

Supporting Information

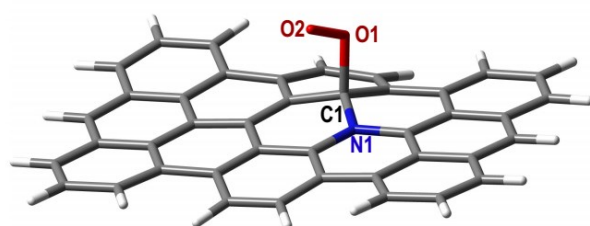
Probing the Effect of Different Graphitic Nitrogen Sites on the Aerobic Oxidation of Thiols to Disulfides: A DFT Study

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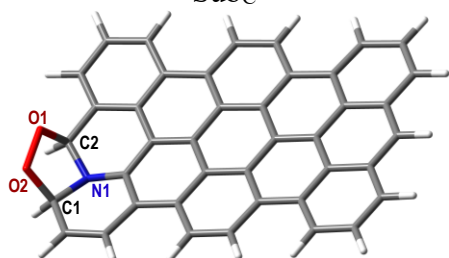
- ESI. 1** Optimized Geometries of AOS used in this study along with important geometrical parameters.
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Sub_C

Bond Length (Å)

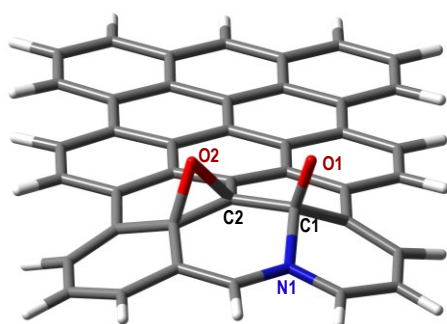
C1–O1	1.55
O1–O2	1.29
N1–C1	1.45



Sub_E

Bond Length (Å)

C1–O2	1.48
C2–O1	1.44
O2–O1	1.45
C1–N1	1.43
C2–N1	1.43

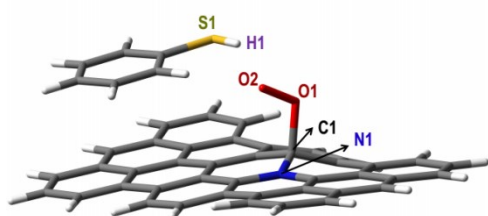


Sub_K

Bond Length (Å)

C1–O1	1.35
O1–O2	2.72
C2–O2	1.46
N1–C1	1.49

ESI. 1 Optimized Geometries of AOS used in this study along with important geometrical parameters



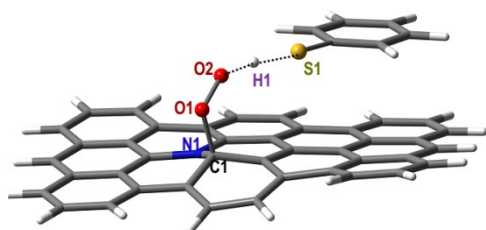
(Ec)TP

Bond Length (Å)

C1–O1	1.59
O1–O2	1.29
O2–H1	2.12
S1–H1	1.34

Spin Density

O2	0.670
O1	0.339



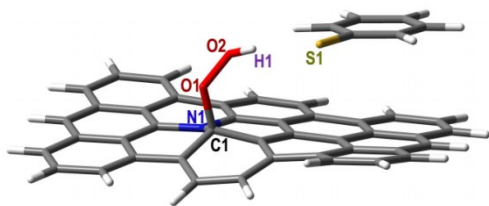
(T1c)TP

Bond Length (Å)

C1–O1	1.51
O1–O2	1.34
O2–H1	1.23
S1–H1	1.56

Spin Density

O2	0.440
O1	0.187
H1	-0.078
S1	0.397



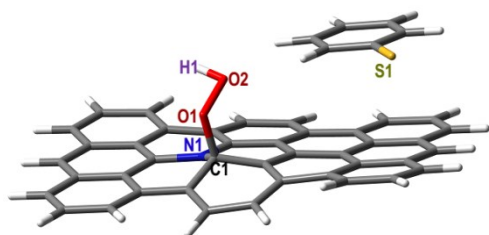
(I1C)TP

Bond Length (Å)

C1–O1	1.44
O1–O2	1.42
O2–H1	0.98
S1–H1	2.35

Spin Density

S1	0.757
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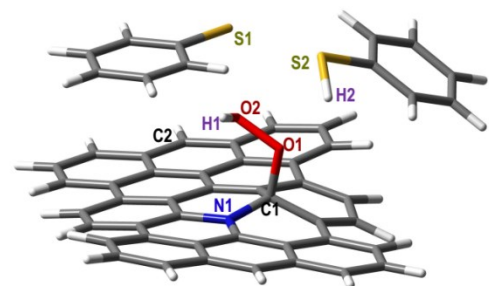
(I2C)TP

Bond Length (Å)

C1–O1	1.44
O1–O2	1.42
O2–H1	0.98

Spin Density

S1	0.750
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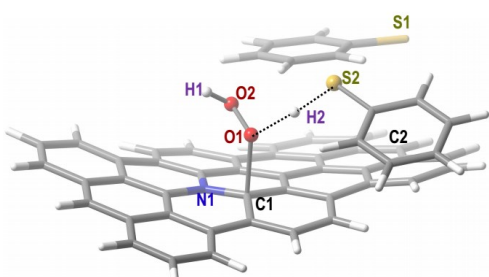
(I3C)TP

**Bond Length
(Å)**

C1–O1	1.44
O1–O2	1.42
O1–H2	2.18
H2–S2	1.34
S1–C2	3.60

Spin Density

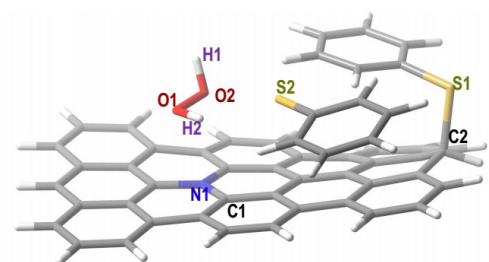
S1	0.740
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(T2C)TP

**Bond Length
(Å)**

C1–O1	2.05
O1–O2	1.42
O1–H2	1.46
H2–S2	1.48



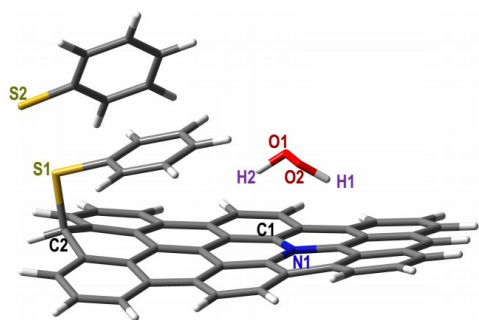
(I4C)TP

**Bond Length
(Å)**

C1–O1	3.01
O1–O2	1.42
O1–H2	0.97
H2–S2	2.44

Spin Density

S2	0.776
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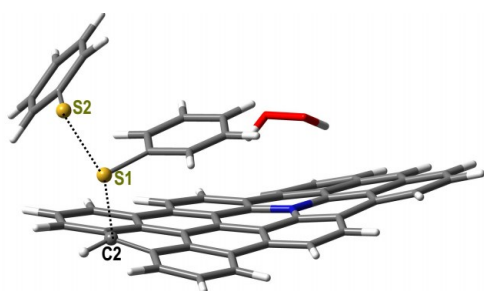
(I5C)TP

Bond Length (Å)

S1–S2	3.64
S1–C2	1.89

Spin Density

S2	0.811
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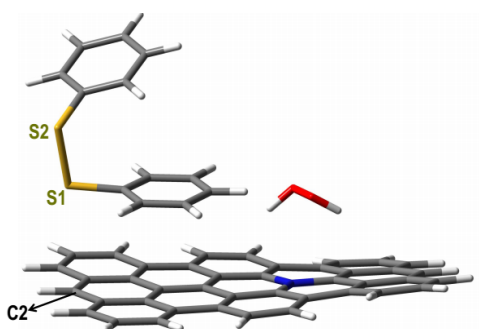
(T3C)TP

Bond Length (Å)

S1–S2	2.43
S1–C2	2.18

Spin Density

S2	0.471
S1	0.036
C2	0.268

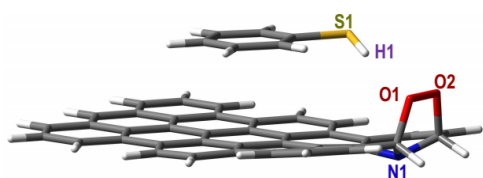


(PC)TP

Bond Length (Å)

S1–S2	2.09
S1–C2	3.37

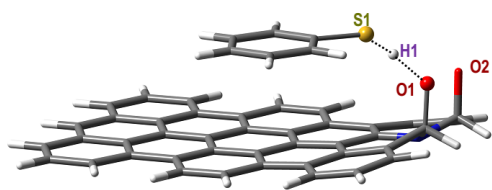
ESI. 2. The optimized geometries corresponding to oxidation of thiophenol by Sub_C with relevant geometrical parameter and Mulliken spin density values.



(EE)TP

Bond Length (Å)

O1–O2	1.45
H1–O1	2.24
S1–H1	1.36



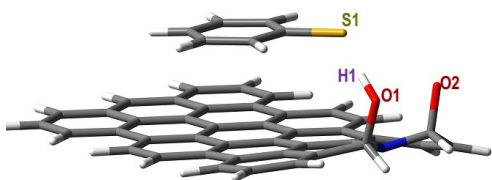
(T_{1E})_{TP}

Bond Length (Å)

O1–O2	2.29
H1–O1	1.64
S1–H1	1.41

Spin Density

O1	-0.296
O2	0.626
S1	0.199
H1	-0.004



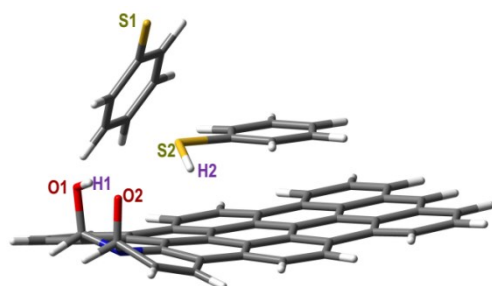
(I_{1E})_{TP}

Bond Length (Å)

O1–O2	2.72
H1–O1	0.97
S1–H1	2.51

Spin Density

O2	0.885
S1	-0.756



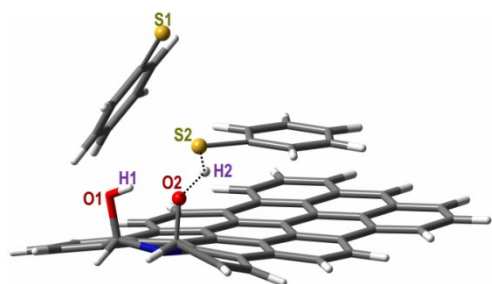
(I_{2E})_{TP}

Bond Length (Å)

O2–H2	2.44
S1–S2	3.81
S2–H2	1.35

Spin Density

S1	0.801
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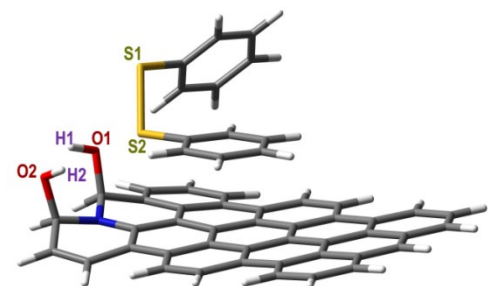
(T_{2E})_{TP}

Bond Length (Å)

O2–H2	1.62
S1–S2	3.66
S2–H2	1.43

Spin Density

S1	0.765
S2	-0.155
O2	-0.046

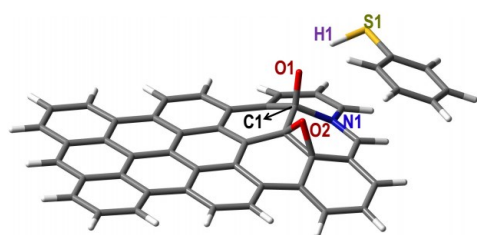


(P_E)_{TP}

Bond Length (Å)

O2–H2	0.97
S1–S2	2.08
S2–H2	2.71

ESI. 3. The optimized geometries corresponding to oxidation of thiophenol by Sub_E with relevant geometrical parameter and Mulliken spin density values.



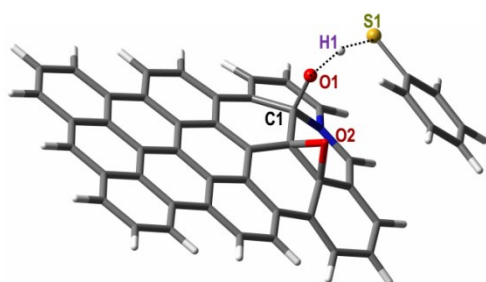
(E_K)TP

Bond Length (Å)

O1-H1	1.77
C1-O1	1.29
S1-H1	1.38

Spin Density

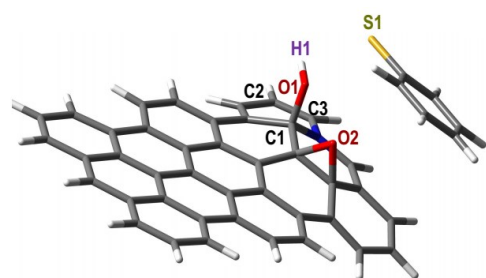
O1	0.550
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(T_{1K})TP

Bond Length (Å)

O1-C1	1.31
O1-H1	1.54
S1-H1	1.44



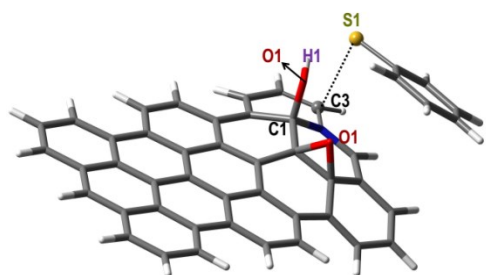
(I_{1K})TP

Bond Length (Å)

O1-C1	1.41
O1-H1	0.97
S1-H1	2.79

Spin Density

S1	0.741
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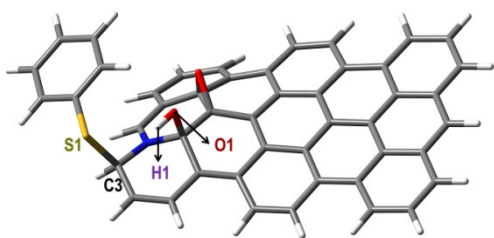
(T_{2K})TP

Bond Length (Å)

O1-C1	1.41
O1-H1	0.97
S1-C3	2.62

Spin Density

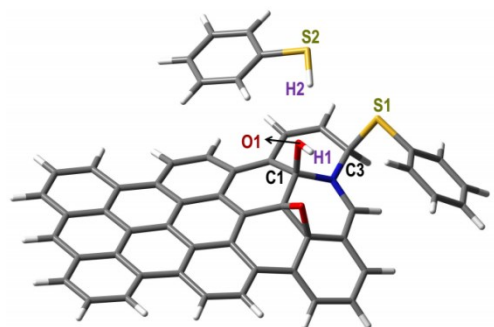
S1	0.504
C3	0.244



(I_{2K})_{TP}

Bond Length (Å)

