

Supplementary materials

Analysis of the sensitivity of the gas electron diffraction method to the determination of the conformational composition of phenyl and thiophenyl substituted aza-BODIPY: theoretical study

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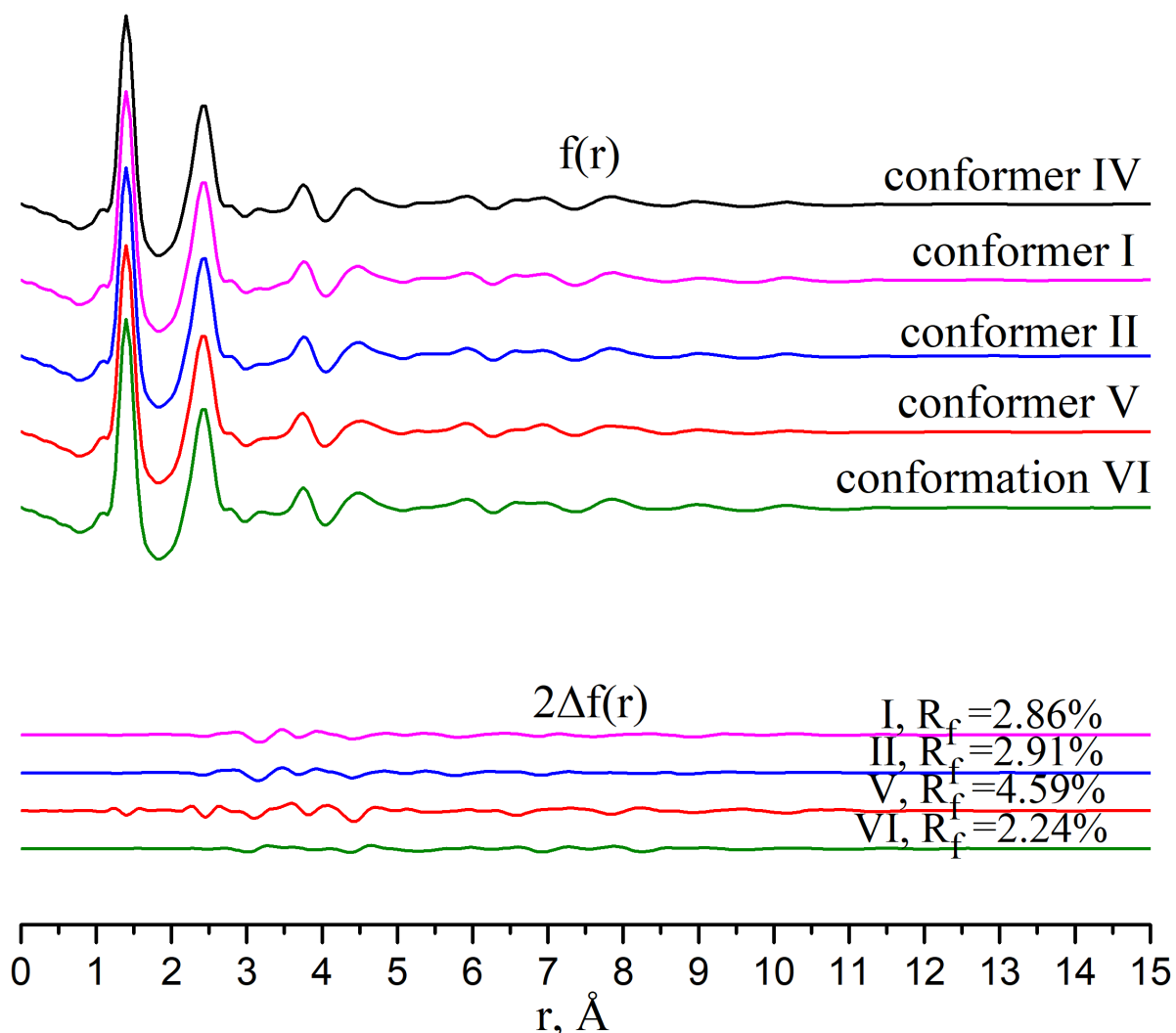


Рис. S1. Сравнение теоретических функций радиального распределения $f(r)$ для **1**. Разностные функции $\Delta f(r)$ рассчитаны относительно конформера IV (Рис. 2). Молекулярные параметры рассчитаны в приближении B3LYP/6-31G*.

Fig. S1. Comparison of theoretical radial distribution functions $f(r)$ of molecule **1**. Differences functions $\Delta f(r)$ were calculated concerning conformer IV (Fig. 2). Molecular parameters were calculated at B3LYP/6-31G* theory level.

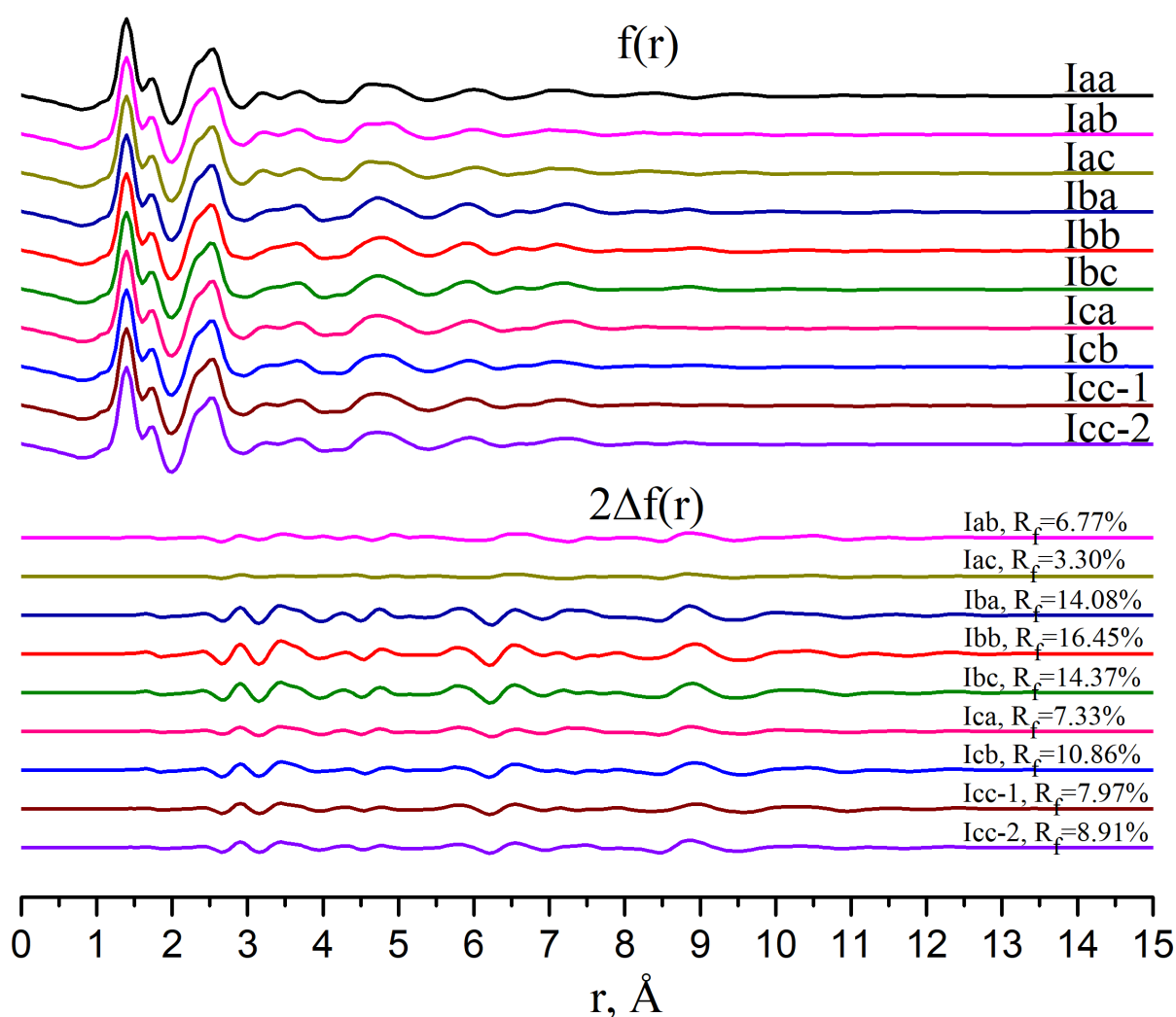


Рис. S2. Сравнение теоретических функций радиального распределения $f(r)$ для конформеров INN молекулы **2**. Разностные функции $\Delta f(r)$ рассчитаны относительно конформера Iaa (Рис. 2, 5). Молекулярные параметры рассчитаны в приближении B3LYP/6-31G*.

Fig. S2. Comparison of theoretical radial distribution functions $f(r)$ of conformers INN of molecule **2**. Differences functions $\Delta f(r)$ were calculated concerning conformer Iaa (Fig. 2, 5). Molecular parameters were calculated at B3LYP/6-31G* theory level.

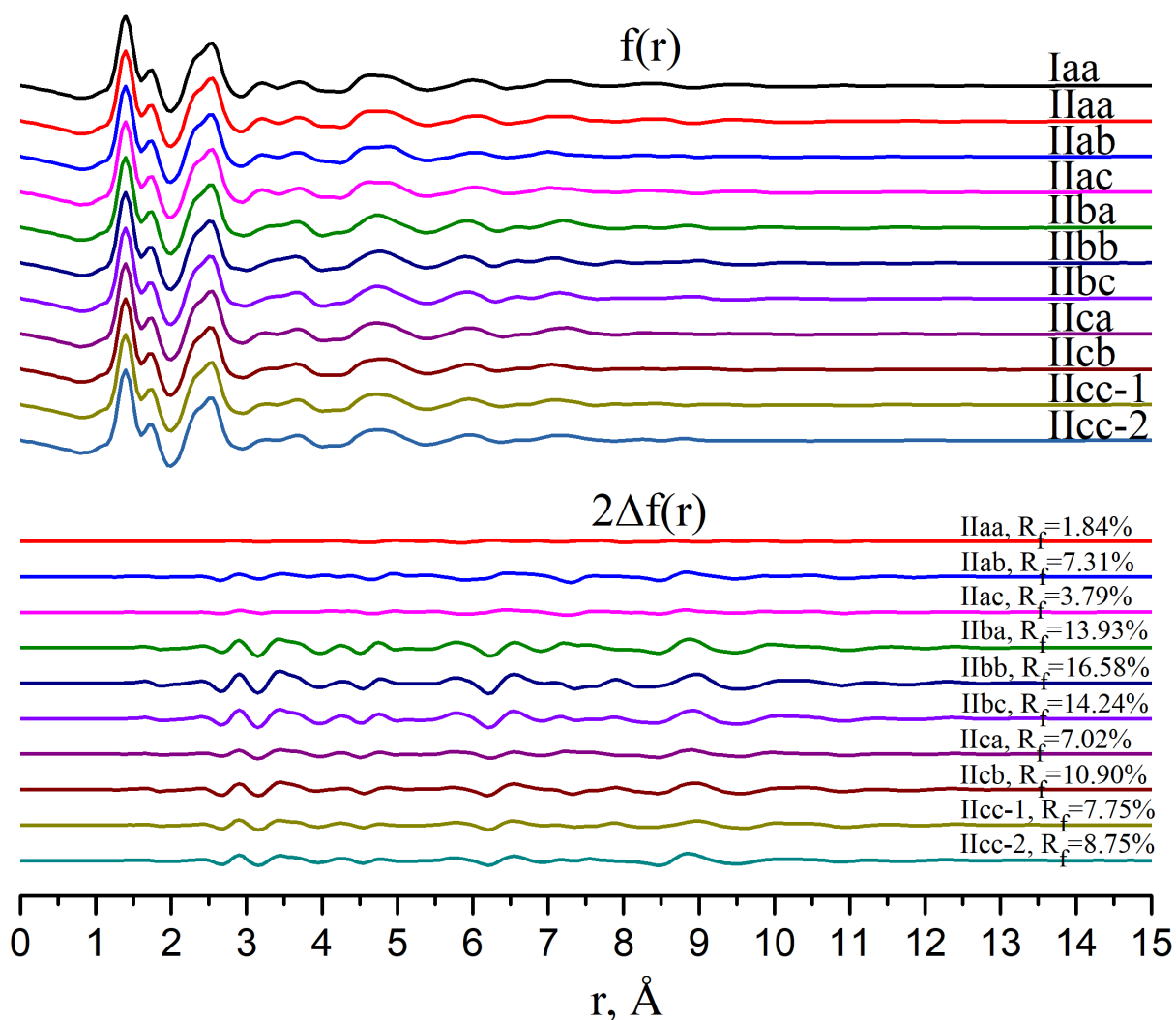


Рис. S3. Сравнение теоретических функций радиального распределения $f(r)$ для конформеров II_{NN} молекулы **2**. Разностные функции $\Delta f(r)$ рассчитаны относительно конформера Iaa (Рис. 2, 5). Молекулярные параметры рассчитаны в приближении B3LYP/6-31G*.

Fig. S3. Comparison of theoretical radial distribution functions $f(r)$ of conformers II_{NN} of molecule **2**. Differences functions $\Delta f(r)$ were calculated concerning conformer Iaa (Fig. 2, 5). Molecular parameters were calculated at B3LYP/6-31G* theory level.

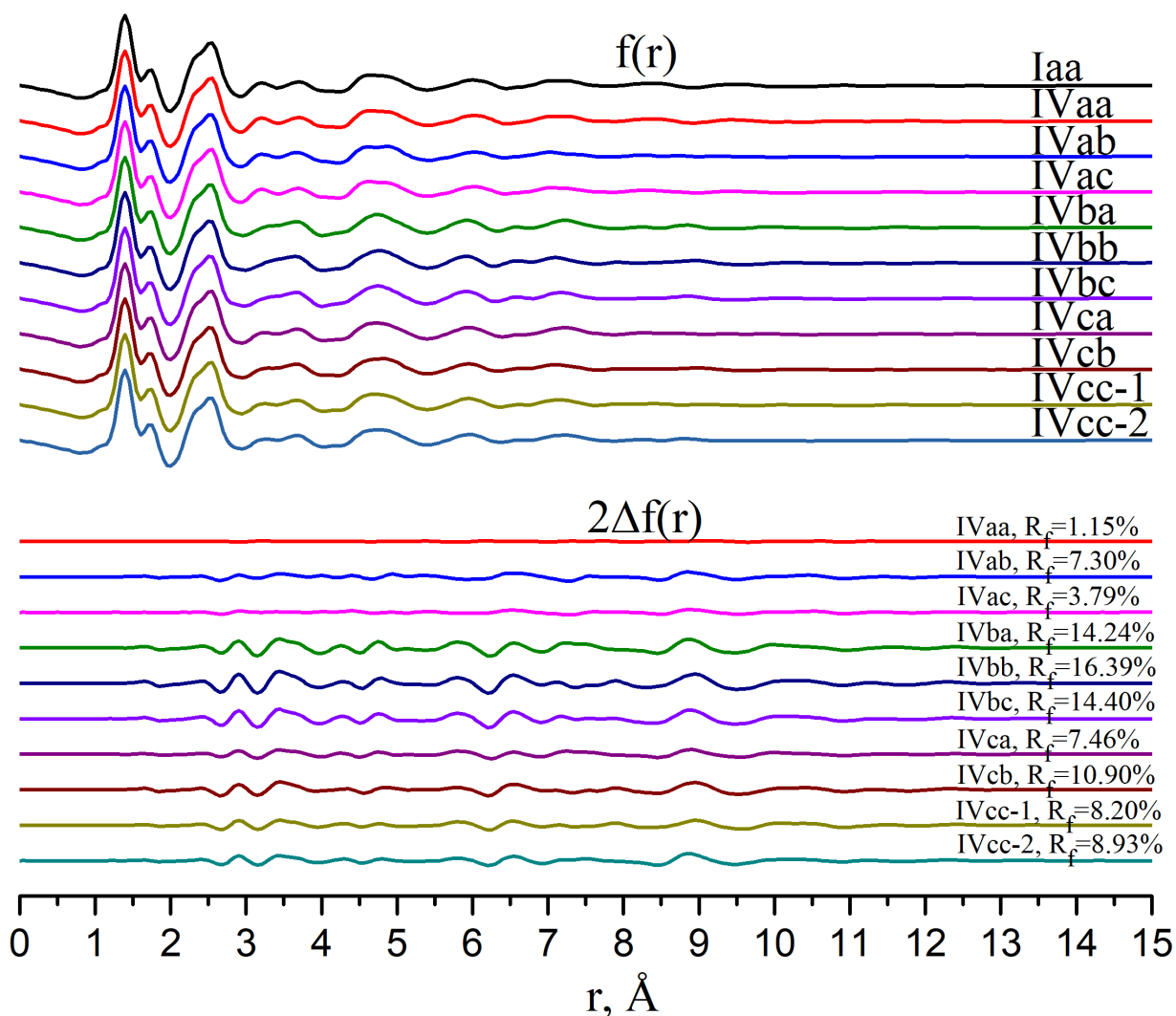


Рис. S4. Сравнение теоретических функций радиального распределения $f(r)$ для конформеров IVNN молекулы **2**. Разностные функции $\Delta f(r)$ рассчитаны относительно конформера Iaa (Рис. 2, 5). Молекулярные параметры рассчитаны в приближении B3LYP/6-31G*.

Fig. S5. Comparison of theoretical radial distribution functions $f(r)$ of conformers IVNN of molecule **2**. Differences functions $\Delta f(r)$ were calculated concerning conformer Iaa (Fig. 2, 5). Molecular parameters were calculated at B3LYP/6-31G* theory level.

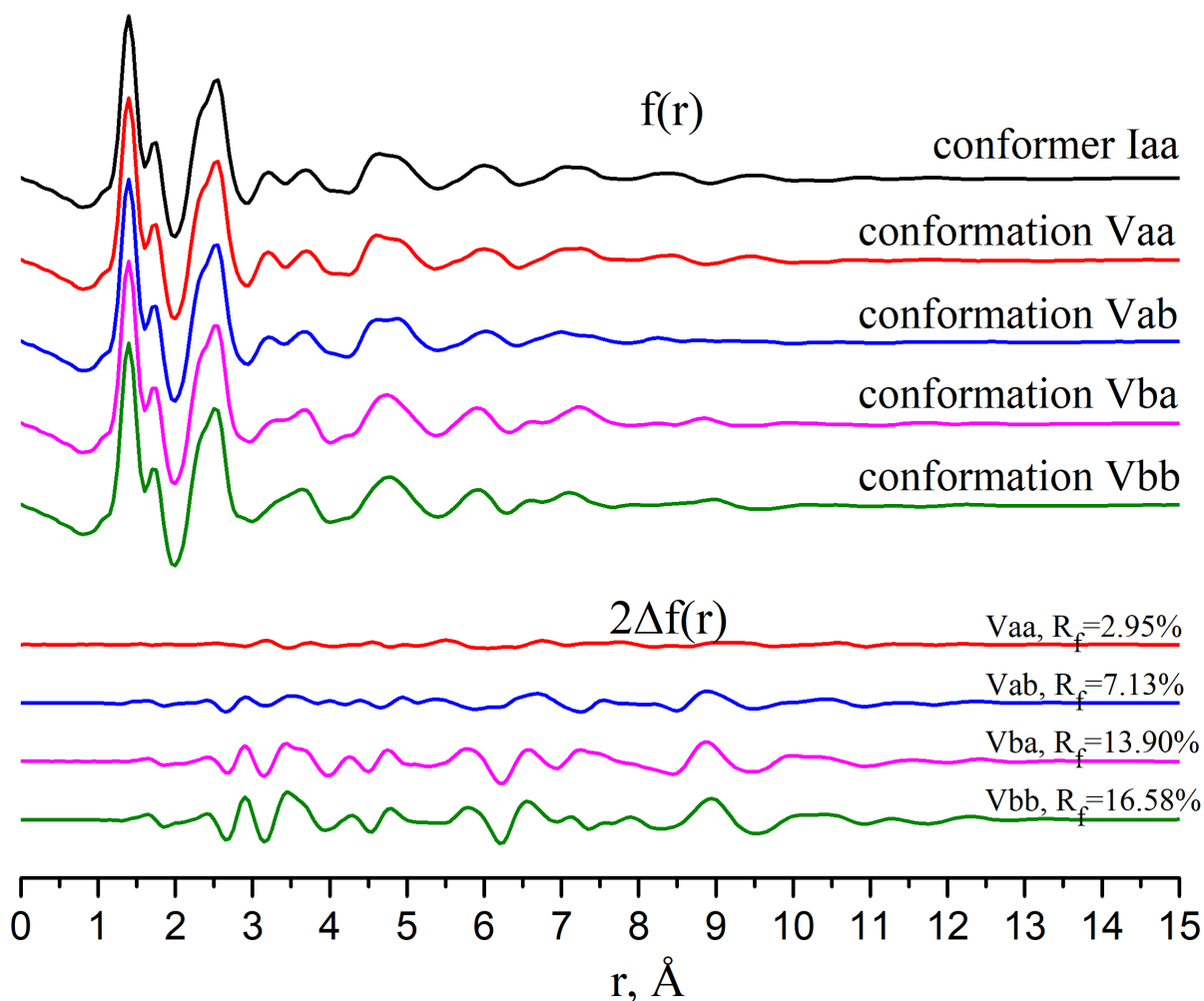


Рис. S5. Сравнение теоретических функций радиального распределения $f(r)$ для конформаций VNN молекулы **2**. Разностные функции $\Delta f(r)$ рассчитаны относительно конформера Iaa (Рис. 2, 5). Молекулярные параметры рассчитаны в приближении B3LYP/6-31G*.

