	4.58089600	1.69588700	-1.86807800
H	3.33132900	2.24291800	-2.98365600
H	4.68365600	4.18859500	-2.25229100
H	4.38628500	3.79456100	-0.55958900
C	-0.26767100	2.59891200	1.50274600
C	-1.65056000	2.42757100	2.16224100
C	0.85138400	2.10139700	2.44512800
H	-0.11661500	3.66733500	1.31172400
C	-1.70202900	3.12517900	3.53132800
H	-1.86468900	1.36281800	2.28674500
H	-2.43614600	2.83283200	1.51618600
C	0.79016300	2.79458900	3.81458300
H	0.73954000	1.01563000	2.57551400
H	1.83650400	2.25793800	1.99142500
C	-0.59059100	2.62313300	4.46451200
H	-2.68609900	2.96132000	3.98702000
H	-1.59416800	4.20999000	3.39080300
H	1.57451100	2.39196000	4.46694700
H	1.00199200	3.86539200	3.68708100
H	-0.62887800	3.15383100	5.42349900
H	-0.75710500	1.55867200	4.68304500

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Sum of electronic and thermal Free Energies= -3696.924475

Ni	-0.35330600	0.17290400	-0.94931600	C	-3.29934300	1.16721200	3.87470700
C	0.26256600	-0.16615800	-3.01415400	H	-1.29467300	1.94661700	3.69426300
C	-0.89611900	0.59432900	-2.95154300	H	-1.35316300	0.20336500	3.94938900
H	-1.79463900	-0.01199900	-3.03548000	C	-3.92262900	2.11902400	1.60704000
C	5.97686400	-3.16907100	-0.48805300	H	-1.93769500	2.92152600	1.31988000
C	5.31483500	-2.58226700	-1.57460300	H	-2.43024100	1.78535900	0.06348500
C	4.92378300	-1.23471100	-1.53733800	C	-4.01529400	2.30465500	3.12953200
C	5.20820300	-0.48790000	-0.38076800	H	-3.33600700	1.33782200	4.95756600
C	5.86733200	-1.06835600	0.70738500	H	-3.82289800	0.22026000	3.68328600
C	6.25520500	-2.41392000	0.65766800	H	-4.39499300	2.96255400	1.08897200
H	6.27225900	-4.21462800	-0.53561600	H	-4.47960100	1.21715200	1.31794500
H	5.09793100	-3.17808500	-2.45933600	H	-5.06500100	2.36077600	3.44251700
H	4.90428100	0.55643600	-0.33138700	H	-3.55064200	3.26216600	3.40476600
H	6.07346300	-0.47423600	1.59463400	C	0.96384100	1.98885400	1.77107400
H	6.76444300	-2.86899400	1.50360400	C	1.65702600	1.77798400	3.13681200
C	4.13367800	-0.61208600	-2.67031900	C	1.98319600	2.49562200	0.73022100
C	2.62897300	-0.67458600	-2.35705400	H	0.21684200	2.78376400	1.89963400
H	4.34505700	-1.12481800	-3.61587300	C	2.34769000	3.06710200	3.61347600
H	4.44206200	0.43327500	-2.78828100	H	2.41468600	0.99001400	3.04471700
C	1.72162500	0.08005300	-3.34438800	H	0.94244300	1.44398000	3.89462000
H	2.31552500	-1.72442900	-2.30985200	C	2.69306100	3.77102100	1.21240400
H	2.45253800	-0.24569400	-1.36893900	H	2.72822200	1.71339800	0.53279200
H	1.85912600	-0.35242500	-4.34974600	H	1.47809000	2.69009300	-0.21900100
O	2.04536600	1.47253800	-3.39601200	C	3.36252000	3.57281900	2.57922500
C	-5.38089400	-4.49963800	-0.76986000	H	2.83996800	2.88241200	4.57594700
C	-4.07761700	-4.02532400	-0.97088700	H	1.58754700	3.84112200	3.78866500
C	-3.74157600	-2.67604800	-0.74174200	H	3.43215400	4.08243000	0.46423100
C	-4.76785800	-1.81645700	-0.29927100	H	1.95556000	4.58277400	1.28537000
C	-6.07308700	-2.27835200	-0.09255600	H	3.82073300	4.50926100	2.91961100
C	-6.38376100	-3.62539000	-0.32903500	H	4.17435500	2.83803300	2.48167400
H	-5.61642900	-5.54605100	-0.95386400	C	0.62757800	-0.98711600	2.03111800
H	-3.30528100	-4.71278700	-1.30965600	C	-0.37394100	-2.15807300	2.07638000
H	-4.52516500	-0.77224900	-0.11415900	C	1.92134300	-1.41315500	1.30430600
H	-6.84753300	-1.59535000	0.25129000	H	0.87429600	-0.71408900	3.06318000
H	-7.39650100	-3.98984100	-0.17041000	C	0.26212400	-3.40141900	2.72095700
B	-2.27308700	-2.10444700	-0.94418800	H	-0.69495500	-2.40000700	1.05958300
O	-1.30691300	-3.05868300	-1.34799000	H	-1.27281900	-1.87636100	2.63436600
H	-0.44619900	-2.60943100	-1.38072800	C	2.55453900	-2.65376800	1.94872900
O	-1.99696400	-0.82724100	-0.72231400	H	1.67260800	-1.63780000	0.25976300
H	2.87900200	1.56972700	-3.88254000	H	2.64844600	-0.59463800	1.27801000
H	0.83124600	0.97504700	-0.98955600	C	1.55398900	-3.81738200	2.00134300
P	-0.07010100	0.52435800	1.19067800	H	-0.46185500	-4.22527200	2.71292700
C	-1.76325700	0.82398700	1.89515800	H	0.48778300	-3.18780100	3.77531100
C	-1.83547600	1.03222500	3.41858100	H	3.45227100	-2.93608500	1.38755200
C	-2.46490000	1.97453300	1.14088600	H	2.88261000	-2.40611800	2.96822700
H	-2.29481300	-0.09522600	1.62540100	H	2.00337900	-4.68611300	2.49761800

H	1.31025400	-4.12795700	0.97534900
H	0.05114000	-1.22941900	-3.13972300
C	-1.22868500	2.03168600	-2.85382000
C	-0.31657900	3.08114400	-2.60988800
C	-2.60368300	2.35339800	-2.91275600
C	-0.76738700	4.39163000	-2.44155000
H	0.73803800	2.85582100	-2.54609400
C	-3.05309200	3.66529000	-2.74817200
H	-3.32880700	1.55897700	-3.07425000
C	-2.13448100	4.69456200	-2.50890000
H	-0.04664600	5.18256200	-2.24653500
H	-4.11755400	3.88155500	-2.79510000
H	-2.47853900	5.71655300	-2.36992400

dist-7

Sum of electronic and thermal Free Energies= -4010.068658

Ni	-0.34920500	0.38502200	-0.73697000
P	-1.61889400	-1.24736700	-0.08356300
C	-2.25679800	-0.75986700	1.61056900
C	-3.23722300	-1.70820100	2.32761300
C	-1.13550900	-0.34102100	2.57980300
H	-2.80357600	0.15790500	1.36042200
C	-3.84651200	-1.01119800	3.55748300
H	-2.69714100	-2.60001900	2.66525700
H	-4.03035600	-2.05132200	1.65536400
C	-1.71676100	0.34596500	3.82612100
H	-0.57395200	-1.22963700	2.89157600
H	-0.43115800	0.32898300	2.07782700
C	-2.75333800	-0.54231400	4.53107500
H	-4.53909100	-1.69364700	4.06471500
H	-4.43823700	-0.14672800	3.22534700
H	-0.90474600	0.60746700	4.51543700
H	-2.18878800	1.29033900	3.52329000
H	-3.20120800	-0.00575500	5.37610800
H	-2.24572300	-1.42340700	4.94816600
C	-0.86567600	-2.96735700	0.00251700
C	-1.80732500	-4.15361800	0.30348800
C	-0.06405900	-3.27855200	-1.28414000
H	-0.15273500	-2.88129800	0.83390900
C	-1.00429300	-5.45834100	0.46123100
H	-2.51622400	-4.27611000	-0.52482700
H	-2.39948700	-3.97776200	1.20253500
C	0.74432900	-4.57835800	-1.14624800
H	-0.76042000	-3.40609400	-2.11879500
H	0.57842600	-2.43445000	-1.55258400
C	-0.16556400	-5.76300900	-0.78857700
H	-1.69074700	-6.28782200	0.66997600
H	-0.34198100	-5.36889800	1.33371400
H	1.28439500	-4.77686600	-2.07986300
H	1.50335000	-4.46137900	-0.36389800
H	0.43335900	-6.66853500	-0.63398300
H	-0.83962700	-5.96781600	-1.63201700
C	-3.18985600	-1.46172200	-1.10103700
C	-4.24593600	-0.36712100	-0.82751900
C	-2.85685500	-1.50055200	-2.61030000
H	-3.62519300	-2.42579100	-0.81275900
C	-5.49811000	-0.54927800	-1.70281800
H	-3.80553800	0.61835700	-1.02774400
H	-4.55240400	-0.37037600	0.22178400
C	-4.11273200	-1.67592800	-3.47921400
H	-2.35052500	-0.56348300	-2.87647700
H	-2.15589300	-2.30731200	-2.83337400
C	-5.15067200	-0.58318300	-3.19616600
H	-6.20694800	0.26048200	-1.49107700
H	-5.99811200	-1.48809400	-1.42571600
H	-3.82614400	-1.66968600	-4.53797700
H	-4.55796100	-2.66046400	-3.27745500
H	-6.05436100	-0.74697400	-3.79581100
H	-4.74095800	0.39182200	-3.49509100
P	1.90903100	0.10642900	-0.06517600
C	2.57587500	-1.58173000	0.50825000
C	4.04105300	-1.94097100	0.16940600
C	2.30496600	-1.83881800	2.00673600
H	1.95387000	-2.28450500	-0.04846400
C	4.37617000	-3.38483400	0.58832900
H	4.72879100	-1.25217200	0.67326800
H	4.22769100	-1.84537800	-0.90354900
C	2.62492700	-3.28783900	2.40780700
H	2.92499000	-1.17094700	2.61635400
H	1.26625500	-1.60936000	2.25250100
C	4.07857200	-3.64546600	2.07087400
H	5.43147900	-3.58889100	0.36947600
H	3.78957800	-4.08025800	-0.02671200
H	2.43587600	-3.41984400	3.48014300
H	1.94650700	-3.97366700	1.88319000
H	4.28356600	-4.69327300	2.32162500
H	4.75100600	-3.03312500	2.68811700
C	2.33159100	1.25814600	1.35287300
C	3.83263200	1.45005400	1.65388100
C	1.60088100	2.61272100	1.25045100
H	1.89114700	0.74530700	2.21794600

C	4.03791200	2.30757000	2.91575900
H	4.32477500	1.93678100	0.80423400
H	4.32747700	0.48445400	1.78932800
C	1.81551900	3.45150800	2.51896100
H	1.95510400	3.17182200	0.37906800
H	0.53565400	2.44527400	1.08464400
C	3.30912600	3.65565900	2.81280400
H	5.11055100	2.46334300	3.08501300
H	3.65663300	1.75663400	3.78728400
H	1.30949500	4.41877700	2.40992600
H	1.34412700	2.94253200	3.37237300
H	3.44365200	4.23111800	3.73702200
H	3.75780600	4.24718300	2.00204600
C	3.04321700	0.51065100	-1.50441300
C	2.55980700	-0.32343700	-2.71307800
C	3.16067700	1.99958300	-1.88723400
H	4.04812600	0.17605200	-1.22615000
C	3.45654300	-0.12488300	-3.94469400
H	1.53105800	-0.02003900	-2.94882300
H	2.52051400	-1.38939100	-2.45705900
C	4.07324500	2.18062100	-3.11232400
H	2.16491300	2.38957600	-2.09866400
H	3.56246400	2.57843400	-1.05112000
C	3.57748500	1.36089800	-4.31246300
H	3.05706700	-0.69917600	-4.78975000
H	4.45682700	-0.52802000	-3.73164900
H	4.12566100	3.24502300	-3.37376300
H	5.09636100	1.86661200	-2.85905700
H	4.25116800	1.48830000	-5.16887000
H	2.59208000	1.73673900	-4.62290600
C	-2.75935900	5.82697600	0.35403200
C	-1.85183400	5.26629500	-0.55411800
C	-1.46319300	3.91135000	-0.47887200
C	-2.03285700	3.14328700	0.55661000
C	-2.94363900	3.68823100	1.46849100
C	-3.31117100	5.03685400	1.37123500
H	-3.03745400	6.87579500	0.27038200
H	-1.43308200	5.89147300	-1.33907800
H	-1.76062200	2.09603000	0.64366700
H	-3.36739900	3.06481800	2.25345200
H	-4.01750300	5.46644700	2.07844600
B	-0.42327000	3.29854500	-1.52328800
O	0.01408500	4.23531200	-2.49591400
H	0.62754500	3.76888800	-3.08702300
O	0.06313900	2.06388200	-1.54776200
H	-1.71134900	0.70956700	-1.09986500

dist-TS4

Sum of electronic and thermal Free Energies= -4010.043924

Ni	0.04092200	0.16765200	0.47835300
P	2.08602300	-0.17058900	0.03068000
C	2.55913700	0.55472800	-1.63389800
C	3.99376500	0.29640200	-2.12926100
C	1.53305400	0.17622500	-2.72082900
H	2.45641000	1.63442300	-1.46804400
C	4.26792100	1.06538500	-3.43414200
H	4.12675800	-0.77606500	-2.31801500
H	4.72745800	0.58195300	-1.36713200
C	1.80717800	0.92890200	-4.03259800
H	1.58399100	-0.90283100	-2.91517100
H	0.51900300	0.38244700	-2.35893500
C	3.24579900	0.70352500	-4.52285300
H	5.28645400	0.85467200	-3.78269900
H	4.21835400	2.14463800	-3.23210000
H	1.08841000	0.61351900	-4.79894700
H	1.64416300	2.00315200	-3.87088600
H	3.43444700	1.28836100	-5.43140900
H	3.37118200	-0.35418300	-4.79479600
C	2.58522100	-1.99166300	-0.05694400
C	4.06878000	-2.33796200	0.19131100
C	1.69385600	-2.85513000	0.86059800
H	2.34679900	-2.26591300	-1.09492600
C	4.32655100	-3.83757300	-0.04612100
H	4.33105500	-2.09839400	1.22931800
H	4.73120000	-1.74526400	-0.44447900
C	1.94214200	-4.35411000	0.63662700
H	1.90119800	-2.60947900	1.90996600
H	0.64457000	-2.60537600	0.69539800
C	3.42249700	-4.71306000	0.83514200
H	5.38211800	-4.06549000	0.14729800
H	4.14072200	-4.07097900	-1.10403100
H	1.30987000	-4.94224200	1.31350000
H	1.64070800	-4.61757000	-0.38623300
H	3.59119800	-5.77481100	0.61719500
H	3.69175000	-4.55872400	1.88963500
C	3.32213100	0.58835800	1.22245800
C	3.37943900	2.12548300	1.10156500
C	2.94242800	0.17295300	2.66117600
H	4.32009100	0.19552300	0.99493700
C	4.30716000	2.74759100	2.15906500
H	2.37114500	2.54153600	1.22484400

H	3.72409700	2.41985100	0.10474900
C	3.86633900	0.80724800	3.71273400
H	1.90394400	0.47819000	2.84806400
H	2.96969300	-0.91675200	2.76309100
C	3.89939300	2.33595100	3.58028000
H	4.29610200	3.83984700	2.05796000
H	5.33999500	2.42203800	1.97061400
H	3.53526900	0.51618300	4.71735800
H	4.88403900	0.41110500	3.58720600
H	4.58783400	2.76955100	4.31601800
H	2.90094400	2.73955400	3.80040400
P	-1.86514400	-0.99767500	0.04136800
C	-1.73833600	-2.67583500	-0.78521300
C	-3.06493300	-3.38164500	-1.12255500
C	-0.83140000	-2.58955100	-2.02742700
H	-1.21054500	-3.29855200	-0.05251700
C	-2.81100300	-4.77398600	-1.72749900
H	-3.62430800	-2.78287600	-1.85155000
H	-3.69464700	-3.47220100	-0.23037700
C	-0.59406700	-3.97347100	-2.65233900
H	-1.28753500	-1.93049300	-2.77885300
H	0.11832000	-2.12889700	-1.74713800
C	-1.91655600	-4.68566400	-2.97343900
H	-3.76745000	-5.24971000	-1.97698000
H	-2.32539900	-5.41185600	-0.97557200
H	0.01782800	-3.87184700	-3.55723700
H	-0.01768900	-4.58865200	-1.94849500
H	-1.72135400	-5.68776800	-3.37442600
H	-2.44724800	-4.12763700	-3.75795600
C	-3.05141100	-0.04859300	-1.07359900
C	-4.56259100	-0.21337100	-0.80882100
C	-2.66715800	1.44386600	-1.10302300
H	-2.84507000	-0.45360400	-2.07448700
C	-5.38930600	0.56666300	-1.84744100
H	-4.80783200	0.16800500	0.18884900
H	-4.85297200	-1.26738400	-0.81872100
C	-3.50163900	2.23370900	-2.12045000
H	-2.80728100	1.87833200	-0.10577200
H	-1.60164900	1.54651900	-1.32938400
C	-5.00664000	2.05487600	-1.87081100
H	-6.45834500	0.45127000	-1.62947600
H	-5.22033500	0.13227800	-2.84303100
H	-3.22518100	3.29441300	-2.07682300
H	-3.25885600	1.88239300	-3.13359600
H	-5.58740700	2.58508700	-2.63567900
H	-5.26735900	2.50769100	-0.90357400
C	-2.78675700	-1.34236800	1.63309900
C	-1.97981300	-2.33123800	2.50329300
C	-2.99758900	-0.02335300	2.40778800
H	-3.76431600	-1.78707600	1.40688200
C	-2.64652400	-2.56513400	3.86923300
H	-0.96912600	-1.92368700	2.65099300
H	-1.86149200	-3.29300800	1.99287400
C	-3.68148800	-0.26151100	3.76277500
H	-2.02100000	0.44795300	2.56507500
H	-3.58584900	0.68596200	1.81744500
C	-2.87782600	-1.24752000	4.62260000
H	-2.02864400	-3.24557400	4.46823500
H	-3.61197700	-3.06742200	3.71501800
H	-3.80139500	0.69399100	4.28890900
H	-4.69231800	-0.66154100	3.59860800
H	-3.39202200	-1.43736000	5.57281100
H	-1.90564100	-0.79823900	4.87026200
C	-1.16624400	5.98104100	-1.01493700
C	-1.35833900	5.19291900	0.12657600
C	-0.70527200	3.95358000	0.28717300
C	0.15349100	3.53825300	-0.74888800
C	0.35653700	4.31673200	-1.89259000
C	-0.30501200	5.54428600	-2.03007300
H	-1.68612500	6.93149500	-1.11578600
H	-2.03203900	5.54053400	0.90613100
H	0.65176300	2.57624900	-0.66701100
H	1.02326100	3.96748500	-2.67778500
H	-0.15356600	6.15205800	-2.91947300
B	-0.94981300	3.06805600	1.57767000
O	-1.88470800	3.58843800	2.48714900
H	-1.97289200	2.95634600	3.21991600
O	-0.34794000	1.89858100	1.87398200
H	0.64849500	1.39250600	1.06149700

dist-5-toluene

Sum of electronic and thermal Free Energies= -3696.919325

Ni	-0.28128500	-0.51710700	0.29252300
C	1.32314800	-1.95005500	0.37648100
H	1.85906600	-1.97076300	1.32792700
C	-0.07777900	-2.41504600	0.59314600
H	-0.27801900	-2.69518100	1.62836900
C	8.15743800	-1.50797400	-0.35768100
C	6.80565500	-1.32947600	-0.67456300
C	5.81296000	-1.43163800	0.31289900
C	6.20859400	-1.71703900	1.62996600

C	7.55796500	-1.89586400	1.95352100	C	-1.98840000	3.59988500	-1.41478900
C	8.53867300	-1.79289100	0.95890500	C	-1.85048400	1.23944400	-2.35962400
H	8.91201500	-1.42068000	-1.13603100	H	-2.54988400	1.76039500	-0.42169300
H	6.51828000	-1.10364100	-1.70021900	C	-3.34446100	3.79831400	-2.11557500
H	5.45267700	-1.79606400	2.40983900	H	-1.19209100	3.96389100	-2.07767600
H	7.84482100	-2.11189800	2.98008800	H	-1.94603600	4.20794300	-0.50302800
H	9.58818000	-1.92896800	1.20828400	C	-3.20122500	1.44945700	-3.06347700
C	4.34963600	-1.28313700	-0.04103100	H	-1.03850300	1.49318800	-3.05638700
C	3.68325600	-2.64125100	-0.33467500	H	-1.73095000	0.18742700	-2.08200700
H	4.23905600	-0.64277000	-0.91951000	C	-3.45238400	2.93190800	-3.38032100
H	3.82374500	-0.78212600	0.77963400	H	-3.48403400	4.85755400	-2.36482800
C	2.20696100	-2.54179100	-0.74492300	H	-4.15014100	3.52634000	-1.41994100
H	4.23459800	-3.14212300	-1.14145600	H	-3.23984500	0.85022400	-3.98148200
H	3.76301600	-3.29681300	0.54140500	H	-4.00058700	1.07780000	-2.40859900
H	1.83352400	-3.55125500	-0.96057200	H	-4.43824800	3.06028300	-3.84359400
O	2.05153300	-1.72001900	-1.91778000	H	-2.71053700	3.27573700	-4.11578700
C	-6.75222500	-1.63607900	1.86712800	C	1.18703700	2.48679900	-1.12031900
C	-5.39544600	-1.42985300	2.14702500	C	1.52448000	3.94996600	-0.76298500
C	-4.46702400	-1.17612000	1.11980800	C	2.45820300	1.61484000	-1.09461300
C	-4.94526600	-1.14334400	-0.20485800	H	0.81151100	2.47595400	-2.15320400
C	-6.29745600	-1.35146200	-0.49599200	C	2.60804100	4.51217200	-1.69962000
C	-7.20685200	-1.59649900	0.54245100	H	1.89601500	3.99993800	0.26826400
H	-7.45454000	-1.82856400	2.67609700	H	0.63154100	4.58086900	-0.80731200
H	-5.04629200	-1.46732500	3.17685700	C	3.55577600	2.18625500	-2.00677300
H	-4.23353600	-0.96437400	-1.00732600	H	2.84041800	1.55146000	-0.06644300
H	-6.64495100	-1.32760800	-1.52729000	H	2.21568200	0.59638200	-1.40535300
H	-8.25997000	-1.75832200	0.32095100	C	3.87769400	3.64889900	-1.66858200
B	-2.92769700	-0.94648100	1.39557600	H	2.84101800	5.54553700	-1.41508200
O	-2.47860800	-1.22387100	2.69945000	H	2.21589800	4.54780600	-2.72581400
H	-1.52534600	-1.03806700	2.72419000	H	4.46007600	1.56979200	-1.92974900
O	-2.13836600	-0.49316100	0.41880000	H	3.21878500	2.12201800	-3.05117900
H	2.48112400	-2.17473500	-2.66048300	H	4.62627800	4.04625300	-2.36461400
C	-0.90694400	-3.17569900	-0.36231100	H	4.32214600	3.69811100	-0.66440600
C	-1.90856700	-4.02893800	0.14622400	C	-0.31272700	2.63451400	1.47363400
C	-0.83504200	-3.00747100	-1.76285500	C	-1.67297000	2.43772900	2.17451100
C	-2.79714000	-4.69134200	-0.70216900	C	0.83664100	2.15509600	2.38855200
H	-2.00707400	-4.14942700	1.22291400	H	-0.18274300	3.70526400	1.27574800
C	-1.71933400	-3.67673400	-2.61097200	C	-1.70074000	3.13290800	3.54528200
H	-0.10428900	-2.32100300	-2.17743000	H	-1.86559000	1.36793700	2.30131000
C	-2.70570100	-4.52374600	-2.08938500	H	-2.48474400	2.82734200	1.55198700
H	-3.57041000	-5.32847200	-0.27951500	C	0.80375400	2.84725500	3.75980500
H	-1.64984900	-3.52329700	-3.68609400	H	0.73822800	1.06747200	2.52456300
H	-3.40072800	-5.03382100	-2.75201800	H	1.80889900	2.32079400	1.91045100
H	1.35397300	-0.78890400	0.13709600	C	-0.55512600	2.65337600	4.44808400
P	-0.21459000	1.70362200	-0.14214200	H	-2.66811300	2.94825900	4.02696500
C	-1.75796700	2.11375100	-1.09070400	H	-1.61897000	4.22024100	3.40411500

H	1.61341600	2.45940500	4.39012000
H	0.99456400	3.92144700	3.62612500
H	-0.57583400	3.18475900	5.40715900
H	-0.69774900	1.58712500	4.67376500

dist-5^{B}-toluene

Sum of electronic and thermal Free Energies= -3541.191504

Ni	0.75676500	0.83374100	0.36495500
C	-1.13918200	1.83913600	0.46875800
H	-1.70502600	1.64939600	1.38370000
C	0.10487900	2.59725200	0.80348600
H	0.17879000	2.82618600	1.86851400
C	-7.64007800	-0.09337400	-0.75640600
C	-6.26987500	0.07437500	-0.98892800
C	-5.38359700	0.32835000	0.06976800
C	-5.90488500	0.41032600	1.37142300
C	-7.27317400	0.24317300	1.61080000
C	-8.14716600	-0.00895500	0.54575700
H	-8.30993600	-0.29403100	-1.58940600
H	-5.88299000	0.00216500	-2.00409800
H	-5.23177100	0.60251700	2.20563300
H	-7.65707200	0.30571500	2.62645100
H	-9.21051300	-0.14211700	0.72947700
C	-3.90977700	0.54953200	-0.18960500
C	-3.56120400	2.04257800	-0.33859500
H	-3.60696600	0.02913400	-1.10123600
H	-3.32560100	0.11370500	0.62886200
C	-2.08396700	2.31399300	-0.65792000
H	-4.17353900	2.47356200	-1.14147400
H	-3.83062600	2.58540400	0.57606100
H	-1.94352200	3.39665200	-0.77014600
O	-1.68903000	1.65799900	-1.87758000
B	3.23303300	1.66132500	1.62024400
O	2.66356400	1.90188300	2.89105000
H	1.72543600	1.66563100	2.84340000
O	2.57625700	1.16876100	0.56820900
H	-2.14296300	2.09816100	-2.61440800
C	0.71532600	3.65339900	-0.02922000
C	1.33168100	4.75284700	0.60216100
C	0.78365300	3.57917100	-1.43716100
C	1.97351800	5.74790100	-0.13886700
H	1.31594400	4.81944900	1.68814600
C	1.42051200	4.57565100	-2.17792300
H	0.35331900	2.71965400	-1.94078000
C	2.01715200	5.66899900	-1.53609100
H	2.44419900	6.58336000	0.37452700
H	1.46713100	4.49187000	-3.26177200
H	2.51922900	6.44037500	-2.11512500
H	-0.88812700	0.72879400	0.14155700
P	1.14413000	-1.35413900	-0.11191800
C	2.82238200	-1.48311300	-0.89366300
C	3.34784900	-2.90520900	-1.15478200
C	2.87985700	-0.61765400	-2.17067600
H	3.46620600	-0.98391400	-0.16173100
C	4.78038400	-2.85922700	-1.71580900
H	2.70108400	-3.41300300	-1.88266300
H	3.32463600	-3.50392600	-0.23608900
C	4.30863000	-0.58460900	-2.73768600
H	2.19969900	-1.02174200	-2.93454900
H	2.54754300	0.39716300	-1.93118300
C	4.85442500	-1.99928300	-2.98747900
H	5.13321100	-3.87760700	-1.92144400
H	5.45009300	-2.43812500	-0.95348300
H	4.32630100	-0.00020700	-3.66579600
H	4.95737100	-0.06234600	-2.02268300
H	5.88832100	-1.94963300	-3.35049700
H	4.26421800	-2.48096100	-3.78081200
C	0.00882000	-2.36767400	-1.21581800
C	-0.09590600	-3.87083700	-0.88000600
C	-1.39379400	-1.73754300	-1.32214800
H	0.47587400	-2.28174700	-2.20682000
C	-0.96499400	-4.60880300	-1.91334600
H	-0.55111500	-3.99591100	0.11043200
H	0.89491200	-4.33236600	-0.83114400
C	-2.27603600	-2.48563400	-2.33453100
H	-1.88032600	-1.75915100	-0.33754000
H	-1.31119800	-0.68642200	-1.60859300
C	-2.36459400	-3.98506900	-2.01639900
H	-1.03797500	-5.66936200	-1.64307900
H	-0.47332700	-4.56626400	-2.89545700
H	-3.27876000	-2.04063400	-2.35328700
H	-1.85398700	-2.35291600	-3.34081800
H	-2.95785100	-4.50343500	-2.77934600
H	-2.89067200	-4.12078500	-1.06079300
C	1.23743000	-2.26576800	1.51621200
C	2.44769100	-1.81174200	2.35813300
C	-0.07542700	-2.03067300	2.29695800
H	1.34129100	-3.33932500	1.31784100
C	2.46475600	-2.50154700	3.73181700
H	2.40727600	-0.72604300	2.49410100
H	3.38307500	-2.02416100	1.83097100

C	-0.05496400	-2.71831400	3.67092800
H	-0.20730600	-0.94680500	2.43411400
H	-0.93967200	-2.37775200	1.71943900
C	1.15617600	-2.26729800	4.50006700
H	3.31869600	-2.13414400	4.31311100
H	2.61536100	-3.58204100	3.59520500
H	-0.98865500	-2.50524400	4.20588600
H	-0.01403700	-3.80738900	3.52863100
H	1.17734500	-2.79386000	5.46181100
H	1.05991100	-1.19613800	4.72743800
O	4.60195700	1.93681900	1.52949200
H	4.91953500	2.27151600	2.38110300

COD

Sum of electronic and thermal Free Energies= -311.929253

C	1.74200400	0.67127000	-0.11956100
C	1.74175500	-0.67186700	-0.11956200
H	2.58725800	1.17387300	-0.59071000
C	0.65433900	1.57217100	0.42936100
H	1.04380900	2.59366800	0.48406900
H	0.40115600	1.27973600	1.45582000
C	0.65377900	-1.57237600	0.42937300
H	1.04289600	-2.59400400	0.48412200
H	0.40067000	-1.27981900	1.45581500
H	2.58682200	-1.17478200	-0.59071800
C	-0.65407100	-1.57284700	-0.42848800
H	-0.40088700	-1.28201000	-1.45542500
H	-1.04348200	-2.59444400	-0.48166700
C	-0.65351300	1.57305500	-0.42849200
H	-1.04257500	2.59478400	-0.48170300
H	-0.40041800	1.28209800	-1.45541600
C	-1.74214900	-0.67127900	0.11865500
C	-1.74190100	0.67187300	0.11866500
H	-2.58857000	-1.17357400	0.58804200
H	-2.58813700	1.17447400	0.58806300