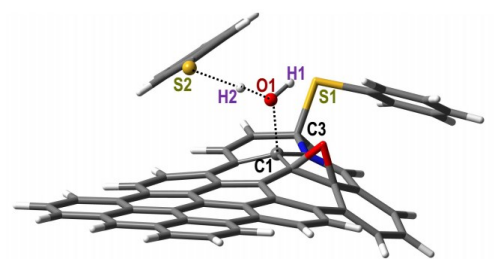
O1–C1	1.41
O1–H1	0.97
S1–C3	1.89



(I_{3K})_{TP}

Bond Length (Å)

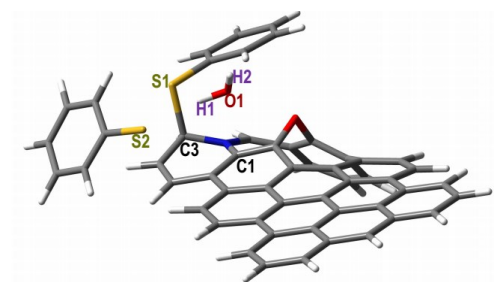
O1–C1	1.41
O1–H2	2.21
S1–C3	1.89
S2–H2	1.35



(T_{3K})_{TP}

Bond Length (Å)

O1–C1	1.83
O1–H2	1.10
S1–C3	1.88
S2–H2	1.83



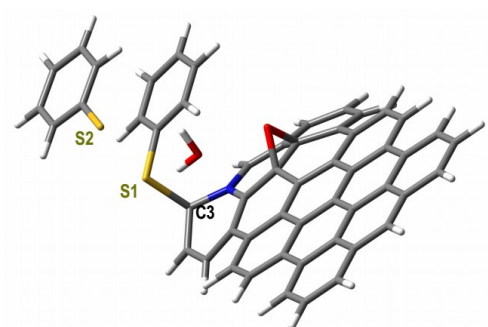
(I_{4K})_{TP}

Bond Length (Å)

O1–C1	2.89
O1–H2	0.98
S1–C3	1.88
S2–H2	2.38

Spin Density

S2	0.694
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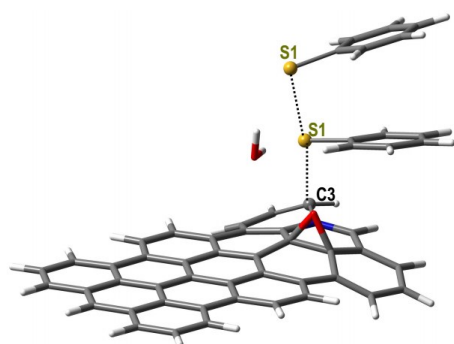
(I5K)_{TP}

Bond Length (Å)

S1-C3	1.89
S2-S1	3.65

Spin Density

S2	0.770
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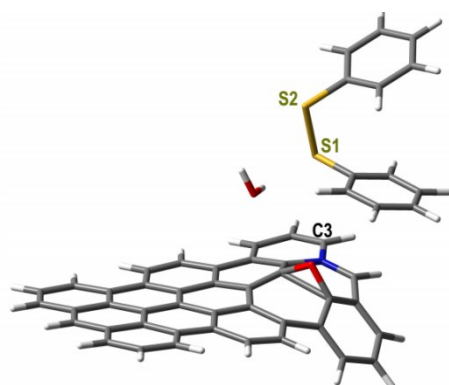
(T4K)_{TP}

Bond Length (Å)

S1-C3	2.21
S2-S1	2.06

Spin Density

S2	0.474
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(PK)_{TP}

Bond Length (Å)

S1-C3	3.27
S2-S1	2.10

ESI. 4. The optimized geometries corresponding to oxidation of thiophenol by Sub_K with relevant geometrical parameter and Mulliken spin density values.

ESI 5 XYZ coordinates for all the structures proposed for methanethiol (MT) oxidation by Sub_C, Sub_E and Sub_K

(E _C) _{MT}				(T _{1C}) _{MT}			
C	5.491349000	0.219466000	-0.635142000	C	5.518482000	0.111823000	-0.593952000
C	1.224500000	0.118294000	-0.393153000	C	1.247242000	0.071352000	-0.388559000
C	-3.033596000	0.061813000	-0.207242000	C	-3.011068000	0.075580000	-0.224914000
C	2.673663000	0.161947000	-0.543109000	C	2.699153000	0.092555000	-0.526703000
C	-5.866399000	0.004922000	-0.026406000	C	-5.845504000	0.056858000	-0.059839000
C	4.763506000	3.824339000	-0.290609000	C	4.831943000	3.738942000	-0.483700000
C	4.833187000	-1.009922000	-0.686853000	C	4.846557000	-1.111112000	-0.577758000
C	0.426631000	3.774570000	-0.385620000	C	0.492757000	3.737236000	-0.481671000
C	0.561159000	-1.078583000	-0.381907000	C	0.569186000	-1.115600000	-0.343757000
C	-3.865612000	3.689485000	-0.121804000	C	-3.784284000	3.710351000	-0.027430000
C	-3.727078000	-1.168022000	-0.205854000	C	-3.721815000	-1.144190000	-0.254612000
C	3.349433000	3.799457000	-0.244174000	C	3.417938000	3.733569000	-0.428572000
C	3.403072000	-1.039360000	-0.647869000	C	3.415914000	-1.120705000	-0.557505000
C	-0.946179000	3.733037000	-0.354354000	C	-0.879677000	3.713735000	-0.415335000
C	-0.892166000	-1.131926000	-0.020806000	C	-0.890653000	-1.152755000	0.012466000
C	-5.276372000	3.646874000	-0.034007000	C	-5.195086000	3.687443000	0.071949000
C	-5.156549000	-1.187864000	-0.100089000	C	-5.152361000	-1.143885000	-0.164728000
C	5.469324000	2.666224000	-0.441409000	C	5.523864000	2.565373000	-0.559215000
C	5.556853000	-2.234432000	-0.752892000	C	5.554449000	-2.346729000	-0.564023000
C	1.166495000	2.590838000	-0.345759000	C	1.219903000	2.546389000	-0.423205000
C	1.263718000	-2.312054000	-0.660942000	C	1.261957000	-2.364620000	-0.575775000
C	-3.116577000	2.535377000	-0.187922000	C	-3.057447000	2.547412000	-0.154420000
C	-3.036350000	-2.410815000	-0.335075000	C	-3.047024000	-2.395026000	-0.394045000
C	2.636035000	2.623917000	-0.358510000	C	2.690081000	2.561734000	-0.465394000
C	2.728923000	-2.297398000	-0.686047000	C	2.726487000	-2.370899000	-0.546089000
C	-1.656911000	2.530503000	-0.281247000	C	-1.601855000	2.522785000	-0.292115000
C	-1.596242000	-2.361835000	-0.504738000	C	-1.600995000	-2.371005000	-0.517248000
C	-5.929585000	2.451505000	-0.007179000	C	-5.868937000	2.503369000	0.049278000
C	-5.836847000	-2.441176000	-0.080534000	C	-5.852517000	-2.385987000	-0.187732000
C	4.787189000	1.418418000	-0.533881000	C	4.827308000	1.322453000	-0.573694000
C	4.890431000	-3.427310000	-0.753856000	C	4.872240000	-3.529478000	-0.507968000
C	0.546735000	-3.428695000	-0.986299000	C	0.541039000	-3.471933000	-0.919870000
C	-3.769280000	1.263867000	-0.156950000	C	-3.730042000	1.286174000	-0.151738000
C	-3.736523000	-3.597755000	-0.288999000	C	-3.767699000	-3.570878000	-0.389446000
C	3.354035000	1.393142000	-0.490806000	C	3.393437000	1.316790000	-0.534406000
C	3.478428000	-3.456623000	-0.708673000	C	3.459014000	-3.539508000	-0.487768000
C	-0.936632000	1.321436000	-0.275314000	C	-0.898070000	1.303382000	-0.289589000
C	-0.872451000	-3.417725000	-0.953164000	C	-0.879506000	-3.434955000	-0.947309000
C	-5.203128000	1.225760000	-0.064920000	C	-5.163989000	1.268068000	-0.057466000
C	-5.144119000	-3.613820000	-0.164879000	C	-5.177313000	-3.567208000	-0.292625000
H	-1.396632000	-4.301503000	-1.302642000	H	-1.403817000	-4.306645000	-1.325685000
H	1.046962000	-4.327756000	-1.326280000	H	1.041645000	-4.380973000	-1.232589000
H	2.984338000	-4.421021000	-0.662546000	H	2.948688000	-4.492717000	-0.399751000
H	5.439325000	-4.363248000	-0.776807000	H	5.409326000	-4.471796000	-0.468861000
H	-5.665401000	-4.565291000	-0.130571000	H	-5.714051000	-4.510634000	-0.291552000
H	-3.202040000	-4.540668000	-0.320850000	H	-3.248416000	-4.521884000	-0.429903000
H	-7.012501000	2.403201000	0.060415000	H	-6.952297000	2.471088000	0.119556000
H	-6.949862000	-0.016049000	0.055270000	H	-6.929365000	0.049029000	0.018707000
H	-6.919248000	-2.434651000	0.010561000	H	-6.935876000	-2.364542000	-0.111040000
H	6.642177000	-2.197586000	-0.782165000	H	6.640478000	-2.325295000	-0.579927000
H	6.578695000	0.242203000	-0.658477000	H	6.606164000	0.121465000	-0.610747000
H	6.555101000	2.669790000	-0.477880000	H	6.609598000	2.553963000	-0.595668000

H	2.834856000	4.742144000	-0.102388000
H	0.917573000	4.736141000	-0.461544000
H	5.277867000	4.775736000	-0.200955000
H	-1.488548000	4.669157000	-0.389081000
H	-3.388739000	4.661311000	-0.128064000
H	-5.831535000	4.578542000	0.013835000
C	0.482073000	1.358004000	-0.315032000
N	-1.615020000	0.093715000	-0.258815000
O	-0.931049000	-1.360874000	1.529006000
O	-0.498203000	-0.323154000	2.166597000
C	2.553654000	0.451751000	2.815193000
S	2.566399000	-1.369814000	2.812650000
H	1.291817000	-1.525736000	3.204444000
H	2.466235000	0.845495000	3.828821000
H	3.506890000	0.772470000	2.388611000
H	1.738660000	0.832791000	2.195757000

H	2.915940000	4.689625000	-0.342742000
H	0.991577000	4.690730000	-0.596344000
H	5.357816000	4.687931000	-0.457791000
H	-1.413832000	4.654017000	-0.468925000
H	-3.288239000	4.672096000	0.009532000
H	-5.733502000	4.625387000	0.166173000
C	0.521246000	1.322051000	-0.343174000
N	-1.593435000	0.087853000	-0.264058000
O	-0.989712000	-1.396682000	1.495380000
O	-0.468041000	-0.367084000	2.189116000
C	2.666894000	0.683677000	2.783117000
S	2.120427000	-1.047984000	2.865073000
H	0.614601000	-0.745404000	2.599781000
H	2.005165000	1.247699000	2.117768000
H	2.665164000	1.149368000	3.769720000
H	3.674958000	0.714632000	2.360791000

(I_{1C'})_{MT}

C	5.468399000	0.214748000	-0.616072000
C	1.195417000	0.115782000	-0.391380000
C	-3.056612000	0.063000000	-0.180543000
C	2.647347000	0.158008000	-0.548647000
C	-5.891723000	0.002848000	0.006566000
C	4.728616000	3.831409000	-0.526026000
C	4.813426000	-1.017918000	-0.588367000
C	0.389754000	3.771948000	-0.439572000
C	0.535946000	-1.078577000	-0.343814000
C	-3.874810000	3.680958000	0.116502000
C	-3.753706000	-1.164925000	-0.237024000
C	3.314839000	3.806926000	-0.451213000
C	3.382040000	-1.045955000	-0.575069000
C	-0.980955000	3.729239000	-0.344996000
C	-0.920610000	-1.151548000	0.052072000
C	-5.283433000	3.637091000	0.233230000
C	-5.182971000	-1.184899000	-0.137996000
C	5.438108000	2.669227000	-0.604355000
C	5.534834000	-2.245071000	-0.555533000
C	1.132604000	2.589702000	-0.406079000
C	1.243444000	-2.316367000	-0.594613000
C	-3.136083000	2.530442000	-0.052929000
C	-3.064776000	-2.403146000	-0.413002000
C	2.602751000	2.625913000	-0.476498000
C	2.707637000	-2.307577000	-0.553484000
C	-1.683717000	2.527508000	-0.219074000
C	-1.618603000	-2.362332000	-0.533050000
C	-5.943543000	2.445685000	0.184751000
C	-5.867807000	-2.434796000	-0.194107000
C	4.759590000	1.415359000	-0.607312000
C	4.867368000	-3.436139000	-0.485489000
C	0.536353000	-3.423365000	-0.963631000
C	-3.792980000	1.261225000	-0.072131000
C	-3.770610000	-3.587524000	-0.442141000
C	3.324991000	1.390937000	-0.559062000
C	3.454667000	-3.466694000	-0.472059000
C	-0.965734000	1.315186000	-0.247026000
C	-0.887114000	-3.402685000	-0.998943000

(I_{2C'})_{MT}

C	5.417699000	0.775463000	-0.605588000
C	1.167543000	0.357948000	-0.351827000
C	-3.076417000	-0.001252000	-0.175473000
C	2.611134000	0.512786000	-0.493693000
C	-5.898591000	-0.266056000	0.001543000
C	4.434104000	4.306793000	-0.150622000
C	4.849452000	-0.496051000	-0.691078000
C	0.111501000	3.946216000	-0.171350000
C	0.590208000	-0.878822000	-0.398016000
C	-4.141283000	3.533031000	0.306025000
C	-3.686083000	-1.271150000	-0.294372000
C	3.025924000	4.178516000	-0.089826000
C	3.425611000	-0.627789000	-0.645039000
C	-1.253723000	3.806687000	-0.108319000
C	-0.856391000	-1.073561000	-0.013129000
C	-5.543896000	3.385974000	0.413178000
C	-5.110482000	-1.394279000	-0.200321000
C	5.220030000	3.207207000	-0.337753000
C	5.656095000	-1.663994000	-0.806152000
C	0.934355000	2.816757000	-0.192383000
C	1.379751000	-2.042653000	-0.742159000
C	-3.324367000	2.446778000	0.082133000
C	-2.911424000	-2.448054000	-0.530975000
C	2.398081000	2.957796000	-0.225459000
C	2.840060000	-1.927933000	-0.736569000
C	-1.874024000	2.553447000	-0.068719000
C	-1.472557000	-2.297874000	-0.651087000
C	-6.120110000	2.155992000	0.302352000
C	-5.708039000	-2.684083000	-0.320584000
C	4.629322000	1.915638000	-0.457743000
C	5.076734000	-2.901296000	-0.842567000
C	0.747274000	-3.179806000	-1.157606000
C	-3.892714000	1.137216000	-0.006753000
C	-3.534933000	-3.674939000	-0.619418000
C	3.202763000	1.786478000	-0.399507000
C	3.669966000	-3.032928000	-0.792046000
C	-1.072471000	1.398625000	-0.158189000
C	-0.672328000	-3.260338000	-1.169750000

