

Supporting Information

**Mechanism and Origins of Enantioselectivity of
Cobalt-Catalyzed Intermolecular
Hydroacylation/Cyclization of 1,6-Enynes with
Aldehydes**

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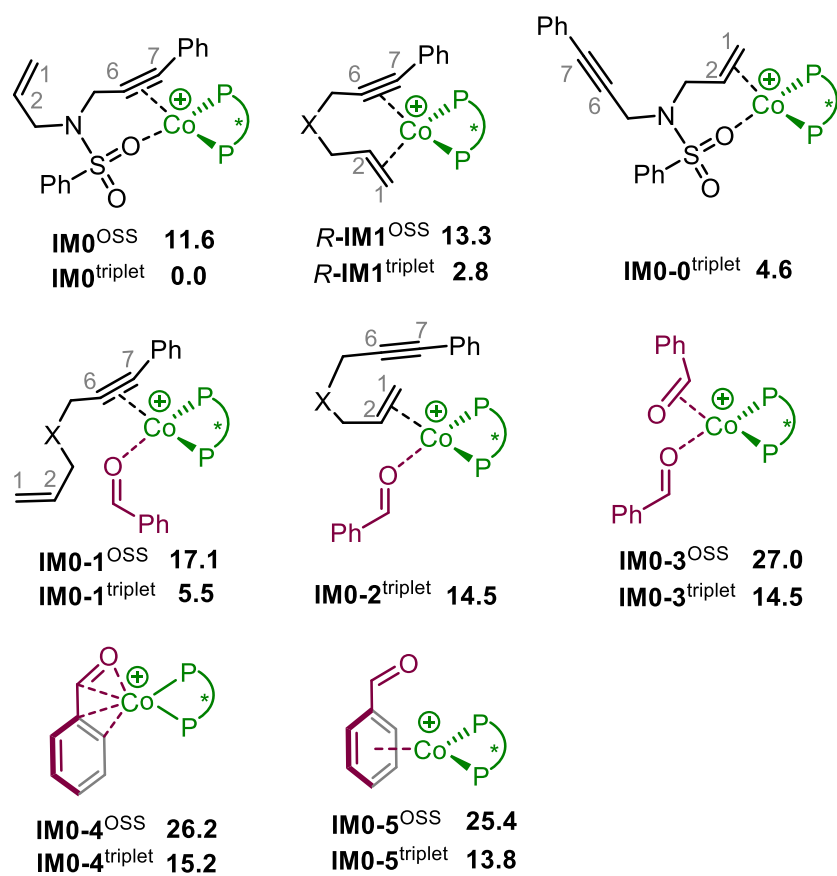
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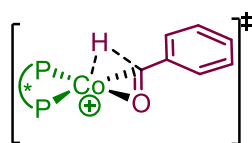
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1. Possible complexations between cobalt catalyst and reactants



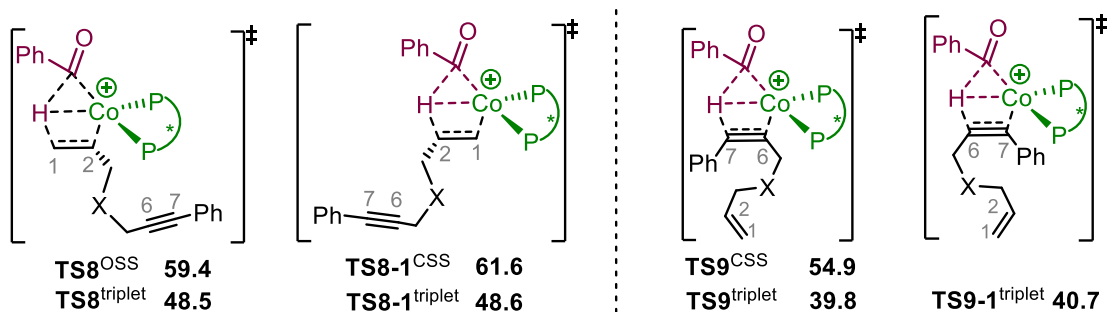
Scheme S1. Possible complexations between cobalt catalyst and reactants. Energies are given in kcal/mol.

2. C(acyl)-H bond cleavage of benzaldehyde



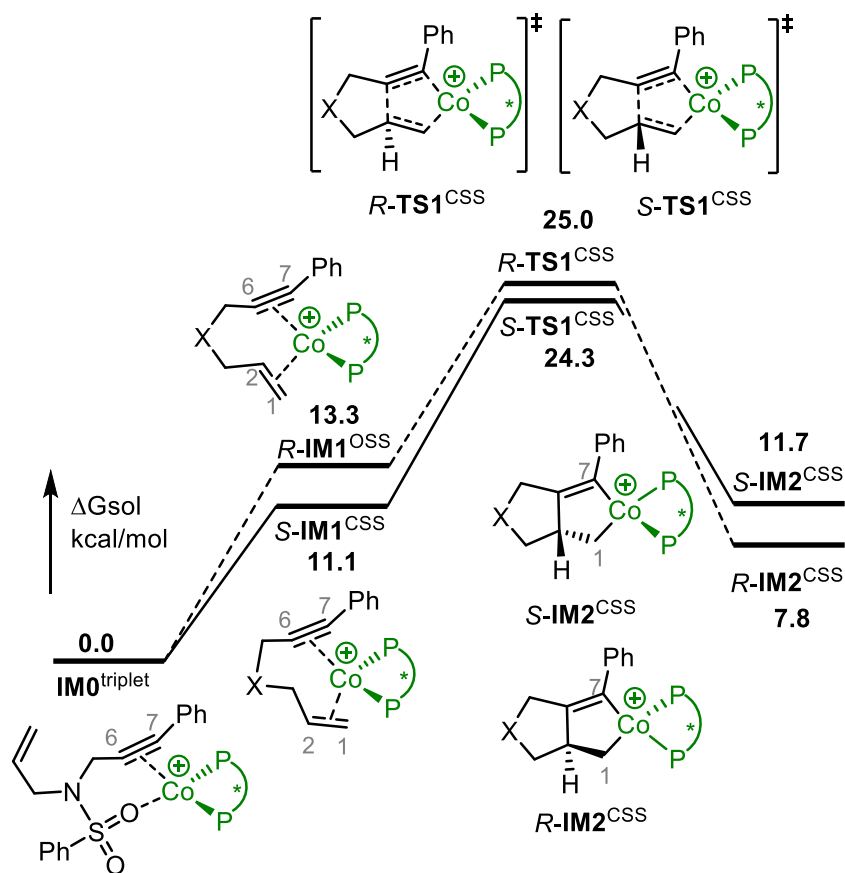
TS7^{CSS}
40.4

Scheme S2. C(acyl)-H bond cleavage via the C-H oxidative addition. Energies are given in kcal/mol.

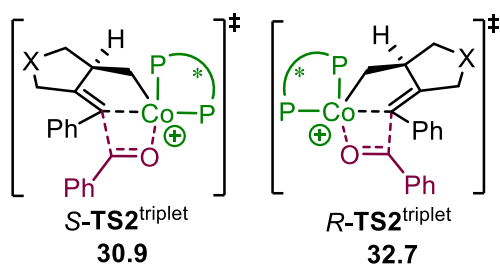


Scheme S3. C(acyl)-H bond cleavage via the ligand-to-ligand hydrogen transfer. Energies are given in kcal/mol.

3. Calculated most favorable pathway with different spin state

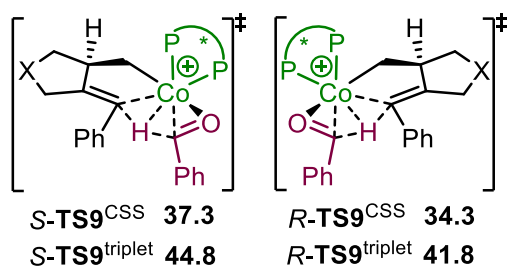


Scheme S4. Oxidative cyclization via the singlet spin state. Energies are given in kcal/mol.

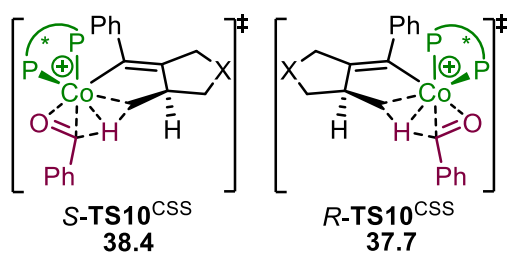


Scheme S5. Migratory insertion via the triplet spin state. Energies are given in kcal/mol.

4. σ -bond metathesis between the Co-C and C(acyl)-H bonds

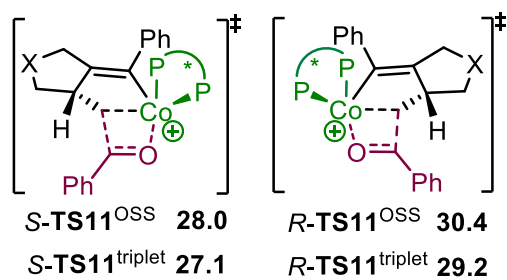


Scheme S6. σ -bond metathesis between the Co-C(sp^2) and C(acyl)-H bonds. Energies are given in kcal/mol.



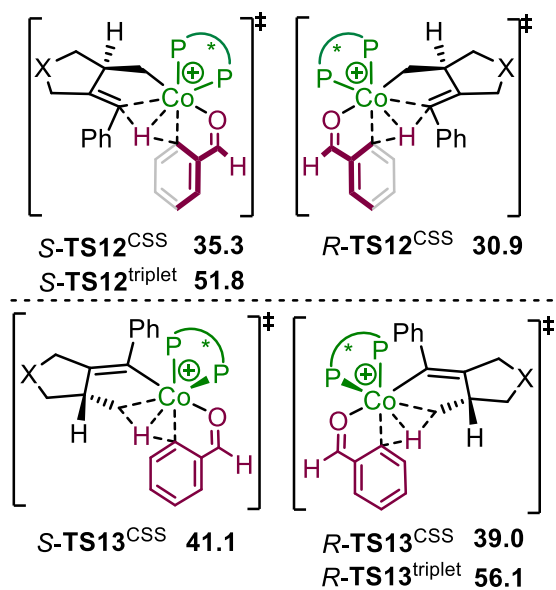
Scheme S7. σ -bond metathesis between the Co-C(sp^3) and C(acyl)-H bonds. Energies are given in kcal/mol.

5. C-O double bond insertion into the Co-C(sp³) bond

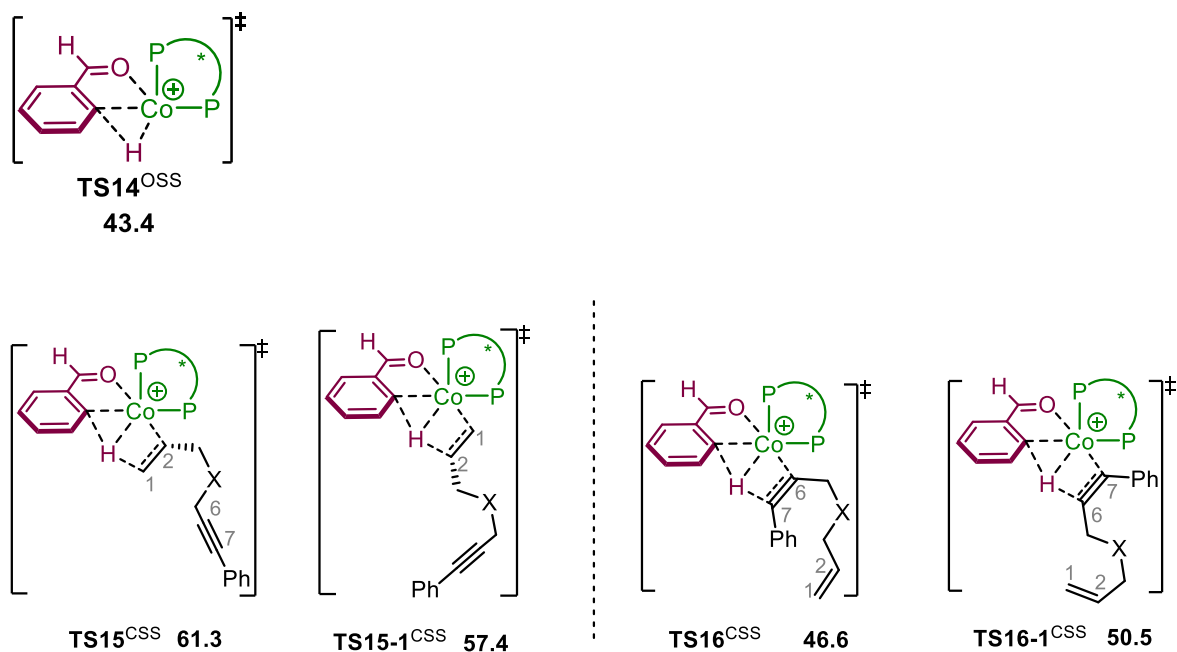


Scheme S8. C-O double bond insertion into the Co-C(sp³) bond. Energies are given in kcal/mol.

6. Possible pathways leading to hydroarylation product



Scheme S9. Hydroarylation initiated by the oxidative cyclization. Energies are given in kcal/mol.



Scheme S10. Hydroarylation initiated by the C(aryl)-H bond cleavage. Energies are given in kcal/mol.

7. Table of calculated energies and energy corrections

Stationary point	Single-point energy-B3LYP-SMD def2-TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)
1a	-1299.927801	0.26187
2a	-345.747569	0.079688
S-3a	-1645.757774	0.373011
R-3a	-1645.757774	0.373011
IM0 ^{triplet}	-4489.269595	0.747226
S-IM1 ^{triplet}	-4489.266931	0.748033
R-IM1 ^{triplet}	-4489.267950	0.749995
S-TS1 ^{triplet}	-4489.240069	0.749232
R-TS1 ^{triplet}	-4489.238183	0.749374
S-IM2 ^{triplet}	-4489.258693	0.749289
R-IM2 ^{triplet}	-4489.261522	0.750287
S-TS2 ^{CSS}	-4835.022884	0.863673
R-TS2 ^{CSS}	-4835.015103	0.863011
S-TS2 ^{triplet}	-4835.001505	0.848381
R-TS2 ^{triplet}	-4834.998599	0.848554
S-IM3 ^{triplet}	-4835.040434	0.845354
R-IM3 ^{triplet}	-4835.041381	0.845294
S-IM3 ^{CSS}	-4835.044834	0.865736
R-IM3 ^{CSS}	-4835.044407	0.866174
S-TS3 ^{CSS}	-4835.032651	0.860851
R-TS3 ^{CSS}	-4835.030894	0.859748
S-IM4 ^{CSS}	-4835.038632	0.858812
R-IM4 ^{CSS}	-4835.034208	0.860737
S-TS4 ^{OSS}	-4835.022539	0.858656
R-TS4 ^{OSS}	-4835.016845	0.857967
S-TS5 ^{triplet}	-4258.056822	0.671895
R-TS5 ^{triplet}	-4258.055075	0.670912
S-TS6 ^{CSS}	-4603.844826	0.783884
R-TS6 ^{CSS}	-4603.842112	0.784551

8. Cartesian coordinates

1a

C	-2.52181000	2.78223700	-6.70928000
C	-2.53005500	3.45588600	-7.96739700
C	-3.55648900	4.36726800	-8.27855600
C	-1.50924100	3.22623300	-8.90832800
C	-3.55882700	5.03032400	-9.50240600
H	-4.34399200	4.54269800	-7.55298500
C	-1.51851900	3.89479300	-10.12919000
H	-0.71820800	2.52421700	-8.66722800
C	-2.54121400	4.79718100	-10.43010700
H	-4.35541400	5.73104100	-9.73333900
H	-0.72605700	3.71131500	-10.84829700
H	-2.54509800	5.31644100	-11.38355800
C	-2.51267700	2.21478900	-5.63922800
C	-2.51379900	1.58354700	-4.32464200
H	-3.49475500	1.74140800	-3.85107100
H	-2.34594600	0.50808100	-4.41836800
N	-1.42714900	2.12162500	-3.48228200
C	-1.39506500	3.59034500	-3.31067300
H	-0.56706200	3.80711900	-2.63295100
H	-1.14444500	4.01013700	-4.28859300
C	-2.69266900	4.17864100	-2.81847300
H	-2.97412100	3.95857200	-1.79119200
C	-3.49464200	4.91728800	-3.58488000
H	-3.24258800	5.13376300	-4.62000300
H	-4.42609900	5.32955400	-3.20819800
S	-0.94282700	1.15925700	-2.19316500
O	-0.92032000	-0.21535400	-2.69736900
O	0.23951800	1.80333000	-1.61837400
C	-2.24805200	1.25769900	-0.96910600
C	-3.38613000	0.46259700	-1.11787000
C	-2.12902000	2.17067400	0.08016600
C	-4.43362600	0.60529200	-0.20844500
H	-3.43307700	-0.26806300	-1.91722500
C	-3.18139400	2.30121400	0.98534100
H	-1.21944700	2.75185200	0.18048100
C	-4.33435200	1.52650400	0.83630200
H	-5.32315800	-0.00814600	-0.31118300
H	-3.09940400	3.00323200	1.80914700
H	-5.15213400	1.63296700	1.54227700

2a

C	0.14850900	-0.42331400	0.49248200
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C	1.45980900	-0.45643300	0.01364900
C	2.06780500	0.70897100	-0.46771800
C	1.36493500	1.90817900	-0.47054900
C	0.04755300	1.94622300	0.00955400
C	-0.55703400	0.77857000	0.49017800
H	-0.31843200	-1.32990400	0.86459100
H	2.01119800	-1.39206000	0.01475600
H	3.08771400	0.67435100	-0.83829000
H	1.80745000	2.82876600	-0.83679500
H	-1.57869400	0.81829300	0.86030600
C	-0.70662300	3.21814100	0.00980400
H	-1.74178000	3.14067500	0.41153800
O	-0.26900100	4.28163300	-0.38651200
S-3a			
C	-1.67946600	0.45108000	0.91119200
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C	-2.30247300	1.76440700	0.37901200
H	-2.07093100	-0.44061700	0.41958800
H	-1.85302000	0.34462500	1.98866200
H	0.19855200	2.14774300	1.99646900
H	1.02471600	2.27001100	0.43875300
N	-0.21733500	0.56126600	0.71936600
S	0.33315700	-0.04566100	-0.77925600
O	-0.63044200	0.19467700	-1.86431200
O	1.71977600	0.41435700	-0.90674800
C	0.30833700	-1.79649300	-0.41720500
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C	0.93509300	4.95999000	1.04843100
C	0.49197000	5.51981100	-1.25457400
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C	1.64510200	6.29948900	-1.28731500

H	-0.12686300	5.43095700	-2.14223200
C	2.44921900	6.41289200	-0.15147400
H	2.70394100	5.82964800	1.90814300
H	1.91812800	6.81738800	-2.20170700
H	3.34741700	7.02217800	-0.17679300
C	-2.33562300	4.58730200	-0.74269700
O	-3.06166100	3.90330900	-1.45617400
C	-2.67114800	6.02869700	-0.51197800
C	-2.19181600	6.75242300	0.58874500
C	-3.55987900	6.64506200	-1.40513400
C	-2.59017000	8.07284400	0.78671600
H	-1.51134900	6.28502900	1.28980200
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H	-3.75938800	9.71809800	0.03197900
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H	-2.61333300	1.62166800	-0.65790400
H	0.30247600	-5.57777400	0.31199900

R-3a

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H	1.02471600	2.27001100	-0.43875300
N	-0.21733500	0.56126600	-0.71936600
S	0.33315700	-0.04566100	0.77925600
O	-0.63044200	0.19467700	1.86431200
O	1.71977600	0.41435700	0.90674800
C	0.30833700	-1.79649300	0.41720500
C	1.15205500	-2.29699400	-0.57608900
C	-0.53039200	-2.62666900	1.15767400
C	1.14393700	-3.66480100	-0.83540300
H	1.79402300	-1.62145600	-1.12968200
C	-0.52876000	-3.99641800	0.88822500
H	-1.16197400	-2.19491200	1.92558300