IM1-PPh$_3$

Sum of electronic and thermal Free Energies= -4616.585383

Ni	-0.02236300	0.07834300	0.03519900
P	-2.01790100	0.88259400	-0.00139800
P	1.74663000	1.30834400	0.03011000
C	2.29675000	1.70345400	1.74868000
C	3.62304700	1.99158600	2.11026600
C	1.31059400	1.68349200	2.75179000
C	3.95542700	2.25524300	3.44389900
H	4.40373700	1.99899300	1.35423500
C	1.63863100	1.95303100	4.08374600
H	0.28609100	1.43212300	2.48180800
C	2.96480800	2.23807800	4.43405700
H	4.98741600	2.47239300	3.70926400
H	0.86430400	1.92812200	4.84678900
H	3.22544200	2.43909500	5.47033700
C	3.28382700	0.64416700	-0.76506500
C	3.69502700	1.05345500	-2.04532400
C	3.95788100	-0.43281100	-0.15716400
C	4.74747900	0.40251400	-2.70243200
H	3.19320100	1.87958600	-2.54143600
C	5.01318300	-1.07534000	-0.80739700
H	3.65631600	-0.77693200	0.82691600
C	5.41073300	-0.66500600	-2.08785900
H	5.04631600	0.73219700	-3.69496800
H	5.51622300	-1.90537100	-0.31685300
H	6.22569400	-1.17215100	-2.59865900
C	1.60149000	2.96147400	-0.78817600
C	2.33025500	4.10199600	-0.41560400
C	0.69329900	3.05511400	-1.85539000
C	2.15338700	5.31075900	-1.09983000
H	3.03294000	4.05622700	0.41208700
C	0.52841700	4.25448700	-2.55323000
H	0.09987000	2.18252800	-2.11968400
C	1.25708800	5.38843400	-2.17391100
H	2.71584100	6.19045900	-0.79527900
H	-0.18357100	4.31050300	-3.37292300
H	1.11981900	6.32857400	-2.70276000
C	-3.05173100	0.57108700	1.50035400
C	-2.66418200	-0.48714800	2.33976000
C	-4.19068400	1.32269900	1.83775200
C	-3.40919700	-0.80557200	3.47955000
H	-1.77639100	-1.05968500	2.08988000
C	-4.93363300	1.01085500	2.98203100
H	-4.49896800	2.15466400	1.20961800
C	-4.54765200	-0.05688100	3.80368800
H	-3.09857700	-1.63322800	4.11285500
H	-5.81353300	1.59942400	3.23124200
H	-5.12703500	-0.29872000	4.69153200
C	-2.33040800	2.68477800	-0.28257700
C	-3.19529300	3.19544600	-1.26207400
C	-1.60891700	3.58689300	0.51987200
C	-3.33985200	4.57958100	-1.43251300
H	-3.75850400	2.51805100	-1.89848000

C	-1.76529100	4.96490200	0.36548900
H	-0.90506800	3.20573500	1.25633400
C	-2.63051300	5.46759400	-0.61695100
H	-4.00901700	4.96062600	-2.20072300
H	-1.19624800	5.64717400	0.99255600
H	-2.74140900	6.54099100	-0.75058200
C	-2.96553700	0.08151900	-1.37184200
C	-4.30534300	-0.32529100	-1.28786900
C	-2.23606000	-0.22248200	-2.53721100
C	-4.90181300	-1.02868000	-2.34266500
H	-4.88383500	-0.11851800	-0.39192300
C	-2.83236800	-0.91046500	-3.59621600
H	-1.18271100	0.04647800	-2.59179500
C	-4.16952800	-1.32256400	-3.49858800
H	-5.93610600	-1.35342300	-2.25619900
H	-2.25014700	-1.14672400	-4.48366200
H	-4.63182600	-1.87567500	-4.31250200
P	0.23321200	-2.06751800	0.00703400
C	1.58898000	-2.60357700	1.14255800
C	2.54499400	-3.58517100	0.84321100
C	1.70662600	-1.88562900	2.34703900
C	3.60627600	-3.83240400	1.72383700
H	2.48473400	-4.14134500	-0.08801700
C	2.75373600	-2.14135200	3.23491100
H	0.99308200	-1.09494000	2.56621800
C	3.71485400	-3.11280400	2.91980600
H	4.35324000	-4.58088000	1.46968100
H	2.83549200	-1.56549300	4.15369600
H	4.54518800	-3.30010500	3.59627000
C	-1.16132400	-3.18471600	0.49517300
C	-2.31538100	-3.19299700	-0.31261200
C	-1.18348500	-3.89919000	1.70418800
C	-3.45555100	-3.89761400	0.07694100
H	-2.32844400	-2.63955200	-1.24695500
C	-2.33154400	-4.59878800	2.10080300
H	-0.30801300	-3.91041400	2.34744000
C	-3.47194800	-4.60025900	1.29080800
H	-4.33577300	-3.88589400	-0.56155600
H	-2.33102800	-5.14159100	3.04338100
H	-4.36386800	-5.13967300	1.60031100
C	0.71991900	-2.74497000	-1.63904400
C	0.52729500	-4.08253000	-2.02445800
C	1.31975800	-1.85557700	-2.54694000
C	0.93332200	-4.52197800	-3.28933800
H	0.05523800	-4.78298800	-1.34026000
C	1.73359000	-2.29441500	-3.80832500
H	1.45915300	-0.81794500	-2.25714500
C	1.54032700	-3.62992100	-4.18360900
H	0.77791500	-5.55949800	-3.57575900
H	2.20146000	-1.59394100	-4.49603400
H	1.85582200	-3.97318400	-5.16598700

1-PPh$_3$

Sum of electronic and thermal Free Energies= -3890.022877

Ni	0.06848200	-0.66819200	-0.89260300
C	2.37487000	-2.46591600	-1.31542800
C	3.65997700	-2.56335100	-1.88388900
C	2.19338600	-3.00506500	-0.02271300
C	4.71770900	-3.16846600	-1.19687900
H	3.83619800	-2.13993500	-2.87057600
C	3.24679700	-3.60500400	0.66901600
H	1.22488100	-2.90883800	0.45978100
C	4.52088900	-3.69176000	0.08653700
H	5.70105100	-3.21742300	-1.65955400
H	3.07961500	-3.99168100	1.67213200
H	5.34441700	-4.15088000	0.62811000
P	1.37656500	0.87373700	-0.04132100
P	-2.00192500	-0.47307100	-0.20098600
C	1.28187400	-1.79070200	-2.05404300
C	-0.06393500	-2.25457100	-2.06908800
H	-0.68387000	-2.04954400	-2.94188800
H	-0.31854700	-3.18742800	-1.56387500
H	1.62407100	-1.20639300	-2.91113000
C	-3.22319500	-0.86227400	-1.52698100
C	-4.41816300	-1.56607300	-1.31401200
C	-2.92913500	-0.39279000	-2.81916400
C	-5.30485100	-1.79304200	-2.37436300
H	-4.66363100	-1.94009500	-0.32382000
C	-3.82052500	-0.60341100	-3.87478200
H	-1.99109800	0.13031900	-2.99488500
C	-5.01207500	-1.30792900	-3.65459500
H	-6.22497500	-2.34510300	-2.19812800
H	-3.58205200	-0.22934000	-4.86749100
H	-5.70327100	-1.48200400	-4.47555000
C	-2.43618100	-1.64526000	1.16362700
C	-3.42138500	-1.37592500	2.12908300
C	-1.72923600	-2.85744800	1.23965900
C	-3.69089000	-2.29920100	3.14563400
H	-3.97826100	-0.44395700	2.09495500
C	-1.99878200	-3.78288600	2.25245900
H	-0.96236800	-3.06937400	0.50236000

C	-2.98072200	-3.50447500	3.21143000
H	-4.45490800	-2.07573700	3.88633400
H	-1.43846100	-4.71360600	2.29616600
H	-3.18844800	-4.21823800	4.00476100
C	-2.67043200	1.11802400	0.46907300
C	-3.79683500	1.76700900	-0.05948000
C	-2.00248900	1.70618900	1.55792100
C	-4.24872200	2.97363200	0.49182200
H	-4.33237600	1.33759700	-0.90072300
C	-2.45643300	2.90263000	2.11451900
H	-1.12259400	1.22914900	1.97885400
C	-3.58361700	3.54334400	1.58214500
H	-5.12214400	3.46370700	0.06798800
H	-1.92253200	3.34195900	2.95349200
H	-3.93384400	4.47985600	2.00930200
C	3.06763000	1.12204200	-0.75154500
C	4.11321500	0.25587400	-0.38682400
C	3.31446600	2.10252500	-1.72892100
C	5.37958400	0.38462400	-0.96413500
H	3.94394400	-0.52741400	0.34652000
C	4.58007200	2.22490000	-2.31377100
H	2.52418600	2.78395400	-2.03157200
C	5.62034000	1.36952700	-1.92917200
H	6.17216900	-0.29802600	-0.66825200
H	4.75328100	2.99320500	-3.06380700
H	6.60538200	1.46776800	-2.37905400
C	0.68168500	2.58091300	-0.16739000
C	1.00720100	3.64705300	0.68489400
C	-0.21174900	2.80770900	-1.22736600
C	0.45193600	4.91405300	0.47815700
H	1.68218200	3.49817100	1.52163100
C	-0.75561800	4.07677200	-1.44665200
H	-0.48774000	1.97725900	-1.87445000
C	-0.42596300	5.13439500	-0.59098100
H	0.70359400	5.72883600	1.15287400
H	-1.44750400	4.23389400	-2.27048300
H	-0.85662700	6.12014300	-0.74907600
C	1.75717200	0.60607300	1.74812100
C	2.77904800	1.28376400	2.43777500
C	0.99617100	-0.34984500	2.44179300
C	3.01098000	1.03194500	3.79307000
H	3.41426100	1.99314400	1.91438100
C	1.22655800	-0.60518900	3.79781900
H	0.22729100	-0.90751000	1.91497300
C	2.23196600	0.08994400	4.47902200
H	3.80330700	1.56594600	4.31199900
H	0.62628400	-1.35008900	4.31457900
H	2.41648700	-0.10709400	5.53219800

H-TS1-PPh$_3$

Sum of electronic and thermal Free Energies= -3277.964795

Ni	0.50054200	-0.14944300	-1.84925500
C	-1.15864300	0.74585800	-2.02443500
O	-1.31048400	1.84905300	-2.55041000
C	2.14435900	-2.49345800	-1.17546800
C	1.17809600	-3.51982100	-1.26324200
C	1.14753400	-4.56099400	-0.33174400
C	2.07892100	-4.60796300	0.71411100
C	3.04761000	-3.59992700	0.80997900
C	3.08050400	-2.56047600	-0.12182800
H	0.42851500	-3.49452200	-2.04968600
H	0.38667700	-5.33370900	-0.41612500
H	2.04751100	-5.41358700	1.44323500
H	3.77563500	-3.62010200	1.61785700
H	3.82880800	-1.77719500	-0.02685700
C	-2.35045900	0.01027800	-1.40494500
H	-2.51143500	-0.89059700	-2.01228400
H	-2.03929500	-0.36337900	-0.42168500
C	-3.64266000	0.83917800	-1.29276100
H	-3.41135600	1.77829600	-0.78069200
H	-3.98496200	1.10522900	-2.29756000
C	-4.71851000	0.08427200	-0.54572600
C	-5.64374700	-0.72482100	-1.22659900
C	-4.78256200	0.13195500	0.85812100
C	-6.60609200	-1.46456300	-0.52813100
H	-5.61087400	-0.77400100	-2.31359800
C	-5.74145500	-0.60542000	1.56220600
H	-4.07668100	0.75470100	1.40513300
C	-6.65835100	-1.40864000	0.87080900
H	-7.31578600	-2.08148900	-1.07467400
H	-5.77575700	-0.55130600	2.64795400
H	-7.40602300	-1.98043700	1.41511000
C	1.44425400	-1.27677300	-3.30932700
H	1.80572900	-0.61148500	-4.09102300
H	0.93255600	-2.15640700	-3.69161100
H	-0.06332000	-0.53141800	-3.17405000
P	1.01385300	0.75242400	0.10390200
C	2.18039300	-1.34722100	-2.10242300
H	3.04821300	-0.70059600	-2.00958900
C	0.24911700	2.40471800	0.42009300
C	0.90444800	3.60580000	0.11034700

C	-1.07914600	2.45635100	0.88005000
C	0.24632900	4.83282400	0.26082800
H	1.93133900	3.59996100	-0.24152800
C	-1.73502200	3.67951600	1.03116900
H	-1.60612900	1.54111000	1.13321800
C	-1.07483300	4.87487100	0.71915100
H	0.77031600	5.75463700	0.02056800
H	-2.76103900	3.69705600	1.39054300
H	-1.58400100	5.82820800	0.83548800
C	2.81891900	1.04864700	0.30255500
C	3.54508100	0.73600400	1.46117500
C	3.50107800	1.57339100	-0.81101600
C	4.92743700	0.95485900	1.50810200
H	3.04902400	0.30300700	2.32364100
C	4.87733500	1.80673100	-0.75815200
H	2.95454200	1.78128600	-1.72920300
C	5.59567800	1.49500600	0.40383400
H	5.48026300	0.69763700	2.40811000
H	5.38869400	2.21595300	-1.62563700
H	6.66892100	1.66281000	0.44359700
C	0.47187200	-0.20905100	1.57003200
C	-0.01170600	-1.51165200	1.38297900
C	0.49760500	0.33496200	2.86816300
C	-0.45015700	-2.26904700	2.47442800
H	-0.04312700	-1.93870400	0.38666100
C	0.06168400	-0.42180800	3.95779200
H	0.84382000	1.35260500	3.02840900
C	-0.41246100	-1.72729100	3.76300100
H	-0.81740200	-3.27898400	2.31275600
H	0.08708500	0.00698100	4.95637100
H	-0.75425100	-2.31370600	4.61227600

dist-TS1-PPh$_3$

Sum of electronic and thermal Free Energies= -3841.23614

C	-0.05731300	-0.03155600	-1.97761900
C	-0.11727200	-1.57571300	-1.99868400
Ni	-0.46955300	-0.37712200	-0.19161000
C	-1.18479800	-2.37165800	-1.01804900
H	-0.92351800	-3.41713700	-1.24071700
C	-2.62697100	-2.08753200	-1.47632000
H	-2.74346300	-2.36417100	-2.53170200
H	-2.81964600	-1.00940200	-1.40850000
C	-3.66999100	-2.82670800	-0.62028200
H	-3.56087700	-3.90800300	-0.76684700
H	-3.44733200	-2.61762500	0.43012200
C	-5.08066300	-2.39052000	-0.95065600
C	-5.90018100	-3.14032600	-1.80940100
C	-5.58588500	-1.18462300	-0.43100400
C	-7.18978200	-2.70242800	-2.14032300
H	-5.52703400	-4.07610600	-2.22187100
C	-6.87231600	-0.74232700	-0.75729100
H	-4.96490800	-0.58967300	0.23619100
C	-7.68118000	-1.50065900	-1.61549800
H	-7.81000900	-3.29970000	-2.80489100
H	-7.24541600	0.19073300	-0.34075500
H	-8.68229200	-1.16018200	-1.86898500
H	-0.46275800	-1.87657500	-2.99264000
H	0.86846300	-2.01956800	-1.83815100
H	-0.90430200	0.43160300	-2.49296600
C	1.21534100	0.66588500	-2.27195700
C	1.19643200	1.87279900	-2.99960200
C	2.45960700	0.20376800	-1.79107600
C	2.37082300	2.59227200	-3.23525900
H	0.24876800	2.25976200	-3.36535500
C	3.63367400	0.92083700	-2.02337000
H	2.50357900	-0.71851100	-1.22095000
C	3.59575900	2.12149800	-2.74799400
H	2.32590900	3.52595100	-3.79067800
H	4.57678800	0.54627300	-1.63645800
H	4.51041400	2.68167900	-2.92686800
O	-1.04161900	-2.15151200	0.37686600
B	3.70116300	-2.39037900	0.43690900
C	5.03880000	-1.78635600	-0.11979200
C	5.52975000	-2.15780300	-1.38705000
C	5.75345700	-0.81214500	0.60440200
C	6.68714500	-1.57622400	-1.91626000
H	4.98763800	-2.89983600	-1.96833800
C	6.91033500	-0.22227200	0.08285000
H	5.38925600	-0.50533500	1.58150700
C	7.37880100	-0.60317300	-1.18197400
H	7.04617400	-1.87100200	-2.89972200
H	7.44263900	0.53505300	0.65389800
H	8.27420400	-0.14298500	-1.59349200
O	2.98553600	-3.26088100	-0.35512300
H	2.15759800	-3.52585300	0.11667900
O	3.26151600	-1.99683200	1.68154000
H	2.38513300	-2.40831700	1.87097800
C	0.45829100	-4.55017100	2.12128700
C	1.66501600	-5.31062300	2.65374800
H	-0.13596900	-5.19120700	1.45551100
H	-0.19128000	-4.23379500	2.94893700

H	1.34419800	-6.19830600	3.20920400
H	2.31154100	-5.63264100	1.83028200
H	2.25397300	-4.67693700	3.32555700
O	0.91333200	-3.39577000	1.39871100
H	0.10569200	-2.88985900	0.99299300
P	-0.65023200	1.52664200	0.70589200
C	-2.24697100	1.62121900	1.61798000
C	-2.83359500	0.41775300	2.04904000
C	-2.88206500	2.84132600	1.90544000
C	-4.03181600	0.43884400	2.77001400
H	-2.36640300	-0.53387900	1.80162300
C	-4.08227800	2.85766500	2.62327800
H	-2.45465600	3.77836400	1.55867600
C	-4.65810100	1.65740800	3.05903300
H	-4.48178800	-0.49642600	3.09330100
H	-4.56829100	3.80608800	2.83778700
H	-5.59361200	1.67185700	3.61253500
C	-0.66285500	2.99889500	-0.38076300
C	-1.71992300	3.12655500	-1.30052500
C	0.37878000	3.93607400	-0.39514300
C	-1.74149100	4.18835300	-2.20619900
H	-2.52702100	2.39730000	-1.30914200
C	0.35706000	4.99827500	-1.30711100
H	1.21359900	3.83998200	0.29275300
C	-0.70083700	5.12858600	-2.21137300
H	-2.56424600	4.27972100	-2.91071800
H	1.17277400	5.71656700	-1.31323000
H	-0.71447900	5.95213200	-2.92075300
C	0.65268800	1.82660500	1.96064500
C	1.76768900	0.97369400	1.97193200
C	0.56167100	2.86143900	2.90797900
C	2.78329800	1.15252000	2.91682000
H	1.84460000	0.16327800	1.25273700
C	1.58112500	3.04317600	3.84626900
H	-0.29974600	3.52380200	2.92022500
C	2.69337500	2.18878700	3.85231600
H	3.62855500	0.47096100	2.91982000
H	1.50579000	3.84596200	4.57536100
H	3.48099500	2.32911200	4.58850600

IM1

Sum of electronic and thermal Free Energies= -2866.894916

C	3.24431000	-1.10204900	0.87471300
C	2.90312400	-1.15489000	-0.47605800
H	2.87697700	-1.91568800	1.50625600
C	4.35908600	-0.25479500	1.47668700
H	5.13717900	-0.07157300	0.73056200
H	4.84568400	-0.81371200	2.28492600
C	3.47907800	-0.24410900	-1.54757200
H	4.44497200	-0.62767000	-1.91091100
H	2.79848100	-0.27585900	-2.40563900
H	2.38135000	-2.03394500	-0.85205100
C	3.67004600	1.24648100	-1.11617000
H	4.66434600	1.37859800	-0.68126500
H	3.65050300	1.86506300	-2.02014400
C	3.83906300	1.09167900	2.04939300
H	3.45713800	0.91606800	3.06206200
H	4.67923700	1.79598100	2.15954500
C	2.61424100	1.75798900	-0.14294600
C	2.70911600	1.70528400	1.24055200
H	1.86235900	2.41897200	-0.57284200
H	2.01257000	2.32357400	1.81076300
Ni	1.55573100	0.06837700	0.50034100
P	-0.56406600	0.00525200	-0.05922100
C	-1.20162100	1.56877700	-0.89477900
C	-1.63721300	-0.18198100	1.48034500
C	-1.11010600	-1.35793700	-1.22730200
C	-2.62353000	1.57547100	-1.48857600
C	-1.01422700	2.79736100	0.02005900
H	-0.49344900	1.68820200	-1.72786900
C	-3.04215200	-0.79110800	1.29610800
C	-0.86224400	-0.91652600	2.59873800
H	-1.77171000	0.85212300	1.82352300
C	-0.44901100	-1.15132400	-2.60715700
C	-0.72690900	-2.73929200	-0.65551300
H	-2.20016700	-1.32398900	-1.35162300
C	-2.88055700	2.87668900	-2.27166500
H	-3.35880500	1.49767300	-0.67809900
H	-2.78331000	0.71438100	-2.14567800
C	-1.25311200	4.10351100	-0.75522100
H	-1.73112400	2.74909200	0.85050500
H	-0.01540100	2.78807100	0.46839500
C	-3.82514900	-0.79241700	2.62135500
H	-2.95772100	-1.82408500	0.93892400
H	-3.60430400	-0.24365900	0.53411300
C	-1.65265200	-0.92969100	3.91766200
H	-0.65377300	-1.94869900	2.29041400
H	0.11286900	-0.43356500	2.75056900
C	-0.77692700	-2.29463300	-3.58132500
H	0.63848100	-1.09192100	-2.46847000
H	-0.76186400	-0.19832600	-3.04735500

C	-1.05659800	-3.87943700	-1.63289200
H	0.34755500	-2.74268400	-0.43412400
H	-1.23736800	-2.91715300	0.29598300
C	-2.64944200	4.11998600	-1.39808100
H	-3.90317000	2.87762200	-2.66938800
H	-2.20433100	2.91041100	-3.13764600
H	-1.13346200	4.96438400	-0.08564500
H	-0.48829800	4.20187800	-1.53844600
C	-3.05476600	-1.52856300	3.72799800
H	-4.80920400	-1.25349900	2.47020700
H	-4.00613200	0.24555500	2.93466800
H	-1.09768800	-1.49029800	4.68014300
H	-1.74796700	0.10078500	4.28843600
C	-0.38822100	-3.66033500	-2.99754500
H	-0.26298200	-2.12606800	-4.53596400
H	-1.85493200	-2.28701600	-3.79626800
H	-0.74145000	-4.83805700	-1.20208200
H	-2.14595500	-3.93643600	-1.76900700
H	-2.78533200	5.03223000	-1.99208600
H	-3.40801500	4.14454800	-0.60274400
H	-3.61467500	-1.49255600	4.67067500
H	-2.96016400	-2.58944900	3.45559400
H	-0.66178500	-4.46468500	-3.69156900
H	0.70360300	-3.70279800	-2.87540300

IM2

Sum of electronic and thermal Free Energies= -3913.738665

C	0.27103600	2.59651400	-1.16188100
C	1.48327200	2.31890900	-0.47419900
H	0.30725200	2.38142600	-2.23900100
C	-0.53402600	3.85667100	-0.89029900
H	-0.58247400	4.06664800	0.17899500
H	-1.57041900	3.74665400	-1.22348100
C	1.83046400	2.95335900	0.86781500
H	1.10028500	2.65382800	1.63008500
H	2.78943300	2.54226900	1.20039400
H	2.36039000	2.11080000	-1.08138400
C	1.91621700	4.52002000	0.90466300
H	0.94776300	4.91919900	1.21824700
H	2.62601400	4.80904100	1.68890300
C	0.05222200	5.08242400	-1.63902600
H	-0.11345000	4.92753100	-2.71393800
H	-0.54248700	5.97478600	-1.38410100
C	2.32021900	5.17417100	-0.39611400
C	1.52454200	5.40490000	-1.45547100
H	3.36618700	5.47157300	-0.48677800
H	1.98489300	5.89908200	-2.31337700
Ni	0.27701400	0.74129100	-0.33077000
P	1.87256200	-0.81778000	-0.00219100
C	3.59967600	-0.19719300	-0.48055500
C	1.81482700	-2.34873600	-1.12114900
C	2.18044700	-1.40396600	1.76646200
C	4.80721000	-1.05173900	-0.03988800
C	3.70856200	0.08859800	-1.99570700
H	3.67823300	0.76826900	0.03117100
C	1.31020600	-3.66245600	-0.50292300
C	1.00297400	-2.00212900	-2.38830800
H	2.85072600	-2.53562600	-1.42904000
C	2.62759200	-0.18647900	2.60924300
C	0.92845400	-2.02763000	2.41283600
H	2.98133400	-2.15439400	1.76526500
C	6.13419300	-0.34527300	-0.37887900
H	4.77907200	-2.02824000	-0.54199100
H	4.78202100	-1.25272900	1.03475200
C	5.01458900	0.82859100	-2.32570000
H	3.69966400	-0.85675300	-2.55219000
H	2.84510500	0.66315100	-2.34393600
C	1.34138000	-4.81111300	-1.52661700
H	0.28397700	-3.53402500	-0.14886300
H	1.91900700	-3.93362200	0.36630000
C	1.01815800	-3.14919600	-3.41110500
H	-0.02524000	-1.77083500	-2.09038100
H	1.38420900	-1.08726400	-2.85149600
C	2.85208400	-0.54572800	4.08649900
H	1.84963900	0.58421100	2.53970900
H	3.54089700	0.25950900	2.20523200
C	1.14280100	-2.38549800	3.89247000
H	0.11095700	-1.30724800	2.33450600
H	0.61159700	-2.92297300	1.87744200
C	6.23507600	0.01560900	-1.86821900
H	6.97830900	-0.98114200	-0.08356500
H	6.20677000	0.57350200	0.22025700
H	5.07063300	1.02573600	-3.40357000
H	5.01344800	1.80628100	-1.82330000
C	0.54003300	-4.47099200	-2.79182600
H	0.95126200	-5.72660200	-1.06422700
H	2.38520900	-5.01626200	-1.80351400
H	0.39487700	-2.88557800	-4.27481300
H	2.04286300	-3.27733800	-3.78836400
C	1.59570800	-1.16862700	4.70890500
H	3.15010600	0.35314300	4.64077700

H	3.68663400	-1.25709300	4.16379600
H	0.21316700	-2.79967800	4.30320000
H	1.90236300	-3.17655700	3.96847900
H	7.16136800	0.57040200	-2.06266600
H	6.28962500	-0.90936600	-2.45989000
H	0.62219000	-5.28523100	-3.52255700
H	-0.52317300	-4.38741700	-2.53334500
H	1.78215300	-1.45198400	5.75218400
H	0.78990200	-0.42073900	4.72028300
P	-1.84702300	-0.00767100	-0.05344700
C	-2.16195700	-1.85023100	0.42370900
C	-3.08802100	0.21302300	-1.45950800
C	-2.59392500	0.90069300	1.42731300
C	-3.16022200	-2.14333400	1.56843400
C	-2.49833600	-2.75856600	-0.78293000
H	-1.17783100	-2.16047600	0.78160400
C	-4.58075700	0.09789600	-1.08553300
C	-2.83732900	1.46784500	-2.31616200
H	-2.84995300	-0.63515800	-2.11343300
C	-1.62341300	0.81482800	2.62558200
C	-2.90962100	2.37851400	1.14292400
H	-3.53350000	0.40385300	1.69380100
C	-3.15788400	-3.63467000	1.95001200
H	-4.17548500	-1.85620000	1.26818200
H	-2.92180600	-1.56130300	2.46100300
C	-2.51562000	-4.25107100	-0.40591700
H	-3.48827600	-2.50372100	-1.17736800
H	-1.78774800	-2.59876300	-1.59865900
C	-5.46913700	0.10327400	-2.34296100
H	-4.86861300	0.93806200	-0.44263600
H	-4.77115400	-0.81105100	-0.50830500
C	-3.72069300	1.46219300	-3.57454000
H	-3.05780000	2.36916100	-1.73630600
H	-1.77881700	1.52219600	-2.58377600
C	-2.16156400	1.53463700	3.87138600
H	-0.66437600	1.25948900	2.32495200
H	-1.40818600	-0.22522000	2.88069300
C	-3.47347600	3.09235800	2.38277300
H	-1.99000400	2.87383800	0.83419700
H	-3.61672000	2.47796000	0.31612900
C	-3.48694300	-4.52818000	0.74808100
H	-3.87412600	-3.80576500	2.76341300
H	-2.16550900	-3.90162300	2.34102300
H	-2.78599900	-4.84493400	-1.28801800
H	-1.50979000	-4.57295800	-0.10978900
C	-5.20953600	1.34168400	-3.21408000
H	-6.52611900	0.05569100	-2.05205400
H	-5.26169700	-0.80231000	-2.93083400
H	-3.54291400	2.37431000	-4.15830300
H	-3.43372500	0.61568600	-4.21503200
C	-2.50479400	2.99944000	3.56985400
H	-1.42260400	1.47015900	4.68020000
H	-3.06409500	1.01595900	4.22497400
H	-3.67866500	4.14242600	2.13881900
H	-4.43525900	2.63821400	2.66145100
H	-3.44969100	-5.58686000	1.03300000
H	-4.51475300	-4.32326600	0.41630100
H	-5.82243600	1.30226100	-4.12321800
H	-5.51904000	2.24067400	-2.66187900
H	-2.93212900	3.48454100	4.45616100
H	-1.58108000	3.54232900	3.32286200

IM3

Sum of electronic and thermal Free Energies= -2129.649281

C	-1.41700000	0.47612400	1.61451100
C	-0.50739100	1.21673500	0.89396000
H	-1.03004600	-0.09895100	2.45619300
C	-2.93129400	0.56314300	1.50681100
H	-3.22859200	1.58062000	1.24529100
H	-3.36798300	0.36096100	2.49022000
C	-0.79908900	2.20713800	-0.21691200
H	-0.97651800	3.20988800	0.19796200
H	0.11158400	2.28108700	-0.82151100
H	0.52778800	1.20078600	1.23306100
C	-1.97969100	1.81332600	-1.14607400
H	-2.92947100	2.12324900	-0.70549600
H	-1.87965600	2.37308600	-2.08164700
C	-3.52939800	-0.45000400	0.49234900
H	-3.60555000	-1.42879000	0.97842100
H	-4.55753000	-0.15160000	0.24122700
C	-2.01258100	0.32603300	-1.46420900
C	-2.71076300	-0.64108100	-0.77019600
H	-1.59317400	0.03648300	-2.42804500
H	-2.82591000	-1.61280500	-1.25051500
Ni	-0.71378000	-0.66565300	-0.08677100
C	3.99626400	0.35413900	1.14206600
C	2.93053400	-0.54861400	1.21014300
C	2.10347500	-0.79877000	0.09334400
C	2.39456200	-0.09779400	-1.10036200
C	3.46032700	0.80228300	-1.16996800
C	4.27158600	1.03781800	-0.05003300

H	4.61437100	0.52402400	2.02116900
H	2.72687200	-1.06785700	2.14509300
H	1.76454900	-0.24352200	-1.97382700
H	3.65611800	1.32977600	-2.10126800
H	5.09877700	1.74113500	-0.10542600
C	0.95221700	-1.71599600	0.22199500
H	0.90077500	-2.24759600	1.17430800
C	0.18776800	-2.22237800	-0.86825000
H	-0.37998600	-3.14229800	-0.72000600
H	0.50225500	-2.06200000	-1.90066600

IM4

Sum of electronic and thermal Free Energies= -2244.190722

C	2.33018800	0.53500500	-1.49754400
C	1.26614700	1.20013900	-0.90025500
H	2.12004000	-0.00158800	-2.42324100
C	3.80412700	0.75242300	-1.17603800
H	3.97337600	1.79572800	-0.90059400
H	4.39303300	0.57672600	-2.08155600
C	1.34274900	2.22278500	0.21940700
H	1.53091600	3.22415500	-0.19354600
H	0.35366900	2.26756500	0.68780800
H	0.30662900	1.16488600	-1.41744100
C	2.39930600	1.90996600	1.31471400
H	3.37889100	2.28672800	1.01455000
H	2.12549500	2.45536800	2.22330900
C	4.33629600	-0.19306400	-0.06294200
H	4.58578400	-1.15890500	-0.51370500
H	5.27528900	0.21014100	0.34105500
C	2.49456900	0.43030600	1.64011100
C	3.35473200	-0.46526000	1.06190800
H	1.90839700	0.08192600	2.49058700
H	3.42366400	-1.45470300	1.51413200
Ni	1.48004900	-0.64678100	-0.03960300
C	-5.56691300	-0.42828500	0.40429200
C	-4.25989900	-0.89275600	0.59531700
C	-3.15246600	-0.09471300	0.26136000
C	-3.38924600	1.18473300	-0.26968200
C	-4.69387800	1.65573000	-0.46207900
C	-5.78936800	0.84944400	-0.12617900
H	-6.41055700	-1.06026200	0.67237100
H	-4.09611800	-1.88546000	1.01104100
H	-2.54367100	1.81864900	-0.53161700
H	-4.85562800	2.65092200	-0.87006100
H	-6.80346100	1.21362400	-0.27210200
C	-1.74183500	-0.61477500	0.42275900
C	-1.26178500	-1.39179800	-0.81734600
H	-1.67090200	-1.26927000	1.29700100
H	-1.05652100	0.22153800	0.60204400
C	0.17774900	-1.87922000	-0.72301800
H	-1.92371200	-2.25675300	-0.97891100
H	-1.35616900	-0.76510900	-1.71290000
H	0.53478200	-2.38921300	-1.63545100
O	0.68281900	-2.28760000	0.43467600