C	-5.225463000	1.222345000	0.036468000
C	-5.179719000	-3.604366000	-0.339357000
H	-1.398575000	-4.266806000	-1.410649000
H	1.050772000	-4.319874000	-1.291807000
H	2.953927000	-4.424347000	-0.375266000
H	5.417588000	-4.370063000	-0.429790000
H	-5.705365000	-4.553750000	-0.364755000
H	-3.239286000	-4.530277000	-0.510951000
H	-7.025661000	2.398641000	0.266028000
H	-6.974712000	-0.021617000	0.093558000
H	-6.950940000	-2.429017000	-0.110271000
H	6.620549000	-2.211055000	-0.566286000
H	6.555753000	0.239458000	-0.632397000
H	6.523422000	2.673995000	-0.651927000
H	2.801420000	4.756161000	-0.359584000
H	0.873421000	4.733031000	-0.556464000
H	5.240707000	4.788309000	-0.510599000
H	-1.529985000	4.661976000	-0.380428000
H	-3.389035000	4.646963000	0.175188000
H	-5.832136000	4.565220000	0.360546000
C	0.452848000	1.356378000	-0.322763000
N	-1.644215000	0.093726000	-0.234037000
O	-1.014266000	-1.429406000	1.465126000
O	-0.404067000	-0.362289000	2.183157000
C	3.052027000	0.445463000	2.673300000
S	2.752451000	-1.334140000	2.644146000
H	0.450329000	-0.776762000	2.426226000
H	2.219011000	1.003050000	2.235655000
H	3.158602000	0.734330000	3.725698000
H	3.984887000	0.685482000	2.156740000

(I3C')MT

C	5.127734000	1.370288000	-0.878350000
C	0.924337000	0.680631000	-0.523803000
C	-3.282369000	0.060169000	-0.226494000
C	2.346955000	0.937515000	-0.711512000
C	-6.081807000	-0.373181000	-0.003032000
C	3.997445000	4.716095000	0.207568000
C	4.615165000	0.107114000	-1.176439000
C	-0.301535000	4.154606000	0.140943000
C	0.414758000	-0.579034000	-0.677207000
C	-4.556730000	3.524833000	0.267788000
C	-3.821064000	-1.240521000	-0.355260000
C	2.599036000	4.508663000	0.270144000
C	3.204418000	-0.117893000	-1.079767000
C	-1.658952000	3.944206000	0.163791000
C	-0.992545000	-0.882788000	-0.214580000
C	-5.949479000	3.296543000	0.355489000
C	-5.231989000	-1.451681000	-0.220368000
C	4.827887000	3.705530000	-0.181160000
C	5.470572000	-0.961187000	-1.565394000
C	0.573302000	3.080465000	-0.034265000
C	1.241233000	-1.652790000	-1.189287000
C	-3.670163000	2.485295000	0.091005000
C	-2.989664000	-2.364651000	-0.646646000
C	2.026848000	3.297007000	-0.058087000

C	-5.318950000	0.993913000	0.094640000
C	-4.939513000	-3.793678000	-0.521485000
H	-1.126235000	-4.138132000	-1.618169000
H	1.315228000	-4.016900000	-1.546568000
H	3.242688000	-4.029992000	-0.775693000
H	5.690170000	-3.795033000	-0.891670000
H	-5.397341000	-4.774952000	-0.597624000
H	-2.941496000	-4.575123000	-0.734816000
H	-7.196423000	2.030161000	0.376263000
H	-6.977360000	-0.369610000	0.083227000
H	-6.788937000	-2.757727000	-0.241181000
H	6.735866000	-1.549514000	-0.838020000
H	6.500037000	0.878341000	-0.638411000
H	6.302150000	3.291252000	-0.384875000
H	2.446796000	5.077875000	0.081684000
H	0.531900000	4.942284000	-0.221546000
H	4.879688000	5.290389000	-0.042119000
H	-1.864263000	4.700938000	-0.100328000
H	-3.723311000	4.526012000	0.413922000
H	-6.156118000	4.266054000	0.584718000
C	0.340245000	1.537921000	-0.207360000
N	-1.667298000	0.130579000	-0.217971000
O	-0.923922000	-1.435608000	1.397064000
O	-0.415751000	-0.355064000	2.172724000
C	2.229497000	-1.746561000	2.571921000
S	3.823876000	-2.577066000	2.443194000
H	-1.240356000	0.086359000	2.441073000
H	1.433410000	-2.312476000	2.082339000
H	1.981567000	-1.683910000	3.638145000
H	2.264486000	-0.730440000	2.172763000

(T2C')MT

C	-5.226093000	-0.105368000	-0.703382000
C	-0.897321000	-0.022989000	-0.625414000
C	3.367389000	0.076843000	-0.328687000
C	-2.283829000	-0.053045000	-0.680118000
C	6.193496000	0.141080000	-0.060663000
C	-4.330937000	-3.776974000	-0.693477000
C	-4.444958000	1.157373000	-0.947577000
C	-0.042049000	-3.661293000	-0.458042000
C	-0.183176000	1.226013000	-0.648525000
C	4.239931000	-3.526621000	-0.683119000
C	4.040891000	1.306520000	-0.148814000
C	-2.954338000	-3.745354000	-0.616476000
C	-3.033200000	1.173377000	-0.850724000
C	1.323558000	-3.605698000	-0.462745000
C	1.235071000	1.248689000	-0.501027000
C	5.649755000	-3.472733000	-0.609281000
C	5.467888000	1.324744000	0.016654000
C	-5.051394000	-2.582555000	-0.731071000
C	-5.134599000	2.326644000	-1.211694000
C	-0.801411000	-2.481010000	-0.527851000
C	-0.901416000	2.434504000	-0.788948000
C	3.480544000	-2.384318000	-0.540570000
C	3.328500000	2.542144000	-0.120673000
C	-2.254841000	-2.524667000	-0.588317000

C	2.682263000	-1.419998000	-1.352407000	C	-2.345917000	2.404434000	-0.965955000
C	-2.220458000	2.670539000	0.022375000	C	2.022453000	-2.388777000	-0.521662000
C	-1.575979000	-2.116774000	-0.857879000	C	1.894829000	2.478704000	-0.385523000
C	-6.447806000	2.031299000	0.271667000	C	6.288545000	-2.287607000	-0.390285000
C	-5.753004000	-2.775572000	-0.325250000	C	6.117760000	2.571514000	0.254271000
C	4.294421000	2.425034000	-0.507790000	C	-4.398712000	-1.363365000	-0.705698000
C	4.946969000	-2.190380000	-1.850321000	C	-4.453284000	3.534461000	-1.377549000
C	0.648305000	-2.821939000	-1.580649000	C	-0.201703000	3.652043000	-0.738423000
C	-4.160284000	1.146249000	-0.021752000	C	4.118653000	-1.119755000	-0.376296000
C	-3.537390000	-3.628125000	-0.717918000	C	3.999863000	3.719229000	0.136378000
C	2.878536000	2.212230000	-0.437362000	C	-2.986932000	-1.316131000	-0.644847000
C	3.558487000	-2.416926000	-1.739320000	C	-3.081512000	3.573097000	-1.241390000
C	-1.360310000	1.569346000	-0.159126000	C	1.293472000	-1.193494000	-0.517945000
C	-0.755601000	-3.006183000	-1.467458000	C	1.149061000	3.661987000	-0.528060000
C	-5.576274000	0.918699000	0.080692000	C	5.549978000	-1.073368000	-0.271564000
C	-4.926037000	-3.835545000	-0.558111000	C	5.399541000	3.728706000	0.326952000
H	-1.185320000	-3.901010000	-1.906278000	H	1.661402000	4.614719000	-0.486836000
H	1.224882000	-3.608874000	-2.051784000	H	-0.721464000	4.596012000	-0.835841000
H	3.190855000	-3.416202000	-1.946047000	H	-2.574584000	4.520717000	-1.373209000
H	5.594108000	-3.008924000	-2.148181000	H	-5.002590000	4.442731000	-1.603462000
H	-5.325070000	-4.843122000	-0.618911000	H	5.899954000	4.672230000	0.522974000
H	-2.892939000	-4.486433000	-0.873099000	H	3.467184000	4.659268000	0.202808000
H	-7.514662000	1.840626000	0.342857000	H	7.370995000	-2.238337000	-0.315741000
H	-7.151592000	-0.539486000	0.091397000	H	7.275258000	0.166228000	0.038911000
H	-6.823869000	-2.915235000	-0.207814000	H	7.196281000	2.570620000	0.382325000
H	6.539154000	-0.776634000	-1.629730000	H	-6.219433000	2.296609000	-1.271182000
H	6.201419000	1.535394000	-0.934859000	H	-6.014340000	-0.194344000	-1.459174000
H	5.902990000	3.851295000	-0.237186000	H	-6.137722000	-2.598999000	-0.761917000
H	1.981479000	5.335681000	0.599418000	H	-2.418352000	-4.685228000	-0.587755000
H	0.072112000	5.165800000	0.237671000	H	-0.521487000	-4.628790000	-0.394008000
H	4.399612000	5.688428000	0.473406000	H	-4.852401000	-4.728375000	-0.720369000
H	-2.308354000	4.799171000	0.301946000	H	1.881904000	-4.530636000	-0.394006000
H	-4.205541000	4.545702000	0.346048000	H	3.770572000	-4.486370000	-0.858312000
H	-6.616510000	4.141713000	0.494695000	H	6.220082000	-4.390167000	-0.720189000
C	0.043312000	1.785622000	-0.208682000	C	-0.130230000	-1.238626000	-0.546328000
N	-1.884054000	0.277484000	-0.304496000	N	1.963684000	0.044795000	-0.470546000
O	-0.952376000	-1.320143000	1.179987000	O	1.211440000	-0.032381000	2.207866000
O	-0.381120000	-0.294787000	1.985540000	O	2.015125000	-1.119741000	2.333882000
C	3.367511000	-0.169196000	2.326016000	C	-4.851116000	0.327933000	2.020975000
S	4.281415000	-1.677704000	1.938190000	S	-6.210959000	0.029199000	0.862199000
H	-1.177375000	0.089726000	2.390735000	H	2.453233000	-0.979357000	3.193653000
C	2.246700000	-4.409637000	1.149053000	C	-1.610326000	1.273443000	2.668436000
S	1.554917000	-3.301976000	2.414438000	S	-1.349869000	-0.500991000	2.967794000
H	0.675790000	-2.666727000	1.617798000	H	0.044374000	-0.452718000	2.344549000
H	2.349512000	-0.232223000	1.929731000	H	-0.654774000	1.799044000	2.763019000
H	3.333637000	0.019596000	3.400088000	H	-2.021429000	1.450420000	1.672329000
H	3.877900000	0.664569000	1.828376000	H	-2.293790000	1.663799000	3.425571000
H	2.724548000	-3.831472000	0.355506000	H	-4.417576000	1.317914000	1.858094000
H	3.008114000	-5.014367000	1.645188000	H	-5.269406000	0.278513000	3.028375000
H	1.479630000	-5.068904000	0.739101000	H	-4.078234000	-0.441819000	1.919681000

(I4C')_{MT}

C	5.253830000	0.297793000	-0.466610000
C	0.946846000	0.230710000	-0.650974000
C	-3.312243000	0.146281000	-0.315629000
C	2.333150000	0.252183000	-0.662743000

(I5C')_{MT}

C	4.885345000	0.773247000	-0.726649000
C	0.601253000	0.322804000	-0.637275000
C	-3.624122000	-0.139895000	-0.156845000
C	1.976445000	0.469563000	-0.732380000

C	-6.131791000	0.083299000	0.004858000
C	4.397104000	3.949383000	-0.951731000
C	4.494553000	-0.976285000	-0.714851000
C	0.114441000	3.873916000	-0.507049000
C	0.224912000	-1.013480000	-0.699979000
C	-4.060134000	3.708999000	0.470879000
C	-4.021266000	-1.066208000	-0.458896000
C	3.018889000	3.932039000	-0.892490000
C	3.080287000	-0.983317000	-0.736839000
C	-1.235732000	3.816453000	-0.295936000
C	-1.200134000	-1.022524000	-0.642431000
C	-5.454243000	3.649309000	0.695887000
C	-5.450352000	-1.082453000	-0.328234000
C	5.114462000	2.757124000	-0.829047000
C	5.196967000	-2.159093000	-0.858371000
C	0.862985000	2.690259000	-0.617982000
C	0.940461000	-2.228745000	-0.819029000
C	-3.356552000	2.584244000	0.096188000
C	-3.343390000	-2.287610000	-0.743508000
C	2.312883000	2.723366000	-0.743141000
C	2.395231000	-2.212953000	-0.868665000
C	-1.930993000	2.598086000	-0.211811000
C	-1.885625000	-2.241386000	-0.743565000
C	-6.132698000	2.477060000	0.537843000
C	-6.148038000	-2.306250000	-0.549566000
C	4.453634000	1.550402000	-0.692573000
C	4.523161000	-3.370551000	-1.028359000
C	0.225610000	-3.437811000	-0.850140000
C	-4.023734000	1.328446000	-0.017956000
C	-4.063799000	-3.438678000	-0.982562000
C	3.040067000	1.512836000	-0.685790000
C	3.143565000	-3.395524000	-1.025587000
C	-1.227322000	1.406532000	-0.424966000
C	-1.142167000	-3.431175000	-0.812545000
C	-5.446041000	1.279797000	0.176477000
C	-5.473397000	-3.442704000	-0.886811000
H	-1.667868000	-4.377638000	-0.818227000
H	0.741419000	-4.388305000	-0.896055000
H	2.644487000	-4.347440000	-1.158650000
H	5.082215000	-4.291910000	-1.156930000
H	-6.014018000	-4.365160000	-1.076211000
H	-3.564167000	-4.360599000	-1.252673000
H	-7.206968000	2.425391000	0.689551000
H	-7.211308000	0.059608000	0.126800000
H	-7.230087000	-2.302911000	-0.455157000
H	6.283041000	-2.136693000	-0.821535000
H	6.148769000	0.315747000	-1.097770000
H	6.201340000	2.769400000	-0.820662000
H	2.485034000	4.870402000	-0.976689000
H	0.595274000	4.842227000	-0.551547000
H	4.922722000	4.890433000	-1.077855000
H	-1.787046000	4.743610000	-0.201768000
H	-3.557905000	4.658387000	0.607266000
H	-5.982503000	4.552525000	0.986446000
C	0.188191000	1.450122000	-0.576511000
N	-1.909427000	0.177895000	-0.483118000
O	-2.225172000	-1.064403000	2.229444000

