

Supporting Information for:

**Computational Study on Cobalt-Catalyzed Allylic
Substitution of Racemic Allylic Carbonates with Amines:
Inner-Sphere C-N Reductive Elimination and Origins of
Regio- and Enantioselectivities**

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Possibility of the Co(0)/NPN complex as the active catalytic species

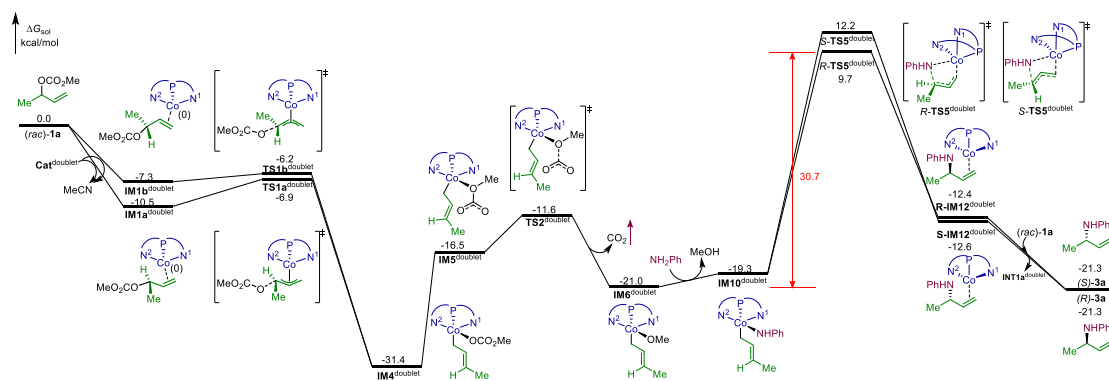


Figure S1. Calculated energy profile of Co(0)/NPN-catalyzed reaction. The energy barrier was calculated relative to $\text{IM6}^{\text{doublet}}$ rather than $\text{IM4}^{\text{doublet}}$, due to that the CO_2 extrusion is irreversible.

C–O oxidative addition via S_N2 front-side attack transition states

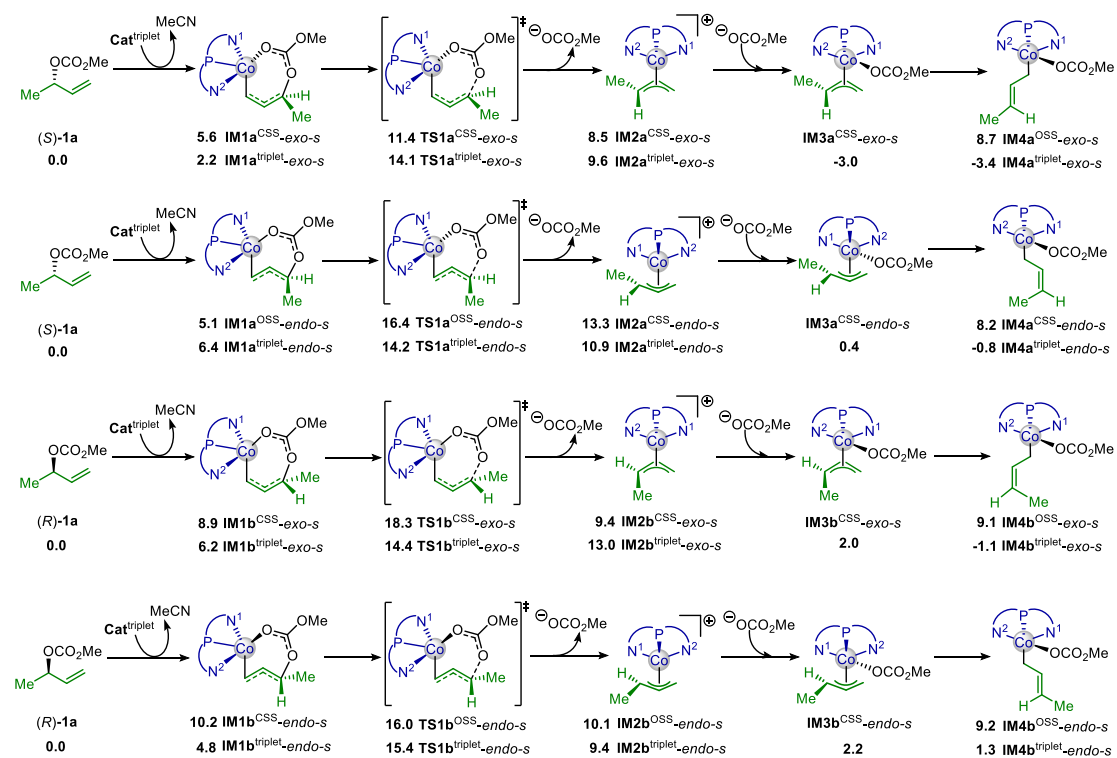


Figure S2. Calculated energies of C–O oxidative addition via S_N2 front-side attack transition states. Gibbs free energies are given in kcal/mol.

Other possibilities of S_N2 back-side attack pathway

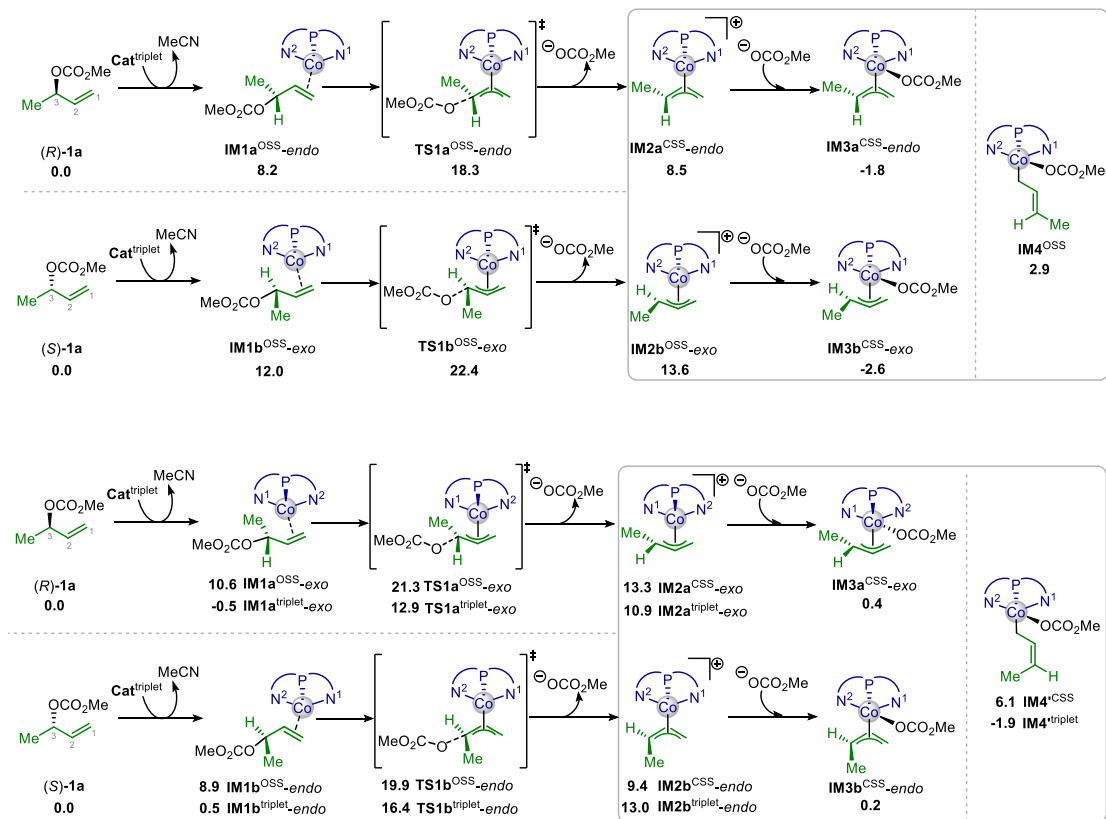


Figure S3. Calculated energies of other possibilities of S_N2 back-side attack pathway. Gibbs free energies are given in kcal/mol.

Other possibilities of outer-sphere nucleophilic attack

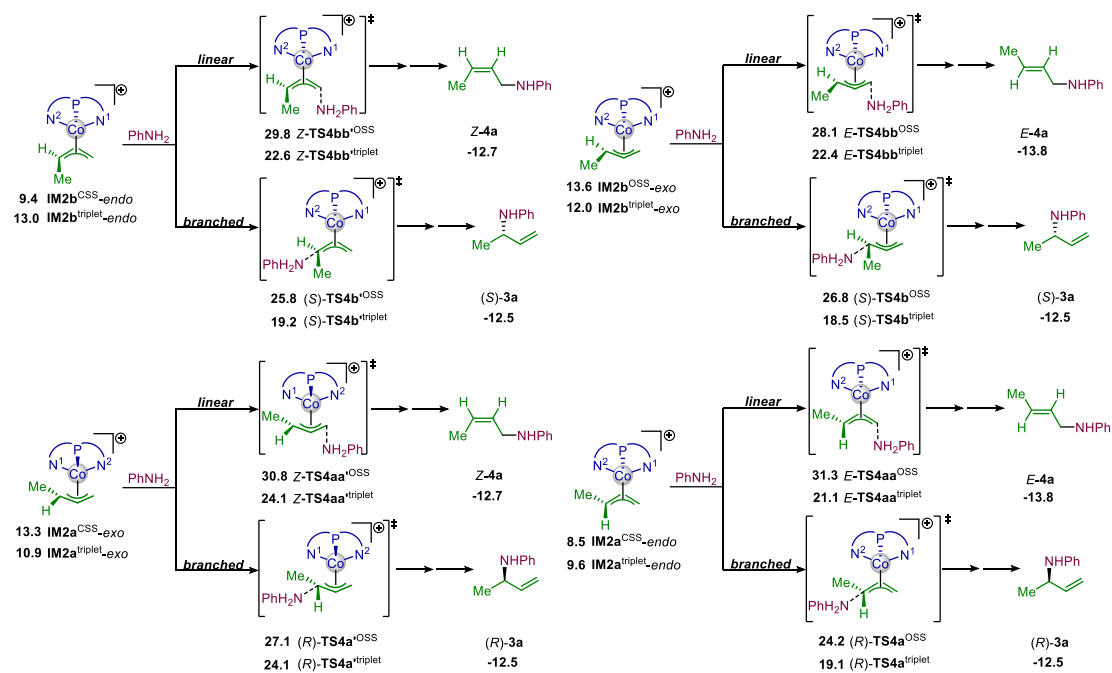


Figure S4. Calculated energies of outer-sphere nucleophilic attack from **IM2**. Gibbs free energies are given in kcal/mol.