IM5

Sum of electronic and thermal Free Energies= -2244.158697

C	2.90607400	-0.36564000	1.43929600
C	1.55451200	-0.70658100	1.53568300
H	3.28765100	0.35744400	2.16462900
C	3.96142200	-1.17914400	0.69755200
H	3.67424400	-2.23415500	0.67982400
H	4.90958800	-1.13400100	1.24512900
C	0.90163500	-1.87065600	0.80576500
H	1.09244300	-2.81819900	1.33138000
H	-0.18138900	-1.71601800	0.84244400
H	0.97116400	-0.28427400	2.35623800
C	1.33740100	-2.03009400	-0.68837700
H	2.19346400	-2.70739200	-0.75196000
H	0.52185000	-2.51897600	-1.23175900
C	4.19775800	-0.66478300	-0.75036200
H	4.92287300	0.15637900	-0.71800100
H	4.66299300	-1.46053100	-1.35225100
C	1.67887100	-0.71403100	-1.37997600
C	2.94273500	-0.13475300	-1.42347300
H	0.93951800	-0.34297400	-2.09234900
H	3.10868500	0.64588400	-2.16871800
Ni	1.78775400	0.73136500	0.10506900
C	-4.62863000	-1.21861800	-1.17828500
C	-3.36219900	-0.62406500	-1.11539100
C	-2.93599600	0.04492400	0.04377000
C	-3.81003200	0.10367700	1.14223100
C	-5.07706600	-0.48884400	1.08544000
C	-5.49181800	-1.15239300	-0.07705000
H	-4.93921900	-1.73605800	-2.08301300
H	-2.69498100	-0.68415600	-1.97343600
H	-3.49338300	0.61359300	2.05038700
H	-5.73803100	-0.43679100	1.94750800
H	-6.47419600	-1.61616200	-0.12217200
C	-1.58094800	0.71380200	0.09587200

C	-1.64515800	2.19737100	-0.30142000
H	-0.88502600	0.19975400	-0.57187200
H	-1.15476800	0.63571100	1.10101700
C	-0.31973700	2.90432100	-0.23881600
H	-2.04166000	2.30627500	-1.32278500
H	-2.35167900	2.74437800	0.33833200
H	-0.32485600	3.99662100	-0.37649500
O	0.77058100	2.33355800	-0.04859400

IM6

Sum of electronic and thermal Free Energies= -2553.761673

C	-1.97408900	-0.21869300	-1.71476000
C	-0.67156700	0.24561200	-1.89512100
H	-2.35936200	-0.84939900	-2.52339900
C	-3.07124700	0.44243300	-0.90819300
H	-2.69541100	0.83191600	0.03350900
H	-3.82248200	-0.30715500	-0.63938100
C	0.00748100	1.40823300	-1.17126200
H	0.52203500	1.04658500	-0.27676200
H	0.79304100	1.79026200	-1.83223300
H	-0.19564800	-0.02313100	-2.83621900
C	-0.88227600	2.59952700	-0.73366500
H	-1.47338000	2.31629300	0.13804500
H	-0.20727600	3.39172500	-0.38874400
C	-3.79289800	1.54896500	-1.70908200
H	-4.28570200	1.08431500	-2.57400700
H	-4.61357900	1.94660800	-1.09291400
C	-1.76269400	3.15337900	-1.83206900
C	-2.96797100	2.70800100	-2.22668700
H	-1.35261900	4.00462500	-2.37730200
H	-3.44516200	3.25471400	-3.04205200
Ni	-0.70096400	-1.52441500	-0.79545800
C	4.81101700	2.16850000	0.60177500
C	3.68049600	1.35439900	0.46062900
C	3.80168700	-0.04278500	0.37098200
C	5.08881600	-0.60435100	0.42666400
C	6.22316500	0.20420800	0.56645500
C	6.08856500	1.59616500	0.65378500
H	4.69489100	3.24754100	0.67336600
H	2.69334500	1.81020100	0.42191300
H	5.20239200	-1.68514600	0.36264400
H	7.21006200	-0.25072100	0.61083600
H	6.96772600	2.22618300	0.76508200
C	2.58529300	-0.91912400	0.16897100
C	2.30009400	-1.17572700	-1.32071700
H	1.70598800	-0.45454100	0.62440200
H	2.71927400	-1.88208900	0.67062500
C	1.07629100	-2.04230200	-1.57284400
H	2.19779200	-0.23087600	-1.86392400
H	3.16629000	-1.68696800	-1.76793100
H	0.89789500	-2.27740400	-2.63722300
O	0.66603800	-2.89535100	-0.68076400
C	-1.35020400	1.16288500	3.05211600
C	-0.96307700	0.00564900	2.37334100
C	-1.92061300	-0.92357300	1.92299500
C	-3.27555300	-0.68764300	2.21832200
C	-3.66479600	0.46451400	2.90766600
C	-2.70619400	1.40010200	3.31779600
H	-0.59796000	1.87977000	3.37169500
H	0.08843600	-0.17341700	2.16368400
H	-4.02686100	-1.40754500	1.90525800
H	-4.71682200	0.63366900	3.12389500
H	-3.01072800	2.29995400	3.84623700
C	-1.47590800	-2.10312900	1.14861700
H	-0.54994400	-2.56515600	1.48882700
C	-2.20291600	-2.74384400	0.17239800
H	-1.89429600	-3.72038600	-0.19145100
H	-3.19865700	-2.41241100	-0.10621000

IM7

Sum of electronic and thermal Free Energies= -2553.761231

C	1.48664700	0.94231200	0.24245000
C	0.49851800	1.09725100	1.21597600
H	2.48483600	0.67441200	0.59746800
C	1.48654400	1.66904700	-1.08419800
H	0.46685600	1.80347000	-1.45009900
H	2.00719900	1.07392000	-1.83995300
C	-0.75388400	1.95996100	1.07366200
H	-1.50312000	1.46577800	0.45186400
H	-1.20285200	2.05546600	2.06691500
H	0.80426300	0.92039000	2.24722900
C	-0.55093300	3.38706900	0.47098900
H	-0.63366000	3.32878800	-0.61695600
H	-1.39367800	4.00492600	0.80128000
C	2.23958000	3.02327900	-0.98218300
H	3.31326200	2.80160200	-0.94160200
H	2.09247300	3.58008700	-1.91942100
C	0.74431800	4.07272200	0.83509100
C	1.91892900	3.91918400	0.20083000
H	0.71793100	4.74368500	1.69449900

H	2.76465900	4.49762500	0.57509600
Ni	0.51717700	-0.82315000	0.41562700
C	-5.78911200	1.09418200	-0.91499900
C	-4.46364800	0.69743300	-0.69895600
C	-4.14917400	-0.63637400	-0.38829500
C	-5.19987700	-1.56542600	-0.29930100
C	-6.52716400	-1.17505600	-0.51354300
C	-6.82746400	0.15846400	-0.82182500
H	-6.01077200	2.13075200	-1.15846000
H	-3.66419400	1.43215500	-0.77671900
H	-4.97511600	-2.60407200	-0.06313000
H	-7.32558500	-1.91025700	-0.44363300
H	-7.85724400	0.46349700	-0.99137900
C	-2.72245100	-1.05258300	-0.10818400
C	-2.37789600	-0.97432100	1.39112700
H	-2.02600500	-0.41604600	-0.66692900
H	-2.54573400	-2.07635100	-0.45158900
C	-0.95191400	-1.38701000	1.71128200
H	-2.56816000	0.02824400	1.78270200
H	-3.04450200	-1.64868500	1.95018600
H	-0.61707600	-1.16874100	2.73818400
O	-0.40589400	-2.38248100	1.08499000
C	5.30832500	-1.33495700	0.81214000
C	4.01985100	-1.85069300	0.65255100
C	3.29568300	-1.63687600	-0.53727000
C	3.91374000	-0.91572100	-1.57655200
C	5.20179300	-0.39774400	-1.41792500
C	5.90350200	-0.59876600	-0.22151000
H	5.84703200	-1.50244100	1.74164700
H	3.55499100	-2.40898800	1.46255100
H	3.39341900	-0.77421300	-2.51968900
H	5.66288000	0.15702900	-2.23154200
H	6.90563100	-0.19530600	-0.10022700
C	1.91565600	-2.15134900	-0.63110500
H	1.71369100	-3.04695400	-0.04651200
C	0.92695200	-1.69660700	-1.47613900
H	0.02024700	-2.28004900	-1.61489900
H	1.10540200	-0.90621100	-2.19905400

IM8

Sum of electronic and thermal Free Energies= -3601.815226

Ni	0.00004800	-0.00065000	0.24975700
P	2.13004700	0.06056700	0.06068200
C	2.84757200	-1.61128800	-0.39077800
C	3.12382700	0.59445100	1.57263300
C	2.66096900	1.20121300	-1.33108700
C	4.37317000	-1.70411200	-0.56919000
C	2.34169200	-2.68486300	0.59599400
H	2.37687100	-1.83272600	-1.35804500
C	4.45509400	1.33240900	1.32410400
C	2.23112400	1.40352400	2.53968200
H	3.36074600	-0.35498300	2.07383200
C	2.21051700	0.63264500	-2.69338100
C	2.02841500	2.59214900	-1.10030600
H	3.75360200	1.30217700	-1.33880500
C	4.79039100	-3.11429100	-1.02431100
H	4.86707800	-1.48087200	0.38523800
H	4.72425700	-0.95832100	-1.29209600
C	2.76315400	-4.09397600	0.14772700
H	2.74890900	-2.49173200	1.59826800
H	1.24939600	-2.61177900	0.68017900
C	5.18334000	1.61854400	2.64988300
H	4.25937100	2.28617400	0.81869000
H	5.10562100	0.75489600	0.66052700
C	2.95713700	1.69978300	3.86150900
H	1.94237400	2.35024000	2.06344600
H	1.29710300	0.85599200	2.71845500
C	2.48961500	1.60910500	-3.84797600
H	1.13320900	0.41713100	-2.64291300
H	2.71400500	-0.31834100	-2.89771100
C	2.32077700	3.56262500	-2.25496200
H	0.94130700	2.45992600	-0.99534300
H	2.37837400	3.02255300	-0.15584100
C	4.28444300	-4.19050600	-0.05060500
H	5.88216900	-3.16924400	-1.11843200
H	4.37585100	-3.30593800	-2.02413700
H	2.42709300	-4.83691800	0.88179000
H	2.25854200	-4.33309200	-0.79913200
C	4.29601700	2.41456800	3.61944300
H	6.11489100	2.16347300	2.45177700
H	5.46740200	0.66500500	3.11725900
H	2.31528400	2.30389000	4.51497200
H	3.14339600	0.75277700	4.38793400
C	1.85270000	2.98320600	-3.59756200
H	2.12027600	1.18150200	-4.78853600
H	3.57622800	1.73132200	-3.96142800
H	1.83125000	4.52535000	-2.06165100
H	3.40131700	3.75983300	-2.30147900
H	4.55852000	-5.18922700	-0.41249300
H	4.78246600	-4.05807600	0.92055300
H	4.82003400	2.57568300	4.56972600

H	4.10082400	3.40876200	3.19264100
H	2.09360200	3.67092000	-4.41757500
H	0.75859700	2.87671000	-3.58152700
P	-2.12997800	-0.06110000	0.06078800
C	-2.84624100	1.61105300	-0.39161500
C	-3.12431700	-0.59351800	1.57286000
C	-2.66152500	-1.20205700	-1.33047500
C	-4.37174000	1.70483700	-0.57039200
C	-2.33984800	2.68480700	0.59470100
H	-2.37515500	1.83165700	-1.35888600
C	-4.45608400	-1.33062800	1.32452000
C	-2.23228700	-1.40277500	2.54036600
H	-3.36061800	0.35632000	2.07358100
C	-2.21050800	-0.63443600	-2.69297700
C	-2.02994000	-2.59330000	-1.09892700
H	-3.75422300	-1.30229500	-1.33828100
C	-4.78787800	3.11505100	-1.02639500
H	-4.86599300	1.48247200	0.38406300
H	-4.72320800	0.95888500	-1.29294600
C	-2.76019700	4.09396400	0.14553000
H	-2.74746700	2.49253000	1.59697500
H	-1.24762800	2.61102700	0.67921700
C	-5.18466700	-1.61564100	2.65035600
H	-4.26099600	-2.28475700	0.81954700
H	-5.10611600	-0.75292700	0.66061700
C	-2.95864100	-1.69792600	3.86225100
H	-1.94416600	-2.34990700	2.06457200
H	-1.29789600	-0.85581900	2.71897200
C	-2.49008100	-1.61126400	-3.84714200
H	-1.13306800	-0.41959400	-2.64243600
H	-2.71334200	0.31678200	-2.89783500
C	-2.32278000	-3.56413200	-2.25316400
H	-0.94276000	-2.46175100	-0.99384600
H	-2.38034800	-3.02300700	-0.15430900
C	-4.28137000	4.19147000	-0.05320500
H	-5.87959800	3.17072100	-1.12076800
H	-4.37300300	3.30583300	-2.02624700
H	-2.42377300	4.83708400	0.87924700
H	-2.25518800	4.33217600	-0.80134600
C	-4.29801000	-2.41185900	3.62036800
H	-6.11658700	-2.15999500	2.45240700
H	-5.46809000	-0.66168600	3.11726900
H	-2.31729000	-2.30220200	4.51605000
H	-3.14427300	-0.75055300	4.38823600
C	-1.85412300	-2.98567000	-3.59597600
H	-2.12031900	-1.18435900	-4.78785300
H	-3.57675900	-1.73281100	-3.96069700
H	-1.83393200	-4.52709600	-2.05932100
H	-3.40344600	-3.76063500	-2.29974500
H	-4.55465100	5.19017600	-0.41573500
H	-4.77970300	4.05996400	0.91791900
H	-4.82224000	-2.57216700	4.57067000
H	-4.10348700	-3.40638700	3.19403800
H	-2.09537200	-3.67361800	-4.41569100
H	-0.75995100	-2.87990200	-3.57983900

IM9

Sum of electronic and thermal Free Energies= -4025.964266

Ni	-0.10060600	0.06049500	-0.73911700
P	0.00914300	2.06540400	0.12782800
C	-0.99243700	3.30863700	-0.86295600
C	1.69530600	2.93728100	0.12149300
C	-0.68391300	2.23127300	1.86478600
C	-1.15788800	4.71823200	-0.25836300
C	-0.45650900	3.41949900	-2.30671500
H	-1.98589000	2.84800000	-0.92370700
C	2.40925600	3.12769900	1.47420200
C	2.61566500	2.24076100	-0.90232000
H	1.49421000	3.94663200	-0.25609000
C	-2.22339900	2.11594600	1.89785400
C	-0.09066900	1.13258200	2.76884700
H	-0.40235100	3.21493100	2.26180700
C	-2.10058800	5.57391600	-1.12534300
H	-0.18143900	5.21609900	-0.19739500
H	-1.54604400	4.66957900	0.76370200
C	-1.40486500	4.25575300	-3.18063500
H	0.52841600	3.90415000	-2.29874900
H	-0.31205200	2.42178500	-2.73419900
C	3.74679600	3.86742800	1.29387700
H	2.61100200	2.16160200	1.94413500
H	1.77135700	3.68563200	2.16781800
C	3.96129100	2.96348300	-1.05941000
H	2.78736000	1.21113400	-0.57881000
H	2.11223200	2.16346100	-1.87190600
C	-2.75913100	2.23385100	3.33515700
H	-2.51428100	1.14269700	1.48861300
H	-2.69782200	2.87557200	1.27038500
C	-0.60931700	1.22764100	4.21098900
H	-0.37121800	0.16166900	2.33973900
H	1.00025800	1.16841800	2.76710300
C	-1.61834900	5.65528700	-2.58214100

H	-2.18813700	6.58032800	-0.69746200	H	-1.34219500	-2.36872600	0.13506300
H	-3.10622600	5.13102900	-1.10046500	H	-0.51172100	-2.85375100	1.61003400
H	-1.00428300	4.33476400	-4.19885200	C	-0.47242100	-5.04195800	-1.67772000
H	-2.37174300	3.73891300	-3.25839800	H	-0.28204400	-2.94823400	-2.20358600
C	4.66195500	3.14222800	0.29557500	H	1.23529500	-3.84396100	-2.23336100
H	4.24463200	3.96720700	2.26631400	C	3.97284900	-1.76583500	3.96844300
H	3.55139300	4.88635200	0.93094600	H	3.06198900	-3.72336700	4.23224000
H	4.60164900	2.40281800	-1.75199300	H	1.93099800	-2.37594900	4.33139800
H	3.79241900	3.95093600	-1.51190100	H	4.52245100	0.25462100	3.36756100
C	-2.14294900	1.17054500	4.25628900	H	2.82724700	0.06356900	3.81066100
H	-3.85241900	2.14324700	3.32788500	C	4.73046200	-2.29001200	-3.48125500
H	-2.52645400	3.23445500	3.72605400	H	5.66247400	-3.62146700	-2.03305900
H	-0.17736900	0.41722800	4.81163600	H	5.71525700	-1.91548400	-1.59326600
H	-0.26464700	2.17112600	4.65708400	H	3.59763500	-0.76342900	-4.54183800
H	-2.33460600	6.22442900	-3.18741800	H	4.44785400	-0.17539400	-3.11335200
H	-0.66775500	6.20648800	-2.61483800	C	-1.77561000	-4.94138500	-0.87143600
H	5.60146200	3.69424700	0.17021300	H	-2.42495700	-4.37166400	1.12814400
H	4.92606400	2.15459400	0.69974200	H	-0.89998400	-5.25378100	1.08191000
H	-2.50199100	1.30032200	5.28457400	H	-0.68631400	-5.34464600	-2.71060800
H	-2.47448000	0.17572800	3.92648300	H	0.15855200	-5.83042800	-1.24190200
P	1.42302700	-1.55252500	-0.12220800	H	4.18438700	-1.61719700	5.03438700
C	2.09981300	-1.58703100	1.64941100	H	4.88128100	-2.19305000	3.52068400
C	2.94376100	-1.59436800	-1.21613900	H	5.64739500	-2.14059200	-4.06467300
C	0.59072900	-3.23125300	-0.24515100	H	4.17902900	-3.11077800	-3.96173600
C	2.43225800	-2.94457100	2.30697900	H	-2.30108200	-5.90451100	-0.86892300
C	3.29623100	-0.62915300	1.81299000	H	-2.44317700	-4.21435600	-1.35548300
H	1.27030400	-1.16109200	2.22319200	C	-1.74940700	0.15069700	-1.74019700
C	3.81720700	-2.86321000	-1.17392400	O	-1.06691100	-0.94407100	-2.05641600
C	2.59285400	-1.19227800	-2.66564900	H	-1.81602200	0.93777500	-2.50996400
H	3.55407600	-0.77365100	-0.81824100	C	-3.02833300	-0.04526600	-0.93674800
C	-0.71808800	-3.15444100	0.57560200	H	-3.46786700	0.92321500	-0.67138800
C	0.29978400	-3.71012300	-1.68264400	H	-2.78775200	-0.56101600	-0.00015300
H	1.25568200	-3.97102200	0.21641700	C	-4.06439300	-0.89834800	-1.70777900
C	2.80983000	-2.75225600	3.78857300	H	-4.40326600	-0.34664000	-2.59276000
H	3.26364000	-3.42925700	1.78131100	H	-3.55173900	-1.79921100	-2.06190300
H	1.58166400	-3.62935600	2.25198300	C	-5.24074300	-1.27925800	-0.83897300
C	3.66344600	-0.42345200	3.29026200	C	-6.43128600	-0.53403900	-0.84589100
H	4.17046800	-1.04052700	1.29236600	C	-5.14074400	-2.36548000	0.04958400
H	3.08005600	0.33237000	1.34397200	C	-7.49366500	-0.86333800	0.00631000
C	5.07875200	-2.69256100	-2.04000600	H	-6.52782800	0.31109000	-1.52531800
H	3.24478600	-3.72548100	-1.53505800	C	-6.19755900	-2.69954400	0.90330100
H	4.11002600	-3.09100000	-0.14444700	H	-4.22483400	-2.95357600	0.06956200
C	3.86542900	-1.02002500	-3.50931800	C	-7.38098800	-1.94798800	0.88538400
H	1.95482600	-1.95450300	-3.12548800	H	-8.40862400	-0.27559300	-0.01753400
H	2.00827500	-0.26541400	-2.65482900	H	-6.10066700	-3.54593800	1.57966500
C	-1.48911800	-4.48258900	0.56521000	H	-8.20497900	-2.20648600	1.54612900

H-3

Sum of electronic and thermal Free Energies= -3288.70192

Ni	-0.19827900	-1.22075800	-0.13947900
C	1.32766400	-1.05880400	-1.14000400
O	1.35086600	-0.84537600	-2.35270600
C	-1.31844600	-3.17718100	0.33379900
C	-2.46857600	-3.54327600	-0.42285800
C	-3.74440600	-3.48189900	0.12899000
C	-3.93897600	-3.02666300	1.44628000
C	-2.83256500	-2.62651200	2.19757000
C	-1.54305700	-2.69562400	1.65238300
H	-2.34591200	-3.89548900	-1.44257100
H	-4.60213100	-3.78046800	-0.46948800
H	-4.94012200	-2.97292800	1.86574400
H	-2.96399800	-2.26110000	3.21322300
H	-0.68612100	-2.43514300	2.27027700
C	2.63558300	-1.18506700	-0.34712000
H	2.50190700	-0.68569900	0.61927400
H	2.74893100	-2.25012700	-0.11021100
C	3.88703200	-0.66431700	-1.07906400
H	4.03988700	-1.26136800	-1.98317200
H	3.70882800	0.36347800	-1.40841700
C	5.10759500	-0.72172100	-0.18919900
C	5.90705800	-1.87600100	-0.13003300
C	5.43917700	0.36211100	0.64244000
C	7.00668200	-1.94731300	0.73384000
H	5.66663900	-2.72490000	-0.76779000
C	6.53741600	0.29689700	1.50822800
H	4.83265300	1.26557800	0.60927000
C	7.32618800	-0.86016600	1.55813500
H	7.61523300	-2.84833000	0.76186700
H	6.77955500	1.14808200	2.14056300
H	8.18107700	-0.91259100	2.22795900
P	-0.87775400	0.92299600	-0.09221800
C	0.16995900	2.06516700	-1.14377200
C	-0.46098900	3.39135200	-1.61451100
C	1.54095600	2.34603800	-0.49358800
H	0.36066300	1.44857900	-2.03093800
C	0.47208500	4.10559900	-2.61017600
H	-0.63202100	4.04815400	-0.75326500
H	-1.43407400	3.22456100	-2.08612500
C	2.48347700	3.04156700	-1.48909100
H	1.40954700	3.00100200	0.37731300
H	1.99222100	1.42252600	-0.12243800
C	1.86658200	4.34797700	-2.01199500
H	0.02189800	5.05610700	-2.92158200
H	0.56677500	3.48822600	-3.51428900
H	3.45048600	3.23954700	-1.01052000
H	2.67808000	2.36574700	-2.33285300
H	2.52511100	4.80790700	-2.75869400
H	1.78207200	5.06195300	-1.18060700
C	-1.00563700	1.75025500	1.58556500
C	-2.02859700	2.90005600	1.70027700
C	-1.20635900	0.71003700	2.70795400
H	-0.00683600	2.18022700	1.73425600
C	-1.97412300	3.54930500	3.09454100
H	-3.04108900	2.51643000	1.53020000
H	-1.84830800	3.65762600	0.93231800
C	-1.16597200	1.36843400	4.09579300
H	-2.16554600	0.19707900	2.57617300
H	-0.43251400	-0.06194700	2.63005800
C	-2.18603500	2.51176200	4.20697900
H	-2.73000400	4.34133000	3.16117900
H	-0.99603200	4.03186600	3.22985700
H	-1.35192000	0.61275600	4.86887200
H	-0.15720400	1.76579500	4.27650400
H	-2.11591200	2.99018700	5.19140700
H	-3.20158900	2.09884800	4.12597800
C	-2.56618300	0.98324800	-0.88558700
C	-2.47002900	0.43423700	-2.32733200
C	-3.57169500	0.14757300	-0.07102200
H	-2.90925300	2.02460800	-0.91898100
C	-3.84827700	0.37937000	-3.00504900
H	-2.04409200	-0.57844500	-2.28728300
H	-1.78556400	1.03866400	-2.93136400
C	-4.94853500	0.08000700	-0.74882800
H	-3.17509800	-0.86522700	0.03600700
H	-3.68293500	0.54670300	0.94107500
C	-4.84236700	-0.45427800	-2.18397400
H	-3.74407000	-0.03436700	-4.01555300
H	-4.23604300	1.40152600	-3.11900800
H	-5.61359800	-0.55686300	-0.15302900
H	-5.39726500	1.08342300	-0.76572200
H	-5.82810200	-0.45698700	-2.66515700
H	-4.49812000	-1.49707100	-2.15247200
C	0.04785600	-3.17259700	-0.20924600
H	0.79156200	-3.42700500	0.55449400
C	0.30941200	-3.88407500	-1.52846600
H	1.37028800	-3.82268300	-1.79002000
H	0.03593200	-4.94911000	-1.49032500

H	-0.24605900	-3.42435400	-2.35284400

H-TS2

Sum of electronic and thermal Free Energies= -3288.682353

Ni	-0.41930400	1.23143500	0.28670500
C	1.14287400	1.21234100	1.34070500
O	1.11400400	0.98605700	2.57055200
C	-0.37118600	3.26994100	-0.10481100
C	-1.64634200	3.73171100	0.32622300
C	-2.65601100	4.02446800	-0.59409000
C	-2.44757000	3.84950200	-1.96920900
C	-1.20975700	3.36918000	-2.41718500
C	-0.18703200	3.08394100	-1.50645000
H	-1.83535200	3.87680900	1.38473300
H	-3.61806100	4.38137400	-0.23380000
H	-3.24031500	4.07307200	-2.67820000
H	-1.03513500	3.21853000	-3.47993600
H	0.78143000	2.74953600	-1.87120800
C	2.33364300	0.67570700	0.52915300
H	2.26984400	-0.41691200	0.56558500
H	2.25427200	0.97072100	-0.52245900
C	3.69960400	1.11409000	1.10103000
H	3.77564800	2.20676200	1.06668100
H	3.73925900	0.81861300	2.15396600
C	4.83866200	0.48894600	0.32816700
C	5.42601200	1.15405200	-0.76114200
C	5.29066900	-0.80477200	0.64204800
C	6.43800300	0.54720400	-1.51561600
H	5.08793500	2.15592500	-1.02035700
C	6.30153900	-1.41653900	-0.10792900
H	4.84555800	-1.33584500	1.48177600
C	6.87970800	-0.74221100	-1.19214200
H	6.88234600	1.08034700	-2.35303600
H	6.63985000	-2.41662300	0.15356200
H	7.66642100	-1.21480400	-1.77523900
P	-1.11739000	-0.80179700	0.00969400
C	0.01025000	-1.80693000	-1.08462400
C	-0.46597700	-3.23158900	-1.42480300
C	0.36409400	-1.02523200	-2.36723400
H	0.93439000	-1.89049700	-0.49927900
C	0.60023200	-3.98030100	-2.24433800
H	-1.39191300	-3.17822800	-2.01129600
H	-0.69874600	-3.79192300	-0.51227100
C	1.42542400	-1.77363300	-3.18994300
H	-0.53673900	-0.88924600	-2.98102800
H	0.71770400	-0.02184800	-2.10481900
C	0.97583800	-3.20634900	-3.51774500
H	0.23551400	-4.98232800	-2.50119700
H	1.49710800	-4.11796100	-1.62432100
H	1.63945300	-1.22082400	-4.11275500
H	2.36196600	-1.80787300	-2.61587700
H	1.76523900	-3.73631100	-4.06445800
H	0.10202500	-3.16519000	-4.18340700
C	-2.79148300	-0.86698100	-0.85442400
C	-3.72316200	-2.03215200	-0.46386300
C	-3.52524800	0.48421500	-0.72556100
H	-2.53027900	-0.99020000	-1.91454900
C	-5.01278100	-2.01051000	-1.30388500
H	-3.99454000	-1.94744100	0.59579100
H	-3.21847400	-2.99565600	-0.58469900
C	-4.82478400	0.50275000	-1.54475200
H	-3.75427700	0.67925600	0.33072900
H	-2.86995600	1.29621000	-1.05339600
C	-5.74683600	-0.66758900	-1.17225400
H	-5.66669700	-2.83526000	-0.99497500
H	-4.75894900	-2.18493400	-2.35894700
H	-5.33961600	1.46026300	-1.39860900
H	-4.57302600	0.43935500	-2.61296800
H	-6.64495200	-0.66164300	-1.80193900
H	-6.08599800	-0.54392500	-0.13398300
C	-1.30405300	-1.78078300	1.58833100
C	0.05090900	-2.26416400	2.14733100
C	-2.03168300	-0.89362400	2.62309200
H	-1.91960300	-2.66445800	1.38228700
C	-0.13388200	-2.98817900	3.49263200
H	0.71290300	-1.40337000	2.28745400
H	0.53794500	-2.94322600	1.43920200
C	-2.20761300	-1.61748800	3.96719600
H	-1.43946200	0.02010600	2.76526800
H	-3.01009600	-0.58144900	2.23996800
C	-0.86045000	-2.10647200	4.51916300
H	0.84510100	-3.29650400	3.88001900
H	-0.71438900	-3.90785200	3.33147600
H	-2.69547700	-0.94818300	4.68654100
H	-2.87768800	-2.47814200	3.82997200
H	-1.01041400	-2.65849400	5.45523600
H	-0.23197400	-1.23789700	4.75852000
C	0.75054900	2.97460600	0.85735600
H	1.69428300	3.16463700	0.34324600
C	0.67243600	3.70979400	2.18863500
H	-0.13211900	3.31062100	2.81173300

H	1.60166300	3.57792100	2.74782400
H	0.49817000	4.78159000	2.03549100

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Sum of electronic and thermal Free Energies= -3288.698098