C	0.30432000	-4.51193700	-0.10505600
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C	0.12203900	4.83163600	0.08790300
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H	0.64542600	4.46548200	-1.97013000
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H	-0.12686300	5.43095700	2.14223200
C	2.44921900	6.41289200	0.15147400
H	2.70394100	5.82964800	-1.90814300
H	1.91812800	6.81738800	2.20170700
H	3.34741700	7.02217800	0.17679300
C	-2.33562300	4.58730200	0.74269700
O	-3.06166100	3.90330900	1.45617400
C	-2.67114800	6.02869700	0.51197800
C	-2.19181600	6.75242300	-0.58874500
C	-3.55987900	6.64506200	1.40513400
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H	-1.51134900	6.28502900	-1.28980200
C	-3.94345200	7.96871600	1.21612900
H	-3.93651000	6.06175900	2.23824000
C	-3.45883600	8.68533600	0.11835700
H	-2.21929100	8.62520200	-1.64466600
H	-4.62207000	8.44290300	1.91871400
H	-3.75938800	9.71809800	-0.03197900
C	-3.50564500	2.21225800	-1.21700400
H	-3.20350500	2.43664500	-2.24608400
H	-3.98012600	3.09761500	-0.79240500
H	-4.25862900	1.41756400	-1.25260600
H	-2.61333300	1.62166800	0.65790400
H	0.30247600	-5.57777400	-0.31199900

S**2 before annihilation 2.0182, after 2.0002

IM0^{triplet}

C	0.65797200	-1.98075700	2.22537800
C	-0.01619600	-3.11706400	1.41912200
C	2.19511100	-1.82269900	2.15552300
H	-1.03854800	-3.18848700	1.81084800
H	0.17322100	-1.02554100	1.99562900
H	0.42706100	-2.17353500	3.28070100

H	2.64123000	-2.81893900	2.24138400
P	2.82241100	-1.20961800	0.49753200
P	-0.19736000	-2.64914200	-0.38205600
C	4.58821400	-1.70930400	0.42429200
C	5.24255300	-1.51857200	-0.80652700
C	5.29249100	-2.31653100	1.47119900
C	6.57374800	-1.89427500	-0.97439200
H	4.69887000	-1.07719000	-1.63675400
C	6.62376000	-2.70550200	1.29894300
H	4.81618100	-2.49408300	2.42766200
C	7.27012100	-2.48848300	0.08234600
H	7.06717800	-1.72656900	-1.92690700
H	7.15484500	-3.17325200	2.12199900
H	8.30804100	-2.77986100	-0.04458900
C	2.86959600	0.61725600	0.66123400
C	4.05783100	1.35664400	0.58783200
C	1.65066300	1.30190600	0.79588700
C	4.02365600	2.75194000	0.63456800
H	5.01059900	0.84816700	0.49344400
C	1.62155100	2.69286800	0.86013200
H	0.71692100	0.75433900	0.83598800
C	2.80848800	3.42391700	0.77226600
H	4.95142300	3.31243100	0.57372000
H	0.66975800	3.20372600	0.96931300
H	2.78697300	4.50828400	0.81561000
C	-1.39065200	-1.25689900	-0.29545000
C	-1.02674400	-0.02424400	-0.85316500
C	-2.64693600	-1.38182200	0.31746300
C	-1.89121200	1.07001400	-0.78456500
H	-0.06342900	0.08497500	-1.33707400
C	-3.51060100	-0.29100400	0.38417300
H	-2.96021600	-2.33436400	0.73274400
C	-3.13185200	0.93866200	-0.16261800
H	-1.59014700	2.01675400	-1.22048400
H	-4.48072900	-0.39874000	0.85910500
H	-3.80707800	1.78688400	-0.10798600
C	-1.13615000	-4.01168300	-1.16258900
C	-2.06206500	-4.82003700	-0.48964800
C	-0.90576800	-4.23128800	-2.52819400
C	-2.74428500	-5.82663400	-1.17190900
H	-2.24918800	-4.67608800	0.56958500
C	-1.59779100	-5.22843300	-3.21344000
H	-0.17270100	-3.61714500	-3.04523500
C	-2.51612900	-6.03025100	-2.53419600

H	-3.45524800	-6.45176800	-0.64092500
H	-1.41891400	-5.38385000	-4.27324600
H	-3.05125800	-6.81285600	-3.06260900
Co	1.80632600	-2.12620700	-1.38742600
C	2.24878800	-1.36242000	-3.35141900
C	1.61647800	-0.07832200	-3.42966900
C	0.42084600	0.07277300	-4.15823800
C	2.15149900	1.01786300	-2.72658500
C	-0.22250400	1.30502200	-4.18094400
H	0.00671200	-0.77848400	-4.68742400
C	1.49622700	2.24534200	-2.75501500
H	3.06174200	0.90015400	-2.15177100
C	0.31183200	2.39098500	-3.48052900
H	-1.14489500	1.41885900	-4.74053400
H	1.90809300	3.07956600	-2.19850700
H	-0.19641000	3.34982400	-3.50140400
C	2.77475600	-2.47582300	-3.34258400
C	3.50249800	-3.73921700	-3.54904700
H	3.76841500	-3.86564400	-4.60291900
H	4.44351200	-3.70617900	-2.98867700
N	2.71772000	-4.91066300	-3.15445800
C	1.97881800	-5.66759200	-4.16373000
H	1.23088600	-6.27181300	-3.64305400
H	1.41006900	-4.94777000	-4.76868200
C	2.84438600	-6.52398400	-5.04987800
H	2.31891600	-6.98013200	-5.88760200
C	4.14579900	-6.74914900	-4.87857600
S	2.70915300	-5.33744800	-1.55301400
O	2.79456500	-4.05215900	-0.81268900
O	1.59693000	-6.25881900	-1.34274900
C	4.24347000	-6.16804000	-1.21340600
C	5.34103400	-5.42008500	-0.78193600
C	4.32244000	-7.54425700	-1.44135000
C	6.55487100	-6.07694600	-0.58311900
H	5.23910600	-4.36108600	-0.58501700
C	5.54226500	-8.18308600	-1.23382600
H	3.44613400	-8.09489200	-1.76302700
C	6.65572300	-7.45057300	-0.81081000
H	7.41461200	-5.51070600	-0.24180800
H	5.62348200	-9.25236300	-1.39791300
H	4.70082800	-7.38601100	-5.55872100
H	4.69826700	-6.31875100	-4.04917900
C	0.66775900	-4.47512800	1.61505700
H	0.12532100	-5.27600000	1.10953700

H	1.68259300	-4.47674000	1.21831500
H	0.71191600	-4.71396800	2.68339900
C	2.67631100	-0.94897500	3.32448600
H	2.16055800	0.01484400	3.32481900
H	2.46557500	-1.44604700	4.27689700
H	3.74764400	-0.74089900	3.27686800
H	7.60263800	-7.95627100	-0.65129300

S**2 before annihilation 2.0266, after 2.0004

S-IM1^{triplet}

C	0.81180300	-2.22962100	2.74217800
C	-0.08098800	-3.11615100	1.84056000
C	2.32860200	-2.14695300	2.46351500
H	-1.07068400	-3.13243900	2.31215200
H	0.41910000	-1.20988800	2.79202900
H	0.70474600	-2.63563600	3.75580900
H	2.69034200	-3.13519200	2.15962100
P	2.69738900	-1.03927500	0.99107500
P	-0.37774200	-2.37758000	0.14563800
C	4.52119700	-0.90739600	0.97551700
C	5.15353600	0.29691500	0.62939100
C	5.30857100	-2.05744100	1.15084800
C	6.53844700	0.34751300	0.46617800
H	4.56317400	1.19567600	0.48601100
C	6.69251800	-2.00273600	0.98839700
H	4.84702900	-3.00287400	1.41990700
C	7.31064400	-0.79976400	0.64641900
H	7.01381000	1.28571600	0.19791100
H	7.28781700	-2.89923400	1.12924500
H	8.38423300	-0.76011500	0.51262900
C	2.09434700	0.61471700	1.49060300
C	2.69981500	1.39684800	2.48896100
C	0.93596000	1.09788600	0.86313800
C	2.14667800	2.62361000	2.85256000
H	3.61035700	1.05603800	2.96898700
C	0.37541300	2.31908900	1.23599800
H	0.45511600	0.51602900	0.08667900
C	0.98097300	3.08338700	2.23305200
H	2.62421400	3.22152400	3.62238700
H	-0.53355900	2.65991700	0.75068400
H	0.55166300	4.03629500	2.52599100
C	-1.63905800	-1.07347600	0.46160000
C	-2.23588100	-0.47361100	-0.65819100
C	-2.02314600	-0.64570400	1.74038400

C	-3.18625700	0.53235100	-0.50034900
H	-1.97017700	-0.80067200	-1.65664900
C	-2.96761800	0.36974600	1.89479500
H	-1.60103000	-1.09227300	2.63069200
C	-3.54997000	0.96403300	0.77639000
H	-3.64001500	0.97679900	-1.37899400
H	-3.25014700	0.68913500	2.89292900
H	-4.28824200	1.75028800	0.89804500
C	-1.35957900	-3.62768700	-0.76131100
C	-0.95979000	-3.99865400	-2.05162500
C	-1.69605900	-4.93378600	-2.78069400
H	-0.07443800	-3.54538100	-2.48893600
C	-3.25106700	-5.13238500	-0.93777400
C	-2.83831100	-5.50518500	-2.22063300
H	-1.37850200	-5.21492400	-3.77990700
H	-4.14603100	-5.56975300	-0.50679800
H	-3.41116900	-6.23564300	-2.78280400
Co	1.59740800	-1.71612400	-0.97196000
C	1.61864300	-0.25128300	-2.62313900
C	0.31480400	0.19413400	-3.01803100
C	-0.14994700	1.46157900	-2.62305000
C	-0.48040900	-0.61274200	-3.85401600
C	-1.38344800	1.91770400	-3.07787100
H	0.46496500	2.07718700	-1.97608200
C	-1.71612200	-0.14924400	-4.29473200
H	-0.11406400	-1.58504200	-4.16466900
C	-2.16736200	1.11751900	-3.91235400
H	-1.73452500	2.90039500	-2.78060900
H	-2.32295700	-0.77059100	-4.94500600
H	-3.12623600	1.48040500	-4.26827200
C	2.81105000	-0.50077500	-2.44809400
C	4.26592100	-0.59600800	-2.64440900
H	4.55284500	0.14343100	-3.39673600
H	4.79660600	-0.37697400	-1.71061100
N	4.60997200	-1.91968800	-3.16555900
C	4.42345000	-3.04321800	-2.25117100
H	4.93961700	-3.89955500	-2.69553800
H	4.86657900	-2.84428600	-1.26718200
S	5.92158000	-1.98791000	-4.23739000
O	5.96024900	-3.37189400	-4.70651000
O	5.74768300	-0.84505000	-5.13220700
C	7.39352700	-1.69811200	-3.26224700
C	8.03977800	-2.78262500	-2.66479300
C	7.88469300	-0.39635800	-3.14349000

C	9.20601000	-2.55316100	-1.93640200
H	7.65892200	-3.78683800	-2.81069200
C	9.05341600	-0.18157800	-2.41415300
H	7.38239600	0.41789800	-3.65283300
H	9.73083100	-3.38823900	-1.48372300
H	9.45935600	0.82147600	-2.33164600
C	-2.52021200	-4.19407100	-0.21316700
H	-2.85893300	-3.89154900	0.77325100
C	2.97441400	-3.43045900	-2.11714100
C	2.44608600	-3.97210600	-0.99526400
H	1.49481600	-4.48776700	-1.01030600
H	3.04448400	-4.06202400	-0.09378000
C	9.71432700	-1.25730200	-1.81677000
H	10.63501500	-1.08750600	-1.26707300
C	3.05990100	-1.72919000	3.74614000
H	2.65254700	-0.79273900	4.13692400
H	2.92675700	-2.49599700	4.51607800
H	4.13134500	-1.59537200	3.58510400
C	0.40685000	-4.56866300	1.78419900
H	1.39013200	-4.66164300	1.32322100
H	0.48117600	-4.96563100	2.80182300
H	-0.28606700	-5.20163600	1.22657700
H	2.41286200	-3.44215800	-3.05023400

S**2 before annihilation 2.0242, after 2.0003

R-IM1^{triplet}

C	-0.66295400	-1.65690500	2.59384000
C	-0.80612500	-3.01909600	1.87163000
C	0.73371700	-1.24245600	3.10972000
H	-1.87999300	-3.22516400	1.81513800
H	-1.08784800	-0.85404600	1.98063500
H	-1.31068000	-1.71702500	3.47703000
H	1.24705100	-2.13565400	3.47911600
P	1.87369100	-0.58468300	1.76382800
P	-0.24240600	-2.82617400	0.09678700
C	3.55738800	-0.69377800	2.48902400
C	4.63910700	-0.39347600	1.64137800
C	3.83034300	-1.11723300	3.79785900
C	5.95044300	-0.47998200	2.10138600
H	4.45817600	-0.10303800	0.61111500
C	5.14742000	-1.22036800	4.25158200
H	3.02616200	-1.37070700	4.47731000
C	6.20922200	-0.89487700	3.40938500
H	6.76729200	-0.23454800	1.43296900

H	5.33902800	-1.55139900	5.26733700
H	7.23134900	-0.96985500	3.76615400
C	1.50015000	1.20740800	1.76702800
C	2.28634900	2.14165100	2.45350900
C	0.35171900	1.64117900	1.08924300
C	1.92559300	3.48918100	2.46021000
H	3.17633400	1.81848300	2.98243600
C	-0.01037200	2.98560500	1.10513800
H	-0.25292400	0.92919900	0.54038400
C	0.77748600	3.91295500	1.78979700
H	2.53959800	4.20722800	2.99506600
H	-0.89889200	3.30979900	0.57305400
H	0.49929800	4.96207800	1.79779800
C	-1.61252600	-1.80352400	-0.56985000
C	-1.32817600	-0.57846500	-1.18562700
C	-2.95183600	-2.21005600	-0.45194000
C	-2.35812600	0.23838700	-1.65542700
H	-0.29977700	-0.26386800	-1.29825400
C	-3.97959700	-1.39851000	-0.92739200
H	-3.19349100	-3.16999000	-0.00562200
C	-3.68489700	-0.16952800	-1.52492200
H	-2.11933800	1.19034500	-2.11956100
H	-5.01072700	-1.72390600	-0.83351800
H	-4.48838300	0.46220300	-1.88989800
C	-0.41916100	-4.41728100	-0.80522400
C	-1.04192600	-4.43162900	-2.06533600
C	-1.02234300	-5.58141200	-2.85583100
H	-1.54682100	-3.54448200	-2.43021200
C	0.23510700	-6.73656900	-1.15383700
C	-0.38526900	-6.73726400	-2.40410100
H	-1.51072000	-5.57217800	-3.82515700
H	0.72959600	-7.63177400	-0.78999800
H	-0.37191300	-7.63062100	-3.01962800
Co	1.85766600	-1.84352600	-0.22109600
C	2.13982500	-0.18385100	-1.90751300
C	2.04886700	1.23642500	-1.80033700
C	1.03396400	1.89309800	-2.52620900
C	2.94217600	1.99240400	-1.02242400
C	0.92345900	3.27863000	-2.47020300
H	0.35350300	1.30832000	-3.13602100
C	2.82425700	3.37608200	-0.97563700
H	3.71625100	1.49049900	-0.45877600
C	1.81605800	4.02168900	-1.69491400
H	0.14496000	3.77946900	-3.03656100

H	3.50929000	3.95173100	-0.36324800
H	1.72575800	5.10205400	-1.65006200
C	2.08594300	-1.37649800	-2.23019300
C	2.19403800	-2.59637400	-3.08575000
H	1.33717000	-3.25447100	-2.90851900
H	2.17253700	-2.29241500	-4.13511800
N	3.40228700	-3.37126500	-2.86227300
C	3.52806800	-4.10620700	-1.60715800
H	2.65157100	-4.75699300	-1.51336300
H	4.40045800	-4.75830100	-1.71137200
S	4.79699600	-2.95764600	-3.72445400
O	5.67661100	-4.11933400	-3.61426900
O	4.31404400	-2.43103000	-5.00005900
C	5.58927000	-1.61032000	-2.84989200
C	6.59813800	-1.90281000	-1.93013200
C	5.18959800	-0.29792100	-3.10689200
C	7.20568000	-0.85341100	-1.24148400
H	6.91648800	-2.92932400	-1.78856800
C	5.80013200	0.74172400	-2.40652500
H	4.43490700	-0.09882100	-3.85784600
H	8.00849200	-1.06533600	-0.54285000
H	5.50270700	1.76635600	-2.60143100
C	0.22743400	-5.58581800	-0.36603300
H	0.72592100	-5.61073300	0.59434800
C	3.68939500	-3.27321800	-0.34783500
H	4.44945300	-2.49457200	-0.36255800
C	3.12138400	-3.63272900	0.83213600
H	2.47035300	-4.49758300	0.88168300
H	3.41742100	-3.17509100	1.76843200
C	6.80202500	0.46437700	-1.47267800
H	7.28570300	1.27900800	-0.94244400
C	0.56094700	-0.24261100	4.26493800
H	-0.06779200	0.59557300	3.95403300
H	0.07486100	-0.73629100	5.11256300
H	1.50748500	0.17597300	4.61116500
C	-0.15467200	-4.16447900	2.65215900
H	-0.49097500	-5.13593200	2.28707600
H	0.93695200	-4.13783400	2.60600200
H	-0.44058800	-4.09648400	3.70726300

S**2 before annihilation 2.0689, after 2.0012

S-TS1^{triplet}

C	0.36352700	-2.30585800	2.86278800
C	-0.31396700	-3.36278900	1.95534600

C	1.89247100	-2.09798500	2.75837600
H	-1.33750500	-3.47896100	2.33261800
H	-0.13943900	-1.33828800	2.76582000
H	0.16894500	-2.63173700	3.89199300
H	2.37042700	-3.06974900	2.59808300
P	2.33498200	-1.09578900	1.24755700
P	-0.50646600	-2.82568200	0.17777800
C	4.14774800	-1.12073000	1.07950700
C	4.72301900	-0.27101100	0.11677200
C	4.95839200	-2.05779400	1.73427100
C	6.08435600	-0.34506200	-0.16631800
H	4.09842400	0.44237000	-0.41271500
C	6.32284700	-2.13128100	1.44537100
H	4.53920900	-2.73150400	2.47316200
C	6.88661000	-1.27552200	0.50093600
H	6.52264400	0.30785000	-0.91339300
H	6.94235600	-2.85638800	1.96347700
H	7.94416800	-1.33330600	0.27331900
C	1.88118900	0.61755000	1.67981000
C	2.79378800	1.50665900	2.26824700
C	0.56520900	1.04113300	1.43670500
C	2.39082300	2.79768500	2.60712700
H	3.81546700	1.19298700	2.45275800
C	0.16388600	2.32873700	1.78918100
H	-0.13822500	0.38133100	0.94601100
C	1.07625600	3.20903000	2.37223900
H	3.10264800	3.48192200	3.05782300
H	-0.85628600	2.64070800	1.59116100
H	0.76781700	4.21490600	2.63910200
C	-1.69220600	-1.43455200	0.20348600
C	-1.76453900	-0.65133100	-0.95967300
C	-2.45674700	-1.07090200	1.32159100
C	-2.56018200	0.49060400	-0.99851300
H	-1.17606500	-0.92268300	-1.82703100
C	-3.25561700	0.07245600	1.28009200
H	-2.43117700	-1.66139800	2.23026000
C	-3.30037800	0.85923300	0.12702600
H	-2.58158600	1.09548300	-1.89876800
H	-3.84066500	0.34964300	2.15124100
H	-3.91452400	1.75395300	0.10553700
C	-1.34991000	-4.19548300	-0.67266600
C	-0.80144900	-4.68509800	-1.86498900
C	-1.42552700	-5.72921600	-2.54820400
H	0.10659100	-4.23857100	-2.25896300

C	-3.15546300	-5.79686900	-0.85535200
C	-2.59888900	-6.28738500	-2.04041600
H	-0.99763000	-6.10422000	-3.47235800
H	-4.07358000	-6.22644700	-0.46766700
H	-3.08478600	-7.10094800	-2.56928700
Co	1.46364200	-2.04006600	-0.68600700
C	1.58950900	-0.83271400	-2.17060700
C	0.97249100	0.41456700	-2.57839800
C	1.06598800	1.56597600	-1.77845700
C	0.22413100	0.46754100	-3.76950800
C	0.42877000	2.74233900	-2.16226500
H	1.63009300	1.53147300	-0.85578900
C	-0.41759100	1.64624500	-4.14279600
H	0.14523400	-0.42087900	-4.38840900
C	-0.32013700	2.78670000	-3.34041700
H	0.51233000	3.62321900	-1.53348500
H	-0.99091600	1.67584000	-5.06400800
H	-0.82133000	3.70317200	-3.63469100
C	2.59231900	-1.58232800	-2.52673100
C	3.76870700	-1.31770900	-3.43355800
H	3.44108200	-1.05855500	-4.44252400
H	4.32402700	-0.46248300	-3.01525700
N	4.56194100	-2.53326100	-3.45406100
C	4.46577400	-3.23483200	-2.18331800
H	4.87518000	-4.23933700	-2.29500900
H	4.97933800	-2.71736200	-1.36106500
S	5.93136100	-2.61817500	-4.41412100
O	6.40531300	-3.99539900	-4.29893000
O	5.54499600	-2.00073500	-5.68066600
C	7.14306500	-1.55223400	-3.64280200
C	8.11455400	-2.11321300	-2.81345200
C	7.09984300	-0.17835400	-3.89684900
C	9.06245100	-1.27565100	-2.22538200
H	8.13821000	-3.18683400	-2.66639400
C	8.04220000	0.64987200	-3.28796200
H	6.36839600	0.22036800	-4.59064800
H	9.84219000	-1.70036800	-1.60087400
H	8.02881200	1.71715400	-3.48402100
C	-2.53741900	-4.75147700	-0.17371900
H	-2.98405400	-4.36295400	0.73690800
C	2.96485500	-3.30219500	-1.91841000
C	2.53755300	-3.73878700	-0.59017500
H	1.87786500	-4.59912300	-0.56221900
H	3.29986300	-3.72290100	0.18409400