Fig. S5. Comparison of theoretical radial distribution functions $f(r)$ of conformations VNN of molecule **2**. Differences functions $\Delta f(r)$ were calculated concerning conformer Iaa (Fig. 2, 5). Molecular parameters were calculated at B3LYP/6-31G* theory level.

Таблица S1. Некоторые межъядерные расстояния (Å) конформеров Iaa, Iab, Ibb молекулы **2** согласно расчетам B3LYP/cc-pVTZ.

Table S1. Comparison of internuclear distances (Å) for conformers Iaa, Iab, Ibb of molecule **2** from B3LYP/cc-pVTZ calculations.

	Iaa	Iab	Ibb
S ₁₂ ⋯S ₂₇	8.78	3.74	3.75
S ₁₇ ⋯S ₂₂	9.72	9.71	5.00
S ₁₇ ⋯F ₉	4.82	4.81	3.24
S ₁₂ ⋯N ₈	4.78	3.17	3.17
S ₁₂ ⋯S ₁₇	5.75	7.21	7.75
S ₂₇ ⋯N _{4a}	6.87	5.54	5.54
S ₂₇ ⋯F ₉	7.34	6.60	6.59
S ₁₇ ⋯N _{4a}	4.05	4.04	3.37
S ₁₇ ⋯N ₈	6.19	6.19	5.73

Optimized structures from B3LYP/6-31G* and B3LYP/cc-pVTZ calculations.
 Оптимизированные структуры согласно B3LYP/6-31G* и B3LYP/cc-pVTZ
 расчетам.

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1 | I B3LYP/6-31G*

N	-0.076083000	1.255082000	-0.703060000
C	-0.071805000	1.145960000	0.688995000
C	-0.054140000	2.462746000	1.271962000
C	0.000000000	3.335432000	0.193842000
C	-0.014428000	2.582746000	-1.009372000
N	0.076083000	-1.255082000	-0.703060000
C	0.071805000	-1.145960000	0.688995000
C	0.054140000	-2.462746000	1.271962000
C	0.000000000	-3.335432000	0.193842000
C	0.014428000	-2.582746000	-1.009372000
B	0.000000000	0.000000000	-1.648276000
N	0.000000000	0.000000000	1.343576000
F	1.145202000	0.121526000	-2.427340000
F	-1.145202000	-0.121526000	-2.427340000
H	-0.029298000	4.414635000	0.235354000
H	0.029298000	-4.414635000	0.235354000
C	-0.031358000	-3.180561000	-2.348383000
C	0.618032000	-2.629417000	-3.469308000
C	-0.725840000	-4.398615000	-2.505232000
C	0.569232000	-3.280943000	-4.699719000
C	-0.776344000	-5.039668000	-3.739002000
C	-0.125134000	-4.483850000	-4.843115000
H	1.164060000	-1.701148000	-3.370594000
H	-1.253946000	-4.825521000	-1.658206000
H	1.081837000	-2.844044000	-5.552341000
H	-1.328387000	-5.970086000	-3.839995000
H	-0.160737000	-4.984066000	-5.807168000
C	0.031358000	3.180561000	-2.348383000
C	-0.618032000	2.629417000	-3.469308000
C	0.725840000	4.398615000	-2.505232000
C	-0.569232000	3.280943000	-4.699719000
C	0.776344000	5.039668000	-3.739002000
C	0.125134000	4.483850000	-4.843115000
H	-1.164060000	1.701148000	-3.370594000
H	1.253946000	4.825521000	-1.658206000
H	-1.081837000	2.844044000	-5.552341000
H	1.328387000	5.970086000	-3.839995000
H	0.160737000	4.984066000	-5.807168000
C	-0.076842000	2.808050000	2.695545000

C	0.459859000	4.037887000	3.125224000
C	-0.646693000	1.954732000	3.660874000
C	0.427786000	4.403582000	4.467989000
C	-0.675423000	2.324203000	5.004205000
C	-0.141521000	3.547829000	5.414727000
H	0.926195000	4.698725000	2.400204000
H	-1.066122000	1.005725000	3.349828000
H	0.853193000	5.354528000	4.777359000
H	-1.124090000	1.654122000	5.732716000
H	-0.167486000	3.832616000	6.463103000
C	0.076842000	-2.808050000	2.695545000
C	0.646693000	-1.954732000	3.660874000
C	-0.459859000	-4.037887000	3.125224000
C	0.675423000	-2.324203000	5.004205000
C	-0.427786000	-4.403582000	4.467989000
C	0.141521000	-3.547829000	5.414727000
H	1.066122000	-1.005725000	3.349828000
H	-0.926195000	-4.698725000	2.400204000
H	1.124090000	-1.654122000	5.732716000
H	-0.853193000	-5.354528000	4.777359000
H	0.167486000	-3.832616000	6.463103000

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1 | II B3LYP/6-31G*

N	-0.075432000	1.255738000	-0.699998000
C	-0.026353000	1.147841000	0.691631000
C	0.005183000	2.465202000	1.272846000
C	0.000000000	3.337115000	0.193410000
C	-0.038533000	2.583770000	-1.008767000
N	0.075432000	-1.255738000	-0.699998000
C	0.026353000	-1.147841000	0.691631000
C	-0.005183000	-2.465202000	1.272846000
C	0.000000000	-3.337115000	0.193410000
C	0.038533000	-2.583770000	-1.008767000
B	0.000000000	0.000000000	-1.645250000
N	0.000000000	0.000000000	1.345843000
F	1.145211000	0.123443000	-2.423648000
F	-1.145211000	-0.123443000	-2.423648000
H	0.015126000	4.416486000	0.235342000
H	-0.015126000	-4.416486000	0.235342000
C	0.015049000	-3.181929000	-2.348836000
C	0.679644000	-2.628541000	-3.459628000
C	-0.671647000	-4.403118000	-2.516515000
C	0.653741000	-3.280821000	-4.690436000
C	-0.699620000	-5.044541000	-3.750827000
C	-0.032892000	-4.486708000	-4.844592000

H	1.218531000	-1.697137000	-3.353067000
H	-1.212766000	-4.832199000	-1.678956000
H	1.177962000	-2.841683000	-5.534811000
H	-1.246605000	-5.976994000	-3.860238000
H	-0.050814000	-4.987486000	-5.808845000
C	-0.015049000	3.181929000	-2.348836000
C	-0.679644000	2.628541000	-3.459628000
C	0.671647000	4.403118000	-2.516515000
C	-0.653741000	3.280821000	-4.690436000
C	0.699620000	5.044541000	-3.750827000
C	0.032892000	4.486708000	-4.844592000
H	-1.218531000	1.697137000	-3.353067000
H	1.212766000	4.832199000	-1.678956000
H	-1.177962000	2.841683000	-5.534811000
H	1.246605000	5.976994000	-3.860238000
H	0.050814000	4.987486000	-5.808845000
C	0.023409000	2.816458000	2.696056000
C	-0.497951000	4.057047000	3.113881000
C	0.570601000	1.960012000	3.671598000
C	-0.474000000	4.429315000	4.455078000
C	0.591905000	2.336828000	5.013251000
C	0.072576000	3.570355000	5.412167000
H	-0.947978000	4.720690000	2.381174000
H	0.980744000	1.004262000	3.369414000
H	-0.888446000	5.388135000	4.754904000
H	1.024021000	1.664257000	5.749484000
H	0.092615000	3.860507000	6.459202000
C	-0.023409000	-2.816458000	2.696056000
C	-0.570601000	-1.960012000	3.671598000
C	0.497951000	-4.057047000	3.113881000
C	-0.591905000	-2.336828000	5.013251000
C	0.474000000	-4.429315000	4.455078000
C	-0.072576000	-3.570355000	5.412167000
H	-0.980744000	-1.004262000	3.369414000
H	0.947978000	-4.720690000	2.381174000
H	-1.024021000	-1.664257000	5.749484000
H	0.888446000	-5.388135000	4.754904000
H	-0.092615000	-3.860507000	6.459202000

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1 | IV B3LYP/6-31G*

N	-0.692060000	-1.255525000	0.135472000
C	0.699257000	-1.151060000	0.160182000
C	1.276545000	-2.467769000	0.066026000
C	0.195385000	-3.331278000	-0.053651000
C	-1.003929000	-2.574656000	0.003398000

N	-0.691738000	1.249542000	0.104905000
C	0.700538000	1.144231000	0.090478000
C	1.275546000	2.459120000	-0.044533000
C	0.190948000	3.322105000	-0.127060000
C	-1.006771000	2.567168000	-0.032996000
B	-1.627741000	-0.001457000	0.266761000
N	1.355522000	-0.003010000	0.143159000
F	-2.172991000	0.012241000	1.562536000
F	-2.608260000	-0.012376000	-0.698182000
H	0.231424000	-4.410363000	-0.097127000
H	0.225595000	4.396123000	-0.239171000
C	-2.354257000	3.145181000	-0.088127000
C	-3.436947000	2.645909000	0.660180000
C	-2.557385000	4.287397000	-0.889415000
C	-4.679267000	3.272868000	0.599512000
C	-3.803911000	4.903104000	-0.951616000
C	-4.871111000	4.398486000	-0.204512000
H	-3.295906000	1.783778000	1.298480000
H	-1.738367000	4.671928000	-1.489675000
H	-5.502913000	2.879032000	1.188644000
H	-3.943401000	5.773471000	-1.586916000
H	-5.844616000	4.879247000	-0.249396000
C	-2.350264000	-3.153571000	-0.054286000
C	-2.546061000	-4.308603000	-0.838562000
C	-3.439297000	-2.641956000	0.676353000
C	-3.792029000	-4.925281000	-0.902077000
C	-4.681162000	-3.269486000	0.614333000
C	-4.865815000	-4.407992000	-0.173245000
H	-1.720597000	-4.702951000	-1.423582000
H	-3.303219000	-1.770360000	1.302947000
H	-3.926070000	-5.806261000	-1.523770000
H	-5.510108000	-2.866356000	1.189556000
H	-5.839040000	-4.889209000	-0.219223000
C	2.698798000	-2.817323000	0.078611000
C	3.134327000	-4.004246000	-0.543014000
C	3.657304000	-2.009588000	0.721706000
C	4.476838000	-4.371812000	-0.523423000
C	5.000525000	-2.380487000	0.737503000
C	5.417048000	-3.561055000	0.118121000
H	2.414257000	-4.628006000	-1.064831000
H	3.340569000	-1.095848000	1.209940000
H	4.791309000	-5.288702000	-1.014725000
H	5.723855000	-1.746800000	1.243728000
H	6.465109000	-3.847654000	0.134461000
C	2.696520000	2.818890000	-0.078476000

C	3.687798000	1.918529000	-0.516117000
C	3.096382000	4.111593000	0.315071000
C	5.026279000	2.304424000	-0.557735000
C	4.434609000	4.492441000	0.271648000
C	5.407111000	3.589973000	-0.166849000
H	3.400240000	0.920874000	-0.824064000
H	2.351856000	4.812300000	0.681671000
H	5.774708000	1.596579000	-0.904062000
H	4.719935000	5.492591000	0.586753000
H	6.451973000	3.886492000	-0.201946000

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1 | V B3LYP/6-31G*

N	-0.154971000	-0.683663000	1.250341000
C	-0.161996000	0.709446000	1.148162000
C	-0.008224000	1.278297000	2.464005000
C	0.124489000	0.192803000	3.319207000
C	0.019381000	-1.002632000	2.561980000
N	-0.154971000	-0.683663000	-1.250341000
C	-0.161996000	0.709446000	-1.148162000
C	-0.008224000	1.278297000	-2.464005000
C	0.124489000	0.192803000	-3.319207000
C	0.019381000	-1.002632000	-2.561980000
B	-0.315410000	-1.617854000	0.000000000
N	-0.174870000	1.367610000	0.000000000
F	-1.616760000	-2.149613000	0.000000000
F	0.639559000	-2.608650000	0.000000000
H	0.207712000	0.226309000	4.396064000
H	0.207712000	0.226309000	-4.396064000
C	0.071535000	-2.351887000	-3.134289000
C	-0.696456000	-3.424597000	-2.643245000
C	0.888508000	-2.566909000	-4.262823000
C	-0.638837000	-4.669599000	-3.264865000
C	0.947366000	-3.816089000	-4.873470000
C	0.181187000	-4.873536000	-4.376911000
H	-1.346989000	-3.273529000	-1.791756000
H	1.501797000	-1.754318000	-4.640619000
H	-1.242792000	-5.485785000	-2.878046000
H	1.594314000	-3.965402000	-5.733563000
H	0.223415000	-5.849130000	-4.853662000
C	0.071535000	-2.351887000	3.134289000
C	0.888508000	-2.566909000	4.262823000
C	-0.696456000	-3.424597000	2.643245000
C	0.947366000	-3.816089000	4.873470000
C	-0.638837000	-4.669599000	3.264865000
C	0.181187000	-4.873536000	4.376911000

H	1.501797000	-1.754318000	4.640619000
H	-1.346989000	-3.273529000	1.791756000
H	1.594314000	-3.965402000	5.733563000
H	-1.242792000	-5.485785000	2.878046000
H	0.223415000	-5.849130000	4.853662000
C	0.019391000	2.696543000	2.829424000
C	0.734111000	3.112085000	3.969835000
C	-0.677672000	3.668483000	2.087916000
C	0.752080000	4.449893000	4.354894000
C	-0.658119000	5.006304000	2.475814000
C	0.054821000	5.403888000	3.609222000
H	1.298357000	2.380241000	4.540717000
H	-1.239802000	3.362900000	1.213993000
H	1.315919000	4.749728000	5.234156000
H	-1.206758000	5.741521000	1.893159000
H	0.068207000	6.448323000	3.908771000
C	0.019391000	2.696543000	-2.829424000
C	-0.677672000	3.668483000	-2.087916000
C	0.734111000	3.112085000	-3.969835000
C	-0.658119000	5.006304000	-2.475814000
C	0.752080000	4.449893000	-4.354894000
C	0.054821000	5.403888000	-3.609222000
H	-1.239802000	3.362900000	-1.213993000
H	1.298357000	2.380241000	-4.540717000
H	-1.206758000	5.741521000	-1.893159000
H	1.315919000	4.749728000	-5.234156000
H	0.068207000	6.448323000	-3.908771000

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1 | VI (TS) B3LYP/6-31G*

N	-0.070096000	-0.680600000	1.251263000
C	-0.067713000	0.713636000	1.148932000
C	-0.002919000	1.280272000	2.473712000
C	0.056420000	0.193753000	3.334368000
C	0.014132000	-1.001495000	2.571099000
N	-0.070096000	-0.680600000	-1.251263000
C	-0.067713000	0.713636000	-1.148932000
C	-0.002919000	1.280272000	-2.473712000
C	0.056420000	0.193753000	-3.334368000
C	0.014132000	-1.001495000	-2.571099000
B	-0.209269000	-1.615497000	0.000000000
N	-0.085111000	1.370828000	0.000000000
F	-1.504712000	-2.164243000	0.000000000
F	0.757290000	-2.594682000	0.000000000
H	0.119440000	0.228025000	4.412474000
H	0.119440000	0.228025000	-4.412474000

C	0.069869000	-2.349825000	-3.148590000
C	-0.644863000	-3.444526000	-2.627043000
C	0.838097000	-2.540137000	-4.315610000
C	-0.583157000	-4.685793000	-3.256083000
C	0.901930000	-3.785618000	-4.933310000
C	0.188734000	-4.864890000	-4.405973000
H	-1.259393000	-3.313452000	-1.746526000
H	1.412106000	-1.711294000	-4.718733000
H	-1.146530000	-5.518777000	-2.844577000
H	1.511997000	-3.914621000	-5.823129000
H	0.234696000	-5.837676000	-4.888087000
C	0.069869000	-2.349825000	3.148590000
C	0.838097000	-2.540137000	4.315610000
C	-0.644863000	-3.444526000	2.627043000
C	0.901930000	-3.785618000	4.933310000
C	-0.583157000	-4.685793000	3.256083000
C	0.188734000	-4.864890000	4.405973000
H	1.412106000	-1.711294000	4.718733000
H	-1.259393000	-3.313452000	1.746526000
H	1.511997000	-3.914621000	5.823129000
H	-1.146530000	-5.518777000	2.844577000
H	0.234696000	-5.837676000	4.888087000
C	-0.016777000	2.695412000	2.858499000
C	-0.574364000	3.073789000	4.095540000
C	0.538022000	3.698270000	2.043185000
C	-0.577538000	4.405626000	4.501759000
C	0.535393000	5.029832000	2.452999000
C	-0.021274000	5.390732000	3.681979000
H	-1.031533000	2.317734000	4.727321000
H	0.979868000	3.420633000	1.094875000
H	-1.020608000	4.675968000	5.456500000
H	0.974376000	5.789024000	1.811094000
H	-0.023249000	6.430408000	3.997887000
C	-0.016777000	2.695412000	-2.858499000
C	0.538022000	3.698270000	-2.043185000
C	-0.574364000	3.073789000	-4.095540000
C	0.535393000	5.029832000	-2.452999000
C	-0.577538000	4.405626000	-4.501759000
C	-0.021274000	5.390732000	-3.681979000
H	0.979868000	3.420633000	-1.094875000
H	-1.031533000	2.317734000	-4.727321000
H	0.974376000	5.789024000	-1.811094000
H	-1.020608000	4.675968000	-5.456500000
H	-0.023249000	6.430408000	-3.997887000

1 | I B3LYP/cc-pVTZ

N	-0.082014000	1.256346000	-0.703813000
C	-0.075568000	1.142596000	0.684909000
C	-0.056351000	2.454802000	1.266199000
C	0.000000000	3.326583000	0.194845000
C	-0.020411000	2.579324000	-1.005498000
N	0.082014000	-1.256346000	-0.703813000
C	0.075568000	-1.142596000	0.684909000
C	0.056351000	-2.454802000	1.266199000
C	0.000000000	-3.326583000	0.194845000
C	0.020411000	-2.579324000	-1.005498000
B	0.000000000	0.000000000	-1.647629000
N	0.000000000	0.000000000	1.332656000
F	1.141506000	0.122874000	-2.429308000
F	-1.141506000	-0.122874000	-2.429308000
H	-0.020905000	4.401098000	0.238647000
H	0.020905000	-4.401098000	0.238647000
C	-0.017438000	-3.182980000	-2.338550000
C	0.679363000	-2.671132000	-3.440896000
C	-0.756018000	-4.365877000	-2.506397000
C	0.634313000	-3.324130000	-4.663999000
C	-0.805661000	-5.007227000	-3.733210000
C	-0.106995000	-4.489553000	-4.818692000
H	1.262769000	-1.771537000	-3.336497000
H	-1.318204000	-4.765267000	-1.674023000
H	1.185116000	-2.917543000	-5.501484000
H	-1.393356000	-5.908638000	-3.843589000
H	-0.141516000	-4.990505000	-5.776884000
C	0.017438000	3.182980000	-2.338550000
C	-0.679363000	2.671132000	-3.440896000
C	0.756018000	4.365877000	-2.506397000
C	-0.634313000	3.324130000	-4.663999000
C	0.805661000	5.007227000	-3.733210000
C	0.106995000	4.489553000	-4.818692000
H	-1.262769000	1.771537000	-3.336497000
H	1.318204000	4.765267000	-1.674023000
H	-1.185116000	2.917543000	-5.501484000
H	1.393356000	5.908638000	-3.843589000
H	0.141516000	4.990505000	-5.776884000
C	-0.084058000	2.799963000	2.685867000
C	0.492897000	4.001148000	3.124526000
C	-0.700011000	1.974410000	3.637417000
C	0.455679000	4.364719000	4.461526000
C	-0.736724000	2.342522000	4.974677000
C	-0.161050000	3.536709000	5.393775000

H	0.994026000	4.641834000	2.411800000
H	-1.153169000	1.048024000	3.321070000
H	0.913361000	5.292487000	4.778117000
H	-1.222725000	1.694479000	5.691806000
H	-0.191843000	3.820175000	6.437294000
C	0.084058000	-2.799963000	2.685867000
C	0.700011000	-1.974410000	3.637417000
C	-0.492897000	-4.001148000	3.124526000
C	0.736724000	-2.342522000	4.974677000
C	-0.455679000	-4.364719000	4.461526000
C	0.161050000	-3.536709000	5.393775000
H	1.153169000	-1.048024000	3.321070000
H	-0.994026000	-4.641834000	2.411800000
H	1.222725000	-1.694479000	5.691806000
H	-0.913361000	-5.292487000	4.778117000
H	0.191843000	-3.820175000	6.437294000

