Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information for:

Catalytic and non-catalytic roles of derivative groups in the decompostion of N@C_{60}: a DFT investigation†

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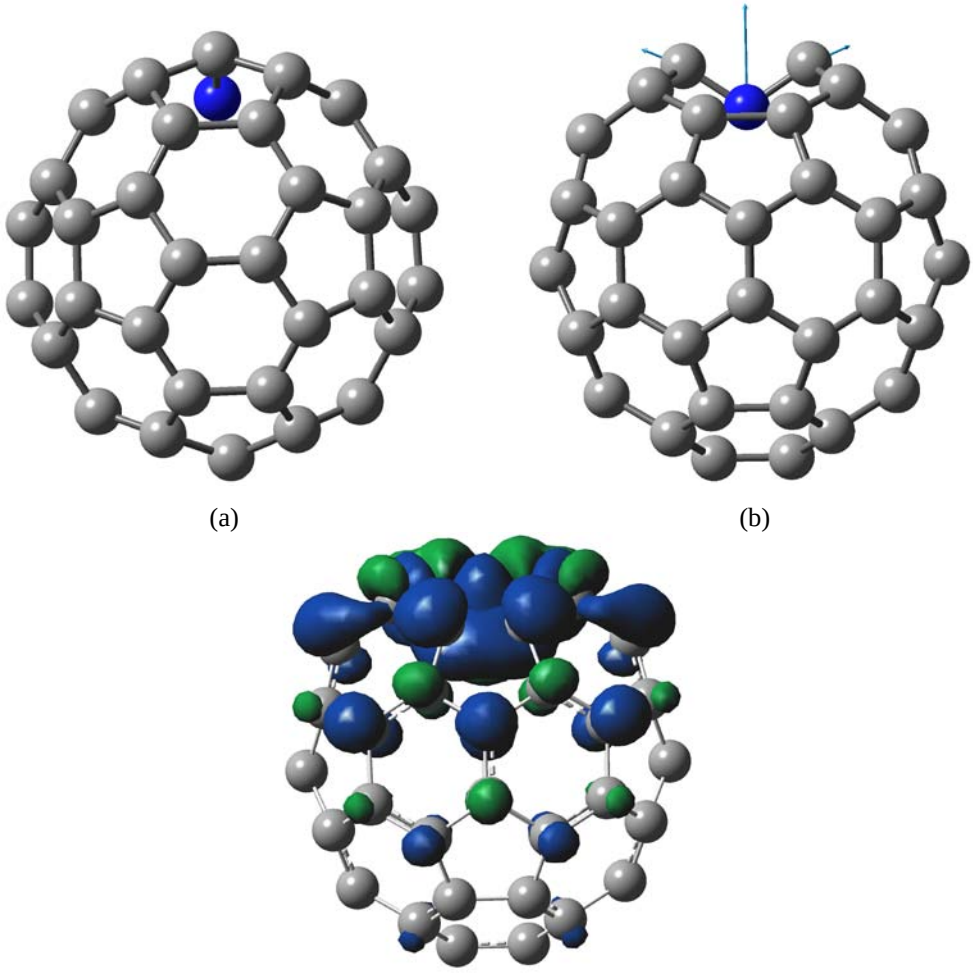
Computational details

Hybrid DFT calculations were carried out with the Gaussian03 programme[1] at the spin-unrestricted B3LYP level[2,3]. Split-valence 6-31G basis set was used for all elements with additional *p* polarization functional applied to N. Stationary points have been optimized using the Berny optimization algorithm with GDIIS step[4]. Analytical frequency calculations were further carried out to verify the nature of these minima. Transition states were obtained using the Berny optimization algorithm with Rational Function Optimization (RFO) step[5] and verified by frequency calculations. Thermal energy calculation was performed with temperature and pressure set to be 298.15 K and 1 atm, respectively. Molecular structure and spin density distribution are visualized using GaussView[6]. All calculations were set to be in the gas phase.

Figure S1 Optimized geometry (a, b) and spin density distribution (c) of the transition state **TS1b** in the decomposition of N@C_{60}. The displacement vectors are shown in (b).



(a) (b)

(c)

Figure S2 Decomposition pathway for pristine N@C_{60} through coordination of four carbon atoms. Proposed by Tsetseris [7], recalculated at the B3LYP/6-31G level.

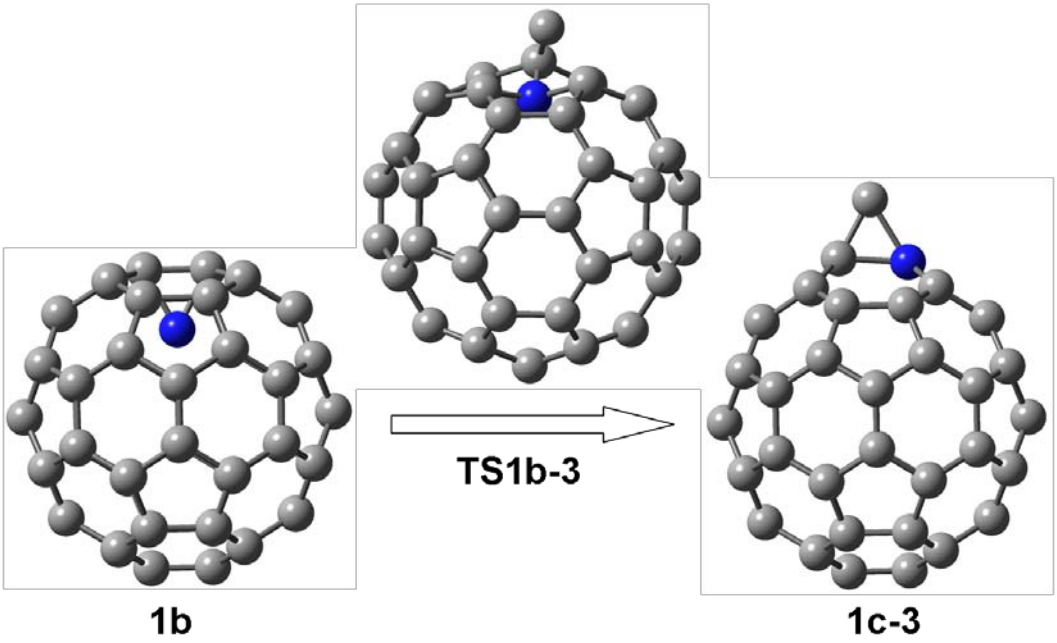
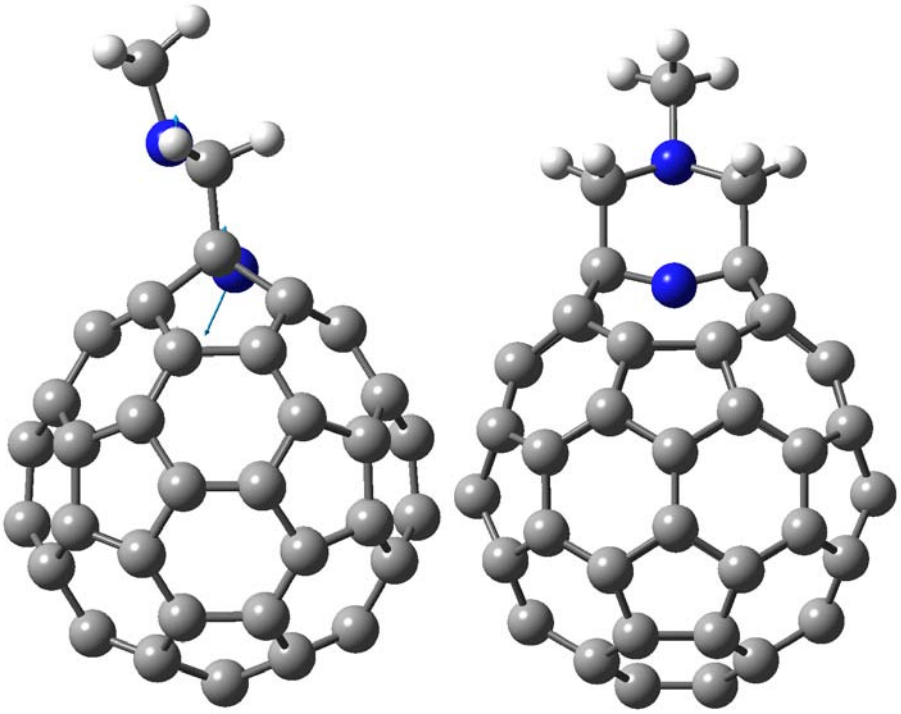
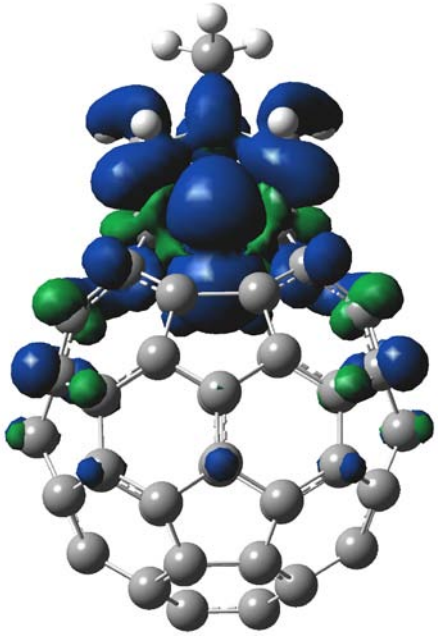