C	-6.420665000	-0.446519000	0.220483000
C	3.686900000	4.343853000	-1.059237000
C	4.229611000	-0.555836000	-0.972424000
C	-0.542759000	3.878594000	-0.421222000
C	-0.007398000	-0.982380000	-0.660245000
C	-4.662664000	3.345762000	0.653347000
C	-4.226388000	-1.412362000	-0.277227000
C	2.322035000	4.202097000	-0.921208000
C	2.824716000	-0.693210000	-0.879898000
C	-1.874925000	3.703362000	-0.168719000
C	-1.421286000	-1.121526000	-0.537907000
C	-6.043528000	3.165794000	0.901028000
C	-5.644969000	-1.552065000	-0.115649000
C	4.512145000	3.217217000	-1.016638000
C	5.021414000	-1.661789000	-1.222562000
C	0.301613000	2.766550000	-0.573980000
C	0.806088000	-2.126287000	-0.824987000
C	-3.870907000	2.289650000	0.259234000
C	-3.448174000	-2.573153000	-0.561587000
C	1.734726000	2.931254000	-0.767282000
C	2.245128000	-1.978203000	-0.980644000
C	-2.457707000	2.427891000	-0.078543000
C	-2.000627000	-2.396345000	-0.613580000
C	-6.621873000	1.940996000	0.749436000
C	-6.236489000	-2.835702000	-0.303174000
C	3.968705000	1.953808000	-0.874218000
C	4.446436000	-2.927114000	-1.368883000
C	0.202837000	-3.395211000	-0.819398000
C	-4.431441000	0.978788000	0.150573000
C	-4.069052000	-3.786788000	-0.763512000
C	2.567158000	1.789795000	-0.778645000
C	3.082138000	-3.082321000	-1.236272000
C	-1.657081000	1.303699000	-0.310354000
C	-1.155197000	-3.514882000	-0.716529000
C	-5.841014000	0.806668000	0.373736000
C	-5.470217000	-3.914051000	-0.634714000
H	-1.589426000	-4.506217000	-0.695942000
H	0.802069000	-4.294179000	-0.877271000
H	2.660676000	-4.073269000	-1.350099000
H	5.075907000	-3.787859000	-1.569442000
H	-5.929817000	-4.884773000	-0.793231000
H	-3.496003000	-4.665982000	-1.029144000
H	-7.684304000	1.795732000	0.921126000
H	-7.490482000	-0.566003000	0.367633000
H	-7.312022000	-2.927104000	-0.183682000
H	6.100586000	-1.544746000	-1.273325000
H	5.746144000	0.886067000	-1.394020000
H	5.592011000	3.326235000	-1.076235000
H	1.705072000	5.091496000	-0.944817000
H	-0.150253000	4.885391000	-0.471212000
H	4.120231000	5.330570000	-1.186543000
H	-2.501515000	4.577990000	-0.049035000
H	-4.241583000	4.334087000	0.786433000
H	-6.641063000	4.019422000	1.205667000
C	-0.258273000	1.470716000	-0.516910000
N	-2.231275000	0.015589000	-0.344571000
O	-2.379057000	-1.144645000	2.497557000

O	-1.662145000	0.245307000	2.287650000
C	4.462668000	0.297151000	2.216381000
S	5.986733000	0.293101000	1.237314000
H	-1.946165000	0.532706000	3.170100000
C	1.961854000	-3.095305000	2.320039000
S	1.021308000	-1.558327000	2.395987000
H	-1.408848000	-1.603610000	2.256613000
H	3.840880000	-0.572709000	1.987332000
H	4.761505000	0.253901000	3.265664000
H	3.886836000	1.210483000	2.046377000
H	1.436497000	-3.838814000	1.715476000
H	2.967061000	-2.931283000	1.924233000
H	2.039059000	-3.479060000	3.344103000

O	-2.354587000	0.274167000	2.669358000
C	4.228263000	0.879331000	2.007837000
S	5.693436000	0.797515000	0.946469000
H	-3.217636000	0.511583000	2.287231000
C	4.538029000	-2.520790000	2.176854000
S	6.307155000	-2.189802000	2.027586000
H	-1.592925000	-1.272829000	1.940912000
H	4.106707000	-2.074043000	3.074816000
H	4.011607000	-2.162977000	1.286149000
H	4.400720000	-3.606708000	2.217880000
H	4.582261000	0.736122000	3.031256000
H	3.736299000	1.850985000	1.923493000
H	3.519996000	0.082238000	1.763819000

(T3C')_{MT}

C	4.739926000	0.442153000	-1.064685000
C	0.482931000	0.178301000	-0.708013000
C	-3.739169000	-0.087396000	-0.088379000
C	1.861332000	0.263400000	-0.869516000
C	-6.533062000	-0.263584000	0.377324000
C	3.729836000	4.047570000	-1.338794000
C	4.061365000	-0.854627000	-1.153448000
C	-0.501721000	3.784958000	-0.569205000
C	-0.173028000	-1.099216000	-0.646669000
C	-4.608644000	3.463652000	0.632491000
C	-4.395352000	-1.336597000	-0.144952000
C	2.363531000	3.970458000	-1.141862000
C	2.655456000	-0.936747000	-0.984915000
C	-1.832420000	3.674822000	-0.276018000
C	-1.588450000	-1.174111000	-0.482698000
C	-5.988296000	3.350507000	0.922132000
C	-5.813367000	-1.411494000	0.059933000
C	4.503917000	2.889980000	-1.325373000
C	4.809673000	-2.012881000	-1.320096000
C	0.291268000	2.633973000	-0.709436000
C	0.590705000	-2.283291000	-0.766642000
C	-3.873339000	2.362084000	0.252286000
C	-3.672753000	-2.538689000	-0.403097000
C	1.723572000	2.731344000	-0.949149000
C	2.030731000	-2.203706000	-0.960807000
C	-2.465590000	2.428926000	-0.127890000
C	-2.220314000	-2.425733000	-0.488277000
C	-6.620555000	2.146626000	0.827770000
C	-6.461401000	-2.675100000	-0.066209000
C	3.909429000	1.645688000	-1.139965000
C	4.189467000	-3.261793000	-1.315688000
C	-0.063795000	-3.524107000	-0.686338000
C	-4.490077000	1.073608000	0.203129000
C	-4.347447000	-3.731755000	-0.545498000
C	2.500976000	1.552377000	-0.974671000
C	2.823102000	-3.355165000	-1.132542000
C	-1.719613000	1.265044000	-0.345812000
C	-1.423044000	-3.582785000	-0.553229000
C	-5.898216000	0.968492000	0.470983000
C	-5.749017000	-3.795404000	-0.378489000
H	-1.897792000	-4.552629000	-0.477526000

(PC')_{MT}

C	4.443873000	-1.659776000	-1.188035000
C	0.368139000	-0.619934000	-0.654075000
C	-3.735512000	0.420562000	-0.129810000
C	1.718398000	-0.966422000	-0.836413000
C	-6.463025000	1.116359000	0.222805000
C	4.575168000	1.974708000	-1.922358000
C	3.529607000	-2.654226000	-0.800016000
C	0.429708000	3.055936000	-1.320989000
C	-0.594384000	-1.615675000	-0.297672000
C	-3.580124000	4.141474000	-0.231580000
C	-4.709218000	-0.584075000	0.066207000
C	3.240667000	2.331207000	-1.737119000
C	2.148618000	-2.314176000	-0.626747000
C	-0.872004000	3.382208000	-1.059579000
C	-1.973159000	-1.265599000	-0.167769000
C	-4.933507000	4.474202000	0.009497000
C	-6.090506000	-0.224609000	0.207632000
C	4.977608000	0.661688000	-1.767915000
C	3.946344000	-3.983744000	-0.576658000
C	0.873809000	1.730774000	-1.178971000
C	-0.179308000	-2.954724000	-0.093112000
C	-3.183628000	2.825825000	-0.336139000
C	-4.346405000	-1.961525000	0.129978000
C	2.268639000	1.375940000	-1.391932000
C	1.222727000	-3.312120000	-0.244903000
C	-1.820011000	2.421365000	-0.663582000
C	-2.919718000	-2.265327000	0.093334000
C	-5.876135000	3.497961000	0.139946000
C	-7.061285000	-1.260428000	0.337501000
C	4.041958000	-0.331728000	-1.408417000
C	3.031625000	-4.947946000	-0.199285000
C	-1.144328000	-3.916183000	0.252378000
C	-4.133136000	1.776205000	-0.136396000
C	-5.323237000	-2.928696000	0.231139000
C	2.669493000	0.030625000	-1.220819000
C	1.687400000	-4.621835000	-0.036513000
C	-1.429645000	1.080314000	-0.595477000
C	-2.465962000	-3.575419000	0.335559000
C	-5.512394000	2.119272000	0.078679000
C	-6.686422000	-2.571935000	0.330804000
H	-3.184535000	-4.337475000	0.609492000

H	0.495841000	-4.449350000	-0.718932000
H	2.369871000	-4.338260000	-1.136440000
H	4.778493000	-4.163004000	-1.454023000
H	-6.251945000	-4.750794000	-0.491977000
H	-3.817325000	-4.642904000	-0.791775000
H	-7.683008000	2.052942000	1.031901000
H	-7.602411000	-0.332095000	0.556574000
H	-7.536132000	-2.716805000	0.083932000
H	5.887222000	-1.932429000	-1.442334000
H	5.662189000	0.502222000	-1.641519000
H	5.582530000	2.946722000	-1.445297000
H	1.789460000	4.888180000	-1.148486000
H	-0.070414000	4.772176000	-0.666745000
H	4.199736000	5.013447000	-1.493118000
H	-2.417745000	4.579360000	-0.170686000
H	-4.143222000	4.436901000	0.722124000
H	-6.541516000	4.238098000	1.213215000
C	-0.321204000	1.364880000	-0.598413000
N	-2.346892000	0.002628000	-0.321968000
O	-2.544405000	-1.028171000	2.595911000
O	-2.296072000	0.377707000	2.664247000
C	4.171545000	0.177227000	1.791305000
S	5.677237000	0.514526000	0.835725000
H	-3.151918000	0.722775000	2.355038000
C	6.524356000	-2.144511000	2.306551000
S	7.180150000	-0.449364000	2.348093000
H	-1.847647000	-1.304819000	1.977303000
H	7.310354000	-2.817444000	2.657399000
H	5.649269000	-2.253482000	2.951204000
H	6.257837000	-2.422502000	1.282383000
H	4.398116000	0.372248000	2.839567000
H	3.378689000	0.851011000	1.458525000
H	3.855856000	-0.861112000	1.658343000

H	-0.859178000	-4.940617000	0.452237000
H	1.002963000	-5.407451000	0.257082000
H	3.357302000	-5.969239000	-0.028593000
H	-7.433530000	-3.355254000	0.414345000
H	-5.064956000	-3.980144000	0.230535000
H	-6.920245000	3.743859000	0.309279000
H	-7.507787000	1.381403000	0.359348000
H	-8.104723000	-0.975763000	0.434971000
H	4.995730000	-4.231846000	-0.707135000
H	5.492514000	-1.918543000	-1.307433000
H	6.019162000	0.380377000	-1.894690000
H	2.969126000	3.371922000	-1.860047000
H	1.109621000	3.837506000	-1.633291000
H	5.302706000	2.738808000	-2.176903000
H	-1.187145000	4.410682000	-1.181983000
H	-2.861034000	4.944787000	-0.329936000
H	-5.215653000	5.520190000	0.080541000
C	-0.064792000	0.731900000	-0.822109000
N	-2.376868000	0.074551000	-0.317853000
O	-2.811653000	-0.221917000	2.756263000
O	-2.123980000	1.007018000	2.512485000
C	4.461968000	0.670668000	1.690311000
S	6.203504000	0.181628000	1.477278000
H	-2.824746000	1.514225000	2.066249000
C	7.421168000	2.711875000	2.606816000
S	7.090886000	1.972988000	0.975745000
H	-2.252501000	-0.844576000	2.261450000
H	6.490248000	2.913379000	3.139769000
H	8.060661000	2.058640000	3.201547000
H	7.937864000	3.657346000	2.421623000
H	3.873625000	-0.251978000	1.689732000
H	4.314218000	1.195052000	2.636095000
H	4.148751000	1.298398000	0.853159000

(E_{E'})_{MT}

C	6.225469000	-0.246130000	0.143901000
C	2.002355000	-0.000125000	-0.224945000
C	-2.231514000	0.234387000	-0.626951000
C	3.407167000	-0.081164000	-0.100743000
C	-5.089475000	0.293065000	-0.614692000
C	5.349733000	-3.850723000	0.052932000
C	5.617150000	1.019393000	0.096573000
C	1.032889000	-3.619992000	-0.299024000
C	1.361102000	1.283185000	-0.265535000
C	-3.266256000	-3.367741000	-0.740555000
C	-2.899450000	1.507918000	-0.548057000
C	3.965551000	-3.785682000	-0.066048000
C	4.193221000	1.113186000	-0.026776000
C	-0.321289000	-3.542531000	-0.432985000
C	-0.062711000	1.366517000	-0.373877000
C	-4.598329000	-3.256593000	-0.690172000
C	-4.307530000	1.562941000	-0.550332000
C	6.103044000	-2.693046000	0.123880000
C	6.386488000	2.200062000	0.167577000
C	1.850085000	-2.460962000	-0.241750000

(T_{1E'})_{MT}

C	6.276946000	-0.312346000	0.182427000
C	2.054304000	0.001064000	-0.162898000
C	-2.196770000	0.332253000	-0.449627000
C	3.457257000	-0.103853000	-0.048219000
C	-5.142856000	0.513939000	-0.299672000
C	5.338707000	-3.900744000	0.236518000
C	5.691192000	0.959025000	0.088525000
C	1.035356000	-3.601419000	-0.142918000
C	1.434043000	1.290391000	-0.237765000
C	-3.096412000	-3.221660000	-1.140669000
C	-2.832780000	1.619820000	-0.399853000
C	3.953206000	-3.813548000	0.115882000
C	4.266868000	1.073477000	-0.025508000
C	-0.324231000	-3.497843000	-0.306912000
C	0.004945000	1.401599000	-0.318006000
C	-4.554198000	-3.183040000	-1.152605000
C	-4.239389000	1.724547000	-0.379907000
C	6.110220000	-2.756154000	0.260318000
C	6.482631000	2.127440000	0.104605000
C	1.857559000	-2.462558000	-0.114300000

C	2.132032000	2.466097000	-0.193212000
C	-2.399207000	-2.198876000	-0.703900000
C	-2.155438000	2.701005000	-0.431191000
C	3.288868000	-2.551169000	-0.117192000
C	3.578242000	2.388105000	-0.074034000
C	-0.985672000	-2.290053000	-0.530122000
C	-0.702572000	2.622992000	-0.385825000
C	-5.227189000	-1.910251000	-0.640031000
C	-4.971773000	2.768032000	-0.452833000
C	5.475578000	-1.430454000	0.074483000
C	5.773269000	3.437164000	0.119446000
C	1.461678000	3.705659000	-0.241416000
C	-2.993803000	-0.949015000	-0.785950000
C	-2.859143000	3.918089000	-0.326039000
C	4.048785000	-1.356231000	-0.048951000
C	4.389431000	3.533884000	0.000408000
C	-0.199780000	-1.115084000	-0.445393000
C	0.097229000	3.783562000	-0.331338000
C	-4.238722000	3.955640000	-0.340092000
H	-0.361624000	4.764175000	-0.369260000
H	2.024656000	4.629945000	-0.205061000
H	3.947213000	4.521714000	-0.033333000
H	6.369096000	4.342931000	0.173448000
H	-4.754820000	4.906140000	-0.253972000
H	-2.318905000	4.850860000	-0.216784000
H	-6.151893000	-1.867765000	-1.228492000
H	-5.986726000	0.415747000	-1.233621000
H	-6.058225000	2.786920000	-0.452638000
H	7.465683000	2.117518000	0.260793000
H	7.306807000	-0.309386000	0.237324000
H	7.184366000	-2.737836000	0.217517000
H	3.412157000	-4.714441000	-0.121902000
H	1.483048000	-4.602559000	-0.229259000
H	5.837684000	-4.819723000	0.090398000
H	-0.890433000	-4.463357000	-0.460170000
H	-2.825727000	-4.356225000	-0.796710000
H	-5.249622000	-4.122317000	-0.685294000
C	1.223392000	-1.199374000	-0.304132000
N	-4.362420000	-0.849002000	-1.088409000
C	-0.838930000	0.156117000	-0.484349000
O	-5.529353000	-0.085908000	0.717990000
O	-5.553511000	-1.535674000	0.722297000
C	-1.820665000	0.704614000	2.931151000
S	-2.707900000	-0.874639000	2.742965000
H	-3.810697000	-0.372022000	2.159287000
H	-2.311184000	1.355407000	3.656650000
H	-0.820055000	0.462565000	3.294019000
H	-1.724405000	1.223096000	1.974757000