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1 | II B3LYP/cc-pVTZ

N	-0.083061000	1.256604000	-0.699585000
C	-0.024066000	1.144604000	0.688452000
C	0.012785000	2.457650000	1.267124000
C	0.000000000	3.328418000	0.194107000
C	-0.051021000	2.579796000	-1.004241000
N	0.083061000	-1.256604000	-0.699585000
C	0.024066000	-1.144604000	0.688452000
C	-0.012785000	-2.457650000	1.267124000
C	0.000000000	-3.328418000	0.194107000
C	0.051021000	-2.579796000	-1.004241000
B	0.000000000	0.000000000	-1.644021000
N	0.000000000	0.000000000	1.336186000
F	1.140984000	0.127359000	-2.425133000
F	-1.140984000	-0.127359000	-2.425133000
H	0.019084000	4.402921000	0.237124000
H	-0.019084000	-4.402921000	0.237124000
C	0.045963000	-3.182884000	-2.338736000
C	0.770532000	-2.670539000	-3.422660000
C	-0.687192000	-4.366367000	-2.525496000
C	0.757616000	-3.323504000	-4.646650000
C	-0.704987000	-5.007231000	-3.753511000
C	0.021196000	-4.489211000	-4.820584000
H	1.349292000	-1.769943000	-3.303299000
H	-1.271140000	-4.766199000	-1.708507000
H	1.329502000	-2.916271000	-5.469566000
H	-1.289623000	-5.908639000	-3.879108000
H	0.011544000	-4.990023000	-5.779423000

C	-0.045963000	3.182884000	-2.338736000
C	-0.770532000	2.670539000	-3.422660000
C	0.687192000	4.366367000	-2.525496000
C	-0.757616000	3.323504000	-4.646650000
C	0.704987000	5.007231000	-3.753511000
C	-0.021196000	4.489211000	-4.820584000
H	-1.349292000	1.769943000	-3.303299000
H	1.271140000	4.766199000	-1.708507000
H	-1.329502000	2.916271000	-5.469566000
H	1.289623000	5.908639000	-3.879108000
H	-0.011544000	4.990023000	-5.779423000
C	0.045611000	2.809131000	2.686130000
C	-0.508448000	4.024874000	3.114540000
C	0.640054000	1.977416000	3.645920000
C	-0.470951000	4.395744000	4.449581000
C	0.677593000	2.353560000	4.981163000
C	0.124093000	3.561457000	5.390205000
H	-0.994020000	4.670605000	2.395645000
H	1.077701000	1.041186000	3.337366000
H	-0.911943000	5.334336000	4.757867000
H	1.147657000	1.700576000	5.704448000
H	0.155493000	3.850803000	6.432090000
C	-0.045611000	-2.809131000	2.686130000
C	-0.640054000	-1.977416000	3.645920000
C	0.508448000	-4.024874000	3.114540000
C	-0.677593000	-2.353560000	4.981163000
C	0.470951000	-4.395744000	4.449581000
C	-0.124093000	-3.561457000	5.390205000
H	-1.077701000	-1.041186000	3.337366000
H	0.994020000	-4.670605000	2.395645000
H	-1.147657000	-1.700576000	5.704448000
H	0.911943000	-5.334336000	4.757867000
H	-0.155493000	-3.850803000	6.432090000

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1 | IV B3LYP/cc-pVTZ

N	-0.689230000	-1.260089000	0.135470000
C	0.698313000	-1.144361000	0.162917000
C	1.280908000	-2.453175000	0.067246000
C	0.211254000	-3.320334000	-0.060022000
C	-0.989858000	-2.575984000	-0.001550000
N	-0.700586000	1.248815000	0.105551000
C	0.688779000	1.144397000	0.088429000
C	1.256741000	2.456267000	-0.049564000
C	0.175890000	3.314227000	-0.131504000
C	-1.016664000	2.560870000	-0.032805000

B	-1.625346000	-0.008257000	0.284741000
N	1.342304000	0.003500000	0.144481000
F	-2.152996000	0.002056000	1.584031000
F	-2.624125000	-0.022536000	-0.663510000
H	0.255979000	-4.393752000	-0.113029000
H	0.210008000	4.382905000	-0.247956000
C	-2.359059000	3.142643000	-0.083953000
C	-3.432335000	2.666745000	0.680263000
C	-2.566729000	4.263674000	-0.903421000
C	-4.667763000	3.294290000	0.620781000
C	-3.806586000	4.878756000	-0.967349000
C	-4.863365000	4.397247000	-0.202256000
H	-3.293510000	1.819685000	1.331891000
H	-1.756749000	4.633393000	-1.516452000
H	-5.482908000	2.917729000	1.223940000
H	-3.949236000	5.731202000	-1.617781000
H	-5.831375000	4.877971000	-0.248123000
C	-2.325701000	-3.170345000	-0.061748000
C	-2.512849000	-4.305149000	-0.866806000
C	-3.412668000	-2.692365000	0.681603000
C	-3.746329000	-4.932139000	-0.937428000
C	-4.641804000	-3.331284000	0.615429000
C	-4.817044000	-4.448111000	-0.193530000
H	-1.690872000	-4.677037000	-1.462440000
H	-3.289290000	-1.834898000	1.322828000
H	-3.873298000	-5.795828000	-1.576169000
H	-5.468034000	-2.953106000	1.202244000
H	-5.780253000	-4.937862000	-0.244656000
C	2.700841000	-2.796058000	0.088142000
C	3.151778000	-3.953451000	-0.563912000
C	3.641049000	-2.010685000	0.770528000
C	4.490019000	-4.313116000	-0.535671000
C	4.979738000	-2.374598000	0.797599000
C	5.411108000	-3.524994000	0.146740000
H	2.447836000	-4.561366000	-1.115712000
H	3.314509000	-1.119721000	1.283784000
H	4.816497000	-5.206329000	-1.051443000
H	5.688054000	-1.758696000	1.335547000
H	6.455535000	-3.805742000	0.170611000
C	2.672584000	2.820397000	-0.090694000
C	3.653268000	1.947854000	-0.583973000
C	3.076508000	4.089218000	0.351552000
C	4.984409000	2.336646000	-0.633823000
C	4.407650000	4.472543000	0.302623000
C	5.368995000	3.597576000	-0.192340000

H	3.364107000	0.969106000	-0.932595000
H	2.341359000	4.769037000	0.760079000
H	5.724080000	1.650789000	-1.024967000
H	4.696546000	5.453101000	0.656913000
H	6.407962000	3.896219000	-0.232447000

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1 | V B3LYP/cc-pVTZ

N	0.158062000	-0.688223000	-1.252554000
C	0.164970000	0.701429000	-1.145030000
C	0.005400000	1.270645000	-2.454225000
C	-0.133249000	0.192996000	-3.308724000
C	-0.022033000	-1.001268000	-2.559515000
N	0.158062000	-0.688223000	1.252554000
C	0.164970000	0.701429000	1.145030000
C	0.005400000	1.270645000	2.454225000
C	-0.133249000	0.192996000	3.308724000
C	-0.022033000	-1.001268000	2.559515000
B	0.335802000	-1.617005000	0.000000000
N	0.178979000	1.352132000	0.000000000
F	1.640468000	-2.130920000	0.000000000
F	-0.602213000	-2.625863000	0.000000000
H	-0.228496000	0.230651000	-4.379536000
H	-0.228496000	0.230651000	4.379536000
C	-0.073509000	-2.342559000	3.141806000
C	0.710927000	-3.408043000	2.681391000
C	-0.911793000	-2.557179000	4.247163000
C	0.652042000	-4.643489000	3.308647000
C	-0.974714000	-3.797050000	4.862291000
C	-0.189981000	-4.846304000	4.396034000
H	1.376984000	-3.262989000	1.846378000
H	-1.538472000	-1.752076000	4.604686000
H	1.270409000	-5.452903000	2.944638000
H	-1.639092000	-3.945802000	5.702852000
H	-0.235078000	-5.814339000	4.876786000
C	-0.073509000	-2.342559000	-3.141806000
C	-0.911793000	-2.557179000	-4.247163000
C	0.710927000	-3.408043000	-2.681391000
C	-0.974714000	-3.797050000	-4.862291000
C	0.652042000	-4.643489000	-3.308647000
C	-0.189981000	-4.846304000	-4.396034000
H	-1.538472000	-1.752076000	-4.604686000
H	1.376984000	-3.262989000	-1.846378000
H	-1.639092000	-3.945802000	-5.702852000
H	1.270409000	-5.452903000	-2.944638000
H	-0.235078000	-5.814339000	-4.876786000

C	-0.021088000	2.686197000	-2.815796000
C	-0.770039000	3.111962000	-3.922461000
C	0.710499000	3.644850000	-2.102772000
C	-0.787928000	4.445303000	-4.301461000
C	0.693223000	4.977879000	-2.485766000
C	-0.054902000	5.385164000	-3.584705000
H	-1.360781000	2.392390000	-4.472772000
H	1.299458000	3.334285000	-1.254190000
H	-1.379243000	4.752968000	-5.153573000
H	1.270465000	5.701998000	-1.926422000
H	-0.067617000	6.425761000	-3.879866000
C	-0.021088000	2.686197000	2.815796000
C	0.710499000	3.644850000	2.102772000
C	-0.770039000	3.111962000	3.922461000
C	0.693223000	4.977879000	2.485766000
C	-0.787928000	4.445303000	4.301461000
C	-0.054902000	5.385164000	3.584705000
H	1.299458000	3.334285000	1.254190000
H	-1.360781000	2.392390000	4.472772000
H	1.270465000	5.701998000	1.926422000
H	-1.379243000	4.752968000	5.153573000
H	-0.067617000	6.425761000	3.879866000

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1 | VI (TS) B3LYP/cc-pVTZ

N	-0.071378000	-0.686109000	1.253645000
C	-0.070427000	0.704606000	1.145690000
C	-0.004059000	1.272104000	2.464086000
C	0.059361000	0.193948000	3.325230000
C	0.015858000	-1.000532000	2.569613000
N	-0.071378000	-0.686109000	-1.253645000
C	-0.070427000	0.704606000	-1.145690000
C	-0.004059000	1.272104000	-2.464086000
C	0.059361000	0.193948000	-3.325230000
C	0.015858000	-1.000532000	-2.569613000
B	-0.227505000	-1.615827000	0.000000000
N	-0.089726000	1.354318000	0.000000000
F	-1.525646000	-2.148683000	0.000000000
F	0.723951000	-2.611871000	0.000000000
H	0.126681000	0.232961000	4.398019000
H	0.126681000	0.232961000	-4.398019000
C	0.071529000	-2.340557000	-3.157755000
C	-0.654519000	-3.431594000	-2.663013000
C	0.857270000	-2.526274000	-4.306622000
C	-0.590532000	-4.662526000	-3.298987000
C	0.926392000	-3.761638000	-4.930139000

C	0.199500000	-4.836198000	-4.429354000
H	-1.281351000	-3.310083000	-1.795098000
H	1.440717000	-1.702041000	-4.692359000
H	-1.164433000	-5.491541000	-2.907278000
H	1.551006000	-3.886654000	-5.804382000
H	0.249176000	-5.800819000	-4.916469000
C	0.071529000	-2.340557000	3.157755000
C	0.857270000	-2.526274000	4.306622000
C	-0.654519000	-3.431594000	2.663013000
C	0.926392000	-3.761638000	4.930139000
C	-0.590532000	-4.662526000	3.298987000
C	0.199500000	-4.836198000	4.429354000
H	1.440717000	-1.702041000	4.692359000
H	-1.281351000	-3.310083000	1.795098000
H	1.551006000	-3.886654000	5.804382000
H	-1.164433000	-5.491541000	2.907278000
H	0.249176000	-5.800819000	4.916469000
C	-0.016237000	2.685040000	2.843727000
C	-0.607025000	3.072562000	4.055298000
C	0.571608000	3.675808000	2.047866000
C	-0.610931000	4.400254000	4.454754000
C	0.570346000	5.002954000	2.451756000
C	-0.020609000	5.372516000	3.654673000
H	-1.088968000	2.327435000	4.673413000
H	1.038752000	3.394299000	1.118104000
H	-1.080925000	4.677578000	5.388888000
H	1.036817000	5.752151000	1.825997000
H	-0.022559000	6.408598000	3.965511000
C	-0.016237000	2.685040000	-2.843727000
C	0.571608000	3.675808000	-2.047866000
C	-0.607025000	3.072562000	-4.055298000
C	0.570346000	5.002954000	-2.451756000
C	-0.610931000	4.400254000	-4.454754000
C	-0.020609000	5.372516000	-3.654673000
H	1.038752000	3.394299000	-1.118104000
H	-1.088968000	2.327435000	-4.673413000
H	1.036817000	5.752151000	-1.825997000
H	-1.080925000	4.677578000	-5.388888000
H	-0.022559000	6.408598000	-3.965511000

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2 | Iaa B3LYP/6-31G*

N	0.046090000	1.249456000	-0.709686000
C	0.046594000	1.143238000	0.678290000
C	0.042353000	2.465337000	1.253620000
C	0.000000000	3.340035000	0.174476000

C	0.011614000	2.581434000	-1.022275000
N	-0.046090000	-1.249456000	-0.709686000
C	-0.046594000	-1.143238000	0.678290000
C	-0.042353000	-2.465337000	1.253620000
C	0.000000000	-3.340035000	0.174476000
C	-0.011614000	-2.581434000	-1.022275000
B	0.000000000	0.000000000	-1.656074000
N	0.000000000	0.000000000	1.340937000
F	1.144530000	-0.068787000	-2.444352000
F	-1.144530000	0.068787000	-2.444352000
H	0.025596000	4.420278000	0.217756000
H	-0.025596000	-4.420278000	0.217756000
C	-0.086255000	-2.786668000	2.660483000
S	0.344191000	-4.396120000	3.222287000
C	-0.467118000	-1.996013000	3.728147000
C	0.002815000	-3.971331000	4.865266000
C	-0.414756000	-2.670912000	4.977315000
H	-0.785565000	-0.969779000	3.598529000
H	0.134006000	-4.703292000	5.650971000
H	-0.683002000	-2.210689000	5.922075000
C	0.086255000	2.786668000	2.660483000
S	-0.344191000	4.396120000	3.222287000
C	0.467118000	1.996013000	3.728147000
C	-0.002815000	3.971331000	4.865266000
C	0.414756000	2.670912000	4.977315000
H	0.785565000	0.969779000	3.598529000
H	-0.134006000	4.703292000	5.650971000
H	0.683002000	2.210689000	5.922075000
C	0.001251000	3.139464000	-2.353398000
S	-0.566934000	4.793622000	-2.574685000
C	0.406779000	2.609050000	-3.564868000
C	-0.244633000	4.729794000	-4.270104000
C	0.265984000	3.514164000	-4.647441000
H	0.817799000	1.613189000	-3.652273000
H	-0.459277000	5.588207000	-4.892779000
H	0.538653000	3.273605000	-5.669090000
C	-0.001251000	-3.139464000	-2.353398000
S	0.566934000	-4.793622000	-2.574685000
C	-0.406779000	-2.609050000	-3.564868000
C	0.244633000	-4.729794000	-4.270104000
C	-0.265984000	-3.514164000	-4.647441000
H	-0.817799000	-1.613189000	-3.652273000
H	0.459277000	-5.588207000	-4.892779000
H	-0.538653000	-3.273605000	-5.669090000

2 | Iab B3LYP/6-31G*

N	0.044947000	1.246183000	-0.747162000
C	0.040619000	1.143859000	0.641671000
C	0.033407000	2.467608000	1.211814000
C	0.000000000	3.338826000	0.127826000
C	0.012928000	2.577239000	-1.064261000
N	-0.044947000	-1.246183000	-0.747162000
C	-0.040619000	-1.143859000	0.641671000
C	-0.033407000	-2.467608000	1.211814000
C	0.000000000	-3.338826000	0.127826000
C	-0.012928000	-2.577239000	-1.064261000
B	0.000000000	0.000000000	-1.693067000
N	0.000000000	0.000000000	1.306562000
F	1.144487000	-0.068959000	-2.482801000
F	-1.144487000	0.068959000	-2.482801000
H	0.035302000	4.418202000	0.167753000
H	-0.035302000	-4.418202000	0.167753000
C	-0.068933000	-2.842577000	2.605462000
S	-0.576200000	-1.757212000	3.885751000
C	0.222644000	-4.091296000	3.127453000
C	-0.395365000	-2.998009000	5.076189000
C	0.040985000	-4.178626000	4.530556000
H	0.573284000	-4.913773000	2.513683000
H	-0.609139000	-2.783349000	6.115066000
H	0.228903000	-5.075741000	5.110157000
C	0.068933000	2.842577000	2.605462000
S	0.576200000	1.757212000	3.885751000
C	-0.222644000	4.091296000	3.127453000
C	0.395365000	2.998009000	5.076189000
C	-0.040985000	4.178626000	4.530556000
H	-0.573284000	4.913773000	2.513683000
H	0.609139000	2.783349000	6.115066000
H	-0.228903000	5.075741000	5.110157000
C	0.005340000	3.132026000	-2.397568000
S	-0.568348000	4.783872000	-2.622785000
C	0.417103000	2.602294000	-3.606842000
C	-0.238887000	4.720253000	-4.317096000
C	0.277340000	3.506149000	-4.690971000
H	0.830861000	1.607383000	-3.691769000
H	-0.454191000	5.577311000	-4.941400000
H	0.554751000	3.265377000	-5.711314000
C	-0.005340000	-3.132026000	-2.397568000
S	0.568348000	-4.783872000	-2.622785000
C	-0.417103000	-2.602294000	-3.606842000
C	0.238887000	-4.720253000	-4.317096000

C	-0.277340000	-3.506149000	-4.690971000
H	-0.830861000	-1.607383000	-3.691769000
H	0.454191000	-5.577311000	-4.941400000
H	-0.554751000	-3.265377000	-5.711314000

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2 | Iab B3LYP/6-31G*

N	-1.512261000	-0.216047000	-0.050445000
C	-0.930056000	1.046991000	-0.028715000
C	-1.964358000	2.047328000	-0.053617000
C	-3.163503000	1.341032000	-0.061207000
C	-2.870824000	-0.043291000	-0.063703000
N	0.824986000	-1.082687000	0.103815000
C	1.213178000	0.255628000	0.108963000
C	2.655298000	0.326916000	0.132001000
C	3.092637000	-0.991582000	0.100959000
C	1.961482000	-1.844009000	0.092657000
B	-0.673932000	-1.536063000	0.023765000
N	0.371760000	1.273618000	0.045955000
F	-0.853377000	-2.306768000	-1.121212000
F	-1.040425000	-2.246119000	1.163434000
H	-4.158501000	1.758112000	-0.124709000
H	4.118080000	-1.331745000	0.147022000
C	3.461294000	1.522388000	0.191122000
S	5.181031000	1.455194000	-0.173701000
C	3.099484000	2.808064000	0.544190000
C	5.369604000	3.143560000	0.156812000
C	4.183954000	3.725261000	0.522956000
H	2.084559000	3.067068000	0.814561000
H	6.341365000	3.608305000	0.056428000
H	4.088330000	4.775907000	0.774460000
C	-1.807720000	3.482438000	-0.077659000
S	-0.291668000	4.282983000	-0.457187000
C	-2.799069000	4.423238000	0.137898000
C	-1.025114000	5.844653000	-0.320825000
C	-2.354764000	5.763548000	0.002781000
H	-3.815574000	4.150923000	0.399939000
H	-0.430950000	6.734904000	-0.480253000
H	-2.993554000	6.628741000	0.142161000
C	-3.858725000	-1.096381000	-0.086117000
S	-5.504001000	-0.725092000	0.427230000
C	-3.772182000	-2.416823000	-0.487721000
C	-6.026832000	-2.336041000	0.087427000
C	-5.003169000	-3.114575000	-0.388062000
H	-2.856081000	-2.847399000	-0.866706000
H	-7.055577000	-2.618856000	0.267263000

H	-5.125541000	-4.156077000	-0.664341000
C	2.016600000	-3.286351000	0.086262000
S	3.498422000	-4.074975000	-0.452766000
C	1.087834000	-4.233990000	0.477301000
C	2.838327000	-5.639396000	-0.138691000
C	1.558398000	-5.565416000	0.348546000
H	0.117136000	-3.965387000	0.869542000
H	3.427579000	-6.524087000	-0.340665000
H	0.970014000	-6.437220000	0.612627000