Figure S3 Optimized geometry (a, b) and spin density distribution (c) of the transition state **TS2b** in the decomposition of the pyrrolidine derivative of N@C_{60}. The displacement vectors are shown in (a).



(a) (b)



(c)

Table S1 The $<S^2>$ value of the ground state of all the optimized structures.

	1a	**1b**	**TS1b**	**1c**	**2a**	**2b**	**TS2b**	**2c**	**3a**	**3b**
S	3/2	1/2	1/2	1/2	3/2	1/2	1/2	1/2	3/2	1/2
$<S^2>$	3.7525	0.7598	0.7566	0.7541	3.7525	0.7591	0.7581	0.7542	3.7525	0.7591

References

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Cartesian coordinates and energy of the optimized structures.

1a

Sum of electronic and zero-point Energies= -2339.790851
Sum of electronic and thermal Energies= -2339.768303
Sum of electronic and thermal Enthalpies= -2339.767359
Sum of electronic and thermal Free Energies= -2339.838866

C	0.33819900	-3.30298000	-1.28920500
C	-0.39914700	-2.63829700	-2.35924600
C	-1.72613000	-2.24880200	-2.15624900
C	-2.37445300	-2.50672500	-0.87423200
C	-1.66831100	-3.14320500	0.15047200
C	-0.28266800	-3.54994900	-0.06149200
C	0.52366400	-1.74922100	-3.05809400
C	-2.18898200	-0.95298300	-2.64312500
C	-3.23802400	-1.37033600	-0.56878400
C	-1.79457000	-2.67150700	1.52595400
C	0.44748600	-3.32961300	1.18300200
C	1.71669400	-2.82466300	-1.32672900
C	-2.62156700	-1.58325200	1.81846100
C	-3.35893700	-0.91859500	0.74843300
C	-2.17746700	-0.56202800	2.76199900
C	-3.37053400	0.51342000	1.03067100
C	0.08040900	-0.50829400	-3.52432700
C	-3.12340000	-0.41006300	-1.66203600
C	-2.64034500	0.73377100	2.27513700
C	-3.13451500	0.96128700	-1.39174000
C	-1.30525000	-0.10156300	-3.31234800
C	-0.48692400	-2.78670100	2.16409300
C	1.76759400	-2.87158000	1.14704100
C	0.92520400	0.67232700	-3.37306100
C	2.41592300	-2.61363700	-0.13496800
C	1.83130700	-1.86437000	-2.41992600
C	2.21169000	-1.85036200	2.09061100
C	3.26074700	-1.43302100	0.01627500
C	2.64035600	-0.73377400	-2.27512800
C	-3.26074200	1.43302000	-0.01626400
C	-0.06164100	-1.80870400	3.06765000
C	-1.31684200	1.33041800	-3.03009900
C	3.13452600	-0.96128700	1.39175400
C	3.37054000	-0.51342000	-1.03065800
C	2.17746900	0.56202600	-2.76198200
C	2.62157900	1.58325100	-1.81845100
C	0.06164800	1.80870300	-3.06763800
C	-2.21167900	1.85036400	-2.09059700
C	-1.76758700	2.87158400	-1.14702800
C	3.35894400	0.91859300	-0.74842000
C	3.23803200	1.37033800	0.56879600
C	2.37446500	2.50672900	0.87424600
C	3.12341000	0.41006300	1.66204800
C	-0.92519600	-0.67232700	3.37306800
C	-0.44747900	3.32961700	-1.18299000
C	1.31685000	-1.33041800	3.03011300
C	1.30525900	0.10156400	3.31236100
C	0.48693200	2.78670000	-2.16407900
C	-2.41591700	2.61363800	0.13497900
C	-1.71668600	2.82466300	1.32673900
C	1.79457700	2.67150400	-1.52594100
C	1.66831800	3.14320200	-0.15045900
C	2.18899300	0.95298200	2.64313900
C	1.72614000	2.24880100	2.15626100
C	0.28267600	3.54995500	0.06150400
C	-0.08040100	0.50829300	3.52433500
C	-1.83129700	1.86436800	2.41993300
C	-0.33819100	3.30297700	1.28921400
C	-0.52365400	1.74921700	3.05809800
C	0.39915600	2.63829500	2.35925600
N	-0.00021700	0.00000600	-0.00029900

1b

Sum of electronic and zero-point Energies= -2339.724863
Sum of electronic and thermal Energies= -2339.703799
Sum of electronic and thermal Enthalpies= -2339.702855
Sum of electronic and thermal Free Energies= -2339.768835