(I_{1E'})_{MT}

C	6.235430000	-0.258009000	0.187916000
C	2.014328000	-0.005956000	-0.197885000
C	-2.232931000	0.232679000	-0.503133000
C	3.418660000	-0.089185000	-0.072385000
C	-5.141197000	0.338490000	-0.419676000
C	5.359486000	-3.860837000	0.048208000

C	2.231310000	2.456056000	-0.215259000
C	-2.378540000	-2.159783000	-0.698201000
C	-2.045247000	2.794879000	-0.349608000
C	3.302941000	-2.573581000	0.020221000
C	3.673900000	2.356566000	-0.115373000
C	-0.938949000	-2.245900000	-0.454966000
C	-0.604050000	2.674506000	-0.342216000
C	-5.169437000	-1.847796000	-0.921603000
C	-4.844561000	2.960464000	-0.308196000
C	5.503636000	-1.485456000	0.164338000
C	5.890705000	3.372820000	0.011854000
C	1.586879000	3.712230000	-0.288120000
C	-3.025339000	-0.852703000	-0.575657000
C	-2.697349000	4.044529000	-0.282800000
C	4.080257000	-1.391082000	0.044986000
C	4.508345000	3.490222000	-0.096104000
C	-0.164073000	-1.084356000	-0.356344000
C	0.227610000	3.819681000	-0.344962000
C	-4.071614000	4.128471000	-0.264456000
H	-0.208852000	4.808568000	-0.399243000
H	2.171686000	4.623322000	-0.291990000
H	4.084855000	4.484038000	-0.165440000
H	6.503125000	4.268814000	0.023469000
H	-4.554158000	5.098733000	-0.202467000
H	-2.121866000	4.959942000	-0.227087000
H	-6.154307000	-1.595723000	-1.304352000
H	-5.930055000	0.611961000	-1.077007000
H	-5.929100000	3.013747000	-0.263651000
H	7.560937000	2.028924000	0.191142000
H	7.357456000	-0.392504000	0.271199000
H	7.190992000	-2.815286000	0.352398000
H	3.383756000	-4.734071000	0.096518000
H	1.462907000	-4.589013000	-0.024491000
H	5.808038000	-4.876507000	0.311608000
H	-0.927724000	-4.397903000	-0.282577000
H	-2.599924000	-4.129430000	-1.466258000
H	-5.103950000	-3.947130000	-1.694169000
C	1.249100000	-1.186288000	-0.206448000
N	-4.318157000	-0.719455000	-0.832754000
C	-0.809523000	0.216999000	-0.382973000
O	-5.592107000	0.204485000	0.889535000
O	-5.141868000	-2.794168000	0.097419000
C	-2.754719000	0.685891000	2.809211000
S	-3.337958000	-0.983624000	2.359582000
H	-4.533986000	-0.481200000	1.688794000
H	-3.511929000	1.418838000	2.516468000
H	-2.594457000	0.749963000	3.887051000
H	-1.814486000	0.922973000	2.299986000

(I_{2E'})_{MT}

C	6.435107000	-0.344556000	0.297190000
C	2.253252000	0.008464000	-0.365947000
C	-1.966621000	0.352253000	-0.909618000
C	3.646557000	-0.109035000	-0.149945000
C	-4.798995000	0.504112000	-0.827405000
C	5.484073000	-3.924774000	0.115129000

C	5.628509000	1.008381000	0.144683000
C	1.046164000	-3.624833000	-0.346600000
C	1.373158000	1.277663000	-0.242991000
C	-3.208875000	-3.357323000	-0.976078000
C	-2.891217000	1.513648000	-0.520129000
C	3.976589000	-3.794071000	-0.082671000
C	4.205555000	1.103928000	0.012279000
C	-0.307594000	-3.543775000	-0.482280000
C	-0.050713000	1.363834000	-0.361770000
C	-4.547022000	-3.303217000	-0.918868000
C	-4.296446000	1.577959000	-0.559363000
C	6.112515000	-2.704348000	0.140371000
C	6.398141000	2.187970000	0.227056000
C	1.862353000	-2.466708000	-0.256064000
C	2.146926000	2.458721000	-0.168343000
C	-2.387815000	-2.201621000	-0.671081000
C	-2.134064000	2.707433000	-0.509070000
C	3.300105000	-2.558820000	-0.122926000
C	3.591823000	2.379037000	-0.035269000
C	-0.971884000	-2.288010000	-0.533737000
C	-0.684098000	2.621833000	-0.408979000
C	-5.182163000	-2.063443000	-0.346976000
C	-4.941272000	2.798307000	-0.614314000
C	5.485525000	-1.441320000	0.101158000
C	5.786067000	3.425798000	0.179272000
C	1.480321000	3.699615000	-0.224566000
C	-3.018808000	-0.956688000	-0.586035000
C	-2.819823000	3.935139000	-0.578334000
C	4.059602000	-1.365254000	-0.031387000
C	4.403451000	3.524040000	0.049386000
C	-0.188696000	-1.116315000	-0.417054000
C	0.118505000	3.780206000	-0.341276000
C	-4.198445000	3.982474000	-0.638609000
H	-0.336703000	4.762355000	-0.374097000
H	2.043894000	4.622898000	-0.174276000
H	3.962564000	4.512391000	0.014722000
H	6.382072000	4.330986000	0.240943000
H	-4.704875000	4.940741000	-0.693814000
H	-2.269431000	4.867976000	-0.588882000
H	-6.195930000	-1.900175000	-0.736487000
H	-5.968010000	0.372084000	-1.139540000
H	-6.027460000	2.826258000	-0.619909000
H	7.476608000	2.104299000	0.327425000
H	7.316047000	-0.322779000	0.288476000
H	7.193038000	-2.750507000	0.242167000
H	3.423658000	-4.722077000	-0.154087000
H	1.496438000	-4.608637000	-0.296915000
H	5.846989000	-4.830356000	0.077882000
H	-0.885798000	-4.459719000	-0.513576000
H	-2.728358000	-4.259874000	-1.339498000
H	-5.186134000	-4.141720000	-1.164813000
C	1.235000000	-1.203968000	-0.289574000
N	-4.393091000	-0.884475000	-0.673231000
C	-0.834573000	0.154013000	-0.436393000
O	-5.784891000	0.297384000	0.831601000
O	-5.230058000	-2.365969000	0.992848000
C	-1.708901000	0.700098000	2.779537000

C	5.862738000	0.934265000	0.210033000
C	1.219621000	-3.582260000	-0.592067000
C	1.647124000	1.303836000	-0.449012000
C	-2.963401000	-3.198920000	-1.533567000
C	-2.587837000	1.652079000	-0.943825000
C	4.113096000	-3.823874000	-0.110431000
C	4.454074000	1.062741000	-0.016352000
C	-0.122760000	-3.468898000	-0.830467000
C	0.233453000	1.423980000	-0.645814000
C	-4.309973000	-3.083748000	-1.739942000
C	-3.990134000	1.751838000	-1.013221000
C	6.255741000	-2.787707000	0.251371000
C	6.654021000	2.096239000	0.341253000
C	2.048857000	-2.448870000	-0.439434000
C	2.444070000	2.467077000	-0.333298000
C	-2.159787000	-2.081523000	-1.172256000
C	-1.804286000	2.823428000	-0.904378000
C	3.474346000	-2.575703000	-0.203492000
C	3.875147000	2.353416000	-0.107263000
C	-0.747508000	-2.203504000	-0.927448000
C	-0.365157000	2.700491000	-0.735748000
C	-5.003253000	-1.819724000	-1.392849000
C	-4.607910000	2.980943000	-1.092025000
C	5.663529000	-1.508877000	0.164177000
C	6.075939000	3.346619000	0.252331000
C	1.813717000	3.722007000	-0.441194000
C	-2.768054000	-0.810169000	-1.106089000
C	-2.460023000	4.068218000	-0.993231000
C	4.253278000	-1.399175000	-0.064030000
C	4.706148000	3.476846000	0.030881000
C	0.046996000	-1.050733000	-0.740340000
C	0.462195000	3.836638000	-0.636972000
C	-3.833499000	4.148402000	-1.098521000
H	0.035686000	4.829419000	-0.706690000
H	2.396478000	4.631928000	-0.369081000
H	4.292163000	4.475421000	-0.029724000
H	6.686682000	4.238182000	0.354016000
H	-4.314468000	5.118751000	-1.166136000
H	-1.888772000	4.988429000	-0.977935000
H	-5.866866000	-1.554443000	-2.017626000
H	-5.749386000	0.575967000	-1.375704000
H	-5.692348000	3.037423000	-1.126008000
H	7.720942000	1.986917000	0.513362000
H	7.504416000	-0.435123000	0.470427000
H	7.325358000	-2.858992000	0.426796000
H	3.544144000	-4.739565000	-0.211587000
H	1.640278000	-4.577091000	-0.514448000
H	5.942911000	-4.905952000	0.184677000
H	-0.710000000	-4.375832000	-0.908748000
H	-2.496880000	-4.159992000	-1.715462000
H	-4.925445000	-3.920425000	-2.040785000
C	1.453708000	-1.169480000	-0.514184000
N	-4.112724000	-0.665318000	-1.352678000
C	-0.573320000	0.237447000	-0.766962000
O	-5.039242000	0.382597000	0.556683000
O	-5.336021000	-2.355285000	-0.180217000
C	-2.515251000	1.648649000	2.346002000

S	-2.966651000	-0.570791000	2.548594000
H	-5.090494000	0.237307000	1.517470000
H	-1.744442000	0.997600000	3.834398000
H	-0.711801000	0.305414000	2.570631000
H	-1.904284000	1.582806000	2.165007000

S	-2.642845000	1.172098000	4.077131000
H	-5.299239000	-0.539606000	0.747632000
C	-1.588730000	-1.720899000	2.312230000
S	-3.347195000	-2.047873000	2.650263000
H	-3.716548000	-2.365859000	1.394122000
H	-1.471413000	-0.899755000	1.601716000
H	-1.144874000	-1.418773000	3.262250000
H	-1.077860000	-2.611258000	1.939518000
H	-1.507248000	1.502537000	1.945950000
H	-3.226553000	1.017207000	1.796227000
H	-2.831072000	2.686260000	2.202333000

(T_{2E'})_{MT}

C	6.568403000	-1.026315000	0.429086000
C	2.488766000	0.024835000	-0.249451000
C	-1.628363000	1.051263000	-0.835969000
C	3.857042000	-0.326514000	-0.027092000
C	-4.439827000	1.625684000	-0.911063000
C	5.176185000	-4.339360000	-0.503597000
C	6.172672000	0.309105000	0.592343000
C	1.018774000	-3.278944000	-1.232386000
C	2.062326000	1.380008000	-0.087580000
C	-3.062845000	-2.177649000	-2.127281000
C	-2.065307000	2.411974000	-0.656686000
C	3.836618000	-4.003067000	-0.735282000
C	4.798639000	0.671132000	0.361887000
C	-0.292842000	-2.933706000	-1.464359000
C	0.684939000	1.730746000	-0.302875000
C	-4.362840000	-1.846773000	-2.326513000
C	-3.432708000	2.732404000	-0.796544000
C	6.079718000	-3.368227000	-0.120377000
C	7.104753000	1.305177000	0.980213000
C	1.975625000	-2.327590000	-0.827789000
C	3.003748000	2.383801000	0.287305000
C	-2.125063000	-1.254238000	-1.562954000
C	-1.128419000	3.441257000	-0.375029000
C	3.365127000	-2.688791000	-0.588932000
C	4.394845000	2.028201000	0.524242000
C	-0.755563000	-1.607226000	-1.307565000
C	0.264919000	3.082947000	-0.162747000
C	-4.958575000	-0.583686000	-1.794627000
C	-3.860872000	4.046286000	-0.710703000
C	5.659724000	-2.024346000	0.042415000
C	6.697188000	2.615031000	1.135511000
C	2.545552000	3.707220000	0.417820000
C	-2.572789000	0.066603000	-1.266543000
C	-1.596767000	4.770144000	-0.295461000
C	4.285697000	-1.676654000	-0.191699000
C	5.362136000	2.971912000	0.910870000
C	0.180952000	-0.626593000	-0.871937000
C	1.228452000	4.044445000	0.197838000
C	-2.936569000	5.071420000	-0.472086000
H	0.939580000	5.080874000	0.322810000
H	3.231635000	4.497013000	0.699375000
H	5.085304000	4.010470000	1.046167000
H	7.409799000	3.378463000	1.433804000

(P_{E'})_{MT}

C	6.364944000	-0.268843000	0.277041000
C	2.185316000	0.065210000	-0.384723000
C	-2.037462000	0.373400000	-0.845056000
C	3.577285000	-0.045115000	-0.174780000
C	-4.867229000	0.508555000	-0.602760000
C	5.464115000	-3.845896000	-0.127917000
C	5.776578000	1.007006000	0.258458000
C	1.199450000	-3.520170000	-0.863586000
C	1.563473000	1.359114000	-0.407509000
C	-3.044402000	-3.149895000	-1.622154000
C	-2.671984000	1.664541000	-0.860995000
C	4.095383000	-3.751731000	-0.356952000
C	4.368483000	1.130487000	0.027900000
C	-0.142768000	-3.410757000	-1.084892000
C	0.150862000	1.470285000	-0.604762000
C	-4.380203000	-3.067041000	-1.584528000
C	-4.076577000	1.745851000	-0.910441000
C	6.220375000	-2.707333000	0.082411000
C	6.550366000	2.169111000	0.461724000
C	2.015109000	-2.385055000	-0.615484000
C	2.344636000	2.524838000	-0.238700000
C	-2.207932000	-2.032424000	-1.221771000
C	-1.900159000	2.844678000	-0.850910000
C	3.437961000	-2.506249000	-0.380203000
C	3.774044000	2.415761000	-0.000605000
C	-0.796309000	-2.148082000	-1.056409000
C	-0.461277000	2.738570000	-0.666143000
C	-5.034102000	-1.882626000	-0.954575000
C	-4.706734000	2.965037000	-1.033066000
C	5.611449000	-1.434716000	0.069008000
C	5.956429000	3.416412000	0.437235000
C	1.700266000	3.777694000	-0.307020000
C	-2.827451000	-0.800948000	-1.016155000
C	-2.568695000	4.078194000	-0.987495000
C	4.200281000	-1.330860000	-0.162173000
C	4.588692000	3.541909000	0.208694000
C	-0.010059000	-1.000386000	-0.802921000
C	0.351100000	3.882555000	-0.518687000
C	-3.942935000	4.138424000	-1.098856000
H	-0.090700000	4.871113000	-0.552815000
H	2.271531000	4.690729000	-0.193080000
H	4.160587000	4.536426000	0.201498000
H	6.554743000	4.307982000	0.597385000

