Supplementary Information for

A Theoretical Insight into the Curing Mechanism of Phthalonitrile Resins Promoted by Aromatic Amines

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1. Transition states in the reaction pathways

The structures of transition states in reaction pathways shown in Schemes 3-8 are presented below. The imaginary vibrational frequency ($v^{\ddagger}$, i cm^{-1}) and atomic distances (Å) of the corresponding transition state are also given.
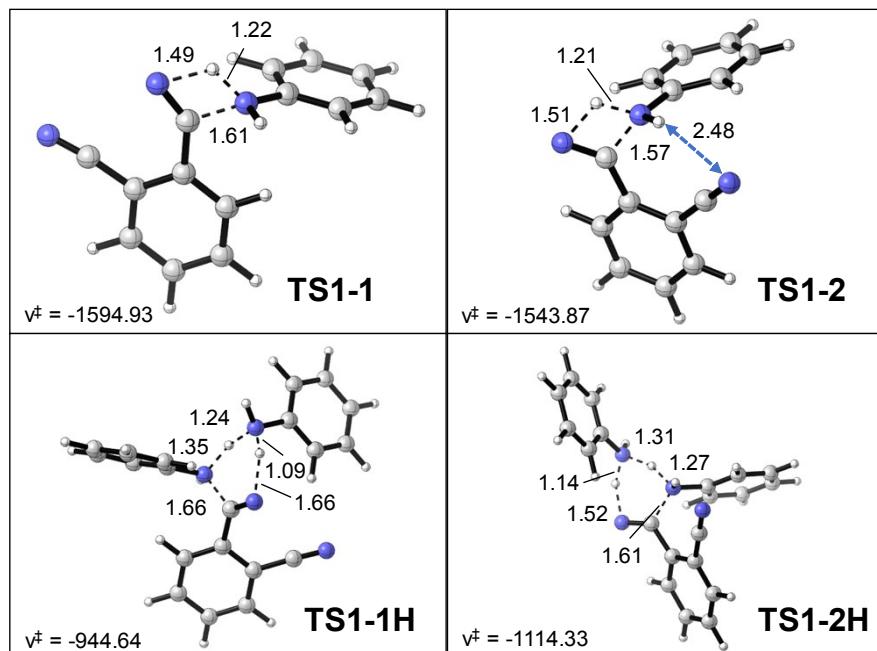
Figure S1. Transition states for the reaction pathways shown in Scheme 3.
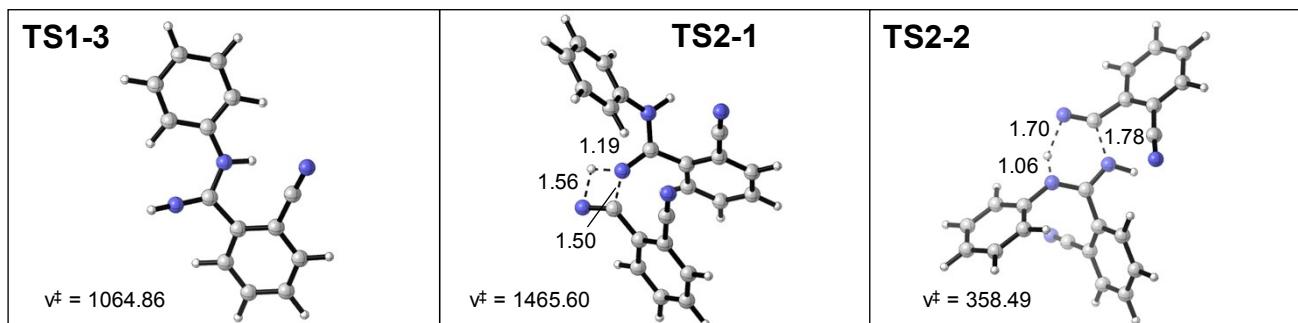
Figure S2. Transition states for the reaction pathways shown in Scheme 4.
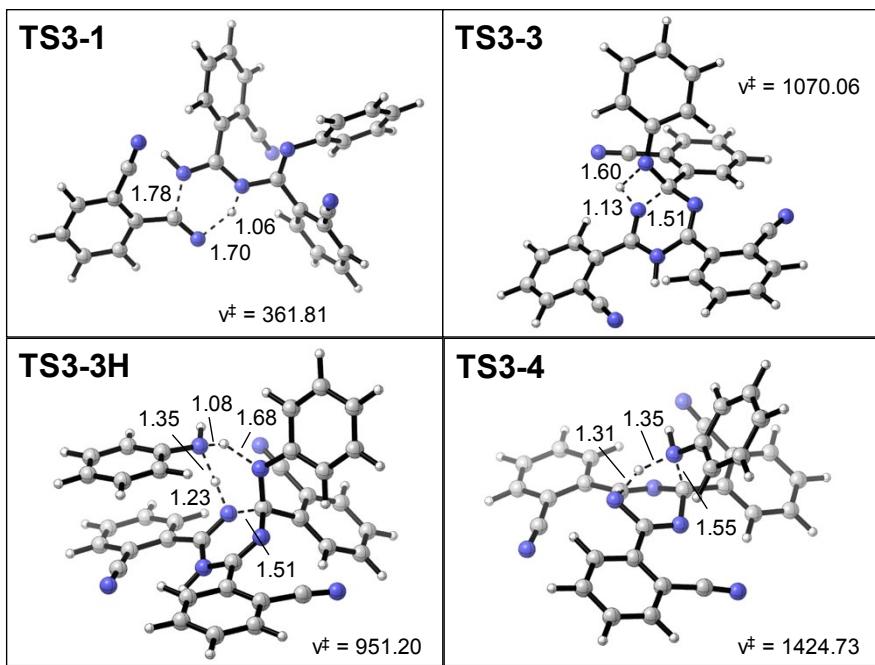
Figure S3. Transition states for the reaction pathways shown in Scheme 5.
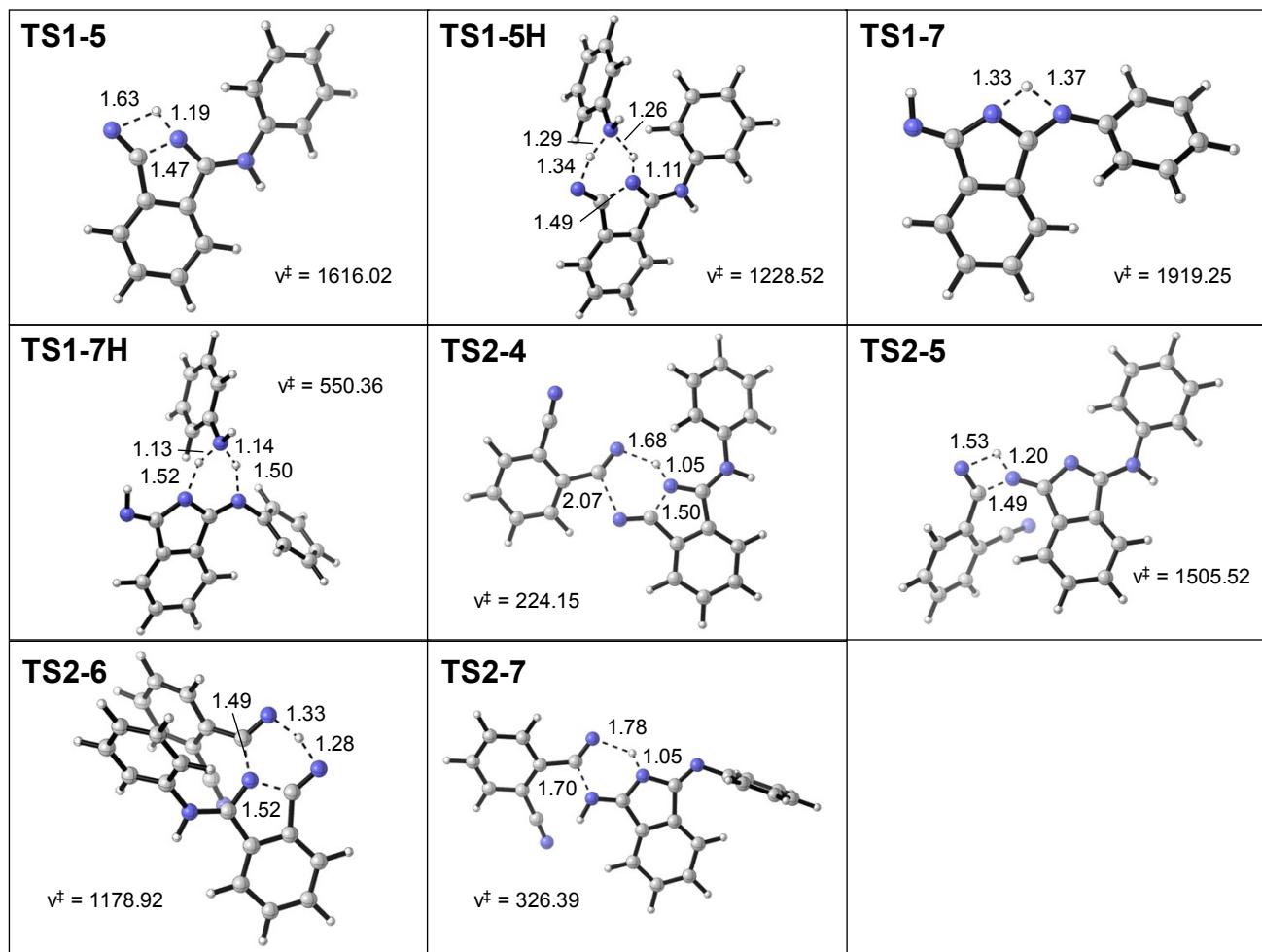
Figure S4. Transition states for the reaction pathways shown in Scheme 6.
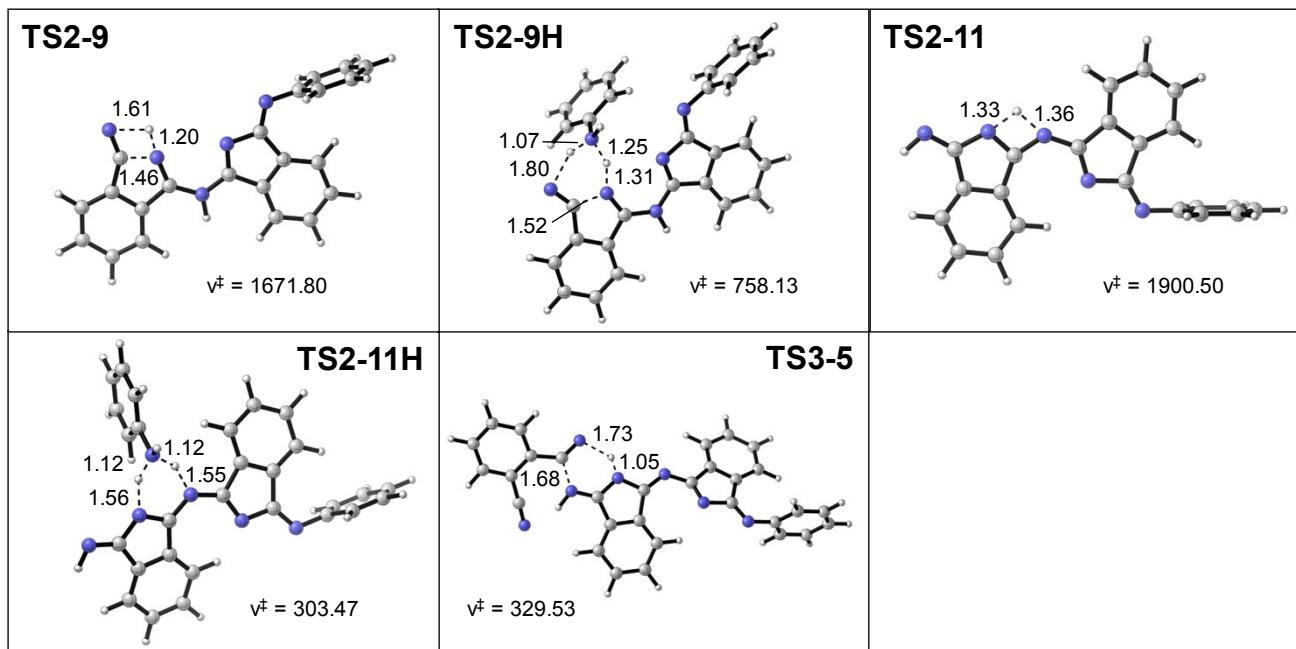
Figure S5. Transition states for the reaction pathways shown in Scheme 7.
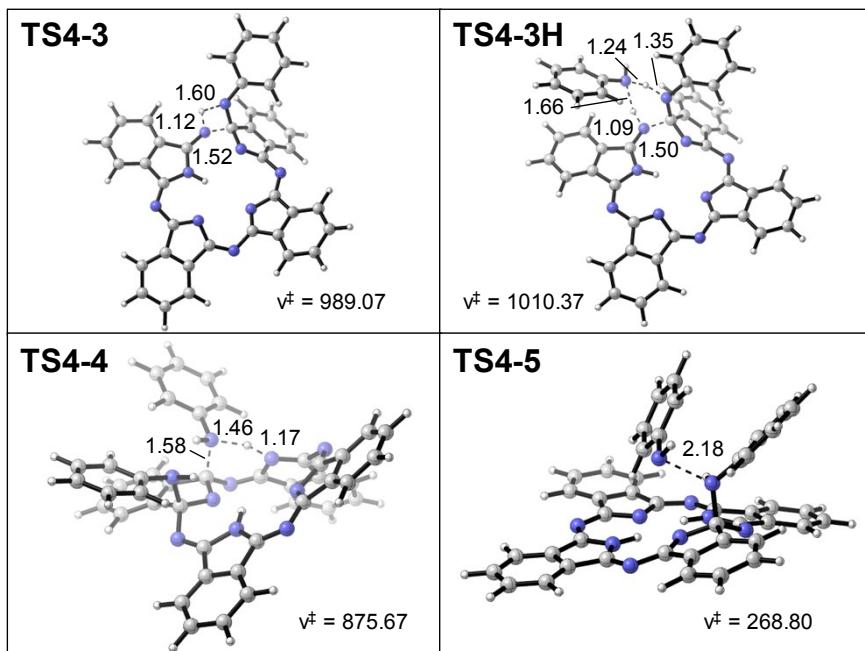
Figure S6. Transition states for the reaction pathways shown in Scheme 8.

2. Free energy surfaces based on the uncorrected free energies in the gas phase

As the entropic contributions to the relative free energies estimated by the ideal gas model were overestimated, the uncorrected activation free energies in the gas phase for bimolecular reaction seem too high to be overcome, as can be seen from Figures S7-S12. It implies that the correction for the free energies of activation is necessary to obtain a reasonable result in kinetics. Nevertheless, the qualitative picture from the uncorrected free energy surfaces is similar to that from the corrected free energy surfaces shown in the text.

The curing of resins is usually an exothermic reaction. The relative enthalpies are also given to understand the heat release of reaction and guide the curing of larger and thick composites. One can see that the formation of triazine is exothermic by 59.3 kcal mol^{-1} (see Figure S9), and the formation of phthalocyanine is exothermic by 101.2 kcal mol^{-1} (see Figure S12). In other words, the heat releases of forming thiazine and phthalocyanine are exothermic by 19.8 kcal and 25.3 kcal per mole of consuming phthalonitrile monomers, respectively. It implies that the curing reaction forming cross-links of triazine has a lower exothermic effect, which is more favorable for phthalonitrile resins to be used in thick composite parts.
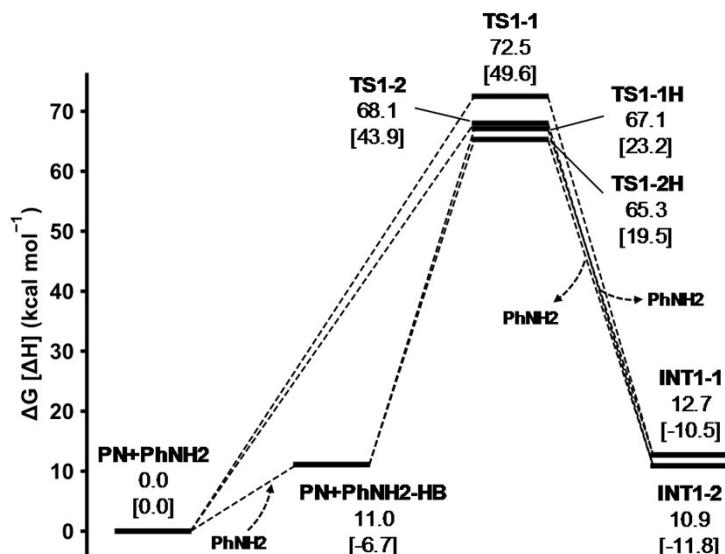
Figure S7. Free energy surfaces of the nucleophilic addition of aniline **PhNH2** or its hydrogen bonding complex **PhNH2-HB** to nitrile group on phthalonitrile **PN**. ΔG presents the relative free energy in the gas phase without correction. Relative enthalpies are given in brackets.
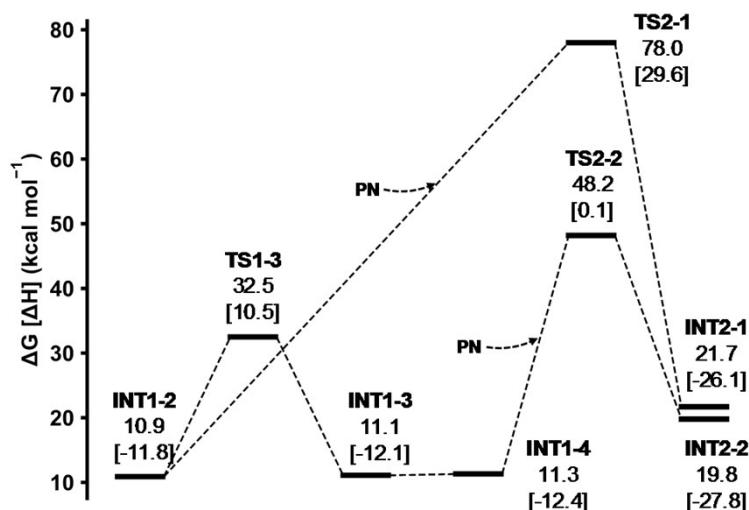
Figure S8. Free energy surfaces of the reaction pathways from amidine intermediate **INT1-2**. ΔG presents the relative free energy in the gas phase without correction. Relative enthalpies are given in brackets.
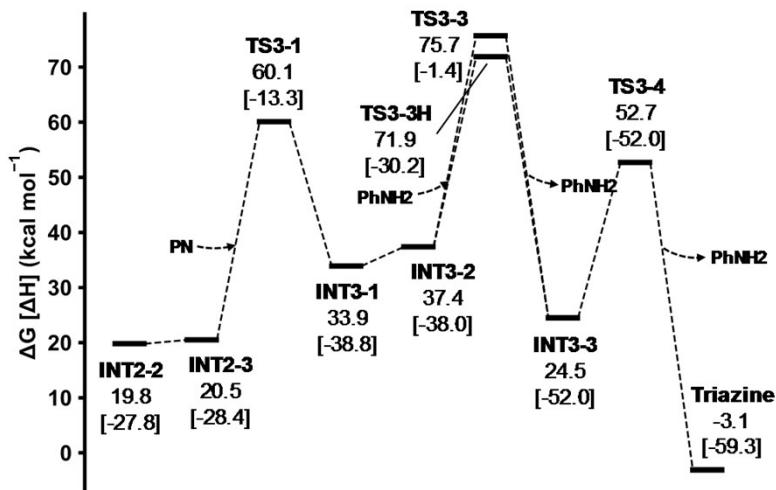
Figure S9. Free energy surfaces of the formation of triazine from amidine intermediate **INT2-2**. ΔG presents the relative free energy in the gas phase without correction. Relative enthalpies are given in brackets.
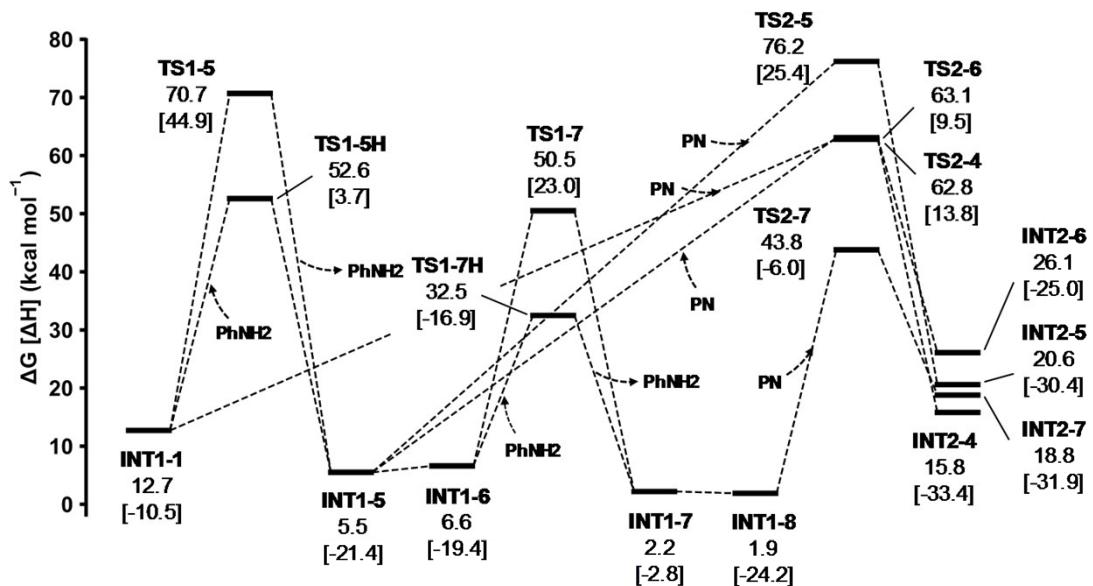
Figure S10. Free energy surfaces of the reaction pathways from amidine intermediate **INT1-1**. ΔG presents the relative free energy in the gas phase without correction. Relative enthalpies are given in brackets.
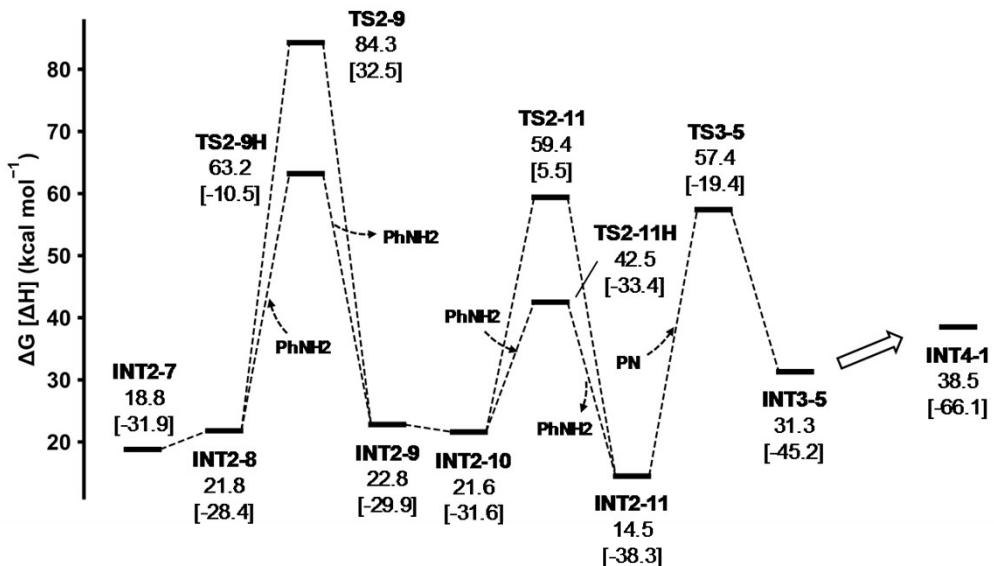
Figure S11. Free energy surfaces of the formation of phthalonitrile tetramer **INT4-1** from amidine intermediate **INT2-7**. Δ*G* presents the relative free energy in the gas phase without correction. Relative enthalpies are given in brackets.
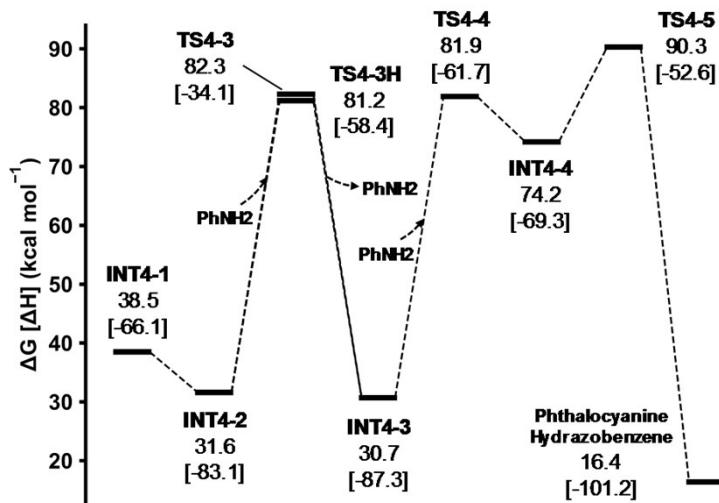
Figure S12. Free energy surfaces of the formation of phthalocyanine from amidine intermediate **INT4-1**. Δ*G* presents the relative free energy in the gas phase without correction. Relative enthalpies are given in brackets.