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2 | Iba B3LYP/6-31G*

N	0.031946000	1.248836000	-0.626382000
C	0.036957000	1.143918000	0.761721000
C	0.037631000	2.468176000	1.332244000
C	0.000000000	3.339601000	0.250874000
C	0.003779000	2.575718000	-0.944985000
N	-0.031946000	-1.248836000	-0.626382000
C	-0.036957000	-1.143918000	0.761721000
C	-0.037631000	-2.468176000	1.332244000
C	0.000000000	-3.339601000	0.250874000
C	-0.003779000	-2.575718000	-0.944985000
B	0.000000000	0.000000000	-1.572070000
N	0.000000000	0.000000000	1.424117000
F	1.147056000	-0.032718000	-2.353002000
F	-1.147056000	0.032718000	-2.353002000
H	0.041925000	4.418689000	0.289496000
H	-0.041925000	-4.418689000	0.289496000
C	-0.086120000	-2.793912000	2.738550000
S	0.339672000	-4.406000000	3.296355000
C	-0.466572000	-2.005806000	3.807778000
C	-0.003789000	-3.985714000	4.940461000
C	-0.418088000	-2.684733000	5.055293000
H	-0.781856000	-0.978249000	3.680696000
H	0.123946000	-4.720457000	5.724116000
H	-0.686752000	-2.226456000	6.000904000
C	0.086120000	2.793912000	2.738550000
S	-0.339672000	4.406000000	3.296355000
C	0.466572000	2.005806000	3.807778000
C	0.003789000	3.985714000	4.940461000
C	0.418088000	2.684733000	5.055293000
H	0.781856000	0.978249000	3.680696000
H	-0.123946000	4.720457000	5.724116000
H	0.686752000	2.226456000	6.000904000
C	-0.015432000	3.163690000	-2.265528000
S	0.603143000	2.432914000	-3.736894000

C	-0.486142000	4.442579000	-2.532275000
C	0.214142000	3.840952000	-4.652559000
C	-0.361266000	4.825602000	-3.887598000
H	-0.935535000	5.068458000	-1.769779000
H	0.429632000	3.864787000	-5.713060000
H	-0.688348000	5.781924000	-4.280129000
C	0.015432000	-3.163690000	-2.265528000
S	-0.603143000	-2.432914000	-3.736894000
C	0.486142000	-4.442579000	-2.532275000
C	-0.214142000	-3.840952000	-4.652559000
C	0.361266000	-4.825602000	-3.887598000
H	0.935535000	-5.068458000	-1.769779000
H	-0.429632000	-3.864787000	-5.713060000
H	0.688348000	-5.781924000	-4.280129000

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2 | Ibb B3LYP/6-31G*

N	0.030531000	1.245427000	-0.664824000
C	0.030890000	1.144437000	0.724030000
C	0.028740000	2.470221000	1.289547000
C	0.000000000	3.338288000	0.203356000
C	0.005062000	2.571286000	-0.987839000
N	-0.030531000	-1.245427000	-0.664824000
C	-0.030890000	-1.144437000	0.724030000
C	-0.028740000	-2.470221000	1.289547000
C	0.000000000	-3.338288000	0.203356000
C	-0.005062000	-2.571286000	-0.987839000
B	0.000000000	0.000000000	-1.610046000
N	0.000000000	0.000000000	1.388622000
F	1.146945000	-0.031990000	-2.392588000
F	-1.146945000	0.031990000	-2.392588000
H	0.051714000	4.416432000	0.238430000
H	-0.051714000	-4.416432000	0.238430000
C	-0.069149000	-2.848118000	2.682940000
S	-0.577801000	-1.763342000	3.963229000
C	0.219502000	-4.097390000	3.204421000
C	-0.401424000	-3.005579000	5.153151000
C	0.034267000	-4.186108000	4.607271000
H	0.570834000	-4.919588000	2.590636000
H	-0.616862000	-2.791474000	6.191792000
H	0.219623000	-5.084137000	5.186336000
C	0.069149000	2.848118000	2.682940000
S	0.577801000	1.763342000	3.963229000
C	-0.219502000	4.097390000	3.204421000
C	0.401424000	3.005579000	5.153151000
C	-0.034267000	4.186108000	4.607271000

H	-0.570834000	4.919588000	2.590636000
H	0.616862000	2.791474000	6.191792000
H	-0.219623000	5.084137000	5.186336000
C	-0.011082000	3.155156000	-2.311107000
S	0.623694000	2.427356000	-3.776968000
C	-0.490246000	4.429452000	-2.583266000
C	0.230585000	3.831232000	-4.697479000
C	-0.358517000	4.812049000	-3.938286000
H	-0.950814000	5.052052000	-1.824747000
H	0.453135000	3.855105000	-5.756528000
H	-0.690920000	5.765019000	-4.334557000
C	0.011082000	-3.155156000	-2.311107000
S	-0.623694000	-2.427356000	-3.776968000
C	0.490246000	-4.429452000	-2.583266000
C	-0.230585000	-3.831232000	-4.697479000
C	0.358517000	-4.812049000	-3.938286000
H	0.950814000	-5.052052000	-1.824747000
H	-0.453135000	-3.855105000	-5.756528000
H	0.690920000	-5.765019000	-4.334557000

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2 | Ibc B3LYP/6-31G*

N	0.979190000	-1.124357000	0.000188000
C	-0.385880000	-1.390446000	0.015286000
C	-0.588419000	-2.815269000	0.021526000
C	0.686671000	-3.372066000	0.032513000
C	1.637008000	-2.321179000	0.016487000
N	0.316869000	1.280542000	0.058571000
C	-0.996644000	0.815325000	0.071955000
C	-1.892823000	1.947793000	0.065169000
C	-1.074737000	3.069213000	0.015615000
C	0.278434000	2.643564000	0.018614000
B	1.559906000	0.327704000	0.023483000
N	-1.330617000	-0.463902000	0.049885000
F	2.297324000	0.563908000	-1.129035000
F	2.329070000	0.509447000	1.165006000
H	0.933990000	-4.422144000	-0.018235000
H	-1.392855000	4.101312000	0.049495000
C	-3.334906000	1.909355000	0.119677000
S	-4.278704000	3.339751000	-0.278261000
C	-4.172061000	0.874419000	0.488008000
C	-5.764047000	2.517694000	0.060430000
C	-5.549132000	1.222488000	0.452626000
H	-3.793824000	-0.096566000	0.778647000
H	-6.706723000	3.035814000	-0.054723000
H	-6.349332000	0.538216000	0.712918000

C	-1.843316000	-3.530394000	0.003012000
S	-3.376316000	-2.779813000	-0.409115000
C	-2.028059000	-4.878777000	0.250630000
C	-4.214853000	-4.284849000	-0.242689000
C	-3.373793000	-5.306754000	0.113838000
H	-1.214747000	-5.536576000	0.536939000
H	-5.283031000	-4.328143000	-0.410311000
H	-3.702627000	-6.327411000	0.275805000
C	3.066998000	-2.538794000	0.017157000
S	4.283609000	-1.449207000	-0.626328000
C	3.669225000	-3.698285000	0.486337000
C	5.544841000	-2.563055000	-0.249542000
C	5.075852000	-3.710914000	0.340081000
H	3.105841000	-4.499879000	0.950208000
H	6.570640000	-2.306840000	-0.481364000
H	5.711891000	-4.527464000	0.663184000
C	1.399045000	3.556394000	-0.012868000
S	3.013044000	3.243930000	0.602780000
C	1.318494000	4.856152000	-0.495316000
C	3.524539000	4.839515000	0.197565000
C	2.525704000	5.583148000	-0.381530000
H	0.416706000	5.255351000	-0.945265000
H	4.542119000	5.143460000	0.406960000
H	2.651820000	6.605924000	-0.718610000

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2 | Ica B3LYP/6-31G*

N	-1.188946000	-0.876547000	-0.004649000
C	-1.316716000	0.509095000	-0.021819000
C	-2.716495000	0.851234000	-0.067829000
C	-3.396684000	-0.360126000	-0.043140000
C	-2.445092000	-1.411814000	-0.009818000
N	1.272108000	-0.461348000	0.121618000
C	0.936315000	0.889835000	0.107884000
C	2.144935000	1.676506000	0.113877000
C	3.187037000	0.757464000	0.093101000
C	2.637217000	-0.548801000	0.107992000
B	0.196599000	-1.601587000	0.089367000
N	-0.300252000	1.352862000	0.037655000
F	0.393480000	-2.402110000	-1.026553000
F	0.239498000	-2.351841000	1.261389000
H	-4.465300000	-0.502003000	-0.117833000
H	4.244708000	0.979808000	0.130217000
C	2.227549000	3.117643000	0.146702000
S	3.727358000	3.935601000	-0.268856000
C	1.265033000	4.042149000	0.505614000

C	3.030563000	5.487961000	0.049180000
C	1.723646000	5.385730000	0.448475000
H	0.270018000	3.746333000	0.811903000
H	3.623679000	6.383282000	-0.080908000
H	1.108902000	6.243040000	0.700385000
C	-3.269811000	2.183133000	-0.143099000
S	-4.964780000	2.467613000	0.227834000
C	-2.658969000	3.365968000	-0.513276000
C	-4.813142000	4.156208000	-0.123188000
C	-3.537065000	4.483201000	-0.500232000
H	-1.615327000	3.409556000	-0.796702000
H	-5.671582000	4.807429000	-0.026894000
H	-3.234292000	5.489970000	-0.766888000
C	-2.807906000	-2.811342000	0.012126000
S	-1.829919000	-4.149635000	-0.566748000
C	-4.038643000	-3.279669000	0.452484000
C	-3.080367000	-5.279862000	-0.202510000
C	-4.192085000	-4.680607000	0.336084000
H	-4.793082000	-2.625737000	0.874627000
H	-2.924945000	-6.331923000	-0.404218000
H	-5.080700000	-5.220755000	0.643029000
C	3.405355000	-1.770286000	0.120734000
S	5.085344000	-1.723163000	-0.411548000
C	3.068781000	-3.049794000	0.524863000
C	5.289214000	-3.405232000	-0.077419000
C	4.139831000	-3.972098000	0.410985000
H	2.091933000	-3.295949000	0.916779000
H	6.241339000	-3.881843000	-0.269710000
H	4.061437000	-5.018120000	0.685945000

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2 | Icb B3LYP/6-31G*

N	-0.562259000	1.381935000	0.021726000
C	0.807901000	1.136593000	0.005716000
C	1.509053000	2.395560000	-0.012807000
C	0.519845000	3.372861000	0.020912000
C	-0.744654000	2.735023000	0.039637000
N	-0.824309000	-1.095338000	0.098224000
C	0.567838000	-1.138929000	0.080609000
C	0.995341000	-2.515473000	0.059372000
C	-0.174315000	-3.267721000	0.032253000
C	-1.279788000	-2.384849000	0.062998000
B	-1.632776000	0.244541000	0.091511000
N	1.348981000	-0.071247000	0.036974000
F	-2.456464000	0.292276000	-1.024904000
F	-2.370280000	0.383172000	1.265145000

H	0.666785000	4.440851000	-0.042956000
H	-0.247745000	-4.345592000	0.059242000
C	2.342584000	-3.034150000	0.077448000
S	3.734527000	-2.090421000	0.574047000
C	2.728513000	-4.328819000	-0.225048000
C	4.787299000	-3.447388000	0.374494000
C	4.116903000	-4.562569000	-0.060040000
H	2.028629000	-5.081271000	-0.571622000
H	5.845225000	-3.343017000	0.576846000
H	4.597810000	-5.514169000	-0.258187000
C	2.933378000	2.625652000	-0.075777000
S	4.086344000	1.408953000	-0.590348000
C	3.586125000	3.816439000	0.192737000
C	5.401408000	2.521990000	-0.442978000
C	4.987703000	3.756870000	-0.012301000
H	3.066422000	4.701242000	0.543735000
H	6.408882000	2.198945000	-0.670280000
H	5.659696000	4.591315000	0.155755000
C	-1.998289000	3.456529000	0.071368000
S	-3.543884000	2.888774000	-0.537837000
C	-2.124561000	4.754933000	0.546048000
C	-4.301664000	4.386227000	-0.140854000
C	-3.432161000	5.281558000	0.431035000
H	-1.296503000	5.294216000	0.991638000
H	-5.355062000	4.523549000	-0.348673000
H	-3.717722000	6.273564000	0.762784000
C	-2.664593000	-2.793012000	0.069163000
S	-3.073705000	-4.411504000	-0.497816000
C	-3.805057000	-2.132845000	0.489142000
C	-4.748071000	-4.161745000	-0.155054000
C	-4.982567000	-2.912906000	0.360521000
H	-3.777869000	-1.134089000	0.901592000
H	-5.464269000	-4.945624000	-0.363046000
H	-5.968114000	-2.560911000	0.644685000

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2 | Icc-1 B3LYP/6-31G*

N	-1.325243000	0.843690000	0.032890000
C	-0.089971000	1.481874000	0.034343000
C	-0.294321000	2.905935000	0.003557000
C	-1.674527000	3.083406000	0.007838000
C	-2.292427000	1.808739000	0.024689000
N	-0.016895000	-1.278993000	0.139375000
C	1.113166000	-0.463059000	0.133163000
C	2.293294000	-1.295736000	0.123723000
C	1.825093000	-2.603269000	0.086867000

C	0.408618000	-2.577979000	0.106528000
B	-1.477645000	-0.710667000	0.112572000
N	1.076304000	0.857717000	0.083898000
F	-2.144595000	-1.185107000	-1.008144000
F	-2.157541000	-1.044480000	1.281216000
H	-2.205865000	4.020533000	-0.068635000
H	2.424063000	-3.503330000	0.109747000
C	3.665554000	-0.850562000	0.160318000
S	4.971904000	-1.959100000	-0.239109000
C	4.178835000	0.382485000	0.513313000
C	6.166322000	-0.747324000	0.077878000
C	5.597449000	0.437941000	0.464748000
H	3.543872000	1.209235000	0.802429000
H	7.216028000	-0.978497000	-0.044824000
H	6.173752000	1.322810000	0.712039000
C	0.709888000	3.943096000	-0.040713000
S	2.392155000	3.641771000	-0.443655000
C	0.509004000	5.295181000	0.172093000
C	2.775033000	5.325187000	-0.320003000
C	1.680941000	6.079383000	0.016266000
H	-0.456342000	5.705851000	0.447064000
H	3.788393000	5.661755000	-0.495507000
H	1.710446000	7.155096000	0.150660000
C	-3.726733000	1.619452000	0.032811000
S	-4.595686000	0.220063000	-0.574694000
C	-4.626063000	2.577687000	0.479947000
C	-6.115821000	0.950301000	-0.213268000
C	-5.981667000	2.197057000	0.345404000
H	-4.306076000	3.515229000	0.920051000
H	-7.030980000	0.414600000	-0.430459000
H	-6.818163000	2.813741000	0.654707000
C	-0.438902000	-3.745914000	0.105472000
S	0.230191000	-5.279475000	-0.450237000
C	-1.750239000	-3.917053000	0.511747000
C	-1.252926000	-6.100952000	-0.122603000
C	-2.206316000	-5.253221000	0.380954000
H	-2.342067000	-3.108206000	0.916561000
H	-1.340447000	-7.159345000	-0.329590000
H	-3.205060000	-5.574828000	0.654785000

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2 | Icc-2 B3LYP/6-31G*

N	0.241264000	1.378387000	-0.021798000
C	1.254478000	0.422717000	-0.047765000
C	2.531372000	1.096284000	-0.076278000
C	2.236864000	2.453238000	-0.033073000

C	0.827752000	2.610528000	-0.005161000
N	-1.336343000	-0.552643000	0.084289000
C	-0.194479000	-1.346747000	0.049994000
C	-0.581277000	-2.733110000	0.039950000
C	-1.972850000	-2.730482000	0.041100000
C	-2.420554000	-1.388259000	0.074078000
B	-1.278868000	1.011269000	0.066812000
N	1.043388000	-0.882178000	-0.010802000
F	-1.953252000	1.496036000	-1.045026000
F	-1.804841000	1.538979000	1.243396000
H	2.943705000	3.268400000	-0.091666000
H	-2.620518000	-3.594818000	0.079728000
C	0.279895000	-3.892176000	0.039431000
S	1.991178000	-3.824655000	0.427176000
C	-0.098076000	-5.199671000	-0.209022000
C	2.149571000	-5.539055000	0.250242000
C	0.962984000	-6.133914000	-0.092236000
H	-1.111615000	-5.472821000	-0.481482000
H	3.112008000	-6.009907000	0.401908000
H	0.850400000	-7.199740000	-0.257735000
C	3.833549000	0.478367000	-0.155188000
S	5.282944000	1.408790000	0.203654000
C	4.173415000	-0.809055000	-0.522230000
C	6.302234000	0.054655000	-0.148525000
C	5.574233000	-1.046293000	-0.516721000
H	3.429173000	-1.546630000	-0.791362000
H	7.376154000	0.148848000	-0.058119000
H	6.024269000	-1.997135000	-0.780643000
C	0.173849000	3.899708000	0.032539000
S	-1.439896000	4.267774000	-0.553060000
C	0.785302000	5.057279000	0.495519000
C	-1.249926000	5.936354000	-0.162008000
C	-0.023723000	6.212243000	0.390804000
H	1.780421000	5.057826000	0.925323000
H	-2.059766000	6.626887000	-0.359566000
H	0.284309000	7.199783000	0.715580000
C	-3.804073000	-0.976692000	0.102855000
S	-5.039506000	-2.115122000	-0.431775000
C	-4.392458000	0.201983000	0.523806000
C	-6.300794000	-0.990027000	-0.074821000
C	-5.807117000	0.188992000	0.421528000
H	-3.817782000	1.027943000	0.918708000
H	-7.332194000	-1.258665000	-0.261087000
H	-6.436097000	1.023793000	0.710405000

2 | IIaa B3LYP/6-31G*

N	-0.073490000	1.249201000	-0.707495000
C	-0.002895000	1.143855000	0.678971000
C	0.049749000	2.465502000	1.252483000
C	0.000000000	3.340082000	0.174043000
C	-0.073754000	2.582000000	-1.020857000
N	0.073490000	-1.249201000	-0.707495000
C	0.002895000	-1.143855000	0.678971000
C	-0.049749000	-2.465502000	1.252483000
C	0.000000000	-3.340082000	0.174043000
C	0.073754000	-2.582000000	-1.020857000
B	0.000000000	0.000000000	-1.653528000
N	0.000000000	0.000000000	1.342034000
F	1.142647000	0.100625000	-2.441151000
F	-1.142647000	-0.100625000	-2.441151000
H	0.006166000	4.420626000	0.218364000
H	-0.006166000	-4.420626000	0.218364000
C	-0.134735000	-2.786888000	2.657707000
S	0.232365000	-4.410305000	3.224980000
C	-0.511817000	-1.986185000	3.719208000
C	-0.127117000	-3.976772000	4.861851000
C	-0.505278000	-2.664014000	4.968028000
H	-0.797695000	-0.951116000	3.584902000
H	-0.034890000	-4.713644000	5.648506000
H	-0.777796000	-2.196662000	5.908051000
C	0.134735000	2.786888000	2.657707000
S	-0.232365000	4.410305000	3.224980000
C	0.511817000	1.986185000	3.719208000
C	0.127117000	3.976772000	4.861851000
C	0.505278000	2.664014000	4.968028000
H	0.797695000	0.951116000	3.584902000
H	0.034890000	4.713644000	5.648506000
H	0.777796000	2.196662000	5.908051000
C	-0.127700000	3.142156000	-2.350042000
S	0.368583000	4.818148000	-2.584709000
C	-0.550153000	2.599189000	-3.550322000
C	-0.003925000	4.744790000	-4.269235000
C	-0.478572000	3.510958000	-4.634007000
H	-0.922939000	1.587768000	-3.628703000
H	0.157195000	5.612247000	-4.895527000
H	-0.773292000	3.261510000	-5.647360000
C	0.127700000	-3.142156000	-2.350042000
S	-0.368583000	-4.818148000	-2.584709000
C	0.550153000	-2.599189000	-3.550322000
C	0.003925000	-4.744790000	-4.269235000

C	0.478572000	-3.510958000	-4.634007000
H	0.922939000	-1.587768000	-3.628703000
H	-0.157195000	-5.612247000	-4.895527000
H	0.773292000	-3.261510000	-5.647360000