C	9.02121100	0.10189300	-2.45378700
H	9.76470500	0.74779000	-1.99756900
C	2.42896000	-1.47094900	4.05292800
H	1.90677600	-0.53681500	4.27651600
H	2.27457900	-2.15563300	4.89286600
H	3.49645800	-1.24765200	3.99045000
C	0.35645700	-4.73966900	2.04645900
H	1.36252700	-4.73410400	1.62469100
H	0.43291300	-5.04175700	3.09579200
H	-0.22379000	-5.49929700	1.51885000
H	2.45434200	-3.83034700	-2.72482600

S**2 before annihilation 2.0646, after 2.0011

R-TS1^{triplet}

C	0.38887500	-1.97414100	2.97884600
C	-0.46935800	-2.97072700	2.15612000
C	1.92971800	-2.00220000	2.83395700
H	-1.48195300	-2.91778900	2.57446300
H	0.03554700	-0.94877300	2.82779200
H	0.18016300	-2.20105800	4.03144900
H	2.26267700	-3.04097200	2.74019500
P	2.49074300	-1.17200000	1.25924100
P	-0.63471100	-2.47565000	0.36691300
C	4.27707800	-1.45563300	1.06874100
C	4.92703100	-0.75967900	0.03368700
C	4.97995400	-2.43597100	1.78219200
C	6.25952300	-1.02954700	-0.26602600
H	4.38470000	-0.01236200	-0.53827200
C	6.31476200	-2.70683700	1.47331200
H	4.50014000	-2.99167400	2.58023400
C	6.95576500	-2.00607200	0.45248300
H	6.75356500	-0.48324400	-1.06306900
H	6.85149900	-3.46525200	2.03408800
H	7.99256800	-2.21955700	0.21423600
C	2.25940900	0.61029100	1.55208700
C	3.25853300	1.40957500	2.12852800
C	1.02223200	1.18146400	1.21795500
C	3.01425300	2.76071300	2.36935700
H	4.22242800	0.97938500	2.37878100
C	0.77862400	2.53027600	1.47269900
H	0.25983600	0.58358100	0.73511900
C	1.77473400	3.32072400	2.04720500
H	3.79099900	3.37706200	2.81056100
H	-0.18279900	2.95695100	1.20666800

H	1.59094100	4.37311200	2.23911600
C	-1.68414700	-0.97695600	0.36062300
C	-1.77327300	-0.28938900	-0.86059600
C	-2.30491500	-0.43663900	1.49530800
C	-2.44693200	0.92568200	-0.94400800
H	-1.29429500	-0.69621100	-1.74262200
C	-2.98193800	0.78093300	1.40956200
H	-2.26280900	-0.94676700	2.45068500
C	-3.04640500	1.46751100	0.19577800
H	-2.48385600	1.45138300	-1.89213400
H	-3.45674000	1.19335400	2.29416600
H	-3.56558300	2.41892500	0.13800500
C	-1.59995400	-3.76938800	-0.47725200
C	-2.76053000	-4.33397900	0.07095500
C	-3.46211800	-5.30667800	-0.63869400
H	-3.11933800	-4.01273600	1.04435100
C	-1.87279600	-5.14336700	-2.45941600
C	-3.01842000	-5.71165100	-1.90119600
H	-4.35787800	-5.74558700	-0.21103800
H	-1.52933200	-5.45038600	-3.44146300
H	-3.57076100	-6.46820600	-2.44964100
Co	1.42497500	-1.98817200	-0.57448100
C	1.55377100	-0.95229200	-2.17157700
C	1.02133200	0.30760200	-2.66506000
C	1.35126300	1.51546400	-2.03096500
C	0.12949900	0.32915800	-3.75342800
C	0.80364000	2.71678100	-2.47325000
H	2.03239300	1.50208200	-1.18936600
C	-0.42806200	1.53141200	-4.18220700
H	-0.13639600	-0.60058800	-4.24720100
C	-0.09363600	2.72864800	-3.54301000
H	1.07107100	3.64288700	-1.97435500
H	-1.11796900	1.53583000	-5.02033400
H	-0.52637100	3.66452500	-3.88168000
C	2.04366100	-2.05080700	-2.68234800
C	2.22078800	-2.53407600	-4.09764600
H	1.21578700	-2.68408900	-4.52757100
H	2.74472700	-1.79535000	-4.70829700
N	2.97713500	-3.77919600	-4.03846000
C	2.66799700	-4.48760600	-2.80316000
H	1.65275200	-4.91627400	-2.79568500
H	3.39109000	-5.29091200	-2.65704600
S	3.09855100	-4.68179100	-5.46134000
O	3.42277200	-3.71369700	-6.50546100

O	3.94372400	-5.82459200	-5.12747400
C	1.43879000	-5.28217100	-5.75109900
C	0.55262200	-4.50514100	-6.50221100
C	1.04753000	-6.49790500	-5.18470000
C	-0.75601800	-4.95503500	-6.67799400
H	0.90189900	-3.58988300	-6.96671900
C	-0.26198900	-6.93930900	-5.37419300
H	1.77033500	-7.09529800	-4.64073400
C	-1.16179800	-6.16753900	-6.11494700
H	-1.45213200	-4.36985400	-7.27003100
H	-0.57479400	-7.89090300	-4.95660600
C	-1.16441000	-4.17687800	-1.74582200
H	-0.27417600	-3.72499000	-2.17192000
C	2.80309300	-3.44704500	-1.70258800
H	3.81710200	-3.05222700	-1.63833400
C	2.24610700	-3.81103600	-0.39850100
H	1.49777800	-4.59984100	-0.40845700
H	2.95291800	-3.86385900	0.42267800
C	2.57910100	-1.36870100	4.07401400
H	2.20163600	-0.35514400	4.23282900
H	2.34356200	-1.96231900	4.96279400
H	3.66625100	-1.30881700	3.98650200
C	0.00799700	-4.42164100	2.30221500
H	0.08159100	-4.67787500	3.36404000
H	-0.68990900	-5.11931600	1.83543700
H	0.98891500	-4.58142200	1.85119300
H	-2.17716000	-6.51974200	-6.26759500

S**2 before annihilation 2.1327, after 2.0026

S-IM2^{triplet}

C	0.23271700	-2.26052100	2.93674800
C	-0.37523300	-3.28192300	1.94328300
C	1.75653900	-2.00834300	2.91004100
H	-1.38033900	-3.51959500	2.31202800
H	-0.29161900	-1.30147600	2.86945400
H	0.00899100	-2.64574200	3.93938000
H	2.27141200	-2.96830500	2.79920600
P	2.26521300	-1.02316500	1.40786900
P	-0.62786300	-2.62241800	0.21054000
C	4.08212300	-1.12014400	1.27416200
C	4.67761200	-0.41469600	0.21289700
C	4.86663700	-2.00230700	2.02885400
C	6.02640300	-0.58329500	-0.08335600
H	4.07985500	0.25371400	-0.39794900

C	6.22117800	-2.17011000	1.72962100
H	4.43466800	-2.56837600	2.84617900
C	6.80045000	-1.46644000	0.67466800
H	6.47338100	-0.03982800	-0.90835500
H	6.81927900	-2.85487100	2.32233900
H	7.84840200	-1.60592700	0.43343400
C	1.85969000	0.71008300	1.79865600
C	2.79514500	1.57758900	2.38172200
C	0.56466500	1.17175900	1.51965200
C	2.43214400	2.88952500	2.68435500
H	3.80180800	1.23070900	2.58886300
C	0.20361700	2.48025700	1.83635600
H	-0.15203900	0.52126100	1.03532500
C	1.13733200	3.34083800	2.41678600
H	3.16001500	3.55917000	3.13121400
H	-0.80256200	2.82318500	1.61742100
H	0.86017000	4.36258500	2.65616500
C	-1.81368800	-1.24279400	0.36543800
C	-1.88302300	-0.32797900	-0.69804800
C	-2.62288900	-1.04355700	1.49408000
C	-2.74016700	0.76856400	-0.62836500
H	-1.26110600	-0.46422900	-1.57609600
C	-3.47127000	0.06161100	1.56407800
H	-2.59552200	-1.73932000	2.32532200
C	-3.52869300	0.97060500	0.50621500
H	-2.78016600	1.46728400	-1.45673500
H	-4.08866700	0.21018100	2.44420600
H	-4.18966900	1.82953000	0.56445400
C	-1.51946600	-3.95046600	-0.66014500
C	-0.85252100	-4.64896100	-1.67660700
C	-1.49412400	-5.69172500	-2.34536800
H	0.16208000	-4.36878100	-1.94525000
C	-3.47441600	-5.33680100	-0.99759900
C	-2.80253700	-6.03629400	-2.00419800
H	-0.97635600	-6.23006700	-3.13284300
H	-4.49522300	-5.60093000	-0.74057400
H	-3.30299300	-6.84548100	-2.52633400
Co	1.52510900	-2.05764300	-0.63091500
C	2.03780300	-1.37438900	-2.33881000
C	1.29877600	-0.15349900	-2.60060900
C	1.39720300	0.96241500	-1.74195000
C	0.36120200	-0.11101100	-3.65927900
C	0.59565800	2.08375900	-1.93791000
H	2.10328300	0.94518900	-0.92215500

C	-0.41977200	1.02033100	-3.86370900
H	0.26632500	-0.97433200	-4.30987400
C	-0.30909900	2.11814900	-3.00012500
H	0.68060400	2.92701200	-1.26077600
H	-1.12103000	1.04957200	-4.69155200
H	-0.92531000	2.99717000	-3.16104200
C	2.95618400	-2.08061700	-3.01219500
C	3.85479400	-1.70674500	-4.16405500
H	3.37581700	-1.74468700	-5.14611400
H	4.25699200	-0.69407500	-4.02246500
N	4.89391000	-2.75801800	-4.06979600
C	4.87490700	-3.42553700	-2.75406100
H	5.30684200	-4.42232700	-2.84136400
H	5.42407100	-2.85373300	-1.98986900
S	6.34443700	-2.53928600	-4.87041600
O	7.04223700	-3.82121300	-4.79824000
O	5.99786000	-1.87915100	-6.12825700
C	7.27500200	-1.37049500	-3.87935900
C	8.19160000	-1.85059800	-2.94179700
C	7.07103900	-0.00039900	-4.06478600
C	8.91943400	-0.93717500	-2.17896700
H	8.35172900	-2.91872300	-2.85042200
C	7.79215900	0.90273800	-3.28340400
H	6.39536800	0.34287400	-4.84001300
H	9.65950500	-1.29610400	-1.47045100
H	7.65356500	1.96963700	-3.42614700
C	-2.83758500	-4.29512000	-0.32701200
H	-3.36792900	-3.74105300	0.44176800
C	3.36451500	-3.40570300	-2.45211600
C	2.88627700	-3.48561600	-1.00038100
H	2.41744700	-4.43219200	-0.71790100
H	3.67258900	-3.21941900	-0.28911200
C	8.71588500	0.43531200	-2.34398600
H	9.29008600	1.14199900	-1.75311800
C	2.20578300	-1.33974900	4.21745600
H	1.65232800	-0.41280600	4.38932800
H	2.01911400	-2.00949700	5.06278400
H	3.27002900	-1.09318700	4.20978900
C	0.41272100	-4.59783100	1.87534600
H	1.39491100	-4.46416800	1.41156600
H	0.56932700	-4.99552600	2.88306800
H	-0.12582100	-5.35002400	1.29524800
H	2.89750900	-4.19939200	-3.05238300

S**2 before annihilation	2.1128,	after	2.0021
<i>R-IM2</i> ^{triplet}			
C	0.33883800	-1.94387500	3.08591900
C	-0.45895700	-2.84501900	2.10602400
C	1.88130400	-1.99168700	3.05395400
H	-1.46951700	-2.94593400	2.51881500
H	0.01767900	-0.90074400	2.99766900
H	0.05037700	-2.25581100	4.09718900
H	2.20103400	-3.03839800	3.02132900
P	2.55769300	-1.24014500	1.48871400
P	-0.67843100	-2.08574700	0.41321500
C	4.34184800	-1.58316500	1.42530500
C	5.09557500	-0.89974300	0.45498800
C	4.95040400	-2.59420300	2.18118500
C	6.43839100	-1.21264200	0.26064500
H	4.63088000	-0.12104100	-0.14283700
C	6.29689400	-2.90484300	1.98056600
H	4.38819400	-3.14194900	2.92950700
C	7.04155200	-2.21669100	1.02307600
H	7.01422100	-0.67469100	-0.48558900
H	6.76174100	-3.68409300	2.57586600
H	8.08746600	-2.46116000	0.86934800
C	2.37427800	0.56497800	1.64540200
C	3.30805000	1.35421100	2.33566200
C	1.25362500	1.17349300	1.05983200
C	3.10673300	2.72852000	2.44852600
H	4.19031600	0.89706800	2.77092000
C	1.05280900	2.54760600	1.18172900
H	0.53468700	0.58349300	0.50618300
C	1.97879800	3.32547000	1.87730200
H	3.83074700	3.33567000	2.98237300
H	0.17595800	3.00015500	0.72983700
H	1.82885100	4.39635200	1.97055500
C	-1.74045700	-0.61884100	0.64875200
C	-1.91988900	0.21895400	-0.46358800
C	-2.35885700	-0.28865400	1.86287500
C	-2.68897700	1.37495800	-0.35676500
H	-1.46002700	-0.03232100	-1.41071500
C	-3.12673100	0.87229400	1.96514900
H	-2.25334700	-0.92464200	2.73413500
C	-3.28807300	1.70854400	0.86010400
H	-2.81566100	2.01154800	-1.22614100
H	-3.59949100	1.12062800	2.90999000
H	-3.88314300	2.61212600	0.94556500

C	-1.71795000	-3.26474200	-0.51251600
C	-3.02709200	-3.55847600	-0.10262600
C	-3.79121000	-4.47618700	-0.81999400
H	-3.45158600	-3.06023000	0.76406100
C	-1.96163400	-4.80064900	-2.37305900
C	-3.25812200	-5.09873600	-1.95270500
H	-4.80352400	-4.70245600	-0.50065400
H	-1.54783800	-5.27058000	-3.25876100
H	-3.85897300	-5.81103100	-2.50948300
Co	1.53623000	-1.97756400	-0.48719200
C	1.64472800	-1.56563300	-2.34907000
C	0.71013700	-0.57223000	-2.87035800
C	0.87612200	0.78848200	-2.54431200
C	-0.39343600	-0.95130700	-3.66237800
C	-0.02163700	1.74467800	-3.01351900
H	1.71771300	1.08425700	-1.92590100
C	-1.28804300	0.00852900	-4.12794500
H	-0.53737100	-1.99837800	-3.90804100
C	-1.10490800	1.35798900	-3.80659900
H	0.12446700	2.79068900	-2.76325000
H	-2.13032800	-0.29290000	-4.74261000
H	-1.80239700	2.10283200	-4.17638800
C	2.54891200	-2.31500500	-3.00390700
C	2.83402800	-2.44605400	-4.47571300
H	1.90627000	-2.41575600	-5.05815500
H	3.49441700	-1.66348900	-4.86258200
N	3.51585300	-3.76261600	-4.54337700
C	3.39892900	-4.49523600	-3.26335800
H	2.47192000	-5.08777500	-3.21447200
H	4.25241900	-5.16035100	-3.13697600
S	3.34335300	-4.64129000	-5.96497700
O	3.58010500	-3.69411900	-7.05207500
O	4.11898100	-5.86500200	-5.77525800
C	1.60787900	-5.08629500	-5.99807800
C	0.69134100	-4.21797900	-6.59856100
C	1.19242600	-6.26378800	-5.37130900
C	-0.66754100	-4.52912300	-6.55140100
H	1.05056100	-3.34076100	-7.12462800
C	-0.16891900	-6.56849900	-5.33868100
H	1.93134100	-6.93944700	-4.95582100
C	-1.09627400	-5.70052000	-5.92173800
H	-1.38804800	-3.87116400	-7.02666500
H	-0.50297600	-7.49118800	-4.87462500
C	-1.19294500	-3.88480700	-1.65440900

H	-0.19125300	-3.63617700	-1.98840100
C	3.32651200	-3.34264300	-2.24092100
H	4.34221400	-2.97015700	-2.05391000
C	2.60560100	-3.60506300	-0.92521900
H	1.79739400	-4.33654800	-1.02792900
H	3.24979400	-3.84845600	-0.07813600
C	2.46097500	-1.32639400	4.31037500
H	2.11648100	-0.29260800	4.39731600
H	2.13518000	-1.86917400	5.20317000
H	3.55326800	-1.31765400	4.30079600
C	0.12452700	-4.25786800	1.96692800
H	0.26977800	-4.70565500	2.95510300
H	-0.54658100	-4.90436900	1.39800300
H	1.09148300	-4.25471000	1.45452600
H	-2.15335300	-5.94774800	-5.90432400

S**2 before annihilation 0.0000, after 0.0000

S-TS2^{CSS}

C	0.93765500	-2.94179600	2.48238300
C	-0.06418900	-3.90660200	1.81866400
C	2.19755900	-2.56471800	1.67707500
H	-0.82782000	-4.14271000	2.56932400
H	0.43370900	-2.02681700	2.81099600
H	1.28081000	-3.43625700	3.39904700
H	2.51987300	-3.43486000	1.09747800
P	1.81050600	-1.24903300	0.40154800
P	-0.97893300	-3.13098200	0.39953100
C	3.42664900	-0.86430400	-0.36433500
C	3.72491500	0.44797200	-0.75915600
C	4.36026700	-1.88125700	-0.62543900
C	4.93840500	0.73718500	-1.38234200
H	3.01707900	1.24682200	-0.57941100
C	5.56991700	-1.59013900	-1.25419800
H	4.15878600	-2.90410800	-0.32613700
C	5.86400500	-0.27676600	-1.62591000
H	5.15242700	1.75886400	-1.67895100
H	6.28182400	-2.38241700	-1.45582100
H	6.80755800	-0.05451200	-2.11004200
C	1.40708800	0.22374300	1.41254300
C	2.40707700	0.97262000	2.05621300
C	0.06659900	0.58860700	1.59385100
C	2.06574700	2.06357800	2.85313300
H	3.45134100	0.71700900	1.92283200
C	-0.27373200	1.67624000	2.39715800

H	-0.71950500	0.02996200	1.10679200
C	0.72576500	2.41807200	3.02597800
H	2.84819300	2.63742400	3.33933100
H	-1.31916600	1.93655500	2.52442400
H	0.46502500	3.26918500	3.64702300
C	-2.15637200	-1.93916000	1.13471100
C	-2.86917900	-1.12360200	0.23606500
C	-2.33121900	-1.75810200	2.51290300
C	-3.72477300	-0.13365000	0.71597200
H	-2.74238700	-1.27335500	-0.83133000
C	-3.19095300	-0.76643900	2.98684100
H	-1.79938700	-2.37586100	3.22695700
C	-3.88165500	0.05189000	2.09192300
H	-4.27139200	0.49061000	0.01612000
H	-3.31863400	-0.63339200	4.05639700
H	-4.54678000	0.82430400	2.46476400
C	-2.05742800	-4.47085100	-0.21756000
C	-2.96602000	-5.06747400	0.67173600
C	-3.77629400	-6.11674700	0.24594900
H	-3.05077300	-4.70488800	1.69197200
C	-2.80354900	-5.97383500	-1.96265500
C	-3.69233100	-6.57440300	-1.07182500
H	-4.47625800	-6.57352100	0.93825000
H	-2.74784600	-6.31787300	-2.99073300
H	-4.32579100	-7.39106300	-1.40302900
Co	0.21029500	-1.91436200	-1.09857700
C	1.05970200	-0.72638400	-2.65021400
C	1.15240800	0.73987900	-2.55650300
C	2.03082000	1.54167000	-3.30885800
C	0.33521600	1.38018400	-1.60775900
C	2.11790000	2.91330600	-3.07756000
H	2.66520900	1.10060400	-4.06482800
C	0.43294400	2.74543100	-1.35940600
H	-0.37014100	0.78356600	-1.03642300
C	1.33432400	3.51937200	-2.09312800
H	2.80792200	3.51074800	-3.66541300
H	-0.18579300	3.19925900	-0.59208900
H	1.41771100	4.58534100	-1.90781700
C	1.92742100	-1.58423700	-3.24602800
C	3.14734700	-1.33125100	-4.09246000
H	2.91684600	-0.71302600	-4.96447900
H	3.93817100	-0.83343400	-3.51141200
N	3.50421300	-2.68048200	-4.53703100
C	3.05338900	-3.68837900	-3.58290200