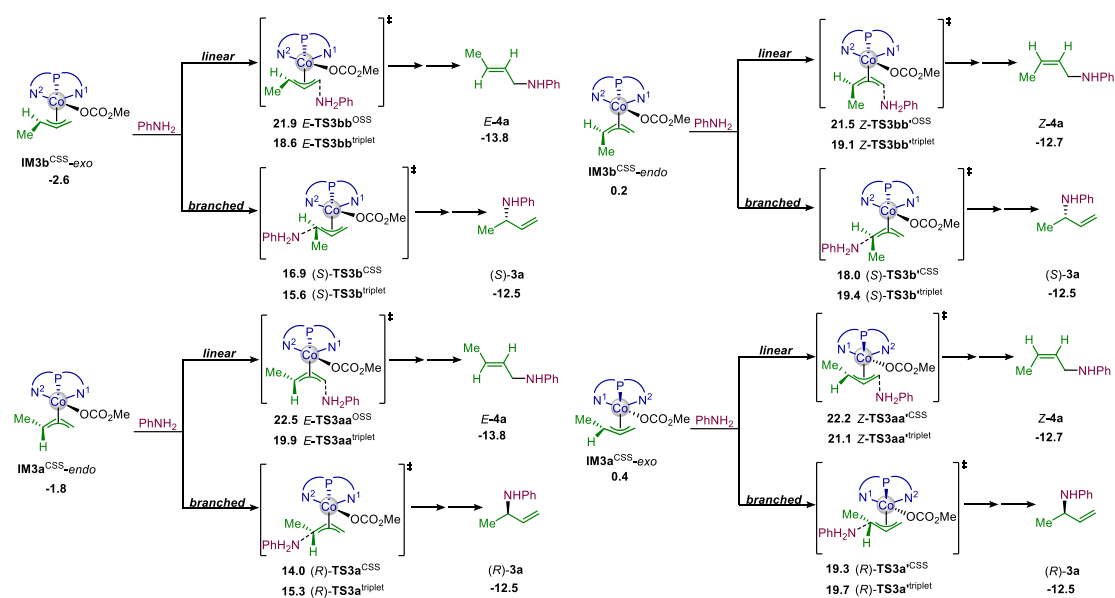


Figure S5. Calculated energies of outer-sphere nucleophilic attack from **IM3**. Gibbs free energies are given in kcal/mol.

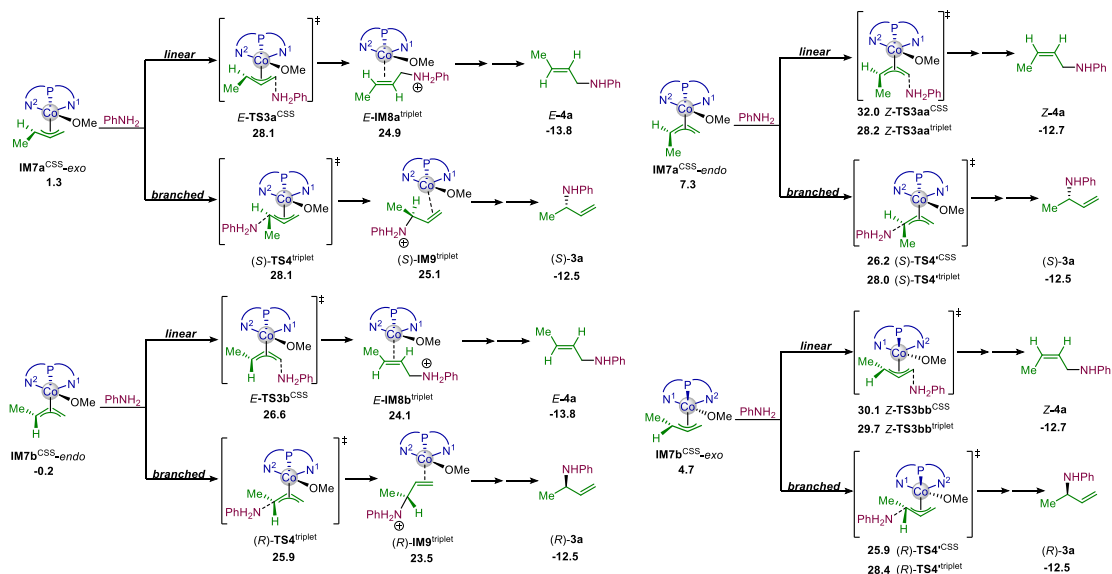


Figure S6. Calculated energies of outer-sphere nucleophilic attack from IM7. Gibbs free energies are given in kcal/mol.

CO₂ extrusion from the carbonate-coordinated η^3 -allyl-Co(III) species

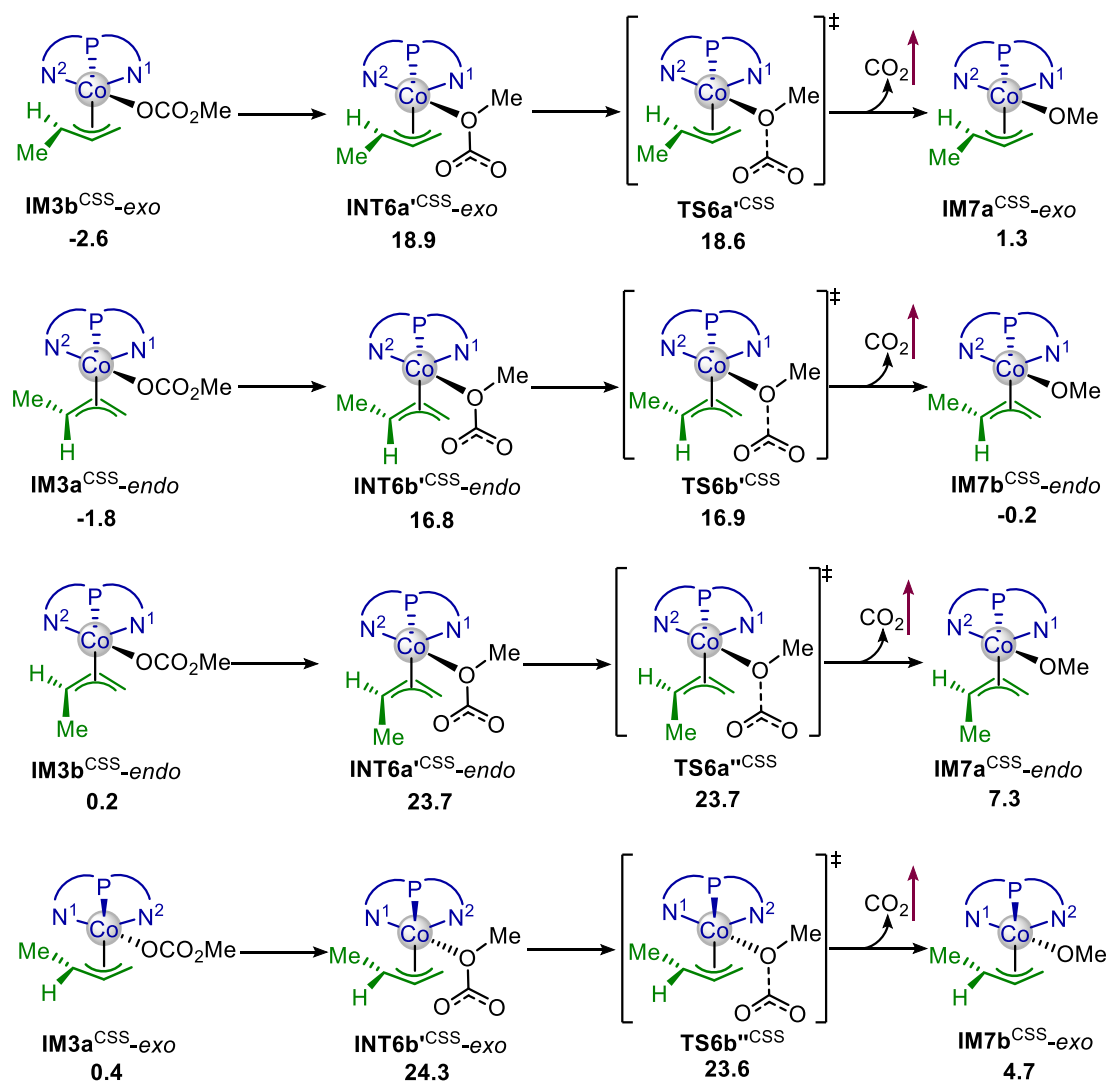


Figure S7. Calculated energies of CO₂ extrusion from the carbonate-coordinated η^3 -allyl-Co(III) species. Gibbs free energies are given in kcal/mol.