3. Cartesian coordinates and associated energies

All calculations were performed using the density functional M06-2X with a D3 dispersion correction. The structures of all reactants, products, intermediates, and transition states were fully optimized with the 6-31G(d,p) basis set in the gas phase. The electronic energies of optimized structures were refined with the larger basis set of 6-311+G(d,p). All thermal dynamic contributions were computed at 260 °C. The Cartesian coordinates of all optimized structures and the associated energies derived from the Gaussian 09 program package are as follows.

PN

C	-2.31080500	-0.69632500	-0.00000300
C	-2.31079800	0.69633700	0.00000000
C	-1.10999600	1.39695600	0.00000600
C	0.10107300	0.70323400	0.00000200
C	0.10106400	-0.70324700	-0.00000300
C	-1.11001100	-1.39695600	-0.00000200
H	-3.24875200	-1.24061200	-0.00000300
H	-3.24874100	1.24063100	0.00000800
H	-1.09748300	2.48085700	0.00001500
H	-1.09751200	-2.48085800	-0.00001100
C	1.33865600	1.43635700	0.00000300
C	1.33865400	-1.43636400	-0.00000300
N	2.31895900	2.05000000	-0.00000800
N	2.31896400	-2.04999600	0.00000800

E(M06-2X-D3/6-31G(d,p)) =   -416.566747994   A.U.

Zero-point correction=   0.098769 (Hartree/Particle)
Thermal correction to Energy=   0.120737
Thermal correction to Enthalpy=   0.122425
Thermal correction to Gibbs Free Energy=   0.028520

E(M06-2X-D3/6-311+G(d,p)) =   -416.669600261   A.U.

PhNH2

C	0.93515300	0.00005600	-0.01031800

C	0.22126400	-1.20490100	-0.00615000
C	0.22130800	1.20489800	-0.00613700
C	-1.16799500	-1.19933800	0.00352100
H	0.76523000	-2.14574000	-0.01564900
C	-1.16807200	1.19928500	0.00354300
H	0.76510300	2.14583100	-0.01566800
C	-1.87560200	0.00002300	0.00910700
H	-1.70176400	-2.14486900	0.00823200
H	-1.70171600	2.14488800	0.00834000
H	-2.95984300	-0.00007500	0.01794600
N	2.32908100	-0.00004300	-0.07625900
H	2.76658000	0.83564500	0.28431700
H	2.76651000	-0.83551300	0.28490200

E(M06-2X-D3/6-31G(d,p)) =   -287.481263191   A.U.

Zero-point correction=   0.118217 (Hartree/Particle)
Thermal correction to Energy=   0.135889
Thermal correction to Enthalpy=   0.137578
Thermal correction to Gibbs Free Energy=   0.057248

E(M06-2X-D3/6-311+G(d,p)) =   -287.553683707   A.U.

PhNH2-HB
C	-1.57903900	-0.79740600	0.57565600
C	-2.83559200	-0.78985900	-0.04031800
C	-0.96861000	0.42141500	0.89071600
C	-3.46684900	0.41374000	-0.33186700
H	-3.31151800	-1.73379900	-0.29353700
C	-1.60339300	1.61945700	0.58305100
H	0.01550200	0.42670200	1.35407800
C	-2.85488000	1.62734700	-0.02705300
H	-4.44372200	0.40028900	-0.80553500
H	-1.10725100	2.55444000	0.82493800
H	-3.34772600	2.56483900	-0.26015200
C	1.43198500	-0.45219000	-0.97714000
C	2.11498500	-1.16029900	0.02280900
C	1.65728200	0.92616400	-1.09277900
C	2.96448000	-0.49806000	0.90193000
H	1.96570200	-2.23393200	0.09972500
C	2.51224400	1.57811600	-0.21384700
H	1.13216000	1.48518500	-1.86272200
C	3.16601400	0.87675800	0.79812100

H	3.47868000	-1.06412700	1.67329800
H	2.66266800	2.64880000	-0.31616500
H	3.82856800	1.39043400	1.48596200
N	0.56731900	-1.11974000	-1.84191300
H	0.09026600	-1.88447300	-1.37516600
H	-0.11023300	-0.50349800	-2.27307000
N	-0.91070000	-2.01371600	0.79928200
H	-0.15234300	-1.93191300	1.46482000
H	-1.52885100	-2.77585500	1.04626900

E(M06-2X-D3/6-31G(d,p)) =   -574.977908081   A.U.

Zero-point correction=	0.238444 (Hartree/Particle)
Thermal correction to Energy=	0.277217
Thermal correction to Enthalpy=	0.278905
Thermal correction to Gibbs Free Energy=	0.146554

E(M06-2X-D3/6-311+G(d,p)) =   -575.121827143   A.U.

TS1-1

C	-1.37524400	2.52764000	-0.31798600
C	-2.63939400	2.46180900	0.25812000
C	-3.21315100	1.22302600	0.51684100
C	-2.52986900	0.04535300	0.19986000
C	-1.25149200	0.10515900	-0.38708400
C	-0.69084500	1.35895700	-0.63503800
H	-0.91606300	3.48986600	-0.51883900
H	-3.17767400	3.36921200	0.50892800
H	-4.19682100	1.14907600	0.96759700
H	0.30036700	1.42569100	-1.07060200
C	-3.19498700	-1.19667300	0.50649800
N	-3.83777500	-2.10893600	0.81110800
C	-0.55732200	-1.15209900	-0.73009100
N	-0.78982400	-2.36316900	-0.68822300
H	0.58510100	-2.17323300	-1.23958600
N	0.93908100	-1.01353300	-1.31865300
H	0.98896100	-0.64040300	-2.26881500
C	1.99475300	-0.50561200	-0.48116900
C	2.01805000	-0.87681700	0.86270300
C	2.97419100	0.33497700	-1.00165400
C	3.03283400	-0.39744500	1.68199600
H	1.24684200	-1.53553500	1.25051100
C	3.98699000	0.80958300	-0.17199200

H	2.94704000	0.61626800	-2.05159200
C	4.01776900	0.44574700	1.17014300
H	3.05335600	-0.68560600	2.72772600
H	4.74940300	1.46561700	-0.57868300
H	4.80541500	0.81687400	1.81685300

E(M06-2X-D3/6-31G(d,p)) =   -703.972803193   A.U.

Zero-point correction=	0.215651 (Hartree/Particle)
Thermal correction to Energy=	0.256198
Thermal correction to Enthalpy=	0.257886
Thermal correction to Gibbs Free Energy=	0.120186

E(M06-2X-D3/6-311+G(d,p)) =   -704.142203359   A.U.

TS1-1H
C	3.00603300	2.84535500	-0.88465000
C	2.34945700	4.06887200	-0.78393600
C	1.07071500	4.12109100	-0.24341500
C	0.45506400	2.95138600	0.21102300
C	1.11316400	1.71204300	0.12038300
C	2.38860200	1.67800400	-0.44491800
H	4.00538600	2.79765400	-1.30518000
H	2.82742800	4.97897100	-1.12980400
H	0.53491900	5.06159000	-0.17330800
H	2.91089600	0.72855600	-0.51732900
C	-0.89600700	3.04659900	0.70689400
N	-1.99659600	3.19721000	1.03265400
C	0.44832300	0.49553600	0.67053500
N	-0.18729700	0.32939000	1.69835000
H	-0.49489800	-1.39907700	-0.06313100
N	0.62369200	-0.73692500	-0.42051900
H	0.61997600	-0.37746600	-1.37401400
N	-1.43380000	-1.74562400	0.66977000
H	-1.06426500	-1.05401700	1.42675200
H	-1.39110000	-2.72096200	0.95175300
C	-2.72426900	-1.35387200	0.17053800
C	-3.52261700	-2.26525200	-0.51620900
C	-3.13739400	-0.03315200	0.33963200
C	-4.74626400	-1.85187300	-1.03429800
H	-3.18694500	-3.29093500	-0.64516100
C	-4.35802700	0.37041800	-0.19125300
H	-2.51484200	0.66681500	0.88902200

C	-5.16528600	-0.53314400	-0.87796700
H	-5.37064000	-2.56407200	-1.56417100
H	-4.67068700	1.40086100	-0.05634900
H	-6.11810700	-0.21300200	-1.28623500
C	1.73999800	-1.59843700	-0.21193200
C	2.56915900	-1.97330100	-1.27305700
C	1.98901800	-2.10094100	1.06966600
C	3.63261100	-2.84292900	-1.05576100
H	2.37659200	-1.58061500	-2.26867300
C	3.05718300	-2.96750400	1.27496100
H	1.36150200	-1.78127000	1.89600400
C	3.88172500	-3.34609800	0.21818700
H	4.26820600	-3.12610700	-1.88874400
H	3.24642900	-3.34758900	2.27392600
H	4.71103400	-4.02449400	0.38632400

E(M06-2X-D3/6-31G(d,p)) =   -991.501505500   A.U.

Zero-point correction=   0.335506 (Hartree/Particle)
Thermal correction to Energy=   0.395944
Thermal correction to Enthalpy=   0.397632
Thermal correction to Gibbs Free Energy=   0.213072

E(M06-2X-D3/6-311+G(d,p)) =   -991.740029372   A.U.

INT1-1

C	-3.09871100	-2.18703500	0.23063500
C	-4.18615900	-1.35603100	-0.01754600
C	-3.98768400	0.00924800	-0.18471900
C	-2.70215800	0.55274300	-0.09716400
C	-1.60014200	-0.28150400	0.15494400
C	-1.81710600	-1.65054500	0.31057900
H	-3.24667200	-3.25292200	0.36915600
H	-5.18763000	-1.76716400	-0.08391700
H	-4.82264900	0.67000800	-0.39061500
H	-0.96940100	-2.29303600	0.52654500
C	-2.57059600	1.97024000	-0.33061100
N	-2.58480500	3.09997700	-0.57872100
C	-0.22257400	0.28346000	0.28679600
N	-0.07506200	1.40012400	0.87588600
H	0.89735800	1.71089100	0.85959600
N	0.76155300	-0.55034500	-0.24879700
H	0.46119500	-1.12128000	-1.02666200

C	2.14719700	-0.31895200	-0.15905400
C	2.73337400	0.04841000	1.05724600
C	2.95583800	-0.51584300	-1.28093800
C	4.10916300	0.23358800	1.13376800
H	2.11151000	0.16262100	1.93927500
C	4.33257100	-0.34844900	-1.18778900
H	2.49914900	-0.79499200	-2.22658300
C	4.91591500	0.03569700	0.01635900
H	4.55326700	0.52085400	2.08144600
H	4.94936200	-0.50958300	-2.06611600
H	5.98913300	0.17614700	0.08425200

E(M06-2X-D3/6-31G(d,p)) =   -704.073838661   A.U.

Zero-point correction=   0.221656 (Hartree/Particle)
Thermal correction to Energy=   0.262468
Thermal correction to Enthalpy=   0.264157
Thermal correction to Gibbs Free Energy=   0.126848

E(M06-2X-D3/6-311+G(d,p)) =   -704.244098173   A.U.

TS1-2

C	3.30228800	-0.90965100	-1.24981900
C	3.40653200	0.45041900	-1.54171700
C	2.58643300	1.35853500	-0.88956700
C	1.64887600	0.90468300	0.04692400
C	1.52313200	-0.46553400	0.33382400
C	2.37315300	-1.35928100	-0.32130300
H	3.94956400	-1.62245700	-1.75018400
H	4.12991800	0.80305600	-2.26861100
H	2.66442800	2.42204900	-1.08691400
H	2.27979300	-2.41064700	-0.06974300
C	0.86331400	1.88416400	0.74850700
N	0.24124500	2.66638100	1.33463000
C	0.57754700	-1.05574700	1.31503800
N	0.56128700	-2.12411600	1.94509800
H	-0.72269300	-1.37709900	2.21564600
N	-0.78946900	-0.33666400	1.59911100
H	-0.72813600	0.52669300	2.14316800
C	-1.72240400	-0.20841400	0.50243500
C	-1.91793700	-1.30401600	-0.33739000
C	-2.42361200	0.97648500	0.30542800
C	-2.82973100	-1.20488300	-1.38126500

H	-1.36085400	-2.21973600	-0.16270400
C	-3.33638100	1.06270500	-0.74279600
H	-2.24403700	1.82732500	0.95583100
C	-3.54092400	-0.02399000	-1.58660700
H	-2.98702000	-2.05576800	-2.03582800
H	-3.88278500	1.98678500	-0.89934300
H	-4.25132800	0.04773800	-2.40334000

E(M06-2X-D3/6-31G(d,p)) =   -703.981683430   A.U.

Zero-point correction=   0.216003 (Hartree/Particle)
Thermal correction to Energy=   0.256241
Thermal correction to Enthalpy=   0.257930
Thermal correction to Gibbs Free Energy=   0.122193

E(M06-2X-D3/6-311+G(d,p)) =   -704.151238340   A.U.

TS1-2H
C	3.85791800	-2.10074300	-1.40937300
C	4.40578200	-2.20163800	-0.13080700
C	3.63297400	-1.87321500	0.97179600
C	2.31740100	-1.42299600	0.79571400
C	1.75955500	-1.29939400	-0.48888400
C	2.55151500	-1.66351900	-1.58048200
H	4.45370700	-2.36551300	-2.27689100
H	5.42576400	-2.54369400	0.00594100
H	4.02921000	-1.96623000	1.97710800
H	2.10057100	-1.59587600	-2.56479200
C	1.54661400	-1.14292600	1.97735600
N	0.92090000	-0.91839400	2.92679800
C	0.35897400	-0.85779800	-0.80072600
N	-0.35661900	-1.25093200	-1.71913500
H	-1.21116500	0.62769300	-0.43514800
N	-0.11624300	0.35769000	0.14370700
H	-0.30153800	0.04366000	1.09684800
N	-2.21956700	0.49101100	-1.26133800
H	-1.58532800	-0.34996300	-1.69473100
H	-2.38346900	1.25966200	-1.90413200
C	-3.40005700	0.04798000	-0.60777700
C	-3.35783500	-1.14979500	0.11230900
C	-4.57756900	0.79552400	-0.63873400
C	-4.48741500	-1.58482600	0.79565100
H	-2.44450800	-1.73870600	0.11104700

C	-5.70324700	0.34962500	0.04596400
H	-4.60829900	1.72644300	-1.19874500
C	-5.66415300	-0.83937800	0.76819300
H	-4.44726200	-2.51669500	1.35059200
H	-6.61476400	0.93807200	0.01456900
H	-6.54279200	-1.18334100	1.30310700
C	0.76766700	1.48669500	0.14735400
C	1.23604900	1.97186000	-1.07487800
C	1.13311500	2.11206100	1.33848900
C	2.06718800	3.08619300	-1.09969700
H	0.95300900	1.46432500	-1.99325000
C	1.96343200	3.22808000	1.30115700
H	0.77500600	1.71844000	2.28545000
C	2.43276800	3.71908400	0.08585100
H	2.43157500	3.45975500	-2.05119400
H	2.24564300	3.71286100	2.23009700
H	3.08129300	4.58823900	0.06304400

E(M06-2X-D3/6-31G(d,p)) =   -991.507184657   A.U.

Zero-point correction=	0.335289 (Hartree/Particle)
Thermal correction to Energy=	0.395333
Thermal correction to Enthalpy=	0.397022
Thermal correction to Gibbs Free Energy=	0.215322

E(M06-2X-D3/6-311+G(d,p)) =   -991.745284288   A.U.

INT1-2

C	4.06527900	-1.22085500	-0.35997200
C	4.51916600	0.08132200	-0.16084500
C	3.60729900	1.09122200	0.10453600
C	2.23551200	0.80760900	0.16240200
C	1.76844000	-0.50254600	-0.04792800
C	2.70742700	-1.50478000	-0.29996200
H	4.77275300	-2.01835700	-0.56173400
H	5.57870400	0.30859500	-0.20603100
H	3.93925800	2.10886900	0.27881700
H	2.33396900	-2.51292400	-0.43760400
C	1.36880900	1.91827900	0.47115900
N	0.72457900	2.85292400	0.69888700
C	0.32649900	-0.91793500	0.00875200
N	0.07657900	-2.11310400	0.38208600
H	-0.92093600	-2.31752700	0.31745200

N	-0.58162300	0.04952200	-0.37907800
H	-0.23307000	0.83666400	-0.90528100
C	-1.97892300	-0.01071200	-0.22213000
C	-2.56183300	-0.56514900	0.92247800
C	-2.79509100	0.54802700	-1.20895500
C	-3.94578700	-0.57460000	1.05692500
H	-1.92969000	-0.95818300	1.71166700
C	-4.17601700	0.55077800	-1.05438300
H	-2.33961300	0.97801200	-2.09637400
C	-4.75986000	-0.01952700	0.07355100
H	-4.38753600	-1.00586700	1.94943000
H	-4.79785400	0.99364100	-1.82569600
H	-5.83825300	-0.02512200	0.18832000

E(M06-2X-D3/6-31G(d,p)) =   -704.076238898   A.U.

Zero-point correction=	0.221732 (Hartree/Particle)
Thermal correction to Energy=	0.262572
Thermal correction to Enthalpy=	0.264260
Thermal correction to Gibbs Free Energy=	0.126183

E(M06-2X-D3/6-311+G(d,p)) =   -704.246370584   A.U.

TS2-1

C	2.60411000	1.71093400	-1.74362900
C	2.65934200	2.84194300	-0.93321400
C	1.61021400	3.13280900	-0.06955500
C	0.50234500	2.28330800	-0.00566700
C	0.45539100	1.12487500	-0.80226200
C	1.50909800	0.85647400	-1.67525600
H	3.41781100	1.48675700	-2.42470500
H	3.51864500	3.50215600	-0.97538700
H	1.63660300	4.01250300	0.56352600
H	1.46624800	-0.03289400	-2.29625800
C	-0.57524600	2.62252500	0.88960300
N	-1.44558500	2.94520500	1.58036000
C	-0.67801600	0.16723300	-0.70779500
N	-0.50282600	-1.10517100	-0.50000800
N	-1.92271500	0.67808800	-0.85658300
H	-1.99174300	1.64959600	-1.12388500
C	0.69393600	-1.99139900	-0.63773900
N	0.31425900	-2.99020300	-1.28130700
H	-0.92528500	-2.08130800	-1.04339800

C	2.01116500	-1.65822200	-0.03909200
C	3.14862600	-2.14353900	-0.68742600
C	2.18141900	-0.91462400	1.14163100
C	4.41945600	-1.86461400	-0.20229600
H	2.99586700	-2.74585900	-1.57752600
C	3.46321700	-0.63496200	1.63152000
C	4.58056700	-1.10070000	0.95402000
H	5.29085600	-2.24488900	-0.72580100
H	3.56454900	-0.06094600	2.54636400
H	5.57272400	-0.88039400	1.33278100
C	1.04743800	-0.44314300	1.89289600
N	0.14291400	-0.05843100	2.50556100
C	-3.12003300	0.03816800	-0.41761200
C	-4.23197500	0.03714900	-1.25377000
C	-3.17868100	-0.52513100	0.85773300
C	-5.42240100	-0.53155600	-0.80929600
H	-4.15746500	0.47443400	-2.24473300
C	-4.36707800	-1.10539600	1.28231400
H	-2.30387200	-0.49345300	1.50130700
C	-5.48928400	-1.10865100	0.45447100
H	-6.29294200	-0.53056600	-1.45664400
H	-4.42082500	-1.54423400	2.27296800
H	-6.41514600	-1.55819300	0.79775900

E(M06-2X-D3/6-31G(d,p)) =   -1120.57786890   A.U.

Zero-point correction=   0.318397 (Hartree/Particle)
Thermal correction to Energy=   0.382923
Thermal correction to Enthalpy=   0.384611
Thermal correction to Gibbs Free Energy=   0.193474

E(M06-2X-D3/6-311+G(d,p)) =   -1120.84782782   A.U.

INT2-1

C	-2.50773900	2.72610400	1.18328300
C	-3.03045400	2.86190100	-0.10078600
C	-2.38130800	2.27788400	-1.18077800
C	-1.19977300	1.55745300	-0.97752900
C	-0.67304000	1.41160700	0.31569600
C	-1.33999300	1.99954900	1.38964700
H	-3.01406400	3.18134600	2.02777400
H	-3.94739300	3.41824500	-0.26182200
H	-2.78179900	2.36366600	-2.18478200

H	-0.94250700	1.86542300	2.39053500
C	-0.56836200	0.92959400	-2.11038400
N	-0.08736900	0.43365600	-3.03888500
C	0.54078900	0.56981300	0.59578400
N	0.51853700	-0.46601600	1.35960100
N	1.67665200	1.03530400	0.01509800
H	1.58443200	1.91542200	-0.47103800
C	-0.70825700	-0.96958500	1.81149400
N	-0.99114300	-1.17360800	3.03628200
H	-0.19639000	-0.87506000	3.60771900
C	-1.73497600	-1.32268400	0.77564300
C	-3.07676100	-1.06317100	1.05608000
C	-1.40034200	-1.84750100	-0.48412200
C	-4.06038200	-1.28143400	0.09881200
H	-3.32231900	-0.67343200	2.03820700
C	-2.39319200	-2.07073600	-1.44635900
C	-3.71856300	-1.77586100	-1.15878700
H	-5.09666400	-1.05856900	0.33178000
H	-2.10499400	-2.46939100	-2.41292100
H	-4.48261600	-1.93816700	-1.91129100
C	-0.05012200	-2.21769500	-0.82979500
N	1.00706300	-2.56005200	-1.15346200
C	2.98976600	0.51638600	0.05532900
C	4.01236200	1.38197300	-0.34684400
C	3.29292700	-0.79030500	0.44454100
C	5.33070600	0.95003700	-0.36027300
H	3.76861800	2.39745400	-0.64977900
C	4.62143700	-1.20527300	0.42903700
H	2.50317400	-1.46795100	0.73270400
C	5.64337500	-0.34833800	0.03394300
H	6.11314700	1.63147000	-0.67794200
H	4.85167400	-2.22406100	0.72310300
H	6.67293100	-0.68969000	0.02551300

E(M06-2X-D3/6-31G(d,p)) =   -1120.67266082   A.U.

Zero-point correction=   0.324485 (Hartree/Particle)
Thermal correction to Energy=   0.389121
Thermal correction to Enthalpy=   0.390810
Thermal correction to Gibbs Free Energy=   0.198947

E(M06-2X-D3/6-311+G(d,p)) =   -1120.94291086   A.U.