C	-2.32940300	-0.69870600	2.60817800
C	-2.31584500	0.75764800	2.60253100
C	-1.18146400	1.45358200	3.03125000
C	0.00000300	0.71990600	3.47704300
C	0.00000300	-0.67482200	3.48949400
C	-1.19108600	-1.40842500	3.05528400
C	-3.04792800	1.21882300	1.42657600
C	-0.73065700	2.63317300	2.30799600
C	1.18146900	1.45358300	3.03124800
C	1.19109200	-1.40842400	3.05528200
C	-0.76402500	-2.59303300	2.35515000
C	-3.07228800	-1.13989100	1.43974000
C	2.32940800	-0.69870500	2.60817400
C	2.31584900	0.75764900	2.60252700
C	3.07229100	-1.13988900	1.43973500
C	3.04793000	1.21882400	1.42657000
C	-2.61098500	2.34833100	0.72920400
C	0.73066000	2.63317400	2.30799400
C	3.51044100	0.04426300	0.69828800
C	1.42893900	3.07348200	1.17914300
C	-1.42893800	3.07348100	1.17914500
C	0.76403100	-2.59303300	2.35514900
C	-1.51063700	-3.00735600	1.24190800
C	-2.61098800	2.34811900	-0.72988900
C	-2.67059400	-2.29188100	0.74441500
C	-3.51044000	0.04426100	0.69829400
C	-0.72582900	-3.24300500	0.00047300
C	-2.67059700	-2.29210000	-0.74373700
C	-3.51044000	0.04405700	-0.69829800
C	2.61098500	2.34833300	0.72919900
C	1.51064100	-3.00735500	1.24190500
C	-0.69919000	3.52471400	-0.00051700
C	-1.51064400	-3.00772500	-1.24102900
C	-3.07229200	-1.14031200	-1.43939800
C	-3.04792800	1.21840300	-1.42692500
C	-2.31585100	0.75688300	-2.60275100
C	-1.42894100	3.07313600	-1.18004500
C	0.69918800	3.52471400	-0.00051800
C	1.42893700	3.07313700	-1.18004800
C	-2.32940700	-0.69947200	-2.60796400
C	-1.19109200	-1.40932000	-3.05486900
C	-0.00000300	-0.67584200	-3.48929000
C	-0.76403100	-2.59372400	-2.35439400
C	2.67059700	-2.29188000	0.74441000
C	0.73065600	2.63249700	-2.30876700
C	0.72583100	-3.24300400	0.00047200
C	1.51064300	-3.00772400	-1.24103200
C	-0.73066100	2.63249700	-2.30876500
C	2.61098600	2.34812100	-0.72989400
C	3.04792500	1.21840500	-1.42693100
C	-1.18147000	1.45269200	-3.03167100
C	-0.00000300	0.71888900	-3.47725100
C	0.76402800	-2.59372300	-2.35439500
C	1.19108800	-1.40931900	-3.05487100
C	1.18146400	1.45269300	-3.03167300
C	2.67059700	-2.29209800	-0.74374200
C	3.51043900	0.04405900	-0.69830400
C	2.31584600	0.75688500	-2.60275500
C	3.07229000	-1.14031000	-1.43940300
C	2.32940200	-0.69947100	-2.60796800
N	0.00000100	-1.88388400	0.00027000

TS1b

Sum of electronic and zero-point Energies= -2339.624051
Sum of electronic and thermal Energies= -2339.602914
Sum of electronic and thermal Enthalpies= -2339.601970
Sum of electronic and thermal Free Energies= -2339.668148

C	2.33256700	-0.67160100	-2.56086000
C	2.31355800	0.78853800	-2.58089700
C	1.17779700	1.47587700	-3.01162600
C	0.00000600	0.73363300	-3.43322600
C	-0.00000800	-0.66260400	-3.38319700
C	1.17831400	-1.38639400	-2.93559600
C	3.05834100	1.27030200	-1.42284400
C	0.72865400	2.67265700	-2.30357400
C	-1.17776900	1.47590100	-3.01162500
C	-1.17834400	-1.38637000	-2.93559600
C	0.77201700	-2.58499000	-2.21431400
C	3.15158400	-1.09441800	-1.42728100
C	-2.33258200	-0.67155400	-2.56085800
C	-2.31354400	0.78858500	-2.58089600
C	-3.15160800	-1.09435400	-1.42727900
C	-3.05831600	1.27036400	-1.42284200
C	2.61712500	2.40182900	-0.72900900
C	-0.72860200	2.67267200	-2.30357400
C	-3.55277200	0.11088100	-0.69688400
C	-1.42949400	3.11944600	-1.17996900
C	1.42955700	3.11941700	-1.17997000
C	-0.77207100	-2.58497600	-2.21431500
C	1.72839000	-3.09020200	-1.23805000
C	2.61712600	2.40182700	0.72901400
C	2.85525500	-2.27563900	-0.75445800
C	3.55277400	0.11080900	-0.69688600
C	1.13824900	-3.51072500	-0.00000500
C	2.85525600	-2.27564100	0.75444900
C	3.55277400	0.11080700	0.69688300
C	-2.61707700	2.40188200	-0.72900700
C	-1.72845400	-3.09016800	-1.23804900
C	0.69877900	3.57161900	0.00000500
C	1.72839300	-3.09020800	1.23804000
C	3.15158600	-1.09442200	1.42727500
C	3.05834200	1.27029800	1.42284500
C	2.31356000	0.78853000	2.58089800
C	1.42955800	3.11941300	1.17997800
C	-0.69870600	3.57163300	0.00000600
C	-1.42949300	3.11944200	1.17997900
C	2.33256900	-0.67160900	2.56085600
C	1.17831600	-1.38640300	2.93559100
C	-0.00000600	-0.66261400	3.38319500
C	0.77201900	-2.58499800	2.21430600
C	-2.85530100	-2.27558100	-0.75445700
C	-0.72860000	2.67266500	2.30358200
C	-1.13832000	-3.51070300	-0.00000400
C	-1.72845500	-3.09017300	1.23804100
C	0.72865600	2.67265000	2.30358100
C	-2.61707600	2.40188000	0.72901600
C	-3.05831500	1.27036000	1.42284700
C	1.17779900	1.47586800	3.01163000
C	0.00000900	0.73362300	3.43322800
C	-0.77207000	-2.58498300	2.21430700
C	-1.17834200	-1.38637900	2.93559300
C	-1.17776700	1.47589200	3.01163100
C	-2.85530100	-2.27558400	0.75445100
C	-3.55277200	0.11087900	0.69688600
C	-2.31354200	0.78857700	2.58089900
C	-3.15160700	-1.09435900	1.42727700
C	-2.33258100	-0.67156200	2.56085800
N	-0.00002800	-2.75103700	-0.00000200

1c

Sum of electronic and zero-point Energies= -2339.860697
Sum of electronic and thermal Energies= -2339.839630
Sum of electronic and thermal Enthalpies= -2339.838686
Sum of electronic and thermal Free Energies= -2339.904705