η^1 - η^3 isomerization

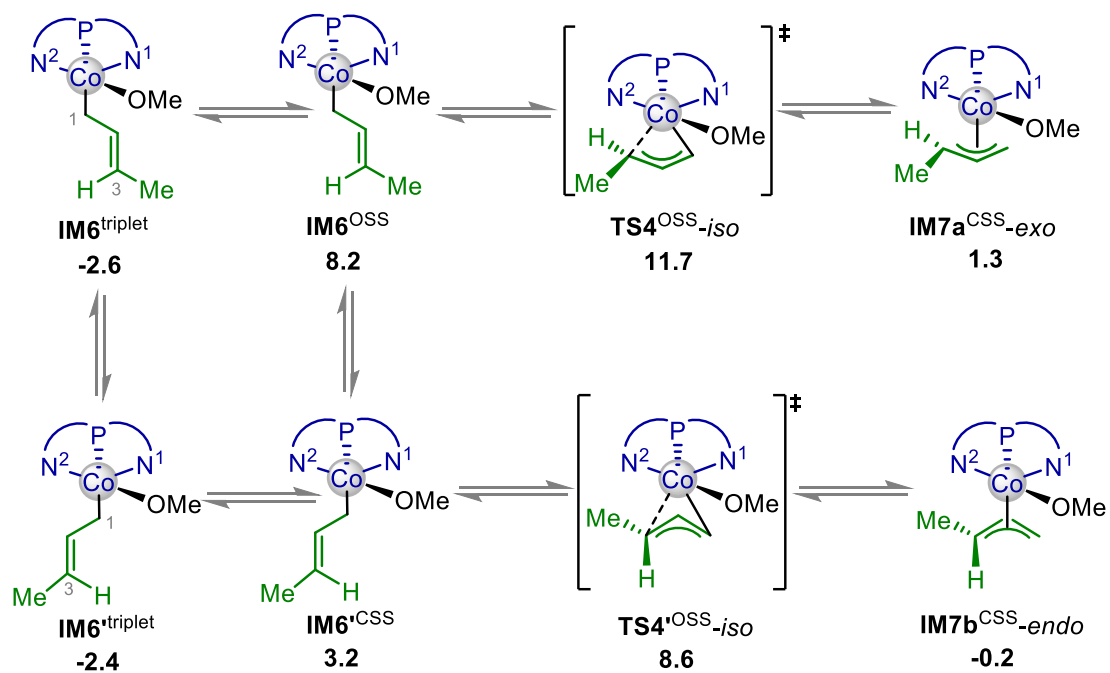


Figure S8. Calculated energies of η^1 - η^3 isomerization. Gibbs free energies are given in kcal/mol.

Proton transfer

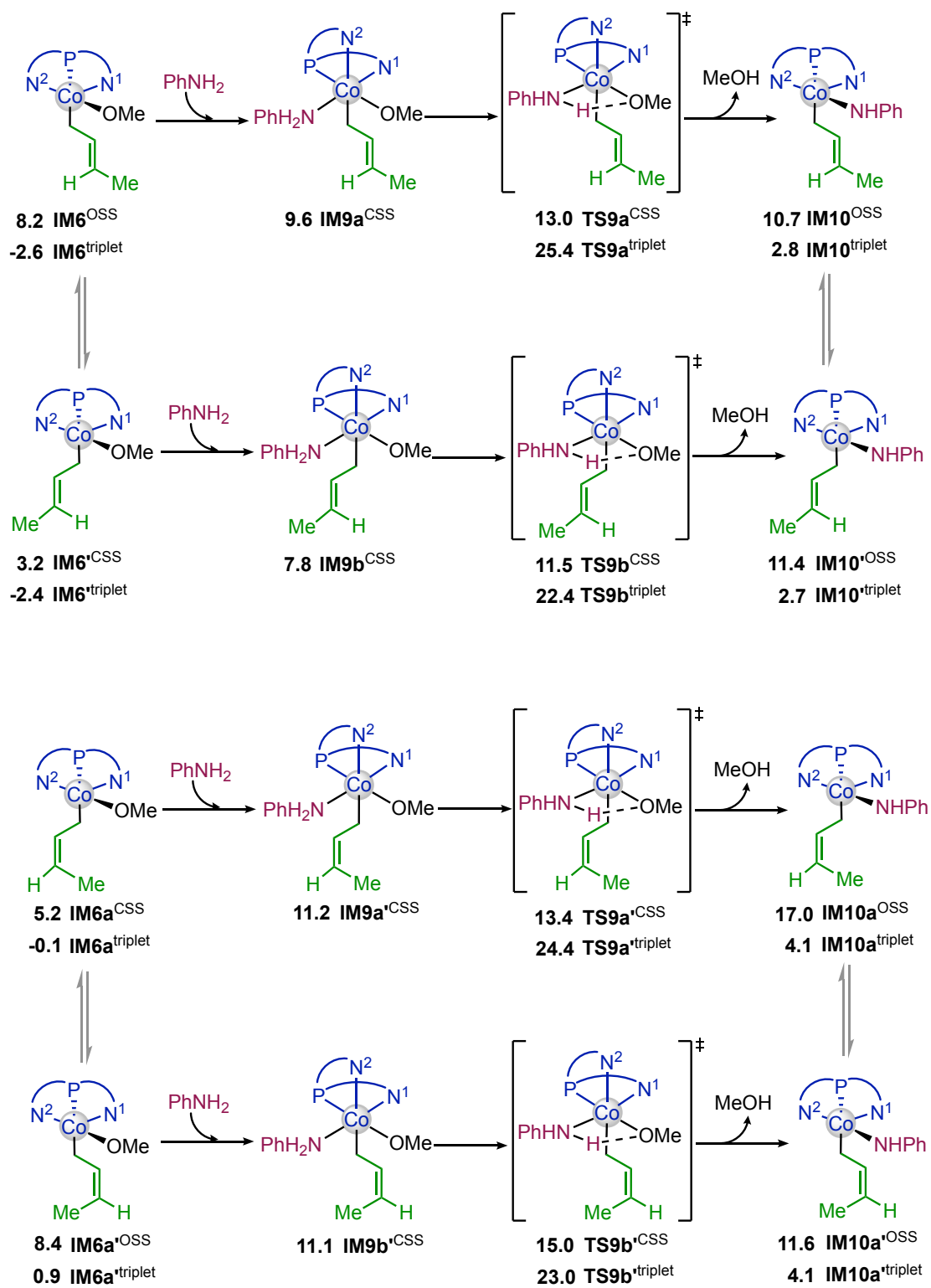


Figure S9. Calculated energies of proton transfer process. Gibbs free energies are given in kcal/mol.

Isomerization between IM10 and IM11

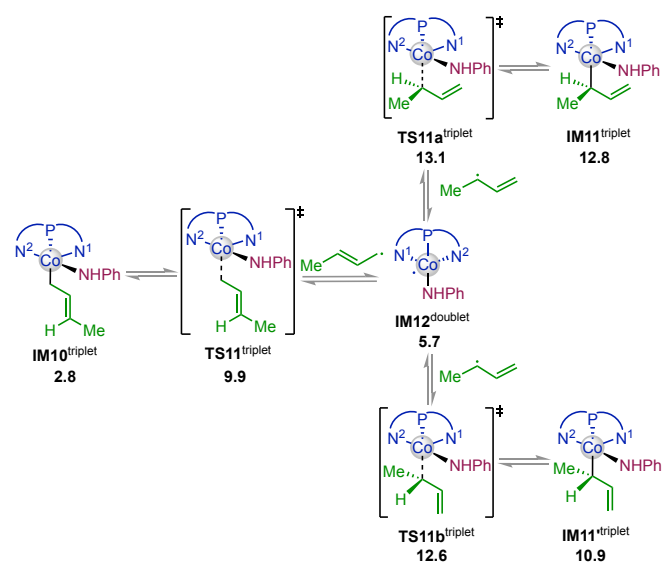


Figure S10. Calculated energies of isomerization between IM10 and IM11. Gibbs free energies are given in kcal/mol.