Ni	0.89908900	1.71084400	0.27555700
C	-2.54478000	2.63322200	-0.72034400
O	-2.81982100	2.85485700	-1.89521600
C	-0.44809400	3.46459300	0.37686300
C	0.07252000	3.17414600	1.66479000
C	1.47132000	3.06811300	1.87340400
C	2.36426500	3.25137400	0.79205600
C	1.85290600	3.48526300	-0.50751200
C	0.45377300	3.58259500	-0.71512300
H	-0.60717200	3.04919000	2.50273600
H	1.85369300	2.83984600	2.86327800
H	3.43359100	3.15356300	0.94741800
H	2.53042300	3.57643400	-1.35077800
H	0.07036200	3.76230400	-1.71463100
C	-2.74731000	1.26750100	-0.09315100
H	-2.94520200	1.37960500	0.97711000
H	-1.77140700	0.76877900	-0.15239600
C	-3.84529800	0.43267800	-0.77091000
H	-3.62549300	0.34978100	-1.83814000
H	-4.79649700	0.97223700	-0.68667500
C	-3.97488300	-0.94370900	-0.15257400
C	-3.64330800	-2.09406500	-0.88173000
C	-4.39991700	-1.09918400	1.17841400
C	-3.70595100	-3.36530100	-0.29747100
H	-3.33000600	-1.99316600	-1.91688800
C	-4.47394000	-2.36545000	1.76570700
H	-4.66926800	-0.22147000	1.76289200
C	-4.11902600	-3.50560400	1.03182900
H	-3.43013800	-4.24140700	-0.87988600
H	-4.80065700	-2.46409600	2.79816800
H	-4.16433300	-4.48945200	1.49226900
P	1.13671800	-0.37775800	-0.06695400
C	0.07228900	-1.12632300	-1.43215500
C	0.38428100	-2.57609200	-1.85198200
C	0.07114000	-0.18620800	-2.65537600
H	-0.94367200	-1.11405200	-1.01899400
C	-0.55796300	-3.07189800	-2.96385000
H	1.41266900	-2.63695400	-2.22725700
H	0.31859700	-3.24668900	-0.98720400
C	-0.88111200	-0.68317300	-3.75422700
H	1.08752800	-0.11811100	-3.06951300
H	-0.20131800	0.82579100	-2.33297300
C	-0.55431200	-2.12476600	-4.17335000
H	-0.26108600	-4.08217000	-3.27270500
H	-1.57659700	-3.15497700	-2.56744900
H	-0.83198100	-0.01355800	-4.62192900
H	-1.91381500	-0.63660300	-3.38238600
H	-1.26707800	-2.47343000	-4.93093400
H	0.44031000	-2.14400700	-4.64145800
C	2.88517300	-0.90121000	-0.60393000
C	3.37542600	-2.29627600	-0.15912100
C	3.93996000	0.16540200	-0.24598400
H	2.81461100	-0.91219100	-1.70123200
C	4.74139100	-2.63167800	-0.78468300
H	3.47803900	-2.32007400	0.93245500
H	2.65353500	-3.07408300	-0.41960000
C	5.31308700	-0.16773500	-0.85220900
H	4.03109300	0.24149700	0.84616500
H	3.59815200	1.14424600	-0.59340600
C	5.79313600	-1.56715400	-0.43984400
H	5.07262900	-3.62031000	-0.44245300
H	4.63200600	-2.69498100	-1.87679000
H	6.04701400	0.59143200	-0.55311700
H	5.23954500	-0.12116400	-1.94831900
H	6.74899900	-1.80250400	-0.92434500
H	5.97505100	-1.58110100	0.64436000
C	0.76944800	-1.44735000	1.43289300
C	-0.73111400	-1.42409100	1.78848300
C	1.59680500	-0.93035300	2.62984600
H	1.05733100	-2.48487900	1.22316400
C	-1.02342700	-2.20987900	3.07747300
H	-1.04748500	-0.38017100	1.91929700
H	-1.33672900	-1.83555000	0.97548100
C	1.31165100	-1.72209500	3.91554700
H	1.34734500	0.12868900	2.78399700
H	2.66815600	-0.96250900	2.40542000
C	-0.18469700	-1.70206000	4.25836700
H	-2.09269200	-2.14564200	3.30744900
H	-0.80291000	-3.27343200	2.90685200
H	1.90044000	-1.30921000	4.74451900
H	1.63959400	-2.76287100	3.78175900
H	-0.38149500	-2.30390700	5.15447400
H	-0.48460900	-0.67117000	4.49590300
C	-1.94159000	3.71555000	0.18061000
C	-2.21721300	5.12882000	-0.35502200
H	-3.29456600	5.31071000	-0.42182600

H	-1.79128200	5.26431000	-1.35177200
H	-1.77913100	5.87474000	0.31514800
H	-2.41862900	3.61099500	1.16079600

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Sum of electronic and thermal Free Energies= -3851.947089

C	2.16044100	1.36156100	-1.79018700
C	1.12977900	1.30441000	-2.94094500
Ni	0.71617000	0.53429700	-0.94502400
C	-0.52460200	1.06181600	-2.70688300
H	-0.80799000	0.88208100	-3.75196900
C	-1.21693000	2.34137600	-2.20605200
H	-0.97549600	3.16979000	-2.88269800
H	-0.83028600	2.61879200	-1.21760600
C	-2.74504500	2.17926600	-2.11112300
H	-3.14644500	1.96215400	-3.10857900
H	-2.96773600	1.31680200	-1.47828800
C	-3.40216300	3.41572800	-1.53758100
C	-3.74960300	4.50041300	-2.36018700
C	-3.63140600	3.52663100	-0.15559600
C	-4.30959000	5.66419800	-1.81916000
H	-3.58220300	4.43143700	-3.43369400
C	-4.18950800	4.68799700	0.39192700
H	-3.37413200	2.69457700	0.49605900
C	-4.53037700	5.76325600	-0.43891900
H	-4.57581500	6.49148400	-2.47309700
H	-4.36184700	4.75202100	1.46392400
H	-4.96677900	6.66539700	-0.01705700
H	1.11639200	2.27881100	-3.43233000
H	1.40763700	0.53950500	-3.66519400
H	2.39248800	2.38170000	-1.47798200
C	3.36268600	0.49296500	-1.88451600
C	4.62321200	0.96032300	-1.46117000
C	3.27707500	-0.83826200	-2.35222700
C	5.74647500	0.12760500	-1.47295600
H	4.72857000	1.98791900	-1.12291700
C	4.39804900	-1.66867000	-2.36593300
H	2.32173400	-1.22672300	-2.69689600
C	5.63998100	-1.19517500	-1.92004000
H	6.70591700	0.51384500	-1.13674800
H	4.30140100	-2.69349400	-2.71694300
H	6.51076300	-1.84597500	-1.92515800
P	1.17573500	0.36089900	1.14062800
C	2.45908800	-0.95864300	1.40775100
C	-0.36661900	-0.14367800	2.09043700
C	1.81016400	1.89852400	1.98274400
C	2.88326800	-1.22866700	2.86405400
C	2.04805700	-2.27227900	0.71114800
H	3.32538000	-0.56429100	0.85883900
C	-0.35057100	0.14922400	3.60668200
C	-1.65439900	0.43917700	1.46261200
H	-0.40538800	-1.23107800	1.94773300
C	3.27344900	2.22295100	1.62730200
C	0.89751900	3.09907000	1.65043200
H	1.75939900	1.70894400	3.06185200
C	4.04036100	-2.24227300	2.90620100
H	2.03339900	-1.64330100	3.41915900
H	3.17587300	-0.30249600	3.37038800
C	3.19006000	-3.29889200	0.76278500
H	1.15738500	-2.69152200	1.19470800
H	1.77787600	-2.06885400	-0.32940700
C	-1.60044700	-0.43982500	4.28541200
H	-0.34242300	1.23414600	3.77009700
H	0.55006200	-0.24840400	4.08156600
C	-2.90776500	-0.13609100	2.13915200
H	-1.65395100	1.52956200	1.57822600
H	-1.68485100	0.24532900	0.38893800
C	3.74780300	3.50092800	2.33826100
H	3.35463200	2.36864400	0.54767900
H	3.93579300	1.39115600	1.88533700
C	1.37864800	4.38484700	2.34191800
H	0.88972300	3.24218400	0.56135200
H	-0.13538100	2.89369600	1.94545800
C	3.65767300	-3.55439700	2.20384700
H	4.32410200	-2.43554500	3.94772800
H	4.91913100	-1.80507300	2.41207800
H	2.86367700	-4.23535100	0.29411000
H	4.03048200	-2.92110900	0.16653600
C	-2.89172900	0.10326100	3.65548000
H	-1.57453500	-0.21416200	5.35837200
H	-1.57952600	-1.53427200	4.18991500
H	-3.80451600	0.30704700	1.68888200
H	-2.95747900	-1.21465800	1.94229600
C	2.84335800	4.69568500	2.00393400
H	4.78482500	3.71355500	2.05191800
H	3.74600400	3.33360900	3.42432900
H	0.73140700	5.22061800	2.05045500
H	1.27407300	4.26692700	3.42939300
H	4.50652600	-4.24878500	2.20912000
H	2.84772600	-4.03904700	2.76703500
H	-3.76760700	-0.36158900	4.12388400

H	-2.96108000	1.18255500	3.85201200
H	3.17703900	5.58997200	2.54368100
H	2.92682000	4.92137400	0.93145900
O	-0.87345900	-0.07476400	-1.93587400
C	-5.80323100	-4.37717900	0.31169700
C	-4.93240900	-3.45251200	-0.27634700
C	-3.56320200	-3.42491200	0.05508700
C	-3.09418200	-4.35861200	1.00112000
C	-3.95761100	-5.28592800	1.59551800
C	-5.31614000	-5.29689800	1.25055900
H	-6.85724700	-4.38269200	0.04282400
H	-5.31625900	-2.73847100	-1.00147200
H	-2.04160700	-4.35247500	1.27466000
H	-3.57719200	-5.99771700	2.32489000
H	-5.99022000	-6.01605000	1.71050500
B	-2.59378300	-2.37305300	-0.59331400
O	-3.08775500	-1.44387900	-1.46855700
H	-2.36739000	-0.81949300	-1.76289900
O	-1.26025200	-2.42753600	-0.22946800
H	-0.74158800	-1.72262000	-0.65796300
C	1.20789500	-4.14239100	-3.92490100
C	0.36881500	-3.26275800	-3.00978700
H	0.74616100	-4.22152000	-4.91508200
H	2.21197900	-3.72145400	-4.04649800
H	1.30347800	-5.15013900	-3.50626300
H	0.83928600	-3.20230600	-2.01795900
H	-0.62980000	-3.70119300	-2.86623400
O	0.26369500	-1.96048600	-3.59815400
H	-0.19603400	-1.35801500	-2.96154600

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Sum of electronic and thermal Free Energies= -3851.937118

C	-0.83185000	0.70411700	-2.14992400
C	0.52007700	1.32890800	-2.06776800
Ni	-0.15268600	0.19080700	-0.45033900
C	1.84211600	0.77313000	-0.83564600
H	2.43167000	1.67547200	-0.99985800
C	2.48963100	-0.49072600	-1.41255900
H	2.90826500	-0.25683100	-2.39699200
H	1.72456200	-1.25776600	-1.57429800
C	3.58450400	-1.07887500	-0.50188000
H	4.41151200	-0.36737900	-0.41236900
H	3.16258700	-1.21085000	0.49814200
C	4.07720900	-2.40733500	-1.03301300
C	5.28375500	-2.51421400	-1.74159700
C	3.29833300	-3.56574300	-0.86024800
C	5.70513900	-3.74527200	-2.26265400
H	5.89956000	-1.62843100	-1.88599500
C	3.71195800	-4.79647500	-1.37939700
H	2.36031100	-3.50035100	-0.31254200
C	4.92022500	-4.89098400	-2.08443800
H	6.64523900	-3.80914400	-2.80572000
H	3.09578700	-5.68062400	-1.23263600
H	5.24621600	-5.84678000	-2.48740900
H	1.15010200	1.06294200	-2.91331100
H	0.51897500	2.40071700	-1.89622400
H	-0.89320900	-0.11840900	-2.86382500
C	-2.05076500	1.55293300	-2.12907500
C	-3.20565000	1.14926800	-2.82929300
C	-2.10900200	2.77070400	-1.41806200
C	-4.37163000	1.92128100	-2.81218800
H	-3.19111300	0.22316000	-3.39801100
C	-3.26775200	3.54735000	-1.40792000
H	-1.24397300	3.10448400	-0.85546200
C	-4.41071700	3.12762300	-2.10240900
H	-5.24839900	1.58194800	-3.35901200
H	-3.28191200	4.47802900	-0.84563600
H	-5.31600000	3.72923300	-2.08771500
P	-1.60096400	-1.12954500	0.48970100
C	-3.21189800	-0.24621600	0.79843700
C	-1.01776100	-1.78798200	2.15226200
C	-2.02650700	-2.64227300	-0.51720700
C	-4.35221800	-1.07336300	1.42245000
C	-2.98123700	1.05194400	1.59996600
H	-3.51798300	0.05710600	-0.21129800
C	-1.69365900	-3.08625500	2.64645200
C	0.51746500	-1.94655700	2.22595600
H	-1.28830400	-0.97895600	2.84405100
C	-2.89284400	-2.32607600	-1.75079600
C	-0.73750800	-3.37702700	-0.94348800
H	-2.60346100	-3.30545700	0.13837400
C	-5.64630600	-0.24423800	1.49070000
H	-4.07479300	-1.36887200	2.44106400
H	-4.52572100	-1.99515500	0.85656600
C	-4.27483200	1.87570600	1.70227700
H	-2.61982400	0.81386700	2.60838400
H	-2.20518200	1.64658100	1.10791800
C	-1.25789400	-3.40618100	4.08814600
H	-1.39892400	-3.92014200	1.99705600
H	-2.78315300	-3.02005500	2.59813200
C	0.96470000	-2.26537900	3.66102700

H	0.83590900	-2.76358400	1.56611000
H	1.00656500	-1.04262400	1.86885900
C	-3.21211300	-3.60242900	-2.54669800
H	-2.35101900	-1.63160400	-2.39869500
H	-3.82391000	-1.82981200	-1.46048300
C	-1.04719000	-4.64486400	-1.75459400
H	-0.12757300	-2.69352700	-1.54881600
H	-0.13728900	-3.64282800	-0.06884900
C	-5.43128100	1.05156000	2.28756900
H	-6.44534400	-0.84356200	1.94354900
H	-5.97136600	0.00264200	0.47041000
H	-4.09404200	2.76948300	2.31164600
H	-4.54806100	2.22537500	0.69947700
C	0.26938600	-3.52190900	4.20571200
H	-1.73686700	-4.33621600	4.41776300
H	-1.61706500	-2.61062000	4.75564400
H	2.05437700	-2.39005500	3.68829800
H	0.72769200	-1.40737100	4.30596900
C	-1.93006800	-4.33365300	-2.97128800
H	-3.81380800	-3.34342200	-3.42619700
H	-3.82601100	-4.27119300	-1.92753100
H	-0.10763400	-5.11409500	-2.07073800
H	-1.56173200	-5.36830700	-1.10709400
H	-6.35154400	1.64801000	2.29896400
H	-5.20544100	0.79648700	3.33259000
H	0.55742100	-3.69795000	5.24927700
H	0.60748700	-4.39597500	3.63133000
H	-2.17765800	-5.25713300	-3.50821100
H	-1.36880300	-3.69910000	-3.67157800
O	1.52215500	0.62676700	0.50840000
B	1.49123500	1.91995100	1.46487600
C	2.97292600	2.56663100	1.41179000
C	4.10358400	1.76624900	1.67534600
C	3.20442500	3.92902400	1.14566200
C	5.40146400	2.29059700	1.67050100
H	3.97085200	0.70491600	1.87883200
C	4.49943900	4.46831000	1.13424700
H	2.36207000	4.58740500	0.94937700
C	5.60555400	3.65034500	1.39529500
H	6.25201700	1.64342400	1.87637600
H	4.64476800	5.52588200	0.92122900
H	6.61146200	4.06450600	1.38560000
O	1.07518400	1.40052300	2.75474200
H	1.77119500	0.85315600	3.14556400
O	0.45621900	2.82475300	0.96487800
H	-0.38800100	2.54123900	1.35019300
C	0.82234900	5.22778600	-1.50171400
C	1.09891700	6.63391200	-2.01557200
H	1.75641700	4.64737100	-1.47159700
H	0.13247600	4.70996800	-2.18630400
H	0.17447500	7.22124000	-2.03995300
H	1.81636200	7.14653800	-1.36576800
H	1.51099100	6.59815800	-3.02999500
O	0.24852100	5.31713200	-0.19267800
H	0.31981900	4.43216600	0.23404300

dist-TS1-4

Sum of electronic and thermal Free Energies= -3696.928145

C	2.31841100	-0.30064100	-1.94727600
C	1.50890700	0.40616200	-3.06453200
Ni	0.68331700	-0.00538000	-1.09099300
C	0.22540200	1.43627300	-2.74105000
H	-0.14026200	1.59117300	-3.76565300
C	0.76960200	2.76310900	-2.16900400
H	1.40557500	3.25127500	-2.91799700
H	1.41317500	2.54919700	-1.30677200
C	-0.34179000	3.72474600	-1.71422000
H	-0.92114600	4.05884900	-2.58286700
H	-1.02269000	3.16976100	-1.06261300
C	0.22780500	4.91089900	-0.96699200
C	0.43047100	6.15106700	-1.59225800
C	0.61928200	4.76993100	0.37690300
C	1.00738900	7.22265000	-0.89677900
H	0.13441900	6.28031500	-2.63174100
C	1.19768400	5.83394200	1.07597900
H	0.46811100	3.81548100	0.87678500
C	1.39496700	7.06785100	0.43994800
H	1.15311800	8.17682200	-1.39809000
H	1.49202400	5.70274800	2.11488500
H	1.84234200	7.89828100	0.98081800
H	2.18614400	1.09421500	-3.57595100
H	1.13186700	-0.31315500	-3.79245600
H	3.13613500	0.32148800	-1.57504800
C	2.74016000	-1.70553300	-2.17378200
C	4.01314100	-2.14414600	-1.75512800
C	1.88548100	-2.65715800	-2.77229800
C	4.41136100	-3.47514700	-1.91301300
H	4.70096600	-1.43404200	-1.30276800
C	2.28428000	-3.98332800	-2.94108200
H	0.88950400	-2.35712700	-3.08830100
C	3.54967700	-4.40439800	-2.50855000

H	5.39805300	-3.78475300	-1.57622700
H	1.60120000	-4.69557000	-3.39757000
H	3.85653100	-5.43982800	-2.63271700
P	0.80576200	-0.76238300	0.90402300
C	1.02600400	-2.61000200	0.89459700
C	-0.77567900	-0.41326500	1.85794400
C	2.19164900	-0.05706500	1.92957200
C	1.20742000	-3.29361100	2.26362600
C	-0.10778300	-3.28809400	0.09527700
H	1.95025000	-2.74096300	0.31595000
C	-0.65409900	-0.42436800	3.39747900
C	-1.47646800	0.88441600	1.39767900
H	-1.42751700	-1.24667300	1.56470500
C	3.57684800	-0.56549100	1.48729200
C	2.14669100	1.48541800	1.88141000
H	2.02173900	-0.38116200	2.96369700
C	1.50261600	-4.79251100	2.07982800
H	0.28723700	-3.18854000	2.85034000
H	2.01025200	-2.82061400	2.83920200
C	0.16628500	-4.79091700	-0.07506000
H	-1.06197800	-3.15880400	0.62195800
H	-0.21787500	-2.80387200	-0.88069900
C	-2.04460800	-0.30495100	4.04774300
H	-0.03860500	0.42392300	3.72201900
H	-0.15666300	-1.32949400	3.75533800
C	-2.86517500	1.01199000	2.04243600
H	-0.86947800	1.75324200	1.68251400
H	-1.55957100	0.91068100	0.31134600
C	4.69469000	0.05539700	2.34094900
H	3.73740100	-0.29233100	0.44084200
H	3.63142400	-1.65718500	1.54133900
C	3.27340700	2.11521400	2.71480400
H	2.23860300	1.80513200	0.83488400
H	1.18094800	1.85441100	2.23850000
C	0.38881200	-5.48368800	1.27813900
H	1.61954000	-5.26887100	3.06074900
H	2.45959400	-4.90867800	1.55226600
H	-0.66854500	-5.25875300	-0.61108500
H	1.05815200	-4.91978900	-0.69999200
C	-2.78385200	0.95589700	3.57491300
H	-1.93915700	-0.29884000	5.13946200
H	-2.63722400	-1.19396700	3.79093500
H	-3.33641800	1.94696800	1.71718600
H	-3.50484700	0.19741500	1.67636600
C	4.65152800	1.58972500	2.28871000
H	5.66729000	-0.31183500	1.99186900
H	4.58412800	-0.27828400	3.38206100
H	3.23100300	3.20684700	2.61785000
H	3.10767600	1.88344200	3.77600800
H	0.63206200	-6.54220700	1.12564900
H	-0.54318600	-5.45296300	1.86011600
H	-3.78896000	0.99223400	4.01245300
H	-2.24705000	1.84342200	3.93901400
H	5.43507200	2.01544300	2.92685400
H	4.86231400	1.92080500	1.26206600
O	-0.81038500	0.90285600	-1.95358600
C	-7.32414100	-0.02108300	-0.09813900
C	-6.07678000	0.38587000	-0.58564100
C	-5.06601800	-0.55017300	-0.88245100
C	-5.34959500	-1.91453800	-0.67226600
C	-6.59390200	-2.33163200	-0.18477600
C	-7.58510200	-1.38352100	0.10357000
H	-8.09079900	0.71731500	0.12646900
H	-5.87650500	1.44461100	-0.73355100
H	-4.58241500	-2.65426900	-0.88988400
H	-6.79295800	-3.38955600	-0.02773000
H	-8.55273400	-1.70363400	0.48360700
B	-3.65684800	-0.08372000	-1.40088500
O	-3.41615800	1.25838100	-1.57851100
H	-2.45521200	1.38483000	-1.80415600
O	-2.69402100	-1.04065200	-1.64631100
H	-1.85248100	-0.59601600	-1.91012000

dist-TS1-5

Sum of electronic and thermal Free Energies= -3443.687157

C	0.40843200	-2.29792400	-0.27518400
C	-0.37374300	-2.90398200	0.92082500
Ni	0.06698000	-0.75062200	0.72033400
C	-1.53763700	-2.03680400	1.70790500
H	-1.78919900	-2.74308300	2.51588100
C	-2.76653300	-1.86455800	0.79556900
H	-3.09669400	-2.84362500	0.42547000
H	-2.48137900	-1.27497100	-0.08497400
C	-3.93320000	-1.16106600	1.51054500
H	-4.28442500	-1.79870300	2.33171900
H	-3.55280300	-0.23772000	1.95632000
C	-5.06877700	-0.86001300	0.55735300
C	-6.00142600	-1.85150900	0.20634400
C	-5.17821300	0.40016400	-0.05302000
C	-7.01038900	-1.59367900	-0.72908900
H	-5.93487200	-2.83422800	0.67026300

C	-6.18183700	0.66399200	-0.99255400
H	-4.46962400	1.18179900	0.21083400
C	-7.10255800	-0.33349500	-1.33617100
H	-7.72400200	-2.37374300	-0.98473600
H	-6.24353800	1.64579100	-1.45661800
H	-7.88413800	-0.13169800	-2.06470800
H	-0.94125800	-3.75740300	0.53764500
H	0.31081900	-3.27481600	1.68692000
H	-0.17461300	-2.33135900	-1.19956400
C	1.78989000	-2.78944300	-0.49740700
C	2.21811800	-3.13024300	-1.79658800
C	2.71559600	-2.93317800	0.55877000
C	3.50862200	-3.61592400	-2.03132100
H	1.52619600	-3.01937500	-2.62934800
C	4.00349500	-3.41700100	0.32754300
H	2.42384700	-2.64556400	1.56547600
C	4.40705700	-3.76949300	-0.96882300
H	3.81202000	-3.87419400	-3.04319500
H	4.69964700	-3.51187400	1.15762800
H	5.41134300	-4.14498100	-1.14795400
P	0.83461100	0.90623200	-0.38337500
C	2.43212600	0.59851700	-1.29959300
C	1.12799000	2.36459300	0.75747000
C	-0.39432000	1.43485100	-1.68329300
C	2.80297900	1.56804100	-2.44141600
C	3.61339100	0.44009400	-0.31885500
H	2.25750200	-0.38727900	-1.74740400
C	1.21207400	3.74625700	0.07536800
C	0.13706800	2.40070800	1.94376300
H	2.11397600	2.14341700	1.18498600
C	-0.61522200	0.29448900	-2.70013100
C	-1.74232200	1.86241700	-1.06621700
H	0.03722400	2.29906100	-2.20416100
C	4.06157100	1.07126400	-3.17551200
H	3.00144000	2.56700700	-2.03730900
H	1.98121500	1.67096800	-3.15673800
C	4.87515600	-0.04245000	-1.05145100
H	3.83025000	1.40537500	0.15629100
H	3.35169400	-0.26291700	0.47737000
C	1.60616900	4.83159500	1.09393200
H	0.24057700	4.00209300	-0.36438600
H	1.93536300	3.73595800	-0.74404800
C	0.54726600	3.47934400	2.95797700
H	-0.87455300	2.61658500	1.58267600
H	0.08357200	1.42228900	2.42695400
C	-1.62620300	0.69305400	-3.78683100
H	-0.99855500	-0.57964900	-2.16092600
H	0.32976700	-0.01027000	-3.16234200
C	-2.75650400	2.25361900	-2.15369200
H	-2.13870000	1.03184800	-0.46920900
H	-1.60572200	2.70386100	-0.38262700
C	5.24411500	0.89413700	-2.21131600
H	4.32174200	1.77514200	-3.97535100
H	3.83816600	0.10963200	-3.65825800
H	5.70636700	-0.11661400	-0.33956700
H	4.69824500	-1.05259800	-1.43676000
C	0.64946600	4.86154600	2.29523400
H	1.62729800	5.80946200	0.59778300
H	2.62739100	4.63362400	1.44815900
H	-0.17487100	3.50311500	3.78301200
H	1.51901000	3.21031900	3.39556100
C	-2.96466200	1.12269800	-3.16896100
H	-1.77388500	-0.14840600	-4.47441400
H	-1.21435800	1.52077800	-4.38079000
H	-3.70906200	2.52713200	-1.68586200
H	-2.39327000	3.15004400	-2.67546400
H	6.11723600	0.50593500	-2.74981500
H	5.53006900	1.87654300	-1.80936600
H	0.98089200	5.61115300	3.02395400
H	-0.34851700	5.17040900	1.95358900
H	-3.66383600	1.43868800	-3.95247300
H	-3.42505300	0.26500200	-2.65991100
O	-1.12193900	-0.81346500	2.27526400
C	1.39919200	-0.24819100	4.51090800
C	2.48801100	-0.14560600	3.44165800
H	1.85794200	-0.36847500	5.49966500
H	0.81795600	0.68647000	4.53893900
H	3.12677700	0.72990500	3.61103500
H	3.11714700	-1.04244500	3.44277600
H	2.03784400	-0.05307100	2.44848600
O	0.53798400	-1.36994000	4.31334600
H	-0.06200600	-1.16009900	3.53884100

dist-TS1-6

Sum of electronic and thermal Free Energies= -3696.920783

C	0.97376700	-0.59140300	-2.39841100
C	-0.32470400	-1.34253000	-2.46865400
Ni	0.24041800	-0.44926700	-0.65895200
C	-1.68467500	-1.16415100	-1.22320800
H	-2.18281300	-2.07881800	-1.54699700
C	-2.48781900	0.09605000	-1.55262500

H	-2.78438100	0.07496800	-2.60643300	C	4.36688700	-2.16045900	1.40646200
H	-1.85637100	0.98151400	-1.41843900	H	2.59751800	-1.38549200	2.38253200
C	-3.73522700	0.23813500	-0.65844800	H	2.30792400	-1.98039000	0.74826300
H	-4.41910800	-0.59611600	-0.84749600	C	0.79917900	2.39662100	4.45174400
H	-3.41850900	0.15918300	0.38467600	H	1.00904400	3.27103600	2.48963200
C	-4.42655900	1.56254000	-0.89365500	H	2.42859100	2.38289400	3.02293300
C	-5.53281300	1.67036200	-1.75098700	C	-1.29579900	1.18697700	3.69324700
C	-3.93273300	2.73232000	-0.28894700	H	-1.09411300	2.05324400	1.72878300
C	-6.13301900	2.91215800	-1.99855400	H	-1.14766500	0.30236700	1.71291200
H	-5.92852900	0.77542100	-2.22772600	C	3.05202200	3.86509000	-1.93684400
C	-4.52690700	3.97507800	-0.53256900	H	2.36580700	1.83305200	-2.15595900
H	-3.07601000	2.66540500	0.37950800	H	3.76722900	1.99480900	-1.10783800
C	-5.63132500	4.06985500	-1.39090900	C	0.76272700	4.58136300	-1.13365800
H	-6.99151700	2.97516700	-2.66328300	H	0.01801200	2.55072500	-1.29785100
H	-4.13221400	4.86774300	-0.05267000	H	-0.13899900	3.24641200	0.30892400
H	-6.09654200	5.03409000	-1.58079800	C	5.42613800	-1.36808400	2.18753600
H	-0.94582100	-0.98956100	-3.28888600	H	6.29898400	0.62551900	2.22758500
H	-0.21287600	-2.42328100	-2.49728400	H	5.96329000	0.01392800	0.60766600
H	0.97438900	0.33978000	-2.96697700	H	4.23128100	-3.15570300	1.84698700
C	2.26193000	-1.32656200	-2.47355500	H	4.71200100	-2.31323700	0.37666200
C	3.39808400	-0.71031700	-3.03699200	C	-0.73662000	2.37809100	4.48569300
C	2.41097500	-2.63871600	-1.97355000	H	1.18022000	3.28896200	4.96309100
C	4.63328600	-1.36393400	-3.08028600	H	1.18770600	1.52696200	4.99956800
H	3.31437400	0.29161300	-3.44950000	H	-2.39188000	1.22480300	3.66902000
C	3.64150800	-3.29548300	-2.02266400	H	-1.02200400	0.25118600	4.20170900
H	1.55599800	-3.14419200	-1.53429000	C	1.73180600	4.54707700	-2.32382600
C	4.76484600	-2.66168200	-2.57129500	H	3.71924300	3.80257900	-2.80497500
H	5.49255600	-0.85983800	-3.51666000	H	3.56951700	4.47267400	-1.18149000
H	3.72791000	-4.30209600	-1.62027400	H	-0.19780800	5.01782700	-1.43291400
H	5.72462500	-3.17118100	-2.60109600	H	1.17491900	5.22944900	-0.34780200
P	1.52098200	0.80570700	0.55452600	H	6.39003900	-1.89009700	2.15267100
C	3.18151500	0.00318700	0.80885900	H	5.13314600	-1.31317300	3.24551800
C	0.79736200	1.12225000	2.26078800	H	-1.09310700	2.35016700	5.52248600
C	1.85781300	2.49356400	-0.16457400	H	-1.11606000	3.31054900	4.04446300
C	4.22048800	0.79169000	1.62853100	H	1.92031800	5.56304000	-2.69092500
C	3.01784400	-1.42506000	1.36963800	H	1.26831200	3.99077600	-3.15075200
H	3.55739100	-0.10136400	-0.21767400	O	-1.38184300	-1.22239200	0.13600500
C	1.33620300	2.36153600	3.00916200	B	-1.28709600	-2.67085200	0.86172700
C	-0.74815000	1.15635500	2.25769200	C	-2.78468300	-3.27861600	0.76057900
H	1.09625200	0.22706800	2.82249200	C	-3.85776700	-2.67868100	1.44959900
C	2.81057800	2.45467500	-1.37418700	C	-3.08604500	-4.40013900	-0.03398300
C	0.52914300	3.17707800	-0.55414700	C	-5.16552000	-3.16952300	1.35730300
H	2.33701300	3.08562000	0.62450000	H	-3.67961100	-1.79506900	2.06249300
C	5.57255100	0.05764600	1.63381300	C	-4.39104800	-4.90452100	-0.13865400
H	3.87243300	0.88730000	2.66373500	H	-2.28103700	-4.88658900	-0.58122200
H	4.34447700	1.80694700	1.23636600	C	-5.43848600	-4.28951800	0.55849000