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2 | IIab B3LYP/6-31G*

N	-0.079033000	1.245517000	-0.743177000
C	-0.009707000	1.144217000	0.644190000
C	0.042988000	2.467591000	1.212395000
C	0.000000000	3.338384000	0.128882000
C	-0.075789000	2.577304000	-1.061129000
N	0.079033000	-1.245517000	-0.743177000
C	0.009707000	-1.144217000	0.644190000
C	-0.042988000	-2.467591000	1.212395000
C	0.000000000	-3.338384000	0.128882000
C	0.075789000	-2.577304000	-1.061129000
B	0.000000000	0.000000000	-1.688833000
N	0.000000000	0.000000000	1.309576000
F	1.142063000	0.106425000	-2.477941000
F	-1.142063000	-0.106425000	-2.477941000
H	0.015784000	4.418252000	0.169223000
H	-0.015784000	-4.418252000	0.169223000
C	-0.128083000	-2.841806000	2.604343000
S	-0.620331000	-1.737184000	3.874029000
C	0.102095000	-4.101049000	3.131862000
C	-0.513106000	-2.983525000	5.067619000
C	-0.112385000	-4.180631000	4.530766000
H	0.432639000	-4.937500000	2.525899000
H	-0.741368000	-2.760470000	6.101638000
H	0.027118000	-5.084518000	5.113524000
C	0.128083000	2.841806000	2.604343000
S	0.620331000	1.737184000	3.874029000
C	-0.102095000	4.101049000	3.131862000
C	0.513106000	2.983525000	5.067619000
C	0.112385000	4.180631000	4.530766000
H	-0.432639000	4.937500000	2.525899000
H	0.741368000	2.760470000	6.101638000
H	-0.027118000	5.084518000	5.113524000
C	-0.127654000	3.133184000	-2.392962000
S	0.380384000	4.804862000	-2.633684000
C	-0.556914000	2.590233000	-3.590399000
C	0.002774000	4.729895000	-4.317329000
C	-0.481550000	3.498593000	-4.677082000
H	-0.935981000	1.580847000	-3.664944000
H	0.168997000	5.594270000	-4.946532000

H	-0.780431000	3.248148000	-5.688989000
C	0.127654000	-3.133184000	-2.392962000
S	-0.380384000	-4.804862000	-2.633684000
C	0.556914000	-2.590233000	-3.590399000
C	-0.002774000	-4.729895000	-4.317329000
C	0.481550000	-3.498593000	-4.677082000
H	0.935981000	-1.580847000	-3.664944000
H	-0.168997000	-5.594270000	-4.946532000
H	0.780431000	-3.248148000	-5.688989000

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2 | Иаc B3LYP/6-31G*

N	0.841111000	-1.065041000	-0.067643000
C	1.209403000	0.276770000	0.013546000
C	2.650091000	0.368997000	0.042533000
C	3.106787000	-0.940834000	-0.030362000
C	1.989444000	-1.808888000	-0.096355000
N	-1.509675000	-0.237736000	0.122049000
C	-0.949195000	1.034214000	0.068491000
C	-2.000299000	2.016631000	0.040823000
C	-3.186856000	1.290831000	0.078610000
C	-2.871344000	-0.087457000	0.129714000
B	-0.650405000	-1.542865000	0.018154000
N	0.350733000	1.281658000	0.047105000
F	-0.802625000	-2.337824000	1.150511000
F	-1.021452000	-2.235476000	-1.130673000
H	4.138784000	-1.263656000	-0.045975000
H	-4.190258000	1.692424000	0.080946000
C	-1.867985000	3.453531000	-0.014128000
S	-0.369920000	4.271193000	-0.427146000
C	-2.871283000	4.382375000	0.198212000
C	-1.125532000	5.823470000	-0.305026000
C	-2.449637000	5.727033000	0.036478000
H	-3.880282000	4.099275000	0.477234000
H	-0.547664000	6.720026000	-0.487378000
H	-3.100340000	6.584286000	0.169718000
C	3.439117000	1.574230000	0.131312000
S	5.161325000	1.537901000	-0.227390000
C	3.058629000	2.847587000	0.508522000
C	5.325198000	3.222129000	0.135989000
C	4.130408000	3.780007000	0.508937000
H	2.039953000	3.086513000	0.782757000
H	6.290843000	3.701968000	0.048425000
H	4.019274000	4.823997000	0.780951000
C	2.069734000	-3.248313000	-0.169267000
S	3.577786000	-4.036638000	0.294652000

C	1.149928000	-4.192458000	-0.589497000
C	2.938901000	-5.594546000	-0.087212000
C	1.647134000	-5.519498000	-0.541702000
H	0.165315000	-3.923076000	-0.944338000
H	3.548721000	-6.477058000	0.054191000
H	1.068358000	-6.387209000	-0.838451000
C	-3.841743000	-1.155901000	0.173258000
S	-5.500469000	-0.816950000	-0.320014000
C	-3.727744000	-2.471312000	0.584807000
C	-5.990966000	-2.433512000	0.040348000
C	-4.947875000	-3.190595000	0.508054000
H	-2.798902000	-2.883919000	0.952604000
H	-7.017168000	-2.735010000	-0.122927000
H	-5.048538000	-4.231751000	0.794192000

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2 | IIba B3LYP/6-31G*

N	-0.058052000	1.248545000	-0.626248000
C	0.005196000	1.144319000	0.760671000
C	0.050568000	2.468409000	1.329575000
C	0.000000000	3.339334000	0.248766000
C	-0.063529000	2.575762000	-0.945707000
N	0.058052000	-1.248545000	-0.626248000
C	-0.005196000	-1.144319000	0.760671000
C	-0.050568000	-2.468409000	1.329575000
C	0.000000000	-3.339334000	0.248766000
C	0.063529000	-2.575762000	-0.945707000
B	0.000000000	0.000000000	-1.571575000
N	0.000000000	0.000000000	1.423324000
F	1.146180000	0.061582000	-2.351938000
F	-1.146180000	-0.061582000	-2.351938000
H	-0.011002000	4.419080000	0.289297000
H	0.011002000	-4.419080000	0.289297000
C	-0.125345000	-2.794456000	2.734944000
S	0.249679000	-4.418266000	3.295922000
C	-0.497519000	-1.997661000	3.800605000
C	-0.101080000	-3.990046000	4.936519000
C	-0.481633000	-2.678672000	5.047989000
H	-0.786013000	-0.962703000	3.670716000
H	-0.001925000	-4.728648000	5.720687000
H	-0.749161000	-2.214062000	5.990823000
C	0.125345000	2.794456000	2.734944000
S	-0.249679000	4.418266000	3.295922000
C	0.497519000	1.997661000	3.800605000
C	0.101080000	3.990046000	4.936519000
C	0.481633000	2.678672000	5.047989000

H	0.786013000	0.962703000	3.670716000
H	0.001925000	4.728648000	5.720687000
H	0.749161000	2.214062000	5.990823000
C	-0.106631000	3.164440000	-2.265573000
S	-0.750560000	2.415464000	-3.717272000
C	0.316307000	4.457058000	-2.547097000
C	-0.435939000	3.835149000	-4.643322000
C	0.134515000	4.836596000	-3.896771000
H	0.772239000	5.097075000	-1.800523000
H	-0.687266000	3.852571000	-5.696039000
H	0.419067000	5.802662000	-4.298476000
C	0.106631000	-3.164440000	-2.265573000
S	0.750560000	-2.415464000	-3.717272000
C	-0.316307000	-4.457058000	-2.547097000
C	0.435939000	-3.835149000	-4.643322000
C	-0.134515000	-4.836596000	-3.896771000
H	-0.772239000	-5.097075000	-1.800523000
H	0.687266000	-3.852571000	-5.696039000
H	-0.419067000	-5.802662000	-4.298476000

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2 | Iibb B3LYP/6-31G*

N	-0.062731000	1.244752000	-0.663584000
C	-0.002267000	1.144704000	0.724232000
C	0.041909000	2.470572000	1.287839000
C	0.000000000	3.337663000	0.201730000
C	-0.063820000	2.570756000	-0.987729000
N	0.062731000	-1.244752000	-0.663584000
C	0.002267000	-1.144704000	0.724232000
C	-0.041909000	-2.470572000	1.287839000
C	0.000000000	-3.337663000	0.201730000
C	0.063820000	-2.570756000	-0.987729000
B	0.000000000	0.000000000	-1.608663000
N	0.000000000	0.000000000	1.389143000
F	1.145775000	0.066327000	-2.390611000
F	-1.145775000	-0.066327000	-2.390611000
H	-0.001708000	4.416956000	0.237745000
H	0.001708000	-4.416956000	0.237745000
C	-0.112408000	-2.849064000	2.680231000
S	-0.598821000	-1.749020000	3.956049000
C	0.129925000	-4.107297000	3.203876000
C	-0.473835000	-2.996356000	5.147178000
C	-0.071404000	-4.190198000	4.604851000
H	0.460264000	-4.940930000	2.593884000
H	-0.693606000	-2.775865000	6.183572000
H	0.078878000	-5.094094000	5.184966000

C	0.112408000	2.849064000	2.680231000
S	0.598821000	1.749020000	3.956049000
C	-0.129925000	4.107297000	3.203876000
C	0.473835000	2.996356000	5.147178000
C	0.071404000	4.190198000	4.604851000
H	-0.460264000	4.940930000	2.593884000
H	0.693606000	2.775865000	6.183572000
H	-0.078878000	5.094094000	5.184966000
C	-0.101927000	3.154253000	-2.310956000
S	-0.764393000	2.410051000	-3.756528000
C	0.338969000	4.439001000	-2.599151000
C	-0.434368000	3.822054000	-4.689192000
C	0.155590000	4.816967000	-3.949326000
H	0.809170000	5.073920000	-1.857036000
H	-0.690669000	3.839484000	-5.740711000
H	0.453234000	5.777021000	-4.356008000
C	0.101927000	-3.154253000	-2.310956000
S	0.764393000	-2.410051000	-3.756528000
C	-0.338969000	-4.439001000	-2.599151000
C	0.434368000	-3.822054000	-4.689192000
C	-0.155590000	-4.816967000	-3.949326000
H	-0.809170000	-5.073920000	-1.857036000
H	0.690669000	-3.839484000	-5.740711000
H	-0.453234000	-5.777021000	-4.356008000

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2 | IIbc B3LYP/6-31G*

N	0.992232000	1.114972000	-0.072488000
C	-0.369097000	1.396989000	-0.029499000
C	-0.553987000	2.823189000	0.024177000
C	0.727485000	3.364548000	0.008928000
C	1.664679000	2.303672000	-0.050660000
N	0.301333000	-1.281698000	0.023446000
C	-1.005503000	-0.801971000	-0.046488000
C	-1.912788000	-1.924436000	-0.098673000
C	-1.108149000	-3.054955000	-0.046931000
C	0.248057000	-2.645036000	0.025390000
B	1.555462000	-0.343480000	-0.020009000
N	-1.324830000	0.481166000	-0.044139000
F	2.314162000	-0.508790000	1.130973000
F	2.297689000	-0.612473000	-1.162048000
H	0.987145000	4.412809000	0.017227000
H	-1.440346000	-4.083091000	-0.039138000
C	-3.353211000	-1.869979000	-0.182604000
S	-4.318399000	-3.305692000	0.138725000
C	-4.173095000	-0.813620000	-0.528108000

C	-5.788783000	-2.456149000	-0.197726000
C	-5.553854000	-1.149059000	-0.534609000
H	-3.779804000	0.163334000	-0.775069000
H	-6.738295000	-2.969037000	-0.122059000
H	-6.342008000	-0.447248000	-0.784751000
C	-1.799990000	3.552698000	0.075703000
S	-3.341878000	2.803646000	0.455902000
C	-1.969104000	4.912269000	-0.115643000
C	-4.163454000	4.323430000	0.349620000
C	-3.310222000	5.349431000	0.036617000
H	-1.148417000	5.572672000	-0.373464000
H	-5.231124000	4.372049000	0.518980000
H	-3.627002000	6.379660000	-0.083352000
C	3.097301000	2.503511000	-0.066449000
S	4.290734000	1.399456000	-0.728893000
C	3.721564000	3.653337000	0.397871000
C	5.571626000	2.495820000	-0.367561000
C	5.126019000	3.647770000	0.232060000
H	3.176419000	4.461333000	0.872189000
H	6.590642000	2.226633000	-0.614107000
H	5.777136000	4.454827000	0.548930000
C	1.356683000	-3.572108000	0.072278000
S	2.955253000	-3.253071000	0.724939000
C	1.274506000	-4.891056000	-0.355676000
C	3.456974000	-4.871277000	0.407099000
C	2.466971000	-5.627346000	-0.170939000
H	0.383137000	-5.299865000	-0.817355000
H	4.463053000	-5.178240000	0.662644000
H	2.589208000	-6.665594000	-0.458517000

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2 | Hca B3LYP/6-31G*

N	1.190994000	-0.875517000	0.000233000
C	1.319604000	0.509436000	0.050049000
C	2.719715000	0.850981000	0.084282000
C	3.398658000	-0.360176000	0.041173000
C	2.447165000	-1.411557000	-0.005504000
N	-1.272173000	-0.460305000	0.118191000
C	-0.936845000	0.888882000	0.036988000
C	-2.145007000	1.672537000	-0.037567000
C	-3.186658000	0.754600000	0.010706000
C	-2.637686000	-0.548679000	0.105875000
B	-0.195316000	-1.600137000	0.091746000
N	0.301265000	1.352921000	0.038119000
F	-0.235301000	-2.348340000	1.265239000
F	-0.394086000	-2.401547000	-1.023078000

H	4.470041000	-0.499589000	0.024443000
H	-4.244766000	0.977147000	-0.011242000
C	-2.228497000	3.110622000	-0.140237000
S	-3.740127000	3.942483000	0.198966000
C	-1.258872000	4.020804000	-0.516070000
C	-3.037694000	5.481018000	-0.169974000
C	-1.720979000	5.364460000	-0.530817000
H	-0.256843000	3.713947000	-0.786080000
H	-3.635464000	6.379585000	-0.095414000
H	-1.101358000	6.211139000	-0.805681000
C	3.274696000	2.183300000	0.142917000
S	4.966510000	2.464011000	-0.245703000
C	2.667834000	3.369651000	0.508362000
C	4.818181000	4.155994000	0.090559000
C	3.545882000	4.486730000	0.476440000
H	1.627635000	3.415677000	0.803521000
H	5.675782000	4.806022000	-0.020205000
H	3.245642000	5.495923000	0.736703000
C	2.810491000	-2.811056000	-0.032356000
S	1.832404000	-4.129777000	-0.655530000
C	4.041508000	-3.294670000	0.391293000
C	3.083859000	-5.271124000	-0.332190000
C	4.195616000	-4.690438000	0.226200000
H	4.796719000	-2.656904000	0.835934000
H	2.928578000	-6.315652000	-0.569973000
H	5.084812000	-5.240250000	0.513696000
C	-3.407719000	-1.767474000	0.167993000
S	-5.097890000	-1.731516000	-0.334147000
C	-3.066992000	-3.036452000	0.601400000
C	-5.298803000	-3.402942000	0.050357000
C	-4.141752000	-3.958827000	0.533065000
H	-2.083301000	-3.274922000	0.980477000
H	-6.255487000	-3.882068000	-0.110515000
H	-4.060133000	-4.997036000	0.835322000

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2 | Hcb B3LYP/6-31G*

N	0.851236000	-1.070188000	0.144617000
C	-0.536953000	-1.153907000	0.061723000
C	-0.923291000	-2.541824000	0.011941000
C	0.265833000	-3.260442000	0.069967000
C	1.343315000	-2.347063000	0.153567000
N	0.521500000	1.395442000	-0.030537000
C	-0.841217000	1.114319000	0.017156000
C	-1.575785000	2.354074000	0.025083000
C	-0.613240000	3.356431000	-0.025156000

C	0.667744000	2.753048000	-0.056818000
B	1.622196000	0.291081000	0.090370000
N	-1.348341000	-0.108570000	0.032899000
F	2.452326000	0.312712000	-1.021912000
F	2.345782000	0.501695000	1.262021000
H	0.369961000	-4.336104000	0.059485000
H	-0.792004000	4.421074000	-0.052297000
C	-3.006676000	2.546625000	0.072339000
S	-4.130978000	1.302909000	0.585444000
C	-3.689333000	3.716490000	-0.213136000
C	-5.475076000	2.377026000	0.413376000
C	-5.091007000	3.619220000	-0.023544000
H	-3.191336000	4.612850000	-0.566248000
H	-6.475513000	2.028057000	0.633293000
H	-5.783951000	4.433167000	-0.206445000
C	-2.252377000	-3.098119000	-0.083403000
S	-3.656372000	-2.169977000	-0.575495000
C	-2.608164000	-4.417607000	0.138650000
C	-4.673474000	-3.564973000	-0.478992000
C	-3.983194000	-4.681964000	-0.082092000
H	-1.897317000	-5.167724000	0.467448000
H	-5.727181000	-3.480589000	-0.710604000
H	-4.440528000	-5.656333000	0.050345000
C	2.737033000	-2.716932000	0.224735000
S	3.208954000	-4.346180000	-0.258094000
C	3.844555000	-2.008991000	0.655372000
C	4.862839000	-4.035825000	0.130905000
C	5.045974000	-2.760652000	0.600592000
H	3.777201000	-0.994477000	1.022106000
H	5.606166000	-4.807661000	-0.018794000
H	6.011229000	-2.369631000	0.902786000
C	1.901681000	3.508157000	-0.088580000
S	3.445720000	2.955657000	-0.716314000
C	2.006366000	4.827975000	0.329594000
C	4.172990000	4.487642000	-0.403227000
C	3.295533000	5.382952000	0.156348000
H	1.177653000	5.364879000	0.776642000
H	5.216320000	4.643267000	-0.645998000
H	3.562933000	6.394873000	0.439540000

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2 | Hcc-1 B3LYP/6-31G*

N	-1.360561000	-0.788770000	-0.039612000
C	-0.154571000	-1.480126000	-0.009011000
C	-0.420796000	-2.894069000	0.009623000
C	-1.807060000	-3.010881000	-0.013201000

C	-2.369014000	-1.710933000	-0.041499000
N	0.038503000	1.274743000	0.102965000
C	1.131046000	0.413362000	0.012021000
C	2.343282000	1.196449000	-0.046415000
C	1.932433000	2.521548000	0.019176000
C	0.518897000	2.555280000	0.110578000
B	-1.445495000	0.769184000	0.070897000
N	1.037884000	-0.905345000	-0.010551000
F	-2.108570000	1.102444000	1.249357000
F	-2.093274000	1.297886000	-1.036582000
H	-2.378713000	-3.926980000	-0.029691000
H	2.569923000	3.395082000	0.012862000
C	3.693109000	0.696395000	-0.152952000
S	5.061309000	1.755990000	0.165441000
C	4.138837000	-0.558773000	-0.519262000
C	6.189211000	0.494872000	-0.199300000
C	5.554906000	-0.670024000	-0.543463000
H	3.457834000	-1.361178000	-0.768998000
H	7.252118000	0.685424000	-0.133711000
H	6.082283000	-1.579112000	-0.811238000
C	0.537343000	-3.974860000	0.038141000
S	2.232771000	-3.751063000	0.436257000
C	0.277909000	-5.314368000	-0.190248000
C	2.543394000	-5.447314000	0.287661000
C	1.416332000	-6.149605000	-0.051934000
H	-0.705245000	-5.680694000	-0.464741000
H	3.542195000	-5.829028000	0.453957000
H	1.399075000	-7.223736000	-0.200417000
C	-3.793745000	-1.458830000	-0.050262000
S	-4.591872000	-0.025791000	-0.676759000
C	-4.740801000	-2.372684000	0.391529000
C	-6.147569000	-0.685574000	-0.331738000
C	-6.076159000	-1.932992000	0.236865000
H	-4.469807000	-3.320582000	0.842091000
H	-7.035043000	-0.111011000	-0.563943000
H	-6.943092000	-2.509658000	0.539494000
C	-0.274090000	3.758596000	0.186837000
S	0.459029000	5.289152000	-0.293512000
C	-1.571564000	3.967817000	0.619576000
C	-0.980530000	6.158202000	0.098259000
C	-1.966516000	5.328556000	0.567813000
H	-2.196639000	3.166212000	0.986734000
H	-1.020797000	7.229350000	-0.049152000
H	-2.946302000	5.679753000	0.872068000

2 | Hcc-2 B3LYP/6-31G*

N	1.348067000	-0.524541000	0.155736000
C	0.225076000	-1.343438000	0.091386000
C	0.643507000	-2.719268000	0.032135000
C	2.034094000	-2.685673000	0.062710000
C	2.451139000	-1.335556000	0.141333000
N	-0.272405000	1.369965000	0.012785000
C	-1.264869000	0.393784000	0.071152000
C	-2.555915000	1.039921000	0.090892000
C	-2.290137000	2.401849000	0.032180000
C	-0.885062000	2.589549000	-0.011265000
B	1.255474000	1.037550000	0.108771000
N	-1.024183000	-0.906497000	0.081294000
F	1.921363000	1.510711000	-1.012980000
F	1.766964000	1.603047000	1.274202000
H	2.701761000	-3.535326000	0.041828000
H	-3.017780000	3.200007000	0.001415000
C	-3.845855000	0.394560000	0.154376000
S	-5.311493000	1.296319000	-0.212589000
C	-4.162079000	-0.901577000	0.511680000
C	-6.305084000	-0.081347000	0.121693000
C	-5.557521000	-1.168567000	0.490938000
H	-3.405167000	-1.623926000	0.786302000
H	-7.379800000	-0.009344000	0.020925000
H	-5.989664000	-2.130210000	0.745456000
C	-0.190719000	-3.895689000	-0.043683000
S	-1.900527000	-3.844462000	-0.440132000
C	0.214760000	-5.206468000	0.134500000
C	-2.022316000	-5.568969000	-0.357064000
C	-0.824728000	-6.155781000	-0.040103000
H	1.232480000	-5.472682000	0.398041000
H	-2.972937000	-6.051686000	-0.542272000
H	-0.689176000	-7.226413000	0.066820000
C	3.824714000	-0.893923000	0.189613000
S	5.094163000	-2.004854000	-0.323833000
C	4.380110000	0.298229000	0.617739000
C	6.323823000	-0.850828000	0.050346000
C	5.796050000	0.317314000	0.537117000
H	3.780854000	1.112258000	1.000729000
H	7.363741000	-1.096376000	-0.119743000
H	6.401344000	1.166781000	0.833717000
C	-0.260266000	3.893269000	-0.052231000
S	1.337598000	4.266434000	-0.677982000
C	-0.891582000	5.060324000	0.358268000
C	1.113888000	5.948619000	-0.373031000