Other possibilities of C-N reductive elimination¹¹

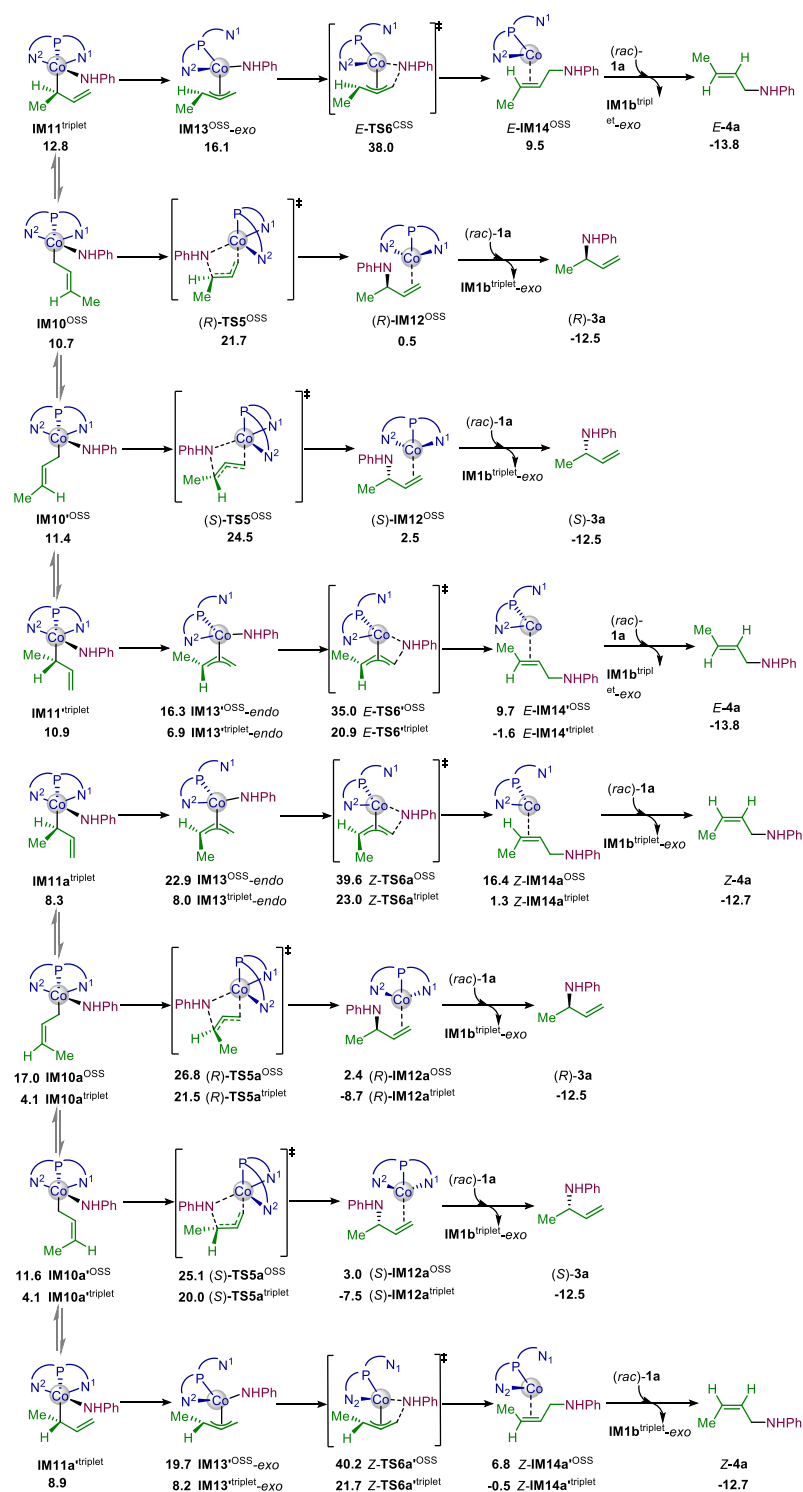


Figure S11. Calculated energies of C-N reductive elimination from **IM10** and **IM11**. Gibbs free energies are given in kcal/mol.

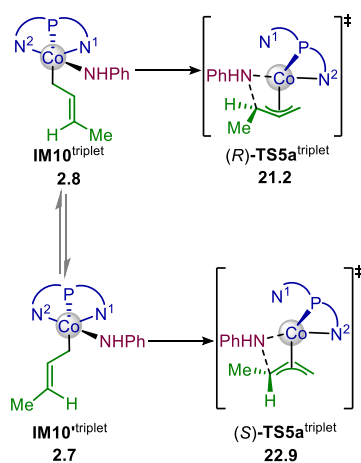


Figure S12. Calculated energies of C-N reductive elimination leading brached products via η^3 -transition states. Gibbs free energies are given in kcal/mol.

Optimized geometries of key transition states

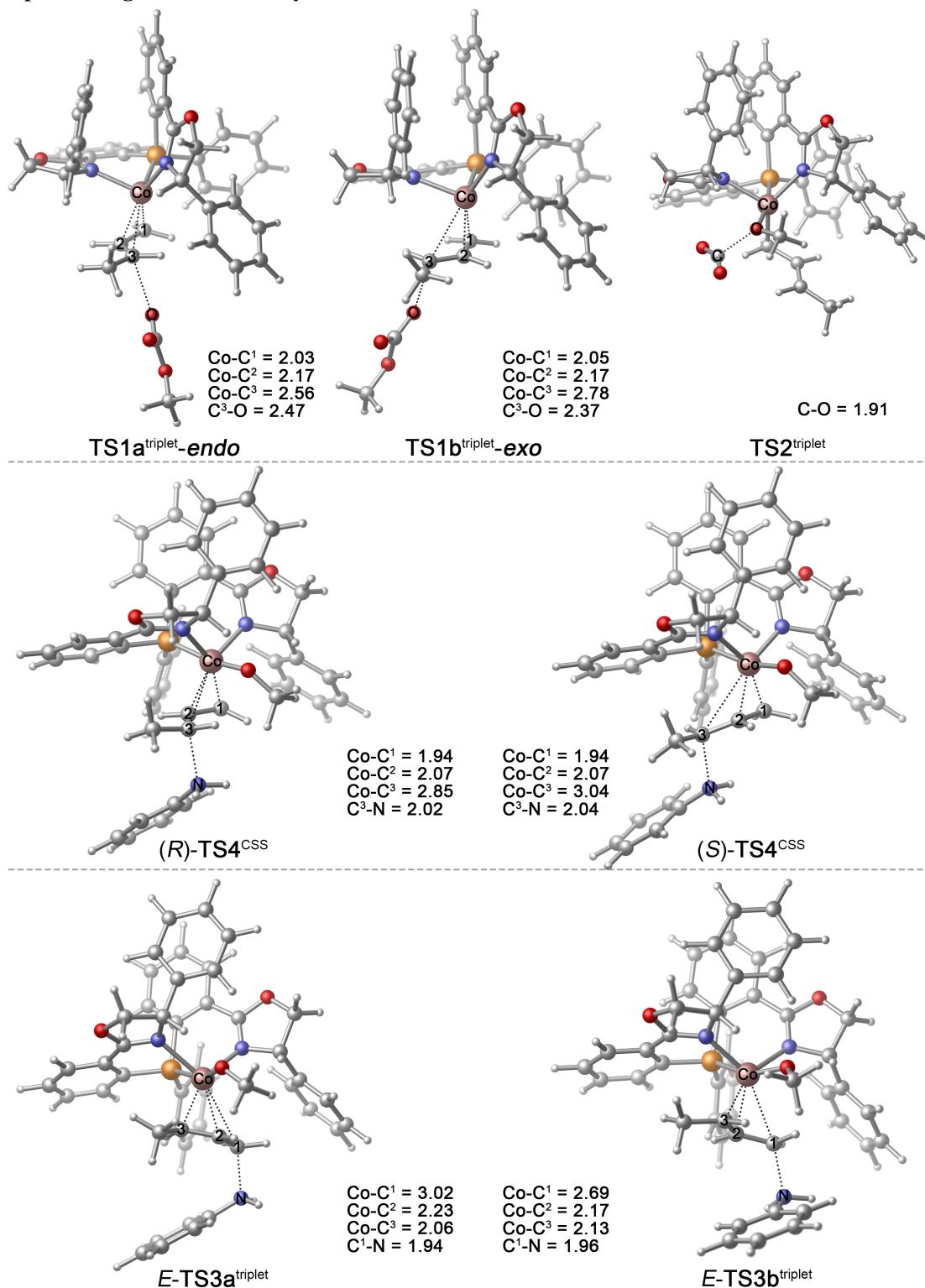


Figure S13. Optimized geometries of key transition states involved in the main pathway. Bond distances are given in Å.

Non-covalent interactions analysis of (*R*)-TS5^{triplet} and (*S*)-TS5^{triplet}

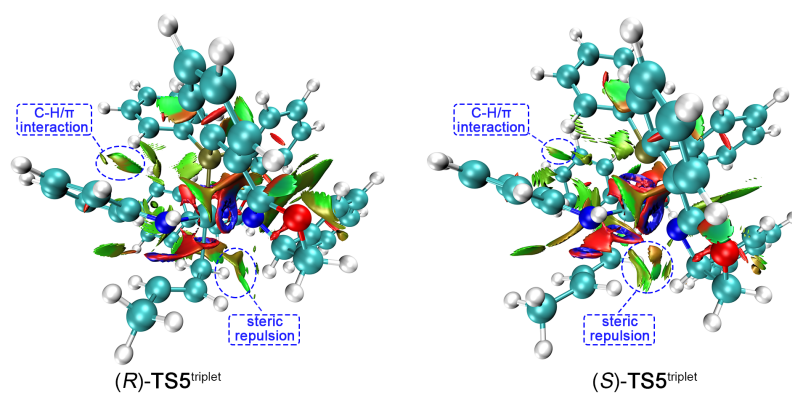


Figure S14. Non-covalent interactions analysis of (*R*)-TS5^{triplet} and (*S*)-TS5^{triplet}.