C	0.62964600	-2.31457900	2.60245700
C	-0.82957900	-2.31411900	2.60804000
C	-1.52501400	-1.18096000	3.03715100
C	-0.79019800	0.00000000	3.48117900
C	0.60716300	0.00000000	3.46990000
C	1.33677100	-1.18022400	3.02172000
C	-1.28604700	-3.04592100	1.42964500
C	-2.70592500	-0.73027400	2.31086000
C	-1.52501400	1.18095900	3.03715200
C	1.33677100	1.18022300	3.02172000
C	2.52442700	-0.74068900	2.30231600
C	1.07131800	-3.04087900	1.42716800
C	0.62964600	2.31457800	2.60245800
C	-0.82957900	2.31411800	2.60804100
C	1.07131900	3.04087900	1.42716900
C	-1.28604700	3.04592100	1.42964600
C	-2.41615500	-2.61165900	0.73019700
C	-2.70592500	0.73027400	2.31086100
C	-0.10804700	3.49697200	0.69813000
C	-3.14155700	1.42908500	1.18072800
C	-3.14155700	-1.42908500	1.18072800
C	2.52442700	0.74068800	2.30231600
C	2.96108300	-1.45966700	1.19664900
C	-2.41615100	-2.61165900	-0.73021200
C	2.20007000	-2.60013500	0.72859100
C	-0.10804800	-3.49697300	0.69812900
C	3.56357400	-0.79229200	0.00001200
C	2.20007500	-2.60013500	-0.72857800
C	-0.10804300	-3.49697300	-0.69813000
C	-2.41615500	2.61165900	0.73019800
C	2.96108300	1.45966700	1.19664900
C	-3.59160000	-0.69866400	-0.00001100
C	2.96108900	-1.45966700	-1.19663100
C	1.07132700	-3.04088000	-1.42716200
C	-1.28603800	-3.04592100	-1.42965300
C	-0.82956300	-2.31411800	-2.60804500
C	-3.14155000	-1.42908500	-1.18074700
C	-3.59160000	0.69866400	-0.00001000
C	-3.14155000	1.42908500	-1.18074600
C	0.62966200	-2.31457800	-2.60245400
C	1.33679000	-1.18022300	-3.02171100
C	0.60718400	0.00000000	-3.46989500
C	2.52444100	-0.74068900	-2.30230000
C	2.20007100	2.60013500	0.72859200
C	-2.70591100	0.73027400	-2.31087600
C	3.56357400	0.79229200	0.00001300
C	2.96108900	1.45966700	-1.19663000
C	-2.70591100	-0.73027400	-2.31087600
C	-2.41615100	2.61165900	-0.73021100
C	-1.28603800	3.04592100	-1.42965200
C	-1.52499500	-1.18095900	-3.03716000
C	-0.79017700	0.00000100	-3.48118300
C	2.52444100	0.74068900	-2.30230000
C	1.33679000	1.18022400	-3.02171000
C	-1.52499500	1.18096000	-3.03716000
C	2.20007500	2.60013500	-0.72857800
C	-0.10804300	3.49697300	-0.69812900
C	-0.82956300	2.31411900	-2.60804500
C	1.07132700	3.04088000	-1.42716100
C	0.62966200	2.31457900	-2.60245300
N	4.78100400	0.00000000	-0.00000400

TS1b-3 (in Fig. S2)

Sum of electronic and zero-point Energies= -2339.647968
Sum of electronic and thermal Energies= -2339.627119
Sum of electronic and thermal Enthalpies= -2339.626175
Sum of electronic and thermal Free Energies= -2339.691794

C	-0.50341400	3.41037700	-0.96088900
C	0.92345800	3.41169700	-0.67226000
C	1.37235400	3.26479400	0.64620700
C	0.40726600	3.10510900	1.73382400
C	-0.95927400	3.11025400	1.45937100
C	-1.42847800	3.28055100	0.08832500
C	1.60357000	2.70512900	-1.75416800
C	2.51600300	2.41538300	0.93743200
C	0.95728200	2.15298600	2.69265600
C	-1.84205700	2.14301200	2.12140100
C	-2.59228600	2.44050600	-0.08283300
C	-0.70978000	2.69059800	-2.20553900
C	-1.31247900	1.22557600	3.05169200
C	0.10826900	1.23080700	3.32774700
C	-1.76895600	-0.17593800	3.05531600
C	0.54409200	-0.15101900	3.50907600
C	2.70519000	1.89188900	-1.47284600
C	2.25609700	1.72654400	2.20187500
C	-0.61475600	-1.02242600	3.34174400
C	2.67321200	0.40231000	2.37474200
C	3.17138300	1.74239600	-0.09934000
C	-2.86234400	1.76498800	1.18749900
C	-2.77937200	1.75118900	-1.28072100
C	2.84659100	0.60158400	-2.13938400
C	-1.82816200	1.84453400	-2.34477800
C	0.59079000	2.25890700	-2.70428300
C	-3.29767200	0.32747100	-1.22390700
C	-1.70069000	0.53924000	-3.00637600
C	0.72003600	1.01955500	-3.33447100
C	1.79764800	-0.55412500	3.04287100
C	-3.27410600	0.35862700	1.11174000
C	3.60490600	0.36143300	0.08168500
C	-2.58994100	-0.42381100	-2.40099100
C	-0.44179600	0.14510100	-3.50527800
C	1.87679300	0.17867600	-3.05444400
C	1.42978500	-1.21033200	-3.05409000
C	3.40356100	-0.34269900	-1.17857500
C	3.35819200	-0.29477800	1.29283400
C	2.91370000	-1.68344000	1.29790300
C	0.00013200	-1.22142400	-3.34141800
C	-0.83251400	-2.15087700	-2.69707900
C	-0.26872100	-3.10844000	-1.74272300
C	-2.13157300	-1.73750600	-2.21448000
C	-2.74148600	-0.62067600	2.15645500
C	2.71917700	-2.36157800	0.08758700
C	-4.32095100	-0.18358800	-0.10610700
C	-2.82288300	-1.71441500	0.09755000
C	2.97083200	-1.67386800	-1.17721900
C	1.95252800	-1.84653700	2.37943300
C	0.84874400	-2.68771900	2.22264700
C	1.96583100	-2.11364100	-2.13158600
C	1.09839300	-3.08074800	-1.45738200
C	-2.38463500	-2.49400000	-0.96671400
C	-1.23219400	-3.30497400	-0.65560100
C	1.57332000	-3.23821200	-0.08747500
C	-2.54278700	-1.90007100	1.50274200
C	-0.45710800	-2.27772300	2.72674400
C	0.64575900	-3.39691100	0.95595200
C	-1.45015800	-2.74071200	1.77416500
C	-0.77321700	-3.44399100	0.67947500
N	-2.64951800	-0.29575200	-0.07348500

1c-3 (in Fig. S2)

Sum of electronic and zero-point Energies= -2339.757869
Sum of electronic and thermal Energies= -2339.736359
Sum of electronic and thermal Enthalpies= -2339.735415
Sum of electronic and thermal Free Energies= -2339.802219