H	-5.97176100	-2.68011900	1.90068500
H	-4.59159300	-5.77332400	-0.76317900
H	-6.45297400	-4.67466700	0.48048100
O	-0.80608600	-2.35466500	2.19774600
H	-1.43543500	-1.79036000	2.66889400
O	-0.31379800	-3.48296100	0.16146300
H	0.56054200	-3.20375600	0.47486400

cat-toluene

Sum of electronic and thermal Free Energies= -2131.990027

C	1.50791900	0.46265500	-1.47943400
C	1.36548800	1.53425500	-0.61247600
H	0.97802200	0.53230600	-2.42662500
C	2.61397500	-0.58565400	-1.42400000
H	3.52770600	-0.13790500	-1.02402700
H	2.85884200	-0.89831500	-2.44521600
C	2.22526000	1.83721400	0.60103400
H	3.13163500	2.38869700	0.30513600
H	1.65476700	2.51551900	1.24583600
H	0.75915000	2.36890800	-0.96153000
C	2.61394200	0.58565900	1.42409900
H	3.52767700	0.13792200	1.02412400
H	2.85880000	0.89830900	2.44532100
C	2.22530300	-1.83720500	-0.60092300
H	1.65484300	-2.51553600	-1.24572700
H	3.13168300	-2.38866000	-0.30499000
C	1.50789500	-0.46265700	1.47951300
C	1.36549400	-1.53425200	0.61256100
H	0.97792400	-0.53226800	2.42666400
H	0.75910800	-2.36888500	0.96157500
C	-1.50788100	-0.46293900	-1.47941100
C	-1.36546100	-1.53437300	-0.61225300
H	-0.97794400	-0.53274500	-2.42656700
C	-2.61394700	0.58537200	-1.42419700
H	-3.52767900	0.13769400	-1.02414600
H	-2.85880400	0.89782900	-2.44547700
C	-2.22526400	-1.83711300	0.60128900
H	-3.13162800	-2.38865400	0.30546600
H	-1.65478600	-2.51529900	1.24623100
H	-0.75908900	-2.36907600	-0.96112700
C	-2.61397400	-0.58541000	1.42411500
H	-3.52770600	-0.13775600	1.02404000
H	-2.85885000	-0.89787300	2.44538900
C	-2.22529200	1.83708400	-0.60136100
H	-1.65480600	2.51528100	-1.24628400
H	-3.13167600	2.38860600	-0.30556600
C	-1.50793900	0.46293000	1.47936000
C	-1.36552000	1.53436500	0.61220800
H	-0.97801400	0.53273900	2.42652200
H	-0.75916600	2.36907700	0.96109200
Ni	0.00000000	0.00001700	-0.00003100

COD-toluene

Sum of electronic and thermal Free Energies= -311.927869

C	1.74173800	0.67097200	-0.12003300
C	1.74162100	-0.67125300	-0.12003100
H	2.58770400	1.17325200	-0.58994200
C	0.65437500	1.57158200	0.42915400
H	1.04423400	2.59313300	0.48485000
H	0.40161700	1.27896700	1.45560100
C	0.65411200	-1.57167500	0.42917000
H	1.04380700	-2.59328700	0.48489200
H	0.40139200	-1.27899400	1.45560600
H	2.58749800	-1.17368100	-0.58994200
C	-0.65417100	-1.57210400	-0.42848300
H	-0.40141400	-1.28071400	-1.45529700
H	-1.04398000	-2.59373700	-0.48299700
C	-0.65390900	1.57219800	-0.42849600
H	-1.04355500	2.59389100	-0.48303300
H	-0.40119400	1.28074300	-1.45530200
C	-1.74185100	-0.67097800	0.11933500
C	-1.74173500	0.67125900	0.11933500
H	-2.58869300	-1.17302000	0.58792500
H	-2.58848800	1.17344700	0.58792900

PCy_3-toluene

Sum of electronic and thermal Free Energies= -1046.840306

P	0.01756900	-0.12631400	-1.07963900
C	-1.50015700	-1.05884500	-0.46021800
C	-1.76944300	-1.07188500	1.05669800
C	-2.76238000	-0.60129100	-1.22456500
H	-1.30509400	-2.09392500	-0.77570600
C	-2.98106500	-1.95513200	1.40525200
H	-1.97230500	-0.04848400	1.39706000
H	-0.88590300	-1.41880200	1.60453100
C	-3.98077100	-1.47381300	-0.87390900
H	-2.99204400	0.44311400	-0.97074000
H	-2.57871100	-0.62824300	-2.30520200
C	-4.23627600	-1.50756200	0.64076200

H	-3.16416500	-1.93015100	2.48689600
H	-2.75190400	-2.99902800	1.14782100
H	-4.86882100	-1.10474500	-1.40204000
H	-3.80276900	-2.49725800	-1.23313100
H	-5.07985900	-2.17025800	0.87006000
H	-4.52366600	-0.50202700	0.98023500
C	-0.20864200	1.59314300	-0.30574900
C	0.30248300	1.82007300	1.13298700
C	0.35392400	2.68322800	-1.24697300
H	-1.30033300	1.72457100	-0.28761100
C	-0.04535000	3.23317600	1.63551800
H	1.39261800	1.70057300	1.16163400
H	-0.10994800	1.07352800	1.81767600
C	0.02454500	4.09881200	-0.74277500
H	1.44460100	2.57250500	-1.32424400
H	-0.04232000	2.54306800	-2.25918000
C	0.51089900	4.31504500	0.69798500
H	0.34395000	3.37227300	2.65204400
H	-1.13820200	3.33502400	1.69967800
H	0.46763300	4.84697200	-1.41197100
H	-1.06422900	4.24731900	-0.78131300
H	0.22389900	5.31274600	1.05255800
H	1.60953200	4.27685400	0.71757300
C	1.41650800	-0.89216800	-0.07613000
C	1.47559100	-2.42489600	-0.24965000
C	2.76173700	-0.26330700	-0.50381500
H	1.26435800	-0.68350600	0.99036300
C	2.66586400	-3.03628200	0.51130800
H	1.56255000	-2.66901900	-1.31810400
H	0.54933800	-2.88917900	0.10549300
C	3.94661900	-0.86768300	0.26771500
H	2.90781000	-0.43082900	-1.57994600
H	2.74453800	0.82257500	-0.36061300
C	3.99860500	-2.39335900	0.10078700
H	2.69652700	-4.11985600	0.34182600
H	2.51265000	-2.89056000	1.59013100
H	4.88495200	-0.41371500	-0.07455900
H	3.84714600	-0.62176300	1.33460000
H	4.82253500	-2.81562700	0.68919800
H	4.20594300	-2.63296800	-0.95180000

R1-toluene

Sum of electronic and thermal Free Energies= -309.586462

C	-1.78560200	-1.04849200	0.00004200
C	-0.40713400	-1.28513400	-0.00000200
C	0.51636300	-0.22162400	-0.00004500
C	0.01034300	1.09502600	-0.00006000
C	-1.36432500	1.33313800	-0.00001800
C	-2.27118100	0.26308000	0.00003600
H	-2.47807500	-1.88685000	0.00007800
H	-0.03967200	-2.30956800	0.00000200
H	0.69270000	1.94060600	-0.00012000
H	-1.73354000	2.35603400	-0.00003500
H	-3.34172900	0.45254500	0.00006600
C	1.95899600	-0.53233100	-0.00007500
H	2.19749400	-1.59631700	-0.00025000
C	2.98383900	0.33712500	0.00010400
H	4.01131400	-0.01659300	0.00005900
H	2.84371100	1.41541800	0.00030700

R2-toluene

Sum of electronic and thermal Free Energies= -424.132666

C	-2.53444900	1.20941300	0.08430500
C	-1.16268300	1.20617000	-0.19309600
C	-0.45772000	-0.00003600	-0.33530200
C	-1.16266200	-1.20622500	-0.19285500
C	-2.53442900	-1.20943500	0.08454800
C	-3.22581500	-0.00000300	0.22546800
H	-3.06384000	2.15401400	0.18570900
H	-0.63411200	2.15129400	-0.30636200
H	-0.63407500	-2.15136300	-0.30592800
H	-3.06380300	-2.15402500	0.18614200
H	-4.29221700	0.00000900	0.43766200
C	1.03529700	-0.00004400	-0.58744300
C	1.83225400	0.00021100	0.72580200
H	1.32428600	0.87609400	-1.17654400
H	1.32433100	-0.87637700	-1.17623000
C	3.33050300	0.00023000	0.54957400
H	1.57561800	0.87095100	1.34679400
H	1.57565800	-0.87032100	1.34710400
H	3.91294900	0.00010800	1.49716200
O	3.90667800	-0.00025800	-0.52519000

PhB(OH)$_2$-toluene

Sum of electronic and thermal Free Energies= -408.249158

C	-1.93270200	-1.22247400	0.00000100
C	-0.53495800	-1.20118200	0.00000700
C	0.17938700	0.01451400	0.00000500
C	-0.56591400	1.21078600	-0.00000600

C	-1.96470800	1.19936300	-0.00001300
C	-2.65150400	-0.02037700	-0.00001000
H	-2.46272600	-2.17211300	0.00000400
H	0.01710300	-2.13745900	0.00001500
H	-0.06320600	2.17774300	-0.00001000
H	-2.51780000	2.13568200	-0.00002100
H	-3.73898700	-0.03343600	-0.00001500
B	1.74822300	-0.00116500	0.00001400
O	2.54090500	1.12888600	0.00001300
H	2.03722600	1.95536400	0.00002600
O	2.39095000	-1.21693800	-0.00001000
H	3.35483600	-1.09932500	-0.00001000

$B(OH)_3$-toluene

Sum of electronic and thermal Free Energies= -252.526964

B	-0.00001400	0.00003300	0.00014700
O	1.01636000	0.92859100	-0.00001000
H	0.66749700	1.83301800	0.00030500
O	-1.31242100	0.41585900	-0.00004100
H	-1.92112200	-0.33859700	-0.00000700
O	0.29605300	-1.34445900	-0.00007400
H	1.25376700	-1.49451600	-0.00003200

1-toluene

Sum of electronic and thermal Free Energies= -3911.411866

Ni	0.01790900	0.66503300	0.71019100
C	2.07239500	2.82836600	1.11165600
C	3.44396000	2.94278000	1.42586500
C	1.57709400	3.67256600	0.09177000
C	4.27516600	3.85288500	0.76523000
H	3.86408200	2.31622000	2.20940100
C	2.39948200	4.59367900	-0.55684900
H	0.53465000	3.58916400	-0.19973500
C	3.75941200	4.69288000	-0.22856800
H	5.32792600	3.91160400	1.03457100
H	1.98328300	5.22682400	-1.33796800
H	4.40236900	5.40312000	-0.74263900
P	1.57281500	-0.79594600	-0.04287300
C	2.86076800	0.15521600	-1.03135700
C	4.19701800	-0.47351400	-1.48719700
C	2.16553400	0.84801800	-2.22403500
H	3.11312900	0.94884200	-0.31920800
C	5.11749500	0.61282300	-2.07123500
H	4.03084400	-1.21878400	-2.26688000
H	4.69719000	-0.99670500	-0.66821400
C	3.08639300	1.87743400	-2.90113100
H	1.85522000	0.09098300	-2.95915900
H	1.25525500	1.34700600	-1.87085900
C	4.45141200	1.28535900	-3.28187600
H	6.07852500	0.16982900	-2.36207500
H	5.33095300	1.36877900	-1.30297400
H	2.58879900	2.29075300	-3.78803200
H	3.24110100	2.71053300	-2.20799100
H	5.10046000	2.07028500	-3.68969500
H	4.32149700	0.53747500	-4.07788700
C	1.05696600	-2.28496100	-1.10311900
C	2.12492600	-3.02566000	-1.93209600
C	0.25943500	-3.30354900	-0.26290700
H	0.36044600	-1.83594300	-1.81682900
C	1.51616800	-4.16761200	-2.77015500
H	2.90630700	-3.42601000	-1.27183300
H	2.61118900	-2.33382400	-2.61947700
C	-0.37478300	-4.40629100	-1.12357000
H	0.93209700	-3.78475200	0.45803300
H	-0.50853000	-2.79194300	0.31752600
C	0.69795400	-5.15274700	-1.92675000
H	2.31686700	-4.69316500	-3.30535200
H	0.86380500	-3.72926600	-3.53856900
H	-0.93112400	-5.10111500	-0.48204300
H	-1.10439300	-3.96250500	-1.81436600
H	0.24060400	-5.91619300	-2.56796800
H	1.36584100	-5.68087900	-1.23138100
C	2.49613800	-1.61407500	1.39291100
C	3.68347600	-0.80359900	1.95722900
C	1.50280300	-1.89762300	2.54765500
H	2.89061000	-2.57223400	1.02495500
C	4.37173700	-1.54539200	3.11604000
H	3.31934600	0.15925300	2.32178300
H	4.42101800	-0.57959400	1.18580400
C	2.17304400	-2.63147500	3.71992300
H	1.09273000	-0.93900900	2.89071900
H	0.64729300	-2.47914200	2.20062000
C	3.38692800	-1.85739400	4.25126400
H	5.20839400	-0.94295000	3.49158200
H	4.80337200	-2.48407600	2.73989000
H	1.44121300	-2.79260400	4.52146200
H	2.49623400	-3.62737800	3.38378600
H	3.88546400	-2.42320800	5.04796800
H	3.04411900	-0.91375300	4.69876000
P	-2.08337600	0.30275100	0.06357200

C	-2.32062300	-0.82683500	-1.42803900
C	-3.76094100	-1.22873700	-1.80222800
C	-1.59583600	-0.24658600	-2.66145100
H	-1.78804900	-1.73979500	-1.14430200
C	-3.77030500	-2.22652800	-2.97479600
H	-4.32900200	-0.33817300	-2.09846700
H	-4.28155500	-1.66625900	-0.94340400
C	-1.60786600	-1.22980500	-3.84376500
H	-2.08960600	0.68017600	-2.98170200
H	-0.57167900	0.02997600	-2.39594300
C	-3.03864600	-1.65983400	-4.20107800
H	-4.80411600	-2.48592400	-3.23490500
H	-3.28227700	-3.15898600	-2.65829500
H	-1.11721400	-0.77305500	-4.71216800
H	-1.02043800	-2.12057000	-3.58504800
H	-3.02334500	-2.39913600	-5.01119200
H	-3.59318800	-0.78890200	-4.57857300
C	-3.17493900	1.76976900	-0.48624400
C	-4.66479500	1.73657800	-0.08028900
C	-2.57094700	3.14025100	-0.13867800
H	-3.14921300	1.69458800	-1.58043500
C	-5.44579000	2.87993700	-0.75444800
H	-4.75615400	1.83927800	1.00785400
H	-5.12795600	0.78218300	-0.34508300
C	-3.34208900	4.28512700	-0.81412000
H	-2.59328400	3.28327500	0.94783300
H	-1.51834700	3.16041600	-0.43488000
C	-4.83140600	4.25184000	-0.44099100
H	-6.49471900	2.84894200	-0.43397200
H	-5.44423200	2.72175500	-1.84248700
H	-2.89896400	5.24866400	-0.53353800
H	-3.23902700	4.19601500	-1.90527000
H	-5.37782500	5.04378600	-0.96781000
H	-4.93713400	4.45602600	0.63395600
C	-3.11284100	-0.54118100	1.39455200
C	-2.69071200	-2.00097400	1.64601700
C	-3.04329800	0.23664800	2.72327600
H	-4.15515200	-0.55154300	1.05701400
C	-3.57443500	-2.66107600	2.71911700
H	-1.64512600	-2.01288500	1.97797500
H	-2.74429100	-2.59150200	0.72558600
C	-3.95150700	-0.39544900	3.78921500
H	-2.00697100	0.21673800	3.07603300
H	-3.29774600	1.29202200	2.57929400
C	-3.57032600	-1.86381800	4.03196900
H	-3.23460800	-3.68914900	2.89636500
H	-4.60408600	-2.73065600	2.34036700
H	-3.88200400	0.17467400	4.72385800
H	-4.99889000	-0.33755000	3.46006800
H	-4.25122600	-2.32354600	4.75871700
H	-2.56383300	-1.90268500	4.47220200
C	1.20443300	1.88137400	1.84299100
C	-0.18911100	2.11520500	2.03115500
H	-0.64426300	1.74460500	2.94912800
H	-0.62068300	3.05340300	1.69410700
H	1.72132900	1.32103300	2.62039700

dist-4-toluene

Sum of electronic and thermal Free Energies= -3696.938084

Ni	0.02095600	-0.64252300	-0.29425400
C	1.20978700	-3.09886600	0.28004400
H	1.22730300	-4.19772100	0.31914800
C	-0.22329400	-2.56354600	0.03585700
H	-0.80010600	-2.82830900	0.91769600
C	7.28856600	-0.02370800	0.39607600
C	5.93786900	-0.38759500	0.43522400
C	5.55243800	-1.66981600	0.86183500
C	6.55047900	-2.57793900	1.24856700
C	7.90272700	-2.21809500	1.20979600
C	8.27656400	-0.93839700	0.78178900
H	7.56890900	0.97497900	0.06920000
H	5.17688700	0.33300700	0.13912100
H	6.26692800	-3.57338700	1.58673000
H	8.66262100	-2.93317700	1.51675100
H	9.32606500	-0.65517300	0.75415500
C	4.09324700	-2.07055100	0.85275100
C	3.67395500	-2.72663400	-0.48310300
H	3.47538400	-1.18374500	1.02529100
H	3.88744700	-2.75736600	1.68024600
C	2.18046600	-2.62649800	-0.79130500
H	4.21732700	-2.24773600	-1.30707600
H	3.97000200	-3.78212300	-0.49637700
H	1.96596100	-3.13478200	-1.73716600
O	1.82215700	-1.21221200	-0.95065000
C	2.45624600	5.60271600	-1.58653200
C	2.51991000	4.26805000	-1.16835400
C	1.46434500	3.37003900	-1.41821100
C	0.34016400	3.85946900	-2.11123100
C	0.26496400	5.19116600	-2.53444200
C	1.32552500	6.06864900	-2.27060200
H	3.28178200	6.28089900	-1.37885500

H	3.39536900	3.91265600	-0.62945800
H	-0.48146200	3.17612300	-2.31156600
H	-0.61495800	5.54793700	-3.06673000
H	1.27126300	7.10596300	-2.59477000
B	1.48177800	1.87224500	-0.89947500
O	2.64469900	1.49193900	-0.19671600
H	2.53630600	0.56245400	0.06375400
O	0.43852300	1.06421400	-1.10301700
H	2.11953400	-0.83374600	-1.79677200
C	-0.92158000	-3.16978900	-1.15440800
C	-1.95128600	-4.11102000	-0.95413600
C	-0.64183000	-2.80084600	-2.48813600
C	-2.67904200	-4.64530400	-2.02180000
H	-2.20007000	-4.41168600	0.06217000
C	-1.36413500	-3.33110500	-3.56062000
H	0.11161700	-2.04452400	-2.68833200
C	-2.39120000	-4.25567100	-3.33534900
H	-3.47616100	-5.36001900	-1.82813100
H	-1.13613800	-3.00782200	-4.57396900
H	-2.96159000	-4.65974000	-4.16814100
H	1.54218700	-2.73220700	1.25682000
P	-1.75906100	0.23882600	0.69272500
C	-1.30210200	1.99640700	1.12761100
C	-2.53594900	-0.36423700	2.31158500
C	-3.15408800	0.38725700	-0.54155100
C	-2.44066500	2.89873300	1.63849500
C	-0.10078400	2.03023500	2.09652700
H	-0.95108500	2.39472000	0.17371600
C	-4.06349900	-0.14995600	2.41943000
C	-2.16692100	-1.79873600	2.72886200
H	-2.06891400	0.29905900	3.05077100
C	-2.75265600	1.26570000	-1.74498100
C	-3.59785100	-1.00627900	-1.02655900
H	-3.99720500	0.86967500	-0.03337300
C	-1.93145800	4.34171700	1.81458600
H	-2.81270000	2.53490500	2.60520200
H	-3.28856400	2.88993500	0.94399500
C	0.40276300	3.46998600	2.29097000
H	-0.39121000	1.61915100	3.07381800
H	0.70672200	1.39991400	1.71080100
C	-4.56957900	-0.47286500	3.83637200
H	-4.57980600	-0.79943800	1.70289400
H	-4.33515200	0.87798400	2.16567900
C	-2.68384900	-2.12507700	4.14004600
H	-2.59577900	-2.51208000	2.01347400
H	-1.08084300	-1.92380700	2.69868800
C	-3.89256700	1.34791700	-2.77428800
H	-1.84775100	0.85531500	-2.20631900
H	-2.49418500	2.27499100	-1.41048000
C	-4.75337700	-0.91235300	-2.03318500
H	-2.74934400	-1.49020100	-1.51368000
H	-3.87778400	-1.65019800	-0.18569500
C	-0.72472800	4.39998000	2.76407700
H	-2.74321900	4.97791500	2.18880200
H	-1.63969600	4.73979800	0.83326900
H	1.23181500	3.47765300	3.00893200
H	0.80606700	3.83682500	1.33967500
C	-4.19742100	-1.90097700	4.25705500
H	-5.65643100	-0.33150100	3.87692900
H	-4.13159700	0.24218800	4.54694900
H	-2.42797600	-3.16084600	4.39438200
H	-2.16580600	-1.48501600	4.86820600
C	-4.35527800	-0.04242300	-3.23438600
H	-3.56409300	1.94517100	-3.63378500
H	-4.74439800	1.88117000	-2.32789800
H	-5.02856000	-1.92025900	-2.36593900
H	-5.63913700	-0.48163000	-1.54400800
H	-0.35741800	5.43015100	2.84455200
H	-1.04612400	4.09877600	3.77193900
H	-4.53522300	-2.09795500	5.28155700
H	-4.72119300	-2.61675800	3.60769000
H	-5.19190700	0.04802500	-3.93808200
H	-3.53593200	-0.53728900	-3.77400700

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Sum of electronic and thermal Free Energies= -3541.209703

Ni	0.16874500	-0.33536700	-0.33862200
C	1.65659500	-2.03551300	1.29860600
H	1.80606600	-2.95715800	1.87968600
C	0.16547300	-1.83254100	0.93047100
H	-0.35577700	-1.66131300	1.86836400
C	7.41045100	1.13236400	-0.52877200
C	6.10019100	0.74011600	-0.23316400
C	5.84014600	-0.17261800	0.80309700
C	6.92289800	-0.68231300	1.53656500
C	8.23538800	-0.29341100	1.24348600
C	8.48375400	0.61544800	0.20780300
H	7.59312900	1.84473000	-1.33003100
H	5.27147500	1.15220900	-0.80719700
H	6.73725200	-1.38619500	2.34628900
H	9.06201800	-0.69562200	1.82475400

H	9.50204100	0.92183900	-0.01940400
C	4.42413200	-0.62817500	1.08071700
C	4.04562900	-1.88746900	0.26828600
H	3.72965900	0.18066400	0.83223600
H	4.29724700	-0.82844000	2.14958000
C	2.54339600	-2.07829500	0.06431900
H	4.51191400	-1.83161000	-0.72302500
H	4.45590000	-2.78385500	0.74796300
H	2.36441900	-3.00546900	-0.48974200
O	2.02664800	-0.96624200	-0.74352200
B	1.30466600	1.67260400	-2.18910100
O	2.52415000	1.81257200	-1.48264400
H	2.55786700	1.10546600	-0.81927400
O	0.37684600	0.75185000	-1.92828900
H	2.23438300	-1.05277600	-1.69090800
C	-0.48118700	-3.02178100	0.26799300
C	-1.38762000	-3.81923700	0.99491800
C	-0.27440400	-3.36010100	-1.08703000
C	-2.06893600	-4.88680700	0.40217900
H	-1.57790100	-3.58177100	2.04013400
C	-0.95017300	-4.42656300	-1.68608200
H	0.37816400	-2.74472700	-1.69983500
C	-1.85595000	-5.19654800	-0.94637600
H	-2.77214100	-5.47227700	0.99077100
H	-0.78358000	-4.64483800	-2.73865700
H	-2.39192600	-6.01835400	-1.41490700
H	1.96129500	-1.19665800	1.93309000
P	-1.71520500	0.71885300	0.16731600
C	-1.46058600	2.49506000	-0.34818800
C	-2.44517600	0.92869500	1.90387400
C	-3.10167400	0.08258100	-0.91083600
C	-2.69356800	3.41575300	-0.28593200
C	-0.27279400	3.12027900	0.41490200
H	-1.15306100	2.39831200	-1.39177700
C	-3.98796900	1.02614300	1.95094600
C	-1.94016200	-0.06786500	2.96234000
H	-2.05559900	1.91143400	2.19905400
C	-2.77255900	0.23495500	-2.41085100
C	-3.41217100	-1.39218300	-0.58666200
H	-3.99074600	0.68612000	-0.69257600
C	-2.35088800	4.80333400	-0.85986200
H	-3.02766300	3.53798600	0.75258000
H	-3.53152200	2.98408700	-0.84517300
C	0.06677800	4.50911100	-0.15052900
H	-0.51829500	3.22068900	1.48178100
H	0.60143900	2.46454700	0.34841600
C	-4.47783400	1.40391400	3.35964400
H	-4.42873500	0.06220000	1.67248600
H	-4.35790600	1.76070200	1.23136700
C	-2.44587500	0.29673100	4.36850200
H	-2.27731600	-1.08037700	2.70602300
H	-0.84685100	-0.08127200	2.96251000
C	-3.91761400	-0.31023400	-3.28099400
H	-1.83972500	-0.29466200	-2.63104600
H	-2.58783800	1.28337900	-2.66320300
C	-4.57065400	-1.92318100	-1.44342500
H	-2.52206400	-1.98877900	-0.79423100
H	-3.63382000	-1.53029700	0.47696800
C	-1.15758900	5.43690900	-0.12789600
H	-3.22931500	5.45748800	-0.79551700
H	-2.10856000	4.69828700	-1.92585400
H	0.89244400	4.95046300	0.42079400
H	0.41963000	4.39046300	-1.18255700
C	-3.97541900	0.40950900	4.41486600
H	-5.57367800	1.44887100	3.36514400
H	-4.11927800	2.41256700	3.60898400
H	-2.09342100	-0.45043100	5.09002400
H	-2.00378000	1.25719400	4.66914400
C	-4.25552800	-1.76894800	-2.93853000
H	-3.64460900	-0.21980300	-4.33938800
H	-4.81283900	0.31119800	-3.13275300
H	-4.75205500	-2.97644100	-1.19780400
H	-5.49235000	-1.37349800	-1.20299900
H	-0.90933600	6.40580700	-0.57811900
H	-1.44115900	5.63738800	0.91567900
H	-4.30635600	0.71284700	5.41538300
H	-4.41827600	-0.57754600	4.22011200
H	-5.09887500	-2.11857100	-3.54691900
H	-3.39630000	-2.40737200	-3.18690700
O	1.12510200	2.60494500	-3.22158400
H	1.90326100	3.17992300	-3.27433500

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Sum of electronic and thermal Free Energies= -3696.912889

Ni	0.28606500	-0.17710000	-0.93404100
C	-0.68929200	-0.10266700	-2.87375900
C	0.62664500	-0.51405800	-2.99531700
H	1.31143100	0.32222300	-3.13023400
C	-6.30359900	1.92851000	0.26266700
C	-5.54668200	1.36754300	-0.77035300
C	-5.26353600	-0.00898800	-0.79237400

C	-5.75899200	-0.80705500	0.24967500	H	3.90155900	1.59335000	4.51599000
C	-6.52211800	-0.25163000	1.28353500	H	3.12679900	2.62933600	3.31791900
C	-6.79670700	1.11931000	1.29439800	H	5.32657300	1.45646300	0.43295400
H	-6.50794900	2.99654400	0.26348600	H	3.99809600	2.54468400	0.82488800
H	-5.17170900	2.00766200	-1.56658000	H	5.53582000	2.37542800	2.76811200
H	-5.54195900	-1.87358400	0.25674800	H	5.37830000	0.61987600	2.77406300
H	-6.89152600	-0.88819000	2.08408500	C	1.53661800	-2.30819300	1.48304200
H	-7.38242700	1.55525800	2.09993000	C	1.31928800	-2.81641900	2.92624500
C	-4.42094900	-0.61109400	-1.89962200	C	1.09346400	-3.37733300	0.46358300
C	-2.98250900	-0.06789900	-1.90629500	H	2.61661100	-2.16589100	1.34441700
H	-4.88502700	-0.41339900	-2.87531800	C	2.06865300	-4.14074100	3.15717700
H	-4.40289400	-1.69838000	-1.76796300	H	0.24946800	-2.98248700	3.10039300
C	-2.04292400	-0.77760900	-2.90294000	H	1.64515300	-2.07593200	3.66214300
H	-3.00237200	1.00257000	-2.14085900	C	1.83228600	-4.70344800	0.69973100
H	-2.54755700	-0.17665100	-0.90777900	H	0.01110600	-3.53953100	0.54640700
H	-2.43889600	-0.62714200	-3.92304100	H	1.27360700	-3.02347300	-0.55275400
O	-1.96445100	-2.17913100	-2.62979300	C	1.65002700	-5.21036000	2.13768300
C	1.44233900	6.56344900	-0.92032100	H	1.88550200	-4.49314400	4.17967400
C	0.68015100	5.38865500	-0.89430900	H	3.14990400	-3.96131100	3.07395200
C	1.27537600	4.12336000	-1.06269100	H	1.47987200	-5.45068400	-0.02106100
C	2.66907700	4.08007900	-1.26355600	H	2.90233800	-4.55562500	0.49666300
C	3.44082700	5.24679800	-1.29442900	H	2.22463200	-6.13119600	2.29601300
C	2.82734100	6.49513900	-1.12041800	H	0.59297700	-5.46555400	2.29909200
H	0.96128900	7.53048700	-0.78531000	C	-0.58491800	-0.31455700	2.29093600
H	-0.39496200	5.44763300	-0.73939400	C	-0.99914700	1.17242300	2.27515900
H	3.14160700	3.10974900	-1.39773800	C	-1.78101200	-1.21783700	1.91995100
H	4.51631900	5.18768300	-1.45197400	H	-0.25408700	-0.57318000	3.30465500
H	3.42277700	7.40574600	-1.14153000	C	-2.21955500	1.42951300	3.17222600
B	0.44437800	2.77256300	-1.01267000	H	-1.23333600	1.47123700	1.24692900
O	-0.95847800	2.93716800	-0.92242300	H	-0.16900000	1.80919100	2.59660000
H	-1.36226900	2.05666700	-0.87130300	C	-2.99585800	-0.94992300	2.82188100
O	1.05001400	1.59006100	-1.04848200	H	-2.05522800	-1.02942800	0.87680500
H	-2.80321000	-2.58213200	-2.90199200	H	-1.49950300	-2.27469300	1.97257600
H	-0.33297400	-1.46875800	-0.76362400	C	-3.40114600	0.52973000	2.78824400
P	0.84458400	-0.59791500	1.13091300	H	-2.50429600	2.48594900	3.10255400
C	2.18279700	0.58716400	1.65848800	H	-1.94309400	1.24349200	4.22004200
C	2.58923400	0.54110700	3.14333200	H	-3.83457800	-1.57805300	2.49966900
C	3.41993300	0.46809600	0.74279900	H	-2.75562300	-1.24177000	3.85441400
H	1.73620500	1.56291400	1.43656100	H	-4.25142500	0.70675700	3.45677900
C	3.60676700	1.65155600	3.46089600	H	-3.74479500	0.78690100	1.77826500
H	3.04762800	-0.42997600	3.37015700	H	-0.80669900	0.97377900	-2.99981800
H	1.71411000	0.64207400	3.79548800	C	1.32448800	-1.81646500	-3.04908400
C	4.44054200	1.57112900	1.06984900	C	0.75187500	-3.04404700	-3.42763100
H	3.89874200	-0.51189400	0.87639400	C	2.68732000	-1.80106900	-2.67717100
H	3.09988100	0.54908400	-0.29900000	C	1.51168900	-4.21597700	-3.40704000
C	4.84187600	1.55397200	2.55244400	H	-0.29230000	-3.07510100	-3.70821600

C	3.44168300	-2.97462400	-2.64361100
H	3.14344800	-0.85748400	-2.38629400
C	2.85377000	-4.19220200	-3.00635800
H	1.05199600	-5.15730100	-3.69952900
H	4.48362900	-2.93987100	-2.33479900
H	3.43442000	-5.11105700	-2.98027800

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Sum of electronic and thermal Free Energies= -3541.186411