Rearrangement of the coordinating O atom of the OCO₂Me anion

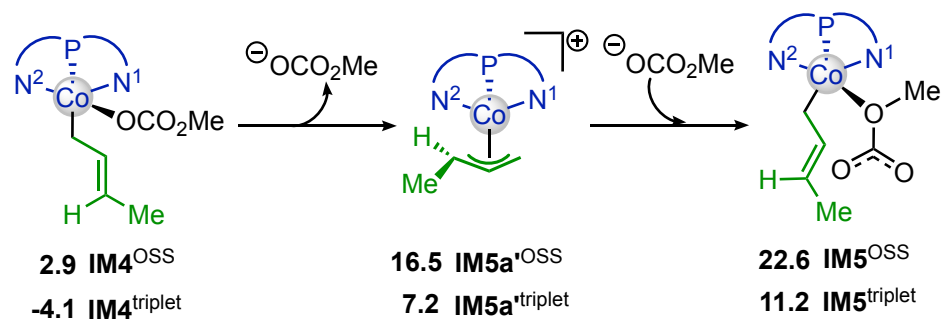
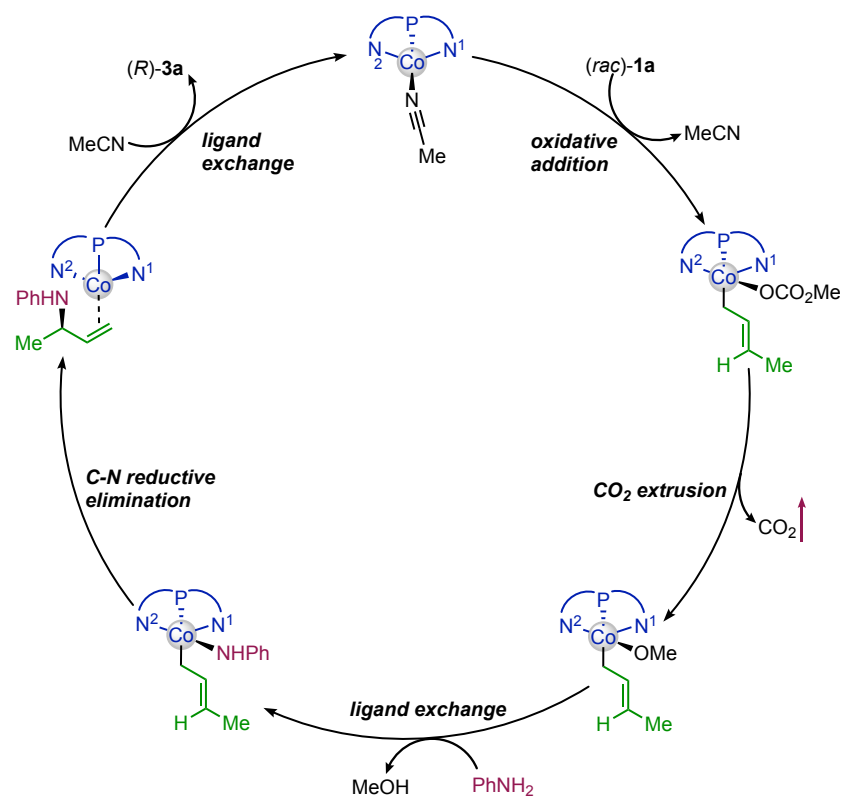


Figure S15. Calculated energies of rearrangement of the coordinating O atom of the OCO₂Me anion. Gibbs free energies are given in kcal/mol.

Overall catalytic cycle



Scheme S1. Overall catalytic cycle.

Table of calculated energies and energy corrections

Stationary point	Single-point energy (U)TPSSh-SMD/ Def2-TZVPP (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	DFT-D3(BJ) correction (kcal/mol)
(<i>R</i>)- 1a	-460.5335721	0.119379	-10.9859
(<i>S</i>)- 1a	-460.5335721	0.119379	-10.9859
Cat ^{triplet}	-3506.9661900	0.527605	-101.9035
MeCN	-132.8225051	0.021037	-1.9484
PhNH ₂	-287.7456990	0.087366	-9.5631
CO ₂	-188.6682277	-0.009138	-0.6493
MeOH	-115.7799784	0.028080	-1.2594
⁻ OCO ₂ Me	-303.9739983	0.025487	-3.1462
(<i>R</i>)- 3a	-443.8282030	0.168005	-18.8082
(<i>S</i>)- 3a	-443.8282030	0.168005	-18.8082
<i>E</i> - 4a	-443.8331260	0.167889	-17.0113
IM1a ^{triplet} - <i>endo</i>	-3834.6741615	0.634581	-119.7908
IM1b ^{triplet} - <i>exo</i>	-3834.6732431	0.632843	-119.4720
TS1a ^{triplet} - <i>endo</i>	-3834.6482408	0.629611	-120.8347
TS1b ^{triplet} - <i>exo</i>	-3834.6443486	0.628535	-119.2921
IM2a ^{triplet} - <i>endo</i>	-3530.6651443	0.587475	-114.0060
IM2b ^{triplet} - <i>exo</i>	-3530.6609962	0.587294	-114.0250
IM3a ^{CSS} - <i>endo</i>	-3834.6672304	0.641757	-128.9139
IM3b ^{CSS} - <i>exo</i>	-3834.6681535	0.640358	-128.2663
IM4 ^{triplet}	-3834.6681421	0.631628	-124.2928
IM5 ^{triplet}	-3834.6397999	0.633222	-127.7682
TS2 ^{triplet}	-3834.6377792	0.632627	-128.0152
IM6 ^{triplet}	-3645.9844678	0.621328	-119.7097
IM6 ^{*triplet}	-3645.9843424	0.621821	-119.9093
IM7a ^{CSS} - <i>exo</i>	-3645.9795718	0.629704	-124.0849
IM7b ^{CSS} - <i>endo</i>	-3645.9816606	0.630106	-124.5684
(<i>R</i>)- TS4 ^{CSS}	-3933.7037524	0.738034	-140.5110
(<i>S</i>)- TS4 ^{CSS}	-3933.7001459	0.736709	-140.2193
<i>E</i> - TS3a ^{triplet}	-3933.6901733	0.730429	-138.7210
<i>E</i> - TS3b ^{triplet}	-3933.6895668	0.727649	-138.2684

<i>(R)</i> - IM9 ^{CSS}	-3933.7106148	0.741671	-140.5289
<i>(S)</i> - IM9 ^{CSS}	-3933.7077722	0.741399	-140.6046
<i>E</i> - IM8a ^{CSS}	-3933.7014636	0.741083	-140.4012
<i>E</i> - IM8b ^{CSS}	-3933.7038229	0.742441	-142.1036
IM10 ^{triplet}	-3817.9347473	0.682055	-133.1782
IM10' ^{triplet}	-3817.9353065	0.682023	-132.8749
IM11 ^{triplet}	-3817.9132049	0.682676	-137.0865
IM13 ^{triplet} - <i>exo</i>	-3817.9305957	0.683598	-133.9308
<i>(R)</i> - TS5 ^{triplet}	-3817.9061460	0.683423	-138.0581
<i>(S)</i> - TS5 ^{triplet}	-3817.9035598	0.683281	-136.9066
<i>E</i> - TS6 ^{triplet}	-3817.9094865	0.680753	-131.1895
<i>(R)</i> - IM12 ^{triplet}	-3817.9666316	0.684026	-129.5879
<i>(S)</i> - IM12 ^{triplet}	-3817.9662107	0.684812	-129.1044
<i>E</i> - IM14 ^{triplet}	-3817.9492710	0.684067	-131.1320

Cartesian coordinates**(R)-1a**

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C	-2.90750000	1.91170300	3.24703500
H	-2.96148200	1.57597400	2.20358600
C	-2.92548300	3.40284700	3.44790600
H	-2.92900700	3.63995700	4.52141100
O	-4.15935800	3.93994900	2.86959700
C	-5.24352000	3.93444600	3.65091800
O	-5.29787100	3.58684400	4.81087900
O	-6.26980600	4.39627500	2.92968700
C	-7.52449200	4.47836800	3.62420100
H	-7.44660100	5.15743500	4.48594000
H	-8.24028200	4.87423900	2.89398400
H	-7.84301600	3.48296500	3.96698400
C	-1.78816500	4.11873500	2.73614600
H	-1.86897500	5.20654000	2.88493100
H	-0.82479400	3.77868100	3.14491100
H	-1.80483700	3.90599800	1.65565900

(S)-1a

C	-2.81128700	1.02211400	-4.24126800
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C	-2.90750000	1.91170300	-3.24703500
H	-2.96148200	1.57597400	-2.20358600
C	-2.92548300	3.40284700	-3.44790600
H	-2.92900700	3.63995700	-4.52141100
O	-4.15935800	3.93994900	-2.86959700
C	-5.24352000	3.93444600	-3.65091800
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H	-1.80483700	3.90599800	-1.65565900

Cat^{triplet}

Co	9.06692900	6.75438300	3.68451300
C	6.17510100	7.53336400	2.23996400

O	8.43980900	10.38030000	5.78003300
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P	6.85166500	6.61504500	3.70685700
N	9.11877100	6.78324400	1.67357200
O	8.51542800	6.65779700	-0.48376300
C	4.93626700	8.19082700	2.32617800
H	4.39365700	8.18578400	3.27370800
N	9.81096100	5.93059100	5.28416600
C	4.37079700	8.84205500	1.22500000
H	3.40676200	9.34558400	1.32935900
C	5.03673800	8.83492400	-0.00390200
H	4.60288700	9.33383200	-0.87339700
C	6.26914400	8.19188800	-0.11608900
H	6.80161000	8.19405900	-1.06808100
C	6.86054500	7.55488200	0.99419600
C	8.19681700	6.97078400	0.78477000
C	10.32762600	6.26809500	0.98818100
H	11.09815900	7.05315300	1.02819200
C	9.83906400	6.06151200	-0.46662700
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H	9.73185400	5.00202600	-0.74065300
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H	3.38690000	7.42783300	7.20106300
C	4.91174900	7.11330000	5.70443800
H	4.40485200	6.23859800	5.29235600
C	6.12336900	7.53747300	5.13078300
C	6.16130200	9.35819900	6.76301300
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H	4.51116100	9.46179000	8.14712100
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H	9.55623800	11.64080800	4.57873300
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H	10.94345700	8.96028400	4.92157800
C	5.89903800	5.03411400	3.67738800
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C	4.87499500	4.73262100	2.76226700