C	0.65306500	2.31355500	-2.60427300
C	-0.80448500	2.32410500	-2.60830800
C	-1.50908400	1.19522100	-3.03644600
C	-0.78444700	0.00696100	-3.47904100
C	0.61319800	-0.00472900	-3.46631600
C	1.34889600	1.17056300	-3.01890200
C	-1.25439300	3.06036400	-1.42941200
C	-2.69369400	0.75565300	-2.31068900
C	-1.53125700	-1.16736700	-3.03660800
C	1.33275800	-1.19273900	-3.01465100
C	2.52750000	0.72358300	-2.29331100
C	1.10291100	3.03536000	-1.42892200
C	0.61129000	-2.32402700	-2.60341500
C	-0.84785600	-2.30820300	-2.60912100
C	1.04148700	-3.05563200	-1.43153300
C	-1.31257300	-3.03702700	-1.43097700
C	-2.38786000	2.63470900	-0.73014000
C	-2.70726700	-0.70503400	-2.31036500
C	-0.13997000	-3.50234200	-0.69887400
C	-3.15010100	-1.39954100	-1.18045500
C	-3.12343000	1.45854000	-1.18066200
C	2.51403200	-0.75161100	-2.28677900
C	2.96466700	1.42217300	-1.18265400
C	-2.38785500	2.63470900	0.73015500
C	2.22295300	2.57757600	-0.72773400
C	-0.07268900	3.50280500	-0.69826100
C	3.63189100	0.76357600	-0.00001000
C	2.22295800	2.57757600	0.72772200
C	-0.07268500	3.50280500	0.69826300
C	-2.43665300	-2.58959800	-0.73037700
C	2.90246700	-1.46196800	-1.16341200
C	-3.58008000	0.73251400	0.00001000
C	2.96467300	1.42217300	1.18263800
C	1.10291900	3.03535900	1.42891600
C	-1.25438500	3.06036300	1.42942000
C	-0.80447000	2.32410500	2.60831300
C	-3.12342300	1.45854000	1.18068100
C	-3.59304300	-0.66494100	0.00001000
C	-3.15009500	-1.39954200	1.18047300
C	0.65308000	2.31355400	2.60427000
C	1.34891400	1.17056200	3.01889500
C	0.61321800	-0.00473000	3.46631200
C	2.52751400	0.72358200	2.29329700
C	2.16371500	-2.61279100	-0.72260100
C	-2.70725400	-0.70503500	2.31038100
C	2.90247300	-1.46196800	1.16339500
C	-2.69368100	0.75565200	2.31070400
C	-2.43664800	-2.58959800	0.73039100
C	-1.31256500	-3.03702800	1.43098400
C	-1.50906700	1.19522000	3.03645600
C	-0.78442700	0.00696000	3.47904600
C	2.51404500	-0.75161200	2.28676400
C	1.33277500	-1.19274000	3.01464300
C	-1.53123900	-1.16736800	3.03661700
C	2.16371900	-2.61279200	0.72258800
C	-0.13996600	-3.50234200	0.69887400
C	-0.84784100	-2.30820400	2.60912500
C	1.04149500	-3.05563300	1.43152600
C	0.61130500	-2.32402800	2.60341000
C	4.96710500	0.00246600	-0.00001400
N	3.50353800	-0.83204000	-0.00001000

2a

Sum of electronic and zero-point Energies= -2512.928983
Sum of electronic and thermal Energies= -2512.901955
Sum of electronic and thermal Enthalpies= -2512.901011
Sum of electronic and thermal Free Energies= -2512.980813

C	-0.38379200	-0.00001300	3.42327900
C	-1.08753400	1.18043800	2.93695400
C	-0.36109000	2.31939800	2.56379500
C	1.09463700	2.31686200	2.64529300
C	1.76708600	1.18197300	3.10958300
C	1.01074300	-0.00001300	3.51411500
C	-2.22978900	0.74299100	2.15244900
C	-0.74367100	3.04236500	1.36827500
C	1.61146800	3.04792500	1.49133900
C	2.98230900	0.73084900	2.44530100
C	1.76708600	-1.18199600	3.10957400
C	-1.08753400	-1.18046000	2.93694600
C	3.47720500	1.42986100	1.33935900
C	2.77667700	2.61275300	0.85195600
C	3.98746900	0.69900800	0.18383000
C	2.85265500	2.61279100	-0.60648100
C	-2.60470700	1.44114000	1.02326200
C	0.47204200	3.49902300	0.69996800
C	3.59973200	1.42983400	-1.01854800
C	0.54496100	3.49982500	-0.69451700
C	-1.83225400	2.58958500	0.61062700
C	2.98230900	-0.73086800	2.44529500
C	1.09463700	-2.31688200	2.64527600
C	-3.29948500	0.81094900	-0.19823900
C	-0.36109100	-2.31941800	2.56377700
C	-2.22978900	-0.74300700	2.15244300
C	1.61146700	-3.04793600	1.49131500
C	-0.74367200	-3.04237500	1.36825200
C	-2.60470700	-1.44114700	1.02325100
C	1.76007200	3.04826000	-1.36325500
C	3.47720500	-1.42987100	1.33934900
C	-1.75675000	2.59236100	-0.84495800
C	0.47204100	-3.49902800	0.69994200
C	-1.83225500	-2.58958900	0.61060800
C	-3.29948500	-0.81094600	-0.19824500
C	-2.48449700	-1.44634600	-1.33661200
C	-2.48449700	1.44635700	-1.33660200
C	-0.59477100	3.04331500	-1.48527000
C	-0.09070200	2.31931900	-2.63443100
C	-1.75675100	-2.59235400	-0.84497800
C	-0.59477100	-3.04330300	-1.48529200
C	-0.09070200	-2.31929900	-2.63444900
C	0.54496100	-3.49981900	-0.69454400
C	3.98746900	-0.69900800	0.18382500
C	-0.77452000	1.18048700	-3.08126100
C	2.77667700	-2.61275900	0.85193700
C	2.85265500	-2.61278600	-0.60650100
C	-1.99220100	0.74348300	-2.41915200
C	1.36579200	2.31705500	-2.56449700
C	2.08260200	1.18204100	-2.95634000
C	-1.99220100	-0.74346400	-2.41915800
C	-0.77452000	-1.18046300	-3.08126900
C	1.76007200	-3.04824900	-1.36327800
C	1.36579100	-2.31703500	-2.56451400
C	-0.02411400	0.00001400	-3.49142400
C	3.59973200	-1.42982500	-1.01855800
C	3.22246700	0.73086800	-2.16995000
C	1.37214500	0.00001300	-3.43708100
C	3.22246700	-0.73085100	-2.16995500
C	2.08260200	-1.18201800	-2.95634900
N	-5.47018700	-0.00000100	0.36418300
C	-6.92887800	0.00000000	0.23813100
C	-4.82367100	1.15380700	-0.26401400
C	-4.82367100	-1.15380400	-0.26402300
H	-7.33783500	-0.88620800	0.73388200
H	-7.27040800	0.00000400	-0.81479900
H	-7.33783500	0.88620300	0.73388900
H	-5.05980400	2.07828500	0.27088400
H	-5.12583500	1.27841100	-1.32258200
H	-5.12583500	-1.27839900	-1.32259200
H	-5.05980500	-2.07828600	0.27086700
N	0.46767000	-0.00001600	0.00111400

2b

Sum of electronic and zero-point Energies= -2512.896841
Sum of electronic and thermal Energies= -2512.871327
Sum of electronic and thermal Enthalpies= -2512.870382
Sum of electronic and thermal Free Energies= -2512.944862