H	2.93827600	-4.65100600	-4.08038700
H	3.75031300	-3.79632700	-2.73802800
S	4.76478400	-2.95577500	-5.58701200
O	4.57618400	-4.31700100	-6.08436300
O	4.81043600	-1.78040100	-6.45724400
C	6.25390500	-2.95691000	-4.59334300
C	6.58858700	-4.10620000	-3.87196100
C	7.05396900	-1.81506100	-4.56011100
C	7.74063700	-4.09895900	-3.08658600
H	5.97508300	-4.99598900	-3.95783200
C	8.21179500	-1.82474400	-3.78137200
H	6.77920800	-0.95426400	-5.15874300
C	8.54969700	-2.95936700	-3.04000000
H	8.01922700	-4.98742000	-2.52899800
H	8.85711800	-0.95198000	-3.76372900
C	-1.98774000	-4.92318900	-1.54053900
H	-1.32695100	-4.43007400	-2.23900000
C	1.71524800	-3.07876500	-3.11168300
C	1.28039400	-3.43760600	-1.70736300
C	3.32948400	-2.16571000	2.63287900
H	3.01184300	-1.36048800	3.30016900
H	3.60055600	-3.02583400	3.25322100
H	4.22533200	-1.83803600	2.10204100
C	0.57894900	-5.23695100	1.39655800
H	1.14274300	-5.65350600	2.23731600
H	-0.17969200	-5.96461200	1.10331000
H	1.26695200	-5.12129300	0.55652500
H	0.94492200	-3.36449100	-3.84128100
H	2.13793500	-3.56216900	-1.04524200
H	0.66634300	-4.33600000	-1.66968400
H	9.45389300	-2.96322600	-2.43956700
C	-0.96264400	-3.19929900	-6.42623600
C	-0.52213700	-2.25389200	-7.35174000
C	-0.20609900	-0.95554600	-6.93355200
C	-0.31983700	-0.60993800	-5.59249700
C	-0.73264500	-1.56784900	-4.65254300
C	-1.06569900	-2.86037100	-5.07650700
H	-1.22456900	-4.20001400	-6.75453400
H	-0.43068700	-2.52143000	-8.39936700
H	0.12643600	-0.21866100	-7.65739800
H	-0.06708800	0.39324300	-5.26045800
H	-1.42567200	-3.57631200	-4.34632200
C	-0.80855800	-1.20284300	-3.21907100
O	-1.20000300	-2.10351800	-2.34436700

H	-1.12977600	-0.17057400	-3.04472300
S**2 before annihilation	0.0000,	after	-0.0000
R-TS2^{CSS}			
C	-0.25267100	-2.48399600	2.90016700
C	-0.30787600	-3.32318000	1.60691200
C	1.13276200	-1.98691100	3.35215600
H	-1.32843600	-3.71275900	1.51755900
H	-0.93780500	-1.63185200	2.83836500
H	-0.64275200	-3.12218700	3.70252000
H	1.86846500	-2.77599200	3.16652300
P	1.69724700	-0.55951400	2.30014500
P	-0.08821800	-2.29416900	0.06214400
C	3.38059300	-0.16118800	2.87374700
C	3.88220500	1.13413600	2.66581200
C	4.22827500	-1.14420700	3.40748500
C	5.20268200	1.43633000	2.99266500
H	3.24312300	1.89802700	2.24109300
C	5.54928600	-0.83624400	3.73355800
H	3.86845400	-2.15349800	3.57719300
C	6.03931100	0.45312900	3.52523600
H	5.57785200	2.44182200	2.83044000
H	6.19180200	-1.60367700	4.15313800
H	7.06689200	0.69182100	3.78006500
C	0.67396600	0.86730600	2.78812700
C	0.88924400	1.55798700	3.99216800
C	-0.36686800	1.27207700	1.94220700
C	0.06016500	2.62066000	4.34468400
H	1.70942200	1.27483200	4.64201100
C	-1.19790300	2.33315000	2.29958500
H	-0.53317400	0.76141200	1.00349400
C	-0.98666500	3.00636900	3.50266200
H	0.23218800	3.15052200	5.27613000
H	-2.00299100	2.62863900	1.63471300
H	-1.62930000	3.83495200	3.78297100
C	-1.62182500	-1.29067000	-0.02269100
C	-1.65947300	-0.25418800	-0.97004200
C	-2.72803000	-1.47337700	0.82023700
C	-2.76858400	0.58295400	-1.06821500
H	-0.82363300	-0.10126600	-1.63731700
C	-3.83376200	-0.62759400	0.72716500
H	-2.74654500	-2.26781800	1.55585000
C	-3.85706200	0.40368000	-0.21288900
H	-2.77547500	1.37059500	-1.81473600

H	-4.67930300	-0.77864000	1.39055600
H	-4.72063800	1.05752600	-0.28136300
C	-0.26230300	-3.51046400	-1.29031800
C	-1.47243800	-3.67938700	-1.97566600
C	-1.55667400	-4.58202400	-3.03715700
H	-2.34019500	-3.09132400	-1.70016100
C	0.76738300	-5.17209500	-2.73244300
C	-0.43806300	-5.32195000	-3.42229300
H	-2.49696300	-4.69920500	-3.56663700
H	1.63578900	-5.75210400	-3.01829200
H	-0.49921900	-6.01612800	-4.25413100
Co	1.65060200	-0.82926900	0.03084500
C	1.88842300	-0.75267400	-2.11495900
C	0.89182700	-0.43627500	-3.16973500
C	0.24838000	-1.50260000	-3.83195400
C	0.47952700	0.86704100	-3.51608700
C	-0.76035800	-1.28363300	-4.76501100
H	0.52126900	-2.51862500	-3.58913700
C	-0.52949800	1.08728200	-4.45353900
H	0.93762800	1.73784300	-3.06518500
C	-1.16225200	0.01425300	-5.07991100
H	-1.23614900	-2.13622700	-5.23918800
H	-0.81445200	2.10618000	-4.69717100
H	-1.95013900	0.18788100	-5.80554400
C	2.88126100	-1.65483700	-2.31226400
C	3.30016500	-2.35994400	-3.57854600
H	2.55662500	-3.10669500	-3.89257300
H	3.45174000	-1.66096000	-4.40568800
N	4.56842000	-2.98603500	-3.17912400
C	4.52881300	-3.30314900	-1.74738200
H	3.94395300	-4.21370100	-1.53751900
H	5.53935800	-3.43856500	-1.36498500
S	5.33339700	-4.01285500	-4.25660400
O	5.35348500	-3.30049800	-5.53269000
O	6.54006200	-4.47416300	-3.57307300
C	4.23761500	-5.41758000	-4.44927800
C	3.29129500	-5.40753300	-5.47674600
C	4.34710800	-6.49671700	-3.56802800
C	2.43977700	-6.50317200	-5.62267300
H	3.25721300	-4.57103700	-6.16529600
C	3.48884800	-7.58546600	-3.72369900
H	5.11887100	-6.49252100	-2.80659100
H	1.71282200	-6.51602400	-6.42844800
H	3.57281900	-8.43768900	-3.05713300

C	0.85268000	-4.27024500	-1.67550500
H	1.79585100	-4.15248400	-1.16029600
C	3.82235000	-2.04443400	-1.19962400
H	4.58977600	-1.26009500	-1.14778900
C	3.10733500	-2.14442000	0.12961100
H	2.68325000	-3.13016000	0.31148000
H	3.75076400	-1.85877200	0.96002000
C	4.25775100	1.27441600	-3.31413600
C	5.51182600	1.37354800	-3.90368500
C	6.66561800	1.27832500	-3.11594400
C	6.56146000	1.09147700	-1.73759200
C	5.30584300	0.97599400	-1.14123800
C	4.14923800	1.05970200	-1.93061300
H	3.35944900	1.33039100	-3.92244500
H	5.59767900	1.52105700	-4.97517300
H	7.64323100	1.35320000	-3.58103900
H	7.45730800	1.03039400	-1.12799600
H	5.19976000	0.83798600	-0.07028500
O	2.74778000	0.69241700	-0.01524000
C	2.82333200	0.92358100	-1.29699400
H	2.04256100	1.54925800	-1.72689000
C	2.53833600	-7.58882100	-4.74909400
H	1.88222000	-8.44456600	-4.87323300
C	1.12473600	-1.66194200	4.85175000
H	0.35514500	-0.92224500	5.08690100
H	0.90589200	-2.56965900	5.42297000
H	2.08704000	-1.27309600	5.19132600
C	0.61571000	-4.54826900	1.66174500
H	0.41191100	-5.11077800	2.57862700
H	0.44277500	-5.21500500	0.81579000
H	1.67528800	-4.28321200	1.66870500

S**2 before annihilation 2.0652, after 2.0007

S-TS2^{triplet}

C	0.96273800	-2.95582900	2.38251200
C	0.03673100	-3.92022200	1.61260000
C	2.20496500	-2.41751300	1.65076100
H	-0.71842100	-4.27450100	2.32479000
H	0.39399300	-2.11197900	2.78507500
H	1.32359400	-3.51326300	3.25549100
H	2.60881400	-3.20786700	1.01159000
P	1.78008100	-1.02847100	0.45981200
P	-0.94447500	-3.08544200	0.27110800
C	3.41422900	-0.62211900	-0.25641300

C	3.80693600	0.70311700	-0.48143000
C	4.26958600	-1.66103400	-0.66320100
C	5.03778600	0.98217500	-1.07606100
H	3.15044900	1.52024300	-0.21038000
C	5.49516900	-1.38034700	-1.26174700
H	3.99296600	-2.69845700	-0.51019400
C	5.88426400	-0.05394100	-1.46491000
H	5.32264500	2.01554000	-1.24455100
H	6.14537400	-2.19136300	-1.56860100
H	6.83925300	0.16076000	-1.93121100
C	1.29785500	0.37937400	1.51631400
C	2.22657400	1.10836400	2.27804600
C	-0.05992400	0.72166400	1.58456800
C	1.79665800	2.15708900	3.08892700
H	3.28245800	0.87138800	2.22543100
C	-0.48790700	1.76543000	2.40361100
H	-0.78621500	0.17579400	0.99711300
C	0.44044500	2.48604000	3.15528700
H	2.52178700	2.71842500	3.66951500
H	-1.54406400	2.00952100	2.44738300
H	0.11170700	3.30387200	3.78871600
C	-2.11509400	-1.98168500	1.15311900
C	-2.90526600	-1.11091600	0.38144500
C	-2.25522300	-1.97063800	2.54900400
C	-3.79293400	-0.23328700	1.00140800
H	-2.80630500	-1.11020200	-0.69684100
C	-3.14528500	-1.08927000	3.16297000
H	-1.68035800	-2.64113500	3.17540000
C	-3.91041100	-0.21368000	2.39294500
H	-4.39510500	0.43522300	0.39409000
H	-3.23924400	-1.09040600	4.24419800
H	-4.60121500	0.47209100	2.87318900
C	-2.03086400	-4.39924400	-0.38450100
C	-2.98508300	-4.98601600	0.46167800
C	-3.80888900	-6.00379100	-0.01351600
H	-3.09795700	-4.63631400	1.48322000
C	-2.75980200	-5.84657300	-2.18569400
C	-3.69642800	-6.43665800	-1.33741100
H	-4.54451500	-6.45328200	0.64575300
H	-2.67541900	-6.17196400	-3.21790200
H	-4.34322500	-7.22624300	-1.70617800
Co	0.26982300	-1.89556400	-1.26114500
C	1.20612800	-0.74131500	-2.81863700
C	1.44888200	0.70346600	-2.61906300

C	2.43245300	1.45162300	-3.29026300
C	0.64506300	1.38151700	-1.68124000
C	2.61997900	2.80377100	-3.00824200
H	3.07010200	0.99047400	-4.02993400
C	0.84689800	2.72461900	-1.37962800
H	-0.14376100	0.83736300	-1.17307700
C	1.84173100	3.44495300	-2.04359800
H	3.38674500	3.35608500	-3.54259700
H	0.22869500	3.20284400	-0.62665600
H	2.00149600	4.49472500	-1.81986200
C	2.00705900	-1.63872000	-3.45582300
C	3.26958300	-1.42534800	-4.25093600
H	3.13495000	-0.71840600	-5.07293600
H	4.08299900	-1.05719800	-3.60399300
N	3.52372300	-2.76171700	-4.79870100
C	3.01178500	-3.78267700	-3.88601200
H	2.85228800	-4.71927700	-4.41844800
H	3.69372900	-3.95902900	-3.03862800
S	4.88366200	-3.03041700	-5.73195100
O	4.76445000	-4.40576900	-6.21010100
O	4.97824000	-1.87318500	-6.62162700
C	6.27910200	-2.96054400	-4.61168200
C	6.60060800	-4.08867100	-3.85164000
C	7.02732700	-1.78557700	-4.52709600
C	7.68795900	-4.02838500	-2.98069200
H	6.03263100	-5.00364700	-3.97645000
C	8.12191000	-1.74289200	-3.66282900
H	6.76867200	-0.94172800	-5.15615300
C	8.44735400	-2.85792700	-2.88723000
H	7.95721200	-4.90000600	-2.39286100
H	8.72944300	-0.84511500	-3.60649100
C	-1.92861600	-4.83153800	-1.71119500
H	-1.21420200	-4.36404400	-2.37295100
C	1.70475900	-3.11806800	-3.39139400
C	1.26717800	-3.49271700	-1.99023100
C	3.28400900	-2.02032200	2.66628600
H	2.89848200	-1.28850800	3.38090100
H	3.59780100	-2.90459300	3.23016600
H	4.16767900	-1.59944200	2.18237700
C	0.76297900	-5.16514000	1.08468500
H	1.28100900	-5.66299600	1.91044800
H	0.05636700	-5.87646100	0.65156400
H	1.50394600	-4.92634800	0.32019900
H	0.91098800	-3.33741200	-4.12007500

H	2.11889000	-3.46855800	-1.30311800
H	0.77418900	-4.45935300	-1.91622700
H	9.30300400	-2.82167200	-2.22045200
C	-1.76337400	-3.42596900	-5.85825600
C	-1.09929900	-2.94324500	-6.98511200
C	-0.33643900	-1.77154600	-6.90102700
C	-0.22976700	-1.09845700	-5.69053200
C	-0.86486200	-1.60190200	-4.54515500
C	-1.64615800	-2.75834800	-4.63745800
H	-2.37590700	-4.31945900	-5.92870200
H	-1.18037700	-3.46815700	-7.93145700
H	0.17191400	-1.39014500	-7.78039900
H	0.36601900	-0.19238400	-5.61976600
H	-2.17312500	-3.10555900	-3.75808800
C	-0.72890300	-0.88863500	-3.24909700
O	-1.31959400	-1.39326700	-2.18055800
H	-0.77217000	0.20005800	-3.34272500

S**2 before annihilation 2.0708, after 2.0009

R-TS2^{triplet}

C	0.07412000	-2.44583400	2.81881500
C	-0.21198200	-3.21566300	1.51357900
C	1.51852800	-1.96846200	3.07820200
H	-1.24702600	-3.57180200	1.57129800
H	-0.59870000	-1.58931800	2.92411000
H	-0.18377500	-3.13008300	3.63626700
H	2.22443100	-2.72523900	2.71956800
P	1.90193300	-0.45723500	2.05395700
P	-0.20068900	-2.11539700	-0.00970900
C	3.48036900	0.19953900	2.67393600
C	3.68626000	1.58707700	2.71862900
C	4.54205400	-0.66404400	2.99050500
C	4.93286400	2.09826500	3.07821800
H	2.87989500	2.26247100	2.45885900
C	5.78626800	-0.14720700	3.34692700
H	4.40220200	-1.73994900	2.96582700
C	5.98423400	1.23488800	3.38958200
H	5.08289300	3.17254800	3.10808600
H	6.59854200	-0.82279200	3.59512500
H	6.95323700	1.63614600	3.66857100
C	0.65165100	0.79579600	2.49318900
C	0.55448700	1.30943800	3.79886800
C	-0.25205900	1.23590100	1.51700600
C	-0.45476200	2.21370400	4.12124600

H	1.27838000	1.02453100	4.55329000
C	-1.26475200	2.13635500	1.84472100
H	-0.15641800	0.88993500	0.49800300
C	-1.37226100	2.61950700	3.14788400
H	-0.52205500	2.60650600	5.13075700
H	-1.96538500	2.45164600	1.07914400
H	-2.15929700	3.32122000	3.40550800
C	-1.80345100	-1.23540600	0.05856000
C	-2.12327600	-0.41270800	-1.03261700
C	-2.68448900	-1.29086700	1.14668100
C	-3.28766200	0.34960500	-1.03011900
H	-1.46475100	-0.37362200	-1.88828400
C	-3.84824200	-0.52049700	1.14968800
H	-2.48148200	-1.92396400	2.00074000
C	-4.15090500	0.30513300	0.06734500
H	-3.51650400	0.97480100	-1.88740500
H	-4.51887600	-0.56988600	2.00149500
H	-5.05662600	0.90307800	0.07535600
C	-0.37823500	-3.29541900	-1.39988500
C	-1.58912200	-3.49757300	-2.07412600
C	-1.66042000	-4.40573800	-3.13192000
H	-2.47211900	-2.94006100	-1.78587000
C	0.67379600	-4.95093900	-2.83520500
C	-0.53306700	-5.13287300	-3.51433900
H	-2.60269100	-4.54688600	-3.65191900
H	1.54789800	-5.52580000	-3.11362800
H	-0.58836900	-5.84331300	-4.33259600
Co	1.89182700	-0.79078700	-0.21036700
C	2.11505100	-0.74953100	-2.29885700
C	0.93309800	-0.42311300	-3.13389600
C	0.37455500	-1.37447200	-4.01191700
C	0.27393100	0.82319400	-3.03801000
C	-0.73945500	-1.07825000	-4.79261500
H	0.78714500	-2.37071700	-4.06702100
C	-0.82600600	1.12645800	-3.83760000
H	0.58543300	1.55342600	-2.30166800
C	-1.33664200	0.18079900	-4.72708800
H	-1.14108800	-1.84084600	-5.45203900
H	-1.29557200	2.10095300	-3.74635600
H	-2.19528200	0.41563600	-5.34767700
C	3.04822300	-1.71384600	-2.55623800
C	3.28516900	-2.54914600	-3.79153900
H	2.49218700	-3.29813700	-3.93180000
H	3.34701800	-1.94754300	-4.70236200

N	4.57267900	-3.18914500	-3.48338000
C	4.63980700	-3.42438900	-2.03738200
H	4.00845500	-4.27266500	-1.72401600
H	5.66769600	-3.61216000	-1.73182500
S	5.18869200	-4.31941700	-4.55953700
O	5.10787400	-3.69059800	-5.87642200
O	6.43862400	-4.78444500	-3.96322800
C	4.02748200	-5.68298600	-4.54507800
C	3.03936300	-5.74722600	-5.52984500
C	4.12629500	-6.65372800	-3.54401400
C	2.13285600	-6.80806900	-5.50921400
H	3.01440400	-4.99510200	-6.30992900
C	3.20744200	-7.70273300	-3.52840000
H	4.93220000	-6.60255600	-2.82055900
H	1.37387300	-6.88231800	-6.28151500
H	3.27759900	-8.46969100	-2.76393700
C	0.75139400	-4.02815900	-1.79587200
H	1.69729300	-3.88069300	-1.29093000
C	4.07045700	-2.08750400	-1.51268900
H	4.88861500	-1.36095500	-1.57940900
C	3.46487400	-2.05847300	-0.11670400
H	2.96409700	-2.99981400	0.13039800
H	4.19069900	-1.81196400	0.65672800
C	4.98276400	0.97946800	-2.85891500
C	6.37136100	0.96469000	-2.92523900
C	7.12581100	0.92131900	-1.74656900
C	6.48506800	0.89741100	-0.50732200
C	5.09204800	0.89593900	-0.44066000
C	4.33446700	0.92921900	-1.61560500
H	4.39308100	1.00579400	-3.77188800
H	6.86896600	0.98766800	-3.88910200
H	8.20981700	0.91060800	-1.79979600
H	7.06398200	0.87600500	0.41022100
H	4.58460300	0.86973300	0.51124600
O	2.21919000	1.09086400	-0.42173800
C	2.85047700	0.92317500	-1.57744900
H	2.43578900	1.46104600	-2.43315700
C	2.21374400	-7.77977400	-4.50895800
H	1.51016700	-8.60614800	-4.49957900
C	1.72828600	-1.77464200	4.58782800
H	0.94779400	-1.13695200	5.00957800
H	1.66701500	-2.74615100	5.08825600
H	2.69836400	-1.33379000	4.82297100
C	0.67452200	-4.46055800	1.38399800