H	-3.271742000	6.102678000	-0.410061000
H	-0.906338000	5.582244000	-0.099314000
H	-5.595799000	-0.073331000	-2.542757000
H	-5.255311000	1.925180000	-1.587459000
H	-4.918746000	4.272499000	-0.811548000
H	8.138767000	1.019151000	1.152214000
H	7.606944000	-1.295949000	0.605242000
H	7.121345000	-3.618911000	0.061532000
H	3.159642000	-4.794422000	-1.033657000
H	1.301690000	-4.316075000	-1.365620000
H	5.497502000	-5.369287000	-0.627213000
H	-0.981274000	-3.718028000	-1.753866000
H	-2.720299000	-3.155997000	-2.445882000
H	-5.066065000	-2.556684000	-2.748928000
C	1.548426000	-0.978598000	-0.649078000
N	-3.867364000	0.414528000	-1.496911000
C	-0.262381000	0.716594000	-0.670795000
O	-4.955975000	1.375073000	0.381879000
O	-5.655185000	-0.966821000	-0.694249000
C	-3.091540000	-0.115505000	3.078435000
S	-4.058437000	-1.322136000	4.048219000
H	-5.459371000	0.523523000	0.281935000
C	-3.439622000	-3.664202000	1.338451000
S	-5.083371000	-2.966537000	1.737957000
H	-5.180382000	-2.101858000	0.669112000
H	-2.680502000	-2.880383000	1.289044000
H	-3.180103000	-4.355762000	2.142393000
H	-3.471670000	-4.207939000	0.389859000
H	-2.198710000	-0.565438000	2.631635000
H	-3.699721000	0.355855000	2.300978000
H	-2.766417000	0.671932000	3.770222000

(E_{K'})_{MT}

C	6.431372000	-0.154854000	0.308209000
C	2.195729000	-0.047908000	0.035240000
C	-1.935102000	-0.066653000	0.523300000
C	3.599268000	-0.080680000	0.100909000
C	-5.003034000	0.464543000	-0.900293000
C	5.737032000	-3.711476000	-0.479163000
C	5.765643000	1.069628000	0.479817000
C	1.402388000	-3.672192000	-0.562596000
C	1.497461000	1.215761000	0.116801000
C	-3.004949000	-3.219054000	-0.779086000
C	-2.941383000	1.783123000	-0.341168000
C	4.346102000	-3.698725000	-0.556950000
C	4.340704000	1.122175000	0.349718000
C	0.026370000	-3.660004000	-0.503143000
C	0.075508000	1.271341000	-0.020002000
C	-4.456523000	-3.043749000	-0.863899000
C	-4.162065000	1.679118000	-1.018585000
C	6.428515000	-2.552517000	-0.188570000
C	6.480531000	2.251616000	0.769300000
C	2.154884000	-2.499439000	-0.377983000
C	2.237580000	2.415123000	0.262469000
C	-2.134436000	-2.436010000	-0.109908000

H	-4.433858000	5.099895000	-1.209485000
H	-2.004410000	5.002988000	-1.014186000
H	-5.999704000	-1.654471000	-1.416061000
H	-5.845227000	0.538576000	-1.105831000
H	-5.792111000	3.011347000	-1.050875000
H	7.617232000	2.064387000	0.637510000
H	7.434344000	-0.354899000	0.452904000
H	7.289886000	-2.775052000	0.259971000
H	3.538852000	-4.666855000	-0.515782000
H	1.640914000	-4.509167000	-0.881904000
H	5.937604000	-4.822719000	-0.115246000
H	-0.718679000	-4.314083000	-1.249739000
H	-2.575019000	-4.045588000	-2.015264000
H	-5.018876000	-3.881705000	-1.906592000
C	1.402412000	-1.114434000	-0.602687000
N	-4.206261000	-0.698570000	-1.076741000
C	-0.643402000	0.275000000	-0.751870000
O	-5.044692000	0.517936000	0.798470000
O	-5.378735000	-2.168354000	0.408584000
C	-2.454936000	1.436384000	2.557997000
S	-2.772097000	-0.021570000	3.602966000
H	-5.416573000	-0.349578000	1.045321000
C	-0.666485000	-1.831324000	2.412039000
S	-2.463593000	-1.568019000	2.278340000
H	-4.574373000	-2.502602000	0.845165000
H	-2.457837000	2.299399000	3.229689000
H	-1.476234000	1.362189000	2.075329000
H	-3.249334000	1.532144000	1.817217000
H	-0.401417000	-2.097050000	3.436138000
H	-0.411338000	-2.652206000	1.734863000
H	-0.125146000	-0.935217000	2.099423000

(T_{1K'})_{MT}

C	6.391945000	-0.518572000	0.307828000
C	2.169922000	-0.033563000	-0.039447000
C	-2.112913000	0.436575000	0.075285000
C	3.596554000	-0.193409000	0.058889000
C	-4.826631000	0.747285000	-0.816290000
C	5.358372000	-4.029085000	-0.250610000
C	5.843151000	0.766026000	0.404738000
C	1.059643000	-3.549008000	-0.628543000
C	1.597768000	1.267736000	0.016268000
C	-3.207328000	-3.064389000	-0.959155000
C	-2.689461000	1.782956000	-0.210808000
C	3.970676000	-3.879923000	-0.370674000
C	4.429144000	0.939224000	0.265495000
C	-0.301691000	-3.407798000	-0.698135000
C	0.182582000	1.420890000	-0.094799000
C	-4.569623000	-2.870875000	-1.048518000
C	-4.095212000	1.870009000	-0.681975000
C	6.160205000	-2.934842000	-0.029533000
C	6.666450000	1.897296000	0.639027000
C	1.919105000	-2.456603000	-0.383686000
C	2.431628000	2.417681000	0.154476000
C	-2.342374000	-2.026783000	-0.568779000

C	-1.935944000	2.651759000	-0.744829000
C	3.611312000	-2.521047000	-0.348868000
C	3.677698000	2.365350000	0.466697000
C	-0.667548000	-2.467945000	-0.264502000
C	-0.554811000	2.516315000	-0.218100000
C	-5.104479000	-1.861751000	-0.940749000
C	-4.458277000	2.646727000	-1.979649000
C	5.735553000	-1.340041000	0.014774000
C	5.813951000	3.451639000	0.921288000
C	1.556322000	3.641873000	0.181673000
C	-2.615563000	-1.353805000	0.786040000
C	-2.246244000	3.579012000	-1.749997000
C	4.306668000	-1.319106000	-0.076061000
C	4.431035000	3.512634000	0.766682000
C	0.053507000	-1.271520000	-0.128632000
C	0.211846000	3.687926000	-0.093528000
C	-3.511416000	3.608447000	-2.324582000
H	-0.280864000	4.648700000	-0.206949000
H	2.096136000	4.575396000	0.281958000
H	3.940804000	4.468549000	0.902976000
H	6.365798000	4.355463000	1.159368000
H	-3.739556000	4.344100000	-3.088801000
H	-1.477138000	4.260758000	-2.100157000
H	-6.188460000	-1.834303000	-1.068649000
H	-6.097202000	0.560672000	-0.901688000
H	-5.413536000	2.606624000	-2.496314000
H	7.560445000	2.197904000	0.874267000
H	7.514559000	-0.185131000	0.394739000
H	7.512470000	-2.553831000	-0.117017000
H	3.837520000	-4.627379000	-0.783484000
H	1.899738000	-4.621875000	-0.714791000
H	6.273272000	-4.640585000	-0.644541000
H	-0.526353000	-4.590711000	-0.590765000
H	-2.599075000	-4.018444000	-1.400622000
H	-5.049268000	-3.947677000	-0.978542000
C	1.467719000	-1.276617000	-0.171538000
N	-4.404420000	-0.662199000	-0.907486000
C	-0.654720000	0.000338000	0.088517000
O	-2.701831000	1.029575000	0.795374000
O	-3.464436000	-1.478705000	1.644855000
C	-5.762054000	0.604074000	2.491533000
S	-6.728168000	-0.841873000	1.941653000
H	-5.693126000	-1.699106000	1.927000000
H	-4.812656000	0.647377000	1.956127000
H	-6.356308000	1.493177000	2.271832000
H	-5.572341000	0.558149000	3.564660000

(I1K')MT

C	7.046046000	-0.094048000	0.496255000
C	2.803569000	0.004035000	-0.059086000
C	-1.506320000	0.113879000	-0.188860000
C	4.247915000	-0.028745000	0.123717000
C	-4.144148000	0.147862000	-1.253682000
C	6.355251000	-3.696357000	0.062200000
C	6.384905000	1.133232000	0.507236000
C	2.022150000	-3.615262000	-0.347208000

C	-1.790436000	2.909249000	-0.557898000
C	3.352614000	-2.628652000	-0.273507000
C	3.874073000	2.250365000	0.337859000
C	-0.940540000	-2.161578000	-0.505833000
C	-0.372814000	2.731223000	-0.231187000
C	-5.103316000	-1.578463000	-0.905926000
C	-4.609280000	3.167410000	-1.066652000
C	5.591447000	-1.639194000	0.079269000
C	6.110386000	3.147790000	0.730668000
C	1.837710000	3.672682000	0.103319000
C	-2.986359000	-0.833202000	0.127045000
C	-2.330525000	4.044880000	-1.058001000
C	4.171537000	-1.480086000	-0.043845000
C	4.724528000	3.322652000	0.579635000
C	-0.090425000	-1.004782000	-0.268074000
C	0.470847000	3.824148000	-0.104336000
C	-3.760031000	4.197959000	-1.261587000
H	0.059560000	4.826533000	-0.154830000
H	2.439382000	4.569029000	0.196394000
H	4.326065000	4.326301000	0.667511000
H	6.736897000	4.013351000	0.921381000
H	-4.132345000	5.159969000	-1.597519000
H	-1.693590000	4.885963000	-1.314070000
H	-6.140633000	-1.374934000	-1.154355000
H	-5.860910000	0.791133000	-1.151459000
H	-5.675066000	3.271953000	-1.251162000
H	7.737282000	1.750634000	0.748363000
H	7.467081000	-0.645616000	0.410976000
H	7.236917000	-3.042415000	0.066651000
H	3.379253000	-4.771793000	-0.537143000
H	1.472601000	-4.541025000	-0.762998000
H	5.794712000	-5.019352000	-0.332689000
H	-0.897621000	-4.295030000	-0.873489000
H	-2.813424000	-4.039156000	-1.226157000
H	-5.244896000	-3.680631000	-1.293259000
C	1.342292000	-1.163827000	-0.238827000
N	-4.322757000	-0.533265000	-0.646885000
C	-0.644078000	0.262060000	-0.111049000
O	-2.473117000	1.325804000	1.122200000
O	-3.259704000	-1.182867000	1.362279000
C	-6.224217000	-0.160164000	2.141743000
S	-6.014889000	-1.949409000	1.835244000
H	-4.581222000	-1.781908000	1.617913000
H	-5.245406000	0.320461000	2.060335000
H	-6.915333000	0.283901000	1.419320000
H	-6.621165000	0.004727000	3.145519000

(T2K')MT

C	6.401266000	-0.619354000	0.234621000
C	2.173100000	-0.048673000	-0.031864000
C	-2.096957000	0.517959000	0.130949000
C	3.609387000	-0.241411000	0.049878000
C	-4.796656000	0.889101000	-0.692848000
C	5.298267000	-4.104546000	-0.308417000
C	5.878916000	0.670123000	0.343445000
C	0.985056000	-3.545539000	-0.470415000

C	2.124348000	1.243451000	-0.099856000	C	1.629879000	1.258061000	0.026031000
C	-2.209584000	-3.438951000	-1.232820000	C	-3.235505000	-2.870782000	-1.082661000
C	-2.182728000	1.400512000	-0.542398000	C	-2.652425000	1.885214000	-0.115638000
C	4.953611000	-3.673707000	-0.110400000	C	3.901994000	-3.926861000	-0.388724000
C	4.966218000	1.172946000	0.303377000	C	4.463677000	0.869125000	0.234573000
C	0.632591000	-3.580497000	-0.506396000	C	-0.393546000	-3.358166000	-0.536166000
C	0.699919000	1.271905000	-0.278067000	C	0.210785000	1.444180000	-0.059283000
C	-3.637983000	-3.402701000	-1.371501000	C	-4.631674000	-2.679331000	-1.146984000
C	-3.541275000	1.346100000	-1.123575000	C	-4.055060000	2.006533000	-0.572177000
C	7.044405000	-2.535375000	0.267269000	C	6.120695000	-3.031946000	-0.100441000
C	7.098596000	2.347444000	0.716417000	C	6.730144000	1.789356000	0.559814000
C	2.770841000	-2.461263000	-0.223067000	C	1.863647000	-2.482081000	-0.319082000
C	2.850534000	2.472853000	0.038605000	C	2.490537000	2.394936000	0.161653000
C	-1.513502000	-2.375441000	-0.759055000	C	-2.400822000	-1.916012000	-0.563340000
C	-1.362385000	2.588666000	-0.870955000	C	-1.731287000	2.990521000	-0.467257000
C	4.231601000	-2.495901000	-0.074643000	C	3.313664000	-2.678923000	-0.259699000
C	4.297976000	2.440219000	0.287861000	C	3.935978000	2.196958000	0.317979000
C	-0.068653000	-2.393665000	-0.533393000	C	-0.968618000	-2.100539000	-0.435899000
C	0.043608000	2.539601000	-0.471849000	C	-0.316514000	2.777412000	-0.164826000
C	-4.268502000	-2.213693000	-1.258618000	C	-5.157043000	-1.444418000	-0.835052000
C	-4.140566000	2.567080000	-1.601797000	C	-4.542606000	3.305699000	-0.973888000
C	6.356296000	-1.289253000	0.296806000	C	5.575228000	-1.724102000	0.027566000
C	6.435942000	3.541317000	0.722526000	C	6.200954000	3.045410000	0.663637000
C	2.157027000	3.663392000	-0.067343000	C	1.924200000	3.657953000	0.138420000
C	-2.296042000	-1.203512000	-0.200397000	C	-3.017843000	-0.711404000	0.122703000
C	-1.970733000	3.658346000	-1.442291000	C	-2.252341000	4.137196000	-0.967662000
C	4.934182000	-1.262310000	0.118197000	C	4.156482000	-1.539151000	-0.057318000
C	5.040643000	3.584986000	0.507291000	C	4.809949000	3.246368000	0.541882000
C	0.655707000	-1.168344000	-0.341397000	C	-0.102712000	-0.971750000	-0.223509000
C	0.785000000	3.694345000	-0.333296000	C	0.552029000	3.843536000	-0.037605000
C	-3.384121000	3.677707000	-1.754342000	C	-3.674843000	4.321820000	-1.170425000
H	0.296660000	4.658674000	-0.427663000	H	0.163455000	4.856089000	-0.065651000
H	2.672967000	4.610991000	0.031835000	H	2.545537000	4.540710000	0.231456000
H	4.559186000	4.555606000	0.523693000	H	4.435530000	4.258777000	0.635570000
H	6.973657000	4.469219000	0.889936000	H	6.845939000	3.900615000	0.839305000
H	-3.815197000	4.590722000	-2.150940000	H	-4.027843000	5.288194000	-1.513993000
H	-1.388674000	4.540514000	-1.691369000	H	-1.594398000	4.958714000	-1.234570000
H	-5.327919000	-2.079994000	-1.453871000	H	-6.177508000	-1.176726000	-1.084858000
H	-5.138945000	0.071377000	-1.684652000	H	-5.824624000	0.940317000	-1.041851000
H	-5.192856000	2.554120000	-1.876159000	H	-5.605939000	3.427089000	-1.163313000
H	8.172510000	2.299480000	0.873392000	H	7.800080000	1.621253000	0.644831000
H	8.123432000	-0.119354000	0.643206000	H	7.476298000	-0.766028000	0.310610000
H	8.122083000	-2.537830000	0.404699000	H	7.197954000	-3.155844000	-0.033525000
H	4.451494000	-4.619458000	-0.276268000	H	3.291309000	-4.805548000	-0.559462000
H	2.500194000	-4.587053000	-0.314891000	H	1.358404000	-4.560433000	-0.532773000
H	6.876909000	-4.647693000	0.029788000	H	5.712090000	-5.102375000	-0.413355000
H	0.103474000	-4.523599000	-0.587781000	H	-1.025178000	-4.233761000	-0.637436000
H	-1.688258000	-4.338889000	-1.542422000	H	-2.825486000	-3.793569000	-1.478218000
H	-4.198798000	-4.290947000	-1.631352000	H	-5.300935000	-3.471281000	-1.458272000
C	2.086234000	-1.200997000	-0.219296000	C	1.320909000	-1.162163000	-0.201016000
N	-3.572316000	-1.063448000	-0.939684000	N	-4.328880000	-0.398475000	-0.505689000
C	-0.019986000	0.060013000	-0.291851000	C	-0.635501000	0.314355000	-0.074799000
O	-2.013711000	0.984572000	0.817199000	O	-2.434258000	1.387218000	1.203486000
O	-2.564901000	-1.475072000	1.157230000	O	-3.209559000	-1.027566000	1.477075000
C	-6.067280000	2.175289000	1.149409000	C	-6.349899000	-0.511285000	1.971321000
C	-7.059579000	1.355105000	0.601362000	S	-6.202039000	-2.242463000	1.449726000
C	-6.979733000	-0.019603000	0.750608000	H	-3.798761000	-1.807368000	1.536467000