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C	12.23905700	4.91867200	1.96128700
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C	12.42078200	9.95297300	1.35850000
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C	10.18555000	10.65673900	0.74762300
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C	11.53192500	10.46500200	0.40705900
H	13.47257000	9.80166000	1.10201300
H	9.48526300	11.05535700	0.00891900
H	11.88514100	10.71522700	-0.59662700
H	3.46901600	3.25129100	2.05673800
H	4.18046100	1.52117000	3.70945400
H	6.00520900	2.03789100	5.33716800
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H	13.56713000	5.16469900	5.82853300
H	13.41301600	6.72680700	6.69412100
H	14.14166900	6.67730400	5.05707900
PhNH ₂			
N	0.73405600	6.29562200	-1.66347400
H	0.20911900	6.59322400	-0.84429400
C	2.10342400	6.48598200	-1.61169000
C	2.97184900	5.75081100	-2.45206600
C	2.66971800	7.46321300	-0.75994600

C	4.34779500	5.99174200	-2.43977800
H	2.55226800	4.98807400	-3.11455500
C	4.04741900	7.69401900	-0.75779900
H	2.01382200	8.03843500	-0.09984100
C	4.90208200	6.96431000	-1.59588600
H	4.99564000	5.40656900	-3.09901200
H	4.45802700	8.45460900	-0.08727400
H	5.97916500	7.14785900	-1.58937700
H	0.41990100	5.39806900	-2.02537400
CO ₂			
C	-0.83769600	0.56282700	0.00000000
O	0.32840700	0.56282700	0.00000000
O	-2.00379900	0.56282700	0.00000000
MeOH			
C	-0.64698700	5.77471000	0.24391300
H	-0.29064400	6.34254900	1.12597100
H	-0.27731600	6.28756900	-0.65785300
H	-1.75374500	5.82358800	0.23097000
O	-0.15564000	4.44824700	0.20984600
H	-0.48793500	3.99880200	1.00438200
⁻ OCO ₂ Me			
O	9.20119600	3.35531000	26.15117000
C	9.93555800	3.65568500	25.19658300
O	10.90472500	3.06730100	24.67798600
O	9.57767200	4.91587300	24.60365300
C	10.36900500	5.32325400	23.51303000
H	10.32756000	4.60920400	22.66870200
H	9.97737200	6.29744500	23.17307500
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C	-2.87921100	1.22459200	2.71362800
H	-2.13749900	1.20532800	1.90466700
C	-3.05447200	2.57912300	3.37722200
H	-2.05102800	2.92537800	3.68421200
N	-3.90080000	2.56529200	4.55622100
H	-4.89583800	2.70586100	4.40287800
C	-3.52744200	2.13607500	5.80963900
C	-4.48803100	2.11180200	6.85411500
C	-2.20551300	1.73072100	6.11848400
C	-4.13583800	1.71445400	8.14315600
H	-5.51577900	2.41515500	6.63274500

C	-1.86897100	1.34017000	7.41883300
H	-1.44103100	1.71381700	5.33959500
C	-2.82119100	1.32631600	8.44519400
H	-4.90140200	1.70890700	8.92464200
H	-0.83913200	1.03440000	7.62597500
H	-2.54866200	1.01578100	9.45661300
C	-3.60113400	3.60653200	2.37464500
H	-2.96591000	3.64730000	1.47702200
H	-4.62132500	3.33122800	2.05935600
H	-3.63069500	4.60859400	2.83008200
(S)-3a			
C	-3.55210100	0.10975200	-3.02045000
H	-3.37821800	-0.82672700	-2.48157000
H	-4.29922400	0.09318000	-3.82084300
C	-2.87921100	1.22459200	-2.71362800
H	-2.13749900	1.20532800	-1.90466700
C	-3.05447200	2.57912300	-3.37722200
H	-2.05102800	2.92537800	-3.68421200
N	-3.90080000	2.56529200	-4.55622100
H	-4.89583800	2.70586100	-4.40287800
C	-3.52744200	2.13607500	-5.80963900
C	-4.48803100	2.11180200	-6.85411500
C	-2.20551300	1.73072100	-6.11848400
C	-4.13583800	1.71445400	-8.14315600
H	-5.51577900	2.41515500	-6.63274500
C	-1.86897100	1.34017000	-7.41883300
H	-1.44103100	1.71381700	-5.33959500
C	-2.82119100	1.32631600	-8.44519400
H	-4.90140200	1.70890700	-8.92464200
H	-0.83913200	1.03440000	-7.62597500
H	-2.54866200	1.01578100	-9.45661300
C	-3.60113400	3.60653200	-2.37464500
H	-2.96591000	3.64730000	-1.47702200
H	-4.62132500	3.33122800	-2.05935600
H	-3.63069500	4.60859400	-2.83008200
E-4a			
C	10.32832800	4.36236000	8.24006500
C	10.29475300	4.12433200	6.76100800
C	10.68554300	5.00116200	5.82316800
H	11.08148500	5.98097300	6.12278300
C	10.61327500	4.75046300	4.34281700
H	9.92566700	5.48530300	3.88780400
H	10.18642900	3.74649600	4.14618400
H	9.90924100	3.14798700	6.43549600

H	10.73407600	5.35590300	8.48608300
N	11.92421100	4.92022800	3.73203200
C	12.13808000	4.93290700	2.36883500
C	11.08459700	5.04598000	1.42945300
C	13.46456500	4.85781900	1.87106000
C	11.36037300	5.10393600	0.05833900
H	10.04814500	5.08828400	1.76884300
C	13.72073000	4.91132600	0.50207300
H	14.29062200	4.76077000	2.58201200
C	12.67269400	5.03882200	-0.42330200
H	10.52556400	5.19411400	-0.64300400
H	14.75548200	4.85141100	0.15224600
H	12.87712700	5.08053500	-1.49577800
H	12.70352800	4.57352000	4.28678300
H	9.31579800	4.28347500	8.67435300
H	10.94327000	3.59832400	8.74783900
IM1a ^{triplet} -endo			
C	12.76338300	7.77763800	23.46127900
O	11.44817600	6.15940400	29.37972300
N	10.92765700	5.56493000	27.27622400
P	12.28341000	6.83942700	24.97213400
N	11.00730100	4.16870400	24.28206800
O	12.34067200	2.64381900	23.32304700
C	13.85639000	7.41297500	22.65503900
H	14.50258800	6.58239300	22.94544300
C	14.12916900	8.11228000	21.47270000
C	13.59011100	10.07040900	27.21549100
H	14.11300800	11.00806600	27.01304800
C	13.31536600	9.19014200	26.16282900
H	13.63700500	9.45387400	25.15387600
C	12.64614000	7.97555800	26.37800900
C	11.94513400	8.85241000	23.05539600
H	11.08732600	9.14969200	23.66313500
C	12.22960800	9.55589200	21.88181400
C	13.32101600	9.18569600	21.08492100
C	13.20342800	9.74020800	28.51584600
H	13.41517200	10.41604900	29.34721600
C	12.54012100	8.53585200	28.75333800
H	12.23457600	8.27474400	29.76663500
C	11.52051200	6.40844200	28.06010900
C	12.24318400	7.64550800	27.70205900
C	10.73158500	4.91491700	29.55601000
H	9.89430000	5.09460300	30.24264000
H	11.42592300	4.18780200	30.00032900

C	10.27974500	4.53123600	28.12516600
H	9.19136200	4.65680900	28.01963800
C	13.63023000	5.57799200	25.13294100
C	14.86489400	5.94501000	25.69309500
H	15.01044800	6.96541700	26.05291600
C	15.92182400	5.03422100	25.79151200
H	16.86905300	5.35081400	26.23428000
C	15.76391200	3.73024700	25.31490300
H	16.58361900	3.01164000	25.38212800
C	14.54666600	3.34387900	24.75430400
H	14.41185800	2.32447700	24.39170000
C	13.46885300	4.24780400	24.66760000
C	12.21224200	3.72810600	24.09893800
C	11.00654700	2.18188000	22.99292000
H	10.83142100	1.24306700	23.53676000
H	10.96850000	2.00297000	21.91149500
C	10.08797400	3.33251400	23.47695100
H	9.30358400	2.93301300	24.13408900
C	9.28220900	7.61028500	25.34200500
H	9.78715000	8.30257200	26.02268800
H	9.14759800	7.97150600	24.31514100
C	8.43428200	6.60981400	25.83309900
H	8.31941700	6.49700600	26.91857500
C	7.28209300	6.08959700	25.01509600
O	6.17869000	7.05366900	25.21520500
C	5.35312300	7.25546500	24.19006400
O	5.41759100	6.74254900	23.09153400
O	4.42469900	8.14001600	24.57424300
C	3.44658800	8.48068000	23.57985800
H	2.88779600	7.58776300	23.26309200
H	2.77171100	9.19722400	24.06316800
H	3.92692100	8.94351800	22.70519900
H	7.52373800	6.11023700	23.94335500
Co	10.27871100	5.79358800	25.29153300
C	10.63190300	3.10832300	27.73362600
C	9.61341100	2.17082700	27.50152200
C	11.97168600	2.69187600	27.64879000
C	9.92459900	0.84110400	27.18935900
H	8.56791400	2.48353000	27.57244000
C	12.28429700	1.36615500	27.33254700
H	12.77594900	3.40978600	27.83168900
C	11.26113100	0.43598800	27.10310100
H	9.12026800	0.12167200	27.01535100
H	13.33039200	1.05609400	27.26763300