TS1-3

C	-4.09061100	-1.17899300	0.30946700
C	-4.51296400	0.14457000	0.19859700
C	-3.57864700	1.14507600	-0.01979800
C	-2.21614900	0.82754600	-0.11300400
C	-1.77851900	-0.50469300	0.00242500
C	-2.74226200	-1.49334800	0.20102600
H	-4.81651900	-1.96810200	0.47610900
H	-5.56543300	0.39501000	0.27482400
H	-3.88614100	2.17957200	-0.12750500
H	-2.39688600	-2.51995400	0.25925400
C	-1.31151600	1.92438900	-0.35396600
N	-0.60807100	2.82990800	-0.51606200
C	-0.33589100	-0.97503800	-0.15060000
N	-0.07579100	-2.07415700	-0.66935500
H	0.14275700	-2.75528900	-1.35318500
N	0.57868400	-0.10278900	0.41195000
H	0.21188200	0.72654600	0.85367700
C	1.97675800	-0.09203900	0.24595100
C	2.73307800	-1.24948500	0.04162300
C	2.61804000	1.14996600	0.32544500
C	4.11506900	-1.14674900	-0.09294900
H	2.23896200	-2.20914100	-0.00139500
C	3.99754800	1.23432800	0.20044100
H	2.02101800	2.04840400	0.46202600
C	4.75567900	0.08548100	-0.01475500
H	4.69597800	-2.05008000	-0.25211700
H	4.47948700	2.20484300	0.26213700
H	5.83347000	0.15140100	-0.11899000

E(M06-2X-D3/6-31G(d,p)) =   -704.036846555   A.U.

Zero-point correction=   0.218769 (Hartree/Particle)
Thermal correction to Energy=   0.260027
Thermal correction to Enthalpy=   0.261715
Thermal correction to Gibbs Free Energy=   0.122602

E(M06-2X-D3/6-311+G(d,p)) =   -704.208340361   A.U.

INT1-3

C	-4.06115800	-1.13739200	0.51781500
C	-4.48566700	0.17228300	0.30857500
C	-3.56379800	1.14491600	-0.05151900

C	-2.21221300	0.81145900	-0.20064500
C	-1.77438800	-0.50973300	0.00258800
C	-2.72051000	-1.47042300	0.36156400
H	-4.77454100	-1.90138300	0.80856400
H	-5.53085100	0.43610600	0.42666500
H	-3.87492800	2.16916400	-0.22571800
H	-2.38493500	-2.48808900	0.53567000
C	-1.30455600	1.86889900	-0.57151100
N	-0.60326900	2.75134200	-0.83485400
C	-0.34877000	-0.95304000	-0.18651500
N	-0.02655500	-2.02442900	-0.80727200
H	-0.85897600	-2.45544300	-1.20395800
N	0.57464900	-0.12177900	0.39309500
H	0.20637900	0.67699500	0.88595000
C	1.97450100	-0.10947500	0.25100700
C	2.71707200	-1.19082400	-0.23241200
C	2.63015400	1.06547400	0.64076600
C	4.10262900	-1.07480000	-0.31783300
H	2.20792400	-2.09319400	-0.53783600
C	4.01093300	1.15977800	0.55477700
H	2.04501300	1.91242200	0.99120200
C	4.75846200	0.08717100	0.07317400
H	4.67416700	-1.91714100	-0.69533700
H	4.50236500	2.07901100	0.85712500
H	5.83845900	0.15983400	0.00189900

E(M06-2X-D3/6-31G(d,p)) =   -704.076719978   A.U.

Zero-point correction=   0.221872 (Hartree/Particle)
Thermal correction to Energy=   0.262690
Thermal correction to Enthalpy=   0.264378
Thermal correction to Gibbs Free Energy=   0.127081

E(M06-2X-D3/6-311+G(d,p)) =   -704.246915145   A.U.

INT1-4
C	3.08636000	-1.17588300	0.96838300
C	2.92956700	-1.88830500	-0.21730800
C	2.04308100	-1.43339900	-1.18531800
C	1.29794500	-0.27106300	-0.96400000
C	1.44345900	0.44715700	0.23506200
C	2.35229200	-0.01425200	1.18613700
H	3.77892600	-1.52614500	1.72653300

H	3.49870500	-2.79481400	-0.39187800
H	1.92012700	-1.96659100	-2.12156100
H	2.46203200	0.54225300	2.11245200
C	0.41965800	0.17739100	-2.01532500
N	-0.25693300	0.50181800	-2.89611900
C	0.70428400	1.72566100	0.49554500
N	1.26810900	2.81429600	0.85729700
H	2.27993200	2.69558600	0.86895000
N	-0.65029000	1.71693900	0.25106900
H	-1.05739100	2.64199000	0.21368300
C	-1.52896100	0.61896900	0.36696800
C	-1.32498600	-0.38803000	1.31367200
C	-2.63731500	0.55562400	-0.48155900
C	-2.21336700	-1.45592100	1.39257600
H	-0.48137700	-0.32481100	1.99340200
C	-3.53366800	-0.50027700	-0.37687300
H	-2.76817400	1.32433700	-1.23665500
C	-3.32243700	-1.51508800	0.55437200
H	-2.04522300	-2.23462300	2.12961700
H	-4.39122400	-0.53973200	-1.04052200
H	-4.01801900	-2.34432100	0.62627000

E(M06-2X-D3/6-31G(d,p)) =   -704.075655091   A.U.

Zero-point correction=	0.221751 (Hartree/Particle)
Thermal correction to Energy=	0.262601
Thermal correction to Enthalpy=	0.264290
Thermal correction to Gibbs Free Energy=	0.127846

E(M06-2X-D3/6-311+G(d,p)) =   -704.247322697   A.U.

TS2-2
C	-1.51474900	3.55778500	-0.41361700
C	-2.57064400	3.65473000	0.48828500
C	-2.89258700	2.57522000	1.30283900
C	-2.16824100	1.38472800	1.20276000
C	-1.11314400	1.28017500	0.28112200
C	-0.78173600	2.37815900	-0.51189800
H	-1.25650000	4.40212300	-1.04360700
H	-3.14018800	4.57449100	0.56571000
H	-3.69869900	2.64341400	2.02477100
H	0.04655400	2.29776000	-1.21239700
C	-2.49640300	0.29820200	2.08937000

N	-2.76736800	-0.55105300	2.82687400
C	-0.28816200	0.03893200	0.15950300
N	1.00857400	0.12726900	0.29310400
H	1.34474700	1.04680200	0.55697200
N	-0.85318100	-1.14879300	-0.06529100
C	-2.18336900	-1.39680200	-0.48281200
C	-2.79517400	-0.63853900	-1.48185200
C	-2.86482600	-2.46372300	0.10445400
C	-4.09829700	-0.93531400	-1.86899300
H	-2.24717700	0.16720600	-1.95976000
C	-4.15883500	-2.76324600	-0.30171000
H	-2.37803900	-3.02865000	0.89264300
C	-4.78246900	-1.99689400	-1.28375100
H	-4.57197800	-0.34297800	-2.64511200
H	-4.68556600	-3.59067400	0.16179400
H	-5.79574900	-2.22898100	-1.59413500
H	-0.14205900	-1.92948500	-0.03761000
C	2.03088200	-1.31102700	0.08316400
C	3.42283400	-0.80856000	0.12260700
C	4.34546700	-1.60010200	0.81082900
C	3.89114500	0.34306600	-0.53342600
C	5.68683500	-1.24699900	0.87370000
H	3.97671200	-2.50104700	1.28875200
C	5.24738700	0.69336000	-0.47495100
C	6.14139600	-0.09549700	0.23278300
H	6.38146900	-1.87366900	1.42337700
H	5.58318800	1.58230500	-0.99796500
H	7.18873600	0.18230500	0.27738300
N	1.50034300	-2.38296600	-0.00223100
C	3.02995900	1.19309600	-1.31522100
N	2.37891000	1.92048300	-1.93815800

E(M06-2X-D3/6-31G(d,p)) =   -1120.62712030   A.U.

Zero-point correction=   0.321105 (Hartree/Particle)
Thermal correction to Energy=   0.385290
Thermal correction to Enthalpy=   0.386979
Thermal correction to Gibbs Free Energy=   0.195530

E(M06-2X-D3/6-311+G(d,p)) =   -1120.89734054   A.U.

INT2-2

C	-1.30053100	3.44354000	-0.43377400

C	-2.23895800	3.62057000	0.57874900
C	-2.56318900	2.56228700	1.41969700
C	-1.95857000	1.31622700	1.23601600
C	-1.02923400	1.12737700	0.19998500
C	-0.69350200	2.20375400	-0.61916000
H	-1.03474800	4.27096100	-1.08282300
H	-2.71234500	4.58573400	0.72243800
H	-3.27717600	2.68966200	2.22563200
H	0.04470200	2.06912500	-1.40434700
C	-2.26290800	0.25141100	2.15666200
N	-2.49837400	-0.57811700	2.92813300
C	-0.38147700	-0.20916100	-0.02142900
N	0.99710600	-0.15202300	0.09002400
H	1.36669400	0.73258000	0.40629600
N	-0.97803100	-1.30789500	-0.27958100
C	-2.36427500	-1.35349200	-0.54092400
C	-2.95791600	-0.56844200	-1.53437600
C	-3.14164400	-2.27762500	0.16319900
C	-4.31801900	-0.69246700	-1.79971800
H	-2.34449300	0.12278700	-2.10445700
C	-4.50148300	-2.38483300	-0.09807900
H	-2.66659800	-2.88015900	0.93006800
C	-5.09588800	-1.59501000	-1.08034600
H	-4.76840100	-0.08211400	-2.57623600
H	-5.09952100	-3.09186900	0.46771900
H	-6.15671500	-1.68797800	-1.28798500
H	0.62821900	-2.56024900	-0.37591200
C	1.90736100	-1.20253700	-0.10409700
C	3.35079200	-0.80887400	0.02583300
C	4.21098100	-1.74578500	0.60066500
C	3.89812700	0.40655100	-0.42312800
C	5.56564200	-1.47915800	0.75017500
H	3.78381900	-2.69032100	0.91791200
C	5.26646500	0.67297400	-0.27614100
C	6.09670000	-0.26571500	0.31651000
H	6.21167800	-2.22165400	1.20683400
H	5.66084400	1.61495800	-0.64103400
H	7.15420700	-0.05514200	0.43242600
N	1.63961400	-2.41937300	-0.34007800
C	3.10742200	1.41389500	-1.08372400
N	2.50174900	2.25323100	-1.60308500

E(M06-2X-D3/6-31G(d,p)) =   -1120.67686213   A.U.

Zero-point correction=   0.324752 (Hartree/Particle)
Thermal correction to Energy=   0.389230
Thermal correction to Enthalpy=   0.390918
Thermal correction to Gibbs Free Energy=   0.198695

E(M06-2X-D3/6-311+G(d,p)) =   -1120.94573461   A.U.

INT2-3

C	3.11547300	-2.37153300	-1.48219900
C	4.22396400	-1.92772400	-0.76650300
C	4.05125000	-1.12301000	0.35282800
C	2.76496900	-0.74864700	0.75050800
C	1.64481500	-1.18161200	0.02151000
C	1.83132900	-2.00889900	-1.08496500
H	3.24788000	-3.00083000	-2.35602100
H	5.22409100	-2.21237000	-1.07472900
H	4.90283500	-0.78437200	0.93235600
H	0.96357600	-2.33181700	-1.65241400
C	2.61688900	0.04144000	1.94580700
N	2.53547900	0.65204800	2.92525200
C	0.26039400	-0.78427700	0.43785500
N	-0.56628500	-1.87852500	0.65121200
N	-0.18471700	0.39780300	0.60200500
C	0.52553800	1.52295500	0.14209900
C	0.97810700	1.61636100	-1.17931100
C	0.69273300	2.60928600	1.00685300
C	1.61249100	2.77513800	-1.61620000
H	0.80856500	0.78638500	-1.86011900
C	1.34047100	3.75549000	0.56541300
H	0.33160400	2.52179800	2.02591000
C	1.80252600	3.84528800	-0.74693100
H	1.95592500	2.83988000	-2.64402200
H	1.48240400	4.58531100	1.25039600
H	2.30004100	4.74640200	-1.09026100
H	-3.42160400	-2.78873700	1.61414800
C	-1.93155400	-1.86358600	0.92223600
C	-2.76639400	-0.73875200	0.39402800
C	-3.70202400	-0.16136200	1.24784100
C	-2.71772300	-0.30272000	-0.94136200
C	-4.56012400	0.83774500	0.79762800
H	-3.73304800	-0.48519100	2.28337600
C	-3.58346600	0.69453000	-1.39520800
C	-4.50287400	1.26697200	-0.52412000

H	-5.27110500	1.28353800	1.48512900
H	-3.52509800	1.01319800	-2.43008000
H	-5.16871600	2.04590200	-0.87843400
N	-2.40597200	-2.85833500	1.56211400
C	-1.77470300	-0.85989900	-1.87499100
N	-1.02158200	-1.28683000	-2.64391800
H	-0.12833800	-2.76131400	0.88121300

E(M06-2X-D3/6-31G(d,p)) =   -1120.67586261   A.U.

Zero-point correction=   0.324662 (Hartree/Particle)
Thermal correction to Energy=   0.389052
Thermal correction to Enthalpy=   0.390741
Thermal correction to Gibbs Free Energy=   0.200455

E(M06-2X-D3/6-311+G(d,p)) =   -1120.94639063   A.U.

TS3-1

C	2.24945400	-3.61024400	-1.81056400
C	2.98096500	-4.28308900	-0.83611100
C	3.10976800	-3.73819900	0.43563800
C	2.52135500	-2.50551800	0.72834900
C	1.80065200	-1.81313900	-0.25915000
C	1.65209400	-2.38719100	-1.52084300
H	2.13935800	-4.03813300	-2.80119900
H	3.44324700	-5.23822600	-1.06061100
H	3.65491600	-4.26038400	1.21384700
H	1.09070100	-1.85356200	-2.28116600
C	2.62724700	-1.99614200	2.07119100
N	2.71133400	-1.62781400	3.16483400
C	1.16976900	-0.48925700	0.03998200
N	-0.19819700	-0.47846700	-0.24506700
N	1.72517000	0.54686800	0.52505700
C	3.12386400	0.67758300	0.61375000
C	3.96079600	0.41048700	-0.47619400
C	3.66908800	1.18438700	1.79771500
C	5.33081700	0.62670800	-0.36621800
H	3.52884000	0.05507900	-1.40759600
C	5.03961600	1.37914800	1.90280800
H	3.00387300	1.38915700	2.62966800
C	5.87649900	1.10344600	0.82211800
H	5.97232900	0.42155800	-1.21757500
H	5.45626500	1.75249300	2.83271700

H	6.94605100	1.26634300	0.90486000
H	-2.82354400	1.27332100	-0.46987500
C	-0.98845800	0.60881800	-0.33318500
C	-0.46015300	1.99416900	-0.52385900
C	-0.94765700	3.00125300	0.30387400
C	0.43436500	2.32399600	-1.55629900
C	-0.52852600	4.31818200	0.12473000
H	-1.64114000	2.74828000	1.10199100
C	0.84238800	3.64509800	-1.73708900
C	0.36363500	4.64082000	-0.89138800
H	-0.90339000	5.09035700	0.78779500
H	1.53345300	3.87948200	-2.53905800
H	0.68966400	5.66568100	-1.03006500
N	-2.27852800	0.43583300	-0.29171800
C	0.95148500	1.31318900	-2.43995400
N	1.37813300	0.51032100	-3.15682900
H	-0.77511900	-1.37754500	-0.26006500
N	-2.24859100	-2.11729000	-0.22460400
C	-2.97587200	-1.16358700	-0.13729400
C	-4.43646600	-0.96962500	0.02923100
C	-5.24959200	-1.93375000	-0.57268000
C	-5.05315900	0.03565900	0.79479800
C	-6.63119700	-1.88970700	-0.44465800
H	-4.76010400	-2.72099900	-1.13532000
C	-6.44855900	0.07374300	0.92800900
C	-4.31088200	1.05047200	1.49714100
C	-7.23586300	-0.88169000	0.30491200
H	-7.23927200	-2.64641000	-0.92934100
H	-6.89662300	0.85536900	1.53192400
N	-3.76500300	1.90582500	2.05497200
H	-8.31455100	-0.84490800	0.40999700

E(M06-2X-D3/6-31G(d,p)) =   -1537.22295843   A.U.

Zero-point correction=   0.423560 (Hartree/Particle)
Thermal correction to Energy=   0.511336
Thermal correction to Enthalpy=   0.513024
Thermal correction to Gibbs Free Energy=   0.267881

E(M06-2X-D3/6-311+G(d,p)) =   -1537.59181640   A.U.

INT3-1

C	2.54115200	-3.52811000	-1.76119900

C	3.43827800	-4.09314000	-0.85812000
C	3.61402500	-3.51703500	0.39287200
C	2.90912000	-2.35813400	0.73227300
C	2.02477200	-1.76723900	-0.18581800
C	1.82938300	-2.38192800	-1.42167800
H	2.39199000	-3.98170600	-2.73540800
H	3.99189600	-4.98762900	-1.12210100
H	4.28765000	-3.95638200	1.12017200
H	1.13285900	-1.93929700	-2.12565300
C	3.06958100	-1.83005800	2.06269800
N	3.20224100	-1.45161900	3.14817000
C	1.26117700	-0.52416600	0.16819600
N	-0.12537700	-0.71114700	0.06290400
N	1.75419000	0.56899100	0.60200700
C	3.13349600	0.84506200	0.56361300
C	3.88308200	0.67103800	-0.60621300
C	3.73461500	1.41254900	1.69192900
C	5.22437500	1.03953300	-0.63151100
H	3.40356500	0.26440400	-1.49251700
C	5.07924200	1.75680300	1.66281300
H	3.13699400	1.54404700	2.58758700
C	5.82948800	1.57474700	0.50186500
H	5.79610100	0.90676100	-1.54471700
H	5.54296900	2.17500000	2.55042300
H	6.87747300	1.85539500	0.48011700
H	-2.83449100	0.89648800	-0.33737400
C	-0.92164500	0.28111500	-0.12697500
C	-0.56692900	1.71191100	-0.41871800
C	-1.05961400	2.71184900	0.41431300
C	0.20039200	2.07392500	-1.53825100
C	-0.77204900	4.05029100	0.15397000
H	-1.66164600	2.44418800	1.27659800
C	0.48598500	3.41486900	-1.79692900
C	0.00151000	4.40279600	-0.94639300
H	-1.15814300	4.81471000	0.81956400
H	1.08481800	3.67035000	-2.66391400
H	0.22708300	5.44410600	-1.14785100
N	-2.28212300	0.08950700	-0.08326500
C	0.71159900	1.07135700	-2.43324300
N	1.12988500	0.28129500	-3.16922100
H	-1.44841000	-2.20839800	0.34858000
N	-2.46831800	-2.25403800	0.38937800
C	-2.97312600	-1.11082000	0.18264700
C	-4.47063300	-0.99104700	0.16168400

C	-5.17785700	-2.09588900	-0.31583300
C	-5.20535000	0.11825200	0.61805200
C	-6.56561100	-2.09591900	-0.36243700
H	-4.60309800	-2.95668700	-0.63779900
C	-6.60639000	0.11558000	0.57466900
C	-4.57909400	1.28765800	1.17981800
C	-7.28470100	-0.98689800	0.07902900
H	-7.08902000	-2.96607200	-0.74458800
H	-7.14460500	0.98255300	0.94182200
N	-4.10979700	2.25241600	1.61578400
H	-8.36852300	-0.98338000	0.04402700

E(M06-2X-D3/6-31G(d,p)) =   -1537.26881047   A.U.

Zero-point correction=   0.427450 (Hartree/Particle)
Thermal correction to Energy=   0.515648
Thermal correction to Enthalpy=   0.517336
Thermal correction to Gibbs Free Energy=   0.271040

E(M06-2X-D3/6-311+G(d,p)) =   -1537.63676112   A.U.

INT3-2
C	-2.29858500	-3.92342900	1.72795300
C	-3.30142500	-3.29611500	2.46205400
C	-3.46123000	-1.91926000	2.37484100
C	-2.62538600	-1.17028100	1.54083900
C	-1.61915100	-1.79834400	0.78882200
C	-1.45644400	-3.17963600	0.90688400
H	-2.16620200	-4.99821700	1.79591100
H	-3.95422900	-3.87551900	3.10587300
H	-4.22680700	-1.40960300	2.94939000
H	-0.66823800	-3.66086000	0.33541300
C	-2.82186000	0.25497800	1.50874100
N	-3.01258500	1.39677300	1.53631800
C	-0.70481000	-1.05405900	-0.13447400
N	0.61457700	-1.49087900	-0.02000400
N	-1.01076800	-0.22601300	-1.05693000
C	-2.33045500	0.03156300	-1.46371200
C	-2.66009600	1.35587100	-1.77451100
C	-3.28830000	-0.97197600	-1.65803400
C	-3.94055300	1.68134600	-2.20010800
H	-1.89314500	2.11589000	-1.66292600
C	-4.56340600	-0.64053400	-2.10351000

H	-3.02366000	-2.00822000	-1.47303000
C	-4.90125000	0.68496800	-2.36254500
H	-4.18736300	2.71586500	-2.41746600
H	-5.29645400	-1.42709700	-2.25291100
H	-5.89946500	0.93787300	-2.70407300
H	2.34682200	1.12622200	-0.51754000
C	1.64545500	-0.74988400	-0.05973400
C	2.97866300	-1.39096300	-0.24552200
C	4.14407300	-0.71148700	0.11137800
C	3.09427300	-2.69199200	-0.77586400
C	5.39711900	-1.29113000	-0.06570100
H	4.07659600	0.27712300	0.55208100
C	4.35519600	-3.26923400	-0.94869500
C	5.50497900	-2.56980700	-0.59960200
H	6.28443100	-0.73716600	0.22112800
H	4.41998000	-4.26949400	-1.36265100
H	6.47809200	-3.02736400	-0.74141300
N	1.66492200	0.64269700	0.04826900
C	1.96720400	-3.50350100	-1.16818000
N	1.16152700	-4.25882000	-1.51592200
H	-0.47053700	1.51296400	2.22802100
N	0.10322100	0.82925200	1.73757100
C	0.80788400	1.39488100	0.84377200
C	0.75745400	2.86281200	0.53773200
C	-0.50352200	3.45751900	0.46734100
C	1.89123400	3.67302300	0.35008300
C	-0.63348000	4.81697200	0.20091600
H	-1.38805000	2.84239200	0.61558300
C	1.75796600	5.04197800	0.09203200
C	3.22165900	3.13045000	0.44191200
C	0.49459100	5.61112400	0.01249900
H	-1.62463000	5.25406400	0.14085300
H	2.65072800	5.64413300	-0.03676700
N	4.29378500	2.69564400	0.49501200
H	0.39259500	6.67131000	-0.19132200

E(M06-2X-D3/6-31G(d,p)) =   -1537.26825131   A.U.

Zero-point correction=   0.427651 (Hartree/Particle)
Thermal correction to Energy=   0.515592
Thermal correction to Enthalpy=   0.517280
Thermal correction to Gibbs Free Energy=   0.275378

E(M06-2X-D3/6-311+G(d,p)) =   -1537.63539334   A.U.

TS3-3

C	3.17391700	1.53795200	2.69709500
C	4.01199100	0.46790500	2.98630000
C	3.80055000	-0.75264600	2.35709200
C	2.75624700	-0.89909600	1.43933300
C	1.90319000	0.18130600	1.14149900
C	2.13242600	1.39240700	1.78332500
H	3.32351200	2.49981500	3.17668900
H	4.82521200	0.57746900	3.69541100
H	4.43857500	-1.60422000	2.56724300
H	1.49672200	2.23833500	1.55484300
C	2.58554200	-2.20681000	0.85639800
N	2.45326800	-3.28234500	0.44631700
C	0.78530400	0.04092700	0.10420500
N	-0.00504000	1.25420200	0.04306700
N	1.14236500	-0.42688700	-1.19268400
C	2.38881300	-0.14697000	-1.73447000
C	2.97927800	-1.10839700	-2.57546000
C	3.07192300	1.06943200	-1.54036200
C	4.20409000	-0.87019000	-3.18126900
H	2.45710900	-2.04923500	-2.72003000
C	4.29939000	1.29643100	-2.15206800
H	2.61113000	1.84681200	-0.93882600
C	4.87928400	0.33215200	-2.97224100
H	4.64027600	-1.63393700	-3.81871100
H	4.80210500	2.24582900	-1.99067000
H	5.83773400	0.51555100	-3.44633500
H	-2.97346700	0.01356300	0.39337000
C	-1.27171000	1.17552100	0.08125700
C	-2.14310300	2.35654300	-0.16099100
C	-3.32802900	2.20914400	-0.88382200
C	-1.78731000	3.63981600	0.28989600
C	-4.14256500	3.30439900	-1.15528500
H	-3.61286500	1.23489100	-1.26813000
C	-2.60719900	4.73746700	0.01285300
C	-3.78256700	4.57092700	-0.70909800
H	-5.05517800	3.16081000	-1.72354300
H	-2.31265500	5.71531800	0.37741400
H	-4.41196800	5.42823600	-0.92081200
N	-1.96928100	-0.02738000	0.28958900
C	-0.61460700	3.88919900	1.08787600
N	0.27659900	4.19142900	1.76142700

H	0.55894400	-1.69023500	-0.40124200
N	-0.00039500	-1.20424200	0.45452800
C	-1.30848400	-1.20479900	0.36176100
C	-1.99573100	-2.51640400	0.32004700
C	-1.23433200	-3.64317800	0.65725300
C	-3.34111600	-2.71432100	-0.05701400
C	-1.78529000	-4.91722100	0.61532500
H	-0.19690800	-3.51177700	0.94870400
C	-3.89162700	-3.99965300	-0.08712700
C	-4.21201300	-1.63670300	-0.44172400
C	-3.11542800	-5.10032500	0.24715000
H	-1.16755100	-5.76957200	0.87557800
H	-4.92763500	-4.11843400	-0.38433400
N	-4.93331100	-0.77817200	-0.73362200
H	-3.54752400	-6.09434400	0.21662700

E(M06-2X-D3/6-31G(d,p)) =   -1537.20675297   A.U.