C	-5.896794000	-0.605639000	1.449866000
C	-4.900364000	0.239562000	1.991178000
C	-4.993103000	1.615632000	1.840469000
H	-6.126288000	3.252403000	1.023145000
H	-7.894750000	1.796141000	0.065242000
H	-7.745972000	-0.671353000	0.341017000
H	-4.043294000	-0.203471000	2.483572000
H	-4.206158000	2.249766000	2.235619000
S	-5.794132000	-2.321012000	1.601991000
H	-3.034652000	-2.326343000	1.203467000

H	-5.370067000	-0.026123000	2.004723000
H	-7.032211000	0.048894000	1.325573000
H	-6.767654000	-0.510341000	2.983610000

(I_{2K'})_{MT}

C	6.361855000	-0.601194000	0.286651000
C	2.159909000	-0.042581000	0.009057000
C	-2.093231000	0.485476000	0.175211000
C	3.571757000	-0.223952000	0.074000000
C	-4.750300000	0.706039000	-0.746049000
C	5.261327000	-4.072259000	-0.429914000
C	5.835055000	0.693515000	0.438188000
C	0.970254000	-3.491497000	-0.842192000
C	1.608178000	1.272372000	0.107594000
C	-3.313437000	-3.036826000	-0.696256000
C	-2.654930000	1.819909000	-0.226990000
C	3.884274000	-3.901212000	-0.539082000
C	4.424949000	0.896146000	0.314442000
C	-0.374388000	-3.337021000	-0.869438000
C	0.199655000	1.446219000	-0.001576000
C	-4.645797000	-2.889914000	-0.607636000
C	-4.014413000	1.846424000	-0.793285000
C	6.087780000	-2.997203000	-0.160925000
C	6.673697000	1.800262000	0.705559000
C	1.866929000	-2.429793000	-0.481155000
C	2.455447000	2.403252000	0.239476000
C	-2.379773000	-1.972055000	-0.397139000
C	-1.728038000	2.906219000	-0.612729000
C	3.282823000	-2.633082000	-0.381446000
C	3.890526000	2.208198000	0.424426000
C	-1.011636000	-2.101508000	-0.484466000
C	-0.336107000	2.747215000	-0.197990000
C	-5.268903000	-1.587298000	-0.229405000
C	-4.465973000	3.042718000	-1.446859000
C	5.544212000	-1.701877000	0.011429000
C	6.136781000	3.061556000	0.841013000
C	1.877314000	3.674661000	0.158216000
C	-2.976511000	-0.753387000	0.275446000
C	-2.225085000	3.977084000	-1.283528000
C	4.124194000	-1.516045000	-0.095424000
C	4.760395000	3.266132000	0.698686000
C	-0.119260000	-0.972685000	-0.216610000
C	0.525494000	3.840883000	-0.087680000
C	-3.611662000	4.071307000	-1.672770000
H	0.124696000	4.844439000	-0.187021000
H	2.496491000	4.560627000	0.239088000
H	4.373024000	4.270894000	0.819850000
H	6.781101000	3.907662000	1.058680000
H	-3.949009000	4.965069000	-2.185945000

(I_{3K'})_{MT}

C	6.554545000	-0.916226000	0.233256000
C	2.437347000	0.069318000	-0.115047000
C	-1.753546000	0.948638000	0.010255000
C	3.823693000	-0.250788000	-0.027146000
C	-4.340725000	1.520082000	-0.936358000
C	5.184406000	-4.142836000	-0.985584000
C	6.138479000	0.390991000	0.541154000
C	0.987264000	-3.114096000	-1.463421000
C	1.998902000	1.402489000	0.155572000
C	-3.246172000	-2.363154000	-1.209090000
C	-2.192669000	2.366366000	-0.183255000
C	3.835185000	-3.828270000	-1.120530000
C	4.759875000	0.741214000	0.396672000
C	-0.337066000	-2.837858000	-1.500105000
C	0.615430000	1.717042000	0.040127000
C	-4.559294000	-2.105484000	-1.113896000
C	-3.519707000	2.593115000	-0.778360000
C	6.089699000	-3.195829000	-0.544283000
C	7.058844000	1.367623000	0.987177000
C	1.957293000	-2.195445000	-0.933901000
C	2.934356000	2.420427000	0.477070000
C	-2.230696000	-1.397872000	-0.850303000
C	-1.167314000	3.417276000	-0.362101000
C	3.343113000	-2.540606000	-0.815309000
C	4.339293000	2.070679000	0.671074000
C	-0.878370000	-1.614989000	-0.956860000
C	0.195888000	3.074368000	0.041904000
C	-5.089664000	-0.764435000	-0.729982000
C	-3.850166000	3.909479000	-1.245698000
C	5.656607000	-1.888323000	-0.218367000
C	6.631213000	2.644764000	1.274969000
C	2.468582000	3.735259000	0.578702000
C	-2.745237000	-0.211341000	-0.071549000
C	-1.554003000	4.617948000	-0.865382000
C	4.265882000	-1.555054000	-0.351030000
C	5.286443000	2.995678000	1.115732000
C	0.098294000	-0.610077000	-0.530102000
C	1.143485000	4.056746000	0.336912000
C	-2.912122000	4.888586000	-1.272060000
H	0.833507000	5.095559000	0.388893000
H	3.156323000	4.540003000	0.811658000
H	4.986851000	4.007762000	1.361098000
H	7.337522000	3.389598000	1.628068000
H	-3.158545000	5.877794000	-1.641364000

H	-1.560481000	4.788282000	-1.567367000
H	-6.083728000	-1.342666000	-0.916276000
H	-5.758246000	0.697540000	-1.155362000
H	-5.498915000	3.090680000	-1.783897000
H	7.742920000	1.635557000	0.805260000
H	7.435415000	-0.748494000	0.377978000
H	7.162416000	-3.130196000	-0.075061000
H	3.272945000	-4.773365000	-0.735060000
H	1.376970000	-4.456847000	-1.119266000
H	5.685723000	-5.063608000	-0.554739000
H	-0.983720000	-4.184410000	-1.157881000
H	-2.928315000	-4.006039000	-0.992088000
H	-5.320236000	-3.722228000	-0.780725000
C	1.314077000	-1.153849000	-0.238794000
N	-4.325748000	-0.499020000	-0.272487000
C	-0.639149000	0.286068000	0.001837000
O	-2.498413000	1.442481000	1.142109000
O	-3.062410000	-0.997802000	1.665521000
C	-6.244324000	-0.127029000	1.981886000
S	-6.062890000	-1.851805000	1.449944000
H	-3.517798000	-1.846658000	1.798802000
H	-5.261319000	0.345690000	2.050983000
H	-6.899007000	0.435581000	1.311655000
H	-6.701645000	-0.159252000	2.972986000

H	-0.815627000	5.402843000	-1.002630000
H	-5.780177000	-0.415457000	-1.507731000
H	-5.322321000	1.655137000	-1.386171000
H	-4.860663000	4.093533000	-1.603306000
H	8.103286000	1.091049000	1.100218000
H	7.605261000	-1.174457000	0.341663000
H	7.142830000	-3.439781000	-0.438424000
H	3.157048000	-4.604860000	-1.451512000
H	1.322105000	-4.062557000	-1.866290000
H	5.523448000	-5.145257000	-1.227571000
H	-1.009265000	-3.571090000	-1.929105000
H	-2.944759000	-3.354055000	-1.530631000
H	-5.299220000	-2.873488000	-1.311846000
C	1.510108000	-0.916265000	-0.539059000
N	-4.042512000	0.232037000	-0.617913000
C	-0.316466000	0.648040000	-0.151224000
O	-2.117324000	1.765145000	1.125101000
O	-2.938274000	-0.706696000	1.236377000
C	-6.911367000	0.656045000	0.837835000
S	-6.131962000	-0.979617000	0.786126000
H	-3.127837000	0.065555000	1.799546000
C	-1.930454000	-3.805077000	1.701313000
S	-3.668490000	-3.868106000	2.245158000
H	-3.989789000	-2.638640000	1.806257000
H	-7.628085000	0.634338000	1.661316000
H	-6.179712000	1.444180000	1.032775000
H	-7.453553000	0.869428000	-0.088651000
H	-1.831713000	-4.044470000	0.640059000
H	-1.514348000	-2.813904000	1.886558000
H	-1.378079000	-4.545931000	2.281812000

(T_{3K'})_{MT}

C	6.516464000	-0.779130000	0.032731000
C	2.349064000	0.099048000	-0.205878000
C	-1.868828000	0.885920000	-0.059379000
C	3.752139000	-0.190131000	-0.143378000
C	-4.543999000	1.481655000	-0.754488000
C	5.197603000	-4.072697000	-1.077764000
C	6.075932000	0.520282000	0.336463000
C	0.939140000	-3.187704000	-1.325668000
C	1.885680000	1.425094000	0.056806000
C	-3.305575000	-2.337901000	-1.496594000
C	-2.349509000	2.333854000	-0.124633000
C	3.830948000	-3.797832000	-1.163688000
C	4.675314000	0.830564000	0.235439000
C	-0.404542000	-2.929418000	-1.346090000
C	0.481996000	1.712849000	-0.024200000
C	-4.626952000	-2.107336000	-1.395663000
C	-3.723111000	2.565913000	-0.606421000
C	6.090286000	-3.090488000	-0.686470000
C	6.985605000	1.530884000	0.736401000
C	1.899081000	-2.219676000	-0.927521000
C	2.810185000	2.465711000	0.367739000
C	-2.322884000	-1.398578000	-1.008693000
C	-1.351285000	3.408247000	-0.266353000
C	3.310629000	-2.521910000	-0.859455000

(I_{4K'})_{MT}

C	6.417562000	-1.026426000	0.273969000
C	2.325371000	0.031386000	-0.105661000
C	-1.764676000	0.803546000	0.126729000
C	3.690084000	-0.311623000	-0.009923000
C	-4.434491000	1.771713000	-0.710266000
C	5.020890000	-4.225846000	-0.985132000
C	6.020653000	0.286578000	0.582301000
C	0.819373000	-3.174328000	-1.367985000
C	1.902242000	1.383170000	0.179781000
C	-3.429343000	-2.045314000	-1.590268000
C	-2.307985000	2.828424000	-0.113461000
C	3.677991000	-3.893276000	-1.128131000
C	4.649029000	0.662067000	0.425433000
C	-0.510055000	-2.864750000	-1.399842000
C	0.524207000	1.737525000	0.080487000
C	-4.719194000	-1.719669000	-1.408265000
C	-3.531514000	2.871160000	-0.805314000
C	5.929138000	-3.290948000	-0.523059000
C	6.954138000	1.242954000	1.036736000
C	1.804574000	-2.248461000	-0.926236000
C	2.864920000	2.375575000	0.487373000
C	-2.372631000	-1.243616000	-0.989471000
C	-1.180807000	3.570928000	-0.422850000
C	3.201767000	-2.606601000	-0.810199000

C	4.227249000	2.156319000	0.512192000
C	-0.937754000	-1.667172000	-0.962640000
C	0.029938000	3.071594000	0.041823000
C	-5.170697000	-0.856725000	-0.801442000
C	-4.110907000	3.900215000	-0.934216000
C	5.628785000	-1.788138000	-0.368280000
C	6.532502000	2.803904000	1.023459000
C	2.312205000	3.771618000	0.514237000
C	-2.824071000	-0.205208000	-0.398830000
C	-1.803196000	4.646193000	-0.651992000
C	4.221155000	-1.495623000	-0.455687000
C	5.172453000	3.115562000	0.910430000
C	0.017002000	-0.643169000	-0.574737000
C	0.973667000	4.067719000	0.332265000
C	-3.179981000	4.903866000	-0.946322000
H	0.646614000	5.097078000	0.436666000
H	2.986486000	4.586717000	0.749409000
H	4.857544000	4.124188000	1.150894000
H	7.231164000	3.573976000	1.338536000
H	-3.471908000	5.911668000	-1.225132000
H	-1.099205000	5.465517000	-0.761937000
H	-5.953982000	-0.444118000	-1.444305000
H	-5.585304000	1.610770000	-1.028212000
H	-5.143912000	4.094730000	-1.212008000
H	8.041340000	1.285390000	0.815473000
H	7.577135000	-1.007335000	0.106753000
H	7.153814000	-3.302327000	-0.615894000
H	3.166301000	-4.598650000	-1.463855000
H	1.265652000	-4.181693000	-1.606917000
H	5.556249000	-5.069807000	-1.317743000
H	-1.075994000	-3.730292000	-1.629139000
H	-2.972183000	-3.262421000	-1.952942000
H	-5.356511000	-2.837202000	-1.730568000
C	1.431887000	-0.924472000	-0.576283000
N	-4.137423000	0.175684000	-0.675840000
C	-0.424214000	0.633942000	-0.230300000
O	-2.240855000	1.606378000	1.123140000
O	-3.128627000	-0.958925000	1.447632000
C	-7.770568000	-1.151097000	0.237393000
S	-6.041327000	-1.158255000	0.848257000
H	-3.172304000	-0.172122000	2.020801000
C	-2.266456000	-4.070061000	2.819252000
S	-1.131820000	-2.635137000	2.644048000
H	-2.227368000	-1.656667000	1.951716000
H	-8.404507000	-1.284399000	1.118579000
H	-8.038259000	-0.200846000	-0.237631000
H	-7.971293000	-1.976420000	-0.452920000
H	-2.880343000	-3.976321000	3.721491000
H	-2.934872000	-4.152560000	1.956016000
H	-1.680461000	-4.990916000	2.899281000