Ni	0.91518800	-0.53758600	-0.77971800
C	0.66486800	-2.48892700	-1.62989300
C	2.00210600	-2.30582100	-1.31515700
H	2.58027100	-1.87933300	-2.13241500
C	-5.84735100	-0.78250400	-0.52757200
C	-4.93315900	-1.77618100	-0.89654600
C	-4.03200500	-2.31065000	0.03750600
C	-4.07315400	-1.82608500	1.35557900
C	-4.98088500	-0.82987900	1.72962100
C	-5.87144100	-0.30118900	0.78686800
H	-6.53690600	-0.38059000	-1.26638800
H	-4.91357100	-2.13534700	-1.92416200
H	-3.38062800	-2.22869700	2.09240600
H	-4.99192600	-0.46599000	2.75478500
H	-6.57679600	0.47525900	1.07292300
C	-2.95635800	-3.29079700	-0.38154000
C	-1.70953200	-2.50732300	-0.82818300
H	-3.31015700	-3.93336100	-1.19658900
H	-2.68591700	-3.94103000	0.45555200
C	-0.44572000	-3.34557700	-1.04249200
H	-1.93181100	-1.96369800	-1.75409300
H	-1.47422800	-1.75360800	-0.07425600
H	-0.65888400	-4.10779100	-1.81343700
O	-0.15278300	-4.00386200	0.18942300
B	1.17077900	0.37388100	-3.57461200
O	-0.14755900	-0.00171100	-3.95301600
H	-0.65717700	-0.16438700	-3.14554000
O	1.61589300	0.38183200	-2.32402600
H	0.64146500	-4.54784200	0.06448600
H	0.47463200	-1.14419500	0.43651600
P	0.35161700	1.27254200	0.31958400
C	1.89253900	2.31117000	0.28437100
C	1.81225500	3.68589000	0.97277600
C	3.10453100	1.50446900	0.80260400
H	2.04505700	2.44793400	-0.79323900
C	3.11652100	4.47496900	0.76177500
H	1.65526700	3.54878000	2.05066800
H	0.95944200	4.26311200	0.59698800
C	4.40756300	2.29709900	0.60932800
H	2.97591600	1.27372500	1.86923900
H	3.17101800	0.54671600	0.27521200
C	4.33363800	3.68412000	1.26595100
H	3.05096300	5.44342700	1.27274400
H	3.23775900	4.68765400	-0.30915600
H	5.25009900	1.72592700	1.01728600
H	4.59379700	2.41203300	-0.46667800
H	5.25611400	4.24521000	1.07379900
H	4.25774000	3.56503800	2.35644300
C	-0.15728700	1.14042800	2.12979600
C	-1.00865700	2.32437500	2.64476700
C	-0.85641600	-0.18774500	2.48953500
H	0.80469300	1.15930900	2.66151100
C	-1.25274000	2.21910800	4.16004300
H	-1.98230000	2.31557800	2.13890200
H	-0.53968300	3.28426400	2.41187900
C	-1.12954800	-0.29779000	3.99777800
H	-1.80544600	-0.26058500	1.94545100
H	-0.24757700	-1.03397600	2.16265700
C	-1.94004800	0.89543200	4.52155400
H	-1.85987600	3.06987200	4.49232800
H	-0.29208400	2.28995300	4.68914700
H	-1.65440800	-1.23858300	4.20480600
H	-0.17096300	-0.34810700	4.53331400
H	-2.07826800	0.81871000	5.60671200
H	-2.94273100	0.87642900	4.07095500
C	-1.00519800	2.24668800	-0.51608000
C	-0.54571400	2.92847000	-1.82049100
C	-2.20831300	1.30947700	-0.76592100
H	-1.31924900	3.03590800	0.17636800
C	-1.71579100	3.64361200	-2.51591800
H	-0.11892100	2.18305700	-2.49385400
H	0.24997900	3.65080300	-1.61148900
C	-3.36084200	2.02927400	-1.47995600
H	-1.87293900	0.46227800	-1.37814700
H	-2.57001300	0.87397200	0.17163900
C	-2.88599500	2.68625900	-2.78319300
H	-1.36176400	4.08628000	-3.45444200
H	-2.06461800	4.47404800	-1.88500600
H	-4.16827700	1.31399400	-1.67104800
H	-3.77367000	2.79866700	-0.81200300
H	-3.71420000	3.22062500	-3.26423800
H	-2.55827300	1.90751500	-3.48574000

H	0.41269800	-2.19050300	-2.64883200
C	2.86863600	-2.74659700	-0.19454300
C	2.45830900	-2.93749800	1.14146700
C	4.23485900	-2.93141000	-0.49609500
C	3.37184100	-3.33344200	2.12038100
H	1.42618200	-2.75391600	1.40832900
C	5.14809500	-3.33152700	0.48218300
H	4.58302000	-2.75855500	-1.51214600
C	4.71941500	-3.53891500	1.79835300
H	3.03098200	-3.47058600	3.14408700
H	6.19357800	-3.47207900	0.21881600
H	5.42785700	-3.84210200	2.56542400
O	1.98394500	0.75677700	-4.65075600
H	1.47123000	0.72347600	-5.47199500

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Sum of electronic and thermal Free Energies= -3696.918791

C	2.06992600	-1.10374400	-1.91162800
C	1.60963400	-0.17295500	-3.06744900
Ni	0.63813200	-0.23073500	-1.08726300
C	0.80601200	1.25144000	-2.78591000
H	0.55009600	1.53601800	-3.81707500
C	1.78339900	2.28616400	-2.18635600
H	2.58451900	2.49785400	-2.90624400
H	2.26968100	1.85481100	-1.30191100
C	1.09291500	3.59432600	-1.76407400
H	0.71697800	4.11843300	-2.65061800
H	0.22508200	3.33520100	-1.15125800
C	2.03101400	4.48370700	-0.97792000
C	2.71666300	5.55015900	-1.57867300
C	2.27476900	4.21692700	0.38113200
C	3.62071800	6.32989300	-0.84551400
H	2.53967100	5.77490900	-2.62906300
C	3.17711500	4.98916300	1.11813800
H	1.74699400	3.39635600	0.86276200
C	3.85623000	6.05127200	0.50583400
H	4.13861200	7.15544200	-1.32864300
H	3.34756900	4.76751200	2.16955800
H	4.55627500	6.65672700	1.07663700
H	2.50968200	0.18059200	-3.57840700
H	1.00204200	-0.72209100	-3.78814700
H	3.04709500	-0.81211400	-1.51699300
C	1.96865500	-2.56951200	-2.12194600
C	2.99512200	-3.42801400	-1.67936700
C	0.84046800	-3.15979100	-2.73156300
C	2.89654300	-4.81449600	-1.82673500
H	3.88441600	-3.00423100	-1.21912700
C	0.74414100	-4.54201600	-2.88990500
H	0.02183600	-2.52785100	-3.06670400
C	1.77017200	-5.38114500	-2.43456700
H	3.70424700	-5.45199600	-1.47444200
H	-0.13975000	-4.96836800	-3.35805000
H	1.69176200	-6.45889900	-2.55297100
P	0.44474100	-0.97804800	0.90036600
C	-0.01504700	-2.78136200	0.89674300
C	-0.92723800	-0.06892500	1.80713800
C	1.96718900	-0.81036200	1.96189600
C	-0.11501500	-3.47210200	2.27081800
C	-1.30458400	-3.01215800	0.07896100
H	0.80880400	-3.24323500	0.33617100
C	-0.86362800	-0.11532200	3.34961700
C	-1.09253500	1.39304000	1.33360600
H	-1.82926400	-0.60667900	1.48721300
C	3.08973600	-1.78041800	1.54731000
C	2.47738500	0.64634400	1.92425300
H	1.66821400	-1.05040400	2.99010000
C	-0.37762900	-4.97829200	2.09704600
H	-0.94483800	-3.03612700	2.83957300
H	0.79458900	-3.31534600	2.86100500
C	-1.58719300	-4.51425200	-0.08227500
H	-2.15681600	-2.54192300	0.58518200
H	-1.22144900	-2.52860900	-0.89958400
C	-2.13161100	0.50954500	3.96042500
H	0.01080600	0.45001600	3.69658500
H	-0.74256700	-1.13787900	3.71754900
C	-2.35739600	2.02061900	1.93814600
H	-0.21861200	1.98230900	1.64034900
H	-1.13152100	1.44424000	0.24566000
C	4.33655100	-1.59809000	2.42828900
H	3.35956700	-1.58422800	0.50582500
H	2.74962400	-2.81970300	1.59338600
C	3.73677900	0.83419100	2.78412100
H	2.69893200	0.91424000	0.88263300
H	1.69883100	1.33522400	2.26377600
C	-1.65223800	-5.22852400	1.27638800
H	-0.45609800	-5.45603200	3.08120300
H	0.48135800	-5.43680300	1.58761400
H	-2.52526400	-4.65394600	-0.63284500
H	-0.79128300	-4.96206000	-0.68937300
C	-2.34462700	1.95037100	3.47183100
H	-2.06288200	0.48200500	5.05491700

H	-3.00129000	-0.10156000	3.68202600
H	-2.44832000	3.05831300	1.59826200
H	-3.23845400	1.49245000	1.55155400
C	4.84532600	-0.14966800	2.38464100
H	5.12186600	-2.28946900	2.09954400
H	4.09163100	-1.86832500	3.46501200
H	4.08979600	1.86825000	2.69133300
H	3.47752200	0.68029000	3.84094000
H	-1.80462600	-6.30489500	1.13174500
H	-2.52035000	-4.85943300	1.84071000
H	-3.27912200	2.35341000	3.88013900
H	-1.53200400	2.58340700	3.85663100
H	5.71517100	-0.03049500	3.04133200
H	5.18391200	0.08319000	1.36523100
O	-0.37624300	1.13931600	-2.03138400
C	-6.79478200	2.49795000	-0.07490900
C	-5.49277700	2.45777600	-0.58574300
C	-4.87609800	1.23576100	-0.91868500
C	-5.61085400	0.05038800	-0.72144100
C	-6.91368700	0.08051500	-0.21073500
C	-7.50878200	1.30696200	0.11382900
H	-7.25419300	3.45175000	0.17682500
H	-4.93757400	3.38237600	-0.72560800
H	-5.14969100	-0.90258900	-0.97155400
H	-7.46610600	-0.84570700	-0.06556300
H	-8.52145000	1.33456500	0.51095600
B	-3.40247900	1.19635700	-1.46375300
O	-2.72185400	2.37714100	-1.63815900
H	-1.78282000	2.17974100	-1.88602400
O	-2.82771800	-0.03097600	-1.72293300
H	-1.89518400	0.10484600	-2.01189000

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Sum of electronic and thermal Free Energies= -3696.908678

C	0.95109300	-0.41051800	-2.43518300
C	-0.31224900	-1.22146400	-2.55085000
Ni	0.20989200	-0.40570400	-0.69541500
C	-1.69164100	-1.13554000	-1.32550600
H	-2.16397500	-2.05250400	-1.68249100
C	-2.51146400	0.12343900	-1.63040500
H	-2.87904300	0.07512200	-2.66146000
H	-1.86366200	1.00546300	-1.57106100
C	-3.69149200	0.31860700	-0.65894100
H	-4.40777200	-0.50133300	-0.77652200
H	-3.30394000	0.25703500	0.36112900
C	-4.36075600	1.65751400	-0.87782400
C	-5.56387700	1.77343800	-1.58946800
C	-3.75119300	2.83190600	-0.40124700
C	-6.14610200	3.02688800	-1.81929900
H	-6.05123600	0.87527600	-1.96451400
C	-4.32604300	4.08553800	-0.62835600
H	-2.81798600	2.75832200	0.15469600
C	-5.52863600	4.18800300	-1.34077700
H	-7.08165500	3.09586300	-2.36970800
H	-3.84062500	4.98164400	-0.24789100
H	-5.98009700	5.16140800	-1.51693900
H	-0.93527300	-0.86632100	-3.36955800
H	-0.14579800	-2.29346500	-2.61573900
H	0.90217000	0.54919300	-2.95378700
C	2.27208600	-1.07537300	-2.56788600
C	3.35989600	-0.38373700	-3.13757500
C	2.49534600	-2.39419900	-2.11634000
C	4.62249300	-0.97493800	-3.24073100
H	3.21501000	0.62714500	-3.51136700
C	3.75259300	-2.98838800	-2.22997500
H	1.67789300	-2.94177400	-1.65584000
C	4.82783600	-2.28337600	-2.78790500
H	5.44383900	-0.41605000	-3.68384500
H	3.89870500	-4.00427400	-1.86978900
H	5.80777500	-2.74724500	-2.86904800
P	1.43050800	0.78393500	0.62711600
C	3.10749300	0.00009000	0.82458900
C	0.70792700	0.95237900	2.35461900
C	1.72552900	2.52911100	0.03688200
C	4.13491800	0.75151400	1.69146300
C	2.96355300	-1.46347600	1.29457700
H	3.48198500	-0.03382100	-0.20738200
C	1.21113400	2.15501900	3.18278300
C	-0.83676200	0.92010400	2.36468300
H	1.04057600	0.02938500	2.84679600
C	2.66924700	2.59744900	-1.17825300
C	0.37576400	3.20150400	-0.29649900
H	2.19502400	3.07764900	0.86274800
C	5.49786400	0.03858900	1.65217000
H	3.78551600	0.77856500	2.73060300
H	4.24399800	1.79157800	1.36335200
C	4.32404400	-2.17787200	1.28372500
H	2.54526400	-1.49303200	2.30851100
H	2.25244900	-1.98622000	0.64808700
C	0.68593300	2.07650000	4.62784200
H	0.84968300	3.08706500	2.72927500

H	2.30283300	2.21327200	3.19086300
C	-1.37040800	0.84758000	3.80339600
H	-1.23023700	1.82508100	1.88253800
H	-1.19310900	0.06643900	1.79263800
C	2.86292600	4.04625600	-1.65483300
H	2.23959500	2.00853100	-1.99308500
H	3.64095800	2.15072000	-0.94589500
C	0.56141500	4.64436100	-0.79116800
H	-0.12767200	2.60735200	-1.07135700
H	-0.28366400	3.19641200	0.57652600
C	5.37222200	-1.42157600	2.11409200
H	6.21727000	0.57812500	2.28030700
H	5.88848400	0.06450600	0.62536900
H	4.20566300	-3.20147100	1.65997800
H	4.67152600	-2.25869000	0.24678100
C	-0.84796200	2.00439400	4.66764900
H	1.04261000	2.94392700	5.19690100
H	1.10605700	1.18494200	5.11393100
H	-2.46746200	0.84721000	3.78986600
H	-1.05962600	-0.10967000	4.24454200
C	1.51935900	4.71080500	-1.98895700
H	3.52406800	4.05951500	-2.52986200
H	3.36925600	4.62301100	-0.86808200
H	-0.41444100	5.06901600	-1.05617300
H	0.96184800	5.25731700	0.02849100
H	6.34416300	-1.92532100	2.04733900
H	5.07965100	-1.43848000	3.17365600
H	-1.19606000	1.89941900	5.70245600
H	-1.26098400	2.95080600	4.29008300
H	1.67377800	5.75192600	-2.29633700
H	1.06353500	4.19238100	-2.84435100
O	-1.40345300	-1.23105200	0.03304100
B	-1.16325900	-2.69222900	0.67729200
C	-2.60511700	-3.42353800	0.59264900
C	-3.75019800	-2.84630800	1.17840500
C	-2.77268800	-4.65631500	-0.06176900
C	-5.00258500	-3.46877000	1.12172800
H	-3.66558400	-1.88066800	1.67653200
C	-4.02121200	-5.29082800	-0.13035700
H	-1.90324700	-5.11897600	-0.52448500
C	-5.14261900	-4.69844300	0.46315800
H	-5.86872200	-2.99763500	1.58338700
H	-4.12112700	-6.24475100	-0.64551200
H	-6.11385600	-5.18643300	0.41273300
O	-0.68030500	-2.41984600	2.01846500
H	-1.39212800	-2.53700800	2.66162900
O	-0.11924800	-3.32383300	-0.12344200
H	0.59754000	-3.54377800	0.48842100

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Sum of electronic and thermal Free Energies= -3696.909752

Ni	-0.12145300	-0.48530300	0.28264000
C	1.18310600	-2.12844600	0.34962200
H	1.75643700	-2.04109600	1.27097000
C	-0.15211400	-2.52272800	0.54535400
H	-0.45841400	-2.65470500	1.58225000
C	8.02775000	-1.70394100	-0.27619000
C	6.69428800	-1.46274200	-0.62788600
C	5.66353800	-1.59158200	0.31649500
C	6.00257000	-1.96882500	1.62640200
C	7.33311100	-2.21057700	1.98480700
C	8.35219300	-2.07967800	1.03278700
H	8.81251700	-1.59459700	-1.02123000
H	6.45139200	-1.16602700	-1.64701700
H	5.21642000	-2.06977900	2.37318400
H	7.57569900	-2.49724400	3.00551500
H	9.38735900	-2.26447000	1.30938400
C	4.21887400	-1.37233600	-0.07533100
C	3.52118000	-2.68918200	-0.46867000
H	4.16031400	-0.67881100	-0.91749000
H	3.68012600	-0.89999100	0.75306300
C	2.04178100	-2.53265300	-0.85407000
H	4.05861800	-3.13685100	-1.31499800
H	3.59446900	-3.41187900	0.35347800
H	1.66873200	-3.51238900	-1.18527900
O	1.88421800	-1.59691400	-1.94012800
C	-6.62777900	-1.55662500	1.98833300
C	-5.27136400	-1.32343800	2.24969200
C	-4.34829100	-1.12523100	1.20574700
C	-4.83193300	-1.17675100	-0.11634500
C	-6.18293300	-1.41311900	-0.38942800
C	-7.08721400	-1.60135000	0.66551100
H	-7.32582500	-1.70499700	2.81023000
H	-4.91840200	-1.29649900	3.27867300
H	-4.12340100	-1.04472000	-0.93052500
H	-6.53338800	-1.45608200	-1.41915100
H	-8.13976000	-1.78466500	0.45830900
B	-2.80691400	-0.87093300	1.45527200
O	-2.34944900	-1.09655500	2.77219400
H	-1.40223500	-0.88265000	2.79351900
O	-2.01943100	-0.46859300	0.46194000

H	2.32889200	-1.97734700	-2.71584600
C	-1.08569700	-3.12411900	-0.42836000
C	-2.14257600	-3.91313200	0.06438000
C	-1.02185900	-2.88773700	-1.81710400
C	-3.09260000	-4.46604600	-0.79618100
H	-2.23441700	-4.07245000	1.13636100
C	-1.97103100	-3.44333900	-2.67713500
H	-0.25258900	-2.23114700	-2.20946700
C	-3.00943900	-4.23818400	-2.17455600
H	-3.90976700	-5.05558800	-0.38823300
H	-1.91217700	-3.23873400	-3.74414700
H	-3.75514300	-4.65729800	-2.84582500
H	1.31433300	-0.34007800	0.13364400
P	-0.12364700	1.68238100	-0.12495200
C	-1.68325300	2.06171300	-1.06019300
C	-1.93104900	3.54255700	-1.39781000
C	-1.78307600	1.17375400	-2.31920300
H	-2.46174500	1.70829700	-0.37690100
C	-3.30188700	3.71729600	-2.07613600
H	-1.15186400	3.90653100	-2.08039400
H	-1.87959300	4.16300200	-0.49499500
C	-3.14745700	1.36081800	-3.00253600
H	-0.98515100	1.43078200	-3.03065800
H	-1.64728800	0.12635400	-2.03406400
C	-3.42187300	2.83675200	-3.32993100
H	-3.45748000	4.77228400	-2.33364400
H	-4.09174800	3.44360600	-1.36338100
H	-3.19338700	0.75186500	-3.91383200
H	-3.93093000	0.98580900	-2.33086700
H	-4.41731300	2.94893400	-3.77657700
H	-2.69734700	3.18187900	-4.08184700
C	1.24791300	2.47728000	-1.13998200
C	1.55013000	3.95333900	-0.79848500
C	2.54881600	1.65326600	-1.14801400
H	0.84547700	2.45023200	-2.16215200
C	2.57814300	4.54611000	-1.77810500
H	1.96035800	4.01677800	0.21728700
H	0.63899400	4.55861300	-0.81002500
C	3.59242500	2.25283100	-2.10393300
H	2.96683400	1.61556900	-0.13290300
H	2.32894800	0.62444700	-1.43562500
C	3.87765200	3.72832800	-1.79074900
H	2.78448500	5.58872200	-1.50715300
H	2.14635400	4.56194900	-2.78878400
H	4.51786800	1.66526600	-2.05218400
H	3.22190000	2.16693700	-3.13551700
H	4.58379300	4.14566000	-2.51878800
H	4.35868400	3.80197000	-0.80516500
C	-0.20072400	2.62720700	1.48139200
C	-1.55504500	2.46348000	2.20022400
C	0.95790500	2.16150400	2.39111900
H	-0.06445800	3.69164700	1.25743200
C	-1.55786600	3.19492000	3.55238800
H	-1.75963200	1.40134500	2.35895500
H	-2.36915700	2.84616000	1.57647500
C	0.94644100	2.88918500	3.74403800
H	0.85663200	1.07864200	2.55242500
H	1.92376500	2.30892600	1.89442400
C	-0.40596400	2.72577700	4.45272100
H	-2.52108300	3.03338100	4.05034100
H	-1.46621900	4.27731000	3.38216500
H	1.75976800	2.50984100	4.37465700
H	1.14536800	3.95786700	3.58104300
H	-0.40992900	3.28046100	5.39870100
H	-0.55619200	1.66681900	4.70604800

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Sum of electronic and thermal Free Energies= -3541.190876

C	-0.57184600	-1.98830500	-1.49498500
C	0.24178000	-1.61433700	-2.76383700
Ni	-0.05337900	-0.26194500	-1.01510100
C	1.37307300	-0.40109100	-2.77319700
H	1.57111500	-0.34267400	-3.85441100
C	2.66530500	-0.83073500	-2.05243000
H	3.02588600	-1.78084700	-2.46704000
H	2.45391400	-1.01112500	-0.99005200
C	3.76577800	0.24016800	-2.16177000
H	4.06084900	0.34491000	-3.21328500
H	3.33823300	1.19818700	-1.85356400
C	4.96924300	-0.09944900	-1.31081000
C	5.99447900	-0.92553500	-1.79961500
C	5.06226500	0.36262000	0.01270200
C	7.08068700	-1.28183300	-0.99200000
H	5.94287600	-1.28932400	-2.82461500
C	6.14483300	0.00963700	0.82601600
H	4.28131900	1.00955800	0.40565200
C	7.15939500	-0.81641800	0.32657400
H	7.86702300	-1.91834900	-1.39163900
H	6.20024700	0.38343800	1.84613500
H	8.00402700	-1.08914300	0.95481200
H	0.83152600	-2.48867000	-3.05307400
H	-0.43928000	-1.37352300	-3.58177800

H	-0.11036600	-2.79919200	-0.92521500
C	-2.03921500	-2.16723000	-1.65447000
C	-2.70251000	-3.26090100	-1.06472700
C	-2.82049200	-1.23004500	-2.36640500
C	-4.08982500	-3.40523300	-1.16011400
H	-2.12473300	-4.01253400	-0.53158800
C	-4.20410800	-1.37423500	-2.46533300
H	-2.34295400	-0.36526400	-2.82175800
C	-4.85010200	-2.46032100	-1.85884800
H	-4.57588700	-4.25964700	-0.69460200
H	-4.78226600	-0.63129700	-3.00946100
H	-5.92923700	-2.56915000	-1.93366000
P	-0.70653500	0.09217300	0.98031500
C	-2.54890900	0.35580400	1.02247000
C	0.11892800	1.67257000	1.56633500
C	-0.33138000	-1.20854300	2.26216600
C	-3.18660700	0.64076200	2.39603700
C	-2.96983300	1.42864000	-0.00290300
H	-2.93281700	-0.60610100	0.65458300
C	0.10166400	1.92839700	3.08874700
C	1.56715300	1.81569600	1.03980000
H	-0.47285900	2.45234500	1.07016200
C	-1.23896800	-2.44718500	2.12941800
C	1.15446300	-1.62181400	2.18647300
H	-0.51815200	-0.75061000	3.24229300
C	-4.71994100	0.68998400	2.27370400
H	-2.83550900	1.61105000	2.76616100
H	-2.89135400	-0.11018200	3.13725700
C	-4.49969100	1.50565500	-0.11770000
H	-2.58075400	2.40931000	0.29550400
H	-2.53275700	1.20112500	-0.97878000
C	0.65011800	3.33226200	3.40532000
H	0.72922500	1.18033000	3.59105000
H	-0.90431500	1.82434200	3.50319000
C	2.11749800	3.21805700	1.34010900
H	2.20725500	1.06873200	1.52448600
H	1.61852400	1.61093400	-0.03227200
C	-0.89336300	-3.51145600	3.18338000
H	-1.10818300	-2.87724200	1.13319300
H	-2.29489600	-2.17381700	2.21467300
C	1.50043900	-2.70104600	3.22493800
H	1.36361500	-1.99704500	1.17539300
H	1.80395700	-0.75516400	2.33538900
C	-5.16148200	1.74558800	1.24774200
H	-5.16276300	0.90146200	3.25463200
H	-5.08819000	-0.29819400	1.96439100
H	-4.77198300	2.30296100	-0.81948500
H	-4.87104100	0.56409500	-0.54221000
C	2.06642700	3.52828200	2.84356500
H	0.64454600	3.49288000	4.49041500
H	-0.02186200	4.08396100	2.96958000
H	3.14733300	3.29749100	0.96995100
H	1.52357600	3.95523600	0.78531100
C	0.58274100	-3.92474800	3.09900100
H	-1.54436300	-4.38385400	3.04935800
H	-1.10348500	-3.11184100	4.18542300
H	2.55064700	-2.99443900	3.11061600
H	1.39932700	-2.27502300	4.23302300
H	-6.25354900	1.74190900	1.14678300
H	-4.88121100	2.74250300	1.61584300
H	2.41053900	4.55177700	3.03427600
H	2.75847400	2.85807400	3.37375100
H	0.81910400	-4.66036000	3.87696800
H	0.76546400	-4.41604700	2.13270400
O	0.91135900	0.85100700	-2.32139100
B	-1.21088200	3.10715400	-2.33106700
O	-0.15582400	3.28982300	-1.46172000
H	0.50038300	2.57923400	-1.59950600
O	-1.28511800	2.06078700	-3.22200900
H	-0.47843700	1.48642900	-3.08685700
O	-2.23629400	4.03350500	-2.26553800
H	-2.91969600	3.80151800	-2.91156000

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Sum of electronic and thermal Free Energies= -3541.181699

C	-0.75332500	-1.76142200	1.73246100
C	0.14685900	-2.81816500	1.14784600
Ni	-0.09622700	-1.01108100	0.12799800
C	1.43860200	-2.47575200	-0.12754700
H	1.56040200	-3.52494400	-0.39961200
C	2.67137300	-1.88068300	0.55522500
H	2.95574400	-2.49698500	1.41488700
H	2.42796300	-0.88538400	0.94535100
C	3.86131400	-1.75194800	-0.41777800
H	4.19410600	-2.75022200	-0.72217600
H	3.51027300	-1.24430400	-1.32038000
C	4.99772500	-0.97587900	0.21012800
C	6.08730500	-1.62424100	0.81101900
C	4.95341700	0.42886800	0.24790300
C	7.10738600	-0.89244100	1.43216400
H	6.14023800	-2.71135900	0.78910000

C	5.96805400	1.16527100	0.86690400
H	4.11558300	0.94620800	-0.21684300
C	7.05097700	0.50575000	1.46352700
H	7.94633900	-1.41329100	1.88813000
H	5.91828800	2.25184600	0.88070600
H	7.84334200	1.07568800	1.94284100
H	0.87174500	-3.16978700	1.87936700
H	-0.38881200	-3.64768700	0.69284300
H	-0.36059200	-1.30933800	2.64586600
C	-2.22082300	-1.98704800	1.77798400
C	-2.98466400	-1.48804900	2.85172900
C	-2.90076400	-2.67899300	0.75226600
C	-4.37208900	-1.65517100	2.89499200
H	-2.48705400	-0.96887900	3.66758500
C	-4.28386600	-2.85570300	0.80123800
H	-2.33640000	-3.05689800	-0.09601100
C	-5.03216700	-2.34090000	1.86876800
H	-4.93608500	-1.25749300	3.73586500
H	-4.78393400	-3.38822700	-0.00466900
H	-6.11069100	-2.47466600	1.90037200
P	-0.86228500	0.99116700	-0.11960000
C	-2.70508600	0.94741500	-0.38308100
C	-0.12282900	1.87193700	-1.60631200
C	-0.56437700	2.11896300	1.33598000
C	-3.42661000	2.30117400	-0.51941800
C	-3.05718400	0.02128700	-1.56651800
H	-3.06708800	0.45014000	0.52708500
C	-0.20233000	3.41418100	-1.58382600
C	1.32679800	1.42750800	-1.90470000
H	-0.73839300	1.50305900	-2.43715300
C	-1.43987300	1.76324700	2.55233800
C	0.92991100	2.08506100	1.72470000
H	-0.82088700	3.13711400	1.01786900
C	-4.94897400	2.09433600	-0.60446400
H	-3.09139000	2.80282300	-1.43511800
H	-3.18240800	2.96579200	0.31693900
C	-4.57772900	-0.17237300	-1.67712600
H	-2.67655400	0.44819700	-2.50306800
H	-2.55782900	-0.94286100	-1.43394400
C	0.27509400	4.00353000	-2.92352800
H	0.44189600	3.79980100	-0.78295500
H	-1.21503500	3.76457500	-1.36728300
C	1.81493900	2.01686800	-3.23693000
H	1.98992500	1.76799800	-1.09809300
H	1.38594600	0.34132700	-1.93565000
C	-1.14538400	2.68865300	3.74416500
H	-1.23567400	0.72974600	2.84378600
H	-2.50344800	1.81324900	2.29953500
C	1.22834300	2.99563900	2.92626800
H	1.20336200	1.04886300	1.96764600
H	1.55633500	2.38029500	0.87773400
C	-5.31758000	1.17041500	-1.77566400
H	-5.44999200	3.06437200	-0.71017900
H	-5.30553700	1.65203100	0.33619200
H	-4.80737500	-0.79905700	-2.54769200
H	-4.92903900	-0.71629200	-0.79192200
C	1.70228900	3.54804000	-3.26257100
H	0.22240200	5.09857500	-2.88349300
H	-0.40964500	3.68267600	-3.72088100
H	2.85178300	1.70741000	-3.41776400
H	1.21214900	1.59050300	-4.05061600
C	0.34036700	2.65078700	4.13008900
H	-1.76995500	2.39741600	4.59748200
H	-1.42803600	3.71830300	3.48340100
H	2.28828200	2.91285500	3.19482500
H	1.05599400	4.04175700	2.63648500
H	-6.40146600	1.00500300	-1.80159700
H	-5.05070900	1.66525400	-2.72036200
H	2.00309400	3.93957700	-4.24196300
H	2.39839900	3.97316300	-2.52521300
H	0.53762800	3.34034400	4.95951900
H	0.59420200	1.64322700	4.48888700
O	1.09748300	-1.72577600	-1.24926400
B	0.37694900	-2.46061800	-2.45977200
O	0.10433400	-1.41151600	-3.42217100
H	0.86457700	-1.34849300	-4.01723200
O	-0.87222400	-3.03441400	-1.96132200
H	-1.58830000	-2.63316300	-2.47344500
O	1.34188200	-3.46516900	-2.87090200
H	0.84381700	-4.23999800	-3.16618100

dist-TS3^{B}-toluene

Sum of electronic and thermal Free Energies= -3541.179828

Ni	0.53896800	0.72946400	0.42902800
C	-1.11155400	2.03020200	0.53490100
H	-1.69865200	1.71320800	1.39497600
C	0.07801900	2.69707900	0.86073600
H	0.29256800	2.79124800	1.92422500
C	-7.61119600	0.11584300	-0.72981500
C	-6.23394600	0.20741100	-0.96372800
C	-5.34197600	0.50331100	0.07922700