H	11.50652400	-0.60113100	26.86051500
C	9.42515600	4.10952800	22.35046200
C	8.17360700	3.68454200	21.87268600
C	10.05203900	5.20487300	21.73489100
C	7.56277600	4.33704700	20.79689100
H	7.67421800	2.83601800	22.34880200
C	9.43661000	5.86349100	20.66305900
H	11.02262800	5.55150900	22.09778300
C	8.19267200	5.43061500	20.18966100
H	6.58820900	3.99637400	20.43797400
H	9.93366900	6.71827400	20.19708600
H	7.71352500	5.94585000	19.35328900
C	6.77170700	4.71797300	25.42716100
H	5.91044500	4.42149400	24.80946400
H	7.56362600	3.96523600	25.29954700
H	6.46390100	4.72294300	26.48487600
H	14.98191400	7.81581500	20.85671400
H	13.53842400	9.73247600	20.16399600
H	11.59265900	10.39348000	21.58658200
IM1b^{triplet}-exo			
Co	9.57200300	5.22181400	4.06976200
C	7.91003600	5.91863700	1.21280000
O	6.47877800	7.86414800	5.42532600
N	8.27858900	6.79645500	4.60671600
P	7.93700600	4.66199700	2.57303800
N	10.69694800	5.98855900	2.57217500
O	11.45984400	6.70922200	0.59394000
C	6.69699100	6.20682800	0.56608400
H	5.78017900	5.71782200	0.90136700
C	6.63496800	7.09861700	-0.50905000
H	5.67498300	7.30164800	-0.98938300
C	7.80199000	7.71443400	-0.96895300
H	7.76847200	8.40812800	-1.81188500
C	9.01761400	7.44470800	-0.34143600
H	9.92928100	7.93196700	-0.68788500
C	9.08953300	6.56357000	0.75673200
C	10.41817900	6.38457500	1.37148800
C	12.16974200	5.98913300	2.73643400
H	12.42741000	6.69600100	3.53825700
C	12.67175600	6.52590700	1.36999500
H	13.17230600	7.49978000	1.45118600
H	13.31283200	5.81922200	0.82681300
C	3.94300700	4.06322100	3.52310400
H	3.15438400	3.37561700	3.20886800

C	5.21444900	3.96663300	2.94640500
H	5.39280400	3.20560300	2.18513400
C	6.25815000	4.82779700	3.32064700
C	4.70822000	5.91457900	4.86633100
H	4.51581200	6.68207500	5.61605000
C	3.68962300	5.03954500	4.48845800
H	2.70202500	5.12505700	4.94681400
C	6.99213800	6.81162900	4.76031800
C	5.99584500	5.82485700	4.30094000
C	7.59604100	8.62149700	5.94944700
H	7.66473700	8.41919000	7.02852000
H	7.39595800	9.68632800	5.77970400
C	8.80968200	8.07062000	5.17004300
H	9.63078400	7.83862400	5.85811500
C	7.90586900	3.06365900	1.65893700
C	7.69673100	1.86937900	2.38037800
H	7.46194600	1.90550100	3.44662900
C	7.76591000	0.63035700	1.73791300
C	8.06191600	0.56030200	0.37050000
C	8.28231700	1.73826300	-0.35042600
C	8.20258400	2.98323200	0.28591100
H	8.37225500	3.89163600	-0.29559500
C	12.70026900	4.61859100	3.11836200
C	13.72400900	4.50695900	4.07235500
C	12.20436900	3.45257900	2.51034200
C	14.24400400	3.25308100	4.41501900
H	14.11272900	5.40919200	4.55307700
C	12.71835400	2.19846800	2.85789000
H	11.40749800	3.52312300	1.76523100
C	13.73998300	2.09532300	3.81071400
H	15.04029400	3.18076700	5.16034100
H	12.31938900	1.29881600	2.38222000
H	14.14076000	1.11529000	4.08182900
C	9.34381800	9.00181800	4.09410100
C	10.67458600	9.44453100	4.15170200
C	8.51506900	9.47374200	3.06093800
C	11.17407200	10.33594100	3.19385300
H	11.32340200	9.09277600	4.95871300
C	9.01090400	10.36730300	2.10618200
H	7.47354100	9.14583400	2.99939100
C	10.34254200	10.79919600	2.16837500
H	12.21273400	10.67132400	3.25301400
H	8.35519700	10.72830900	1.30979900
H	10.72814400	11.49749100	1.42114900

C	11.27641200	6.00807300	7.37837700
C	10.00648400	5.21769600	7.10253300
C	10.08595100	4.33598100	5.88533300
H	11.07076100	3.88488600	5.69985800
C	8.96668300	3.69224500	5.34238900
H	7.96481700	3.86555100	5.75251700
H	9.10070200	2.74477800	4.81173900
O	9.77438900	4.32708900	8.25920800
C	9.04859900	4.82304600	9.25989800
O	8.54271300	5.92608100	9.31475800
O	8.95921000	3.88741500	10.21208600
C	8.19666600	4.25708900	11.37167900
H	7.15765900	4.48890000	11.09501700
H	8.22560500	3.38393900	12.03442800
H	8.64769500	5.12721500	11.87105100
H	11.51657200	6.65538300	6.52151100
H	9.13138100	5.87922200	7.05289000
H	8.51300900	1.69419900	-1.41784000
H	8.12010200	-0.40941700	-0.12996100
H	7.58920600	-0.28411800	2.30969900
H	11.15816500	6.64042600	8.27086300
H	12.12414900	5.32309300	7.53789900
TS1a^{triplet}-endo			
C	12.86123300	7.78917800	23.52719900
O	11.38474400	6.08735700	29.37196600
N	10.94441800	5.56448200	27.23770100
P	12.40192600	6.85018100	25.03440200
N	11.04707500	4.26781800	24.24647200
O	12.30263400	2.63972500	23.37269100
C	13.80803000	7.28524200	22.61664900
H	14.33901300	6.35524400	22.82833200
C	14.08084100	7.97542100	21.42979400
C	13.78836200	9.94703200	27.39342600
H	14.36496100	10.86058200	27.23233100
C	13.49695800	9.11416700	26.30665700
H	13.85953600	9.38981300	25.31516700
C	12.75810000	7.93411200	26.47386900
C	12.19103400	8.99321300	23.22701500
H	11.45874900	9.40904400	23.92142800
C	12.47580200	9.68082200	22.04459300
C	13.41786100	9.17243200	21.14137000
C	13.34852400	9.60211900	28.67213500
H	13.57202100	10.24292500	29.52759600
C	12.61843600	8.42724200	28.85926200

H	12.27389500	8.15386800	29.85659900
C	11.52536200	6.36841800	28.07154600
C	12.30792200	7.58428400	27.77567700
C	10.57708800	4.88888300	29.48637300
H	9.69216000	5.13244500	30.08836600
H	11.18006700	4.12807400	29.99991100
C	10.23585500	4.51862700	28.02000300
H	9.15860200	4.64105400	27.83399400
C	13.69238500	5.53675600	25.16821300
C	14.93998600	5.87549400	25.71491000
H	15.11255000	6.88806600	26.08363800
C	15.97710400	4.93965200	25.78957400
H	16.93622200	5.23140500	26.22314000
C	15.78387500	3.64426600	25.30442800
H	16.58831900	2.90752900	25.35494000
C	14.55225100	3.28929500	24.75399500
H	14.39183100	2.27767900	24.38068200
C	13.49605500	4.21812000	24.68745500
C	12.22676800	3.74685300	24.10951600
C	10.95777300	2.28671100	22.94960300
H	10.70063200	1.33003400	23.42272500
H	10.97043500	2.17747600	21.85805700
C	10.08234800	3.46303600	23.45334700
H	9.30345500	3.08733400	24.13097000
C	9.58267800	7.75431800	25.15374100
H	10.07930900	8.57699500	25.67458000
H	9.44969300	7.88954700	24.07283100
C	8.61082300	6.98295900	25.85585000
H	8.51012600	7.09325400	26.94065500
C	7.82027100	6.04783500	25.19290500
O	6.08283800	7.55494100	24.28852100
C	4.95798200	7.09966500	23.96863500
O	4.52489300	5.93033600	24.00585700
O	4.08772500	8.09691100	23.50802400
C	2.79111700	7.66330000	23.13351700
H	2.25399200	7.19281500	23.97510800
H	2.24228600	8.56102300	22.80969500
H	2.82209100	6.93747000	22.30246800
H	7.93318200	5.96312400	24.10957000
Co	10.37568300	5.88428100	25.23939300
C	10.62672700	3.10225700	27.63944400
C	9.63059900	2.14638400	27.38512000
C	11.97515800	2.70955700	27.59173400
C	9.97317800	0.82128600	27.08700500