Zero-point correction=   0.423803 (Hartree/Particle)
Thermal correction to Energy=   0.510115
Thermal correction to Enthalpy=   0.511803
Thermal correction to Gibbs Free Energy=   0.272592

E(M06-2X-D3/6-311+G(d,p)) =   -1537.57165514   A.U.

TS3-3H
C	-3.79899200	-0.90802400	-2.91637800
C	-3.77680400	-2.27637100	-3.15844800
C	-2.85926000	-3.07128100	-2.48348000
C	-1.98022200	-2.49614500	-1.56053400
C	-1.99931200	-1.11321800	-1.30482700
C	-2.91439500	-0.33574500	-2.00421800
H	-4.51386100	-0.27233400	-3.42881700
H	-4.46727300	-2.72442500	-3.86461800
H	-2.81412100	-4.14088700	-2.65828800
H	-2.96074800	0.72882200	-1.81278200
C	-1.02882500	-3.38145600	-0.93745700
N	-0.25505500	-4.14477300	-0.53466800
C	-1.06125500	-0.51861300	-0.23201100
N	-1.25219800	0.94827800	-0.18714300
N	-1.17858100	-1.09727200	1.04578500
C	-2.40896100	-1.15850500	1.66977900
C	-2.51927500	-2.02292400	2.78301600

C	-3.56398200	-0.42348900	1.32135400
C	-3.70158100	-2.15632200	3.49151700
H	-1.64239200	-2.59819500	3.07066600
C	-4.74835700	-0.57213400	2.03677200
H	-3.52765100	0.29564400	0.51202000
C	-4.83875700	-1.43543400	3.12331800
H	-3.73902400	-2.83615700	4.33869500
H	-5.61389600	0.01291600	1.73665500
H	-5.76745400	-1.54151600	3.67393100
H	1.58471400	2.01450600	-1.35429700
C	-0.33048200	1.74912600	-0.50986900
C	-0.45382100	3.21508300	-0.27934100
C	0.66381800	3.96173000	0.09519400
C	-1.69686700	3.86609700	-0.37190600
C	0.55734100	5.32337200	0.36505900
H	1.62827900	3.47877300	0.21578800
C	-1.79825800	5.23339900	-0.10266400
C	-0.67309500	5.96196500	0.26499200
H	1.44146100	5.87746900	0.66137200
H	-2.76685500	5.71299100	-0.19035300
H	-0.76179200	7.02242000	0.47370000
N	0.91257500	1.32925200	-1.04197500
C	-2.90356700	3.19529900	-0.78337900
N	-3.91755700	2.77069900	-1.14582600
N	0.33649100	-0.87141800	-0.66677700
C	1.21934900	0.01136100	-0.99678300
C	2.59595300	-0.48594600	-1.27956800
C	2.71478900	-1.80521100	-1.72721700
C	3.77198000	0.24781000	-1.03443900
C	3.96436700	-2.38468200	-1.91429100
H	1.81282900	-2.37690100	-1.92219800
C	5.02566600	-0.34149600	-1.22164600
C	3.75934600	1.61601300	-0.58977700
C	5.12190300	-1.65610700	-1.65783100
H	4.02904300	-3.41005300	-2.26190600
H	5.91476400	0.24140700	-1.00824200
N	3.78620400	2.73306200	-0.28463700
H	6.09815700	-2.10703900	-1.79787700
H	0.79800100	-1.78662400	0.01000800
N	1.15556800	-2.33769000	1.18867100
H	0.15808600	-2.01959700	1.47191200
H	1.30017700	-3.34194300	1.17816200
C	2.20532100	-1.54435100	1.70794800
C	1.92006100	-0.22500400	2.08246600

C	3.52453900	-2.00157300	1.71357000
C	2.95896300	0.62616700	2.44476400
H	0.88135900	0.10142600	2.08154000
C	4.55322500	-1.14063300	2.08150400
H	3.73967600	-3.02231900	1.40842100
C	4.27926000	0.17785200	2.43933500
H	2.73528300	1.65048200	2.72730300
H	5.57711900	-1.50256200	2.08111500
H	5.08509600	0.84907700	2.71694100

E(M06-2X-D3/6-31G(d,p)) =   -1824.73920343   A.U.

Zero-point correction=	0.543179 (Hartree/Particle)
Thermal correction to Energy=	0.649261
Thermal correction to Enthalpy=	0.650949
Thermal correction to Gibbs Free Energy=	0.371370

E(M06-2X-D3/6-311+G(d,p)) =   -1825.17283734   A.U.

INT3-3

C	3.30295400	-0.21695300	2.98604700
C	3.76172000	-1.52864600	3.02120200
C	3.20809700	-2.47213400	2.16390000
C	2.19313500	-2.09709100	1.28096400
C	1.71638400	-0.77451100	1.24886900
C	2.28818500	0.15725400	2.10616700
H	3.73960500	0.52892200	3.64215800
H	4.55300500	-1.81787800	3.70422300
H	3.55704000	-3.49902600	2.16472900
H	1.94498700	1.18503500	2.06424000
C	1.67555300	-3.10259000	0.38648500
N	1.29365800	-3.92508100	-0.33498600
C	0.61800500	-0.39452300	0.25287200
N	0.25725200	1.00660400	0.43904600
N	1.03052100	-0.61136600	-1.14281000
C	2.34661100	-0.33144600	-1.56269400
C	2.98093400	-1.21317200	-2.44478000
C	3.02026200	0.82017500	-1.14354200
C	4.25999800	-0.93734000	-2.91311400
H	2.46842600	-2.12223700	-2.75024600
C	4.30599500	1.07616100	-1.60590200
H	2.53764400	1.51333800	-0.46477200
C	4.93359500	0.20739200	-2.49507400

H	4.73541400	-1.63153400	-3.59930500
H	4.81304700	1.97434700	-1.26653500
H	5.93486600	0.41761100	-2.85578700
H	-2.68180400	0.69448700	-0.85356900
C	-0.89249400	1.34700500	0.01323200
C	-1.31715900	2.77526800	0.03654300
C	-2.65481400	3.13395000	-0.13540400
C	-0.37817700	3.80547700	0.24965400
C	-3.05563100	4.46649400	-0.12842600
H	-3.42522200	2.37954600	-0.24211700
C	-0.78677100	5.14251900	0.25395900
C	-2.12071700	5.47666100	0.05761600
H	-4.10547100	4.70378900	-0.26220700
H	-0.04044600	5.91241600	0.41532500
H	-2.42429300	6.51776000	0.06079700
N	-1.81314800	0.40252600	-0.43478000
C	1.02716800	3.59701200	0.49873100
N	2.16217800	3.60339300	0.72803600
H	0.73786900	-1.53970200	-1.43043300
N	-0.50312600	-1.30461300	0.45116600
C	-1.62162200	-0.90556800	-0.01911600
C	-2.73283100	-1.90393100	-0.10045300
C	-2.34816600	-3.24826400	-0.12985900
C	-4.10806500	-1.60893900	-0.14869100
C	-3.29507000	-4.26278700	-0.19453100
H	-1.28788100	-3.47951800	-0.10193900
C	-5.05972200	-2.63444100	-0.21591600
C	-4.62314600	-0.26643600	-0.13291000
C	-4.65379300	-3.95999600	-0.23777500
H	-2.96502400	-5.29580600	-0.21789000
H	-6.11156100	-2.37273800	-0.24728300
N	-5.07427600	0.80026800	-0.15635200
H	-5.39413600	-4.75053900	-0.29296400

E(M06-2X-D3/6-31G(d,p)) =   -1537.29331591   A.U.

Zero-point correction=   0.429156 (Hartree/Particle)
Thermal correction to Energy=   0.515971
Thermal correction to Enthalpy=   0.517660
Thermal correction to Gibbs Free Energy=   0.277487

E(M06-2X-D3/6-311+G(d,p)) =   -1537.65810290   A.U.

TS3-4

C	3.83640600	0.66780500	-2.53240700
C	4.25734400	1.98400200	-2.37704500
C	3.52373400	2.85388200	-1.57866200
C	2.36330800	2.39852500	-0.94944300
C	1.92699100	1.07236000	-1.11321300
C	2.67858500	0.21057500	-1.90371800
H	4.41066800	-0.01694400	-3.14755100
H	5.15788700	2.33485100	-2.86936800
H	3.83972000	3.88118500	-1.43391300
H	2.34801300	-0.81594900	-2.02508100
C	1.65435800	3.29947300	-0.07771000
N	1.11865000	3.99491300	0.67952500
C	0.66481800	0.58943500	-0.43561700
N	0.36874200	-0.78400700	-0.76715200
N	0.80193300	0.63500300	1.10655900
C	1.96841000	0.03362700	1.69178400
C	2.87993000	0.86636700	2.34156200
C	2.19847300	-1.33953600	1.61633400
C	4.01836300	0.32486400	2.92657500
H	2.69393900	1.93732000	2.38222700
C	3.35051500	-1.86740900	2.19193800
H	1.49506400	-1.98904200	1.11013900
C	4.25937600	-1.04412900	2.84956400
H	4.72085300	0.97757400	3.43407200
H	3.53135300	-2.93501400	2.12581200
H	5.15133900	-1.46698500	3.29914400
H	-0.42874700	0.10685300	1.23869900
C	-0.71688600	-1.15888100	-0.18946800
C	-1.12094300	-2.58438300	-0.20510400
C	-2.26674600	-2.96970400	0.48897100
C	-0.37187600	-3.57119000	-0.88127000
C	-2.68769600	-4.29538300	0.49446900
H	-2.82951900	-2.20640500	1.00900300
C	-0.80275200	-4.90112700	-0.87229700
C	-1.95977000	-5.26178500	-0.19059600
H	-3.59171700	-4.56437200	1.02995200
H	-0.21841200	-5.64417600	-1.40388400
H	-2.28561700	-6.29647300	-0.19585500
N	-1.49581900	-0.25454200	0.56447800
C	0.85418000	-3.31115900	-1.59619200
N	1.85008400	-3.24115800	-2.18285400
H	0.74312300	1.61518800	1.38573900
N	-0.46710800	1.46201000	-0.69076000

C	-1.51103700	0.99016300	-0.10196600
C	-2.72282700	1.84435100	-0.01487400
C	-2.54047400	3.22909700	-0.07702000
C	-4.02535700	1.34241000	0.14384800
C	-3.62138000	4.09679300	0.01472800
H	-1.52921200	3.60791400	-0.18322300
C	-5.11162900	2.22172800	0.23140400
C	-4.35286400	-0.06044400	0.17295100
C	-4.91041300	3.59376600	0.17082900
H	-3.45441900	5.16779900	-0.02827200
H	-6.10891200	1.81069300	0.34261100
N	-4.77078800	-1.14006700	0.18366000
H	-5.75811700	4.26637000	0.24541200

E(M06-2X-D3/6-31G(d,p)) =   -1537.24694155   A.U.

Zero-point correction=	0.424987 (Hartree/Particle)
Thermal correction to Energy=	0.510186
Thermal correction to Enthalpy=	0.511874
Thermal correction to Gibbs Free Energy=	0.274114

E(M06-2X-D3/6-311+G(d,p)) =   -1537.60979066   A.U.

Triazine

C	-2.72927500	4.19513300	0.00123900
C	-4.07353500	3.83768400	0.00089000
C	-4.42842800	2.49469100	0.00043300
C	-3.44469000	1.49970100	0.00023400
C	-2.08142100	1.85805700	0.00063900
C	-1.74466600	3.21410400	0.00102300
H	-2.43801200	5.23994600	0.00169200
H	-4.84685900	4.59829600	0.00097900
H	-5.47109400	2.19666800	0.00000400
H	-0.69671200	3.49323100	0.00131100
C	-3.94271200	0.14619400	-0.00051500
N	-4.48650500	-0.87587000	-0.00142300
C	-0.98153500	0.85906100	0.00033700
N	0.27109700	1.33398500	0.00034600
C	1.23494100	0.42082500	-0.00026200
C	2.65015700	0.87377800	-0.00046400
C	3.65558200	-0.09643300	-0.00072000
C	3.02184600	2.23349300	-0.00036400
C	4.99761600	0.26522700	-0.00085100

H	3.37259000	-1.14323400	-0.00092600
C	4.37543600	2.58748700	-0.00045400
C	5.36051500	1.60801900	-0.00061700
H	5.75665700	-0.50951400	-0.00112400
H	4.63948400	3.63925100	-0.00055500
H	6.40605900	1.89706100	-0.00064400
N	1.01991600	-0.90144600	-0.00025600
C	2.09909000	3.34187700	-0.00024800
N	1.48439700	4.32297200	-0.00107700
N	-1.29044700	-0.43214400	-0.00010800
C	-0.25280900	-1.27941300	-0.00034200
C	-0.56819100	-2.73142600	-0.00031900
C	-1.91123200	-3.11679200	-0.00156600
C	0.42322100	-3.73334700	0.00076300
C	-2.26907800	-4.45986700	-0.00157300
H	-2.67611300	-2.34812000	-0.00239000
C	0.05288800	-5.08257900	0.00085700
C	1.84452700	-3.48867800	0.00184600
C	-1.28789600	-5.44581500	-0.00039600
H	-3.31961900	-4.72983200	-0.00238700
H	0.83180200	-5.83696900	0.00163000
N	3.00161200	-3.44849500	0.00327800
H	-1.56078700	-6.49567300	-0.00035000

E(M06-2X-D3/6-31G(d,p)) =   -1249.81769575   A.U.

Zero-point correction=	0.307312 (Hartree/Particle)
Thermal correction to Energy=	0.372655
Thermal correction to Enthalpy=	0.374343
Thermal correction to Gibbs Free Energy=	0.182187

E(M06-2X-D3/6-311+G(d,p)) =   -1250.11041585   A.U.

TS2-4

C	3.52265600	-4.12565200	0.32814400
C	2.27348100	-4.74845900	0.21240100
C	1.10765700	-4.00367500	0.05655700
C	1.21908500	-2.62243900	0.01357500
C	2.46397000	-2.00366700	0.12617800
C	3.63354300	-2.73905100	0.28868600
H	4.41389100	-4.73131200	0.45285600
H	2.21880000	-5.83182300	0.24840400
H	0.13023300	-4.46685100	-0.02932800

H	4.60816800	-2.26854100	0.39013200
C	0.15345900	-1.58761200	-0.12548100
N	-1.07802500	-1.65471500	-0.20818400
C	2.22667600	-0.54777200	0.04070200
N	0.95541900	-0.32062300	-0.10941800
H	0.38446900	0.55465300	-0.18703500
N	-1.18076500	1.15584000	-0.12056300
C	-1.92533100	0.23624600	-0.16171100
C	-3.35273400	-0.10333600	-0.16598800
C	-3.85503900	-1.36162800	-0.49331000
C	-4.26075800	0.93017600	0.14809400
C	-5.22802500	-1.58725900	-0.51617900
H	-3.14613900	-2.14831200	-0.71087000
C	-5.63732200	0.69058400	0.13105200
C	-6.12137700	-0.56734700	-0.20425800
H	-5.60036800	-2.57249300	-0.77759400
H	-6.31383000	1.50016900	0.38208200
H	-7.19085800	-0.74828900	-0.21873900
C	-3.82673600	2.25641300	0.50809600
N	-3.57625100	3.34353700	0.81529400
N	3.21010100	0.36017900	0.10784100
H	4.15039400	-0.00834600	0.12031000
C	3.08670900	1.77238500	0.01256500
C	1.97220300	2.44998200	0.50700200
C	4.13851100	2.47635100	-0.57562100
C	1.90523900	3.83354400	0.37183100
H	1.16169000	1.92813000	1.00120200
C	4.06888700	3.85924400	-0.68215400
H	5.00031300	1.93748600	-0.96020700
C	2.94694700	4.54198800	-0.21784900
H	1.02519400	4.35081800	0.73842000
H	4.88855200	4.40076800	-1.14247200
H	2.88591500	5.62032400	-0.31596600

E(M06-2X-D3/6-31G(d,p)) =   -1120.60871236   A.U.

Zero-point correction=   0.322145 (Hartree/Particle)
Thermal correction to Energy=   0.385342
Thermal correction to Enthalpy=   0.387031
Thermal correction to Gibbs Free Energy=   0.196924

E(M06-2X-D3/6-311+G(d,p)) =   -1120.87546184   A.U.

INT2-4

C	-5.13131100	-0.61639100	-0.52383200
C	-5.16190800	0.73117400	-0.16089200
C	-3.99750600	1.39981300	0.22716200
C	-2.82039500	0.67528000	0.23643100
C	-2.78693000	-0.66970300	-0.12572600
C	-3.93586400	-1.34076000	-0.51107500
H	-6.05114600	-1.11031100	-0.81886200
H	-6.10668600	1.26443100	-0.17952400
H	-4.00557400	2.44598100	0.51466700
H	-3.93305900	-2.39016100	-0.79358600
C	-1.41857500	1.03774400	0.58156000
N	-1.04413400	2.19785000	0.95861100
C	-1.35421700	-1.06099800	0.02385900
N	-0.59082000	-0.08138600	0.42982400
H	0.11116600	2.31885200	3.09777700
N	0.84374600	2.42976200	2.39272300
C	0.33779400	2.34061200	1.23401400
C	1.21658500	2.47126300	0.03515900
C	0.79605300	3.22396900	-1.06013800
C	2.47374000	1.85024900	-0.01286500
C	1.62009200	3.38923600	-2.16846300
H	-0.18502100	3.68639100	-1.02606400
C	3.29534100	2.00660600	-1.13370300
C	2.87274200	2.78311600	-2.20501400
H	1.28298300	3.99098800	-3.00617200
H	4.25689900	1.50542600	-1.15592000
H	3.51641300	2.90446900	-3.06963000
C	2.93907500	0.97331000	1.03249100
N	3.38177200	0.21315100	1.78479200
N	-0.94713900	-2.31175500	-0.24681700
H	-1.65812500	-2.93903500	-0.59418400
C	0.35014600	-2.86721400	-0.14826300
C	1.40192100	-2.22596400	0.51048000
C	0.54452600	-4.12444400	-0.72863100
C	2.64271100	-2.85317200	0.57027300
H	1.25668500	-1.25709500	0.96655100
C	1.78749500	-4.73787300	-0.65645400
H	-0.27860100	-4.61736600	-1.24079200
C	2.84467000	-4.10289800	-0.00798700
H	3.44829200	-2.33886800	1.08461600
H	1.92805300	-5.71335700	-1.11065700
H	3.81663900	-4.58143100	0.04752300

E(M06-2X-D3/6-31G(d,p)) =   -1120.68921687   A.U.

Zero-point correction=   0.326959 (Hartree/Particle)
Thermal correction to Energy=   0.389707
Thermal correction to Enthalpy=   0.391395
Thermal correction to Gibbs Free Energy=   0.201707

E(M06-2X-D3/6-311+G(d,p)) =   -1120.95512225   A.U.

TS1-5

C	-3.56599200	-1.96172800	0.15247800
C	-2.18475800	-1.78909000	0.16214500
C	-1.69218300	-0.49227000	0.05510300
C	-2.55332200	0.61208300	-0.04915900
C	-3.92988100	0.43355200	-0.06047500
C	-4.42616800	-0.86346000	0.04003100
N	-0.33660700	1.31449100	-0.02758500
C	-0.29479200	0.01740700	0.02570000
H	-3.98159600	-2.96018000	0.23669400
H	-1.53085600	-2.65180700	0.26092000
H	-4.58882100	1.29124400	-0.14392400
H	-5.49848000	-1.03042900	0.03374000
C	-1.71306600	1.82782400	-0.14098300
C	2.14101200	-0.46029900	0.03421300
C	2.59498900	0.80103800	0.42461100
C	3.05561900	-1.44171000	-0.35706400
C	3.96050400	1.06817200	0.40311100
H	1.89645600	1.55731400	0.75574500
C	4.41527400	-1.16241400	-0.36543600
H	2.69623600	-2.42075100	-0.66322400
C	4.87561100	0.09736800	0.00970600
H	4.30718400	2.05029400	0.70718000
H	5.11535900	-1.93197800	-0.67354200
H	5.93716100	0.31823600	-0.00259200
N	0.77460400	-0.80651900	0.04541400
H	0.56760900	-1.79172900	-0.03008000
N	-1.69956800	3.05980400	-0.33963800
H	-0.18632000	2.47651100	-0.23214400

E(M06-2X-D3/6-31G(d,p)) =   -703.982225528   A.U.

Zero-point correction=   0.217079 (Hartree/Particle)
Thermal correction to Energy=   0.256298

Thermal correction to Enthalpy=   0.257986
Thermal correction to Gibbs Free Energy=   0.124886

E(M06-2X-D3/6-311+G(d,p)) =   -704.149778577   A.U.

TS1-5H

C	-5.09172500	0.51204600	0.88938900
C	-3.85300900	1.14036500	0.79519700
C	-2.81675200	0.43287000	0.19576300
C	-2.99839000	-0.86458900	-0.28815200
C	-4.23117500	-1.49180800	-0.19089500
C	-5.27669000	-0.78696000	0.40069900
N	-0.79892300	-0.20144400	-0.64478500
C	-1.40381600	0.78834900	-0.05972500
H	-5.92335000	1.03302800	1.35157800
H	-3.71950200	2.14453200	1.18883700
H	-4.35450100	-2.50115000	-0.56913000
H	-6.25399300	-1.25023300	0.49136600
C	-1.71192200	-1.36336700	-0.84272900
N	-1.33848800	-2.44071400	-1.33983000
H	0.19785500	-0.43157700	-1.06784600
N	1.09297100	-1.59177800	-1.61023500
H	1.53549300	-1.49516100	-2.51860900
H	-0.04358200	-2.20004800	-1.57149400
C	2.00812900	-1.86270700	-0.60113700
C	3.39581300	-1.69439600	-0.76057000
C	1.53596800	-2.24885100	0.66998000
C	4.26676400	-1.88754900	0.30580100
H	3.78100900	-1.40058400	-1.73407300
C	2.41558500	-2.43028800	1.73036100
H	0.47014600	-2.41696200	0.80165300
C	3.78735900	-2.24670600	1.56408300
H	5.33387000	-1.75318400	0.14993600
H	2.02313900	-2.72821500	2.69856100
H	4.47016600	-2.39317600	2.39378000
C	0.50219500	2.33737300	0.11192900
C	0.79724600	3.64665200	-0.26587000
C	1.52588500	1.42003200	0.35128900
C	2.12357300	4.03610000	-0.41294800
H	-0.00927700	4.34967400	-0.45456500
C	2.84845300	1.81641200	0.18059800
H	1.30777300	0.40955700	0.68205400
C	3.15172000	3.12066000	-0.20012600

H	2.35136100	5.05573900	-0.70572700
H	3.63339900	1.08771200	0.35592500
H	4.18496000	3.42542700	-0.32717200
N	-0.86143000	1.96876200	0.27813100
H	-1.49515700	2.67901200	0.61433000

E(M06-2X-D3/6-31G(d,p)) =   -991.535552214   A.U.