C	0.35698100	-0.00000300	3.30106800
C	1.05428400	-1.18014700	2.81385800
C	0.30603400	-2.33810000	2.51010300
C	-1.14910300	-2.32037400	2.62530200
C	-1.80410000	-1.18018700	3.09038900
C	-1.02877400	-0.00000300	3.45685800
C	2.21618300	-0.79188600	2.03628300
C	0.64700800	-3.13372200	1.35494800
C	-1.70432600	-3.06634000	1.50022700
C	-3.03547700	-0.73060900	2.45828500
C	-1.80410000	1.18018100	3.09039100
C	1.05428400	1.18014200	2.81386000
C	-3.55637200	-1.43131900	1.36455000
C	-2.87376200	-2.62101500	0.87321000
C	-4.07672800	-0.69846900	0.21390200
C	-2.96157600	-2.62109800	-0.58485500
C	2.63965100	-1.71585900	1.03799300
C	-0.59017600	-3.55613600	0.70291400
C	-3.69781000	-1.43121400	-0.99086900
C	-0.67450800	-3.55706900	-0.68953800
C	1.77483500	-2.78949000	0.60526400
C	-3.03547700	0.73060400	2.45828600
C	-1.14910300	2.32036900	2.62530600
C	3.38267700	-1.22333300	-0.23675000
C	0.30603400	2.33809600	2.51010700
C	2.21618300	0.79188300	2.03628500
C	-1.70432600	3.06633700	1.50023200
C	0.64700800	3.13372000	1.35495300
C	2.63965100	1.71585700	1.03799600
C	-1.87598800	-3.06697500	-1.34752900
C	-3.55637200	1.43131700	1.36455200
C	1.68561200	-2.79295700	-0.87592400
C	-0.59017600	3.55613500	0.70292000
C	1.77483500	2.78948900	0.60526800
C	3.38267700	1.22333300	-0.23674800
C	2.49438100	1.72375600	-1.41104600
C	2.49438100	-1.72375400	-1.41104900
C	0.47534000	-3.13489600	-1.48503300
C	-0.00075800	-2.33876600	-2.59086900
C	1.68561200	2.79295800	-0.87591900
C	0.47534000	3.13489800	-1.48502800
C	-0.00075800	2.33877000	-2.59086500
C	-0.67450800	3.55707000	-0.68953200
C	-4.07672800	0.69846900	0.21390300
C	0.70657000	-1.18093000	-2.98304300
C	-2.87376200	2.62101400	0.87321400
C	-2.96157600	2.62109900	-0.58485100
C	1.95373400	-0.79522000	-2.35116900
C	-1.45930300	-2.32085200	-2.53098500
C	-2.16474300	-1.18018800	-2.91372100
C	1.95373400	0.79522400	-2.35116800
C	0.70657000	1.18093500	-2.98304100
C	-1.87598800	3.06697700	-1.34752400
C	-1.45930300	2.32085600	-2.53098100
C	-0.04406700	0.00000300	-3.38162900
C	-3.69781000	1.43121600	-0.99086600
C	-3.31193100	-0.73061800	-2.13928600
C	-1.43837200	0.00000300	-3.36967500
C	-3.31193100	0.73062200	-2.13928400
C	-2.16474300	1.18019300	-2.91371900
N	5.40538800	0.00000000	0.36259800
C	6.86857900	0.00000000	0.47424900
C	4.91459800	-1.21484500	-0.31833500
C	4.91459800	1.21484500	-0.31833300
H	7.19029900	0.88688300	1.02945400
H	7.37932500	0.00000000	-0.50719400
H	7.19029900	-0.88688400	1.02945200
H	5.33216600	-2.09375100	0.18190300
H	5.23028400	-1.24776700	-1.37947000
H	5.23028400	1.24776900	-1.37946800
H	5.33216600	2.09375000	0.18190700
N	2.74576900	0.00000000	-0.20569400

TS2b

Sum of electronic and zero-point Energies= -2512.862673
Sum of electronic and thermal Energies= -2512.837193
Sum of electronic and thermal Enthalpies=-2512.836249
Sum of electronic and thermal Free Energies=-2512.910791

C	-3.26631200	0.39201700	0.00000000
C	-2.75629400	1.07229600	1.17201000
C	-2.48529500	0.32954100	2.33177800
C	-2.63491000	-1.12072700	2.32026600
C	-3.11408200	-1.76968400	1.18017100
C	-3.46547100	-0.99124500	0.00000000
C	-1.93643400	2.21469200	0.77224800
C	-1.32662100	0.65686800	3.13453800
C	-1.52005700	-1.69309600	3.06912900
C	-2.50237300	-3.01213300	0.73081800
C	-3.11408200	-1.76968400	-1.18017100
C	-2.75629400	1.07229600	-1.17201000
C	-1.41629200	-3.54752700	1.43160500
C	-0.91353000	-2.87280300	2.62278200
C	-0.27419000	-4.08506000	0.69884500
C	0.54305100	-2.98623500	2.62318000
C	-0.95561000	2.63620100	1.68766700
C	-0.70383800	-0.59225100	3.56405400
C	0.93644300	-3.72695500	1.43218100
C	0.68741200	-0.70386500	3.56860400
C	-0.55891700	1.76780900	2.78923200
C	-2.50237300	-3.01213300	-0.73081800
C	-2.63491000	-1.12072700	-2.32026600
C	0.28785500	3.43313300	1.27426300
C	-2.48529500	0.32954100	-2.33177800
C	-1.93643400	2.21469200	-0.77224800
C	-1.52005700	-1.69309600	-3.06912900
C	-1.32662100	0.65686800	-3.13453800
C	-0.95561000	2.63620100	-1.68766700
C	1.32298000	-1.91427100	3.07157000
C	-1.41629200	-3.54752700	-1.43160500
C	0.91911600	1.66281700	2.83270600
C	-0.70383800	-0.59225100	-3.56405400
C	-0.55891700	1.76780900	-2.78923200
C	0.28785500	3.43313300	-1.27426300
C	1.46345300	2.48167300	-1.78298100
C	1.46345300	2.48167300	1.78298100
C	1.50206800	0.43417500	3.15711300
C	2.59456500	-0.05599000	2.34780500
C	0.91911600	1.66281700	-2.83270600
C	1.50206800	0.43417500	-3.15711300
C	2.59456500	-0.05599000	-2.34780500
C	0.68741200	-0.70386500	-3.56860400
C	-0.27419000	-4.08506000	-0.69884500
C	2.97684900	0.64946200	1.18492900
C	-0.91353000	-2.87280300	-2.62278200
C	0.54305100	-2.98623500	-2.62318000
C	2.35260200	1.90549800	0.80589600
C	2.51069800	-1.51299800	2.32356500
C	2.87982000	-2.22102200	1.18025400
C	2.35260200	1.90549800	-0.80589600
C	2.97684900	0.64946200	-1.18492900
C	1.32298000	-1.91427100	-3.07157000
C	2.51069800	-1.51299800	-2.32356500
C	3.36085300	-0.10435900	0.00000000
C	0.93644300	-3.72695500	-1.43218100
C	2.08988200	-3.35713200	0.73048400
C	3.34102600	-1.49844500	0.00000000
C	2.08988200	-3.35713200	-0.73048400
C	2.87982000	-2.22102200	-1.18025400
N	-0.37584800	5.42981300	0.00000000
C	-0.67254400	6.86831500	0.00000000
C	0.28797700	5.00443700	1.26419300
C	0.28797700	5.00443700	-1.26419300
H	-1.26563100	7.11584900	-0.88618300
H	0.23092200	7.50471600	0.00000000
H	-1.26563100	7.11584900	0.88618300
H	-0.27808300	5.41749800	2.10283400
H	1.33493400	5.34479900	1.33702900
H	1.33493400	5.34479900	-1.33702900
H	-0.27808300	5.41749800	-2.10283400
N	0.56518900	3.11576000	0.00000000