H	0.62775300	-5.02911200	2.31851700
H	0.33848800	-5.11162700	0.57708800
H	1.72410100	-4.21709500	1.20250100
S**2 before annihilation	2.2921,	after	2.0047
S-IM3 ^{triplet}			
C	0.98234700	-2.89513900	2.57793100
C	0.16908900	-4.00416100	1.86021800
C	2.28523200	-2.38765500	1.91873600
H	-0.50692400	-4.42951500	2.61130300
H	0.33889000	-2.04160300	2.81739900
H	1.28036300	-3.31760100	3.54467700
H	2.79116800	-3.23317300	1.44226000
P	1.98044000	-1.16996000	0.52493300
P	-0.88640900	-3.31637400	0.49772900
C	3.62781300	-0.75476600	-0.12866600
C	3.86198200	0.50947000	-0.69190300
C	4.63221100	-1.73468200	-0.19756400
C	5.08744900	0.79000300	-1.29473400
H	3.09242600	1.27043200	-0.67153100
C	5.85372300	-1.44923800	-0.80520400
H	4.47071000	-2.72380200	0.21864600
C	6.08396200	-0.18477000	-1.35061300
H	5.25031200	1.76979200	-1.73126600
H	6.61743900	-2.21595800	-0.87023900
H	7.03257100	0.03090800	-1.82908200
C	1.32291600	0.33451200	1.31248500
C	2.14629500	1.27110400	1.95656000
C	-0.06316200	0.54636500	1.27510000
C	1.58399100	2.40076500	2.54826400
H	3.22062800	1.12841400	1.97916300
C	-0.62314300	1.67205500	1.87663900
H	-0.71204000	-0.15998100	0.77209800
C	0.20134900	2.60243400	2.51105200
H	2.22573700	3.12498000	3.03971900
H	-1.69821100	1.81503600	1.84340700
H	-0.22949200	3.48407300	2.97483300
C	-2.16908400	-2.28303000	1.28702000
C	-2.89359300	-1.42131100	0.44464800
C	-2.43571500	-2.29052300	2.66237200
C	-3.86993200	-0.58210800	0.97823400
H	-2.66788000	-1.39302800	-0.61787500
C	-3.40836200	-1.44103300	3.19080400
H	-1.89479000	-2.95162000	3.33050400

C	-4.12484100	-0.58631500	2.35217800
H	-4.42785600	0.07853200	0.32199900
H	-3.60762200	-1.45061600	4.25767500
H	-4.88112800	0.07216300	2.76740000
C	-1.77183600	-4.70760300	-0.27478400
C	-2.31449600	-5.76486600	0.46996900
C	-3.00344900	-6.78865300	-0.17713700
H	-2.20765900	-5.78844800	1.55053300
C	-2.64306700	-5.69852100	-2.30821400
C	-3.16624300	-6.75731400	-1.56541100
H	-3.41894600	-7.60837800	0.40022400
H	-2.77573700	-5.66313400	-3.38507600
H	-3.70565400	-7.55647100	-2.06370500
Co	0.39758500	-2.01795600	-1.02864100
C	1.00901800	-0.33932100	-3.31610500
C	1.39528600	1.07842700	-3.09490000
C	2.29238000	1.77307400	-3.91730100
C	0.85505200	1.73837500	-1.97813600
C	2.67846500	3.07552600	-3.59808100
H	2.67597500	1.30454600	-4.81769900
C	1.24726200	3.03497100	-1.65325200
H	0.14866200	1.21715300	-1.34161200
C	2.17107800	3.70490800	-2.45919900
H	3.37044000	3.60257000	-4.24750200
H	0.83636700	3.51386000	-0.76972700
H	2.47866800	4.71631100	-2.21331900
C	1.90695000	-1.33371800	-3.43564400
C	3.40361000	-1.24239800	-3.61744800
H	3.76436600	-0.29447900	-3.99975400
H	3.94178800	-1.47600400	-2.68977400
N	3.57645000	-2.29961800	-4.61914400
C	2.77812700	-3.46709600	-4.24716400
H	2.47681300	-4.01752100	-5.13798600
H	3.32892900	-4.14862900	-3.58111200
S	4.97416600	-2.43521500	-5.51493900
O	4.73481700	-3.54657200	-6.43363200
O	5.29279700	-1.07913800	-5.96254400
C	6.26854000	-2.92968700	-4.37843200
C	6.28445400	-4.23483700	-3.87788400
C	7.25555100	-2.00645600	-4.03336400
C	7.29608500	-4.60734500	-2.99400300
H	5.54421200	-4.95465300	-4.20892300
C	8.27756900	-2.39867700	-3.16831500
H	7.22497600	-1.01231300	-4.46363500

C	8.29277600	-3.69216600	-2.64198800
H	7.32455100	-5.61948900	-2.60326700
H	9.06665800	-1.69812900	-2.91319300
C	-1.94354900	-4.67594700	-1.66685500
H	-1.54973700	-3.84290300	-2.23922200
C	1.56391900	-2.82670100	-3.49888700
C	1.41684000	-3.38348400	-2.09994000
C	3.21759000	-1.79698400	2.98749900
H	2.72371100	-0.98671700	3.53060000
H	3.48550100	-2.57288200	3.71125600
H	4.14184200	-1.40674200	2.55590700
C	1.04500200	-5.14631800	1.32504500
H	1.72037300	-5.50260200	2.10941200
H	0.43507800	-5.98860400	0.99409500
H	1.65541400	-4.83185800	0.47318500
H	0.64131500	-2.99112400	-4.05416900
H	2.34998200	-3.43838500	-1.53165200
H	0.81234800	-4.28606600	-2.00614600
H	9.09228900	-3.99509700	-1.97312300
C	-2.65152400	-2.79270400	-5.58874000
C	-2.03860600	-2.60467900	-6.82853300
C	-0.92843100	-1.76475300	-6.92768700
C	-0.42563900	-1.12676400	-5.79330900
C	-1.02324200	-1.32789900	-4.54419700
C	-2.14922100	-2.15487500	-4.45416500
H	-3.52587700	-3.43165800	-5.50461600
H	-2.42564200	-3.10338400	-7.71142900
H	-0.44743900	-1.60837600	-7.88813200
H	0.44767100	-0.48882700	-5.88065300
H	-2.62568800	-2.29574500	-3.49097200
C	-0.50244100	-0.63692000	-3.28612800
O	-0.85588000	-1.37109100	-2.12942800
H	-1.01038400	0.33468800	-3.21234700

S**2 before annihilation 2.2272, after 2.0034

R-IM3^{triplet}

C	-0.14105600	-2.56409800	2.96094300
C	-0.19276000	-3.44996000	1.69186700
C	1.23848400	-2.05873300	3.44185200
H	-1.20164100	-3.87687800	1.64428800
H	-0.83090600	-1.71824600	2.87186300
H	-0.54495800	-3.18790500	3.76749900
H	1.99490300	-2.81491500	3.20695600
P	1.75283600	-0.55597800	2.46101100

P	-0.00324600	-2.50802700	0.08650600
C	3.43616200	-0.11726000	3.00339600
C	3.85967300	1.21737100	2.89530700
C	4.36827100	-1.10398100	3.35923800
C	5.18784800	1.55606700	3.14957500
H	3.15161000	1.98877800	2.61154000
C	5.69592600	-0.75950300	3.61391700
H	4.06697200	-2.14329600	3.44382800
C	6.10877400	0.56965800	3.50802800
H	5.50178900	2.59172000	3.06659300
H	6.40601600	-1.52970000	3.89768700
H	7.14213800	0.83514600	3.70599700
C	0.66999200	0.80132600	3.00791400
C	0.83017700	1.42286100	4.25800300
C	-0.36851400	1.21252700	2.16084900
C	-0.05030800	2.42638900	4.65520900
H	1.64889700	1.13422800	4.90792600
C	-1.25171000	2.21290900	2.56636600
H	-0.48120900	0.76164700	1.18394100
C	-1.09524500	2.81788700	3.81320000
H	0.07942600	2.90546900	5.62039400
H	-2.05231500	2.52024200	1.90161200
H	-1.77835200	3.60062700	4.12756500
C	-1.43942700	-1.38946200	-0.02626900
C	-1.35826300	-0.33482500	-0.95220000
C	-2.58488700	-1.51314200	0.77368900
C	-2.40260700	0.57935400	-1.07367600
H	-0.48117500	-0.22359800	-1.57807600
C	-3.62118800	-0.58696500	0.65920600
H	-2.68048700	-2.32438500	1.48629700
C	-3.53174900	0.45984800	-0.26108300
H	-2.32730100	1.38309600	-1.79865000
H	-4.50093500	-0.68619200	1.28678500
H	-4.34262200	1.17614100	-0.34697500
C	-0.22000800	-3.73391600	-1.24283400
C	-1.40309000	-3.81569900	-1.99060100
C	-1.51077500	-4.75026700	-3.02162500
H	-2.22890900	-3.14673600	-1.77589900
C	0.72823000	-5.54041700	-2.55714400
C	-0.45057300	-5.61349300	-3.30209500
H	-2.42641500	-4.80522200	-3.60189700
H	1.55452200	-6.20478900	-2.77618600
H	-0.53297200	-6.33922200	-4.10383600
Co	1.76295600	-0.95523300	0.08535800

C	2.15865000	-0.27106800	-2.78346600
C	1.08190500	-0.03682900	-3.77422400
C	0.09763300	-1.01511700	-4.00363200
C	0.99763100	1.17092500	-4.48851800
C	-0.93223300	-0.79640500	-4.91496800
H	0.12202900	-1.93969700	-3.43853500
C	-0.02767000	1.38524700	-5.40785000
H	1.75131900	1.93913200	-4.34522800
C	-0.99854500	0.40487500	-5.62234000
H	-1.68588700	-1.56342600	-5.06565000
H	-0.06622100	2.31872300	-5.96028100
H	-1.79929000	0.57725500	-6.33434400
C	2.79778400	-1.45519900	-2.70915600
C	2.72114300	-2.55697500	-3.75214100
H	1.92717900	-3.28684900	-3.54542400
H	2.58339500	-2.16492500	-4.76002300
N	4.04695900	-3.15993400	-3.60778800
C	4.40381600	-3.20430300	-2.19989800
H	3.88030600	-4.01591300	-1.66693200
H	5.47792100	-3.34238800	-2.08273500
S	4.68913400	-4.19144200	-4.74384800
O	4.35921900	-3.60858900	-6.04272100
O	6.05869900	-4.45054400	-4.30229700
C	3.78265300	-5.73198400	-4.61534000
C	2.71488600	-5.96793300	-5.48258600
C	4.17689300	-6.67876600	-3.66635000
C	2.03075800	-7.18098100	-5.39733100
H	2.45738500	-5.22432100	-6.22790400
C	3.47852000	-7.88345400	-3.58393200
H	5.03905200	-6.48495700	-3.03797500
H	1.21456500	-7.38781800	-6.08237700
H	3.78126500	-8.63425900	-2.86113900
C	0.84753300	-4.59410300	-1.54304400
H	1.77751400	-4.51978500	-0.98951100
C	3.91164900	-1.81864900	-1.70653500
H	4.71734200	-1.09354000	-1.85294100
C	3.52702200	-1.80338000	-0.24214000
H	3.32478800	-2.78734900	0.19637700
H	4.16720600	-1.19537300	0.39636100
C	4.68213000	1.35831900	-3.09317200
C	6.04376300	1.65563700	-3.11505700
C	6.73871900	1.85428100	-1.91896600
C	6.05976800	1.76331100	-0.70375000
C	4.69548200	1.46991300	-0.68183400

C	4.00037500	1.25442900	-1.87439300
H	4.15622200	1.17744400	-4.02648400
H	6.56463900	1.72296000	-4.06497800
H	7.80066600	2.07785800	-1.93795800
H	6.58910600	1.91416000	0.23258500
H	4.16466900	1.39348600	0.25810200
O	2.06652100	0.67649300	-0.53694900
C	2.51821400	0.90310800	-1.85075400
H	1.95965900	1.77651200	-2.21440500
C	2.40868000	-8.13445000	-4.44891500
H	1.87929300	-9.08028500	-4.39172600
C	1.23784500	-1.82330400	4.95707100
H	0.45564900	-1.11481500	5.24161300
H	1.04835700	-2.76537700	5.48144600
H	2.19705700	-1.43087600	5.30347800
C	0.79413300	-4.62491400	1.76125400
H	0.72077500	-5.10778300	2.74072700
H	0.57502400	-5.37573100	1.00108700
H	1.83296400	-4.30664000	1.62652700

S**2 before annihilation 0.0000, after 0.0000

S-IM3^{CSS}

C	1.02040800	-2.96520600	2.53020800
C	0.15340200	-3.93797300	1.70469400
C	2.33651900	-2.48210800	1.89546600
H	-0.63094900	-4.30741100	2.37537400
H	0.43612900	-2.09312200	2.84230100
H	1.28796600	-3.49162600	3.45441900
H	2.82839900	-3.33188000	1.41180600
P	2.00793600	-1.26895400	0.51865500
P	-0.77130500	-3.09415300	0.32867500
C	3.65264000	-0.81708600	-0.12000100
C	3.84789000	0.45091900	-0.69110100
C	4.69788700	-1.75409500	-0.15390300
C	5.07301500	0.77562200	-1.27088300
H	3.04682800	1.18001800	-0.69434000
C	5.91952900	-1.42519800	-0.74006000
H	4.56605200	-2.74425700	0.26910600
C	6.10898600	-0.15890500	-1.29586000
H	5.20720600	1.75708800	-1.71364000
H	6.71483800	-2.16095000	-0.78132200
H	7.05823400	0.09126400	-1.75594800
C	1.39760300	0.24610500	1.33978700
C	2.25629200	1.12874600	2.01569400

C	0.02670700	0.53274200	1.29187700
C	1.74376700	2.26954900	2.62993700
H	3.32249800	0.93627200	2.04565700
C	-0.48607700	1.67124700	1.91219200
H	-0.64864900	-0.12419100	0.76106400
C	0.37350700	2.54222300	2.58168800
H	2.41496300	2.94826800	3.14638100
H	-1.55186000	1.86962200	1.86583700
H	-0.01887000	3.43252600	3.06282200
C	-2.07032200	-2.08961100	1.13930600
C	-2.87995200	-1.29361000	0.30943000
C	-2.28220300	-2.07615600	2.52481600
C	-3.87328900	-0.49109100	0.86557500
H	-2.70297100	-1.29630800	-0.76057400
C	-3.27942500	-1.26914300	3.07401200
H	-1.68380600	-2.68599800	3.19064000
C	-4.07247900	-0.47250800	2.24861700
H	-4.49434400	0.11935800	0.21748700
H	-3.43460100	-1.26605200	4.14815000
H	-4.84619600	0.15483600	2.67961900
C	-1.71085900	-4.42878800	-0.49398300
C	-2.46862100	-5.30544500	0.30047700
C	-3.20046000	-6.33050800	-0.29354300
H	-2.50246000	-5.18340000	1.37891000
C	-2.46105000	-5.59963800	-2.47566100
C	-3.19399300	-6.48196600	-1.68300200
H	-3.78159300	-7.00579400	0.32618500
H	-2.46842700	-5.69469600	-3.55697400
H	-3.76873500	-7.27951300	-2.14293700
Co	0.47352500	-1.86890600	-1.04719900
C	0.88459200	-0.48202600	-3.07380700
C	1.23580100	0.95533800	-2.93010300
C	2.11845200	1.61296000	-3.79858600
C	0.67126200	1.67588800	-1.86641800
C	2.47078600	2.94314700	-3.56770600
H	2.51797400	1.09541300	-4.66452600
C	1.03595500	2.99805000	-1.62518900
H	-0.03319300	1.18440400	-1.20535700
C	1.94784600	3.63293700	-2.47200300
H	3.15164700	3.44169900	-4.25030100
H	0.61219700	3.52502200	-0.77612000
H	2.23399000	4.66406300	-2.29102600
C	1.81792500	-1.46483500	-3.16211800
C	3.30695100	-1.33930400	-3.39024400

H	3.64358700	-0.37282400	-3.74453700
H	3.87984000	-1.61360300	-2.49813200
N	3.43487200	-2.35701500	-4.43881100
C	2.71880200	-3.56348900	-4.01829300
H	2.39640600	-4.12864400	-4.89210300
H	3.33858300	-4.21061500	-3.38004800
S	4.76455000	-2.39964100	-5.44274100
O	4.50930000	-3.49687500	-6.37308700
O	4.97720500	-1.01679000	-5.87351100
C	6.15657000	-2.85200000	-4.41154200
C	6.26847700	-4.16641400	-3.94880100
C	7.10966500	-1.88420200	-4.09524700
C	7.34618700	-4.50511600	-3.13240200
H	5.54650800	-4.91459600	-4.25617600
C	8.19765600	-2.24214400	-3.29833300
H	7.00051600	-0.88219700	-4.49312100
C	8.31034900	-3.54533100	-2.80961100
H	7.44946900	-5.52310000	-2.77068200
H	8.96154200	-1.50641000	-3.06648000
C	-1.71913000	-4.57577300	-1.88580300
H	-1.18773300	-3.86494500	-2.50033100
C	1.52942600	-2.97016800	-3.20504600
C	1.46433400	-3.40999200	-1.74941700
C	3.26919600	-1.92096200	2.97747300
H	2.78286700	-1.11442700	3.53229200
H	3.52135700	-2.71328100	3.68909200
H	4.20155500	-1.53529600	2.55988300
C	0.93542100	-5.16483200	1.21456200
H	1.42868900	-5.64325800	2.06681000
H	0.27182100	-5.89808200	0.75302500
H	1.70392500	-4.90616700	0.48498300
H	0.58508300	-3.17363400	-3.70850000
H	2.45800500	-3.47338300	-1.29905500
H	0.92114900	-4.34116600	-1.59613900
H	9.16048900	-3.82041500	-2.19314100
C	-2.53271500	-2.89757200	-5.74441800
C	-1.77344500	-2.71959400	-6.90252900
C	-0.63496000	-1.91381400	-6.86389700
C	-0.25084800	-1.29728400	-5.67230900
C	-0.99932700	-1.48349800	-4.50547800
C	-2.15018000	-2.27993800	-4.55395000
H	-3.42555900	-3.51547800	-5.76770500
H	-2.06739300	-3.20324700	-7.82867100
H	-0.03782900	-1.76962900	-7.75875200

H	0.64746700	-0.68892200	-5.65547400
H	-2.73250000	-2.42331900	-3.65082600
C	-0.62058700	-0.83409000	-3.17734600
O	-0.99439500	-1.64789600	-2.08514500
H	-1.16791500	0.11475100	-3.08920500

S**2 before annihilation -0.0000, after -0.0000

R-IM3^{CSS}

C	-0.10201200	-2.56428100	2.94561600
C	-0.18503800	-3.49991200	1.72390900
C	1.29522400	-2.01252200	3.29475800
H	-1.20500600	-3.89768500	1.68352000
H	-0.80977300	-1.73399100	2.84671500
H	-0.44519500	-3.14744300	3.80819800
H	2.04877500	-2.76992600	3.05542300
P	1.72876500	-0.56373900	2.20896100
P	0.02859500	-2.55279900	0.13046800
C	3.38360500	-0.02299500	2.73655300
C	3.73253600	1.33140700	2.62463900
C	4.34437900	-0.94627700	3.17759900
C	5.01827600	1.75228500	2.96058200
H	3.00530000	2.04816800	2.26404900
C	5.63006400	-0.52033800	3.50821600
H	4.09885800	-1.99907400	3.27011200
C	5.96898600	0.82926100	3.39959400
H	5.27850500	2.80191100	2.87013900
H	6.36352700	-1.24179400	3.85336400
H	6.96949700	1.16016100	3.65880100
C	0.61107100	0.78954900	2.69497000
C	0.74890800	1.43240300	3.93780700
C	-0.41508300	1.18413700	1.82938600
C	-0.14733200	2.43222800	4.30827500
H	1.56291500	1.16866200	4.60268600
C	-1.31183300	2.18348100	2.20455500
H	-0.51137000	0.71797200	0.86057500
C	-1.18235200	2.80482700	3.44620500
H	-0.03405500	2.92571500	5.26819100
H	-2.10359300	2.47371200	1.52174700
H	-1.87699000	3.58529800	3.74011800
C	-1.49266200	-1.54239400	-0.01253300
C	-1.46597900	-0.49060900	-0.94321800
C	-2.64851700	-1.73425000	0.75637000
C	-2.56767500	0.34543900	-1.11111200
H	-0.58063100	-0.31763900	-1.54118100