Zero-point correction=   0.336469 (Hartree/Particle)
Thermal correction to Energy=   0.395269
Thermal correction to Enthalpy=   0.396957
Thermal correction to Gibbs Free Energy=   0.220395

E(M06-2X-D3/6-311+G(d,p)) =   -991.770486809   A.U.

INT1-5

C	-3.52977700	-2.01505400	-0.00011200
C	-2.14291100	-1.84796500	-0.00011700
C	-1.65558500	-0.54958200	-0.00009000
C	-2.51374600	0.54596400	-0.00004100
C	-3.88788500	0.39023600	0.00003000
C	-4.38872100	-0.91350200	-0.00002400
N	-0.29006400	1.34980000	0.00023700
C	-0.28961300	0.04894100	0.00002000
H	-3.94665400	-3.01682600	-0.00016900
H	-1.49176900	-2.71823500	-0.00025300
H	-4.53959200	1.25745100	0.00005700
H	-5.46131800	-1.07823600	0.00001200
C	-1.64634500	1.75708200	0.00003900
C	2.16620600	-0.40624900	-0.00004800
C	2.62229100	0.91544200	-0.00034300
C	3.08617100	-1.46093200	0.00024000
C	3.99361000	1.15561800	-0.00031100
H	1.90848300	1.72680100	-0.00052600
C	4.44924400	-1.20165400	0.00025300
H	2.72795100	-2.48769800	0.00043000
C	4.91266100	0.11177300	-0.00000700
H	4.34271900	2.18332400	-0.00052000
H	5.14938100	-2.03067600	0.00047700
H	5.97761300	0.31697100	0.00006200
N	0.80133000	-0.75054700	-0.00003000
H	0.61051900	-1.74157600	0.00030000
N	-2.08801800	2.94597500	0.00020800

| H | -1.29367700 | 3.59139200 | 0.00030000 |

E(M06-2X-D3/6-31G(d,p)) =   -704.094939996   A.U.

Zero-point correction=	0.223964 (Hartree/Particle)
Thermal correction to Energy=	0.263019
Thermal correction to Enthalpy=	0.264708
Thermal correction to Gibbs Free Energy=	0.133287

E(M06-2X-D3/6-311+G(d,p)) =   -704.262018635   A.U.

TS2-5

C	-0.36218100	3.73241000	-0.44336300
C	0.83037600	3.02628500	-0.27185500
C	0.76142500	1.64480000	-0.24034200
C	-0.45304200	0.95822200	-0.35974200
C	-1.63369900	1.65943800	-0.56283600
C	-1.56999800	3.05549700	-0.59689500
N	1.29984800	-0.62166600	-0.21356800
C	1.79668500	0.58466600	-0.15345500
H	-0.34583500	4.81658300	-0.47208700
H	1.77101800	3.56202600	-0.17669300
H	-2.58299200	1.15997000	-0.70805700
H	-2.48270100	3.62114700	-0.75158300
C	-0.08005000	-0.48182300	-0.29065400
H	-0.68403200	-2.54103900	-0.93485700
N	3.10046900	0.89637400	-0.03878700
H	3.30823700	1.88342600	0.00533200
C	4.22585000	0.04973600	0.03786500
C	5.47609000	0.67273900	0.11595000
C	4.13597000	-1.34510700	0.04010700
C	6.63230100	-0.08975100	0.19468200
H	5.53925000	1.75837200	0.11431900
C	5.30750100	-2.09277200	0.11914000
H	3.16808000	-1.82264400	-0.01852800
C	6.55403800	-1.48036500	0.19554800
H	7.59559900	0.40589300	0.25556700
H	5.23505700	-3.17547100	0.12086100
H	7.45663500	-2.07869600	0.25515700
N	-0.81506900	-1.54747200	-0.27562100
C	-2.18903500	-1.82322900	-0.76700300
N	-2.05990700	-2.78280500	-1.55775800
C	-3.41120500	-1.14260900	-0.27940500

C	-4.52298900	-1.15258600	-1.12638400
C	-3.54156200	-0.55653200	0.99259800
C	-5.72255900	-0.57314100	-0.73606100
H	-4.41002200	-1.63495900	-2.09169500
C	-4.75656000	0.01996600	1.38645600
C	-2.44899400	-0.50728200	1.92977300
C	-5.84153800	0.01718100	0.52261400
H	-6.57085200	-0.58408100	-1.41253200
H	-4.83236800	0.46299900	2.37351800
N	-1.59783900	-0.42379200	2.70988000
H	-6.77855200	0.46754000	0.83184300

E(M06-2X-D3/6-31G(d,p)) =   -1120.58957470   A.U.

Zero-point correction=   0.320690 (Hartree/Particle)
Thermal correction to Energy=   0.383352
Thermal correction to Enthalpy=   0.385041
Thermal correction to Gibbs Free Energy=   0.197844

E(M06-2X-D3/6-311+G(d,p)) =   -1120.85495607   A.U.

INT2-5

C	0.01188300	3.99483300	-0.66930700
C	-1.07010700	3.11214400	-0.61390100
C	-0.85063800	1.86419800	-0.05797400
C	0.39868200	1.48519700	0.43171900
C	1.47581000	2.35668500	0.37830200
C	1.26197700	3.62097700	-0.18121900
N	-1.10647300	-0.32278500	0.72730900
C	-1.72310900	0.67849900	0.16866700
H	-0.12290600	4.98177200	-1.09920300
H	-2.03827700	3.41451500	-1.00404400
H	2.45121900	2.08306200	0.76443300
H	2.08645100	4.32422400	-0.23448300
C	0.22538500	0.06311700	0.89437100
H	2.12807400	0.39688600	3.16363500
N	-3.02276400	0.71004400	-0.18190100
H	-3.33627400	1.56854400	-0.61046600
C	-4.00645900	-0.29389100	-0.07257700
C	-5.29776000	0.04345500	-0.49194800
C	-3.74189400	-1.57521200	0.41969500
C	-6.32175300	-0.89003000	-0.42266100
H	-5.49633100	1.04195200	-0.87443600

C	-4.78259000	-2.49765800	0.48171900
H	-2.74156000	-1.83117100	0.73995800
C	-6.06900300	-2.16926500	0.06644400
H	-7.31834700	-0.61474400	-0.75182700
H	-4.57488600	-3.49235900	0.86294700
H	-6.86735100	-2.90135200	0.12297800
N	1.09960200	-0.76925100	1.30311900
C	2.42974500	-0.40264300	1.48879100
N	2.89621500	0.17899700	2.52508900
C	3.40208600	-0.87438200	0.44697400
C	4.72647000	-1.07096500	0.84528800
C	3.06782000	-1.11676700	-0.89794200
C	5.69205400	-1.50856500	-0.05124700
H	4.97056000	-0.86916200	1.88198100
C	4.04654900	-1.55450000	-1.80092900
C	1.75868200	-0.89110400	-1.46131600
C	5.35190000	-1.75615900	-1.37936300
H	6.71136800	-1.66064200	0.28824700
H	3.76385600	-1.72851900	-2.83337300
N	0.75779500	-0.69952600	-2.01093200
H	6.09939600	-2.10315100	-2.08465300

E(M06-2X-D3/6-31G(d,p)) =   -1120.68467387   A.U.

Zero-point correction=	0.326702 (Hartree/Particle)
Thermal correction to Energy=	0.389427
Thermal correction to Enthalpy=	0.391116
Thermal correction to Gibbs Free Energy=	0.204264

E(M06-2X-D3/6-311+G(d,p)) =   -1120.95008162   A.U.

TS2-6

C	-4.61587200	1.39433400	-1.22065400
C	-3.22734900	1.48927200	-1.21350400
C	-2.53044700	0.65484100	-0.34789200
C	-3.18899100	-0.23441100	0.49925600
C	-4.57224600	-0.31618100	0.50974100
C	-5.27793300	0.50360000	-0.36832500
N	-0.87096300	-0.44309100	0.77494700
C	-1.08692000	0.52595800	-0.07903200
H	-5.19300200	2.02042400	-1.89239000
H	-2.72617400	2.18986600	-1.87575800
H	-5.06906000	-1.00363700	1.18582700

H	-6.36180500	0.45626600	-0.39214600
C	-2.19520500	-0.94598100	1.33589100
N	-2.25727500	-1.69666900	2.31679700
H	-1.01320300	-1.81922700	2.57054200
N	-0.17031300	1.34261600	-0.62220400
H	-0.49260400	1.91308300	-1.39166900
N	0.29386800	-1.80054300	2.30998500
C	0.33502100	-1.19361300	1.22505400
C	1.46121100	-1.27491700	0.23564500
C	1.30843700	-1.47752500	-1.14703300
C	2.75620600	-1.24086000	0.75746000
C	2.43099200	-1.60966500	-1.97831900
C	3.86592000	-1.36031200	-0.06625100
H	2.85867400	-1.12263000	1.83109800
C	3.70655900	-1.53983300	-1.44115000
H	2.28177300	-1.77725400	-3.03984200
H	4.86172600	-1.31468900	0.36323900
H	4.57206200	-1.63726400	-2.08775900
C	0.01418400	-1.56783500	-1.77331100
N	-1.00767400	-1.61708600	-2.31686300
C	1.11626000	1.64628600	-0.08851900
C	2.18564200	1.81965200	-0.96271800
C	1.28559300	1.79281800	1.28800300
C	3.44031900	2.13322600	-0.45263400
H	2.03616500	1.67606700	-2.02873200
C	2.54839800	2.09126700	1.78642600
H	0.44363300	1.65540200	1.95882200
C	3.62632400	2.26302800	0.92146800
H	4.27660000	2.25796800	-1.13245300
H	2.68613300	2.19381400	2.85759300
H	4.60897300	2.49632100	1.31740200

E(M06-2X-D3/6-31G(d,p)) =   -1120.61109536   A.U.

Zero-point correction=   0.319600 (Hartree/Particle)
Thermal correction to Energy=   0.382051
Thermal correction to Enthalpy=   0.383740
Thermal correction to Gibbs Free Energy=   0.201004

E(M06-2X-D3/6-311+G(d,p)) =   -1120.87901930   A.U.

INT2-6
C	4.30348300	2.03812500	0.81536500

C	2.95280600	1.86326400	0.53033300
C	2.47462600	0.66247100	0.00449000
C	3.39014800	-0.37607900	-0.24839800
C	4.74401600	-0.19800300	0.04739000
C	5.20000800	1.00251600	0.57979200
N	0.70395200	-0.27867300	-1.26366600
C	1.02137500	0.50006900	-0.29817500
H	4.65270600	2.98487700	1.21338800
H	2.25932700	2.68325600	0.68665200
H	5.43100600	-1.01488500	-0.14362000
H	6.25415500	1.12728100	0.80252800
C	3.02036800	-1.65498600	-0.80461400
N	2.86681500	-2.71295500	-1.24656500
H	-0.24446300	-0.40970900	-3.40024300
N	0.19016400	1.23570100	0.52033200
H	0.55742700	1.43835300	1.43993200
N	-0.98792700	-0.76562600	-2.79510200
C	-0.57964100	-0.71976300	-1.58794000
C	-1.51951000	-1.22364200	-0.52567700
C	-1.14380600	-1.70407500	0.74126900
C	-2.88329200	-1.17882000	-0.83125100
C	-2.11878800	-2.11318300	1.66367700
C	-3.84524900	-1.57457400	0.08678700
H	-3.16305400	-0.81272900	-1.81193800
C	-3.46499000	-2.04205100	1.34296500
H	-1.79629700	-2.48519100	2.63019300
H	-4.89597900	-1.51538400	-0.17794600
H	-4.21063500	-2.35468700	2.06619400
C	0.21560400	-1.79119800	1.21209300
N	1.26089800	-1.85650800	1.70681200
C	-1.15040100	1.60976600	0.27583900
C	-2.07331400	1.56126400	1.32156800
C	-1.54572700	2.04991800	-0.98859900
C	-3.39140900	1.94064200	1.09851800
H	-1.75785400	1.19668700	2.29527700
C	-2.87218900	2.40440600	-1.20642900
H	-0.81930000	2.09326600	-1.79369700
C	-3.79883700	2.35332400	-0.16806600
H	-4.10546000	1.89395800	1.91432500
H	-3.17911600	2.73041300	-2.19472600
H	-4.83146400	2.63456700	-0.34462200

E(M06-2X-D3/6-31G(d,p)) =   -1120.67103116   A.U.

Zero-point correction=   0.324613 (Hartree/Particle)
Thermal correction to Energy=   0.388751
Thermal correction to Enthalpy=   0.390439
Thermal correction to Gibbs Free Energy=   0.203710

E(M06-2X-D3/6-311+G(d,p)) =   -1120.94072731   A.U.

INT1-6

C	1.33364700	2.58914300	-0.44731200
C	0.47433100	1.48815800	-0.42833700
C	1.03166700	0.24244100	-0.16374900
C	2.40480500	0.10403300	0.03931900
C	3.26115800	1.18971400	0.02216400
C	2.70343300	2.44674100	-0.21706500
N	1.44695800	-2.05175700	0.08061900
C	0.51758500	-1.16119100	-0.10463700
H	0.92617700	3.57490700	-0.64726200
H	-0.58530900	1.61656200	-0.61678500
H	4.32552700	1.05019800	0.17971700
H	3.34065700	3.32503700	-0.23649400
C	2.66974700	-1.35271000	0.19391500
C	-1.92759400	-0.75321700	-0.07571400
C	-3.02235100	-0.88891600	-0.93045400
C	-2.00219200	0.11004000	1.02023300
C	-4.18084200	-0.15653300	-0.69584000
H	-2.95054100	-1.56097300	-1.78003800
C	-3.15372000	0.86082400	1.23006600
H	-1.15907000	0.18598700	1.69976000
C	-4.24716800	0.72805000	0.37774000
H	-5.02877000	-0.26809600	-1.36366400
H	-3.20227200	1.53630300	2.07791800
H	-5.14844400	1.30549700	0.55364600
N	-0.77170000	-1.53427100	-0.31335300
H	-0.89317100	-2.53709000	-0.38208200
N	3.82035500	-1.84843700	0.39552300
H	3.73088600	-2.86653200	0.45377900

E(M06-2X-D3/6-31G(d,p)) =   -704.090955082   A.U.

Zero-point correction=   0.223755 (Hartree/Particle)
Thermal correction to Energy=   0.262795
Thermal correction to Enthalpy=   0.264483
Thermal correction to Gibbs Free Energy=   0.131755

E(M06-2X-D3/6-311+G(d,p)) =   -704.258691275   A.U.

TS1-7

C	1.97831100	2.60236200	-0.32560300
C	0.89516400	1.72683700	-0.24185000
C	1.17527800	0.37864300	-0.05855200
C	2.49545700	-0.08836600	0.01731600
C	3.56928400	0.77927900	-0.06417300
C	3.29255900	2.13753500	-0.23154400
N	1.13321900	-1.93748300	0.15575000
C	0.35884200	-0.84515000	0.03184700
H	1.79641600	3.66230200	-0.46852400
H	-0.12372100	2.08856900	-0.32616800
H	4.58301300	0.39759500	-0.00478900
H	4.11097700	2.84728100	-0.29840200
C	2.48161600	-1.58224300	0.14839600
C	-2.07595200	-0.58552700	0.01585800
C	-3.18995300	-1.11027600	-0.64692000
C	-2.20497500	0.60467200	0.74292000
C	-4.40372000	-0.43562900	-0.60957800
H	-3.08094500	-2.04221100	-1.19165100
C	-3.42087200	1.27847500	0.76460000
H	-1.35726300	0.97543800	1.31173600
C	-4.52420400	0.76483600	0.08772800
H	-5.26107600	-0.84941800	-1.13086600
H	-3.50985400	2.20071300	1.33021500
H	-5.47324800	1.28939000	0.11358200
N	-0.87234500	-1.29255400	-0.03059900
H	-0.10480500	-2.42223200	0.09304100
N	3.53497000	-2.28761900	0.22998300
H	3.28858900	-3.27652000	0.30322400

E(M06-2X-D3/6-31G(d,p)) =   -704.019608320   A.U.

Zero-point correction=   0.218014 (Hartree/Particle)
Thermal correction to Energy=   0.256553
Thermal correction to Enthalpy=   0.258242
Thermal correction to Gibbs Free Energy=   0.127816

E(M06-2X-D3/6-311+G(d,p)) =   -704.184919874   A.U.

TS1-7H

C	-4.00420900	-0.99290200	1.14444600
C	-2.94647900	-0.23109000	0.64475400
C	-1.88523600	-0.91012900	0.05201100
C	-1.88170500	-2.30301000	-0.00864900
C	-2.92716200	-3.06402100	0.48359800
C	-4.00139700	-2.38719400	1.06038400
N	0.13641600	-1.58115000	-0.91575700
C	-0.57881800	-0.48833500	-0.55237000
H	-4.84491100	-0.48908300	1.61060100
H	-2.96404100	0.84914000	0.72712800
H	-2.88849700	-4.14648300	0.42042200
H	-4.84239800	-2.94664900	1.45828900
C	-0.59508000	-2.72914100	-0.62385800
C	-0.82320000	1.87634700	-0.42021800
C	-0.43598700	2.70168000	0.63921600
C	-1.90878200	2.25377500	-1.21917700
C	-1.14435500	3.86614400	0.91663800
H	0.41694800	2.40632600	1.24280700
C	-2.61492700	3.41819300	-0.93619900
H	-2.19453600	1.61579800	-2.05021400
C	-2.23899300	4.22722600	0.13427300
H	-0.84153300	4.49254800	1.74986900
H	-3.46172100	3.69578600	-1.55622400
H	-2.79075200	5.13539600	0.35284800
N	-0.07990700	0.71493200	-0.70485100
N	-0.28688100	-3.95157900	-0.81110400
H	0.64225400	-4.00463800	-1.23526700
H	1.30768000	0.51979800	-1.24292800
N	2.17987200	-0.17493600	-1.50237300
H	2.53098200	-0.04776800	-2.44760300
H	1.49227900	-1.06838100	-1.38839400
C	3.20889700	-0.12400700	-0.50129000
C	4.52078000	0.19882900	-0.83097300
C	2.85008000	-0.38699300	0.82039900
C	5.48521800	0.25825600	0.17098900
H	4.78676400	0.40432100	-1.86438200
C	3.82170500	-0.32372100	1.81286300
H	1.82176000	-0.64787100	1.05192900
C	5.13884100	-0.00069900	1.49344300
H	6.50910000	0.50888900	-0.08614900
H	3.54683100	-0.53128300	2.84176500
H	5.89215100	0.04803400	2.27242500

E(M06-2X-D3/6-31G(d,p)) =   -991.569884717   A.U.

Zero-point correction=   0.339234 (Hartree/Particle)
Thermal correction to Energy=   0.397055
Thermal correction to Enthalpy=   0.398743
Thermal correction to Gibbs Free Energy=   0.222844

E(M06-2X-D3/6-311+G(d,p)) =   -991.805059177   A.U.

INT1-7

C	0.94176300	2.62262600	0.00006900
C	0.20255900	1.43940400	-0.00003000
C	0.90677800	0.23834300	-0.00007200
C	2.30278400	0.23642900	0.00000100
C	3.04138800	1.40745900	0.00013500
C	2.33902200	2.61078900	0.00016600
C	0.45989300	-1.18701100	-0.00012000
H	0.41743100	3.57264400	0.00008200
H	-0.88069400	1.46551700	-0.00015400
H	4.12539500	1.36687800	0.00019800
H	2.88068600	3.55113200	0.00026400
C	2.79210500	-1.16330700	-0.00003500
C	-1.83671100	-0.94344700	-0.00000300
C	-2.42739900	-0.56112900	1.20766500
C	-2.42712600	-0.56075700	-1.20766200
C	-3.57527700	0.22491700	1.20314600
H	-1.96922600	-0.87831100	2.13905000
C	-3.57502100	0.22531700	-1.20315800
H	-1.96872700	-0.87759200	-2.13905300
C	-4.15131400	0.62649900	-0.00002100
H	-4.02036700	0.52660700	2.14629900
H	-4.01986700	0.52727900	-2.14634100
H	-5.04609400	1.23976500	-0.00000100
N	-0.67936200	-1.74945000	0.00000700
N	4.01552800	-1.50299200	0.00005000
H	4.12433800	-2.51830400	0.00001300
N	1.63399100	-1.93718100	-0.00016700
H	1.60535000	-2.94506500	-0.00006700

E(M06-2X-D3/6-31G(d,p)) =   -704.098109580   A.U.

Zero-point correction=   0.223269 (Hartree/Particle)
Thermal correction to Energy=   0.262567

Thermal correction to Enthalpy=   0.264255
Thermal correction to Gibbs Free Energy=   0.131570

E(M06-2X-D3/6-311+G(d,p)) =   -704.265523245   A.U.

INT1-8

C	0.92514900	2.61431500	0.00338700
C	0.19652500	1.42420600	0.00219300
C	0.90729500	0.22782600	0.00044800
C	2.30492700	0.23177300	0.00031700
C	3.02946200	1.41245100	0.00137700
C	2.32089300	2.61260400	0.00286000
C	0.46243500	-1.20138100	-0.00107000
H	0.39345500	3.56008700	0.00471600
H	-0.88680300	1.44211100	0.00265100
H	4.11559000	1.40667700	0.00118300
H	2.85824700	3.55521400	0.00369500
C	2.79038500	-1.17660000	-0.00079700
C	-1.83475000	-0.94703700	-0.00081500
C	-2.42802300	-0.56721500	1.20667300
C	-2.42079900	-0.55635600	-1.20853500
C	-3.57114000	0.22584400	1.20222200
H	-1.97504400	-0.89202700	2.13795800
C	-3.56393800	0.23656800	-1.20395900
H	-1.96188300	-0.87256700	-2.13990200
C	-4.14106200	0.63675000	-0.00075900
H	-4.01768500	0.52525700	2.14545600
H	-4.00464600	0.54468000	-2.14713900
H	-5.03228300	1.25519500	-0.00070000
N	-0.68128800	-1.75652300	-0.00105600
N	3.95492400	-1.68246600	-0.00053100
H	4.65724300	-0.94331000	0.00057900
N	1.63346000	-1.94282500	-0.00255400
H	1.63998400	-2.95111200	-0.00076500

E(M06-2X-D3/6-31G(d,p)) =   -704.098488209   A.U.

Zero-point correction=   0.223301 (Hartree/Particle)
Thermal correction to Energy=   0.262560
Thermal correction to Enthalpy=   0.264248
Thermal correction to Gibbs Free Energy=   0.131657

E(M06-2X-D3/6-311+G(d,p)) =   -704.266071784   A.U.

TS2-7

C	2.76474400	2.97169300	-0.32347200
C	2.97457700	1.59866600	-0.17427900
C	1.85495100	0.77665000	-0.11851000
C	0.57372400	1.32789000	-0.21109500
C	0.35634200	2.68888800	-0.34561900
C	1.48067500	3.51218800	-0.40464500
C	1.68961900	-0.70102700	0.07206300
H	3.62310200	3.63376200	-0.36839200
H	3.97928900	1.19933700	-0.10068500
H	-0.64707100	3.10463300	-0.38272200
H	1.35542700	4.58476400	-0.50738300
C	-0.39113400	0.21179500	-0.10161700
C	3.89443200	-1.36016400	0.15336700
C	4.54547600	-1.33161200	-1.08268500
C	4.61905100	-1.13719200	1.32661600
C	5.90453800	-1.04189900	-1.14344400
H	3.97318800	-1.52766500	-1.98373700
C	5.97753300	-0.84503300	1.25463900
H	4.10346000	-1.18198400	2.28036300
C	6.62481200	-0.78976200	0.02222600
H	6.40181500	-1.01041100	-2.10785000
H	6.53205100	-0.65865600	2.16899400
H	7.68414500	-0.56186600	-0.02834300
N	2.51455800	-1.65107300	0.21508600
N	0.30716600	-0.92475500	0.08088900
N	-1.68318600	0.27187000	-0.16888900
H	-2.05707300	1.20406700	-0.30962000
C	-2.58067300	-1.15183700	0.07406300
N	-1.98328700	-2.18789400	0.23923600
H	-0.25021900	-1.80295300	0.19473300
C	-4.03842100	-0.84558500	-0.02480000
C	-4.69829200	0.37022500	0.23913000
C	-4.83178500	-1.94804100	-0.36695000
C	-6.09636000	0.46535400	0.14545600
C	-6.21148600	-1.85063800	-0.46427800
H	-4.31734900	-2.88563700	-0.54482900
C	-6.85239500	-0.63878100	-0.20882300
H	-6.57052600	1.41707800	0.35968800
H	-6.79153800	-2.72526100	-0.74006700
H	-7.93126500	-0.55653700	-0.28174900
C	-4.01761100	1.57965500	0.61873100

N	-3.48972800	2.57738800	0.88155700

E(M06-2X-D3/6-31G(d,p)) = -1120.64167715   A.U.