C	-0.111143000	6.225883000	0.181583000
H	-1.880468000	5.062971000	0.801965000
H	1.905057000	6.645599000	-0.617975000
H	-0.438066000	7.221982000	0.458192000

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2 | IVaa B3LYP/6-31G*

N	-1.255853000	-0.696780000	0.126338000
C	-1.133419000	0.689452000	0.077775000
C	-2.445726000	1.277216000	-0.032866000
C	-3.331901000	0.207099000	-0.039075000
C	-2.589748000	-0.995944000	0.057782000
N	1.245562000	-0.722396000	0.128724000
C	1.153685000	0.666092000	0.149544000
C	2.480815000	1.228496000	0.120374000
C	3.343529000	0.141611000	0.043057000
C	2.573065000	-1.047428000	0.058260000
B	-0.014555000	-1.656050000	0.156147000
N	0.016674000	1.340317000	0.114043000
F	-0.024525000	-2.505385000	-0.929333000
F	-0.017943000	-2.380226000	1.359787000
H	-4.410251000	0.261553000	-0.100435000
H	4.424450000	0.173772000	0.039885000
C	2.815162000	2.631825000	0.173560000
S	4.410613000	3.189415000	-0.310214000
C	2.047687000	3.698590000	0.601573000
C	4.011253000	4.829797000	0.072412000
C	2.728846000	4.944118000	0.541759000
H	1.034303000	3.570985000	0.959640000
H	4.743318000	5.612532000	-0.074969000
H	2.286324000	5.887577000	0.842392000
C	-2.750869000	2.686080000	-0.117960000
S	-4.391427000	3.259967000	0.150708000
C	-1.920620000	3.747049000	-0.426473000
C	-3.925108000	4.898323000	-0.156376000
C	-2.589774000	5.000230000	-0.446727000
H	-0.869713000	3.609044000	-0.644700000
H	-4.661434000	5.688941000	-0.101007000
H	-2.099736000	5.940613000	-0.674485000
C	-3.164875000	-2.319992000	0.068372000
S	-4.805599000	-2.537631000	-0.539566000
C	-2.662797000	-3.525762000	0.523186000
C	-4.773114000	-4.223584000	-0.167410000
C	-3.577410000	-4.600948000	0.388033000
H	-1.680895000	-3.613413000	0.965351000
H	-5.633069000	-4.841629000	-0.389105000

H	-3.357609000	-5.617274000	0.695783000
C	3.117216000	-2.383883000	0.017695000
S	4.745648000	-2.618153000	-0.615002000
C	2.590924000	-3.591982000	0.437048000
C	4.677298000	-4.314761000	-0.299426000
C	3.478610000	-4.682945000	0.255860000
H	1.612315000	-3.671366000	0.888120000
H	5.519979000	-4.944870000	-0.551394000
H	3.238212000	-5.703759000	0.531719000

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2 | IVab B3LYP/6-31G*

N	1.251854000	-0.744497000	0.145049000
C	-0.017093000	-1.315801000	0.088410000
C	0.113523000	-2.748344000	-0.005648000
C	1.482189000	-2.996765000	-0.001235000
C	2.165718000	-1.762271000	0.093682000
N	0.061545000	1.447109000	0.097014000
C	-1.110430000	0.695279000	0.106695000
C	-2.242007000	1.585808000	0.043946000
C	-1.703761000	2.865889000	-0.037288000
C	-0.293203000	2.765424000	0.002909000
B	1.487418000	0.803457000	0.161669000
N	-1.147766000	-0.628135000	0.093721000
F	2.257769000	1.196093000	-0.912479000
F	2.098643000	1.167462000	1.374155000
H	1.963021000	-3.963135000	-0.054503000
H	-2.253766000	3.796047000	-0.052432000
C	-3.646512000	1.252853000	0.074066000
S	-4.263792000	-0.268277000	0.689385000
C	-4.694900000	2.075590000	-0.300528000
C	-5.898159000	0.236351000	0.438691000
C	-5.972996000	1.496788000	-0.097913000
H	-4.540480000	3.061338000	-0.725513000
H	-6.712795000	-0.430552000	0.688907000
H	-6.906651000	1.991314000	-0.342467000
C	-0.933142000	-3.738803000	-0.092187000
S	-2.601737000	-3.354726000	-0.471632000
C	-0.782042000	-5.107102000	0.057904000
C	-3.046936000	-5.025064000	-0.427372000
C	-1.982396000	-5.837162000	-0.129184000
H	0.167012000	-5.566792000	0.310938000
H	-4.072750000	-5.314166000	-0.615072000
H	-2.053703000	-6.915901000	-0.043752000
C	3.602288000	-1.615183000	0.120019000
S	4.602122000	-2.937863000	-0.479508000

C	4.402292000	-0.589013000	0.587494000
C	6.052417000	-2.085948000	-0.086735000
C	5.789399000	-0.860278000	0.468773000
H	3.992253000	0.309192000	1.026257000
H	7.014834000	-2.532745000	-0.298304000
H	6.564241000	-0.171960000	0.787871000
C	0.615187000	3.887534000	-0.036249000
S	0.046819000	5.414004000	-0.709972000
C	1.916188000	4.020390000	0.412224000
C	1.556026000	6.182790000	-0.370937000
C	2.444814000	5.322611000	0.221041000
H	2.448621000	3.210522000	0.889784000
H	1.705130000	7.220699000	-0.637655000
H	3.447417000	5.611860000	0.516192000

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2 | IVac B3LYP/6-31G*

N	-1.525063000	-0.146050000	0.156732000
C	-0.884005000	1.087997000	0.122810000
C	-1.868287000	2.133127000	0.021341000
C	-3.098113000	1.482352000	-0.004192000
C	-2.872349000	0.088436000	0.081695000
N	0.775310000	-1.119906000	0.144110000
C	1.224314000	0.198770000	0.168645000
C	2.667449000	0.205418000	0.124287000
C	3.042377000	-1.129499000	0.034139000
C	1.874041000	-1.929973000	0.056466000
B	-0.745081000	-1.504178000	0.177795000
N	0.428413000	1.254635000	0.149962000
F	-1.081373000	-2.282748000	-0.909012000
F	-1.018508000	-2.178367000	1.380096000
H	-4.073318000	1.943825000	-0.068028000
H	4.052141000	-1.516115000	0.018254000
C	3.527206000	1.362864000	0.179097000
S	5.216158000	1.241614000	-0.297161000
C	3.243767000	2.645749000	0.606183000
C	5.497513000	2.905485000	0.087693000
C	4.363183000	3.518653000	0.551904000
H	2.260275000	2.933686000	0.952765000
H	6.480248000	3.334396000	-0.056008000
H	4.328887000	4.560534000	0.851169000
C	-1.642866000	3.557908000	-0.041606000
S	-0.067809000	4.276835000	-0.335359000
C	-2.601381000	4.549088000	0.075588000
C	-0.734567000	5.873490000	-0.293962000
C	-2.086085000	5.863017000	-0.064923000

H	-3.645782000	4.332108000	0.271071000
H	-0.089631000	6.730520000	-0.437509000
H	-2.691852000	6.759944000	0.002935000
C	-3.908212000	-0.917892000	0.080640000
S	-5.501663000	-0.497298000	-0.545371000
C	-3.906307000	-2.222643000	0.537880000
C	-6.116571000	-2.068777000	-0.175971000
C	-5.159558000	-2.870512000	0.390813000
H	-3.035310000	-2.675499000	0.989356000
H	-7.144361000	-2.314376000	-0.408230000
H	-5.345187000	-3.893692000	0.698441000
C	1.862709000	-3.372617000	0.006559000
S	3.270058000	-4.209357000	-0.646485000
C	0.918094000	-4.289309000	0.430702000
C	2.559899000	-5.751862000	-0.332740000
C	1.317738000	-5.635952000	0.236982000
H	-0.011302000	-3.990091000	0.893413000
H	3.093664000	-6.655327000	-0.596370000
H	0.707406000	-6.488348000	0.514213000

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2 | IVba B3LYP/6-31G*

N	-0.643453000	1.240614000	-0.003837000
C	0.746170000	1.151671000	-0.019971000
C	1.301487000	2.480993000	-0.083277000
C	0.209790000	3.339564000	-0.090686000
C	-0.977500000	2.563624000	-0.047286000
N	-0.612052000	-1.259315000	0.000401000
C	0.773487000	-1.136182000	0.050694000
C	1.361590000	-2.452260000	0.066823000
C	0.294134000	-3.338195000	-0.007728000
C	-0.911391000	-2.590520000	-0.043826000
B	-1.572361000	-0.021441000	-0.043665000
N	1.421816000	0.016130000	0.025351000
F	-2.330150000	-0.031221000	-1.196710000
F	-2.375822000	-0.033099000	1.098380000
H	0.237465000	4.419594000	-0.109333000
H	0.346323000	-4.416802000	0.031259000
C	2.770049000	-2.757787000	0.160840000
S	3.368220000	-4.353579000	-0.270836000
C	3.812268000	-1.959911000	0.592388000
C	4.992302000	-3.913830000	0.137811000
C	5.071621000	-2.618458000	0.577083000
H	3.657799000	-0.940486000	0.921575000
H	5.791633000	-4.634178000	0.026238000
H	5.999585000	-2.150347000	0.887123000

C	2.704491000	2.823204000	-0.121731000
S	3.230741000	4.469017000	0.205517000
C	3.793029000	2.027414000	-0.423274000
C	4.888004000	4.050708000	-0.070262000
C	5.029883000	2.726642000	-0.392490000
H	3.686697000	0.979462000	-0.671677000
H	5.658503000	4.803977000	0.025676000
H	5.987603000	2.265202000	-0.607476000
C	-2.303936000	3.139100000	-0.071147000
S	-3.772375000	2.395272000	0.538808000
C	-2.581037000	4.415095000	-0.544636000
C	-4.699186000	3.794311000	0.144182000
C	-3.940334000	4.785702000	-0.427430000
H	-1.823404000	5.048717000	-0.991103000
H	-5.761029000	3.808093000	0.353858000
H	-4.339634000	5.738227000	-0.757361000
C	-2.221527000	-3.197808000	-0.116273000
S	-3.727382000	-2.492030000	0.444495000
C	-2.450000000	-4.478386000	-0.602499000
C	-4.605811000	-3.911264000	0.012719000
C	-3.803413000	-4.881976000	-0.534540000
H	-1.660777000	-5.090970000	-1.023084000
H	-5.673732000	-3.951483000	0.184679000
H	-4.167923000	-5.842498000	-0.881134000

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2 | IVbb B3LYP/6-31G*

N	-0.678095000	1.243612000	0.017023000
C	0.711799000	1.155720000	-0.002479000
C	1.265194000	2.486008000	-0.043792000
C	0.170686000	3.343672000	-0.041903000
C	-1.013245000	2.566795000	-0.006916000
N	-0.652198000	-1.248615000	-0.034735000
C	0.734909000	-1.133958000	0.009300000
C	1.314322000	-2.453511000	-0.008881000
C	0.239054000	-3.331340000	-0.091669000
C	-0.959932000	-2.576606000	-0.105154000
B	-1.609882000	-0.011615000	-0.041569000
N	1.387659000	0.017855000	0.011815000
F	-2.381203000	0.005829000	-1.186245000
F	-2.403242000	-0.047272000	1.108244000
H	0.196400000	4.423207000	-0.050699000
H	0.284652000	-4.410049000	-0.066989000
C	2.709671000	-2.819161000	0.065415000
S	3.956682000	-1.746363000	0.671814000
C	3.256106000	-4.048842000	-0.258616000

C	5.167224000	-2.966788000	0.485291000
C	4.651997000	-4.131535000	-0.024184000
H	2.665539000	-4.860027000	-0.670205000
H	6.194374000	-2.752226000	0.749720000
H	5.248371000	-5.014137000	-0.227868000
C	2.655767000	2.875480000	-0.076837000
S	3.958839000	1.773162000	-0.479648000
C	3.159035000	4.145844000	0.145219000
C	5.133115000	3.036039000	-0.349696000
C	4.565697000	4.236606000	-0.006361000
H	2.529932000	4.983598000	0.425437000
H	6.178943000	2.819252000	-0.523795000
H	5.131595000	5.150692000	0.136257000
C	-2.341678000	3.140153000	-0.019764000
S	-3.801857000	2.395787000	0.608345000
C	-2.625213000	4.414999000	-0.491237000
C	-4.734567000	3.794060000	0.224304000
C	-3.983543000	4.784991000	-0.358012000
H	-1.873115000	5.047913000	-0.948074000
H	-5.793903000	3.807051000	0.446330000
H	-4.387659000	5.736554000	-0.684945000
C	-2.274972000	-3.174440000	-0.182350000
S	-3.770567000	-2.481873000	0.420429000
C	-2.514865000	-4.437467000	-0.706644000
C	-4.660198000	-3.883515000	-0.044954000
C	-3.868984000	-4.838645000	-0.634015000
H	-1.733274000	-5.038209000	-1.157531000
H	-5.726027000	-3.925290000	0.139227000
H	-4.241796000	-5.785976000	-1.007151000

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2 | IVbc B3LYP/6-31G*

N	-0.306788000	1.283462000	-0.019833000
C	1.003344000	0.807864000	-0.047262000
C	1.907934000	1.932982000	-0.094211000
C	1.098029000	3.060820000	-0.082602000
C	-0.258120000	2.646875000	-0.041785000
N	-0.986912000	-1.118526000	-0.043545000
C	0.375991000	-1.394083000	-0.014283000
C	0.568888000	-2.820150000	-0.019071000
C	-0.708730000	-3.368113000	-0.074276000
C	-1.651898000	-2.310824000	-0.088575000
B	-1.556210000	0.338524000	-0.063868000
N	1.327484000	-0.473701000	-0.027802000
F	-2.295161000	0.561669000	-1.207924000
F	-2.321176000	0.541935000	1.087242000

H	1.425846000	4.090377000	-0.084574000
H	-0.964373000	-4.416753000	-0.036818000
C	1.817173000	-3.544743000	0.039183000
S	3.335081000	-2.812977000	0.532112000
C	2.004099000	-4.889558000	-0.225156000
C	4.171258000	-4.320125000	0.373860000
C	3.340114000	-5.329146000	-0.038388000
H	1.199944000	-5.536019000	-0.559180000
H	5.230887000	-4.373797000	0.586563000
H	3.669586000	-6.348769000	-0.205511000
C	3.350334000	1.884225000	-0.138277000
S	4.298922000	3.336200000	0.159607000
C	4.185008000	0.822051000	-0.425870000
C	5.782227000	2.485278000	-0.109327000
C	5.563448000	1.166072000	-0.407867000
H	3.803519000	-0.165367000	-0.648554000
H	6.726574000	3.006477000	-0.026165000
H	6.361817000	0.461219000	-0.613019000
C	-1.369845000	3.571795000	-0.047678000
S	-2.986478000	3.263876000	0.563292000
C	-1.277363000	4.880889000	-0.502973000
C	-3.482036000	4.872822000	0.193106000
C	-2.476355000	5.618110000	-0.371534000
H	-0.373262000	5.281389000	-0.946792000
H	-4.496028000	5.182721000	0.411017000
H	-2.591785000	6.649157000	-0.686492000
C	-3.082164000	-2.520369000	-0.145794000
S	-4.317936000	-1.427845000	0.453529000
C	-3.671172000	-3.674213000	-0.644880000
C	-5.569088000	-2.532384000	0.020038000
C	-5.082646000	-3.679907000	-0.555780000
H	-3.093795000	-4.476565000	-1.089817000
H	-6.602004000	-2.271506000	0.211495000
H	-5.709336000	-4.491342000	-0.908641000

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2 | IVca B3LYP/6-31G*

N	-1.214929000	-0.842118000	0.032511000
C	-1.298602000	0.547009000	0.005136000
C	-2.684161000	0.933050000	-0.096284000
C	-3.400624000	-0.257062000	-0.114287000
C	-2.485247000	-1.338056000	-0.039083000
N	1.261983000	-0.503800000	0.080730000
C	0.966462000	0.856304000	0.115267000
C	2.197572000	1.606878000	0.126982000
C	3.211672000	0.659342000	0.060638000

C	2.623685000	-0.630179000	0.040156000
B	0.151164000	-1.610331000	0.047096000
N	-0.256004000	1.357905000	0.066198000
F	0.279261000	-2.401498000	-1.075316000
F	0.217285000	-2.376609000	1.217601000
H	-4.474905000	-0.364180000	-0.159895000
H	4.275887000	0.849752000	0.086124000
C	2.321819000	3.043190000	0.204579000
S	3.831101000	3.833999000	-0.228170000
C	1.395952000	3.980578000	0.621746000
C	3.186769000	5.393120000	0.160080000
C	1.889499000	5.312747000	0.594197000
H	0.402859000	3.701605000	0.949385000
H	3.800464000	6.276100000	0.041594000
H	1.306247000	6.177310000	0.891997000
C	-3.196317000	2.282314000	-0.157853000
S	-4.902643000	2.602479000	0.122949000
C	-2.534054000	3.459041000	-0.451174000
C	-4.685958000	4.296727000	-0.159895000
C	-3.381789000	4.599591000	-0.450787000
H	-1.475030000	3.481874000	-0.672888000
H	-5.531132000	4.968428000	-0.090712000
H	-3.037292000	5.605573000	-0.664522000
C	-2.892382000	-2.725842000	-0.061423000
S	-2.002286000	-4.082636000	0.608254000
C	-4.104544000	-3.164225000	-0.577645000
C	-3.261065000	-5.180174000	0.179127000
C	-4.312208000	-4.556886000	-0.446406000
H	-4.806261000	-2.496542000	-1.064110000
H	-3.154708000	-6.232227000	0.410425000
H	-5.194920000	-5.074485000	-0.804874000
C	3.357040000	-1.872188000	-0.006476000
S	5.027801000	-1.850797000	-0.569008000
C	2.992477000	-3.156514000	0.355287000
C	5.190605000	-3.549293000	-0.302563000
C	4.034884000	-4.102809000	0.186148000
H	2.016974000	-3.391009000	0.756891000
H	6.125228000	-4.044087000	-0.531312000
H	3.932032000	-5.156102000	0.422562000

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2 | IVcb B3LYP/6-31G*

N	-0.605482000	1.368879000	0.050423000
C	0.771201000	1.164480000	0.018276000
C	1.433500000	2.441819000	-0.066247000
C	0.414221000	3.388217000	-0.076735000

C	-0.829215000	2.714767000	-0.005831000
N	-0.792541000	-1.117250000	0.051507000
C	0.600227000	-1.117881000	0.077197000
C	1.070480000	-2.480513000	0.058123000
C	-0.073613000	-3.268016000	-0.012127000
C	-1.206365000	-2.419696000	-0.010696000
B	-1.642072000	0.197664000	0.052555000
N	1.348570000	-0.026231000	0.051041000
F	-2.455697000	0.260263000	-1.060080000
F	-2.394550000	0.270927000	1.232707000
H	0.529341000	4.461248000	-0.115888000
H	-0.113988000	-4.347874000	0.002623000
C	2.431652000	-2.958571000	0.115591000
S	3.770700000	-1.989439000	0.699900000
C	2.870410000	-4.230965000	-0.208225000
C	4.873638000	-3.306431000	0.505049000
C	4.257517000	-4.427189000	0.008654000
H	2.209537000	-4.992753000	-0.607065000
H	5.918340000	-3.176285000	0.755395000
H	4.776412000	-5.356880000	-0.197512000
C	2.850888000	2.712767000	-0.125838000
S	4.053318000	1.493642000	-0.504226000
C	3.460282000	3.943404000	0.049914000
C	5.329589000	2.657955000	-0.426114000
C	4.867675000	3.911968000	-0.117273000
H	2.906098000	4.839154000	0.308060000
H	6.351712000	2.349522000	-0.602748000
H	5.508991000	4.779915000	-0.010023000
C	-2.105023000	3.398131000	-0.017240000
S	-3.606278000	2.809673000	0.676056000
C	-2.291154000	4.672069000	-0.536019000
C	-4.426813000	4.266397000	0.253447000
C	-3.609321000	5.163374000	-0.387970000
H	-1.499794000	5.218175000	-1.036516000
H	-5.474910000	4.380037000	0.498801000
H	-3.939025000	6.132071000	-0.746547000
C	-2.576900000	-2.871453000	-0.057051000
S	-2.913940000	-4.493835000	-0.659411000
C	-3.751729000	-2.254450000	0.332138000
C	-4.606170000	-4.302702000	-0.371226000
C	-4.898365000	-3.069608000	0.152717000
H	-3.771341000	-1.262046000	0.759500000
H	-5.289192000	-5.105741000	-0.614674000
H	-5.903893000	-2.753254000	0.407212000