C	-3.74416500	-0.88400900	0.60314100
H	-2.71080300	-2.53934200	1.47874300
C	-3.70861900	0.15411400	-0.32989400
H	-2.52653700	1.14208500	-1.84689600
H	-4.63022300	-1.03838500	1.21045300
H	-4.56748800	0.80691800	-0.44848200
C	-0.12542200	-3.80311800	-1.19669300
C	-1.22417100	-3.80856600	-2.06792700
C	-1.29849400	-4.74794300	-3.09800400
H	-2.01883000	-3.08190600	-1.94626500
C	0.81046000	-5.69748800	-2.39933600
C	-0.28798700	-5.69466300	-3.26143600
H	-2.15252600	-4.74079400	-3.76793000
H	1.60717100	-6.41953500	-2.53551300
H	-0.34368500	-6.42370200	-4.06162800
Co	1.67811300	-0.97579300	0.01375500
C	2.12188900	-0.21401500	-2.38067400
C	1.11058600	0.17838800	-3.39174500
C	0.10939800	-0.71739200	-3.81621800
C	1.13357600	1.46089000	-3.97165100
C	-0.82682800	-0.34877300	-4.77734100
H	0.03816900	-1.69936200	-3.36397800
C	0.20310200	1.82464100	-4.94283400
H	1.90230900	2.17191400	-3.69177300
C	-0.78339800	0.92461600	-5.34760300
H	-1.59320300	-1.05682900	-5.07681100
H	0.25299700	2.81386800	-5.38624600
H	-1.51034300	1.21267600	-6.10006700
C	2.62367300	-1.48276500	-2.32747600
C	2.44662500	-2.52993200	-3.41509000
H	1.63756100	-3.23827600	-3.20669900
H	2.27797800	-2.08092300	-4.39378200
N	3.75751300	-3.17375700	-3.37669600
C	4.26161300	-3.26689200	-2.01688800
H	3.86800200	-4.15182300	-1.49352300
H	5.34996700	-3.32084900	-2.02374500
S	4.40670100	-3.99727500	-4.66174500
O	3.89863400	-3.33550800	-5.86321700
O	5.83088800	-4.13685500	-4.36281100
C	3.68813500	-5.63668700	-4.61195000
C	2.61411200	-5.93649900	-5.44936600
C	4.21810800	-6.58488100	-3.73300500
C	2.05954200	-7.21615300	-5.40381000
H	2.24803000	-5.18293700	-6.13692000

C	3.64631400	-7.85579000	-3.68648900
H	5.08264900	-6.33644300	-3.12749100
H	1.23976200	-7.47151600	-6.06804800
H	4.05361700	-8.60663600	-3.01701200
C	0.89616400	-4.75069900	-1.38160600
H	1.77047900	-4.74189400	-0.74245600
C	3.73366300	-1.96139300	-1.36775700
H	4.52267900	-1.20563000	-1.38397600
C	3.23531300	-2.12629500	0.05939600
H	2.95667200	-3.15165800	0.30571100
H	3.93543600	-1.73305700	0.79297200
C	4.66838000	1.16638700	-3.11153800
C	6.02080100	1.37780400	-3.37686400
C	6.92255200	1.55896000	-2.32588200
C	6.46173800	1.52783700	-1.00955000
C	5.10841700	1.31606500	-0.74270600
C	4.20285400	1.13369600	-1.79085000
H	3.98319900	1.00200900	-3.93825800
H	6.37152900	1.39019300	-4.40401400
H	7.97600100	1.71729700	-2.53393600
H	7.15575500	1.66206400	-0.18483000
H	4.74509300	1.27242000	0.27489000
O	2.49367600	0.62002700	-0.13185000
C	2.72588800	0.90273900	-1.48712700
H	2.17756900	1.82470500	-1.71787000
C	2.56862200	-8.17079300	-4.52058900
H	2.13756600	-9.16654300	-4.49256500
C	1.38205500	-1.69223600	4.79389000
H	0.58168500	-1.01187200	5.09445600
H	1.26840300	-2.61761400	5.36709100
H	2.33872100	-1.24206100	5.06631900
C	0.75415000	-4.70769700	1.85290400
H	0.63758100	-5.14859000	2.84817700
H	0.51481400	-5.47738300	1.11877100
H	1.80799600	-4.44293900	1.73152600

S**2 before annihilation -0.0000, after -0.0000

S-TS3^{CSS}

Co	2.84172200	-0.86859000	0.09195100
C	1.30363400	0.43460100	2.63977300
C	0.38198600	1.49727000	3.12419100
C	0.88724700	2.65015300	3.74139300
C	-1.00458500	1.37150600	2.95484600
C	0.02515600	3.65139900	4.18365100

H	1.95924000	2.75957000	3.87457300
C	-1.86696600	2.37476100	3.39457600
H	-1.40040900	0.49317000	2.45535400
C	-1.35383300	3.51742000	4.01023100
H	0.42929900	4.53598000	4.66542800
H	-2.93844800	2.26625900	3.25566600
H	-2.02404300	4.29888900	4.35369800
C	1.20124700	-0.83818100	3.07180500
C	0.19331300	-1.29516100	4.09702700
H	-0.79651900	-1.40725500	3.62454800
H	0.08619800	-0.61210300	4.94067200
N	0.72977500	-2.59176500	4.53350700
C	1.40628700	-3.22062600	3.39405700
H	0.68838400	-3.71973100	2.72310800
H	2.13064000	-3.95661200	3.74179800
S	-0.28619600	-3.55949400	5.46474400
O	-0.80083200	-2.69459600	6.52375800
O	0.46122900	-4.78899400	5.72028000
C	-1.65567400	-3.96352300	4.37947800
C	-2.76367000	-3.11320400	4.33282800
C	-1.57698100	-5.10166700	3.57309000
C	-3.80784900	-3.40985700	3.45670100
H	-2.81424800	-2.26214900	5.00260100
C	-2.62851200	-5.38813400	2.70219200
H	-0.72373500	-5.76399600	3.66517500
H	-4.68418100	-2.76980600	3.42774300
H	-2.59068100	-6.28258300	2.08816300
C	2.05843500	-2.02157400	2.66128000
H	3.06211400	-1.86390400	3.06237800
C	2.14704100	-2.34437900	1.16683800
H	1.15981500	-2.61553700	0.79309000
H	2.83322700	-3.18213400	1.02515300
O	3.51738900	0.20572500	1.65339000
H	1.59322900	-0.02053700	0.46848000
C	2.35389100	0.80236200	1.62835000
C	2.30328400	2.12693700	0.91485100
C	1.11320900	2.64657800	0.38429800
C	3.50106100	2.82342700	0.72123800
C	1.12761800	3.82951000	-0.34471300
H	0.17969200	2.12215400	0.54472200
C	3.51141300	4.02070300	0.00652300
H	4.41317000	2.42351800	1.14590700
C	2.32774700	4.52098100	-0.53548100
H	0.20422000	4.21557800	-0.76382600

H	4.44295800	4.56195200	-0.12628300
H	2.33611600	5.44857000	-1.09913400
C	-3.74020400	-4.54357600	2.64311300
H	-4.56413400	-4.78060600	1.97673200
C	3.39617200	-2.71087900	-3.08056700
C	4.39074200	-3.18937200	-1.99487700
C	1.90050800	-2.69519400	-2.71073100
H	5.35203900	-3.34322300	-2.49909500
H	3.68341400	-1.72530400	-3.46234200
H	3.50415200	-3.40005100	-3.92679900
H	1.67627700	-3.58737000	-2.11875600
P	1.50007200	-1.26788600	-1.59305300
P	4.69759300	-1.89458200	-0.69393100
C	-0.22266800	-1.52073800	-1.04087400
C	-0.98183300	-0.40854200	-0.64629400
C	-0.72263500	-2.80793900	-0.79499200
C	-2.21043400	-0.58220000	-0.01322500
H	-0.60651300	0.59181300	-0.82879000
C	-1.94447700	-2.97844200	-0.14214700
H	-0.15755500	-3.68669200	-1.08690900
C	-2.68667600	-1.86780400	0.25614900
H	-2.78943000	0.28795000	0.27962900
H	-2.30637600	-3.97777000	0.07206900
H	-3.62707000	-2.00572900	0.77805300
C	1.52598900	0.24695900	-2.60281800
C	0.45133900	0.62994800	-3.42074500
C	2.65860400	1.07203500	-2.52100100
C	0.51681400	1.81995400	-4.14297400
H	-0.43692700	0.01047000	-3.47903800
C	2.72007900	2.26041100	-3.24547600
H	3.49868700	0.79919700	-1.89334200
C	1.64884600	2.63510100	-4.05613300
H	-0.31703400	2.11284200	-4.77293800
H	3.59885600	2.88986800	-3.16128500
H	1.69076000	3.56294800	-4.61774400
C	5.63822200	-0.55666700	-1.51649300
C	5.84183900	0.60759900	-0.75587500
C	6.08804800	-0.59871500	-2.84251300
C	6.46924900	1.71526200	-1.32099200
H	5.48572900	0.64079400	0.26820800
C	6.71351800	0.51482400	-3.40470700
H	5.95850100	-1.48889900	-3.44698300
C	6.89879700	1.67389500	-2.64960500
H	6.61901300	2.61081000	-0.72641000

H	7.05708200	0.47490100	-4.43344600
H	7.38271600	2.53835200	-3.09282600
C	5.84742100	-2.62511300	0.51309600
C	6.89843500	-3.46796800	0.12016000
C	7.77221300	-3.98200700	1.07526200
H	7.04176500	-3.72082000	-0.92605600
C	6.58183600	-2.79339800	2.81459400
C	7.61135100	-3.64931800	2.42330300
H	8.58075200	-4.63807600	0.76918400
H	6.46349400	-2.52403600	3.85935300
H	8.29372500	-4.05255200	3.16465400
C	5.69878500	-2.28053600	1.86349400
H	4.91239600	-1.59470400	2.15612700
C	1.01904400	-2.70287700	-3.96708200
H	1.23850900	-1.84334100	-4.60594800
H	1.20851400	-3.61210900	-4.54577500
H	-0.04445000	-2.68005300	-3.71580500
C	3.97947600	-4.52947300	-1.36673600
H	3.76786700	-5.25784700	-2.15625900
H	4.77290400	-4.93419200	-0.73681300
H	3.08397900	-4.43856900	-0.74731600

S**2 before annihilation 0.0000, after -0.0000

R-TS3^{CSS}

C	3.85756400	-2.93979500	2.98447000
C	2.33250700	-2.69439300	3.04326800
C	4.45594500	-3.38980600	1.63873300
H	4.40660200	-2.06146400	3.33881100
H	4.06933500	-3.73553800	3.70910900
H	3.76986800	-4.10603300	1.17603200
P	4.54055900	-1.97169800	0.44018300
P	1.80278300	-1.13487000	2.17898900
C	5.05563500	-2.69224600	-1.15040700
C	5.62297400	-1.84644700	-2.11784600
C	4.74187400	-4.01515400	-1.49618900
C	5.87167800	-2.32046200	-3.40389200
H	5.85115500	-0.81725600	-1.86762800
C	4.99016400	-4.48378800	-2.78661800
H	4.30133200	-4.68872100	-0.76954100
C	5.55211800	-3.63747000	-3.74310300
H	6.31165000	-1.65914300	-4.14352600
H	4.74781100	-5.51078100	-3.04082800
H	5.74494300	-4.00321200	-4.74655700
C	5.90710400	-0.88853600	0.96788500

C	7.25379800	-1.22053100	0.74781400
C	5.59228300	0.32207000	1.60239200
C	8.26340200	-0.35964600	1.17320500
H	7.50934500	-2.13896400	0.23093700
C	6.60537300	1.17960600	2.02930100
H	4.55941800	0.60366100	1.76223600
C	7.94115700	0.83833400	1.81722100
H	9.30229600	-0.62113400	0.99915900
H	6.34391800	2.11081200	2.52124100
H	8.73196400	1.50564900	2.14518700
C	2.46394100	0.24584900	3.18323700
C	2.28509200	1.54283400	2.67371000
C	3.17143600	0.07552800	4.38209500
C	2.82533300	2.64342200	3.33591900
H	1.72756600	1.69443600	1.75710700
C	3.71299000	1.17916200	5.04061700
H	3.30676400	-0.90819700	4.81466700
C	3.55033800	2.46207500	4.51501900
H	2.68148800	3.63457700	2.92158200
H	4.26072900	1.03518800	5.96649800
H	3.97726000	3.31725100	5.02939100
C	-0.00275900	-1.05581100	2.40858400
C	-0.54434900	-1.18578900	3.69884000
C	-1.92330900	-1.14710400	3.88295300
H	0.10805200	-1.30197300	4.55942400
C	-2.23874900	-0.84524400	1.50350700
C	-2.77238200	-0.98366000	2.78346300
H	-2.33707500	-1.24405600	4.88164500
H	-2.88479100	-0.73580100	0.63950500
H	-3.84776600	-0.96548600	2.92985200
Co	2.65195000	-0.75968200	0.18941000
C	1.23956200	0.44080600	-2.38500900
C	0.34979200	1.49497600	-2.95095300
C	0.87567200	2.55637900	-3.69719900
C	-1.03324800	1.44653400	-2.71194800
C	0.03703200	3.55112100	-4.19928300
H	1.94550800	2.60559500	-3.87710600
C	-1.86952800	2.44330400	-3.21328200
H	-1.43711100	0.62739600	-2.12472500
C	-1.33647800	3.49802000	-3.95758100
H	0.45635000	4.36839400	-4.77765300
H	-2.93686600	2.40156300	-3.01681500
H	-1.98753300	4.27507600	-4.34548100
C	1.14499300	-0.84049000	-2.78837200

C	0.21535500	-1.33479800	-3.87760600
H	-0.69407400	-0.75272200	-4.00304100
H	0.73931200	-1.33903100	-4.84280800
N	-0.06764100	-2.74081500	-3.52741200
C	1.20262000	-3.24580800	-2.96656800
H	1.01672600	-4.11322600	-2.33413800
H	1.82489600	-3.56035700	-3.81004400
S	-1.41799000	-2.90128100	-2.48794700
O	-1.30939900	-4.22950900	-1.87924700
O	-1.56064000	-1.71102900	-1.62263000
C	-2.75112200	-2.86661300	-3.66702900
C	-3.03854000	-4.02931600	-4.38421900
C	-3.46917400	-1.68530600	-3.85327500
C	-4.07221200	-3.99924000	-5.31683400
H	-2.46890900	-4.93351100	-4.20255500
C	-4.49788200	-1.66938500	-4.79515800
H	-3.22890800	-0.80687400	-3.26625200
H	-4.31494500	-4.89398600	-5.88046300
H	-5.06767500	-0.75990600	-4.95489700
C	-0.85622600	-0.87120300	1.31586400
H	-0.45839400	-0.76238400	0.31623200
C	1.87056100	-2.04678700	-2.22066800
H	2.92939800	-2.00123600	-2.47491800
C	1.72459600	-2.21097500	-0.70616500
H	0.67855800	-2.23362800	-0.40447200
H	2.19669900	-3.14701100	-0.40024500
O	3.37770000	0.15374800	-1.30641400
H	1.44479200	0.14628600	-0.04812000
C	2.25618200	0.82329000	-1.34722200
C	2.30893500	2.21418700	-0.77985900
C	1.15960600	2.93962900	-0.43209500
C	3.57234200	2.77176300	-0.54326800
C	1.27710300	4.20943800	0.12570800
H	0.17751700	2.51153700	-0.58833500
C	3.68641600	4.04907200	0.00332200
H	4.45388600	2.19338900	-0.79204100
C	2.54015400	4.77226900	0.33545100
H	0.38259200	4.76279400	0.39268800
H	4.66964300	4.47772200	0.16982900
H	2.62705800	5.76868900	0.75781200
C	-4.79677700	-2.82175300	-5.52371500
H	-5.60044900	-2.80532200	-6.25292300
C	5.81323100	-4.07373900	1.84864400
H	6.51167900	-3.40729000	2.36165900

H	5.68566100	-4.96868300	2.46560500
H	6.26662600	-4.37857400	0.90236800
H	2.08118500	-2.53652500	4.09907900
C	1.50901300	-3.89640800	2.55591200
H	1.85273300	-4.80595200	3.05883300
H	0.44957900	-3.76380700	2.78189600
H	1.59418100	-4.05478100	1.47883900

S**2 before annihilation 0.0000, after -0.0000

S-IM4^{CSS}

C	0.67398600	-3.59402600	2.69485700
C	-0.27887200	-4.20883900	1.64349300
C	2.15110700	-3.39625600	2.29634200
H	-1.22039300	-4.44128400	2.15476300
H	0.27827700	-2.64525900	3.07205700
H	0.66903400	-4.27756300	3.55282000
H	2.46964300	-4.24928500	1.68867500
P	2.37196600	-1.91093100	1.19094400
P	-0.71627700	-2.99786500	0.29391900
C	4.13920100	-1.89698700	0.73712300
C	4.71121900	-0.69518300	0.29256800
C	4.89089500	-3.07772200	0.66959300
C	6.01496100	-0.67600300	-0.19650500
H	4.13226200	0.22183900	0.32272500
C	6.19342100	-3.05644600	0.17026900
H	4.46843100	-4.02215500	0.99423900
C	6.75698500	-1.85781400	-0.26315000
H	6.45004500	0.26058600	-0.53066500
H	6.76017300	-3.97884700	0.11111000
H	7.76834400	-1.84365400	-0.65521000
C	2.09113200	-0.46242500	2.26153100
C	3.07947600	0.05424600	3.11303300
C	0.82249100	0.13787800	2.23608900
C	2.79425400	1.14706300	3.93008400
H	4.06930200	-0.38877300	3.12859500
C	0.53946100	1.22780700	3.05827200
H	0.04501100	-0.24778700	1.58570500
C	1.52557900	1.73239200	3.90659500
H	3.56299100	1.54276800	4.58616900
H	-0.44915800	1.67467300	3.03332400
H	1.30964900	2.58202800	4.54652700
C	-1.89560500	-1.82579300	1.06747000
C	-2.39301400	-0.79339900	0.25184700
C	-2.26594900	-1.85767200	2.41900300

C	-3.22791900	0.18778400	0.78096300
H	-2.11803200	-0.76248400	-0.79483400
C	-3.09473400	-0.86653600	2.94826700
H	-1.91822500	-2.64796900	3.07281300
C	-3.57304400	0.16043700	2.13445300
H	-3.60810800	0.97136600	0.13274400
H	-3.36973400	-0.90312100	3.99759000
H	-4.21849800	0.92797300	2.54954900
C	-1.74666900	-3.95177400	-0.88143300
C	-3.14724700	-3.92225000	-0.83494000
C	-3.89636300	-4.66220400	-1.75043600
H	-3.65337100	-3.31915200	-0.08967800
C	-1.86372100	-5.48354400	-2.76434500
C	-3.25862700	-5.44103300	-2.71646700
H	-4.98041400	-4.63027700	-1.70604300
H	-1.36119700	-6.09192900	-3.50986100
H	-3.84465000	-6.01382000	-3.42795900
Co	1.05972100	-1.66328100	-0.53884000
C	1.40554300	-0.37199600	-3.70112400
C	1.92394600	0.80263800	-4.46314400
C	2.06383400	0.76211100	-5.85795500
C	2.26063900	1.97699200	-3.77796600
C	2.53689400	1.87422800	-6.55196400
H	1.78926700	-0.13944200	-6.39844200
C	2.73358200	3.08940700	-4.47284900
H	2.14862500	2.01594300	-2.69797900
C	2.87253300	3.04014300	-5.86065600
H	2.63915100	1.83125500	-7.63158100
H	2.99239000	3.99392500	-3.93141300
H	3.23848500	3.90659400	-6.40211900
C	2.04972100	-1.56680800	-3.70014400
C	3.33027000	-1.85126000	-4.43283700
H	3.54643000	-1.19172200	-5.26770800
H	4.16929600	-1.78795500	-3.71247800
N	3.08985600	-3.22056100	-4.89565500
C	2.34952000	-3.96762900	-3.86767200
H	1.66255000	-4.66866900	-4.34414200
H	3.02588700	-4.53491700	-3.21307500
S	4.31289000	-4.00136500	-5.74172700
O	3.77523200	-5.31873800	-6.07541100
O	4.77181600	-3.04131900	-6.74373200
C	5.63127700	-4.22458700	-4.55251600
C	5.66704300	-5.38974000	-3.78246500
C	6.58693900	-3.21667600	-4.39862600