Zero-point correction=	0.322911 (Hartree/Particle)
Thermal correction to Energy=	0.385482
Thermal correction to Enthalpy=	0.387171
Thermal correction to Gibbs Free Energy=	0.198367

E(M06-2X-D3/6-311+G(d,p)) = -1120.90715695   A.U.

INT2-7

C	2.55322100	2.96087800	-0.23755900
C	2.87786100	1.60539500	-0.11934500
C	1.83214700	0.69249000	-0.06889300
C	0.50929400	1.13649400	-0.13111300
C	0.17588800	2.47670100	-0.23421200
C	1.22897700	3.39247800	-0.29208600
C	1.74382900	-0.80087300	0.10116300
H	3.35298200	3.69314100	-0.28016100
H	3.91402200	1.29222600	-0.06703500
H	-0.85532100	2.82104300	-0.24352600
H	1.01278300	4.45265500	-0.37087800
C	-0.31380400	-0.09273200	-0.01728200
C	3.99944000	-1.28929200	0.11607800
C	4.59181100	-1.13496400	-1.14114700
C	4.76422900	-1.10291800	1.27039100
C	5.92740000	-0.75989500	-1.23786600
H	3.99065000	-1.30348500	-2.02899800
C	6.09750000	-0.72089700	1.16244300
H	4.29727200	-1.24521500	2.23937700
C	6.68438400	-0.54275700	-0.08867400
H	6.37731900	-0.63372300	-2.21775100
H	6.68098500	-0.56190900	2.06402900
H	7.72519900	-0.24721200	-0.16676900
N	2.65027200	-1.68178200	0.21628900
N	0.37883900	-1.17651500	0.13315800
N	-1.67238200	-0.02809200	-0.07547800
H	-2.04945200	0.88730300	-0.26862100
C	-2.55659400	-1.10971900	0.08382500
N	-2.22038800	-2.31467300	0.28684100
H	-1.20340700	-2.41899300	0.31808900
C	-4.02677100	-0.79368200	-0.02122800

C	-4.63625300	0.46203700	0.17176700
C	-4.86091500	-1.87653500	-0.31375200
C	-6.02720600	0.61147600	0.07007000
C	-6.23659500	-1.72717500	-0.41706200
H	-4.38927900	-2.84275400	-0.44727800
C	-6.82734300	-0.47985300	-0.22537000
H	-6.46080300	1.59268600	0.22913700
H	-6.85119200	-2.59009500	-0.65090600
H	-7.90189400	-0.35762700	-0.30537100
C	-3.89971700	1.66019000	0.48027500
N	-3.31413500	2.63833000	0.68692300

E(M06-2X-D3/6-31G(d,p)) =   -1120.68807244   A.U.

Zero-point correction=   0.327041 (Hartree/Particle)
Thermal correction to Energy=   0.389668
Thermal correction to Enthalpy=   0.391356
Thermal correction to Gibbs Free Energy=   0.203943

E(M06-2X-D3/6-311+G(d,p)) =   -1120.95265091   A.U.

INT2-8

C	-2.84842400	2.93144700	0.76888900
C	-3.06199900	1.59582400	0.41363600
C	-1.94734000	0.80615800	0.16135600
C	-0.66316300	1.34625100	0.26276400
C	-0.44394100	2.66808200	0.61177900
C	-1.56353200	3.46251000	0.86715800
C	-1.74562600	-0.63164200	-0.23940700
H	-3.70338200	3.56753200	0.97317000
H	-4.06942500	1.20272400	0.34147300
H	0.55444300	3.09044000	0.68917600
H	-1.43185500	4.50299800	1.14471000
C	0.25094700	0.22575500	-0.07639300
C	-3.95845800	-1.27407000	-0.32922900
C	-4.59852100	-1.45979900	0.89931300
C	-4.69364600	-0.84620600	-1.43808200
C	-5.95466200	-1.17586400	1.02291700
H	-4.01890600	-1.81114400	1.74680600
C	-6.04915400	-0.56477700	-1.30303500
H	-4.18774900	-0.72556300	-2.39040100
C	-6.68455400	-0.72008400	-0.07275000
H	-6.44203200	-1.31059200	1.98350100

H	-6.61137400	-0.22119500	-2.16581500
H	-7.74178100	-0.49935600	0.02840400
N	-2.58422000	-1.55743800	-0.46100000
N	-0.35743500	-0.88116700	-0.35816400
N	1.60089900	0.39371200	-0.08961600
H	1.95164000	1.28034300	0.24210800
C	2.56340200	-0.61432400	-0.33383800
N	2.35080700	-1.83954100	-0.55389900
H	1.35304900	-2.06280700	-0.52650700
C	3.95992200	-0.08266700	-0.33600400
C	5.00339200	-0.81095800	0.25827700
C	4.25799000	1.12878500	-0.96013500
C	6.31170200	-0.31954000	0.22163200
C	5.56263400	1.61186700	-1.00171100
H	3.46263100	1.68104100	-1.45275100
C	6.59105200	0.88737900	-0.40828900
H	7.10037000	-0.89241900	0.69682600
H	5.77450800	2.54889400	-1.50570000
H	7.60974800	1.25836000	-0.43517700
C	4.77800700	-2.04696100	0.96615900
N	4.70479900	-3.01731700	1.59126900

E(M06-2X-D3/6-31G(d,p)) =   -1120.68100659   A.U.

Zero-point correction=   0.326553 (Hartree/Particle)
Thermal correction to Energy=   0.389391
Thermal correction to Enthalpy=   0.391080
Thermal correction to Gibbs Free Energy=   0.202923

E(M06-2X-D3/6-311+G(d,p)) =   -1120.94685121   A.U.

TS2-9
C	-3.03265400	3.06283200	0.04010500
C	-3.14053500	1.66824900	0.04061600
C	-1.96536100	0.92721900	0.03528000
C	-0.72639200	1.57316800	0.03466700
C	-0.61159300	2.95297800	0.03347100
C	-1.79251600	3.69834100	0.03515900
C	-1.64377000	-0.54464100	0.04716300
H	-3.93671800	3.66259500	0.04378800
H	-4.11556600	1.19495100	0.04510300
H	0.35092100	3.45776300	0.03380300
H	-1.74399400	4.78205200	0.03465100

C	0.26917100	0.47439000	0.04427200
C	-3.79762000	-1.36409100	0.00062900
C	-4.54669300	-1.35291800	1.18000600
C	-4.43849600	-1.22352300	-1.23342400
C	-5.92255600	-1.15519900	1.12146900
H	-4.03810400	-1.48528600	2.12922300
C	-5.81518500	-1.03111800	-1.28000800
H	-3.84459200	-1.25492400	-2.14111000
C	-6.56234300	-0.98719400	-0.10479000
H	-6.49777900	-1.13354200	2.04176200
H	-6.30498600	-0.91213600	-2.24138800
H	-7.63560800	-0.83515900	-0.14462400
N	-2.40238600	-1.56050900	0.04960800
N	-0.23305500	-0.70946700	0.05870200
N	1.61623300	0.74145200	0.03489900
H	1.89788300	1.71025200	0.02023400
C	2.61967300	-0.18878200	0.02434000
C	4.05392000	0.18892800	-0.00852700
N	2.52359300	-1.47443700	0.03761800
C	4.67210600	1.43522400	-0.03349300
C	4.80109600	-1.00174700	-0.01275500
C	3.83655600	-2.12327100	0.01812100
C	6.06286000	1.46816500	-0.06296600
H	4.10834100	2.36470400	-0.03095600
C	6.18857400	-0.96156800	-0.04240400
N	3.69112000	-3.36612800	0.03568400
C	6.80978900	0.28392600	-0.06729600
H	6.57595900	2.42368500	-0.08355200
H	6.76004000	-1.88351400	-0.04587300
H	7.89313000	0.34307200	-0.09108900
H	2.25433800	-2.64710600	0.05663300

E(M06-2X-D3/6-31G(d,p)) =   -1120.57981068   A.U.

Zero-point correction=   0.321343 (Hartree/Particle)
Thermal correction to Energy=   0.382734
Thermal correction to Enthalpy=   0.384423
Thermal correction to Gibbs Free Energy=   0.198825

E(M06-2X-D3/6-311+G(d,p)) =   -1120.84305644   A.U.

TS2-9H

C	-3.22762700	-3.66695400	1.07988500

C	-3.28957300	-2.40561500	0.47861200
C	-2.09106400	-1.77620200	0.16968000
C	-0.87231100	-2.40072400	0.44755500
C	-0.80355500	-3.64768400	1.04476600
C	-2.00823300	-4.27936600	1.36214000
C	-1.72422200	-0.47149400	-0.48478900
H	-4.15035800	-4.17867700	1.33241600
H	-4.24810900	-1.94574900	0.26797200
H	0.14219400	-4.13579300	1.26433900
H	-1.99401000	-5.25771700	1.83079900
C	0.16276400	-1.45080700	-0.03543400
C	-3.85251200	0.37811000	-0.78975300
C	-4.65555600	-0.06512700	-1.84294700
C	-4.44067600	0.79172500	0.40940700
C	-6.03514400	-0.13491600	-1.67689100
H	-4.18560200	-0.36500600	-2.77388800
C	-5.82144200	0.72428500	0.56205700
H	-3.80119700	1.14950600	1.21079000
C	-6.62368500	0.25324700	-0.47517600
H	-6.65360900	-0.49374400	-2.49359100
H	-6.27139300	1.03890600	1.49856700
H	-7.70003200	0.19938700	-0.35172300
N	-2.45400300	0.46055200	-0.94705100
N	-0.31695600	-0.37318300	-0.56560100
N	1.49174500	-1.73405400	0.09224800
H	1.74134000	-2.62088700	0.50376500
C	2.53046500	-0.88300700	-0.24235900
C	3.94857400	-1.27088200	-0.09769000
N	2.39008500	0.30593100	-0.68763200
C	4.56708700	-2.44298400	0.32713800
C	4.68592100	-0.15519700	-0.50104600
C	3.75746300	0.94413800	-0.90593100
H	1.47504500	1.19377400	-0.98772800
C	5.95855900	-2.47065900	0.34193500
H	4.00346600	-3.32064600	0.63546500
C	6.07307600	-0.18498000	-0.48504300
N	3.91601400	2.10291000	-1.31319600
N	1.17278100	2.36606500	-1.29257400
C	6.70103700	-1.35237500	-0.05921400
H	6.47515000	-3.36831200	0.66547600
H	6.63055200	0.69127400	-0.80058000
H	2.19839000	2.60363200	-1.50544000
H	0.55596100	2.42013200	-2.09746500
C	0.66518400	3.05544200	-0.14499800

H	7.78521500	-1.40378700	-0.03660900
C	-0.70806300	3.13362400	0.07706700
C	1.56756100	3.58318500	0.77739700
C	-1.17837500	3.76470000	1.22392200
H	-1.39441900	2.67822900	-0.63165200
C	1.08283300	4.20579500	1.92378400
H	2.63320700	3.50082800	0.58138100
C	-0.28761300	4.30274600	2.15040900
H	-2.24884000	3.83416200	1.39284900
H	1.78384100	4.62111700	2.64085600
H	-0.65969300	4.79366300	3.04374800

E(M06-2X-D3/6-31G(d,p)) =   -1408.13712108   A.U.

Zero-point correction=   0.442202 (Hartree/Particle)
Thermal correction to Energy=   0.523265
Thermal correction to Enthalpy=   0.524954
Thermal correction to Gibbs Free Energy=   0.293948

E(M06-2X-D3/6-311+G(d,p)) =   -1408.46828441   A.U.

INT2-9

C	-2.98650200	3.05408200	-0.04904600
C	-3.13420000	1.66326800	-0.05211100
C	-1.98123700	0.88827600	-0.04723200
C	-0.72355600	1.49518900	-0.04638100
C	-0.56990500	2.87131200	-0.04234500
C	-1.72815800	3.65207500	-0.04229300
C	-1.70046200	-0.59191100	-0.06543800
H	-3.87281300	3.67985800	-0.05214600
H	-4.12268400	1.21903600	-0.05805800
H	0.40647100	3.34923600	-0.04256100
H	-1.64693100	4.73392900	-0.03958500
C	0.24368700	0.36534300	-0.06172700
C	-3.87885600	-1.34971000	-0.00348400
C	-4.49824000	-1.17394700	1.23763200
C	-4.64750400	-1.34017900	-1.17069000
C	-5.86935400	-0.95097000	1.30283600
H	-3.89048500	-1.20305700	2.13622900
C	-6.01738600	-1.11019000	-1.09410600
H	-4.15678800	-1.49833200	-2.12537000
C	-6.63425900	-0.90908800	0.13893500
H	-6.34129100	-0.80628200	2.26970600

H	-6.60633500	-1.08958900	-2.00578800
H	-7.70321300	-0.73273400	0.19289700
N	-2.49162200	-1.58410600	-0.06966100
N	-0.29753400	-0.80132300	-0.08216500
N	1.59188700	0.62701200	-0.05024000
H	1.85147700	1.60171000	-0.03150600
C	2.63456200	-0.26707700	-0.03479000
C	4.03620300	0.23720900	0.00699300
N	2.52754500	-1.55068200	-0.05032500
C	4.61207200	1.49804600	0.03609000
C	4.81465200	-0.91746900	0.01747500
C	3.85785300	-2.05857900	-0.01901100
C	6.00667600	1.56727900	0.07662100
H	4.02371900	2.41216700	0.02911200
C	6.19557700	-0.85804400	0.05749900
N	4.19339000	-3.27930600	-0.02002400
C	6.78547200	0.40796600	0.08710000
H	6.49305300	2.53687300	0.10130800
H	6.78691500	-1.76746600	0.06560600
H	7.86648500	0.49676900	0.11958100
H	3.34394900	-3.85056400	-0.04768900

E(M06-2X-D3/6-31G(d,p)) =   -1120.68620009   A.U.

Zero-point correction=	0.328198 (Hartree/Particle)
Thermal correction to Energy=	0.389534
Thermal correction to Enthalpy=	0.391222
Thermal correction to Gibbs Free Energy=	0.207084

E(M06-2X-D3/6-311+G(d,p)) =   -1120.94932447   A.U.

INT2-10
C	-3.28378400	2.99768200	0.00018900
C	-3.18025700	1.60305600	-0.00002600
C	-1.90678100	1.04819700	-0.00002400
C	-0.77941300	1.87303200	0.00016600
C	-0.87332500	3.25425000	0.00038300
C	-2.15319900	3.81273000	0.00039600
C	-1.36810700	-0.35727900	-0.00024800
H	-4.26819100	3.45412700	0.00020300
H	-4.07260000	0.98864600	-0.00018500
H	0.00253000	3.89714400	0.00053900
H	-2.26858900	4.89135700	0.00056300

C	0.37905400	0.94172600	0.00002200
C	-3.37240100	-1.50012000	-0.00027900
C	-4.07206300	-1.53184200	1.20900400
C	-4.07236500	-1.53197500	-1.20938900
C	-5.46297600	-1.55257900	1.20348200
H	-3.51379100	-1.52526000	2.13948300
C	-5.46327500	-1.55269600	-1.20350800
H	-3.51432200	-1.52549600	-2.14000400
C	-6.16493200	-1.55562900	0.00007600
H	-6.00066700	-1.56465800	2.14642600
H	-6.00120800	-1.56486300	-2.14631200
H	-7.24952400	-1.57127100	0.00021100
N	-1.96269100	-1.47920900	-0.00043500
N	0.04499400	-0.30442700	-0.00025300
N	1.64386600	1.44044800	0.00023900
H	1.73183700	2.44950700	0.00005000
C	2.89774800	0.85444800	-0.00003300
C	3.28977100	-0.58894800	0.00020100
N	3.89556000	1.67635400	-0.00038000
C	2.62778800	-1.81138600	0.00044000
C	4.68951900	-0.53890900	0.00001200
C	5.07836600	0.90241500	-0.00039700
C	3.41020700	-2.97066500	0.00055000
H	1.54717200	-1.86042700	0.00048600
C	5.46122400	-1.68523300	0.00010200
N	6.22489300	1.44580500	-0.00074100
C	4.80202100	-2.91608800	0.00039200
H	2.91451300	-3.93594600	0.00075300
H	6.54658700	-1.63411000	-0.00007300
H	5.37738800	-3.83614200	0.00048100
H	6.94560700	0.71948500	-0.00068700

E(M06-2X-D3/6-31G(d,p)) =   -1120.68961985   A.U.

Zero-point correction=   0.328458 (Hartree/Particle)
Thermal correction to Energy=   0.389516
Thermal correction to Enthalpy=   0.391205
Thermal correction to Gibbs Free Energy=   0.207826

E(M06-2X-D3/6-311+G(d,p)) =   -1120.95202064   A.U.

TS2-11

C	-3.29114800	2.99968200	0.00003300

C	-3.19156300	1.60408600	-0.00001100
C	-1.91871600	1.04757600	-0.00002700
C	-0.79193100	1.87334400	-0.00000100
C	-0.87967000	3.25367900	0.00003900
C	-2.15901200	3.81378000	0.00005700
C	-1.37513300	-0.35765200	-0.00010100
H	-4.27502900	3.45772400	0.00004400
H	-4.08607300	0.99254100	-0.00002100
H	0.01053700	3.87423300	0.00006600
H	-2.27538800	4.89257500	0.00009300
C	0.36818600	0.95367000	-0.00006200
C	-3.37907400	-1.50304500	-0.00004500
C	-4.08017300	-1.53704000	1.20873600
C	-4.08032500	-1.53648900	-1.20875400
C	-5.47092700	-1.56244900	1.20337500
H	-3.52200100	-1.52765600	2.13927700
C	-5.47108100	-1.56192400	-1.20322300
H	-3.52227900	-1.52669000	-2.13936800
C	-6.17313300	-1.56794400	0.00011900
H	-6.00858400	-1.57582600	2.14641100
H	-6.00886500	-1.57488200	-2.14619200
H	-7.25771500	-1.58708800	0.00018300
N	-1.97032400	-1.48143500	-0.00009700
N	0.03614500	-0.30243200	-0.00012800
N	1.63969400	1.42055500	-0.00004900
C	2.77069100	0.70673500	0.00002000
H	2.62836200	2.35548300	0.00007000
C	3.29526100	-0.66376900	-0.00002600
N	3.73507200	1.61259000	0.00012700
C	2.70728100	-1.92019100	-0.00011600
C	4.68964100	-0.48987600	0.00003900
C	4.99201900	0.98606000	0.00011300
C	3.56932800	-3.01995100	-0.00013700
H	1.62697600	-2.01614400	-0.00017600
C	5.53535100	-1.58321400	0.00001100
N	6.09337300	1.61238900	0.00014100
C	4.95441700	-2.85564900	-0.00007500
H	3.15263800	-4.02148600	-0.00020000
H	6.61521100	-1.46611800	0.00005200
H	6.86885200	0.94754000	0.00012100
H	5.59390400	-3.73240800	-0.00009000

E(M06-2X-D3/6-31G(d,p)) =   -1120.62594448   A.U.

Zero-point correction=   0.322851 (Hartree/Particle)
Thermal correction to Energy=   0.383395
Thermal correction to Enthalpy=   0.385084
Thermal correction to Gibbs Free Energy=   0.202839

E(M06-2X-D3/6-311+G(d,p)) =   -1120.88680177   A.U.

TS2-11H

C	2.72787000	-3.22332400	0.02442900
C	3.21220300	-1.91174300	-0.02312600
C	2.28366400	-0.88453800	-0.13812500
C	0.91909300	-1.16773100	-0.20495900
C	0.43094300	-2.46154900	-0.14117400
C	1.36185600	-3.49733700	-0.02923300
C	2.36765200	0.61877400	-0.18719400
H	3.43264400	-4.04387800	0.11305700
H	4.27761600	-1.71943800	0.03141000
H	-0.63594800	-2.66933600	-0.15532500
H	1.01855800	-4.52559600	0.02407900
C	0.23229200	0.15139000	-0.31496200
C	4.66211800	0.83301400	-0.02927500
C	5.24952100	0.62900300	1.22337600
C	5.38194700	0.52125400	-1.18714100
C	6.52470900	0.08071300	1.31237500
H	4.68739500	0.89052100	2.11401200
C	6.65746500	-0.02446300	-1.08779900
H	4.92134100	0.69921800	-2.15353200
C	7.23287800	-0.25454900	0.16016500
H	6.96708800	-0.08617300	2.28979200
H	7.20357700	-0.27455600	-1.99220400
H	8.22733300	-0.68166100	0.23468300
N	3.37567000	1.39408600	-0.12676100
N	1.06935200	1.14850400	-0.30585200
N	-1.11172200	0.16504100	-0.45878200
C	-1.93136500	1.22890400	-0.40677200
H	-1.94423800	-0.99569900	-1.07301900
C	-1.73657200	2.65011900	0.04778900
N	-3.20295400	1.02731700	-0.74850500
N	-2.93149600	-1.43892100	-1.37397600
C	-0.65846900	3.39318400	0.51884200
C	-3.00409900	3.23612400	-0.05134000
C	-3.93935900	2.20171300	-0.57693100
H	-3.41554900	-0.44149400	-1.23944200

H	-2.95290100	-1.76612000	-2.33637300
C	-3.36513300	-2.42652500	-0.41994800
C	-0.89263500	4.71999600	0.88916500
H	0.33289800	2.96284500	0.56268000
C	-3.23560900	4.55109400	0.30845000
N	-5.18002000	2.26704800	-0.85150500
C	-3.62843900	-3.73447100	-0.81042900
C	-3.47435600	-2.03854700	0.91413300
C	-2.15755200	5.29608200	0.78814100
H	-0.06303700	5.31587500	1.25565300
H	-4.22479400	4.99270300	0.22291000
H	-5.52273900	3.20949700	-0.65462800
C	-4.01561200	-4.66716700	0.14790000
H	-3.53430100	-4.02207900	-1.85401900
C	-3.86080800	-2.97939900	1.86160200
H	-3.26151700	-1.00994700	1.18948600
H	-2.30365300	6.33125100	1.07988600
C	-4.13250800	-4.29254900	1.48268200
H	-4.22644100	-5.68786900	-0.15324000
H	-3.95000000	-2.68296400	2.90125100
H	-4.43530900	-5.02145100	2.22672900

E(M06-2X-D3/6-31G(d,p)) =   -1408.17518241   A.U.

Zero-point correction=   0.444130 (Hartree/Particle)
Thermal correction to Energy=   0.524094
Thermal correction to Enthalpy=   0.525783
Thermal correction to Gibbs Free Energy=   0.298328

E(M06-2X-D3/6-311+G(d,p)) =   -1408.50556969   A.U.

INT2-11
C	-3.21521100	3.00072100	-0.41598700
C	-3.14493400	1.62130300	-0.19248300
C	-1.88529200	1.06248000	-0.01539200
C	-0.74421400	1.86454300	-0.05897200
C	-0.80319000	3.22850100	-0.27928300
C	-2.06806200	3.79322900	-0.46034200
C	-1.36872700	-0.32302400	0.25120300
H	-4.18677300	3.46344600	-0.55667000
H	-4.04943100	1.02496500	-0.16019100
H	0.10300800	3.82434200	-0.30282500
H	-2.16280300	4.86019000	-0.63506500

C	0.40676100	0.95652100	0.18046800
C	-3.37466100	-1.45925900	0.21845200
C	-4.19524500	-1.37693100	1.34671000
C	-3.94899200	-1.60873900	-1.04732100
C	-5.57817900	-1.40215600	1.20094500
H	-3.73533500	-1.27684600	2.32439800
C	-5.33307600	-1.63595100	-1.18169700
H	-3.29934100	-1.68477700	-1.91333600
C	-6.15420800	-1.52550600	-0.06174000
H	-6.20915600	-1.32442600	2.08095200
H	-5.77175700	-1.74067300	-2.16920300
H	-7.23327400	-1.54508300	-0.17111200
N	-1.97283400	-1.43613900	0.36397100
N	0.04160400	-0.27356100	0.37185100
N	1.66119200	1.49633300	0.22918600
C	2.77125200	0.83752200	0.19125300
C	3.20989500	-0.58159500	-0.01998200
C	2.51733600	-1.77715700	-0.19378900
C	4.61290900	-0.57823000	-0.03497000
C	5.09789500	0.80564600	0.19214500
C	3.26190000	-2.94075400	-0.39741800
H	1.43718900	-1.79782300	-0.14141500
C	5.35065800	-1.73196900	-0.22899500
N	6.25294500	1.32212700	0.27454600
C	4.65546800	-2.92580100	-0.41696000
H	2.73773000	-3.88071300	-0.53440900
H	6.43653600	-1.71056600	-0.23460700
H	5.20201000	-3.85011500	-0.57292200
H	6.96751500	0.60509700	0.15035700
N	3.93345500	1.55646100	0.32064700
H	3.92885100	2.55606200	0.45956900

E(M06-2X-D3/6-31G(d,p)) =   -1120.70093843   A.U.