C	-5.86541900	0.70486100	1.36705800
C	-7.24054500	0.61418900	1.60799500
C	-8.12005300	0.31990100	0.55829100
H	-8.28539500	-0.11831100	-1.55052900
H	-5.84604800	0.04255300	-1.96771100
H	-5.18816700	0.93132400	2.18921600
H	-7.62588200	0.76947200	2.61313100
H	-9.18899600	0.24662900	0.74331500
C	-3.85934000	0.64683900	-0.18496600
C	-3.45812800	2.11358300	-0.43525400
H	-3.57493700	0.05183600	-1.05589100
H	-3.29182700	0.24718100	0.66238900
C	-1.96029100	2.32502500	-0.70501700
H	-4.02517300	2.49547700	-1.29456000
H	-3.75141100	2.73357600	0.42108700
H	-1.80394100	3.38703400	-0.94299700
O	-1.51996400	1.53961800	-1.83178400
B	2.99666100	1.54709500	1.84083600
O	2.38161100	1.64308500	3.11784500
H	1.47843100	1.30170100	3.04017700
O	2.38805300	1.12408200	0.73891300
H	-1.98334200	1.87617900	-2.61675600
C	0.87472400	3.60777100	0.01486700
C	1.63243700	4.61146200	0.64728400
C	0.94720100	3.50151600	-1.38894400
C	2.41328100	5.50040400	-0.09453700
H	1.61653400	4.68708700	1.73246500
C	1.72822300	4.39010600	-2.12950800
H	0.42156800	2.69411900	-1.88775800
C	2.46089200	5.39814800	-1.48977100
H	2.99327900	6.26514200	0.41665800
H	1.78108900	4.28488700	-3.21107100
H	3.07498100	6.08307400	-2.06959100
H	-0.79461500	0.22021400	0.18901700
P	1.05403900	-1.34759600	-0.09990600
C	2.71978400	-1.31694700	-0.91815500
C	3.31895500	-2.68308400	-1.29645900
C	2.70089700	-0.35631000	-2.12682700
H	3.34719500	-0.83776200	-0.16034700
C	4.73714000	-2.50681100	-1.86878600
H	2.69229000	-3.17046800	-2.05490600
H	3.34761700	-3.35223800	-0.42797100
C	4.11497300	-0.19400400	-2.70720300
H	2.03145500	-0.74224200	-2.90916300
H	2.31468200	0.61628000	-1.80799800
C	4.73956900	-1.54991300	-3.07133900
H	5.14605800	-3.48358000	-2.15604100
H	5.39251400	-2.10525100	-1.08393100
H	4.08175500	0.45915500	-3.58784300
H	4.74243000	0.31138500	-1.96180900
H	5.76282700	-1.41087800	-3.44116200
H	4.16627700	-2.00482600	-3.89239400
C	-0.03142800	-2.34950200	-1.26700100
C	-0.02081500	-3.87599000	-1.02779400
C	-1.47918600	-1.83112100	-1.34655500
H	0.42806000	-2.16633900	-2.24806100
C	-0.81559600	-4.61037200	-2.12183200
H	-0.47965800	-4.09714900	-0.05591800
H	1.00061600	-4.26575800	-0.99103000
C	-2.28842800	-2.57667000	-2.41982600
H	-1.96936700	-1.95760900	-0.37176200
H	-1.47454800	-0.76109800	-1.55847300
C	-2.26007300	-4.09680200	-2.20714000
H	-0.80379400	-5.68893400	-1.92268000
H	-0.31763800	-4.46259800	-3.09048800
H	-3.32282600	-2.21003000	-2.42024200
H	-1.87053600	-2.34178700	-3.40928500
H	-2.79926400	-4.60743500	-3.01423900
H	-2.78451500	-4.34055300	-1.27237800
C	1.21556100	-2.36022300	1.45786700
C	2.43196600	-1.94404600	2.30871000
C	-0.08736900	-2.23601000	2.27867300
H	1.34858700	-3.40938500	1.16894800
C	2.50039300	-2.75654300	3.61195900
H	2.36323400	-0.87885400	2.54626200
H	3.35994100	-2.07751700	1.74380300
C	-0.01409900	-3.04226300	3.58431300
H	-0.25119400	-1.17345500	2.50829200
H	-0.95139000	-2.55920200	1.68705200
C	1.20374500	-2.63211500	4.42513400
H	3.35702600	-2.41842100	4.20685100
H	2.67796800	-3.81506200	3.37339800
H	-0.94005400	-2.90501700	4.15611800
H	0.05292600	-4.11287200	3.34446300
H	1.26221800	-3.24281200	5.33413700
H	1.08335500	-1.58937800	4.75130500
O	4.34892200	1.91448600	1.82846000
H	4.62180600	2.16780900	2.72252400

prox-3

Sum of electronic and thermal Free Energies= -3696.953192

Ni	-0.29463300	-0.61828600	-0.87565500	H	-2.01012300	6.49311800	-0.99613000
C	4.33816200	-2.81768400	2.15723300	H	-2.43548500	6.73172900	1.44597400
C	3.67497900	-2.97675900	0.93506000	B	0.74601500	2.66392500	-0.39678300
C	2.49770300	-2.26617800	0.64333700	O	1.32403500	1.81385900	0.52180700
C	1.98938200	-1.40669700	1.63269600	H	1.65366200	1.00531500	0.05770100
C	2.64811800	-1.23925100	2.85445200	O	0.82348800	2.43451400	-1.75279000
C	3.83043800	-1.94015400	3.12318200	H	1.20289700	1.53055300	-1.91260000
H	5.25139100	-3.37514700	2.35306100	P	-2.37237500	-0.87351200	-0.18915800
H	4.08784200	-3.65456500	0.19038000	C	-3.15778800	-2.50665600	-0.59434000
H	1.07943100	-0.85023700	1.44006000	C	-4.58467400	-2.70922100	-0.04887800
H	2.24074100	-0.55613700	3.59620800	C	-3.11260700	-2.77673900	-2.11439800
H	4.34507700	-1.80872400	4.07191300	H	-2.49830100	-3.24177700	-0.11495400
C	1.86235000	-2.40107100	-0.72757900	C	-5.08865500	-4.12887200	-0.36340000
H	2.22254300	-3.34794300	-1.15552800	H	-5.25980600	-1.98077300	-0.51504700
C	0.31785700	-2.41826800	-0.72063200	H	-4.61980700	-2.53200000	1.03146500
H	-0.05810200	-2.88483700	-1.64181700	C	-3.61349500	-4.19640100	-2.42823700
H	-0.09565100	-2.95386800	0.14027700	H	-3.75088700	-2.05368700	-2.63852300
C	7.70743000	1.33570200	-1.87939000	H	-2.09619800	-2.63360000	-2.49573600
C	6.31573200	1.20713500	-1.78967100	C	-5.02614200	-4.42801900	-1.86933700
C	5.72808100	0.32700700	-0.86515500	H	-6.11426500	-4.24672500	0.00632200
C	6.57349800	-0.42360800	-0.02970700	H	-4.46959800	-4.85671000	0.17916200
C	7.96558800	-0.29931300	-0.11423000	H	-3.60070600	-4.36157200	-3.51218300
C	8.53915400	0.58130500	-1.04120300	H	-2.92131400	-4.92663900	-1.98689900
H	8.14240900	2.02607600	-2.59866000	H	-5.34684800	-5.45835300	-2.06430300
H	5.67654200	1.79979000	-2.44207700	H	-5.73273500	-3.77106300	-2.39579300
H	6.13289900	-1.10748100	0.69318800	C	-3.49248100	0.43832600	-0.94175500
H	8.60236700	-0.88569300	0.54463900	C	-4.62059500	0.96133100	-0.02682700
H	9.61994800	0.68179400	-1.10660500	C	-2.64990100	1.60167000	-1.50983600
C	4.22681300	0.15250300	-0.79842500	H	-3.96445900	-0.06940000	-1.79254500
C	3.73264900	-0.89879700	-1.81531700	C	-5.48430500	2.00566200	-0.75561400
H	3.73085900	1.10418900	-1.01252300	H	-4.19255500	1.43285000	0.86444900
H	3.93726500	-0.13754600	0.21332000	H	-5.24905400	0.13671200	0.32358700
C	2.23885100	-1.26214800	-1.71384400	C	-3.51788700	2.66403600	-2.19989300
H	3.93567100	-0.51340700	-2.82212800	H	-2.08031000	2.07482600	-0.70214200
H	4.32640300	-1.81506500	-1.71104100	H	-1.91346400	1.21362600	-2.22469000
H	1.92719400	-1.63439900	-2.70472300	C	-4.63039700	3.17254600	-1.27339600
O	1.44008200	-0.13495000	-1.37636100	H	-6.26268700	2.37178500	-0.07535900
C	-1.18189600	5.05302200	1.98317900	H	-5.99922300	1.52733800	-1.60040500
C	-0.34758900	4.03512800	1.50802900	H	-2.88112000	3.49422400	-2.52641000
C	-0.09509200	3.88037500	0.13050700	H	-3.96867000	2.22977300	-3.10327500
C	-0.70653800	4.78624800	-0.75841600	H	-5.25928900	3.90116400	-1.79904100
C	-1.54043800	5.80875800	-0.29307600	H	-4.17741900	3.69883400	-0.42143400
C	-1.78142900	5.94285700	1.08121800	C	-2.47081500	-0.66306400	1.66057400
H	-1.37160900	5.15003200	3.04996800	C	-1.88140100	-1.87728300	2.40829600
H	0.10147500	3.33591700	2.20914800	C	-1.73373000	0.63311300	2.06922300
H	-0.53906200	4.67373900	-1.82701500	H	-3.52753600	-0.57044900	1.93852100

C	-1.91749300	-1.66042200	3.93069000
H	-0.84334700	-2.03147800	2.09250300
H	-2.43038900	-2.79109900	2.15720400
C	-1.76712600	0.84381000	3.59016600
H	-0.69221600	0.58253100	1.72889900
H	-2.16572700	1.50575600	1.57029900
C	-1.19294500	-0.36859500	4.33654500
H	-1.46723000	-2.52478800	4.43329100
H	-2.96405200	-1.60957000	4.26190900
H	-1.20732300	1.75179900	3.84460200
H	-2.80527600	1.01075200	3.90967500
H	-1.26341700	-0.21821800	5.42051500
H	-0.12511900	-0.46558600	4.09874500

prox-TS2

Sum of electronic and thermal Free Energies= -3696.936068

Ni	0.07449100	-0.34201400	0.60271800
C	-4.72249000	-3.20012900	-1.37615300
C	-4.07699000	-2.90588100	-0.16929700
C	-2.84341100	-2.23372500	-0.14523600
C	-2.25783300	-1.88758500	-1.37624700
C	-2.89719900	-2.17822900	-2.58552600
C	-4.13723400	-2.83067500	-2.59298000
H	-5.68057200	-3.71494400	-1.36522300
H	-4.54737100	-3.19300000	0.76916900
H	-1.29720400	-1.38092400	-1.38863400
H	-2.42780300	-1.89301900	-3.52454000
H	-4.63573000	-3.05413600	-3.53313500
C	-2.21193700	-1.86574100	1.18715500
H	-2.63836900	-2.53833400	1.94542800
C	-0.67310400	-2.00464400	1.20953300
H	-0.32749500	-2.02901700	2.25368700
H	-0.34933300	-2.92242500	0.72121300
C	-7.83374500	2.35207200	0.80237000
C	-6.45375100	2.11672500	0.76489800
C	-5.93865300	0.91209400	0.25693600
C	-6.84409900	-0.05458800	-0.21371500
C	-8.22493500	0.17497200	-0.17936100
C	-8.72605600	1.38021800	0.33046800
H	-8.21230100	3.29303100	1.19531700
H	-5.76690000	2.87835800	1.13035200
H	-6.45969000	-0.99147200	-0.61237000
H	-8.90928500	-0.58366600	-0.55277700
H	-9.79790300	1.56176000	0.35562800
C	-4.45078200	0.63775400	0.25877600
C	-3.98994900	0.03673900	1.60428400
H	-3.89712600	1.56574800	0.08484700
H	-4.19708900	-0.03971300	-0.55868000
C	-2.52091700	-0.41779000	1.64064100
H	-4.15245500	0.78761900	2.38659600
H	-4.62625600	-0.81825600	1.86050200
H	-2.15462800	-0.33910000	2.67368800
O	-1.69868100	0.41067600	0.79990400
C	1.93418700	5.78821400	-1.53740300
C	0.96400000	4.79856600	-1.34198000
C	1.05199600	3.88848500	-0.27020800
C	2.14172500	4.01779800	0.61297300
C	3.12140700	4.99874000	0.42351300
C	3.02051400	5.88609400	-0.65658500
H	1.85147400	6.47644000	-2.37582900
H	0.13413600	4.71637000	-2.04020500
H	2.22101300	3.32766300	1.44854600
H	3.96164000	5.07207300	1.11068200
H	3.78134600	6.64804900	-0.81074100
B	0.01189600	2.72143400	-0.06670100
O	-1.00957900	2.60434400	-1.01131500
H	-1.55428500	1.82092400	-0.80432300
O	0.12073600	1.85828100	0.98090200
H	-1.01889200	1.28067300	1.14414100
P	2.15440000	-0.86901800	0.14705000
C	2.72588700	0.53014300	-0.95238600
C	4.23562800	0.55225200	-1.25963200
C	1.88986300	0.57394600	-2.25291900
H	2.48012800	1.42910100	-0.37848900
C	4.59706100	1.78082800	-2.11268000
H	4.51778600	-0.35327300	-1.81135300
H	4.81927300	0.55681200	-0.33255800
C	2.28375100	1.76886100	-3.13794400
H	2.03623000	-0.35164800	-2.82446000
H	0.82201300	0.62816100	-2.01042100
C	3.79255300	1.80005400	-3.42075100
H	5.67331200	1.77887000	-2.32393500
H	4.38327100	2.69340100	-1.53937700
H	1.71837900	1.72733500	-4.07697900
H	1.99510300	2.69702700	-2.63418500
H	4.04649800	2.68944600	-4.01009600
H	4.07101300	0.92635100	-4.02725600
C	2.69419700	-2.40299000	-0.80401400
C	4.08197100	-2.95738800	-0.41207400
C	1.64530600	-3.53010200	-0.82889100
H	2.77649400	-2.03214300	-1.83307600

C	4.50439500	-4.09320000	-1.36062000
H	4.05158400	-3.34476500	0.61315600
H	4.83912800	-2.16819900	-0.43057500
C	2.07519900	-4.66680300	-1.77037800
H	1.51288700	-3.93124700	0.18385600
H	0.67779800	-3.12909400	-1.14507100
C	3.45920100	-5.21711000	-1.39780600
H	5.47894500	-4.48618200	-1.04686600
H	4.63766600	-3.68549400	-2.37235100
H	1.32493800	-5.46627600	-1.74648400
H	2.10099700	-4.28739700	-2.80159900
H	3.76366500	-5.99614400	-2.10702400
H	3.40488400	-5.69176300	-0.40800300
C	3.19005500	-0.77415800	1.69381800
C	3.15371600	0.64660900	2.29471500
C	2.68986100	-1.80377600	2.72923100
H	4.22687600	-1.01321500	1.43162200
C	3.95413900	0.71722600	3.60591600
H	2.10976100	0.93740300	2.46748800
H	3.56564300	1.37125500	1.58599100
C	3.51678000	-1.74068700	4.02255600
H	1.64293900	-1.57984300	2.96427800
H	2.70856200	-2.81852000	2.31647900
C	3.48260900	-0.32883300	4.62633400
H	3.87374200	1.72647000	4.02777900
H	5.01775700	0.55089100	3.38468400
H	3.13241900	-2.47400800	4.74169800
H	4.55655900	-2.02230100	3.80534300
H	4.10261000	-0.28422800	5.52981400
H	2.45370200	-0.09554800	4.93438300

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Sum of electronic and thermal Free Energies= -3696.948911

Ni	0.19225400	-0.19156100	0.95644000
C	-4.11935700	-3.21293600	-1.57189100
C	-3.58799000	-3.02305900	-0.29036300
C	-2.48481300	-2.18106900	-0.07236800
C	-1.91503700	-1.54768400	-1.19123700
C	-2.44016100	-1.72993900	-2.47346000
C	-3.55042100	-2.56081400	-2.67172200
H	-4.97784500	-3.86637500	-1.70882700
H	-4.04654400	-3.53292200	0.55469600
H	-1.04931800	-0.90452700	-1.06331200
H	-1.98133100	-1.22109700	-3.31816700
H	-3.96173900	-2.70200400	-3.66819800
C	-1.98750500	-1.95526300	1.34994900
H	-2.39333200	-2.77778400	1.95592800
C	-0.44983200	-1.92909500	1.50891400
H	-0.22165600	-1.90940800	2.58872500
H	-0.01605200	-2.84366600	1.11112200
C	-7.94154900	1.75181000	0.80134600
C	-6.55218600	1.66010600	0.95219700
C	-5.82790300	0.61779900	0.35043000
C	-6.53038000	-0.33417300	-0.40830800
C	-7.91908400	-0.24735500	-0.56266800
C	-8.63104100	0.79667000	0.04297100
H	-8.48448000	2.56881100	1.27109400
H	-6.02344300	2.40861600	1.53988100
H	-5.98161900	-1.14588600	-0.88204800
H	-8.44493900	-0.99075400	-1.15764400
H	-9.70930900	0.86763700	-0.07816500
C	-4.33295800	0.48951200	0.54794200
C	-4.00260800	-0.31563800	1.82429600
H	-3.88052500	1.48311900	0.62742700
H	-3.88796400	0.00715300	-0.32390900
C	-2.52083000	-0.67082300	2.01420000
H	-4.34945000	0.25709700	2.69229200
H	-4.57279900	-1.25110900	1.82477500
H	-2.30747900	-0.76529200	3.08467500
O	-1.65312200	0.39242700	1.49524600
C	0.75281800	6.27744400	-1.15175700
C	0.10148000	5.06138900	-0.90686400
C	0.70482600	4.04382100	-0.14178200
C	1.99098500	4.29636300	0.37590800
C	2.65358700	5.50604100	0.13774400
C	2.03441100	6.50240800	-0.63052100
H	0.26796400	7.04706000	-1.74919700
H	-0.88874900	4.89187900	-1.32425600
H	2.47485900	3.51968900	0.96376800
H	3.64932300	5.67412000	0.54354300
H	2.54566800	7.44345000	-0.82198700
B	0.02184600	2.62882500	0.09961100
O	-1.21330000	2.44210900	-0.56002100
H	-1.56597800	1.57193400	-0.30447900
O	0.61473800	1.70422600	0.85378800
H	-1.64646100	1.16825200	2.08384400
P	2.12350300	-0.79624600	0.10964600
C	2.69736400	0.59251200	-0.99835000
C	4.15409600	0.52304300	-1.49292400
C	1.72552700	0.78228800	-2.18380700
H	2.58570400	1.46998200	-0.35742900

C	4.50827200	1.79461500	-2.28584900
H	4.29149800	-0.34667500	-2.14746800
H	4.84757800	0.40625400	-0.65251300
C	2.08687100	2.03753900	-2.99589000
H	1.76368900	-0.09066700	-2.84926800
H	0.69802300	0.85738700	-1.81459400
C	3.54841500	2.00230200	-3.46739400
H	5.54411300	1.73227500	-2.64153100
H	4.45217900	2.66296900	-1.61487600
H	1.41047400	2.12777200	-3.85487500
H	1.92677000	2.92378000	-2.37051500
H	3.79741100	2.92848300	-3.99972700
H	3.67949400	1.17910300	-4.18437900
C	2.42787900	-2.31347300	-0.97712000
C	3.83960900	-2.93045600	-0.83818400
C	1.36230200	-3.42358900	-0.92078600
H	2.36636600	-1.88327600	-1.98433000
C	4.08545100	-3.98353700	-1.93343400
H	3.93817900	-3.40855400	0.14355500
H	4.61701800	-2.16464500	-0.89523300
C	1.60535800	-4.47356500	-2.01775900
H	1.39660900	-3.91841700	0.05763600
H	0.36323000	-2.99669600	-1.03213000
C	3.01177800	-5.08069000	-1.91765500
H	5.08231000	-4.42134200	-1.80096500
H	4.08529200	-3.48688100	-2.91379000
H	0.84300000	-5.25898400	-1.94793600
H	1.48175300	-3.99969700	-3.00182700
H	3.18155100	-5.79113500	-2.73576000
H	3.09246900	-5.64972600	-0.98075500
C	3.35267300	-0.87839200	1.50927800
C	3.47126900	0.48331800	2.22511700
C	2.94984500	-1.97324500	2.51930400
H	4.33181500	-1.13369400	1.08838500
C	4.46489200	0.40662200	3.39619100
H	2.47946000	0.78125700	2.58659600
H	3.79155300	1.26133800	1.52489100
C	3.95697800	-2.05892800	3.67681200
H	1.95976600	-1.72855400	2.92016000
H	2.85605200	-2.94770300	2.02768700
C	4.09424500	-0.70493000	4.38921500
H	4.50477000	1.37649800	3.90701000
H	5.47247600	0.21637400	3.00030800
H	3.63960100	-2.83325400	4.38581800
H	4.93633200	-2.36817800	3.28558300
H	4.84371200	-0.76735100	5.18755600
H	3.13786900	-0.45455000	4.86965800

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Sum of electronic and thermal Free Energies=-3696.93931

Ni	-0.33185200	-0.48065900	-0.07945400
C	1.28798500	-1.99990700	-0.54261600
C	-0.19844900	-2.22452900	-0.79704300
H	-0.62248100	-3.05653800	-0.23022000
C	7.54712500	0.77968700	-1.33241400
C	6.15725400	0.63485000	-1.43016200
C	5.46179300	-0.24038500	-0.58036100
C	6.19344300	-0.97067200	0.37201000
C	7.58222600	-0.83031300	0.47454800
C	8.26534900	0.04652800	-0.37922800
H	8.06775700	1.46604700	-1.99630800
H	5.60566600	1.21031800	-2.17140800
H	5.66822600	-1.65162400	1.03988800
H	8.13073000	-1.40041900	1.22089700
H	9.34384600	0.15964200	-0.29958500
C	3.96703100	-0.43324600	-0.71196500
C	3.63305700	-1.65565700	-1.59086600
H	3.50582500	0.46244900	-1.13682900
H	3.53807400	-0.57163000	0.28585000
C	2.13644900	-1.89559500	-1.83067500
H	4.11851900	-1.54025100	-2.56869700
H	4.06386500	-2.55633200	-1.14120100
H	2.01668700	-2.82345700	-2.40449500
O	1.54293300	-0.81015200	-2.58032700
C	1.97361700	5.89929100	0.12234800
C	1.78002800	4.61058800	-0.39271200
C	1.19077800	3.58852900	0.37879700
C	0.80813400	3.91151400	1.69596100
C	0.99678600	5.19413100	2.22392500
C	1.58070100	6.19539800	1.43493700
H	2.42847400	6.67204300	-0.49446000
H	2.08848100	4.39047000	-1.41247900
H	0.35559600	3.13576900	2.30787200
H	0.69047100	5.41593900	3.24450100
H	1.72852100	7.19489700	1.83847300
B	0.93534800	2.12386100	-0.19085000
O	1.40919700	1.91764500	-1.49829200
H	1.29721900	0.98813100	-1.77959000
O	0.31266900	1.20731500	0.55647100
H	2.00711300	-0.73407400	-3.43054300
H	1.42215000	-0.95751400	-0.10579800

H	-0.45532200	-2.29591800	-1.85777500
C	1.85048000	-2.91982100	0.52479900
C	2.21846100	-4.24131500	0.22426300
C	1.96561400	-2.47070200	1.84830100
C	2.70906100	-5.08745400	1.22399500
H	2.12338000	-4.61403500	-0.79274800
C	2.45140600	-3.31616600	2.85254700
H	1.66825900	-1.45193600	2.09176300
C	2.82934600	-4.62774600	2.54265200
H	2.99566100	-6.10632700	0.97473700
H	2.53543500	-2.95011200	3.87292500
H	3.21098800	-5.28619200	3.31895100
P	-2.46836200	-0.28365700	-0.06975400
C	-3.39117400	-1.89618000	0.24991400
C	-4.73712600	-1.80643900	1.00365200
C	-3.57085400	-2.72798500	-1.03983600
H	-2.68995800	-2.43978600	0.89537300
C	-5.27855400	-3.21381200	1.31678400
H	-5.47175300	-1.26144300	0.39876800
H	-4.63005000	-1.25706900	1.94234000
C	-4.09444000	-4.13742100	-0.71913000
H	-4.29398500	-2.22823800	-1.69661000
H	-2.63327700	-2.79756900	-1.59603300
C	-5.41973300	-4.07331000	0.05302400
H	-6.24396200	-3.12633300	1.82964500
H	-4.59196400	-3.70921000	2.01736700
H	-4.22081300	-4.70276600	-1.65027300
H	-3.34498600	-4.67333400	-0.12044800
H	-5.75831700	-5.08263100	0.31625300
H	-6.19270000	-3.63786600	-0.59572200
C	-3.08391900	0.37626800	-1.70120700
C	-4.55603200	0.83743000	-1.70227900
C	-2.13918700	1.45275100	-2.28213400
H	-3.00356500	-0.49312800	-2.36610000
C	-4.99159600	1.28556300	-3.10859000
H	-4.68688200	1.67161200	-1.00334600
H	-5.21078200	0.03172500	-1.35573500
C	-2.59984900	1.88651300	-3.68252700
H	-2.10638000	2.32841800	-1.62656500
H	-1.11726000	1.06307900	-2.32197700
C	-4.05868300	2.36763500	-3.67208400
H	-6.02530700	1.65010000	-3.07340800
H	-4.98430700	0.41570600	-3.78017500
H	-1.93840500	2.67674500	-4.05764800
H	-2.50408700	1.03727400	-4.37380400
H	-4.37414500	2.64948600	-4.68391400
H	-4.13663700	3.27145300	-3.05140300
C	-3.01876300	0.84773300	1.30685600
C	-2.38074100	0.34703700	2.62390800
C	-2.69201400	2.33928000	1.09288900
H	-4.10913700	0.74931500	1.37680500
C	-2.85715700	1.17851300	3.82484000
H	-1.29134800	0.42775600	2.52277600
H	-2.60649300	-0.71202600	2.79359000
C	-3.15403100	3.17813600	2.29800000
H	-1.61498700	2.44893600	0.94901800
H	-3.18504300	2.71611800	0.19258400
C	-2.56024900	2.67093000	3.62030600
H	-2.37478400	0.81499500	4.74039600
H	-3.93892200	1.03537200	3.95759700
H	-2.87594500	4.22678700	2.13590100
H	-4.25129600	3.14740500	2.36132800
H	-2.95205500	3.25632200	4.46124000
H	-1.47289200	2.82107600	3.61033900

prox-TS3

Sum of electronic and thermal Free Energies=-3696.920667

Ni	-0.47662000	-0.59368400	-0.74955200
C	1.11232500	-1.94460200	-1.28119700
C	-0.10782700	-2.16191800	-1.93861100
H	-0.76801200	-2.96500700	-1.62547900
C	7.84050500	-0.80052800	-0.13137700
C	6.71450200	-1.12100900	-0.89714200
C	5.90635400	-0.11326700	-1.45251500
C	6.25945200	1.22567600	-1.22273500
C	7.38497100	1.55351900	-0.45530500
C	8.17936500	0.54093300	0.09529300
H	8.45460800	-1.59474100	0.28684600
H	6.45977600	-2.16548400	-1.06819800
H	5.65301100	2.01986700	-1.65299100
H	7.64058700	2.59763400	-0.29013500
H	9.05416400	0.79208300	0.69014300
C	4.66413000	-0.47071800	-2.24201600
C	3.53485900	-0.98827800	-1.33150000
H	4.90561500	-1.24206900	-2.98522700
H	4.31783100	0.41070600	-2.79118200
C	2.28479200	-1.39211800	-2.12009300
H	3.89735700	-1.85829800	-0.77583900
H	3.28242800	-0.22092000	-0.59652400
H	2.56374500	-2.22107100	-2.78872900
O	1.77707400	-0.30213700	-2.90692300

C	-7.00990000	-2.49137200	-0.60621100
C	-5.63327000	-2.58442000	-0.36160300
C	-4.72760600	-1.63959400	-0.88441600
C	-5.25863700	-0.59293700	-1.66464100
C	-6.63181000	-0.48726300	-1.91456800
C	-7.51366900	-1.44002600	-1.38435800
H	-7.68998400	-3.23286800	-0.19155000
H	-5.25277900	-3.40142800	0.24785900
H	-4.57331600	0.14538600	-2.07305900
H	-7.01669900	0.33225900	-2.51846300
H	-8.58207100	-1.36331300	-1.57470300
B	-3.16585800	-1.69848800	-0.60269100
O	-2.75400900	-2.76375200	0.23107300
H	-1.79884500	-2.68645700	0.39225000
O	-2.34951700	-0.77878200	-1.10828200
H	2.29189600	-0.25588200	-3.72761500
H	0.93890500	-0.41786400	-0.42532200
P	-0.81477700	1.25709200	0.43732100
C	-2.26726000	2.15428700	-0.30133500
C	-2.71463500	3.42702800	0.44130300
C	-2.01469400	2.43807700	-1.79765300
H	-3.06734900	1.40805000	-0.25736800
C	-3.96450900	4.03131600	-0.22257900
H	-1.91100800	4.17413200	0.41911800
H	-2.91982100	3.21138500	1.49611000
C	-3.25406200	3.06689200	-2.45631600
H	-1.16577600	3.12528400	-1.91513600
H	-1.74966100	1.50278900	-2.30113800
C	-3.71750500	4.32718900	-1.70984400
H	-4.25892200	4.94662500	0.30534600
H	-4.80037000	3.32449700	-0.12566400
H	-3.03715000	3.30203200	-3.50551700
H	-4.07007100	2.33217700	-2.45930400
H	-4.62642900	4.72999200	-2.17316100
H	-2.94515700	5.10457500	-1.79788700
C	0.52866300	2.57484200	0.53631300
C	0.58987000	3.36161600	1.86394200
C	1.92117400	2.03474700	0.16298800
H	0.24271700	3.28532400	-0.25030700
C	1.63127600	4.49170100	1.78793300
H	0.86621500	2.68533900	2.68211600
H	-0.38805500	3.78207700	2.11665600
C	2.97212800	3.15447700	0.11251500
H	2.22935600	1.28328400	0.90283100
H	1.86999500	1.52437000	-0.80275700
C	3.02099500	3.95056500	1.42399600
H	1.66539500	5.02228900	2.74721200
H	1.31496000	5.22344000	1.03142100
H	3.95445500	2.72219200	-0.10908100
H	2.72955500	3.83478700	-0.71599200
H	3.74195600	4.77314900	1.34392900
H	3.37549000	3.29497900	2.23193900
C	-1.28454200	0.84720900	2.19660100
C	-2.67877300	0.19772000	2.30427700
C	-0.21572400	-0.08701500	2.80133000
H	-1.30229700	1.78154100	2.76863700
C	-3.00534900	-0.16595500	3.76251100
H	-2.70399600	-0.70959100	1.69423200
H	-3.45109700	0.86712100	1.91246900
C	-0.53944500	-0.45499000	4.25666600
H	-0.17506900	-1.00201000	2.19742100
H	0.77981500	0.36804200	2.74259000
C	-1.93524800	-1.08558300	4.36941800
H	-3.99027500	-0.64644900	3.80639100
H	-3.07416500	0.75445100	4.35940800
H	0.22416700	-1.14301000	4.63970600
H	-0.49479400	0.44957900	4.87917700
H	-2.17122000	-1.30567700	5.41758300
H	-1.93994100	-2.04510000	3.83332300
H	-0.24321300	-1.79608200	-2.95372800
C	1.47278900	-2.86466400	-0.13996100
C	1.93905000	-2.39177900	1.09793400
C	1.36709700	-4.25354300	-0.32761800
C	2.27858200	-3.27683400	2.12335200
H	2.02560700	-1.32346000	1.26256600
C	1.70931700	-5.14453800	0.69673500
H	1.01784300	-4.63899300	-1.28195500
C	2.16400900	-4.65952500	1.92808000
H	2.62469800	-2.88609500	3.07714200
H	1.61864700	-6.21528600	0.53138500
H	2.42422000	-5.34961200	2.72678800

prox-6

Sum of electronic and thermal Free Energies=-3696.923988

Ni	-0.38391300	-0.40795900	-0.99577700
C	0.88235900	-2.03499200	-1.89692500
C	-0.23418600	-1.73328300	-2.64006800
H	-1.14953600	-2.30289100	-2.52624200
C	7.22907600	-1.22565500	1.02831000
C	6.41144400	-1.47931800	-0.07987300
C	5.57626500	-0.47927800	-0.60455200