C	6.68136900	-5.54271500	-2.83747700
H	4.93691300	-6.17128700	-3.95929400
C	7.59671600	-3.38387700	-3.45209200
H	6.55421000	-2.34351800	-5.04019700
C	7.64314300	-4.54316100	-2.67444900
H	6.73412700	-6.45139700	-2.24622100
H	8.35763800	-2.61867700	-3.33703500
C	-1.11303800	-4.74068900	-1.85561800
H	-0.03139100	-4.78705000	-1.89611700
C	1.61841400	-2.86076700	-3.04916600
C	2.05998700	-2.92149200	-1.58186200
C	3.03315100	-3.31840800	3.55117500
H	2.69922500	-2.51363200	4.21154600
H	2.96845800	-4.25934900	4.10636500
H	4.08267100	-3.14212700	3.30644400
C	0.26120300	-5.52574700	1.06878800
H	0.58330200	-6.17965800	1.88574400
H	-0.50388600	-6.05144400	0.49634100
H	1.12021300	-5.37245100	0.40879700
H	0.53526300	-2.98255400	-3.11256200
H	3.13351300	-2.74015000	-1.50667000
H	1.84503900	-3.91169500	-1.16393700
H	8.44314900	-4.67650500	-1.95250100
C	-2.37571300	2.53281100	-2.46688300
C	-2.72302500	2.81053200	-3.79197600
C	-2.10570200	2.12146800	-4.83890000
C	-1.13133900	1.16578200	-4.56808100
C	-0.79032500	0.87021200	-3.23882500
C	-1.42427200	1.55732600	-2.18938400
H	-2.84323200	3.08105000	-1.65500700
H	-3.47012300	3.56733900	-4.00913600
H	-2.37957200	2.33465200	-5.86676500
H	-0.64678200	0.64014600	-5.38159000
H	-1.14453000	1.33403700	-1.16644400
C	0.19170100	-0.17968000	-2.90249100
O	-0.05810200	-0.87361800	-1.87964400
H	2.11051600	-0.71122200	-0.89163200

S**2 before annihilation 0.0000, after 0.0000

R-IM4^{CSS}

C	3.92277200	-2.92589300	3.07794200
C	2.38313100	-2.79558600	3.14640500
C	4.53545100	-3.36171700	1.73338300
H	4.40708700	-2.00146400	3.40985400

H	4.19781200	-3.68770500	3.81778500
H	3.88589000	-4.12267400	1.28978300
P	4.50098600	-1.95239600	0.51988800
P	1.70905000	-1.29708500	2.27420500
C	4.99976300	-2.67474500	-1.07843900
C	5.55329600	-1.83778500	-2.06167100
C	4.66617000	-3.99455800	-1.41851800
C	5.76832900	-2.31468300	-3.35289800
H	5.80149100	-0.81171700	-1.81722200
C	4.87901500	-4.46702400	-2.71420500
H	4.23698200	-4.66418600	-0.68135400
C	5.42710600	-3.62820300	-3.68496700
H	6.20098100	-1.65898100	-4.10204900
H	4.62039400	-5.49197600	-2.96087600
H	5.59412300	-3.99694800	-4.69195800
C	5.85256500	-0.81967600	0.99074900
C	7.20251900	-1.09883800	0.72278600
C	5.51709500	0.37919200	1.63719000
C	8.19410100	-0.19841600	1.10741800
H	7.47419800	-2.00988400	0.20092500
C	6.51179900	1.27712700	2.02367800
H	4.48070000	0.62010200	1.83600300
C	7.85097500	0.98867400	1.76061300
H	9.23508600	-0.42122500	0.89564400
H	6.23265900	2.19847700	2.52472300
H	8.62726900	1.68708000	2.05721200
C	2.32216300	0.16592700	3.18884000
C	2.14381000	1.42392300	2.58387200
C	3.02618700	0.08610400	4.39938200
C	2.68238400	2.57035100	3.16591900
H	1.59319500	1.50141300	1.65254100
C	3.56158900	1.23582700	4.97871100
H	3.16400200	-0.86573700	4.89859800
C	3.39988600	2.47696900	4.35940200
H	2.54394100	3.52841300	2.67802200
H	4.10558700	1.16135300	5.91495400
H	3.82297100	3.36814800	4.81227300
C	-0.08823400	-1.36360600	2.56546700
C	-0.57652100	-1.56088500	3.86834200
C	-1.94818800	-1.63096900	4.09585800
H	0.10819000	-1.64687400	4.70712300
C	-2.36202900	-1.30752800	1.73513800
C	-2.84266100	-1.51153100	3.02754100
H	-2.32054400	-1.77783000	5.10475000

H	-3.04195100	-1.22199600	0.89425000
H	-3.91110000	-1.57650800	3.20800400
Co	2.49139600	-0.83708800	0.31463900
C	1.31468600	0.55358800	-2.45694700
C	0.43212600	1.58475800	-3.08015700
C	0.95125300	2.55066900	-3.94914800
C	-0.93903500	1.60068000	-2.77562800
C	0.11701000	3.52139000	-4.50440800
H	2.01170800	2.54580700	-4.18348500
C	-1.77019400	2.57255200	-3.33067500
H	-1.33648300	0.85096300	-2.09739400
C	-1.24352100	3.53570300	-4.19518700
H	0.52987900	4.26615100	-5.17751600
H	-2.82753900	2.58383700	-3.08352500
H	-1.89066300	4.29359800	-4.62512300
C	1.14383100	-0.75861700	-2.77303100
C	0.17943800	-1.22523600	-3.84668800
H	-0.72524000	-0.63158300	-3.94438900
H	0.69254500	-1.19701700	-4.81851600
N	-0.10722300	-2.63404200	-3.53558300
C	1.16784100	-3.15566900	-3.00271400
H	0.99223000	-4.05117800	-2.40830400
H	1.78858900	-3.42620600	-3.86294000
S	-1.45211500	-2.80122500	-2.48518200
O	-1.34008900	-4.13169200	-1.88325300
O	-1.58570800	-1.60947800	-1.62012000
C	-2.79245400	-2.76021700	-3.65580300
C	-3.08383600	-3.91754700	-4.38002500
C	-3.51052800	-1.57692800	-3.82947800
C	-4.12186100	-3.87976500	-5.30747200
H	-2.51404300	-4.82352200	-4.20786200
C	-4.54369400	-1.55346200	-4.76639500
H	-3.26740300	-0.70418300	-3.23490200
H	-4.36796600	-4.77011000	-5.87657100
H	-5.11423900	-0.64277800	-4.91628600
C	-0.98868200	-1.22412600	1.50381600
H	-0.63220500	-1.05455000	0.49746500
C	1.82117700	-1.98701000	-2.20144000
H	2.89137200	-1.94045800	-2.40536400
C	1.62558500	-2.22565300	-0.68892500
H	0.57198500	-2.30898000	-0.43459800
H	2.12031200	-3.16957100	-0.43951900
O	3.28502800	0.14395100	-1.19344900
H	1.21421100	-0.08968700	0.24187300

C	2.36658300	0.96376800	-1.51746800
C	2.50501100	2.33753600	-0.97090300
C	1.42106500	3.20238500	-0.74061300
C	3.79515500	2.73433500	-0.57081800
C	1.63244300	4.43995000	-0.13710200
H	0.41753200	2.90712900	-1.01293500
C	4.00437600	3.98184000	0.00439400
H	4.62054900	2.04874900	-0.71752300
C	2.92246800	4.84016600	0.22018600
H	0.78814900	5.09659600	0.04552200
H	5.00724200	4.28282500	0.28988700
H	3.08275200	5.81543800	0.66971800
C	-4.84646000	-2.70016300	-5.50226300
H	-5.65346300	-2.67784300	-6.22762400
C	5.93147200	-3.96269700	1.92986700
H	6.60314800	-3.24661500	2.41107900
H	5.87032800	-4.85035800	2.56761100
H	6.37860100	-4.26119600	0.97823700
H	2.12598700	-2.66488200	4.20445900
C	1.65467800	-4.05453500	2.64844100
H	2.09596000	-4.94493600	3.10754100
H	0.59606100	-4.02579600	2.91138600
H	1.71744300	-4.16773600	1.56293200

S**2 before annihilation 0.2320, after 0.0041

S-TS4^{OSS}

C	0.81114200	-3.57112300	2.62926900
C	0.09727000	-4.34407400	1.49553600
C	2.29870900	-3.21611900	2.43295200
H	-0.80695600	-4.79359700	1.91957500
H	0.25855200	-2.65847900	2.87855600
H	0.76291400	-4.19771700	3.52858000
H	2.83928700	-4.12890500	2.16101600
P	2.56830400	-2.04835100	1.00111400
P	-0.46852900	-3.17297700	0.16029800
C	4.38079500	-1.99202500	0.74683500
C	4.88850800	-0.99392900	-0.10230000
C	5.27865200	-2.85192500	1.39187500
C	6.26156500	-0.82641300	-0.25733400
H	4.20189100	-0.33084400	-0.62019200
C	6.65615700	-2.69102800	1.22524400
H	4.91990800	-3.64282900	2.03973000
C	7.15071800	-1.66947200	0.41562000
H	6.63895500	-0.03751700	-0.90035200

H	7.34004000	-3.35724800	1.74162300
H	8.22170800	-1.53387200	0.30306900
C	2.16076300	-0.39160900	1.68682000
C	3.13586600	0.47403900	2.20482900
C	0.81762000	0.02167900	1.68537000
C	2.77173700	1.72480300	2.70241300
H	4.17755800	0.17597400	2.21935100
C	0.45780200	1.27350300	2.18365600
H	0.04240300	-0.62580800	1.29942200
C	1.43502400	2.12998700	2.69058400
H	3.53529500	2.38380100	3.10360300
H	-0.58741900	1.56749200	2.17530900
H	1.15938300	3.10517000	3.07915100
C	-1.82469600	-2.20432000	0.92426300
C	-2.25807200	-1.06488300	0.22360000
C	-2.42005700	-2.51209000	2.15520400
C	-3.25501400	-0.24653200	0.74940100
H	-1.79782700	-0.81935100	-0.72562800
C	-3.41561700	-1.68672600	2.68178300
H	-2.11821800	-3.39033900	2.71440400
C	-3.83239900	-0.55268000	1.98401900
H	-3.57309500	0.63078800	0.19445800
H	-3.86600900	-1.93340000	3.63801800
H	-4.60555200	0.08618900	2.39898200
C	-1.32970700	-4.21975900	-1.07892300
C	-2.72676900	-4.22507200	-1.19658100
C	-3.34900400	-4.99886100	-2.17747500
H	-3.33024300	-3.62365500	-0.52684200
C	-1.19689100	-5.78440900	-2.93732200
C	-2.58881800	-5.77787900	-3.04960400
H	-4.43150800	-4.99206600	-2.25702700
H	-0.59737400	-6.39066800	-3.60948700
H	-3.07631000	-6.37710000	-3.81182700
Co	1.27539300	-1.97008700	-0.76978300
C	1.32706900	-0.27477000	-3.87026800
C	1.85462600	0.92400200	-4.58755900
C	1.71087200	1.07214200	-5.97396000
C	2.50805200	1.92715900	-3.85996100
C	2.21482900	2.19998700	-6.61976200
H	1.18588500	0.31023300	-6.54310700
C	3.01224000	3.05504400	-4.50574000
H	2.61126900	1.82464800	-2.78310800
C	2.86720800	3.19324700	-5.88689800
H	2.09427100	2.30500200	-7.69320900

H	3.51594000	3.82605300	-3.93124500
H	3.25809800	4.07167600	-6.39012200
C	1.82250000	-1.51451900	-4.12069300
C	2.93066000	-1.82360300	-5.09919800
H	2.85336600	-1.27409700	-6.03674500
H	3.89743200	-1.54413500	-4.65212200
N	2.81797000	-3.27139400	-5.32107000
C	1.77569100	-3.87706000	-4.47957900
H	0.88981900	-4.10828800	-5.08022800
H	2.12126300	-4.80736500	-4.02460900
S	4.18137400	-4.16525200	-5.70158000
O	3.69976100	-5.43737800	-6.23287400
O	5.05082000	-3.25284300	-6.44241900
C	4.93206300	-4.49897300	-4.11375900
C	4.55244700	-5.64228800	-3.40553100
C	5.81101100	-3.56109500	-3.56719300
C	5.03717200	-5.82843900	-2.11092700
H	3.91567800	-6.37908800	-3.88182700
C	6.29422400	-3.76355700	-2.27579400
H	6.12732100	-2.71153100	-4.16197000
C	5.89752000	-4.88547600	-1.54434600
H	4.75955400	-6.71843400	-1.55468000
H	6.98217300	-3.05076200	-1.83973800
C	-0.57274300	-5.00753800	-1.96375600
H	0.50813600	-5.02053400	-1.89353700
C	1.45405900	-2.79836600	-3.42987700
C	2.32530700	-2.90202100	-2.15935900
C	2.86655800	-2.65936600	3.74834100
H	2.28550200	-1.79624600	4.08270600
H	2.81408300	-3.42623400	4.52757000
H	3.90686600	-2.34210100	3.65573400
C	0.95122700	-5.48691400	0.93250600
H	1.33980100	-6.09942200	1.75281200
H	0.36387700	-6.13557600	0.28126400
H	1.80639200	-5.11588400	0.35827500
H	0.40153500	-2.84173400	-3.15607500
H	3.38669800	-2.79281400	-2.39409700
H	2.21903500	-3.87153900	-1.66127300
H	6.27844700	-5.03132400	-0.53951200
C	-1.62662800	2.79058100	-1.36227800
C	-2.13412700	3.40943800	-2.50809700
C	-1.82390100	2.90448600	-3.77332700
C	-0.99824500	1.79143400	-3.89995800
C	-0.49693000	1.15612300	-2.75263500

C	-0.82288100	1.66215700	-1.48159300
H	-1.85432400	3.19070600	-0.37924700
H	-2.76598300	4.28723500	-2.41624400
H	-2.22232600	3.38226300	-4.66216900
H	-0.75553200	1.40860200	-4.88314200
H	-0.41930500	1.17761600	-0.60093500
C	0.32309100	-0.07207900	-2.81732700
O	0.12591200	-0.91131000	-1.89556000
H	2.46145800	-1.49590900	-1.49787700

S**2 before annihilation 0.2203, after 0.0036

R-TS4^{OSS}

C	4.07780300	-2.88701500	3.30672800
C	2.53399000	-2.91038100	3.39082800
C	4.70776500	-3.29307400	1.95991700
H	4.46692900	-1.90921000	3.61015800
H	4.43543300	-3.59743800	4.06236900
H	4.10436300	-4.09885800	1.53092100
P	4.54033800	-1.90002500	0.73900100
P	1.69812800	-1.60178100	2.36567500
C	4.98272300	-2.61587300	-0.88373300
C	5.52339200	-1.79191700	-1.88456500
C	4.58231200	-3.91778700	-1.22431400
C	5.66309000	-2.26175600	-3.18903500
H	5.82597500	-0.77981000	-1.64204900
C	4.72122500	-4.38497800	-2.53181600
H	4.15489900	-4.57741800	-0.47656500
C	5.25852500	-3.55774600	-3.51887600
H	6.08905200	-1.61467900	-3.94964600
H	4.41292200	-5.39688500	-2.77563800
H	5.36880600	-3.92209600	-4.53525000
C	5.85474200	-0.69464500	1.12767400
C	7.20989400	-0.92531000	0.83705200
C	5.48092000	0.51139800	1.73801600
C	8.16959100	0.03113800	1.16226300
H	7.51047500	-1.84317600	0.34353900
C	6.44534100	1.46378500	2.06861400
H	4.43777500	0.71336500	1.94025100
C	7.78932300	1.22522600	1.78193300
H	9.21411700	-0.15342300	0.93178200
H	6.13769100	2.39062700	2.54216400
H	8.54078000	1.96694000	2.03439900
C	2.16613600	0.02297200	3.07006900
C	1.88863700	1.14796100	2.27069900

C	2.86584200	0.19608500	4.27137600
C	2.33669900	2.41301500	2.64597700
H	1.33106900	1.02118700	1.34697900
C	3.30350800	1.46567100	4.65094000
H	3.07947200	-0.65113000	4.91343700
C	3.05093600	2.57105200	3.83573800
H	2.13595900	3.26553800	2.00661500
H	3.84661500	1.59008400	5.58244800
H	3.40298200	3.55432600	4.13166500
C	-0.08368900	-1.79329400	2.73340400
C	-0.51659500	-1.97425700	4.05800800
C	-1.87366300	-2.10159600	4.34257000
H	0.20082200	-2.00816500	4.87231400
C	-2.39336000	-1.85501500	1.99574600
C	-2.81472400	-2.04768500	3.31023500
H	-2.19796900	-2.24101300	5.36901000
H	-3.11011000	-1.81196000	1.18224800
H	-3.87143600	-2.15314600	3.53487900
Co	2.42321100	-1.18358500	0.36059600
C	1.27976300	0.57130900	-2.43131300
C	0.44731100	1.64234900	-3.05942800
C	0.98022000	2.50373200	-4.02450700
C	-0.89674600	1.78087600	-2.68002100
C	0.18719400	3.50156100	-4.59185900
H	2.02035600	2.40041600	-4.31884200
C	-1.68749700	2.77905600	-3.24782100
H	-1.30958000	1.09942500	-1.94094900
C	-1.14529600	3.64379100	-4.20196800
H	0.61012900	4.16763900	-5.33722300
H	-2.72447700	2.88492000	-2.94420900
H	-1.75995500	4.42276000	-4.64167200
C	1.03389700	-0.72169400	-2.78670900
C	0.02374600	-1.08674400	-3.85975200
H	-0.88661700	-0.49248600	-3.84810600
H	0.48718100	-0.94667400	-4.84650500
N	-0.24820600	-2.52062600	-3.68128600
C	1.03697300	-3.08491200	-3.21531900
H	0.87694500	-4.04200400	-2.72050100
H	1.65558700	-3.25009900	-4.10305200
S	-1.58442300	-2.79596500	-2.63955700
O	-1.46405500	-4.18348500	-2.18581000
O	-1.70679800	-1.70784300	-1.64459600
C	-2.93259900	-2.62501200	-3.78856400
C	-3.15073800	-3.64172700	-4.72044200

C	-3.73607800	-1.48686900	-3.72986700
C	-4.20312000	-3.50419500	-5.62122400
H	-2.51263100	-4.51802700	-4.72903400
C	-4.78479000	-1.36237400	-4.64169800
H	-3.54188000	-0.72960000	-2.97948700
H	-4.39267200	-4.28413200	-6.35120500
H	-5.42262200	-0.48509000	-4.61266800
C	-1.03441500	-1.72328300	1.70752800
H	-0.73711500	-1.56163500	0.68108100
C	1.66866500	-2.00327600	-2.29632700
H	2.75265400	-1.95660900	-2.42042800
C	1.36823600	-2.33733500	-0.81861500
H	0.32530000	-2.61542100	-0.68681900
H	1.97127600	-3.20802500	-0.52957700
O	3.09866000	0.02323700	-1.00465200
H	1.03833600	-1.03542000	-0.11613300
C	2.36603900	0.91921500	-1.51101200
C	2.71801000	2.30886400	-1.12012000
C	1.78793500	3.35797400	-1.00497100
C	4.04782600	2.53069000	-0.71178900
C	2.19029200	4.59637300	-0.50683500
H	0.75214700	3.20977500	-1.27366900
C	4.44760000	3.77295700	-0.23745100
H	4.75279100	1.71082700	-0.76236400
C	3.51863100	4.81265000	-0.13562000
H	1.46133600	5.39475400	-0.41295600
H	5.47931200	3.92652200	0.06160300
H	3.82693800	5.78448500	0.23729600
C	-5.01535900	-2.36646100	-5.58302600
H	-5.83385900	-2.26608500	-6.28864300
C	6.14124000	-3.80104900	2.13515500
H	6.77685100	-3.04088400	2.59704100
H	6.14948300	-4.68573000	2.78011000
H	6.58491900	-4.07960400	1.17550400
H	2.27339300	-2.70704100	4.43626100
C	1.94399400	-4.28037600	3.01640900
H	2.48772000	-5.07737500	3.53324900
H	0.89162500	-4.34776800	3.29731300
H	2.00636600	-4.47192900	1.94056200