2c

Sum of electronic and zero-point Energies= -2512.883181
Sum of electronic and thermal Energies= -2512.857546
Sum of electronic and thermal Enthalpies= -2512.856602
Sum of electronic and thermal Free Energies= -2512.931412

N	3.55352400	0.00000000	-1.11493300
C	-0.26360500	0.00000000	-3.37695100
C	0.50349300	1.17775900	-3.02063200
C	-0.17655200	2.34189100	-2.61753900
C	-1.62813100	2.32407500	-2.47076300
C	-2.35469700	1.18084600	-2.80691100
C	-1.65759800	0.00000000	-3.30119100
C	1.79563400	0.79667200	-2.46296900
C	0.37072500	3.14631100	-1.54729400
C	-1.96801000	3.07004700	-1.26224600
C	-3.45221700	0.73069500	-1.96316100
C	-2.35469700	-1.18084600	-2.80691100
C	0.50349300	-1.17775900	-3.02063200
C	-3.76297400	1.43154100	-0.79283300
C	-3.00217500	2.62212700	-0.43373000
C	-4.06557000	0.69900700	0.43281700
C	-2.82288900	2.62163700	1.01637700
C	2.41467300	1.75170600	-1.60428200
C	-0.72545200	3.56073200	-0.68112600
C	-3.47659400	1.43180100	1.54916500
C	-0.54971700	3.55258000	0.70358500
C	1.61642000	2.80088700	-1.02207700
C	-3.45221700	-0.73069500	-1.96316100
C	-1.62813100	-2.32407500	-2.47076300
C	3.41770400	1.23551500	-0.50561700
C	-0.17655200	-2.34189100	-2.61753900
C	1.79563400	-0.79667200	-2.46296900
C	-1.96801000	-3.07004700	-1.26224600
C	0.37072500	-3.14631100	-1.54729400
C	2.41467300	-1.75170600	-1.60428200
C	-1.61716900	3.06679200	1.56997300
C	-3.76297400	-1.43154100	-0.79283300
C	1.78140200	2.72651500	0.43777000
C	-0.72545200	-3.56073200	-0.68112600
C	1.61642000	-2.80088700	-1.02207700
C	3.41770400	-1.23551500	-0.50561700
C	2.61256800	-1.57209600	0.75496100
C	2.61256800	1.57209600	0.75496100
C	0.72269100	3.10624400	1.26653300
C	0.44111600	2.32806500	2.45164900
C	1.78140200	-2.72651500	0.43777000
C	0.72269100	-3.10624400	1.26653300
C	0.44111600	-2.32806500	2.45164900
C	-0.54971700	-3.55258000	0.70358500
C	-4.06557000	-0.69900700	0.43281700
C	1.19157800	1.17283000	2.70443400
C	-3.00217500	-2.62212700	-0.43373000
C	-2.82288900	-2.62163700	1.01637700
C	2.27728000	0.75358000	1.82370100
C	-1.00139700	2.32068100	2.66356700
C	-1.63016500	1.18155200	3.17272800
C	2.27728000	-0.75358000	1.82370100
C	1.19157800	-1.17283000	2.70443400
C	-1.61716900	-3.06679200	1.56997300
C	-1.00139700	-2.32068100	2.66356700
C	0.53576600	0.00000000	3.25010900
C	-3.47659400	-1.43180100	1.54916500
C	-2.89586900	0.73089800	2.61165800
C	-0.83920000	0.00000000	3.49742800
C	-2.89586900	-0.73089800	2.61165800
C	-1.63016500	-1.18155200	3.17272800
N	5.32682500	0.00000000	0.44236500
C	6.70106400	0.00000000	0.95821700
C	5.00121500	1.31591500	-0.24222300
C	5.00121500	-1.31591500	-0.24222300
H	6.85499000	-0.88529800	1.58409600
H	6.85499000	0.88529800	1.58409600
H	5.51581700	1.45459400	-1.20299300
H	5.28115000	2.11302100	0.45366100
H	5.28115000	-2.11302100	0.45366100
H	5.51581700	-1.45459400	-1.20299400
H	7.47203100	0.00000000	0.16658200

3a

Sum of electronic and zero-point Energies= -2913.096163
Sum of electronic and thermal Energies= -2913.060013
Sum of electronic and thermal Enthalpies= -2913.059069
Sum of electronic and thermal Free Energies= -2913.162485