C	5.57962200	0.78414400	0.01066200	H	-4.24311100	4.82188000	0.88998700
C	6.39298900	1.04343900	1.11990000	H	-4.73287500	3.14878000	0.62096000
C	7.22168000	0.03766000	1.63419900	H	-3.91171700	3.17340600	-3.09630900
H	7.87175100	-2.01183600	1.41778500	H	-4.56327500	2.16336100	-1.81038900
H	6.42157000	-2.46433100	-0.54320200	H	-5.21409700	4.51452000	-1.40879400
H	4.94164100	1.57230800	-0.38270300	H	-3.52878700	5.02700000	-1.48420500
H	6.38182100	2.02899700	1.57973000	C	0.65056500	2.84352900	-0.22911000
H	7.85631800	0.23657900	2.49435700	C	0.95237100	3.78056000	0.96354500
C	4.63948700	-0.77144900	-1.75789200	C	1.96476300	2.36837300	-0.88145300
C	3.28905300	-1.30278700	-1.24288700	H	0.11834100	3.43862500	-0.98224400
H	5.09129500	-1.50575000	-2.43638900	C	1.81912600	4.97230600	0.52018000
H	4.47392400	0.14692200	-2.33048700	H	1.49108400	3.22814000	1.74172300
C	2.27440400	-1.58581300	-2.36113600	H	0.03055000	4.14935800	1.42141600
H	3.46585500	-2.22291800	-0.67782600	C	2.83465000	3.55950000	-1.31347200
H	2.86099300	-0.57134600	-0.55256000	H	2.52396900	1.75546700	-0.16283900
H	2.65381800	-2.43732700	-2.95022700	H	1.75419400	1.72085800	-1.73693200
O	2.11570000	-0.45277700	-3.22743100	C	3.12462400	4.50551400	-0.13987700
C	-6.62406800	-2.38690100	0.91940100	H	2.03460800	5.60888200	1.38686800
C	-5.23581800	-2.49643300	0.76159900	H	1.25061400	5.58698400	-0.19157700
C	-4.51671700	-1.61001400	-0.06521000	H	3.77065700	3.19229200	-1.75258600
C	-5.24864100	-0.60829500	-0.73232800	H	2.31416900	4.11413500	-2.10691200
C	-6.63531000	-0.48749100	-0.58476700	H	3.70986700	5.36867500	-0.47922700
C	-7.32879800	-1.37966400	0.24570100	H	3.73784000	3.97912600	0.60566600
H	-7.15733100	-3.08170600	1.56541300	C	-0.47168200	1.12842300	1.97447700
H	-4.69763700	-3.27991000	1.29086200	C	-1.63772800	0.23017900	2.43585000
H	-4.70625400	0.08181200	-1.37237400	C	0.87940400	0.47479800	2.33291700
H	-7.17577700	0.29712700	-1.11103000	H	-0.54561500	2.09284800	2.49117300
H	-8.40635400	-1.29086000	0.36679700	C	-1.53915900	-0.08709200	3.93670400
B	-2.93665800	-1.68012100	-0.23971200	H	-1.61465500	-0.70497500	1.86616800
O	-2.32452800	-2.74681900	0.45595300	H	-2.60060500	0.70600300	2.22292400
H	-1.36479500	-2.72673300	0.30426800	C	0.97658000	0.15852200	3.83290900
O	-2.28984600	-0.77836100	-0.97043900	H	0.96904600	-0.45461100	1.76182800
H	2.86369600	-0.44101300	-3.84424000	H	1.71863700	1.10766600	2.02811800
H	0.98200300	-0.01225300	-0.80425500	C	-0.18980500	-0.72977200	4.28959600
P	-0.56041200	1.44875100	0.14272400	H	-2.36458000	-0.74981500	4.22336500
C	-2.23791200	2.18822100	-0.19405500	H	-1.66142300	0.84050900	4.51336800
C	-2.58820500	3.44422100	0.62502800	H	1.93585400	-0.33001300	4.04241800
C	-2.41879000	2.43575400	-1.70784000	H	0.96650600	1.09764700	4.40340500
H	-2.92244900	1.37644800	0.07317000	H	-0.12677300	-0.91777000	5.36817700
C	-4.01639000	3.92065700	0.30735000	H	-0.11452200	-1.70648200	3.79080300
H	-1.89057200	4.25466700	0.38056700	H	-0.15794900	-1.07151000	-3.49840600
H	-2.49047800	3.24886300	1.69890200	C	0.81334900	-3.17136800	-0.91838100
C	-3.83274300	2.95303600	-2.02471800	C	1.16270600	-3.01902900	0.43564600
H	-1.69058900	3.17840600	-2.05992800	C	0.35451600	-4.42832100	-1.35238400
H	-2.22386500	1.50355000	-2.24754700	C	1.03919600	-4.08192800	1.33413800
C	-4.18689300	4.19552600	-1.19417300	H	1.50365700	-2.05405300	0.78841900

C	0.23970700	-5.49737300	-0.45708600
H	0.08239900	-4.56463400	-2.39567400
C	0.57747900	-5.32747400	0.89080500
H	1.29404500	-3.93236200	2.38028100
H	-0.12009000	-6.45983600	-0.81204200
H	0.47800300	-6.15485000	1.58863300

prox-TS1-2

Sum of electronic and thermal Free Energies=-3696.907014

C	-0.37866300	-0.18106000	2.47644500
C	0.99944800	-0.76448700	2.23689000
Ni	-0.44211000	-0.43022700	0.64078100
C	1.72137000	-0.65663500	0.55953200
H	2.56426900	-1.31020300	0.79067000
C	2.17999100	0.75880000	0.19629900
H	2.85635900	1.13795300	0.96413200
H	1.32165300	1.44148300	0.16670800
C	2.88472500	0.79429000	-1.17446400
H	3.78834500	0.17645800	-1.13464800
H	2.22284200	0.34003600	-1.91596900
C	3.22256900	2.21256500	-1.57436900
C	4.49142000	2.76066200	-1.32798700
C	2.24216000	3.03363300	-2.15946600
C	4.77731400	4.09176200	-1.65890600
H	5.26207500	2.13986300	-0.87459900
C	2.52089600	4.36392800	-2.49144100
H	1.25280200	2.62368400	-2.35672700
C	3.79230200	4.89909200	-2.24169300
H	5.76752000	4.49719700	-1.46389200
H	1.75025300	4.98177200	-2.94684400
H	4.01276500	5.93179400	-2.50092300
H	0.96886800	-1.85025000	2.33397200
H	-0.40974100	0.83632700	2.86596500
P	-2.42791000	0.11371800	0.07755000
C	-3.68206500	-1.07764800	0.76188000
C	-2.60808600	0.07599800	-1.79393400
C	-2.94207000	1.81766200	0.63150800
C	-5.12491300	-0.88332600	0.25731600
C	-3.21785300	-2.53671800	0.56882400
H	-3.66174800	-0.87665200	1.84076900
C	-3.70204900	0.99213200	-2.38409600
C	-1.26457000	0.33492900	-2.51462600
H	-2.88837900	-0.96743300	-1.99478900
C	-3.35064900	1.87355600	2.11840200
C	-1.79871100	2.81269800	0.33119500
H	-3.81762500	2.10123000	0.03580900
C	-6.08426700	-1.86427300	0.95311000
H	-5.16022800	-1.06604800	-0.82350300
H	-5.45835200	0.14787700	0.41990100
C	-4.18775600	-3.51963600	1.24461900
H	-3.14526100	-2.77170100	-0.50068200
H	-2.21306900	-2.65398200	0.99060700
C	-3.84637700	0.75772700	-3.89863400
H	-3.42700700	2.04101000	-2.21536000
H	-4.66607200	0.83497600	-1.89290300
C	-1.40029200	0.11078300	-4.02879600
H	-0.94535800	1.36928400	-2.33114000
H	-0.48208600	-0.30737200	-2.10793300
C	-3.69611800	3.31082800	2.54546200
H	-2.53294400	1.49812200	2.74322000
H	-4.21483000	1.22719100	2.30207400
C	-2.15414500	4.24069100	0.77176500
H	-0.89684700	2.47938500	0.86165700
H	-1.55331100	2.80504200	-0.73606300
C	-5.63063400	-3.31880500	0.75745700
H	-7.09945100	-1.72442800	0.56306200
H	-6.12087000	-1.63352200	2.02674800
H	-3.85925600	-4.54846600	1.05594300
H	-4.14832800	-3.36738800	2.33197600
C	-2.51529500	0.97665400	-4.63307400
H	-4.61789200	1.42587300	-4.29992300
H	-4.19515500	-0.26983900	-4.07104000
H	-0.44223300	0.32389900	-4.51848800
H	-1.62151400	-0.95003200	-4.21338000
C	-2.54471300	4.28400400	2.25557400
H	-3.94840200	3.32183600	3.61249500
H	-4.59353000	3.64076700	2.00394400
H	-1.30372000	4.90520400	0.57788700
H	-2.99155200	4.60977700	0.16362000
H	-6.30658700	-4.00178600	1.28556700
H	-5.69106600	-3.57414200	-0.30978500
H	-2.63113000	0.75953000	-5.70174600
H	-2.23109200	2.03536700	-4.55296400
H	-2.82653200	5.30302800	2.54626100
H	-1.67393500	4.00758000	2.86678100
O	0.96981700	-1.20171800	-0.49857500
B	1.04738100	-2.78320600	-0.77222800
C	2.59184200	-3.06331900	-1.18373900
C	3.11705500	-2.59058100	-2.40291200
C	3.48399800	-3.73603000	-0.32738900
C	4.45912500	-2.77707300	-2.75581400

H	2.47327600	-2.04587500	-3.09353200
C	4.83178000	-3.93107200	-0.66433100
H	3.11433100	-4.11159600	0.62466000
C	5.32626500	-3.45046500	-1.88325300
H	4.83200300	-2.39508300	-3.70449400
H	5.49567200	-4.45309800	0.02266000
H	6.37094200	-3.59594400	-2.15003000
O	0.04987400	-2.99681500	-1.81581900
H	0.25415800	-2.46147200	-2.59596500
O	0.68017700	-3.50463700	0.43066800
H	-0.27995100	-3.41992800	0.53891500
H	-1.06171900	-0.83741800	3.02232500
C	2.12351000	-0.21265400	3.08815600
C	2.19629900	1.13144000	3.49230100
C	3.15807100	-1.08137200	3.47489300
C	3.27155200	1.59185800	4.25771100
H	1.42272900	1.83360800	3.19531300
C	4.23483900	-0.62498600	4.24389000
H	3.12014400	-2.12609800	3.17227800
C	4.29689000	0.71610700	4.63919300
H	3.30991900	2.63704600	4.55517600
H	5.02155000	-1.31722600	4.53406800
H	5.13100000	1.07481500	5.23700500

prox-TS1-3

Sum of electronic and thermal Free Energies=-3288.653145

C	-0.01493800	0.98240900	1.79334000
C	1.49088600	0.82125400	1.56538300
Ni	-0.18295600	-0.28122000	0.43843200
C	2.01968000	-0.74659600	0.93252200
O	1.39488500	-1.27723600	-0.18088800
H	1.86880700	-1.37715800	1.83196300
C	3.52743000	-0.57491500	0.70486800
H	3.99772900	-0.09931800	1.57458400
H	3.68744700	0.08469000	-0.15403700
C	4.20385500	-1.93319700	0.43497200
H	4.04530000	-2.59216100	1.29756900
H	3.71047200	-2.39845100	-0.42376600
C	5.68517700	-1.77579000	0.16955000
C	6.62422200	-1.87284400	1.21030500
C	6.15285100	-1.47261100	-1.12127500
C	7.99034400	-1.67616600	0.97132500
H	6.28224800	-2.10649100	2.21715200
C	7.51655600	-1.27450000	-1.36719500
H	5.44018600	-1.39248700	-1.94036000
C	8.44250700	-1.37533700	-0.31996200
H	8.70078600	-1.75996200	1.79070400
H	7.85737500	-1.04453300	-2.37422000
H	9.50266200	-1.22429800	-0.50878700
H	-0.35859200	0.60216500	2.76193300
H	-0.39587500	1.99029800	1.61616000
H	1.97669300	0.72402200	2.54017400
C	2.09755100	1.96781800	0.79418300
C	3.11430400	2.75137000	1.36527700
C	1.67425100	2.28533600	-0.50923900
C	3.68504500	3.82055000	0.66424200
H	3.46543200	2.52262400	2.36959700
C	2.24041600	3.35046000	-1.21531700
H	0.89846600	1.68785100	-0.97880000
C	3.25029400	4.12652700	-0.63145400
H	4.46886100	4.41365000	1.12996000
H	1.89478000	3.57333700	-2.22239700
H	3.69180100	4.95644300	-1.17781100
P	-2.26421200	-0.20148400	0.02409700
C	-3.28694700	0.15317200	1.53833200
C	-4.79884900	0.35335000	1.32047800
C	-3.03468500	-0.90330400	2.63572300
H	-2.86548700	1.09961600	1.90070200
C	-5.47985900	0.77130400	2.63634900
H	-5.24663700	-0.58513600	0.97185900
H	-4.98900600	1.10681800	0.54836700
C	-3.71047300	-0.48771600	3.95288800
H	-3.44414400	-1.87126200	2.31914100
H	-1.95866700	-1.04776400	2.78149000
C	-5.21572100	-0.24659500	3.75690700
H	-6.55813300	0.88677300	2.47341100
H	-5.09725400	1.75561200	2.93988400
H	-3.54446800	-1.25935700	4.71413100
H	-3.23763700	0.43214100	4.32385100
H	-5.67050500	0.09578100	4.69419600
H	-5.70059700	-1.19852900	3.49861900
C	-2.92155900	-1.81483900	-0.67721900
C	-4.15315800	-1.69481900	-1.60087900
C	-1.80697600	-2.64265500	-1.35624100
H	-3.23099700	-2.36982900	0.21818300
C	-4.66794300	-3.08832200	-2.00311000
H	-3.88383000	-1.14524400	-2.51030800
H	-4.95506800	-1.12933500	-1.11791400
C	-2.32635400	-4.02841800	-1.77202300
H	-1.44124800	-2.11112500	-2.24404300
H	-0.94850200	-2.74140300	-0.68314300

C	-3.56597100	-3.92261000	-2.67306600
H	-5.52808100	-2.98104600	-2.67502600
H	-5.02835300	-3.61196200	-1.10677600
H	-1.52958400	-4.58328600	-2.28191500
H	-2.58293000	-4.60009500	-0.86902400
H	-3.94379900	-4.92223800	-2.91960000
H	-3.28240100	-3.44720400	-3.62264700
C	-2.66550800	1.13577300	-1.21175800
C	-2.42084600	2.54014700	-0.62074000
C	-1.83263100	0.94113400	-2.49852800
H	-3.72877400	1.04496600	-1.46649000
C	-2.71010000	3.64084700	-1.65458900
H	-1.37496900	2.61573800	-0.30114700
H	-3.03970400	2.70045500	0.26839400
C	-2.11357400	2.04874500	-3.52642600
H	-0.76679800	0.94484800	-2.23673700
H	-2.03424700	-0.03545000	-2.94801800
C	-1.87935000	3.44412900	-2.93072600
H	-2.50281100	4.62177600	-1.21041700
H	-3.77883100	3.62662800	-1.90976000
H	-1.48071600	1.89709900	-4.40895500
H	-3.15581600	1.96854800	-3.86536200
H	-2.12365400	4.21849300	-3.66772000
H	-0.81361800	3.56050800	-2.68868700

dist-5'

Sum of electronic and thermal Free Energies=-3696.938226

Ni	0.13412200	-0.39353700	-0.58810500
C	-1.26539100	-2.06002900	-1.08275200
H	-1.67810800	-2.35670800	-2.05194700
C	0.26401500	-2.23410600	-1.10737000
H	0.59107500	-2.24430600	-2.15399700
C	-7.92005100	-1.30524900	0.38115800
C	-6.52601200	-1.20182300	0.46016600
C	-5.72183000	-1.38695500	-0.67715600
C	-6.35066000	-1.68018900	-1.89873600
C	-7.74449600	-1.78483200	-1.98440000
C	-8.53534100	-1.59809400	-0.84313900
H	-8.52545500	-1.15343300	1.27185200
H	-6.05575600	-0.97035600	1.41428200
H	-5.74383300	-1.82389100	-2.79109200
H	-8.21275600	-2.00798000	-2.94034000
H	-9.61796100	-1.67568300	-0.90778200
C	-4.21353700	-1.31807900	-0.57437700
C	-3.60038300	-2.69803900	-0.25779000
H	-3.92536900	-0.60859200	0.20675400
H	-3.80250000	-0.94016500	-1.51673900
C	-2.09557700	-2.67983800	0.04332600
H	-4.11450400	-3.12903900	0.61080500
H	-3.78057100	-3.38491000	-1.09381100
H	-1.75927100	-3.71128400	0.20422300
O	-1.81674600	-1.91279800	1.24087400
C	-3.43596900	5.07618000	1.47096300
C	-3.06860900	3.72414000	1.44742200
C	-2.12993100	3.23142500	0.51863000
C	-1.57336100	4.15302900	-0.39040900
C	-1.93003900	5.50670000	-0.37748500
C	-2.86554000	5.97316800	0.55711600
H	-4.16292900	5.43281400	2.19814000
H	-3.51478100	3.03571000	2.16200500
H	-0.84866100	3.79110700	-1.11489700
H	-1.48312700	6.19740400	-1.09006400
H	-3.14705700	7.02395600	0.57313200
B	-1.67416100	1.70704600	0.48909000
O	-2.24257900	0.89985600	1.48535100
H	-1.96647200	-0.03242600	1.36756300
O	-0.79532400	1.28437200	-0.42353000
H	-2.25246200	-2.34549700	1.99427600
C	0.89241100	-3.38037000	-0.38767100
C	1.61519800	-4.34324600	-1.12196000
C	0.82907200	-3.54427900	1.01014500
C	2.26484300	-5.40854900	-0.49200200
H	1.68450700	-4.24369000	-2.20344700
C	1.47379800	-4.60854400	1.64541800
H	0.27650500	-2.81976200	1.59492600
C	2.20200400	-5.54613800	0.90069800
H	2.82309800	-6.12769300	-1.08731700
H	1.41549600	-4.70136100	2.72789800
H	2.71076300	-6.36938400	1.39654000
H	-1.53869400	-0.96105700	-1.07876500
P	2.10144000	0.47397600	-0.18609700
C	2.06076800	2.16418000	-0.96801500
C	3.73904900	-0.24511000	-0.78022500
C	2.29025000	0.75663700	1.64981800
C	3.27762800	3.06239600	-0.67850300
C	1.79457000	2.05399700	-2.48464200
H	1.16674000	2.61190300	-0.52450800
C	4.94706700	0.01808500	0.14688700
C	3.65128400	-1.73735800	-1.13495100
H	3.92124200	0.29848900	-1.71661500
C	1.28593900	1.78087400	2.21289600

C	2.13872400	-0.58492000	2.39430600
H	3.30050100	1.14552100	1.81839600
C	3.08046600	4.45466200	-1.30390700
H	4.18534000	2.61426800	-1.10194900
H	3.44205400	3.15926500	0.40056400
C	1.63131100	3.44451700	-3.12158800
H	2.62652900	1.53474800	-2.97944900
H	0.89385200	1.45295800	-2.65140500
C	6.25134100	-0.48613100	-0.49563300
H	4.80134200	-0.50480800	1.09981200
H	5.04345100	1.08242100	0.37932000
C	4.95807600	-2.25286400	-1.75610100
H	3.42206700	-2.31743600	-0.23454000
H	2.82450300	-1.90019600	-1.82799300
C	1.48524200	1.96410700	3.72681800
H	0.26927400	1.42621400	2.02133900
H	1.38619100	2.74721600	1.70920000
C	2.34022700	-0.41392800	3.90711200
H	1.12768800	-0.96295200	2.20400000
H	2.82870600	-1.33958600	2.00181900
C	2.83032500	4.35505200	-2.81630100
H	3.95940800	5.07902200	-1.10225500
H	2.22279600	4.94622100	-0.82395200
H	1.49619400	3.34126100	-4.20517800
H	0.71700500	3.91243600	-2.73365300
C	6.16487500	-1.97772400	-0.84860300
H	7.08874300	-0.30138400	0.18814000
H	6.45209000	0.09398700	-1.40720300
H	4.86509700	-3.32695200	-1.95815700
H	5.11511500	-1.75932800	-2.72577900
C	1.36839700	0.62949100	4.47856200
H	0.74733000	2.68088200	4.10720300
H	2.47678300	2.40066200	3.91252000
H	2.20341200	-1.37992500	4.40850500
H	3.37454700	-0.09796100	4.10250500
H	2.66617200	5.35280500	-3.24111600
H	3.72785500	3.94687500	-3.30245600
H	7.09170200	-2.30954400	-1.33211100
H	6.06196600	-2.56152800	0.07700800
H	1.55270100	0.77740400	5.54956000
H	0.34050500	0.25254800	4.38125100

dist-TS3'

Sum of electronic and thermal Free Energies=-3696.907038

Ni	-0.14822200	-0.74658300	-0.34598400
C	0.22897200	-2.69379200	0.13514300
H	0.44516700	-2.55926500	1.19835200
C	-1.14532200	-2.54775200	-0.14899700
H	-1.78295300	-2.48296500	0.72272700
C	6.92474800	-2.28686500	1.23457600
C	5.75137700	-2.35284800	0.47395800
C	4.52078000	-1.93203600	1.00597000
C	4.49533300	-1.44150000	2.32216000
C	5.66569800	-1.37257400	3.08827900
C	6.88610500	-1.79653700	2.54687600
H	7.86854100	-2.61285400	0.80338900
H	5.79076700	-2.73026300	-0.54644100
H	3.55141000	-1.10508600	2.74799100
H	5.62605900	-0.98481800	4.10366400
H	7.79694900	-1.74107800	3.13811200
C	3.24743800	-2.03641600	0.19680900
C	2.63261400	-3.44940500	0.27042800
H	3.44567000	-1.78552900	-0.84962200
H	2.52383400	-1.30054400	0.55937900
C	1.29516800	-3.60265400	-0.47641500
H	3.34506600	-4.17773400	-0.13748200
H	2.47700500	-3.72885600	1.31960400
H	0.93602900	-4.63283400	-0.32793400
O	1.45304400	-3.37026300	-1.88562300
C	3.73348700	3.70523700	-3.75685100
C	3.23411300	2.44513900	-3.40208800
C	2.19483000	2.30134900	-2.46033300
C	1.67115100	3.47957200	-1.89122100
C	2.15896600	4.74467300	-2.23842000
C	3.19649400	4.86124500	-3.17402500
H	4.53854500	3.78872200	-4.48427200
H	3.65814700	1.55451600	-3.86058700
H	0.86739000	3.39733700	-1.16570400
H	1.73542200	5.63725500	-1.78205300
H	3.58157000	5.84157100	-3.44648300
B	1.63109100	0.87507200	-2.03354300
O	2.16251300	-0.20533600	-2.75317500
H	1.78760600	-1.03692200	-2.40403300
O	0.72380400	0.78615300	-1.05234600
H	2.11196600	-4.00226700	-2.21986300
C	-1.89857500	-2.86664600	-1.38195600
C	-3.23105500	-3.30821700	-1.23810000
C	-1.40412100	-2.66795400	-2.68726500
C	-4.03629600	-3.55839500	-2.35097700
H	-3.64249300	-3.44293200	-0.23999000
C	-2.21392600	-2.90520800	-3.80098600

H	-0.39178000	-2.31172100	-2.82364200
C	-3.53130400	-3.35416700	-3.64199600
H	-5.05947900	-3.89899000	-2.21197600
H	-1.81628200	-2.73231400	-4.79831400
H	-4.15881900	-3.53447800	-4.51131800
H	0.82228500	-1.47659200	-1.09935300
P	-1.50640400	0.66367700	0.92485500
C	-0.41438600	2.11109300	1.34263100
C	-2.28992000	0.24183900	2.58993500
C	-2.87011000	1.34186500	-0.15410400
C	-1.07551000	3.30490500	2.05256100
C	0.84741800	1.63922700	2.09612900
H	-0.07180300	2.42930900	0.35630400
C	-3.61657800	0.97049000	2.89787100
C	-2.43557400	-1.26950300	2.85259000
H	-1.54337900	0.61016800	3.30621600
C	-2.29940700	2.12752600	-1.35389500
C	-3.74099800	0.17111100	-0.65557800
H	-3.49242700	2.02195100	0.43905600
C	-0.07070900	4.46143900	2.20677000
H	-1.42467000	3.00550300	3.04912900
H	-1.95484800	3.64928900	1.49567800
C	1.84564000	2.79765700	2.25668700
H	0.57870000	1.25619300	3.09070300
H	1.31476900	0.81748000	1.54343800
C	-4.07939200	0.69321900	4.33890900
H	-4.39464800	0.62811700	2.20477200
H	-3.51398000	2.04886600	2.74867800
C	-2.90668400	-1.54724000	4.29002900
H	-3.16395800	-1.69726300	2.15111100
H	-1.47823800	-1.77284600	2.67961500
C	-3.42042500	2.60130600	-2.29379600
H	-1.59300100	1.48983300	-1.89826000
H	-1.72814100	2.99458100	-1.00662000
C	-4.86693600	0.65177100	-1.58236900
H	-3.10085900	-0.52361700	-1.20911900
H	-4.16035300	-0.39605100	0.18353500
C	1.19855000	4.00894700	2.94609500
H	-0.54351300	5.29701400	2.73754600
H	0.20337500	4.83335700	1.20946700
H	2.72216800	2.45921600	2.82307900
H	2.20471600	3.09337600	1.26151200
C	-4.21673600	-0.81225700	4.60695500
H	-5.03311400	1.20301200	4.52183500
H	-3.35031800	1.12323300	5.03983000
H	-3.02743100	-2.62747900	4.43597100
H	-2.12720300	-1.21752500	4.99109400
C	-4.29653800	1.43480200	-2.77390500
H	-2.98081200	3.12648100	-3.15072200
H	-4.05026600	3.33088200	-1.76507000
H	-5.44587800	-0.21130200	-1.93326500
H	-5.55845600	1.29367500	-1.01853300
H	1.91476000	4.83727800	3.01054300
H	0.93435100	3.73743300	3.97820800
H	-4.51003900	-0.98917900	5.64875800
H	-5.02069100	-1.21862800	3.97712700
H	-5.10736400	1.80498800	-3.41317600
H	-3.68941600	0.75599300	-3.38950300

dist-6'

Sum of electronic and thermal Free Energies=-3696.908107

Ni	-0.94116700	0.11922800	-0.95016200
C	-1.20074400	-1.84476600	-1.38196800
H	-0.62628900	-2.28442400	-0.57123400
C	-2.44490300	-1.35836700	-0.97118100
H	-2.65899900	-1.48168400	0.08679900
C	4.95310600	-4.16725400	-1.09064700
C	4.00127300	-3.48055200	-1.85751600
C	2.77855100	-3.08095800	-1.29824700
C	2.53074600	-3.38577300	0.05249200
C	3.47557500	-4.06795700	0.82349700
C	4.69418700	-4.46294800	0.25288600
H	5.89641300	-4.46660300	-1.54159300
H	4.21413700	-3.24914900	-2.89945200
H	1.59119300	-3.07673300	0.50673800
H	3.26598200	-4.28592700	1.86824700
H	5.43325400	-4.99131900	0.85022700
C	1.73544700	-2.34313300	-2.10713200
C	0.53790500	-3.22978000	-2.52217000
H	2.18628800	-1.89697300	-2.99719400
H	1.36248100	-1.50390700	-1.51205300
C	-0.74679200	-2.41330400	-2.72921000
H	0.77774000	-3.77853100	-3.44075600
H	0.33971400	-3.98830600	-1.75649400
H	-1.54635500	-3.07899000	-3.08692100
O	-0.53663300	-1.38464600	-3.72237000
C	4.17634000	4.13748500	-2.53951700
C	3.24427200	3.10976400	-2.73480900
C	2.08601200	3.00652600	-1.93971500
C	1.89040400	3.98506200	-0.94433300
C	2.81135200	5.01901100	-0.74228200

C	3.96238800	5.09577000	-1.53939400
H	5.06822700	4.19200500	-3.16064200
H	3.42114800	2.36635600	-3.50917400
H	1.00381200	3.92225400	-0.31805400
H	2.63914500	5.76045300	0.03546400
H	4.68509200	5.89367600	-1.38253000
B	1.05966400	1.80419500	-2.09349700
O	1.26667600	0.96032100	-3.18705200
H	0.60966000	0.23483900	-3.19990000
O	0.10225100	1.65355400	-1.16414800
H	-0.26986000	-1.82878400	-4.54607000
C	-3.63932600	-0.99888800	-1.75758600
C	-4.84767700	-0.80264200	-1.05634600
C	-3.65014400	-0.85129300	-3.16128600
C	-6.02943600	-0.47894300	-1.72782700
H	-4.86030900	-0.90777100	0.02617600
C	-4.83354500	-0.53460900	-3.83123400
H	-2.72812100	-0.96000400	-3.72084800
C	-6.02825300	-0.34562600	-3.12169000
H	-6.94785800	-0.33108000	-1.16515200
H	-4.82396900	-0.42506400	-4.91314900
H	-6.94462000	-0.09240400	-3.64900200
H	-1.26366500	0.32816400	-2.32799400
P	-0.43072800	0.27583000	1.42057900
C	1.24891700	1.06628300	1.57476300
C	-0.39409800	-1.10562200	2.70723900
C	-1.65197600	1.53962200	2.06451300
C	1.68337100	1.51956600	2.97960000
C	2.32502100	0.17374800	0.92430600
H	1.15441700	1.94697900	0.93477800
C	-0.80074200	-0.70039000	4.14139400
C	-1.17482800	-2.36817200	2.28622300
H	0.66836800	-1.38505800	2.73230800
C	-1.45083800	2.92958300	1.42497800
C	-3.08544600	1.03412500	1.78985800
H	-1.51741600	1.64284200	3.14730600
C	3.03558900	2.25266900	2.91412300
H	1.78835300	0.64858300	3.63919300
H	0.92614500	2.17241500	3.42924400
C	3.68505000	0.88932400	0.87754900
H	2.43365800	-0.76566200	1.48234900
H	2.01287300	-0.09107200	-0.08938200
C	-0.55786600	-1.85297400	5.13171800
H	-1.86658700	-0.43963100	4.15768800
H	-0.25459700	0.18703900	4.47119400
C	-0.94202100	-3.52539500	3.27218800
H	-2.24875200	-2.14392400	2.24446900
H	-0.87629300	-2.68902400	1.28519700
C	-2.51482200	3.92462600	1.91856000
H	-1.49585400	2.83738200	0.33425500
H	-0.45514700	3.31801600	1.66269900
C	-4.14603300	2.02578100	2.29032200
H	-3.20743200	0.90257000	0.70660200
H	-3.24790100	0.05116100	2.24786400
C	4.11775400	1.37141100	2.27046800
H	3.34210000	2.55854900	3.92218100
H	2.91723300	3.17149100	2.32315900
H	4.44060700	0.21624400	0.45344000
H	3.60783000	1.75044700	0.20160400
C	-1.30517500	-3.12599400	4.70916500
H	-0.86813100	-1.54438000	6.13745300
H	0.51989300	-2.06183500	5.18233800
H	-1.52371200	-4.40047600	2.95825000
H	0.11701500	-3.81728400	3.23144200
C	-3.94002000	3.41223300	1.66310500
H	-2.36494500	4.89392300	1.42727100
H	-2.37985700	4.09224000	2.99660300
H	-5.14737100	1.64379800	2.05634300
H	-4.08225800	2.10480100	3.38458700
H	5.06485800	1.92101500	2.20473600
H	4.30076300	0.49991000	2.91549900
H	-1.08188500	-3.94733400	5.40070300
H	-2.38752200	-2.94479900	4.77015700
H	-4.67699700	4.12296500	2.05643100
H	-4.11024000	3.34388800	0.57935200