(I5K')MT

C	6.533654000	-1.139854000	0.396524000
C	2.448578000	-0.010879000	-0.176844000
C	-1.697604000	1.018752000	-0.408085000
C	3.839889000	-0.393541000	0.012345000

C	4.256272000	1.995836000	0.692414000
C	-0.980477000	-1.586489000	-0.990296000
C	0.147728000	3.108263000	0.051041000
C	-5.102577000	-0.574511000	-0.516236000
C	-3.711261000	4.003829000	-1.629474000
C	5.505780000	-1.985222000	-0.195026000
C	6.550306000	2.532298000	1.321903000
C	2.444740000	3.713850000	0.560610000
C	-2.749553000	-0.018078000	-0.439586000
C	-1.382392000	4.654472000	-1.294525000
C	4.122381000	-1.634404000	-0.340189000
C	5.219570000	2.908424000	1.148355000
C	-0.006480000	-0.633824000	-0.589630000
C	1.139442000	4.069004000	0.301573000
C	-2.652723000	4.884198000	-1.833693000
H	0.857646000	5.117880000	0.304256000
H	3.161238000	4.499129000	0.769906000
H	4.934937000	3.924114000	1.394924000
H	7.268875000	3.260838000	1.684130000
H	-2.797066000	5.732412000	-2.495689000
H	-0.545761000	5.280670000	-1.588088000
H	-6.020278000	-0.098452000	-0.870324000
H	-5.466617000	1.892480000	-1.018573000
H	-4.652121000	4.147479000	-2.152972000
H	7.991570000	0.944965000	1.159636000
H	7.462278000	-1.303562000	0.391268000
H	6.978778000	-3.545426000	-0.406639000
H	2.995028000	-4.652766000	-1.487525000
H	1.116801000	-4.170342000	-1.672158000
H	5.352957000	-5.228038000	-1.237655000
H	-1.221414000	-3.625312000	-1.702281000
H	-3.164910000	-2.884638000	-2.224753000
H	-5.521459000	-2.284010000	-1.872074000
C	1.385464000	-0.954978000	-0.558961000
N	-4.067317000	0.444470000	-0.502025000
C	-0.417733000	0.646534000	-0.129675000
O	-2.187901000	1.869654000	0.869173000
O	-2.678975000	-0.475847000	2.707423000
C	-5.577724000	0.321423000	2.086453000
S	-5.445566000	-1.244202000	1.177203000
H	-1.725856000	-0.365891000	2.586767000
C	-4.234957000	-4.446922000	1.506494000
S	-2.632740000	-3.700570000	1.151756000
H	-2.882240000	-1.316501000	2.264359000
H	-5.820890000	0.061005000	3.118285000
H	-4.610553000	0.828128000	2.073552000
H	-6.372123000	0.949754000	1.674972000
H	-4.683332000	-4.050976000	2.417999000
H	-4.899955000	-4.233100000	0.662249000
H	-4.118700000	-5.532450000	1.574706000

(T3K')MT

C	6.471174000	-0.978299000	0.264118000
C	2.349597000	0.044082000	-0.204223000
C	-1.822416000	0.979365000	-0.317497000
C	3.749587000	-0.302060000	-0.049046000

C	-4.311531000	1.796687000	-1.175260000
C	5.154738000	-4.309576000	-0.906721000
C	6.137330000	0.161922000	0.700423000
C	0.980117000	-3.170625000	-1.472968000
C	2.036958000	1.312663000	0.112386000
C	-3.139210000	-1.892078000	-2.344092000
C	-2.137869000	2.453416000	-0.306287000
C	3.804230000	-3.946579000	-1.103894000
C	4.770992000	0.548395000	0.502643000
C	-0.361876000	-2.799785000	-1.650054000
C	0.664720000	1.684281000	-0.064911000
C	-4.450929000	-1.614182000	-2.295351000
C	-3.460915000	2.807007000	-0.869430000
C	6.050671000	-3.403368000	-0.416621000
C	7.070337000	1.114189000	1.201949000
C	1.933165000	-2.291867000	-0.996286000
C	2.974810000	2.284005000	0.591467000
C	-2.190104000	-1.123779000	-1.550454000
C	-1.090171000	3.491267000	-0.238232000
C	3.338069000	-2.679414000	-0.810750000
C	4.374997000	1.893580000	0.806686000
C	-0.804297000	-1.533898000	-1.337093000
C	0.260633000	3.053015000	0.130848000
C	-4.923709000	-0.581944000	-1.319690000
C	-3.768472000	4.202495000	-1.046106000
C	5.630774000	-2.079649000	-0.100425000
C	6.667905000	2.387057000	1.488565000
C	2.522513000	3.566730000	0.844433000
C	-2.614785000	0.076540000	-1.061282000
C	-1.443859000	4.767563000	-0.533641000
C	4.259948000	-1.706833000	-0.297299000
C	5.324325000	2.774012000	1.288968000
C	0.147402000	-0.589395000	-0.812469000
C	1.196752000	3.947372000	0.606926000
C	-2.800086000	5.134588000	-0.882978000
H	0.904433000	4.972445000	0.812045000
H	3.201175000	4.320889000	1.224779000
H	5.053103000	3.795189000	1.529774000
H	7.376424000	3.114613000	1.872034000
H	-3.021528000	6.183712000	-1.048547000
H	-0.692468000	5.551786000	-0.530857000
H	-5.864735000	-0.119859000	-1.626280000
H	-5.336077000	1.982690000	-1.485341000
H	-4.774480000	4.483825000	-1.346335000
H	8.101321000	0.804210000	1.348243000
H	7.571484000	-1.428273000	0.547562000
H	7.092365000	-3.669372000	-0.260319000
H	3.130158000	-4.699625000	-1.494892000
H	1.254549000	-4.188221000	-1.726065000
H	5.471234000	-5.318949000	-1.150859000
H	-1.059746000	-3.544129000	-2.019843000
H	-2.764379000	-2.649309000	-3.025529000
H	-5.182771000	-2.127419000	-2.908546000
C	1.522631000	-0.957606000	-0.665845000
N	-3.938564000	0.467066000	-1.182795000
C	-0.257323000	0.702346000	-0.462254000
O	-2.178542000	1.563668000	0.814345000

C	-4.485767000	1.661263000	-0.978680000
C	5.107871000	-4.234434000	-0.830127000
C	6.061118000	0.331445000	0.515567000
C	0.879134000	-3.233221000	-1.180449000
C	1.923966000	1.378043000	0.020048000
C	-3.263284000	-2.083214000	-2.002551000
C	-2.284197000	2.415058000	-0.261747000
C	3.744365000	-3.909731000	-0.981772000
C	4.681475000	0.683529000	0.348981000
C	-0.471763000	-2.898058000	-1.318383000
C	0.537541000	1.714635000	-0.122566000
C	-4.580509000	-1.794226000	-1.956491000
C	-3.645376000	2.706428000	-0.757773000
C	6.003584000	-3.287346000	-0.417530000
C	6.992417000	1.323536000	0.931018000
C	1.841538000	-2.295378000	-0.841731000
C	2.861031000	2.389756000	0.400287000
C	-2.318593000	-1.246354000	-1.291651000
C	-1.258618000	3.474048000	-0.308172000
C	3.260982000	-2.639549000	-0.716916000
C	4.271620000	2.034806000	0.590018000
C	-0.920340000	-1.609860000	-1.102329000
C	0.116022000	3.083989000	0.009058000
C	-5.025433000	-0.707362000	-1.100720000
C	-3.997661000	4.078616000	-0.988824000
C	5.568508000	-1.960158000	-0.146407000
C	6.576184000	2.604500000	1.165914000
C	2.396309000	3.683919000	0.586104000
C	-2.750777000	-0.018179000	-0.864327000
C	-1.662781000	4.727255000	-0.648908000
C	4.182864000	-1.624717000	-0.300522000
C	5.222047000	2.957464000	0.993337000
C	0.034240000	-0.614679000	-0.700208000
C	1.058638000	4.025136000	0.383093000
C	-3.041632000	5.041028000	-0.935821000
H	0.754367000	5.055582000	0.537451000
H	3.076588000	4.471520000	0.887134000
H	4.939786000	3.984718000	1.191445000
H	7.283952000	3.362489000	1.486611000
H	-3.300119000	6.073034000	-1.148513000
H	-0.933205000	5.526898000	-0.731831000
H	-6.031970000	-0.324432000	-1.253395000
H	-5.525109000	1.812909000	-1.252122000
H	-5.025181000	4.321024000	-1.246004000
H	8.033687000	1.040119000	1.056158000
H	7.520054000	-1.238705000	0.386510000
H	7.056603000	-3.524741000	-0.295058000
H	3.072513000	-4.690758000	-1.317546000
H	1.158905000	-4.267058000	-1.345309000
H	5.438128000	-5.245723000	-1.045979000
H	-1.177071000	-3.682168000	-1.574853000
H	-2.898185000	-2.912992000	-2.597929000
H	-5.325178000	-2.401075000	-2.459362000
C	1.421481000	-0.949812000	-0.591284000
N	-4.083599000	0.339975000	-0.970658000
C	-0.379983000	0.692345000	-0.422536000
O	-2.244670000	1.583801000	0.903794000

O	-2.005464000	-1.226726000	1.541939000
C	-5.299882000	0.019193000	1.412740000
S	-5.234830000	-1.432160000	0.321821000
H	-2.371055000	-1.135274000	2.433348000
C	-6.050338000	-3.125932000	3.340610000
S	-4.276437000	-3.141683000	3.012286000
H	-2.711686000	-1.680268000	1.055302000
H	-6.372765000	-4.092843000	3.733711000
H	-6.336341000	-2.327076000	4.027749000
H	-6.560950000	-2.969926000	2.382075000
H	-5.542544000	-0.354445000	2.410863000
H	-4.324633000	0.513456000	1.438923000
H	-6.076874000	0.720935000	1.097420000

O	-1.780606000	-0.935252000	1.897474000
C	-5.210309000	-0.077245000	1.764203000
S	-5.174962000	-1.647312000	0.849896000
H	-1.668238000	-0.031776000	2.224622000
C	-3.122680000	-3.812902000	1.627548000
S	-4.277293000	-2.902329000	2.698876000
H	-2.503901000	-1.312448000	2.430147000
H	-2.606531000	-4.547169000	2.251485000
H	-3.666502000	-4.340857000	0.839894000
H	-2.390367000	-3.132707000	1.184041000
H	-5.611005000	-0.258155000	2.762119000
H	-4.203243000	0.343408000	1.825474000
H	-5.872321000	0.624334000	1.248320000

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C	6.366729000	-1.202297000	0.465097000
C	2.340784000	-0.003722000	-0.164767000
C	-1.742861000	0.844446000	-0.304590000
C	3.684194000	-0.393591000	0.024181000
C	-4.313223000	1.999635000	-1.146063000
C	5.097995000	-4.127531000	-1.432039000
C	5.944042000	0.049577000	0.942262000
C	0.950570000	-2.977535000	-1.998284000
C	1.897109000	1.292377000	0.292333000
C	-3.243315000	-1.846057000	-2.342369000
C	-2.246009000	2.872533000	-0.176823000
C	3.774931000	-3.752770000	-1.646548000
C	4.596876000	0.473899000	0.709123000
C	-0.367524000	-2.628800000	-2.123173000
C	0.538152000	1.691539000	0.105246000
C	-4.566928000	-1.428518000	-2.264186000
C	-3.393844000	3.088083000	-0.942076000
C	5.955060000	-3.297250000	-0.735298000
C	6.829025000	0.898758000	1.641300000
C	1.890706000	-2.132487000	-1.357200000
C	2.825036000	2.193219000	0.871140000
C	-2.266828000	-1.049900000	-1.727624000
C	-1.085851000	3.633635000	-0.218724000
C	3.272728000	-2.528716000	-1.167858000
C	4.184534000	1.754005000	1.151363000
C	-0.856702000	-1.398677000	-1.624597000
C	0.178219000	3.055686000	0.292101000
C	-4.923715000	-0.213299000	-1.729225000
C	-3.492738000	4.357581000	-1.540843000
C	5.503942000	-2.053637000	-0.242022000
C	6.403050000	2.132198000	2.092239000
C	2.407306000	3.507081000	1.143241000
C	-2.673641000	0.154888000	-1.101729000
C	-1.205115000	4.874743000	-0.861391000
C	4.143424000	-1.657814000	-0.464678000
C	5.099228000	2.558800000	1.847800000
C	0.070899000	-0.523442000	-1.008489000
C	1.139765000	3.931404000	0.817851000
C	-2.415766000	5.237394000	-1.459178000
H	0.861165000	4.967451000	0.987713000
H	3.098283000	4.223442000	1.569929000

H	4.794620000	3.526247000	2.227317000
H	7.082740000	2.776952000	2.640658000
H	-2.492295000	6.205535000	-1.944277000
H	-0.345214000	5.533130000	-0.935674000
H	-5.940923000	0.153725000	-1.724057000
H	-5.317995000	2.213571000	-1.487367000
H	-4.377342000	4.623349000	-2.111770000
H	7.846567000	0.561908000	1.818606000
H	7.392814000	-1.516094000	0.640364000
H	6.987580000	-3.585427000	-0.559073000
H	3.132932000	-4.427880000	-2.198419000
H	1.264239000	-3.938370000	-2.386272000
H	5.453411000	-5.079233000	-1.814483000
H	-1.046962000	-3.325485000	-2.601290000
H	-2.995541000	-2.775674000	-2.835495000
H	-5.365419000	-2.055950000	-2.645241000
C	1.445886000	-0.887696000	-0.861329000
N	-3.970533000	0.689552000	-1.282196000
C	-0.375920000	0.687337000	-0.406649000
O	-2.240359000	1.737284000	0.602840000
O	-1.642442000	-1.841223000	1.368807000
C	-4.297051000	-0.285769000	2.022675000
S	-4.830943000	-1.849443000	1.252095000
H	-0.829417000	-2.169705000	0.960593000
C	-6.034136000	-3.158464000	3.683036000
S	-4.457961000	-3.201224000	2.772543000
H	-2.352011000	-2.130777000	0.774216000
H	-4.482605000	0.515162000	1.300552000
H	-4.874852000	-0.092519000	2.928603000
H	-3.229028000	-0.337472000	2.241765000
H	-6.213772000	-2.168628000	4.107302000
H	-6.864995000	-3.444911000	3.037011000
H	-5.941503000	-3.882108000	4.497369000