C	0.43030400	3.03545000	1.58814000
C	-0.33366700	3.12574600	0.34915800
C	0.33567900	3.31102500	-0.86722800
C	1.79158800	3.40475100	-0.89608700
C	2.52041600	3.31564800	0.29329800
C	1.82391800	3.13227400	1.56364700
C	-1.46249900	2.21102000	0.43893700
C	-0.08926900	2.56705500	-2.03732200
C	2.26380300	2.71464000	-2.09314000
C	3.75150300	2.53692100	0.33899900
C	2.63212000	2.24710800	2.39822600
C	-0.22129500	2.05749300	2.45128500
C	4.20269000	1.87364400	-0.80658800
C	3.44306900	1.96421400	-2.04856700
C	4.73829900	0.51984700	-0.70230300
C	3.50708700	0.66488800	-2.71205800
C	-1.88784400	1.52423300	-0.69089400
C	1.09829200	2.19693500	-2.80130300
C	4.30635200	-0.22724000	-1.87957900
C	1.15908800	0.95414100	-3.43486100
C	-1.16453200	1.67638100	-1.93550600
C	3.82037600	1.87601500	1.64026800
C	2.01030800	1.31003500	3.22820800
C	-2.43768300	0.12895600	-0.63356900
C	0.55464600	1.21606800	3.25904000
C	-1.39010600	1.54153400	1.75889500
C	2.55148900	-0.04208400	3.33419800
C	0.19793000	-0.18392400	3.38090100
C	-1.74795400	0.20931600	1.90298700
C	2.38928200	0.17096700	-3.39208000
C	4.33772300	0.58040700	1.73950200
C	-1.10255000	0.37932900	-2.59758600
C	1.42806200	-0.96777500	3.42987000
C	-0.91893800	-0.67349600	2.69302200
C	-2.36141600	-0.58718700	0.79195700
C	-1.65608200	-1.91257000	0.82024700
C	-1.79037300	-0.59610900	-1.77654500
C	0.03516700	0.02776400	-3.33480500
C	0.56413700	-1.31779900	-3.23196500
C	-0.85860000	-1.97018800	2.03034800
C	0.32046100	-2.72335600	2.08336600
C	0.78098600	-3.41266900	0.89386700
C	1.48780500	-2.20965900	2.79454000
C	4.80411500	-0.11239100	0.54237000
C	-0.06810900	-2.24276300	-2.39183700
C	3.68941300	-0.39930900	2.60418500
C	3.75289300	-1.69869700	1.94072400
C	-1.25877200	-1.87095700	-1.64712300
C	2.02069400	-1.23604800	-3.26648600
C	2.78655500	-2.08890400	-2.46669800
C	-1.19248000	-2.54025400	-0.32905000
C	0.04133500	-3.31045300	-0.29051600
C	2.67520100	-2.58523700	2.03473500
C	2.23768800	-3.33069200	0.85831800
C	0.73413100	-3.13363200	-1.56170800
C	4.44084000	-1.52079400	0.66676900
C	3.95355900	-1.57543500	-1.76084600
C	2.12844200	-3.06314200	-1.59967100
C	4.02241100	-2.23657000	-0.45955200
C	2.89752200	-3.15800700	-0.36165200
N	1.26218600	-0.00843500	-0.00129200
C	-3.70504300	-0.26155700	0.12848800
C	-4.52248400	0.86375400	0.72510800
O	-5.09466000	1.60369100	-0.26957500
C	-5.98833000	2.71609100	0.14257500
C	-6.46093200	3.38892600	-1.13140200
C	-4.54839800	-1.40160700	-0.36692500
O	-5.82682800	-1.29578500	0.10720000
C	-6.78418900	-2.37254500	-0.26058000
C	-8.10291200	-2.02484200	0.40167000
O	-4.66597600	1.09325600	1.92649800
O	-4.16290800	-2.33597500	-1.07456000
H	-6.80774400	2.28814700	0.72762500
H	-5.41645200	3.38670500	0.79032200
H	-7.12858600	4.22232600	-0.88569900
H	-7.00655000	2.68408500	-1.76583700
H	-5.61373200	3.78154700	-1.70149700
H	-6.85012900	-2.40531000	-1.35178900
H	-6.37026300	-3.32281500	0.08830200
H	-7.99056800	-1.96967200	1.48836500
H	-8.47806300	-1.06165400	0.04315600
H	-8.84775500	-2.79393300	0.16869100

3c

Sum of electronic and zero-point Energies= -2913.041006
Sum of electronic and thermal Energies= -2913.006425
Sum of electronic and thermal Enthalpies=-2913.005480
Sum of electronic and thermal Free Energies=-2913.103420

C	-0.55145100	2.36530200	-2.44129200
C	0.18085800	2.91517100	-1.30429700
C	-0.54821800	3.46882900	-0.22132900
C	-2.00636200	3.46663500	-0.24514800
C	-2.69204900	2.94478100	-1.34283700
C	-1.94456400	2.39144100	-2.46815600
C	1.38526000	2.15611000	-1.08385800
C	-0.13219900	3.22834200	1.13912700
C	-2.48761700	3.19008500	1.10531700
C	-3.87956400	2.12816600	-1.14628000
C	-2.69294900	1.24992600	-2.98684900
C	0.17882800	1.21117300	-2.95601200
C	-4.33159500	1.84789400	0.14817700
C	-3.61722800	2.38791500	1.29730800
C	-4.78299700	0.50177100	0.48636000
C	-3.61772600	1.37162900	2.34630200
C	1.84917800	2.06989800	0.26703900
C	-1.32391300	3.02652600	1.96294500
C	-4.33220900	0.20611800	1.84266700
C	-1.32467800	2.05646500	2.96464400
C	1.03735100	2.49644700	1.38253400
C	-3.87973100	1.07880400	-2.16344200
C	-2.00784800	0.13614900	-3.47434400
C	2.39247600	0.73537600	0.72038300
C	-0.54999700	0.11193700	-3.47788700
C	1.38197200	1.01329600	-2.19443500
C	-2.48907200	-1.20507700	-3.15524400
C	-0.13362800	-1.23941900	-3.19396400
C	1.84543200	-0.33070200	-2.06553900
C	-2.48907300	1.20507700	3.15524400
C	-4.33220900	-0.20611800	-1.84266700
C	1.03698300	1.45926300	2.45516200
C	-1.32467700	-2.05646500	-2.96464400
C	1.03698300	-1.45926300	-2.45516200
C	2.39247600	-0.73537600	-0.72038300
C	1.84917800	-2.06989900	-0.26703900
C	1.84543200	0.33070200	2.06554000
C	-0.13362900	1.23941900	3.19396400
C	-0.54999800	-0.11193700	3.47788700
C	1.03735100	-2.49644700	-1.38253300
C	-0.13219900	-3.22834200	-1.13912700
C	-0.54821800	-3.46882900	0.22132900
C	-1.32391300	-3.02652600	-1.96294500
C	-4.78299700	-0.50177100	-0.48636100
C	0.17882800	-1.21117300	2.95601200
C	-3.61772600	-1.37162900	-2.34630200
C	-3.61722800	-2.38791500	-1.29730900
C	1.38197100	-1.01329600	2.19443500
C	-2.00784800	-0.13614900	3.47434400
C	-2.69295000	-1.24992600	2.98684900
C	1.38526000	-2.15611000	1.08385800
C	0.18085700	-2.91517100	1.30429700
C	-2.48761700	-3.19008500	-1.10531800
C	-2.00636200	-3.46663500	0.24514700
C	-0.55145100	-2.36530300	2.44129200
C	-4.33159500	-1.84789400	-0.14817700
C	-3.87973100	-1.07880300	2.16344100
C	-1.94456400	-2.39144100	2.46815600
C	-3.87956500	-2.12816600	1.14627900
C	-2.69205000	-2.94478100	1.34283700
N	1.32091900	0.00000000	0.00000000
C	3.54205600	0.00000000	0.00000000
C	4.44341200	0.86172700	-0.87813800
O	5.10890500	1.76485500	-0.10095000
C	6.04597300	2.70095300	-0.78042600
C	6.64252700	3.57808300	0.30234400
C	4.44341200	-0.86172700	0.87813900
O	5.10890500	-1.76485500	0.10095000
C	6.04597300	-2.70095200	0.78042600
C	6.64252700	-3.57808300	-0.30234400
O	4.58187300	0.76112400	-2.09695800
O	4.58187400	-0.76112400	2.09695800
H	6.79489700	2.10262800	-1.30720200
H	5.47329000	3.26733900	-1.52034300
H	7.34472300	4.29093600	-0.14414900
H	7.18190000	2.97610200	1.03946500
H	5.86166200	4.14103300	0.82179700
H	6.79489800	-2.10262700	1.30720100
H	5.47329100	-3.26733900	1.52034300
H	5.86166200	-4.14103400	-0.82179700
H	7.18189900	-2.97610200	-1.03946600
H	7.34472300	-4.29093600	0.14414900