Zero-point correction=   0.328595 (Hartree/Particle)
Thermal correction to Energy=   0.389674
Thermal correction to Enthalpy=   0.391362
Thermal correction to Gibbs Free Energy=   0.207463

E(M06-2X-D3/6-311+G(d,p)) =   -1120.96290369   A.U.

TS3-5
C	4.78425600	-3.16953000	1.21306500

C	5.05116800	-1.94007500	0.60046000
C	3.96608900	-1.19979600	0.14759200
C	2.66770300	-1.68809300	0.30075100
C	2.39221700	-2.90174700	0.90360300
C	3.48138400	-3.64432400	1.36560500
C	3.80030600	0.11496600	-0.56043900
H	5.61369000	-3.76858400	1.57493600
H	6.07188800	-1.59243500	0.48853700
H	1.37102300	-3.25538300	0.99951400
H	3.31558400	-4.60433000	1.84354600
C	1.77818300	-0.66882800	-0.30482800
C	6.00394800	0.78902400	-0.58044100
C	6.47265200	1.12503400	0.69275000
C	6.89097100	0.29354100	-1.53933600
C	7.81205200	0.93046700	1.01227300
H	5.77421400	1.52338000	1.42178800
C	8.22712600	0.09505000	-1.20671400
H	6.51609800	0.05394600	-2.52890300
C	8.69329300	0.40720200	0.06849800
H	8.16669300	1.18525500	2.00608900
H	8.90834700	-0.30622700	-1.95049500
H	9.73672800	0.25216000	0.32129700
N	4.64829100	0.99372400	-0.91120300
N	2.41884400	0.33160200	-0.81787100
N	0.42661000	-0.90571600	-0.34608400
C	-0.47875900	-0.00426800	-0.31646500
C	-0.51668200	1.48325300	-0.11176400
N	-1.80814100	-0.40433900	-0.40684800
C	0.46622500	2.45694500	0.02255900
C	-1.86797800	1.84649800	-0.02759300
C	-2.66492100	0.62236200	-0.23427500
H	-2.24951700	-1.35861700	-0.48846600
C	0.05430100	3.76919900	0.27374700
H	1.51248900	2.21147300	-0.09976200
C	-2.28406000	3.14126000	0.22422100
N	-3.95260300	0.49297000	-0.25011000
N	-3.86112600	-1.99716900	-0.45509200
C	-1.29259300	4.11095900	0.38085600
H	0.80845000	4.54144500	0.38284700
H	-3.33746600	3.39277600	0.31453200
H	-4.46846800	1.35273100	-0.09450200
C	-4.60964500	-1.05552200	-0.32568100
H	-1.57307200	5.13920600	0.58245100
C	-6.10077600	-0.98052800	-0.26282400

C	-6.90353400	0.00706100	0.34062900
C	-6.75249800	-2.08357800	-0.82762200
C	-8.30248700	-0.11336500	0.35774000
C	-6.37050800	1.18270800	0.97566300
C	-8.13442900	-2.19819500	-0.81479100
H	-6.12535900	-2.85027200	-1.26851000
C	-8.91844800	-1.20991200	-0.22071300
H	-8.88730500	0.66432300	0.83702900
N	-5.96019900	2.15638700	1.45208100
H	-8.60376000	-3.06419100	-1.26999700
H	-9.99931700	-1.29549100	-0.20520500

E(M06-2X-D3/6-31G(d,p)) =   -1537.24182176   A.U.

Zero-point correction=   0.427081 (Hartree/Particle)
Thermal correction to Energy=   0.511711
Thermal correction to Enthalpy=   0.513399
Thermal correction to Gibbs Free Energy=   0.273679

E(M06-2X-D3/6-311+G(d,p)) =   -1537.60191900   A.U.

INT3-5

C	-4.98882700	2.71866100	1.73104100
C	-5.17556900	1.63618400	0.86425400
C	-4.04730500	1.09319900	0.26218700
C	-2.78432500	1.62679800	0.52290800
C	-2.58845500	2.69776800	1.37559500
C	-3.72123200	3.24212700	1.98537200
C	-3.79793300	-0.03121300	-0.70465400
H	-5.85330000	3.16219200	2.21451200
H	-6.17049900	1.24787700	0.67809800
H	-1.59404800	3.09554700	1.54972300
H	-3.61711500	4.08354600	2.66276800
C	-1.83357000	0.81670200	-0.27848100
C	-5.96193700	-0.79947200	-0.91034400
C	-6.46069800	-1.47664900	0.20566400
C	-6.83479000	-0.08509100	-1.73539000
C	-7.81580600	-1.40512400	0.51128100
H	-5.77492200	-2.04134700	0.82912100
C	-8.18736500	-0.01684800	-1.41872500
H	-6.43537500	0.42087300	-2.60825500
C	-8.68423500	-0.67049100	-0.29305400
H	-8.19364000	-1.92441600	1.38664500

H	-8.85599200	0.55329400	-2.05619100
H	-9.74003100	-0.61566500	-0.05009400
N	-4.59179300	-0.87069100	-1.23304300
N	-2.40716000	-0.10145700	-0.98816600
N	-0.50594900	1.15742500	-0.30748500
C	0.45731900	0.32420200	-0.23439700
C	0.50109700	-1.15599400	0.04349900
N	1.77431600	0.80894500	-0.34795800
C	-0.45384000	-2.14413700	0.23834400
C	1.86004700	-1.47067100	0.13250600
C	2.56841700	-0.19973000	-0.15036300
H	3.23104800	2.18539900	-0.61087600
C	-0.00487100	-3.43256000	0.54795500
H	-1.50942800	-1.93963500	0.12174500
C	2.31640100	-2.73927400	0.44471900
N	3.92271500	-0.14824200	-0.19320100
N	4.25369400	2.17460800	-0.59482600
C	1.35187600	-3.72830400	0.65600200
H	-0.73527400	-4.21991700	0.70185900
H	3.37411500	-2.96848200	0.54723500
H	4.38810500	-1.03553400	-0.07251500
C	4.70374400	1.00899100	-0.38810900
H	1.66463900	-4.73693900	0.90417500
C	6.19791600	0.81694200	-0.36491500
C	6.90181700	-0.23980000	0.24625000
C	6.94915800	1.81458500	-0.99240800
C	8.30324700	-0.28248100	0.21916700
C	6.25561300	-1.33062500	0.92858400
C	8.33607000	1.77015500	-1.02055700
H	6.40473000	2.63166100	-1.45057800
C	9.02062600	0.71912200	-0.41413400
H	8.81036100	-1.10870300	0.70503900
N	5.74303800	-2.23375000	1.44230700
H	8.88501000	2.56082100	-1.52101800
H	10.10405900	0.67972700	-0.43359100

E(M06-2X-D3/6-31G(d,p)) =   -1537.28754607   A.U.

Zero-point correction=   0.431200 (Hartree/Particle)
Thermal correction to Energy=   0.516075
Thermal correction to Enthalpy=   0.517763
Thermal correction to Gibbs Free Energy=   0.277605

E(M06-2X-D3/6-311+G(d,p)) =   -1537.64739807   A.U.

INT4-1

N	-6.22110800	1.43342900	0.26856300
N	-4.26020000	0.34644000	-0.55320500
N	4.17540200	0.72577000	0.15548500
N	-2.05239900	-0.16263300	-1.02862300
N	2.17813800	-0.36062300	0.84475700
N	-0.04902800	-0.23198500	0.23171100
C	-7.11315700	0.50676100	0.16269800
C	-9.32474300	-0.20083100	0.13342100
C	-4.88039500	1.24859300	0.15421200
C	-2.88251600	0.58808700	-0.41379000
C	3.53467200	-0.27447100	0.67020500
C	-0.69796600	-0.09484300	-0.88506700
C	1.32510400	-0.20590700	-0.09087900
C	-7.11236900	-0.99017600	0.15151500
C	-8.45189100	-1.40119600	0.15646400
C	-3.95416000	2.21136700	0.80034100
C	5.72357000	-0.89888700	0.96176600
C	-2.66833400	1.79308200	0.45758200
C	4.42167400	-1.32808800	1.22303100
C	1.48825400	-0.03624500	-1.57858000
C	0.18365600	0.00320700	-2.07388500
C	-8.80899700	-2.73797800	0.17904300
C	-6.09100700	-1.93538500	0.16337500
C	-4.18947600	3.32092200	1.58925700
C	6.80787000	-1.66745600	1.36712800
C	-1.55822200	2.49271600	0.90633600
C	4.14277600	-2.51304500	1.87889300
C	2.56550200	0.05752100	-2.44839500
C	-0.10408900	0.12464800	-3.42009600
C	-7.78579300	-3.68426500	0.20354300
C	-6.44984300	-3.28364400	0.19635900
C	-3.07314900	4.03086600	2.04031900
C	6.53790500	-2.86983500	2.03022100
C	-1.78396500	3.62220500	1.70123600
C	5.23191900	-3.28918100	2.28284300
C	2.28797900	0.17502800	-3.81523300
C	0.98043800	0.20815200	-4.29726500
H	-9.85139000	-3.04287300	0.17935200
H	-5.05396100	-1.63405600	0.11028900
H	-5.20213700	3.62112900	1.83681000
H	7.83126200	-1.35924100	1.18589800

H	-0.54926000	2.17641900	0.67533400
H	3.11836600	-2.81245000	2.07486900
H	3.58655400	0.07186500	-2.09139900
H	-1.13066200	0.14729700	-3.77073600
H	-8.02993900	-4.74125200	0.22202500
H	-5.66751700	-4.03522100	0.20526000
H	-3.20835800	4.90975000	2.66243100
H	7.36749200	-3.48874300	2.35671000
H	-0.93248500	4.18738300	2.06566300
H	5.06260500	-4.22722200	2.80153800
H	3.11410400	0.25249700	-4.51450200
H	0.80534700	0.30519200	-5.36379600
C	5.55960900	0.42349000	0.26288500
C	7.78268500	0.87219400	-0.15790300
C	8.59151900	1.38190700	0.86108400
C	8.34256500	0.05287500	-1.14275100
C	9.93788800	1.03639900	0.91460900
H	8.14839300	2.03232500	1.60800400
C	9.69113100	-0.28149100	-1.08356200
H	7.70603500	-0.32220500	-1.93782600
C	10.49359500	0.20097800	-0.05216400
H	10.55663600	1.42361200	1.71818100
H	10.11530000	-0.92719300	-1.84627700
H	11.54457600	-0.06404400	-0.00728700
N	-10.58030300	-0.03423200	0.11561600
H	-11.05638600	-0.93617800	0.12074900
N	6.41991200	1.22360200	-0.22080400
N	-8.43183500	0.87133000	0.13357200
H	-8.72605400	1.83709500	0.14642000

E(M06-2X-D3/6-31G(d,p)) =   -1953.90031125   A.U.

Zero-point correction=   0.536367 (Hartree/Particle)
Thermal correction to Energy=   0.642139
Thermal correction to Enthalpy=   0.643828
Thermal correction to Gibbs Free Energy=   0.354526

E(M06-2X-D3/6-311+G(d,p)) =   -1954.35394422   A.U.

INT4-2

N	-0.02323800	3.09409400	-0.18791400
N	-1.90787200	1.62810500	-0.14794100
N	0.22089900	-1.51752900	-0.03836700

N	-4.04595200	0.74848300	0.47765500
N	-1.51621200	-3.14320500	-0.12675700
N	-2.52218200	-1.05531500	0.44539500
C	0.69386500	2.27470200	-0.92125700
C	1.44385700	0.55483600	-2.23621700
C	-1.29378800	2.76043300	0.12478700
C	-3.16856100	1.69240600	0.43625700
C	-0.27599400	-2.67878500	0.25279800
C	-3.66414100	-0.51574500	0.12514000
C	-2.51959800	-2.34334600	-0.09567000
C	2.11317500	2.53627500	-1.23038000
C	2.58112400	1.48795700	-2.01712700
C	-2.16517200	3.70283100	0.87923900
C	1.86597400	-2.82304200	1.07789300
C	-3.37638300	3.03449300	1.04274400
C	0.68760400	-3.56337000	0.95517800
C	-3.84715700	-2.64247000	-0.69954400
C	-4.57554100	-1.45835200	-0.58149400
C	3.91064800	1.42134000	-2.39899500
C	2.94235000	3.56101100	-0.80437300
C	-1.96919000	4.98151100	1.36437200
C	2.95687200	-3.34792400	1.75598800
C	-4.44103200	3.61416000	1.70608800
C	0.56142600	-4.84323000	1.46259600
C	-4.37418400	-3.75667100	-1.32309800
C	-5.86312400	-1.34520300	-1.07008100
C	4.76011900	2.44090500	-1.96480700
C	4.28296500	3.49728400	-1.18376400
C	-3.04483900	5.58327900	2.02819100
C	2.83838800	-4.64107400	2.27802600
C	-4.25760700	4.91293800	2.19513700
C	1.66598500	-5.38104900	2.12857600
C	-5.68148600	-3.65655700	-1.81483200
C	-6.41173700	-2.47439400	-1.68994200
H	4.29286200	0.59572100	-2.99218500
H	2.55169400	4.36303300	-0.18716800
H	-1.01849200	5.48747500	1.23434000
H	3.87594900	-2.78602900	1.87902500
H	-5.37707200	3.08124500	1.83664500
H	-0.36479600	-5.39668100	1.34813200
H	-3.79534600	-4.66933400	-1.41995100
H	-6.42036100	-0.41907000	-0.97578300
H	5.81221900	2.40659500	-2.22790400
H	4.97113300	4.27117600	-0.85978800

H	-2.93549500	6.58773300	2.42437700
H	3.67883600	-5.07715600	2.80841300
H	-5.07075700	5.40883400	2.71528000
H	1.60997100	-6.38274100	2.54246800
H	-6.13684900	-4.51238000	-2.30256800
H	-7.42181200	-2.42998100	-2.08436400
C	1.55576400	-1.50317200	0.42894100
C	3.61999100	-0.36494500	0.50998400
C	4.51724300	-1.20367400	-0.16567300
C	4.11689000	0.68873800	1.28546900
C	5.88791200	-1.00297800	-0.04219500
H	4.12172300	-1.99545500	-0.79634500
C	5.48804700	0.87180300	1.41444400
H	3.40980200	1.35796600	1.76516100
C	6.38023100	0.03121000	0.75049000
H	6.57385900	-1.65591400	-0.57341900
H	5.86251800	1.68708000	2.02580200
H	7.44997300	0.18655400	0.84367200
N	1.32584000	-0.51265300	-2.90478900
H	2.22011300	-0.74057400	-3.34274400
N	2.24362200	-0.44278700	0.27533700
N	0.35969300	1.11898300	-1.52976900
H	-0.47721500	0.59186700	-1.27837400

E(M06-2X-D3/6-31G(d,p)) =   -1953.92713848   A.U.

Zero-point correction=   0.537075 (Hartree/Particle)
Thermal correction to Energy=   0.641581
Thermal correction to Enthalpy=   0.643270
Thermal correction to Gibbs Free Energy=   0.370145

E(M06-2X-D3/6-311+G(d,p)) =   -1954.38056887   A.U.

TS4-3

N	-2.65222600	2.81385300	0.28233500
N	-2.81319700	0.44612900	0.23375200
N	1.37458200	-0.57201700	0.33699100
N	-3.78093900	-1.73892100	-0.05910800
N	0.80340400	-2.81273800	-0.18796000
N	-1.39641600	-1.87909500	-0.30619400
C	-1.36041500	2.82594100	0.19719400
C	0.82988300	2.31761600	-0.13448500
C	-3.33831900	1.64124300	0.19070900

C	-3.85984400	-0.46064800	0.02642800
C	1.43878100	-1.60601500	-0.43014500
C	-2.55683600	-2.36982300	0.01437800
C	-0.45851000	-2.91183200	-0.07951800
C	-0.60074300	4.08450100	0.22167600
C	0.73737800	3.77962700	0.00582900
C	-4.80919100	1.62795700	0.00093700
C	3.05734200	-0.27748900	-1.32857100
C	-5.14348300	0.27955300	-0.09916900
C	2.43943100	-1.50464300	-1.51810000
C	-1.16012800	-4.14764900	0.35284900
C	-2.50327800	-3.79416400	0.43391000
C	1.70994100	4.76708400	-0.04072600
C	-1.03254900	5.38963000	0.39756300
C	-5.76269500	2.62509000	-0.08314300
C	4.09108900	0.13839900	-2.14765900
C	-6.44924200	-0.13056000	-0.28864800
C	2.81441200	-2.36484600	-2.53923400
C	-0.72246500	-5.41748900	0.67987400
C	-3.47188000	-4.69584100	0.83686000
C	1.28673400	6.08237800	0.14583600
C	-0.06219300	6.38943100	0.36072200
C	-7.08915800	2.22028300	-0.27065400
C	4.46855400	-0.70907000	-3.19173500
C	-7.42553400	0.86921600	-0.37147400
C	3.83964400	-1.94166800	-3.38596000
C	-1.69253400	-6.33980000	1.08554700
C	-3.04152300	-5.98585100	1.16291300
H	2.75441000	4.53081900	-0.21657300
H	-2.08288700	5.60535100	0.55926300
H	-5.48906400	3.67204200	-0.00728900
H	4.60633200	1.07777400	-1.97143700
H	-6.69850200	-1.18345000	-0.36771100
H	2.33429100	-3.32990900	-2.66556100
H	0.32884100	-5.67932700	0.62251400
H	-4.51619800	-4.40814900	0.89541600
H	2.01617700	6.88495600	0.12150700
H	-0.35342400	7.42513300	0.49962900
H	-7.87198000	2.96835100	-0.34205900
H	5.27601500	-0.41447900	-3.85440200
H	-8.46429900	0.59160400	-0.51776300
H	4.16384600	-2.58244600	-4.19950200
H	-1.39411700	-7.34961100	1.34791100
H	-3.76615300	-6.72674700	1.48514600

C	2.45658800	0.33612800	-0.06961000
C	4.56763500	0.23114300	1.16758600
C	5.56096300	1.04131000	1.76222600
C	4.90646100	-1.11628700	0.91479000
C	6.81725300	0.54422900	2.06545900
H	5.30492700	2.07480000	1.97775200
C	6.17167000	-1.60375600	1.22308300
H	4.16378100	-1.79198000	0.50501700
C	7.14264600	-0.78579300	1.79284700
H	7.55444800	1.20201700	2.51801700
H	6.39512400	-2.64733700	1.01816700
H	8.12712600	-1.17564800	2.02857500
N	1.95156700	1.73371800	-0.39612800
N	3.33406400	0.80441500	0.94862300
H	2.86765600	2.09934400	0.12993200
N	-0.44224600	1.80266300	0.00911200
H	-0.68179700	0.80565100	0.04118700

E(M06-2X-D3/6-31G(d,p)) =   -1953.84676205   A.U.

Zero-point correction=	0.533829 (Hartree/Particle)
Thermal correction to Energy=	0.636768
Thermal correction to Enthalpy=	0.638456
Thermal correction to Gibbs Free Energy=	0.368016

E(M06-2X-D3/6-311+G(d,p)) =   -1954.29758429   A.U.

TS4-3H

N	1.32831800	3.52607100	0.01585900
N	2.71096100	1.60673400	-0.20711200
N	-0.16196900	-1.40661600	0.12908000
N	4.72830600	0.28537600	-0.19221300
N	1.49285500	-3.02215900	0.69367600
N	2.84195400	-1.06070000	0.44191900
C	0.26087000	2.85384700	0.29156900
C	-1.27734600	1.24802800	0.75358100
C	2.52797100	2.89692600	-0.15392700
C	4.09734100	1.40196800	-0.24925800
C	0.30588400	-2.33834900	0.88957500
C	4.04248900	-0.90082500	-0.03274400
C	2.59468600	-2.44836700	0.41791000
C	-1.00399800	3.52859100	0.61844400
C	-1.93184000	2.55754000	0.96605800

C	3.78841800	3.67489400	-0.23884300
C	-1.83941700	-2.17517500	1.64729700
C	4.79334200	2.71373300	-0.31589900
C	-0.65705800	-2.85554800	1.88848300
C	3.80783400	-3.17409200	-0.03759900
C	4.72738600	-2.17929000	-0.35544900
C	-3.21801800	2.88971100	1.36259800
C	-1.31799500	4.87781800	0.62795000
C	4.07098200	5.02791000	-0.24126200
C	-2.97999300	-2.44246200	2.38369900
C	6.12716400	3.06335000	-0.39627800
C	-0.55308900	-3.82746400	2.87176400
C	4.09706000	-4.51399600	-0.21318400
C	5.98323700	-2.47902000	-0.85096600
C	-3.55126100	4.24414200	1.35546500
C	-2.61897700	5.22156900	0.99263900
C	5.41917800	5.39372700	-0.33198600
C	-2.88662000	-3.40327800	3.39385900
C	6.42686100	4.43085800	-0.40761100
C	-1.69172100	-4.08661900	3.63501000
C	5.36598500	-4.83082400	-0.70984500
C	6.29140200	-3.83272000	-1.02209000
H	-3.94563700	2.13388100	1.63741400
H	-0.57622200	5.61866800	0.35090000
H	3.28066700	5.76778900	-0.17306600
H	-3.91663100	-1.93165500	2.17905600
H	6.90182800	2.30571900	-0.44956300
H	0.37608700	-4.36515500	3.03049400
H	3.36741300	-5.28058100	0.02573800
H	6.69203600	-1.69463000	-1.09407100
H	-4.55935400	4.53872100	1.62595500
H	-2.91646100	6.26482400	0.99598800
H	5.68858000	6.44481800	-0.34060000
H	-3.76071300	-3.63597100	3.99381500
H	7.46143100	4.75111600	-0.47482900
H	-1.65558700	-4.83639600	4.41868700
H	5.63777600	-5.87091100	-0.85780900
H	7.26591300	-4.11572700	-1.40668300
C	-1.59988300	-1.26415300	0.43721300
C	-2.63495900	-2.62165100	-1.34237500
C	-3.67012500	-2.64242100	-2.30548000
C	-1.88413000	-3.80153000	-1.18557100
C	-3.94549500	-3.77329600	-3.05329900
H	-4.24473700	-1.73058600	-2.45079100

C	-2.17016200	-4.93274800	-1.94805500
H	-1.06755900	-3.85450200	-0.47851300
C	-3.19744800	-4.93988300	-2.88255000
H	-4.75172500	-3.74426100	-3.78131500
H	-1.56872400	-5.82551800	-1.79808700
H	-3.41083000	-5.82769200	-3.46816500
N	-1.91495800	0.13876900	0.86767500
N	-2.48669700	-1.42379600	-0.66281400
N	0.03206900	1.48458500	0.39628200
H	0.72011200	0.75805100	0.16469400
H	-2.99829700	0.21989100	0.92743300
N	-4.46396700	-0.05514500	0.19698800
H	-3.64406100	-0.81502800	-0.33506200
H	-5.26230800	-0.47339600	0.66409700
C	-4.81484500	1.06590800	-0.55478500
C	-3.93406000	1.53133500	-1.54974400
C	-5.97152000	1.81651900	-0.28759500
C	-4.18429500	2.73016000	-2.20569600
H	-3.05895000	0.93028600	-1.78806900
C	-6.21454900	3.01118400	-0.95593900
H	-6.66978400	1.45950000	0.46630700
C	-5.31678700	3.48792500	-1.90898400
H	-3.48701000	3.07483300	-2.96406700
H	-7.11429900	3.57553800	-0.72675100
H	-5.50605300	4.42294800	-2.42511200

E(M06-2X-D3/6-31G(d,p)) =   -2241.37175253   A.U.