S**2 before annihilation 2.0783, after 2.0013

S-TS5^{triplet}

C	0.37452300	-2.25062800	2.86534800
C	-0.31401400	-3.33805600	2.00016700

C	1.91090800	-2.09620500	2.77588400
H	-1.32367600	-3.46320500	2.40962300
H	-0.09845200	-1.27591100	2.70361200
H	0.15373100	-2.51392100	3.90674500
H	2.35686100	-3.08918900	2.66227800
P	2.39993500	-1.17683700	1.22941000
P	-0.55513000	-2.83475400	0.22093500
C	4.21180500	-1.24145900	1.09517300
C	4.84168000	-0.34206000	0.21670700
C	4.96945800	-2.25770700	1.69417100
C	6.20458000	-0.45363700	-0.04685900
H	4.26050900	0.44281300	-0.25723100
C	6.33613100	-2.36408900	1.42923800
H	4.50687100	-2.96557700	2.37358300
C	6.95356400	-1.46505100	0.56097000
H	6.68495400	0.23698900	-0.73134800
H	6.91549100	-3.14880500	1.90516800
H	8.01284400	-1.54985600	0.34941800
C	1.96288700	0.56583100	1.52542900
C	2.78879800	1.42950900	2.26228200
C	0.73635100	1.03640500	1.03263900
C	2.38361600	2.74021300	2.50744300
H	3.74654000	1.08014100	2.63304900
C	0.33053200	2.34539700	1.28978400
H	0.10025000	0.38529000	0.44529500
C	1.15350700	3.19767900	2.02703600
H	3.02693200	3.40522800	3.07477400
H	-0.62388700	2.69393200	0.90844400
H	0.84223100	4.21883900	2.22296200
C	-1.74763000	-1.45019400	0.23957300
C	-1.85883800	-0.68894000	-0.93618100
C	-2.51528000	-1.09879500	1.35851700
C	-2.71866000	0.40576900	-0.98850000
H	-1.25672200	-0.95000900	-1.80104600
C	-3.36773200	0.00452100	1.30551300
H	-2.45613600	-1.67278500	2.27617800
C	-3.46849800	0.75924400	0.13614800
H	-2.79954600	0.98516600	-1.90266500
H	-3.95428500	0.27212100	2.17852300
H	-4.13237700	1.61699400	0.09928700
C	-1.39973400	-4.22481200	-0.59335900
C	-0.88618400	-4.70495500	-1.80508700
C	-1.50978100	-5.76741800	-2.45974700
H	-0.00636900	-4.23698400	-2.23663200

C	-3.16919100	-5.87235100	-0.69939800
C	-2.64697900	-6.35363600	-1.90375100
H	-1.10939000	-6.13485100	-3.39906700
H	-4.05962500	-6.32403000	-0.27415300
H	-3.13178100	-7.18213600	-2.40991200
Co	1.41906300	-2.06148700	-0.65569400
C	1.58546200	-0.74408300	-2.01499500
C	2.58456000	-1.44892900	-2.46772900
C	3.75607500	-1.14310100	-3.37416300
H	3.42567200	-0.82774800	-4.36611200
H	4.32250500	-0.31862800	-2.91213300
N	4.53901500	-2.36213200	-3.46770500
C	4.42567700	-3.14827900	-2.25065200
H	4.81481900	-4.15071000	-2.43071200
H	4.94586200	-2.69984900	-1.39314000
S	5.90000600	-2.41685900	-4.44085500
O	6.34345700	-3.80866000	-4.41293600
O	5.52013200	-1.71444100	-5.66418300
C	7.14070100	-1.42760200	-3.61494900
C	8.10224100	-2.05879800	-2.82514600
C	7.13122300	-0.04093700	-3.79035500
C	9.07453700	-1.28003400	-2.19749300
H	8.10035600	-3.13930200	-2.73922900
C	8.09850600	0.72743200	-3.14328600
H	6.40659900	0.41465300	-4.45575900
H	9.84673300	-1.75903900	-1.60367400
H	8.11167200	1.80401200	-3.27930500
C	-2.55227200	-4.80837700	-0.04609800
H	-2.97254700	-4.42841300	0.88047600
C	2.92011700	-3.19341200	-1.99635700
C	2.49551300	-3.73690700	-0.69561900
H	1.83403400	-4.59674400	-0.72794800
H	3.27050000	-3.79065000	0.06497000
C	9.06815600	0.10871700	-2.34854500
H	9.83111400	0.70879000	-1.86284900
C	2.46269800	-1.44247200	4.04967700
H	1.99113800	-0.47235000	4.22722500
H	2.26088500	-2.08123500	4.91530000
H	3.54258000	-1.28638500	3.99049500
C	0.38143100	-4.70283100	2.08560600
H	1.35682600	-4.69496600	1.59513300
H	0.53236800	-4.97609200	3.13477400
H	-0.22108500	-5.48351800	1.61730600
H	2.40383800	-3.66611600	-2.83348500

H	1.25309200	0.26457300	-2.21904300
S**2 before annihilation	2.0678,	after	2.0011
<i>R-TS5</i> ^{triplet}			
C	0.40288000	-1.92686700	2.98983400
C	-0.45361500	-2.95501300	2.20341900
C	1.94424100	-1.98102500	2.86194700
H	-1.46318300	-2.90275400	2.62857500
H	0.06162900	-0.90620500	2.78538200
H	0.17970900	-2.10219900	4.04912800
H	2.25982500	-3.02721400	2.79669100
P	2.52982400	-1.20419600	1.26956800
P	-0.62819000	-2.51121100	0.40434500
C	4.31705200	-1.49861200	1.12065200
C	5.01336100	-0.77018400	0.14014000
C	4.97960500	-2.51848900	1.81828200
C	6.35184300	-1.04996100	-0.12291700
H	4.50519300	0.01400200	-0.41315400
C	6.32103400	-2.79591400	1.54818700
H	4.46331500	-3.09783600	2.57609400
C	7.00801500	-2.06470000	0.57958300
H	6.88286400	-0.47846900	-0.87736800
H	6.82716300	-3.58287800	2.09797000
H	8.05010500	-2.28341700	0.37098600
C	2.29327900	0.58782200	1.47535800
C	3.22750600	1.39077300	2.14787300
C	1.11276500	1.16243100	0.98092800
C	2.97162800	2.74854200	2.33106900
H	4.15239000	0.95852000	2.51501200
C	0.85621900	2.51846300	1.17810600
H	0.39939200	0.55479100	0.43686300
C	1.78510500	3.31151300	1.85333400
H	3.69804900	3.36803300	2.84720600
H	-0.06411200	2.94987400	0.79777400
H	1.59079300	4.36901400	2.00145000
C	-1.67969000	-1.01544500	0.34845200
C	-1.78411900	-0.36512800	-0.89303000
C	-2.32207700	-0.46395100	1.46490700
C	-2.51317700	0.81519400	-1.01266100
H	-1.28582700	-0.78622800	-1.76082900
C	-3.04405400	0.72423500	1.34357300
H	-2.26614700	-0.94619400	2.43396800
C	-3.13804800	1.36702900	0.10898100
H	-2.59097400	1.30698600	-1.97711000

H	-3.53436500	1.14529600	2.21544900
H	-3.69991700	2.29110700	0.01888800
C	-1.59145800	-3.82684400	-0.40548300
C	-2.73080300	-4.40179200	0.17570300
C	-3.43490700	-5.39116600	-0.50777400
H	-3.07102700	-4.07667700	1.15443100
C	-1.89175400	-5.22296700	-2.36739700
C	-3.01546100	-5.80196700	-1.77659000
H	-4.31378900	-5.83853500	-0.05470300
H	-1.56721500	-5.53333900	-3.35487400
H	-3.56981600	-6.57154000	-2.30443300
Co	1.42327100	-2.03210600	-0.53270900
C	1.52028800	-0.97811500	-2.09894100
C	2.06317800	-2.02243100	-2.66214200
C	2.26485500	-2.46410400	-4.09019400
H	1.26712200	-2.55600100	-4.54972300
H	2.83657700	-1.72838400	-4.65943400
N	2.97647300	-3.73772200	-4.05508500
C	2.65524200	-4.46273300	-2.83291400
H	1.63401000	-4.87725000	-2.83252600
H	3.36605300	-5.27929400	-2.70128900
S	3.07429600	-4.61448500	-5.49585500
O	3.41606200	-3.63244100	-6.52116100
O	3.89607600	-5.78101100	-5.18687400
C	1.40136800	-5.17414500	-5.78962700
C	0.52914500	-4.36616600	-6.52416600
C	0.98613000	-6.38997100	-5.24065300
C	-0.79032600	-4.78346900	-6.69906800
H	0.89607600	-3.45185200	-6.97674500
C	-0.33395600	-6.79893000	-5.43004300
H	1.69835500	-7.01233900	-4.71091900
C	-1.22055400	-5.99486100	-6.15226000
H	-1.47616000	-4.17317600	-7.27752400
H	-0.66510700	-7.75102500	-5.02777000
C	-1.17984600	-4.24011300	-1.68014300
H	-0.30664000	-3.78041900	-2.13255900
C	2.80465600	-3.43999000	-1.71689900
H	3.82417300	-3.05956200	-1.64894600
C	2.26152300	-3.83776700	-0.41013200
H	1.51968700	-4.63296500	-0.42941700
H	2.98226500	-3.90933900	0.39781500
C	2.59738200	-1.33267000	4.09160500
H	2.24403300	-0.30666800	4.22327400
H	2.33985100	-1.89879900	4.99215100

H	3.68639500	-1.30479200	4.01084400
C	0.04283000	-4.39702100	2.37390300
H	0.15868700	-4.62340900	3.43864100
H	-0.66449200	-5.11336400	1.95204700
H	1.00756100	-4.55957200	1.88910600
H	-2.24454600	-6.32141500	-6.30415800
H	1.14739200	-0.03970400	-2.48545300

S**2 before annihilation -0.0000, after -0.0000

S-TS6^{CSS}

C	0.93844200	-2.95435300	2.60078600
C	-0.05542800	-3.92419700	1.92966000
C	2.22382100	-2.60601200	1.82612600
H	-0.82464500	-4.15631900	2.67557200
H	0.43779900	-2.02506400	2.89142300
H	1.25101400	-3.43066900	3.53786600
H	2.57525900	-3.50030900	1.30098300
P	1.87879300	-1.38083300	0.46345700
P	-0.95381400	-3.15188400	0.49775400
C	3.51448700	-1.02749700	-0.26565400
C	3.82592700	0.27117100	-0.69503400
C	4.43908900	-2.05918900	-0.49310500
C	5.04690800	0.53502000	-1.31493400
H	3.12170300	1.07920800	-0.53306600
C	5.65655700	-1.79405100	-1.12007100
H	4.22406300	-3.07256600	-0.17098600
C	5.96579700	-0.49441900	-1.52330400
H	5.28055800	1.54694000	-1.63061900
H	6.36309500	-2.59707900	-1.29754600
H	6.91440200	-0.29349100	-2.00595500
C	1.35531500	0.17020500	1.26577700
C	2.20985000	0.93588500	2.07773500
C	0.03655600	0.60241500	1.06551000
C	1.73704700	2.09202300	2.69443900
H	3.24454700	0.64192200	2.20971300
C	-0.43609900	1.75835600	1.68595300
H	-0.63607400	0.03349900	0.43430900
C	0.41338000	2.50045900	2.50599300
H	2.40262500	2.67783500	3.32031000
H	-1.46393100	2.06749100	1.52930800
H	0.05077800	3.40071500	2.99184400
C	-2.14500200	-1.96423500	1.22345200
C	-2.92781100	-1.22430200	0.31847700
C	-2.28017800	-1.72841100	2.59743400

C	-3.81638000	-0.25876700	0.78663500
H	-2.82402600	-1.40426700	-0.74655500
C	-3.17086400	-0.75848700	3.06018900
H	-1.70197000	-2.29234200	3.31952900
C	-3.93489200	-0.01848800	2.15817300
H	-4.41908400	0.30432200	0.08079100
H	-3.26702500	-0.58447100	4.12718300
H	-4.62605000	0.73532000	2.52162900
C	-2.02149100	-4.48750100	-0.14405700
C	-2.88150500	-5.16400400	0.73600300
C	-3.68805500	-6.19842400	0.26911100
H	-2.93139000	-4.87555200	1.78194700
C	-2.81157700	-5.87829700	-1.96164700
C	-3.64974400	-6.56024400	-1.08049000
H	-4.34981300	-6.71860900	0.95420900
H	-2.79242200	-6.14810800	-3.01298600
H	-4.27996300	-7.36601600	-1.44305700
Co	0.29120900	-1.96776900	-1.00014700
C	1.19147200	-0.80252200	-2.43141400
C	1.99134200	-1.63538400	-3.13485100
C	3.15866500	-1.35681400	-4.03816600
H	2.90256100	-0.65915800	-4.84061400
H	4.00014500	-0.93666800	-3.46564600
N	3.43746600	-2.69043500	-4.58681800
C	3.05014300	-3.72617100	-3.62555000
H	2.90962600	-4.67733500	-4.13747700
H	3.79755200	-3.84655700	-2.82595100
S	4.67496300	-2.93616400	-5.67675900
O	4.48785500	-4.29406000	-6.18349600
O	4.68090300	-1.75141900	-6.53443800
C	6.19014700	-2.92503600	-4.72309900
C	6.56786000	-4.08016300	-4.03275400
C	6.96921800	-1.76845900	-4.69261900
C	7.74378300	-4.06536300	-3.28381900
H	5.96886600	-4.97992400	-4.11707200
C	8.15105300	-1.77055200	-3.95065600
H	6.66167400	-0.90315600	-5.26844700
C	8.53320600	-2.91185700	-3.24188000
H	8.05696400	-4.95892500	-2.75329000
H	8.78125700	-0.88664600	-3.93858500
C	-1.99905800	-4.84237500	-1.49809400
H	-1.37544700	-4.28520100	-2.18358700
C	1.74606500	-3.12258600	-3.06227700
C	1.32785000	-3.51127400	-1.65727200

C	3.31729200	-2.15043200	2.80258200
H	2.96183800	-1.32859300	3.42937100
H	3.58208100	-2.98094800	3.46442400
H	4.22490800	-1.82635500	2.28930200
C	0.59696800	-5.25332600	1.51834400
H	1.16709000	-5.65899300	2.36036200
H	-0.15699800	-5.98919700	1.23421100
H	1.28072100	-5.14118600	0.67366000
H	0.94358800	-3.34864900	-3.78006500
H	2.19370700	-3.68142600	-1.01535600
H	0.68037400	-4.38695200	-1.62772300
H	9.45712500	-2.91019600	-2.67214100
C	-0.96425300	-2.98495400	-6.34491800
C	-0.47500200	-2.04487700	-7.25140700
C	-0.09048000	-0.77380300	-6.80765900
C	-0.18426400	-0.45208000	-5.45932800
C	-0.64688000	-1.40501300	-4.53801900
C	-1.04796100	-2.66981100	-4.98854100
H	-1.27908100	-3.96317400	-6.69371100
H	-0.39807700	-2.29503500	-8.30441500
H	0.27991800	-0.04085800	-7.51673400
H	0.11831200	0.53142000	-5.10890300
H	-1.44527700	-3.37980600	-4.27226000
C	-0.69671400	-1.07538600	-3.09763000
O	-1.15563300	-1.95943700	-2.24718100
H	-0.89900400	-0.01690100	-2.88731600
H	1.37013500	0.27157200	-2.41982000

S**2 before annihilation -0.0000, after -0.0000

R-TS6^{CSS}

C	-0.23276700	-2.49114800	2.85898900
C	-0.29615400	-3.33861900	1.56974400
C	1.15767400	-2.00126700	3.31456400
H	-1.32644900	-3.69887400	1.46910300
H	-0.91264200	-1.63489200	2.79239200
H	-0.63058700	-3.12355600	3.66180300
H	1.89928300	-2.77452600	3.08842300
P	1.68670800	-0.52684300	2.30917400
P	-0.00269800	-2.31781400	0.03490900
C	3.37759500	-0.11305500	2.84964800
C	3.85992300	1.18316100	2.60245400
C	4.24414800	-1.07458000	3.39035100
C	5.18232500	1.50709200	2.89991200
H	3.20444600	1.92894600	2.16933200

C	5.56716800	-0.74419500	3.68682200
H	3.89789700	-2.08390800	3.58583400
C	6.03861200	0.54543900	3.44116200
H	5.54356500	2.51250000	2.70816100
H	6.22579900	-1.49466700	4.11205700
H	7.06734700	0.80141000	3.67351600
C	0.65855700	0.86367600	2.88776200
C	0.92881400	1.51808000	4.10124800
C	-0.44124000	1.26818800	2.12043100
C	0.09783800	2.54613200	4.54075200
H	1.79278300	1.23382000	4.69126300
C	-1.27290700	2.29532600	2.56533400
H	-0.64378800	0.79079900	1.17242400
C	-1.00622200	2.93323600	3.77642600
H	0.31368600	3.04811200	5.47848400
H	-2.12100400	2.59654700	1.95909800
H	-1.64961800	3.73598200	4.12246400
C	-1.47995600	-1.24047100	-0.09762800
C	-1.41821100	-0.15655600	-0.99293300
C	-2.62924800	-1.39601600	0.69073300
C	-2.46977900	0.75342600	-1.08500400
H	-0.54174500	-0.02181600	-1.61420900
C	-3.67800900	-0.48086400	0.60153700
H	-2.72111900	-2.22412800	1.38250100
C	-3.59988800	0.59770300	-0.28060700
H	-2.40346700	1.58442200	-1.77983200
H	-4.55779700	-0.61303000	1.22294600
H	-4.41767500	1.30811900	-0.34542700
C	-0.12986900	-3.48011000	-1.36607300
C	-1.24016200	-3.48183600	-2.22035700
C	-1.28726500	-4.35919600	-3.30577900
H	-2.06468700	-2.80093900	-2.04309100
C	0.87453700	-5.24922600	-2.69311400
C	-0.23435100	-5.24239100	-3.54250600
H	-2.15118300	-4.35174600	-3.96283700
H	1.69388200	-5.93481700	-2.87097300
H	-0.26927600	-5.92420400	-4.38541900
Co	1.63522300	-0.80404800	0.04653000
C	1.82463800	-0.83052200	-2.02998700
C	2.81929400	-1.69688200	-2.31210000
C	3.14866900	-2.42648700	-3.58561200
H	2.34064900	-3.12172600	-3.86160800
H	3.31809900	-1.74172600	-4.42183400
N	4.39784800	-3.11060400	-3.22657300

C	4.47404400	-3.34432300	-1.78130700
H	3.90741100	-4.23636800	-1.47173700
H	5.51321600	-3.46598400	-1.47892500
S	5.16568900	-4.10385900	-4.32258400
O	5.09157800	-3.40537100	-5.60502200
O	6.42421000	-4.49138800	-3.68827900
C	4.14670300	-5.57007100	-4.45407300
C	3.17779500	-5.63997200	-5.45672700
C	4.33647300	-6.61553600	-3.54633100
C	2.38241200	-6.78254700	-5.54888600
H	3.08277800	-4.82612300	-6.16617400
C	3.53058000	-7.74969100	-3.64514900
H	5.12665400	-6.54919500	-2.80690700
H	1.64038900	-6.85947600	-6.33730000
H	3.67493700	-8.57566700	-2.95621600
C	0.92906600	-4.36658100	-1.61844500
H	1.80059900	-4.36788400	-0.97658200
C	3.81874900	-2.05121800	-1.24652800
H	4.59368200	-1.27128400	-1.26932100
C	3.15129900	-2.07995200	0.12000600
H	2.78679200	-3.07383100	0.38005200
H	3.81427300	-1.72116400	0.90620300
C	4.14141700	1.27049000	-3.30570500
C	5.43378300	1.37731400	-3.80516800
C	6.52677200	1.32859100	-2.93121800
C	6.32204100	1.17978300	-1.55932500
C	5.02713800	1.05779600	-1.05473200
C	3.93199000	1.09832100	-1.92922100
H	3.28932000	1.30442100	-3.97984500
H	5.59630500	1.49942400	-4.87090200
H	7.53496800	1.41159800	-3.32402400
H	7.16989000	1.15358900	-0.88219500
H	4.84577200	0.94331400	0.00802700
O	2.38560200	0.91034200	-0.10019700
C	2.56117100	0.95447800	-1.39684500
H	1.78594600	1.45809400	-1.98869200
C	2.55545000	-7.83253600	-4.64396900
H	1.94011100	-8.72300900	-4.72457700
C	1.16165900	-1.73350100	4.82533200
H	0.38465300	-1.01344100	5.09447800
H	0.96223200	-2.66443400	5.36542100
H	2.12089300	-1.34161200	5.16997000
C	0.59422100	-4.58725200	1.64755900
H	0.38708200	-5.11747500	2.58261500

H	0.39108100	-5.27226900	0.82358100
H	1.66117000	-4.35156300	1.63383800
H	1.07860100	-0.60005600	-2.79010900