2 | IVcc-1 B3LYP/6-31G*

N	1.335723000	-0.834850000	0.061783000
C	0.104290000	-1.480355000	0.049792000
C	0.315645000	-2.900717000	-0.043436000
C	1.696589000	-3.068182000	-0.082374000
C	2.307416000	-1.792104000	-0.018211000
N	0.011810000	1.281771000	0.095579000
C	-1.111402000	0.457359000	0.134614000
C	-2.298294000	1.280144000	0.131575000
C	-1.842332000	2.589921000	0.052173000
C	-0.425523000	2.576086000	0.038187000
B	1.477049000	0.723322000	0.069353000
N	-1.065655000	-0.863659000	0.102572000
F	2.148916000	1.160657000	-1.053235000
F	2.145618000	1.105140000	1.239894000
H	2.234645000	-4.003271000	-0.132017000
H	-2.448362000	3.485430000	0.064933000
C	-3.664999000	0.823958000	0.211036000
S	-4.989710000	1.902003000	-0.209984000
C	-4.158716000	-0.398379000	0.623995000
C	-6.165434000	0.692406000	0.177716000
C	-5.577341000	-0.470145000	0.602808000
H	-3.510326000	-1.205719000	0.937150000
H	-7.219537000	0.907814000	0.064354000
H	-6.139779000	-1.349577000	0.896960000
C	-0.683648000	-3.943017000	-0.081965000
S	-2.389616000	-3.636098000	-0.363609000
C	-0.463102000	-5.302395000	0.050854000
C	-2.755414000	-5.326615000	-0.297468000
C	-1.638529000	-6.087562000	-0.068757000
H	0.519481000	-5.719098000	0.243247000
H	-3.775897000	-5.662584000	-0.426906000
H	-1.653748000	-7.168798000	0.013649000
C	3.740241000	-1.592101000	-0.055404000
S	4.616379000	-0.234422000	0.629963000
C	4.633072000	-2.507069000	-0.595707000
C	6.131189000	-0.922553000	0.175689000
C	5.989503000	-2.125591000	-0.469866000
H	4.307830000	-3.412200000	-1.095694000
H	7.048319000	-0.396277000	0.406969000
H	6.821096000	-2.710345000	-0.846944000
C	0.410581000	3.750985000	-0.018031000
S	-0.287145000	5.260954000	-0.602715000
C	1.729745000	3.946516000	0.349540000
C	1.195437000	6.105463000	-0.337497000

C	2.169367000	5.282117000	0.167177000
H	2.339482000	3.156432000	0.764100000
H	1.267490000	7.157743000	-0.578756000
H	3.171525000	5.620816000	0.405607000

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2 | IVcc-2 B3LYP/6-31G*

N	0.277594000	1.372291000	0.017375000
C	1.264770000	0.389703000	-0.021587000
C	2.557256000	1.028431000	-0.108052000
C	2.297231000	2.392844000	-0.107611000
C	0.894826000	2.588469000	-0.033989000
N	-1.353268000	-0.518246000	0.040785000
C	-0.231711000	-1.341370000	0.053412000
C	-0.653620000	-2.717514000	0.045328000
C	-2.043753000	-2.679701000	-0.000188000
C	-2.457621000	-1.326240000	0.000962000
B	-1.254423000	1.044048000	0.029933000
N	1.018757000	-0.908972000	0.014577000
F	-1.876868000	1.570623000	-1.082899000
F	-1.807390000	1.559078000	1.209832000
H	3.027110000	3.189024000	-0.137494000
H	-2.714168000	-3.527027000	0.024785000
C	0.176294000	-3.898467000	0.087088000
S	1.867112000	-3.873760000	0.559367000
C	-0.222316000	-5.196478000	-0.177861000
C	1.990847000	-5.591896000	0.392272000
C	0.807763000	-6.156970000	-0.008067000
H	-1.227780000	-5.444193000	-0.500017000
H	2.932401000	-6.086584000	0.591552000
H	0.676551000	-7.219949000	-0.178107000
C	3.843822000	0.376849000	-0.175859000
S	5.321807000	1.298609000	0.074857000
C	4.147487000	-0.941252000	-0.455385000
C	6.302982000	-0.100445000	-0.201577000
C	5.542799000	-1.208724000	-0.468465000
H	3.381036000	-1.679083000	-0.651008000
H	7.380653000	-0.023897000	-0.145691000
H	5.965767000	-2.186331000	-0.672590000
C	0.276073000	3.896041000	-0.039033000
S	-1.290608000	4.311362000	0.635132000
C	0.891806000	5.035196000	-0.540575000
C	-1.077546000	5.972923000	0.227157000
C	0.122532000	6.212721000	-0.395065000
H	1.860074000	5.007817000	-1.026930000
H	-1.855460000	6.686188000	0.467501000

H	0.439151000	7.190249000	-0.741131000
C	-3.830797000	-0.880996000	-0.028272000
S	-5.071447000	-1.995495000	-0.600250000
C	-4.406868000	0.315624000	0.356972000
C	-6.318301000	-0.836991000	-0.305073000
C	-5.816260000	0.335305000	0.198715000
H	-3.829098000	1.131716000	0.766934000
H	-7.347680000	-1.082902000	-0.529888000
H	-6.435702000	1.188080000	0.453683000

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2 | Vaa (TS) B3LYP/6-31G*

N	-0.686882000	-0.175899000	1.247256000
C	0.703143000	-0.172936000	1.146202000
C	1.266425000	-0.078398000	2.473680000
C	0.178543000	-0.004001000	3.335445000
C	-1.010731000	-0.072021000	2.571600000
N	-0.686882000	-0.175899000	-1.247256000
C	0.703143000	-0.172936000	-1.146202000
C	1.266425000	-0.078398000	-2.473680000
C	0.178543000	-0.004001000	-3.335445000
C	-1.010731000	-0.072021000	-2.571600000
B	-1.631817000	-0.218969000	0.000000000
N	1.366495000	-0.179015000	0.000000000
F	-2.495221000	0.855955000	0.000000000
F	-2.342207000	-1.431736000	0.000000000
H	0.213039000	0.039583000	4.415396000
H	0.213039000	0.039583000	-4.415396000
C	2.664373000	-0.063439000	-2.834802000
S	3.154113000	0.388412000	-4.463448000
C	3.775207000	-0.384409000	-2.080829000
C	4.824334000	0.131671000	-4.090688000
C	4.998611000	-0.273324000	-2.793258000
H	3.693396000	-0.695954000	-1.049294000
H	5.578917000	0.299927000	-4.847363000
H	5.969819000	-0.487856000	-2.360890000
C	2.664373000	-0.063439000	2.834802000
S	3.154113000	0.388412000	4.463448000
C	3.775207000	-0.384409000	2.080829000
C	4.824334000	0.131671000	4.090688000
C	4.998611000	-0.273324000	2.793258000
H	3.693396000	-0.695954000	1.049294000
H	5.578917000	0.299927000	4.847363000
H	5.969819000	-0.487856000	2.360890000
C	-2.346102000	-0.047276000	3.119755000
S	-2.590217000	0.628342000	4.729345000

C	-3.544537000	-0.515345000	2.612960000
C	-4.277803000	0.264842000	4.679655000
C	-4.636042000	-0.336840000	3.500476000
H	-3.615759000	-0.996752000	1.648177000
H	-4.910848000	0.525672000	5.517428000
H	-5.650023000	-0.647533000	3.274052000
C	-2.346102000	-0.047276000	-3.119755000
S	-2.590217000	0.628342000	-4.729345000
C	-3.544537000	-0.515345000	-2.612960000
C	-4.277803000	0.264842000	-4.679655000
C	-4.636042000	-0.336840000	-3.500476000
H	-3.615759000	-0.996752000	-1.648177000
H	-4.910848000	0.525672000	-5.517428000
H	-5.650023000	-0.647533000	-3.274052000

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2 | Vab (TS) B3LYP/6-31G*

N	-0.122417000	0.737336000	1.244902000
C	-0.089381000	-0.652419000	1.145961000
C	0.008495000	-1.213472000	2.472368000
C	0.048698000	-0.122334000	3.334974000
C	-0.037104000	1.063042000	2.570500000
N	-0.122417000	0.737336000	-1.244902000
C	-0.089381000	-0.652419000	-1.145961000
C	0.008495000	-1.213472000	-2.472368000
C	0.048698000	-0.122334000	-3.334974000
C	-0.037104000	1.063042000	-2.570500000
B	-0.183341000	1.681313000	0.000000000
N	-0.082186000	-1.317320000	0.000000000
F	0.873525000	2.567497000	0.000000000
F	-1.410320000	2.368486000	0.000000000
H	0.079484000	-0.154152000	4.414597000
H	0.079484000	-0.154152000	-4.414597000
C	0.057314000	-2.600554000	-2.870451000
S	-0.289465000	-3.937417000	-1.793470000
C	0.344744000	-3.075963000	-4.139607000
C	-0.052761000	-5.088450000	-3.062039000
C	0.284131000	-4.487592000	-4.248026000
H	0.603291000	-2.422413000	-4.965284000
H	-0.165019000	-6.145323000	-2.858534000
H	0.484876000	-5.033058000	-5.163533000
C	0.057314000	-2.600554000	2.870451000
S	-0.289465000	-3.937417000	1.793470000
C	0.344744000	-3.075963000	4.139607000
C	-0.052761000	-5.088450000	3.062039000
C	0.284131000	-4.487592000	4.248026000

H	0.603291000	-2.422413000	4.965284000
H	-0.165019000	-6.145323000	2.858534000
H	0.484876000	-5.033058000	5.163533000
C	-0.043030000	2.399383000	3.118823000
S	0.621678000	2.656541000	4.731023000
C	-0.534225000	3.587900000	2.611583000
C	0.222208000	4.336349000	4.681998000
C	-0.382332000	4.682384000	3.500906000
H	-1.012819000	3.649655000	1.644784000
H	0.466385000	4.974024000	5.521266000
H	-0.713643000	5.689704000	3.273881000
C	-0.043030000	2.399383000	-3.118823000
S	0.621678000	2.656541000	-4.731023000
C	-0.534225000	3.587900000	-2.611583000
C	0.222208000	4.336349000	-4.681998000
C	-0.382332000	4.682384000	-3.500906000
H	-1.012819000	3.649655000	-1.644784000
H	0.466385000	4.974024000	-5.521266000
H	-0.713643000	5.689704000	-3.273881000

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2 | Vba (TS) B3LYP/6-31G*

N	-0.040837000	0.607016000	1.246521000
C	-0.071797000	-0.782896000	1.146671000
C	-0.024358000	-1.342986000	2.478062000
C	0.050737000	-0.254489000	3.338189000
C	0.037896000	0.934928000	2.568092000
N	-0.040837000	0.607016000	-1.246521000
C	-0.071797000	-0.782896000	-1.146671000
C	-0.024358000	-1.342986000	-2.478062000
C	0.050737000	-0.254489000	-3.338189000
C	0.037896000	0.934928000	-2.568092000
B	-0.011171000	1.550736000	0.000000000
N	-0.089220000	-1.445564000	0.000000000
F	1.134391000	2.321213000	0.000000000
F	-1.160910000	2.344495000	0.000000000
H	0.052736000	-0.285091000	4.418302000
H	0.052736000	-0.285091000	-4.418302000
C	-0.054182000	-2.739829000	-2.845055000
S	0.330347000	-3.231550000	-4.490456000
C	-0.371460000	-3.847162000	-2.085060000
C	0.051623000	-4.898245000	-4.115839000
C	-0.311166000	-5.069598000	-2.805879000
H	-0.644140000	-3.763626000	-1.042765000
H	0.176905000	-5.652530000	-4.881074000
H	-0.530809000	-6.038009000	-2.369775000

C	-0.054182000	-2.739829000	2.845055000
S	0.330347000	-3.231550000	4.490456000
C	-0.371460000	-3.847162000	2.085060000
C	0.051623000	-4.898245000	4.115839000
C	-0.311166000	-5.069598000	2.805879000
H	-0.644140000	-3.763626000	1.042765000
H	0.176905000	-5.652530000	4.881074000
H	-0.530809000	-6.038009000	2.369775000
C	0.101685000	2.258242000	3.147769000
S	-0.520601000	3.736881000	2.436095000
C	0.624024000	2.521293000	4.407236000
C	-0.065865000	4.650397000	3.825632000
C	0.534548000	3.879415000	4.790351000
H	1.084814000	1.753787000	5.018505000
H	-0.263854000	5.714195000	3.853786000
H	0.903701000	4.269392000	5.732283000
C	0.101685000	2.258242000	-3.147769000
S	-0.520601000	3.736881000	-2.436095000
C	0.624024000	2.521293000	-4.407236000
C	-0.065865000	4.650397000	-3.825632000
C	0.534548000	3.879415000	-4.790351000
H	1.084814000	1.753787000	-5.018505000
H	-0.263854000	5.714195000	-3.853786000
H	0.903701000	4.269392000	-5.732283000

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2 | Vbb (TS) B3LYP/6-31G*

N	-0.011071000	-0.659614000	1.244037000
C	-0.006312000	0.730667000	1.146371000
C	-0.055995000	1.289559000	2.476369000
C	-0.100224000	0.197623000	3.337129000
C	-0.072385000	-0.988920000	2.566472000
N	-0.011071000	-0.659614000	-1.244037000
C	-0.006312000	0.730667000	-1.146371000
C	-0.055995000	1.289559000	-2.476369000
C	-0.100224000	0.197623000	-3.337129000
C	-0.072385000	-0.988920000	-2.566472000
B	-0.025454000	-1.603839000	0.000000000
N	-0.000213000	1.395086000	0.000000000
F	-1.156564000	-2.396063000	0.000000000
F	1.138468000	-2.378153000	0.000000000
H	-0.089806000	0.225750000	4.416484000
H	-0.089806000	0.225750000	-4.416484000
C	-0.055819000	2.676944000	-2.878862000
S	0.287093000	4.007482000	-1.792797000
C	-0.290859000	3.156745000	-4.156826000

C	0.118032000	5.161724000	-3.069532000
C	-0.193665000	4.566609000	-4.265031000
H	-0.537793000	2.507999000	-4.989832000
H	0.248319000	6.216038000	-2.863549000
H	-0.351464000	5.114751000	-5.187361000
C	-0.055819000	2.676944000	2.878862000
S	0.287093000	4.007482000	1.792797000
C	-0.290859000	3.156745000	4.156826000
C	0.118032000	5.161724000	3.069532000
C	-0.193665000	4.566609000	4.265031000
H	-0.537793000	2.507999000	4.989832000
H	0.248319000	6.216038000	2.863549000
H	-0.351464000	5.114751000	5.187361000
C	-0.108871000	-2.314433000	3.145575000
S	0.546970000	-3.779075000	2.435319000
C	-0.627360000	-2.588831000	4.403856000
C	0.110794000	-4.702270000	3.824606000
C	-0.508238000	-3.944673000	4.787939000
H	-1.106861000	-1.831465000	5.013408000
H	0.331923000	-5.761493000	3.853129000
H	-0.870600000	-4.342518000	5.729256000
C	-0.108871000	-2.314433000	-3.145575000
S	0.546970000	-3.779075000	-2.435319000
C	-0.627360000	-2.588831000	-4.403856000
C	0.110794000	-4.702270000	-3.824606000
C	-0.508238000	-3.944673000	-4.787939000
H	-1.106861000	-1.831465000	-5.013408000
H	0.331923000	-5.761493000	-3.853129000
H	-0.870600000	-4.342518000	-5.729256000

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2 | Iaa B3LYP/cc-pVTZ

N	0.033900000	1.252307000	-0.717703000
C	0.044775000	1.140814000	0.666724000
C	0.048333000	2.457604000	1.242572000
C	0.000000000	3.331686000	0.170779000
C	-0.001897000	2.581278000	-1.026129000
N	-0.033900000	-1.252307000	-0.717703000
C	-0.044775000	-1.140814000	0.666724000
C	-0.048333000	-2.457604000	1.242572000
C	0.000000000	-3.331686000	0.170779000
C	0.001897000	-2.581278000	-1.026129000
B	0.000000000	0.000000000	-1.658022000
N	0.000000000	0.000000000	1.321862000
F	1.143015000	-0.052013000	-2.450919000
F	-1.143015000	0.052013000	-2.450919000

H	0.022091000	4.406730000	0.218975000
H	-0.022091000	-4.406730000	0.218975000
C	-0.103718000	-2.781009000	2.644908000
S	0.341074000	-4.375760000	3.208406000
C	-0.504698000	-2.001650000	3.706808000
C	-0.020304000	-3.964462000	4.839860000
C	-0.457036000	-2.675271000	4.949647000
H	-0.835144000	-0.983896000	3.578711000
H	0.113262000	-4.693152000	5.621237000
H	-0.740711000	-2.223589000	5.888463000
C	0.103718000	2.781009000	2.644908000
S	-0.341074000	4.375760000	3.208406000
C	0.504698000	2.001650000	3.706808000
C	0.020304000	3.964462000	4.839860000
C	0.457036000	2.675271000	4.949647000
H	0.835144000	0.983896000	3.578711000
H	-0.113262000	4.693152000	5.621237000
H	0.740711000	2.223589000	5.888463000
C	-0.028701000	3.154716000	-2.345763000
S	-0.514581000	4.831911000	-2.520605000
C	0.288720000	2.628338000	-3.579847000
C	-0.277946000	4.782938000	-4.219332000
C	0.148948000	3.553295000	-4.636590000
H	0.636257000	1.618130000	-3.709447000
H	-0.472998000	5.658657000	-4.815010000
H	0.359267000	3.317251000	-5.668844000
C	0.028701000	-3.154716000	-2.345763000
S	0.514581000	-4.831911000	-2.520605000
C	-0.288720000	-2.628338000	-3.579847000
C	0.277946000	-4.782938000	-4.219332000
C	-0.148948000	-3.553295000	-4.636590000
H	-0.636257000	-1.618130000	-3.709447000
H	0.472998000	-5.658657000	-4.815010000
H	-0.359267000	-3.317251000	-5.668844000

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2 | Iab B3LYP/cc-pVTZ

N	0.031260000	1.249901000	-0.757400000
C	0.041189000	1.140939000	0.627488000
C	0.043940000	2.457648000	1.200768000
C	0.000000000	3.330515000	0.126262000
C	-0.003551000	2.578643000	-1.067743000
N	-0.031260000	-1.249901000	-0.757400000
C	-0.041189000	-1.140939000	0.627488000
C	-0.043940000	-2.457648000	1.200768000
C	0.000000000	-3.330515000	0.126262000

C	0.003551000	-2.578643000	-1.067743000
B	0.000000000	0.000000000	-1.697611000
N	0.000000000	0.000000000	1.284535000
F	1.143019000	-0.050378000	-2.491669000
F	-1.143019000	0.050378000	-2.491669000
H	0.032336000	4.404779000	0.172038000
H	-0.032336000	-4.404779000	0.172038000
C	-0.096539000	-2.822064000	2.593193000
S	-0.664490000	-1.748664000	3.845433000
C	0.222025000	-4.050500000	3.133810000
C	-0.471059000	-2.961049000	5.048687000
C	0.014335000	-4.128029000	4.527509000
H	0.612145000	-4.864155000	2.540821000
H	-0.715244000	-2.743328000	6.074847000
H	0.218241000	-5.007408000	5.119726000
C	0.096539000	2.822064000	2.593193000
S	0.664490000	1.748664000	3.845433000
C	-0.222025000	4.050500000	3.133810000
C	0.471059000	2.961049000	5.048687000
C	-0.014335000	4.128029000	4.527509000
H	-0.612145000	4.864155000	2.540821000
H	0.715244000	2.743328000	6.074847000
H	-0.218241000	5.007408000	5.119726000
C	-0.030296000	3.150321000	-2.388838000
S	-0.526138000	4.824353000	-2.565922000
C	0.293644000	2.625571000	-3.621579000
C	-0.283850000	4.776616000	-4.264153000
C	0.151581000	3.549467000	-4.679313000
H	0.647183000	1.617234000	-3.749584000
H	-0.482423000	5.650888000	-4.860778000
H	0.366423000	3.314095000	-5.710804000
C	0.030296000	-3.150321000	-2.388838000
S	0.526138000	-4.824353000	-2.565922000
C	-0.293644000	-2.625571000	-3.621579000
C	0.283850000	-4.776616000	-4.264153000
C	-0.151581000	-3.549467000	-4.679313000
H	-0.647183000	-1.617234000	-3.749584000
H	0.482423000	-5.650888000	-4.860778000
H	-0.366423000	-3.314095000	-5.710804000