Zero-point correction=   0.652442 (Hartree/Particle)
Thermal correction to Energy=   0.775272
Thermal correction to Enthalpy=   0.776961
Thermal correction to Gibbs Free Energy=   0.463160

E(M06-2X-D3/6-311+G(d,p)) =   -2241.89094009   A.U.

INT4-3
N	-2.83549500	2.30264300	-0.27705100
N	-2.35201300	-0.02699000	-0.15207800
N	1.43657500	0.04553200	-0.42103000
N	-2.66051000	-2.36940000	0.28576200
N	1.79530800	-2.18271700	-1.19414400
N	-0.33327600	-2.03938500	-0.06893500
C	-1.60900700	2.64562100	-0.56477800

C	0.67776000	2.71735600	-0.75148900
C	-3.10626000	1.02318300	0.07865600
C	-3.02714200	-1.13782300	0.35920100
C	2.20421400	-0.93951300	-0.72659400
C	-1.44752300	-2.67586500	-0.27759000
C	0.62896900	-2.63047700	-0.90709400
C	-1.24042800	3.99307300	-1.04490300
C	0.14480000	4.03031400	-1.18646800
C	-4.37355500	0.67258200	0.77463600
C	3.69431600	0.74212900	-0.29091800
C	-4.31694000	-0.70644300	0.96312100
C	3.64507200	-0.59716500	-0.66129800
C	0.04726400	-3.83634500	-1.55849800
C	-1.29410000	-3.84933700	-1.18119400
C	0.79402700	5.17220500	-1.62367300
C	-2.03421500	5.09066100	-1.33621200
C	-5.44921300	1.42338400	1.20881100
C	4.90296000	1.40213800	-0.16519900
C	-5.33578700	-1.39421600	1.59411900
C	4.79218600	-1.32981400	-0.92092900
C	0.56637600	-4.78184300	-2.42138200
C	-2.16977600	-4.81555000	-1.64050200
C	0.00237100	6.28003800	-1.93089900
C	-1.38886000	6.24132200	-1.78865600
C	-6.48675800	0.73697200	1.85075700
C	6.06934700	0.67610100	-0.42622100
C	-6.43053200	-0.64474800	2.04057700
C	6.01556400	-0.67011500	-0.79453300
C	-0.30747300	-5.77218900	-2.88482900
C	-1.64938400	-5.78904400	-2.50118000
H	1.87392500	5.19025000	-1.72343600
H	-3.11079700	5.04138800	-1.21329800
H	-5.48079400	2.49671000	1.05488100
H	4.94520900	2.45210900	0.11100300
H	-5.28211400	-2.46871600	1.73475700
H	4.73168200	-2.37234500	-1.21522000
H	1.60916100	-4.75179500	-2.71949000
H	-3.21361100	-4.81471200	-1.34477600
H	0.47263500	7.19142700	-2.28586500
H	-1.97197900	7.12266700	-2.03434100
H	-7.35165600	1.28667900	2.20802600
H	7.03462100	1.16618600	-0.34517500
H	-7.25205500	-1.14503500	2.54297200
H	6.93901600	-1.20561000	-0.98971300

H	0.06217800	-6.54033700	-3.55638600
H	-2.30071300	-6.56929200	-2.88151100
C	2.26457100	1.17791100	0.00020900
C	2.34450000	0.34122200	2.33271900
C	3.49756800	0.36824900	3.11978000
C	1.45992800	-0.73632400	2.44215800
C	3.75954200	-0.66298300	4.01761000
H	4.19320600	1.19810100	3.02021900
C	1.74315500	-1.77610400	3.31989700
H	0.56554800	-0.75451000	1.82770100
C	2.88739200	-1.74275400	4.11526400
H	4.65495100	-0.62724800	4.63025600
H	1.05347100	-2.61168900	3.39049000
H	3.09654600	-2.55193900	4.80750900
N	1.91208000	2.43483300	-0.64196800
N	2.02652800	1.41191100	1.44684500
H	2.55987900	2.24239400	1.69327900
N	-0.45711600	1.93984700	-0.44311000
H	-0.40246400	0.93653500	-0.24678300

E(M06-2X-D3/6-31G(d,p)) =   -1953.93817787   A.U.

Zero-point correction=	0.539879 (Hartree/Particle)
Thermal correction to Energy=	0.642685
Thermal correction to Enthalpy=	0.644373
Thermal correction to Gibbs Free Energy=	0.376456

E(M06-2X-D3/6-311+G(d,p)) =   -1954.38836245   A.U.

TS4-4

N	2.97213700	-2.57215600	-0.05032300
N	2.77147200	-0.20525400	0.20443800
N	-0.78262900	0.20238800	-0.77856200
N	3.33297800	2.01957900	0.83843900
N	-0.76081100	2.47690200	-1.40150300
C	1.80312600	-2.71625200	-0.64453200
C	-0.38205800	-2.49476300	-1.30013000
C	3.32002700	-1.38241800	0.46038700
C	3.48680800	0.73920400	0.92199700
C	2.37146300	2.47767300	-0.00416900
C	0.42834900	2.76921400	-1.08896200
C	1.38866300	-3.98710500	-1.27501500
C	0.06823400	-3.84495400	-1.70252200

C	4.45730700	-1.26978700	1.41798800
C	-3.09925900	-0.09666600	-0.99059300
C	4.54652700	0.08414300	1.73269100
C	-2.86818900	1.27004900	-0.89307500
C	1.44870500	3.51237500	-1.85211400
C	2.66062300	3.31653800	-1.18399100
C	-0.60731800	-4.89063800	-2.31006300
C	2.08811700	-5.17205600	-1.44604300
C	5.31156500	-2.20208300	1.97434600
C	-4.33776100	-0.59426200	-1.35795400
C	5.49675500	0.56569900	2.61245000
C	-3.87993400	2.18910600	-1.12126000
C	1.39044700	4.23039600	-3.03468100
C	3.85356000	3.83898700	-1.66085000
C	0.09457400	-6.08101000	-2.50114200
C	1.42095200	-6.22129300	-2.07650200
C	6.27563100	-1.72703700	2.87172900
C	-5.36066300	0.32546400	-1.60803600
C	6.36608600	-0.37019500	3.18547300
C	-5.13787700	1.69684200	-1.48098300
C	2.58435500	4.77142600	-3.51435000
C	3.79553000	4.58158600	-2.83938700
H	-1.63995400	-4.77412300	-2.62066000
H	3.11081100	-5.26389900	-1.09623100
H	5.23256500	-3.25356900	1.71963400
H	-4.50052200	-1.66378800	-1.44836600
H	5.56116500	1.62306200	2.84725200
H	-3.69564500	3.25670100	-1.04164400
H	0.44963800	4.35969500	-3.55845000
H	4.78696500	3.67291200	-1.13352500
H	-0.39741200	-6.91894400	-2.98447500
H	1.93257900	-7.16445800	-2.23735400
H	6.96783100	-2.42483500	3.33177000
H	-6.34115800	-0.03036300	-1.90934600
H	7.12515900	-0.03598000	3.88519200
H	-5.94831200	2.39122700	-1.68015100
H	2.57677000	5.34932300	-4.43272400
H	4.70360300	5.01465300	-3.24524700
C	-1.80100800	-0.77867400	-0.60684400
C	-2.80100100	-2.14895700	1.29618700
C	-2.38445400	-3.46905300	1.49252300
C	-4.13413100	-1.81474800	1.55410900
C	-3.28165400	-4.43654300	1.93311000
H	-1.34800200	-3.73309200	1.29224400

C	-5.03390700	-2.78851700	1.97303100
H	-4.45043800	-0.78518700	1.42114200
C	-4.61302900	-4.10222300	2.16661600
H	-2.93987000	-5.45571400	2.08536400
H	-6.06670400	-2.51528600	2.16662000
H	-5.31494700	-4.85715400	2.50570000
N	-1.56395900	-2.04377800	-1.31739900
N	-1.89038100	-1.13325800	0.88394000
H	-0.94106500	-1.41232700	1.12974200
N	0.76386800	-1.87037100	-0.72925000
H	0.69979300	-0.84336200	-0.54128500
C	-1.39617900	1.44267500	-0.57038300
N	1.08707300	2.25937900	0.07582200
H	0.24528100	1.89529100	0.79497200
N	-1.20045300	1.80924100	0.95337300
H	-1.49179800	0.93286800	1.39821100
C	-1.95383100	2.90486200	1.47465000
C	-3.13453100	2.66386400	2.18184400
C	-1.53693000	4.22064500	1.26303100
C	-3.88704300	3.72375000	2.67337500
H	-3.45800400	1.63616100	2.32836700
C	-2.30150900	5.27854600	1.74587200
H	-0.61394100	4.41558000	0.72681800
C	-3.47675200	5.03626300	2.45186600
H	-4.80182900	3.52278000	3.22174500
H	-1.97033700	6.29807400	1.57512800
H	-4.06762200	5.86460200	2.82856500

E(M06-2X-D3/6-31G(d,p)) =   -2241.37822791   A.U.

Zero-point correction=   0.655574 (Hartree/Particle)
Thermal correction to Energy=   0.776885
Thermal correction to Enthalpy=   0.778574
Thermal correction to Gibbs Free Energy=   0.471062

E(M06-2X-D3/6-311+G(d,p)) =   -2241.89776855   A.U.

INT4-4

N	-0.47553300	3.68734700	-0.32599200
N	-1.84304200	1.72920200	-0.21668900
N	0.75256200	-1.00067000	-0.27581600
N	-3.86592100	0.44542400	-0.15921300
N	-0.62711000	-2.95758400	-0.91476100

C	0.60709200	3.00774100	-0.69276100
C	2.17859400	1.38376400	-1.06586000
C	-1.59802400	3.03917100	-0.04822800
C	-3.17260200	1.53857900	0.02608200
C	-3.24828700	-0.68807400	-0.54437400
C	-1.72203300	-2.32970000	-0.97072100
C	1.76940600	3.64961300	-1.32563100
C	2.71634200	2.65720700	-1.58549100
C	-2.80837000	3.76316300	0.42074600
C	2.79954300	-2.13257200	-0.60070900
C	-3.81373500	2.80187900	0.47245800
C	1.79837400	-3.08327300	-0.60677700
C	-3.05018300	-2.84660400	-1.35199400
C	-3.98414100	-1.85043800	-1.05576200
C	3.93279400	2.96287900	-2.17414000
C	1.99090200	4.97986400	-1.65497200
C	-3.04383000	5.08227600	0.75598400
C	4.08934600	-2.44560900	-1.00086900
C	-5.10037700	3.11507200	0.86542800
C	2.04332400	-4.39356500	-0.98293400
C	-3.44960000	-4.07765400	-1.84792400
C	-5.34589300	-2.04065700	-1.24949400
C	4.16107500	4.29633300	-2.51256200
C	3.20686500	5.29026700	-2.25857800
C	-4.34184300	5.41078300	1.16631700
C	4.35242100	-3.76313100	-1.38304600
C	-5.34934500	4.44654400	1.22065700
C	3.34323300	-4.72714900	-1.37011200
C	-4.81488200	-4.27383100	-2.05119500
C	-5.74993700	-3.27265700	-1.75670500
H	4.66841100	2.18670700	-2.35468200
H	1.24111200	5.73455000	-1.44326000
H	-2.25412600	5.82403400	0.70111900
H	4.86323300	-1.68457200	-1.02368100
H	-5.87683900	2.35795900	0.89641900
H	1.24105300	-5.12571300	-1.01101300
H	-2.71870500	-4.84894400	-2.06578000
H	-6.05329100	-1.25453500	-1.00822700
H	5.10011700	4.57417500	-2.98043300
H	3.42386800	6.31707500	-2.53344000
H	-4.57181700	6.43395700	1.44508400
H	5.35095700	-4.03928700	-1.70757300
H	-6.34416800	4.73745700	1.54171000
H	3.56853500	-5.74163100	-1.68492500

H	-5.16500600	-5.22322100	-2.44347800
H	-6.80409200	-3.46510000	-1.92585400
C	2.17100500	-0.82200900	-0.16853100
C	3.92546600	-0.30818900	1.58473600
C	4.50015300	0.96377100	1.67376700
C	4.70891900	-1.42683300	1.88737200
C	5.83218700	1.11557100	2.04588900
H	3.89404300	1.83712400	1.44125300
C	6.04637200	-1.27355200	2.23445500
H	4.24434700	-2.40651000	1.85194200
C	6.61460000	-0.00363100	2.31626700
H	6.26119900	2.11063200	2.11597200
H	6.64325600	-2.15103200	2.46377400
H	7.65550600	0.11282500	2.60027700
N	2.76560000	0.27364600	-0.97766200
N	2.55677700	-0.49155000	1.24903200
H	2.03174400	0.34918300	1.48162200
N	0.88620000	1.70956400	-0.55937900
H	0.28060700	0.94354700	-0.24108600
C	0.52141200	-2.39350300	-0.17841000
N	-1.96031000	-0.98964200	-0.54744400
H	-1.15425500	-0.42218200	-0.26048700
N	0.22830100	-2.92279900	1.24548300
H	0.10970500	-3.93167500	1.17169300
C	-0.88934200	-2.34276500	1.86284000
C	-2.12619000	-2.99871900	1.93758900
C	-0.78823200	-1.02616700	2.34379800
C	-3.24966800	-2.33644000	2.42317700
H	-2.20876800	-4.01745300	1.56559700
C	-1.91748400	-0.36446600	2.80873000
H	0.19110500	-0.56526900	2.32847400
C	-3.15591300	-1.00828500	2.83416100
H	-4.20547700	-2.85087200	2.45517700
H	-1.83364300	0.65967500	3.16157500
H	-4.03839200	-0.48148400	3.18326700

E(M06-2X-D3/6-31G(d,p)) =   -2241.39435842   A.U.

Zero-point correction=   0.659132 (Hartree/Particle)
Thermal correction to Energy=   0.781646
Thermal correction to Enthalpy=   0.783334
Thermal correction to Gibbs Free Energy=   0.475767

E(M06-2X-D3/6-311+G(d,p)) =   -2241.91473298   A.U.

TS4-5

N	-1.12324200	3.17361700	-1.11250800
N	-2.23652900	1.06313000	-0.64402300
N	0.66721300	-1.38780500	-0.86138800
N	-4.03259200	-0.48784200	-0.11747900
N	-0.44813400	-3.51892500	-0.93096100
C	0.04369300	2.67251400	-1.38751900
C	1.78530100	1.18127600	-1.60612500
C	-2.15992600	2.42558500	-0.69197300
C	-3.48664900	0.74922500	-0.23333000
C	-3.37011600	-1.57702400	-0.32627000
C	-1.63586300	-3.02604100	-0.72844700
C	1.17510200	3.39373500	-1.95791100
C	2.22999600	2.48507300	-2.11664800
C	-3.41664800	3.02361100	-0.27813400
C	2.88641700	-2.22526700	-0.93546100
C	-4.26569100	1.94676700	0.02762400
C	1.99215900	-3.28308900	-1.01331800
C	-2.85130400	-3.82324800	-0.51214000
C	-3.90384700	-2.93718900	-0.25358100
C	3.45827000	2.88078000	-2.63427200
C	1.31753600	4.72932600	-2.32841200
C	-3.84978400	4.34363700	-0.14520700
C	4.24789600	-2.41839100	-1.09355100
C	-5.57256200	2.15985600	0.46682200
C	2.41974600	-4.58893600	-1.19791700
C	-3.03913800	-5.19863200	-0.50443600
C	-5.18434000	-3.40499800	0.01874800
C	3.59961900	4.21219500	-3.00607200
C	2.54076600	5.12358500	-2.85440000
C	-5.14928600	4.55346400	0.29502000
C	4.69217200	-3.72951900	-1.28591100
C	-6.00110000	3.47357600	0.59787500
C	3.79317600	-4.79942000	-1.32654400
C	-4.32114500	-5.66931900	-0.23643200
C	-5.37750000	-4.78296300	0.02153700
H	4.26459400	2.16293900	-2.74091000
H	0.49387800	5.42415600	-2.20510200
H	-3.18736300	5.16895200	-0.38561800
H	4.93738300	-1.58055700	-1.07132500
H	-6.22126700	1.32058300	0.69559100
H	1.70247200	-5.40063500	-1.25598100

H	-2.20812800	-5.86760700	-0.70123500
H	-5.99259700	-2.70999500	0.21923000
H	4.54110700	4.55836500	-3.41993600
H	2.68613600	6.15623200	-3.15527100
H	-5.52204800	5.56672900	0.40739500
H	5.75265600	-3.92133900	-1.41536200
H	-7.01137500	3.67773100	0.93857000
H	4.17188600	-5.80503900	-1.47912000
H	-4.51036500	-6.73763800	-0.22448700
H	-6.36483800	-5.18402000	0.22741800
C	2.06628800	-0.97705500	-0.71338400
C	3.37541000	-0.14764700	1.34127800
C	3.65820500	1.19047000	1.63628200
C	4.23967300	-1.15833000	1.78292500
C	4.81230900	1.51832300	2.34054300
H	2.97548100	1.96551500	1.29566200
C	5.39331800	-0.81891300	2.47758200
H	3.99185400	-2.19562500	1.58358100
C	5.68457100	0.51692600	2.75686700
H	5.02913400	2.55859200	2.55958600
H	6.06229000	-1.60280900	2.81727300
H	6.58432200	0.77310800	3.30606400
N	2.52988700	0.13442800	-1.48719100
N	2.14790700	-0.48495200	0.72620100
H	1.53382400	0.32978100	0.73507800
N	0.47773600	1.37276800	-1.19015500
H	-0.15176600	0.62450300	-0.92525500
C	0.63644900	-2.68909000	-0.93909200
N	-2.01870700	-1.71898000	-0.63007000
H	-1.39150400	-0.93974900	-0.78095500
N	0.75999100	-1.22274000	2.24202600
H	1.59152100	-1.53683800	2.75228100
C	0.34979900	-0.03795800	2.73322100
C	1.04112000	0.70134300	3.74065000
C	-0.80403700	0.54488300	2.13420700
C	0.56133600	1.92902000	4.14636700
H	1.93606100	0.27347900	4.18636500
C	-1.26312300	1.78536500	2.54331500
H	-1.30460800	-0.01715800	1.35463700
C	-0.58744600	2.47597500	3.55227200
H	1.07807100	2.48010000	4.92546400
H	-2.14599900	2.21360600	2.07686700
H	-0.95046200	3.44488400	3.87844000

E(M06-2X-D3/6-31G(d,p)) =   -2241.36973641   A.U.

Zero-point correction=   0.658144 (Hartree/Particle)
Thermal correction to Energy=   0.780286
Thermal correction to Enthalpy=   0.781974
Thermal correction to Gibbs Free Energy=   0.473450

E(M06-2X-D3/6-311+G(d,p)) =   -2241.88676952   A.U.

Phthalocyanine

N	-2.37102600	-2.39182900	0.00013300
N	-2.37651000	2.38650000	0.00004200
N	0.00224800	-1.93351100	-0.00001200
N	-0.00226200	1.93348300	0.00002600
N	2.37649800	-2.38654900	0.00001700
N	2.37102000	2.39180000	-0.00009000
C	-2.77245100	-1.14171100	0.00011600
C	-2.77501300	1.13548500	0.00007600
C	-1.08716200	-2.74474700	0.00010900
C	1.09345600	-2.74238000	0.00006500
C	1.08720700	2.74475900	-0.00005600
C	2.77501300	-1.13547100	-0.00003000
C	2.77248500	1.14170800	-0.00007700
C	-4.15796900	-0.70655400	0.00011400
C	-4.15954100	0.69714800	0.00009500
C	-0.69319600	-4.15759000	0.00005100
C	-0.70260100	4.15606700	-0.00001200
C	0.70260700	-4.15611300	0.00001700
C	0.69320300	4.15756600	-0.00005300
C	4.15797900	0.70650800	-0.00010600
C	4.15952900	-0.69718700	-0.00008000
C	-5.35270000	1.41929400	0.00009100
C	-1.41794900	-5.34295400	0.00003700
C	-1.42957000	5.34008600	-0.00000400
C	1.42955600	-5.34013600	-0.00003600
C	1.41793300	5.34295500	-0.00008700
C	5.34977200	1.43093000	-0.00015100
C	5.35276100	-1.41922600	-0.00009600
C	-6.53635500	0.69735100	0.00010700
C	-0.69464700	-6.53272000	-0.00000400
C	-0.70854800	6.53125600	-0.00004000
C	0.70850800	-6.53129900	-0.00004000
C	0.69461400	6.53270000	-0.00008100

C	6.53485700	0.71133400	-0.00016600
C	6.53636200	-0.69723100	-0.00013900
H	-5.33883200	2.50375000	0.00007400
H	-2.50273100	-5.33126900	0.00006700
H	-2.51433600	5.32652200	0.00002700
H	2.51432200	-5.32660300	-0.00005800
H	2.50271600	5.33128500	-0.00012000
H	5.33399400	2.51536800	-0.00017000
H	5.33901700	-2.50368800	-0.00007300
H	-7.48527900	1.22367200	0.00010500
H	-1.22237600	-7.48108600	-0.00000700
H	-1.23820200	7.47855300	-0.00003800
H	1.23815100	-7.47860200	-0.00006900
H	1.22231800	7.48108000	-0.00011000
H	7.48271200	1.23957500	-0.00019900
H	7.48533400	-1.22345500	-0.00015200
C	-1.09341100	2.74233700	0.00000900
N	-2.00943800	-0.00226800	0.00008700
H	-0.99669400	-0.00101700	0.00009200
N	2.00945700	0.00223200	-0.00004600
H	0.99671300	0.00098700	-0.00004400
C	-6.53487800	-0.71121700	0.00012600
H	-7.48281100	-1.23930300	0.00013900
C	-5.34982300	-1.43086000	0.00012900
H	-5.33408100	-2.51530900	0.00014300

E(M06-2X-D3/6-31G(d,p)) =   -1667.70561573   A.U.

Zero-point correction=	0.440345 (Hartree/Particle)
Thermal correction to Energy=	0.525583
Thermal correction to Enthalpy=	0.527272
Thermal correction to Gibbs Free Energy=	0.299953

E(M06-2X-D3/6-311+G(d,p)) =   -1668.08368330   A.U.

Hydrazobenzene

C	1.61900200	-0.57076500	0.03784000
C	2.88516000	-0.96243500	-0.41503600
C	1.41185700	0.75340400	0.43655800
C	3.92363000	-0.04401700	-0.46585400
H	3.04650400	-1.99116600	-0.72698600
C	2.46445400	1.66312300	0.38013000
H	0.43051400	1.07652700	0.76679300

C	3.72302700	1.27673600	-0.06696000
H	4.89956600	-0.36510700	-0.81635500
H	2.28967000	2.68906100	0.68918000
H	4.53688500	1.99215500	-0.10714900
N	0.57655600	-1.51106700	0.04540500
H	0.88223700	-2.47437200	0.07540500
N	-0.51769100	-1.29714300	0.87213600
H	-0.25833700	-0.98916400	1.80696700
C	-1.59096700	-0.56080300	0.33340700
C	-2.52957200	-0.00549300	1.21027500
C	-1.75929100	-0.40672400	-1.04421600
C	-3.62462300	0.68832100	0.71184700
H	-2.39870800	-0.12772700	2.28273700
C	-2.86151700	0.28970800	-1.52856100
H	-1.02158300	-0.82882400	-1.71606900
C	-3.80065600	0.84115600	-0.66144900
H	-4.34430000	1.11288100	1.40491300
H	-2.98181100	0.40556400	-2.60144900
H	-4.65571600	1.38438700	-1.04864600

E(M06-2X-D3/6-31G(d,p)) =   -573.741676462   A.U.

Zero-point correction=   0.217574 (Hartree/Particle)
Thermal correction to Energy=   0.252097
Thermal correction to Enthalpy=   0.253785
Thermal correction to Gibbs Free Energy=   0.132132

E(M06-2X-D3/6-311+G(d,p)) =   -573.879518450   A.U.