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2 | Iac B3LYP/cc-pVTZ

N	-1.501544000	-0.315924000	-0.041313000
C	-0.993856000	0.975571000	-0.028820000
C	-2.082284000	1.909439000	-0.055742000
C	-3.233309000	1.137797000	-0.054479000

C	-2.864150000	-0.223940000	-0.048434000
N	0.891119000	-1.039445000	0.088534000
C	1.189121000	0.318489000	0.105116000
C	2.618603000	0.481950000	0.139881000
C	3.139138000	-0.799490000	0.104780000
C	2.071334000	-1.723478000	0.079675000
B	-0.578300000	-1.577303000	0.016079000
N	0.287123000	1.274818000	0.044344000
F	-0.726052000	-2.351834000	-1.131541000
F	-0.887447000	-2.322506000	1.150961000
H	-4.246191000	1.495582000	-0.111703000
H	4.180179000	-1.069031000	0.149859000
C	3.346747000	1.721610000	0.211815000
S	5.059674000	1.766064000	-0.143480000
C	2.907221000	2.976663000	0.567220000
C	5.144563000	3.451294000	0.192857000
C	3.928264000	3.954920000	0.556130000
H	1.881464000	3.172675000	0.831475000
H	6.082183000	3.972393000	0.099253000
H	3.768378000	4.991843000	0.811149000
C	-2.012497000	3.347959000	-0.086793000
S	-0.573479000	4.231709000	-0.531584000
C	-3.042704000	4.227583000	0.169727000
C	-1.382345000	5.741383000	-0.366408000
C	-2.684774000	5.584762000	0.015033000
H	-4.024616000	3.900295000	0.477176000
H	-0.850545000	6.659110000	-0.553379000
H	-3.361639000	6.409194000	0.181625000
C	-3.796761000	-1.320779000	-0.056300000
S	-5.465145000	-1.004636000	0.386382000
C	-3.643021000	-2.651607000	-0.380363000
C	-5.905810000	-2.642365000	0.123021000
C	-4.838893000	-3.395097000	-0.280299000
H	-2.704509000	-3.066335000	-0.704948000
H	-6.921936000	-2.959173000	0.286869000
H	-4.906807000	-4.449606000	-0.501524000
C	2.234942000	-3.153095000	0.057028000
S	3.799105000	-3.809275000	-0.393323000
C	1.364974000	-4.180245000	0.355525000
C	3.252174000	-5.419716000	-0.168156000
C	1.944993000	-5.460550000	0.229573000
H	0.353233000	-4.009661000	0.680057000
H	3.920499000	-6.244813000	-0.347981000
H	1.413917000	-6.379178000	0.428499000

2 | Iba B3LYP/cc-pVTZ

N	0.026147000	1.252502000	-0.630158000
C	0.039216000	1.141454000	0.754484000
C	0.045226000	2.459669000	1.326847000
C	0.000000000	3.331613000	0.253770000
C	-0.006837000	2.577056000	-0.942898000
N	-0.026147000	-1.252502000	-0.630158000
C	-0.039216000	-1.141454000	0.754484000
C	-0.045226000	-2.459669000	1.326847000
C	0.000000000	-3.331613000	0.253770000
C	0.006837000	-2.577056000	-0.942898000
B	0.000000000	0.000000000	-1.570427000
N	0.000000000	0.000000000	1.408985000
F	1.145417000	-0.028979000	-2.354616000
F	-1.145417000	0.028979000	-2.354616000
H	0.036766000	4.405450000	0.299812000
H	-0.036766000	-4.405450000	0.299812000
C	-0.104618000	-2.786175000	2.728905000
S	0.338188000	-4.382260000	3.290102000
C	-0.506789000	-2.008951000	3.791481000
C	-0.026417000	-3.974481000	4.922104000
C	-0.462135000	-2.685302000	5.033320000
H	-0.835660000	-0.990464000	3.664917000
H	0.104793000	-4.704976000	5.702169000
H	-0.747183000	-2.235097000	5.972451000
C	0.104618000	2.786175000	2.728905000
S	-0.338188000	4.382260000	3.290102000
C	0.506789000	2.008951000	3.791481000
C	0.026417000	3.974481000	4.922104000
C	0.462135000	2.685302000	5.033320000
H	0.835660000	0.990464000	3.664917000
H	-0.104793000	4.704976000	5.702169000
H	0.747183000	2.235097000	5.972451000
C	-0.042379000	3.178283000	-2.252885000
S	0.493089000	2.447540000	-3.745930000
C	-0.474831000	4.471672000	-2.493583000
C	0.127324000	3.867949000	-4.633145000
C	-0.384100000	4.861003000	-3.842334000
H	-0.872629000	5.105694000	-1.716365000
H	0.308192000	3.893311000	-5.694867000
H	-0.686954000	5.828090000	-4.213999000
C	0.042379000	-3.178283000	-2.252885000
S	-0.493089000	-2.447540000	-3.745930000
C	0.474831000	-4.471672000	-2.493583000
C	-0.127324000	-3.867949000	-4.633145000

C	0.384100000	-4.861003000	-3.842334000
H	0.872629000	-5.105694000	-1.716365000
H	-0.308192000	-3.893311000	-5.694867000
H	0.686954000	-5.828090000	-4.213999000

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2 | Ibb B3LYP/cc-pVTZ

N	0.023848000	1.250000000	-0.670481000
C	0.035717000	1.141514000	0.714529000
C	0.040828000	2.459539000	1.284523000
C	0.000000000	3.330398000	0.208728000
C	-0.007987000	2.574275000	-0.985037000
N	-0.023848000	-1.250000000	-0.670481000
C	-0.035717000	-1.141514000	0.714529000
C	-0.040828000	-2.459539000	1.284523000
C	0.000000000	-3.330398000	0.208728000
C	0.007987000	-2.574275000	-0.985037000
B	0.000000000	0.000000000	-1.610728000
N	0.000000000	0.000000000	1.370903000
F	1.145326000	-0.027276000	-2.396131000
F	-1.145326000	0.027276000	-2.396131000
H	0.046859000	4.403415000	0.252072000
H	-0.046859000	-4.403415000	0.252072000
C	-0.097520000	-2.825737000	2.676983000
S	-0.669921000	-1.753208000	3.927935000
C	0.220632000	-4.053666000	3.218265000
C	-0.478913000	-2.965717000	5.131752000
C	0.008798000	-4.131980000	4.611592000
H	0.613587000	-4.866674000	2.626247000
H	-0.725757000	-2.748257000	6.157322000
H	0.211890000	-5.011361000	5.204131000
C	0.097520000	2.825737000	2.676983000
S	0.669921000	1.753208000	3.927935000
C	-0.220632000	4.053666000	3.218265000
C	0.478913000	2.965717000	5.131752000
C	-0.008798000	4.131980000	4.611592000
H	-0.613587000	4.866674000	2.626247000
H	0.725757000	2.748257000	6.157322000
H	-0.211890000	5.011361000	5.204131000
C	-0.042777000	3.173189000	-2.296855000
S	0.510410000	2.447218000	-3.785691000
C	-0.487303000	4.461420000	-2.541410000
C	0.135916000	3.863279000	-4.676457000
C	-0.391526000	4.851170000	-3.889943000
H	-0.897743000	5.090971000	-1.767113000
H	0.323473000	3.889771000	-5.736993000

H	-0.702547000	5.814614000	-4.264375000
C	0.042777000	-3.173189000	-2.296855000
S	-0.510410000	-2.447218000	-3.785691000
C	0.487303000	-4.461420000	-2.541410000
C	-0.135916000	-3.863279000	-4.676457000
C	0.391526000	-4.851170000	-3.889943000
H	0.897743000	-5.090971000	-1.767113000
H	-0.323473000	-3.889771000	-5.736993000
H	0.702547000	-5.814614000	-4.264375000

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2 | Ibc B3LYP/cc-pVTZ

N	1.007151000	-1.105576000	-0.000086000
C	-0.350613000	-1.392856000	0.007811000
C	-0.527537000	-2.816216000	0.008974000
C	0.750894000	-3.349818000	0.027730000
C	1.683119000	-2.288152000	0.021001000
N	0.293531000	1.292745000	0.055195000
C	-1.004657000	0.794909000	0.077276000
C	-1.925135000	1.901210000	0.083935000
C	-1.139636000	3.038361000	0.031218000
C	0.220607000	2.650944000	0.018070000
B	1.551798000	0.360502000	0.019102000
N	-1.305501000	-0.485895000	0.049064000
F	2.284559000	0.612014000	-1.133519000
F	2.322870000	0.558967000	1.156950000
H	1.011913000	-4.391518000	-0.019148000
H	-1.485234000	4.056134000	0.065828000
C	-3.361917000	1.831110000	0.151994000
S	-4.337566000	3.231018000	-0.236047000
C	-4.171463000	0.782320000	0.524083000
C	-5.795009000	2.384035000	0.110480000
C	-5.549871000	1.098585000	0.500210000
H	-3.773633000	-0.177510000	0.808648000
H	-6.744699000	2.879920000	0.002829000
H	-6.329990000	0.400701000	0.765195000
C	-1.766112000	-3.552518000	-0.018434000
S	-3.292304000	-2.848421000	-0.492320000
C	-1.935234000	-4.890873000	0.265093000
C	-4.108440000	-4.351496000	-0.302729000
C	-3.263768000	-5.343528000	0.107521000
H	-1.124131000	-5.523174000	0.593901000
H	-5.165637000	-4.417201000	-0.497642000
H	-3.580407000	-6.358921000	0.292883000
C	3.111158000	-2.491774000	0.035483000
S	4.324934000	-1.372994000	-0.534361000

C	3.717222000	-3.658063000	0.470310000
C	5.586159000	-2.478670000	-0.178899000
C	5.119512000	-3.649414000	0.354077000
H	3.159258000	-4.481628000	0.888398000
H	6.607875000	-2.203060000	-0.380703000
H	5.756119000	-4.467479000	0.655209000
C	1.307276000	3.597503000	-0.027462000
S	2.949787000	3.321652000	0.498025000
C	1.168747000	4.904786000	-0.463365000
C	3.395348000	4.933962000	0.124164000
C	2.352283000	5.660634000	-0.383051000
H	0.241153000	5.291250000	-0.856394000
H	4.407439000	5.259901000	0.297605000
H	2.432649000	6.692366000	-0.689910000

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2 | Ica B3LYP/cc-pVTZ

N	-1.234042000	-0.828240000	-0.011153000
C	-1.291255000	0.559140000	-0.035291000
C	-2.668035000	0.967717000	-0.081727000
C	-3.404929000	-0.203015000	-0.048148000
C	-2.512052000	-1.298952000	-0.008655000
N	1.250176000	-0.525620000	0.100085000
C	0.971895000	0.835406000	0.096977000
C	2.209824000	1.565782000	0.118538000
C	3.207182000	0.607129000	0.096192000
C	2.606368000	-0.672055000	0.092053000
B	0.120241000	-1.610009000	0.070266000
N	-0.238508000	1.347423000	0.025788000
F	0.273690000	-2.416438000	-1.049905000
F	0.142116000	-2.370834000	1.235537000
H	-4.474984000	-0.287932000	-0.114386000
H	4.267992000	0.785184000	0.135383000
C	2.360744000	2.997450000	0.165120000
S	3.884225000	3.745780000	-0.256187000
C	1.451357000	3.960637000	0.540504000
C	3.272226000	5.318570000	0.080460000
C	1.970952000	5.275382000	0.492183000
H	0.450178000	3.713161000	0.853294000
H	3.903853000	6.181107000	-0.047813000
H	1.403821000	6.155052000	0.757551000
C	-3.159892000	2.319241000	-0.164942000
S	-4.823495000	2.686257000	0.230505000
C	-2.506381000	3.465093000	-0.558667000
C	-4.606372000	4.352761000	-0.141128000
C	-3.328889000	4.616071000	-0.544841000

H	-1.471729000	3.460357000	-0.860232000
H	-5.429080000	5.039559000	-0.037169000
H	-2.988108000	5.600619000	-0.828425000
C	-2.953012000	-2.671571000	0.028131000
S	-2.043563000	-4.070672000	-0.487598000
C	-4.215142000	-3.061485000	0.442901000
C	-3.354883000	-5.118119000	-0.136451000
C	-4.441445000	-4.447454000	0.355311000
H	-4.942287000	-2.362537000	0.826382000
H	-3.252242000	-6.176224000	-0.311048000
H	-5.362549000	-4.928949000	0.646591000
C	3.332765000	-1.913851000	0.089914000
S	5.037223000	-1.888261000	-0.327840000
C	2.942218000	-3.203033000	0.384727000
C	5.177987000	-3.582278000	-0.094920000
C	3.989545000	-4.143123000	0.281342000
H	1.941137000	-3.453803000	0.689629000
H	6.124678000	-4.070185000	-0.254600000
H	3.867562000	-5.197172000	0.480199000

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2 | Icb B3LYP/cc-pVTZ

N	-0.559839000	1.394334000	0.019327000
C	0.803778000	1.131808000	-0.006715000
C	1.517637000	2.377364000	-0.026789000
C	0.546319000	3.363649000	0.020503000
C	-0.723808000	2.746226000	0.047076000
N	-0.840748000	-1.089201000	0.076407000
C	0.547907000	-1.136082000	0.073995000
C	0.969452000	-2.509225000	0.069386000
C	-0.196451000	-3.255533000	0.034970000
C	-1.298837000	-2.373845000	0.043914000
B	-1.633968000	0.259215000	0.073984000
N	1.328437000	-0.076283000	0.028173000
F	-2.452664000	0.320695000	-1.046852000
F	-2.383053000	0.389956000	1.240459000
H	0.708558000	4.424828000	-0.034727000
H	-0.271185000	-4.328285000	0.063686000
C	2.313002000	-3.027165000	0.106661000
S	3.683672000	-2.100238000	0.659020000
C	2.709577000	-4.308002000	-0.217083000
C	4.741966000	-3.439148000	0.452660000
C	4.088318000	-4.540543000	-0.025496000
H	2.025116000	-5.050375000	-0.599518000
H	5.788805000	-3.337230000	0.684566000
H	4.576358000	-5.480404000	-0.235482000

C	2.941264000	2.585512000	-0.102890000
S	4.057270000	1.377687000	-0.684686000
C	3.620176000	3.746947000	0.201051000
C	5.391056000	2.449227000	-0.516054000
C	5.010580000	3.668434000	-0.028735000
H	3.127718000	4.622690000	0.596543000
H	6.382653000	2.117674000	-0.774559000
H	5.700074000	4.477149000	0.161597000
C	-1.959236000	3.490042000	0.095860000
S	-3.524779000	2.944839000	-0.453821000
C	-2.051696000	4.794379000	0.549993000
C	-4.244936000	4.451578000	-0.064406000
C	-3.347049000	5.337853000	0.464904000
H	-1.207737000	5.327315000	0.959963000
H	-5.296249000	4.601583000	-0.245651000
H	-3.606052000	6.335746000	0.784730000
C	-2.676277000	-2.790969000	0.031155000
S	-3.047146000	-4.443423000	-0.429492000
C	-3.839383000	-2.119941000	0.343434000
C	-4.727786000	-4.193734000	-0.189207000
C	-4.997105000	-2.917795000	0.220005000
H	-3.850725000	-1.096070000	0.674520000
H	-5.422128000	-4.996966000	-0.369396000
H	-5.993948000	-2.559616000	0.428527000

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2 | Icc-1 B3LYP/cc-pVTZ

N	1.462107000	-0.598640000	0.027278000
C	0.355949000	-1.436151000	0.022489000
C	0.800793000	-2.799246000	-0.003163000
C	2.185153000	-2.738838000	0.013561000
C	2.577240000	-1.382121000	0.031927000
N	-0.202494000	1.267845000	0.116111000
C	-1.165401000	0.264540000	0.122346000
C	-2.470618000	0.871674000	0.130964000
C	-2.245195000	2.235888000	0.092597000
C	-0.851284000	2.466739000	0.090385000
B	1.332949000	0.958380000	0.089429000
N	-0.894054000	-1.022030000	0.073450000
F	1.905996000	1.532092000	-1.038356000
F	1.946706000	1.425602000	1.248393000
H	2.864404000	-3.569425000	-0.051589000
H	-2.993374000	3.009213000	0.118696000
C	-3.739820000	0.194221000	0.183187000
S	-5.217989000	1.048829000	-0.200016000
C	-4.025682000	-1.104742000	0.537475000

C	-6.175348000	-0.343604000	0.124124000
C	-5.406799000	-1.406709000	0.503651000
H	-3.257374000	-1.806330000	0.816651000
H	-7.245360000	-0.299244000	0.012117000
H	-5.815666000	-2.374045000	0.754469000
C	-0.007010000	-3.991539000	-0.052419000
S	-1.687705000	-3.994633000	-0.526521000
C	0.409272000	-5.279830000	0.207124000
C	-1.786968000	-5.705294000	-0.368780000
C	-0.600545000	-6.251420000	0.031458000
H	1.412302000	-5.513113000	0.531646000
H	-2.715767000	-6.210752000	-0.573284000
H	-0.455276000	-7.308336000	0.197150000
C	3.957159000	-0.960947000	0.054296000
S	4.586218000	0.569494000	-0.504637000
C	4.998288000	-1.764288000	0.486153000
C	6.196124000	0.098256000	-0.147991000
C	6.266183000	-1.163127000	0.377024000
H	4.839418000	-2.749128000	0.897521000
H	7.006210000	0.780966000	-0.343571000
H	7.187937000	-1.637698000	0.677580000
C	-0.242441000	3.770114000	0.072947000
S	-1.231508000	5.151401000	-0.368037000
C	1.038551000	4.186673000	0.368156000
C	0.080186000	6.234066000	-0.143681000
C	1.215995000	5.581246000	0.246844000
H	1.812917000	3.510330000	0.685776000
H	-0.056465000	7.287896000	-0.318506000
H	2.151182000	6.083496000	0.443324000

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2 | Icc-2 B3LYP/cc-pVTZ

N	0.367483000	1.361001000	-0.023656000
C	1.280635000	0.313415000	-0.057938000
C	2.611569000	0.859184000	-0.091571000
C	2.451254000	2.232404000	-0.041381000
C	1.069090000	2.527339000	-0.003362000
N	-1.386322000	-0.421965000	0.064622000
C	-0.321244000	-1.311688000	0.041656000
C	-0.829505000	-2.653312000	0.042861000
C	-2.209219000	-2.527510000	0.038741000
C	-2.537865000	-1.154929000	0.055424000
B	-1.178931000	1.128344000	0.054429000
N	0.946568000	-0.959192000	-0.019742000
F	-1.801255000	1.678669000	-1.058872000
F	-1.668918000	1.697220000	1.226819000

H	3.232393000	2.969632000	-0.094640000
H	-2.926841000	-3.327999000	0.077242000
C	-0.078687000	-3.882840000	0.053855000
S	1.607501000	-3.976055000	0.498628000
C	-0.560719000	-5.144082000	-0.224708000
C	1.621661000	-5.685691000	0.304208000
C	0.403969000	-6.166059000	-0.086543000
H	-1.579073000	-5.322424000	-0.536069000
H	2.528217000	-6.239194000	0.482495000
H	0.205328000	-7.211076000	-0.271152000
C	3.846624000	0.124285000	-0.181163000
S	5.371143000	0.905101000	0.177252000
C	4.063992000	-1.182015000	-0.555649000
C	6.255796000	-0.526127000	-0.183938000
C	5.430245000	-1.547810000	-0.556879000
H	3.258032000	-1.844250000	-0.824672000
H	7.328965000	-0.532447000	-0.096327000
H	5.787904000	-2.530013000	-0.827423000
C	0.554827000	3.873744000	0.049439000
S	-1.026819000	4.405908000	-0.466223000
C	1.295404000	4.960663000	0.482399000
C	-0.657831000	6.037743000	-0.091456000
C	0.607351000	6.185633000	0.408418000
H	2.297970000	4.863391000	0.869280000
H	-1.397708000	6.802613000	-0.259366000
H	1.024873000	7.132755000	0.714581000
C	-3.880749000	-0.637134000	0.068748000
S	-5.199009000	-1.713226000	-0.360652000
C	-4.378238000	0.608601000	0.386636000
C	-6.365328000	-0.481407000	-0.100447000
C	-5.784173000	0.691566000	0.292136000
H	-3.750606000	1.424029000	0.701650000
H	-7.410409000	-0.688229000	-0.257822000
H	-6.345143000	1.588095000	0.508996000