H	8.57829200	2.44002100	27.42854100
C	12.31863600	1.38791700	27.28986900
H	12.76238100	3.44155100	27.79129700
C	11.31834900	0.43936500	27.03742400
H	9.18626000	0.08747700	26.89475500
H	13.37123400	1.09596100	27.25400600
H	11.58804500	-0.59400800	26.80503900
C	9.41313900	4.27417500	22.35615000
C	8.04642000	4.08601500	22.09418300
C	10.13604400	5.19385400	21.57748800
C	7.40944500	4.80787800	21.07864000
H	7.47338900	3.37791300	22.69895700
C	9.49890500	5.91810000	20.56365500
H	11.20085200	5.35331300	21.76567300
C	8.13416300	5.72833200	20.31251500
H	6.34179900	4.66022600	20.89761300
H	10.07117100	6.63559100	19.96998200
H	7.63680100	6.29910100	19.52428400
C	6.91270500	5.07869400	25.85219000
H	5.93142700	5.13371000	25.33998800
H	7.28990700	4.05005100	25.71257000
H	6.80120800	5.27502600	26.92845000
H	14.81920200	7.57324200	20.73197900
H	13.63515800	9.71075500	20.21561900
H	11.95668600	10.61775300	21.82880800
TS1b ^{triplet} - <i>exo</i>			
Co	9.47249800	5.34397700	4.05132600
C	7.89296900	5.95621800	1.15318500
O	6.34893700	7.99817000	5.21528800
N	8.16498000	6.93127100	4.44994500
P	7.89255600	4.72585100	2.53218600
N	10.64094000	6.00102900	2.53106400
O	11.44626700	6.75573700	0.58904800
C	6.68645300	6.21639600	0.48495600
H	5.76705500	5.73313700	0.82025800
C	6.63642900	7.07898400	-0.61520600
H	5.68158900	7.26400200	-1.11236800
C	7.80521400	7.68874400	-1.07645900
H	7.77854500	8.35867100	-1.93839800
C	9.01484600	7.44276200	-0.42697100
H	9.92926500	7.92353400	-0.77515700
C	9.07434000	6.59212900	0.69361200
C	10.39072400	6.41928700	1.33089200
C	12.11050500	5.98374200	2.73131800

H	12.35469200	6.66938800	3.55513200
C	12.64303300	6.55044500	1.38878500
H	13.14183900	7.52167600	1.50105200
H	13.29169300	5.85471100	0.84121100
C	3.90101900	4.08388200	3.42197800
H	3.13076500	3.37097600	3.11958400
C	5.18698800	3.98181300	2.87812800
H	5.39431000	3.19357400	2.15317900
C	6.20315900	4.87758100	3.24200100
C	4.60333400	6.00567600	4.70145700
H	4.37973900	6.80204600	5.41132100
C	3.60973800	5.09545700	4.33839900
H	2.61029500	5.18273900	4.76952500
C	6.87660100	6.93527400	4.59534800
C	5.90267300	5.91275700	4.16860000
C	7.44642200	8.82405600	5.68155400
H	7.48272900	8.74494000	6.77708000
H	7.23811500	9.85996700	5.38756500
C	8.69232000	8.21201900	4.99902600
H	9.45711600	7.97581900	5.74894300
C	7.96811200	3.10533800	1.67398300
C	7.69098600	1.91818900	2.38348700
H	7.34077100	1.95828700	3.41684400
C	7.83866500	0.67484700	1.76302600
C	8.27658700	0.59526800	0.43521000
C	8.55924900	1.76780800	-0.27262800
C	8.40466400	3.01734200	0.33888600
H	8.62523700	3.92126400	-0.23210900
C	12.62437200	4.60013800	3.08904900
C	13.60880000	4.45750600	4.07974000
C	12.15411700	3.45500400	2.42377300
C	14.11557700	3.19288200	4.40188900
H	13.97768600	5.34378900	4.60381100
C	12.65495500	2.19016100	2.75057600
H	11.38828000	3.54922900	1.64935600
C	13.63745800	2.05592500	3.73988100
H	14.88118900	3.09588400	5.17588300
H	12.27637600	1.30676200	2.22997000
H	14.02798700	1.06746200	3.99472400
C	9.32927000	9.09252700	3.93727700
C	10.66424100	9.50196100	4.08222900
C	8.59293100	9.55368300	2.83214100
C	11.25662300	10.35366000	3.14120400
H	11.24256300	9.15645700	4.94366200

C	9.18195500	10.40737300	1.89393800
H	7.55063800	9.25002200	2.70006600
C	10.51602400	10.80850500	2.04483600
H	12.29657900	10.66489900	3.26918400
H	8.59731600	10.76076100	1.04091500
H	10.97434600	11.47626000	1.31092500
C	10.96624200	6.04694500	7.46671400
C	9.81801600	5.38029000	6.80843000
C	9.95062300	4.32008000	5.90898300
H	10.94776600	3.88528100	5.77278800
C	8.86219000	3.74879500	5.19092100
H	7.83757200	3.93431800	5.53088500
H	9.03118100	2.78727200	4.69894400
O	8.91621700	4.16153900	8.63065300
C	9.17635400	4.44546500	9.82923400
O	9.92189800	5.32712500	10.29698700
O	8.50293500	3.61610000	10.72704700
C	8.74219400	3.86688100	12.10313400
H	8.43884700	4.88704400	12.39428000
H	8.13935200	3.13526300	12.66205300
H	9.80621400	3.73851400	12.36557800
H	10.98977300	7.12238700	7.21978500
H	8.82967200	5.82322300	6.94255600
H	8.89794100	1.71625200	-1.31018900
H	8.39433200	-0.37867500	-0.04597900
H	7.60931200	-0.23544000	2.32225800
H	10.81035900	5.97319100	8.56398100
H	11.92698700	5.58812000	7.19103800
IM2a^{triplet}-endo			
C	11.77465400	7.12959600	28.48236300
O	8.53463700	1.87900100	27.59327400
N	9.33982700	3.60168500	26.42751600
P	11.07162500	5.57963900	27.80839600
N	11.54581700	5.50700700	24.81672000
O	13.57462000	4.94740000	24.07076600
C	13.15226700	7.40227600	28.40534300
H	13.84325500	6.65848800	28.00363000
C	13.65004900	8.63287300	28.84960200
C	9.54194100	4.67715100	31.54782300
H	9.66093300	5.06421200	32.56219200
C	10.26015600	5.26230700	30.49821700
H	10.93504400	6.09104700	30.71576600
C	10.13259400	4.79622000	29.18158500
C	10.90513900	8.10894900	29.00608200

H	9.83193400	7.91386300	29.07342700
C	11.41151400	9.33057500	29.45676100
C	12.78430600	9.59679700	29.37642300
C	8.68745400	3.60301900	31.29573400
H	8.12259900	3.14047800	32.10758000
C	8.55918600	3.11307200	29.99524700
H	7.89872900	2.26963200	29.79381500
C	9.07342500	3.09646300	27.59515800
C	9.26594400	3.69842600	28.92814200
C	8.29509000	1.48920400	26.21479500
H	7.20797600	1.44690100	26.06551900
H	8.73172500	0.49378000	26.06964200
C	8.97565200	2.59985700	25.38027200
H	8.24973400	3.06924400	24.70251000
C	12.52084500	4.47198300	27.57288200
C	13.04484600	3.80299100	28.68956300
H	12.56615500	3.91956300	29.66363700
C	14.17935600	2.99225000	28.58137400
H	14.56432500	2.48141000	29.46667100
C	14.81518500	2.84764200	27.34639500
H	15.70412600	2.22083900	27.25087800
C	14.30926400	3.50598600	26.22557300
H	14.79921300	3.38836600	25.25929200
C	13.15919700	4.31464400	26.31684700
C	12.69563000	4.95542700	25.07199600
C	12.91196600	5.46421800	22.88665500
H	12.74989800	4.62038100	22.20250000
H	13.57737100	6.20376200	22.42617600
C	11.59280900	6.05838400	23.43324400
H	10.73523500	5.67002000	22.86776800
C	9.26702100	7.47578000	25.97014500
H	9.83094700	8.16540400	26.59983100
H	9.35459800	7.62802800	24.88624000
C	8.13577700	6.78951200	26.46692600
H	7.88547200	6.84080200	27.53206600
C	7.50795300	5.84543600	25.66009400
H	7.70450600	5.88861200	24.57824600
Co	9.77564100	5.48397800	25.83799000
C	10.15682900	2.13195000	24.54828500
C	10.14404500	2.33089100	23.15859700
C	11.23705800	1.44442600	25.12873100
C	11.19088900	1.85363200	22.35998900
H	9.30127500	2.85380400	22.69767800
C	12.28257400	0.96745600	24.33188800

H	11.26399500	1.27079600	26.20820900
C	12.26255900	1.17070900	22.94570600
H	11.16488100	2.01136100	21.27885600
H	13.11531200	0.43258200	24.79510500
H	13.07880100	0.79318800	22.32470200
C	11.54960400	7.57762800	23.41417700
C	10.72676500	8.23902200	22.48909200
C	12.35590200	8.33898600	24.27741200
C	10.70762500	9.63767800	22.42660600
H	10.09549700	7.65358400	21.81447000
C	12.33369200	9.73609400	24.21828600
H	13.00220600	7.84428600	25.00747400
C	11.50972200	10.38930500	23.29264800
H	10.06137400	10.13959900	21.70204100
H	12.96169300	10.31667500	24.89884000
H	11.49272100	11.48116600	23.24811000
C	6.38640200	4.97666000	26.11359900
H	5.44223400	5.41120900	25.73552100
H	6.44846400	3.96387600	25.68910000
H	6.32362900	4.91642500	27.20889300
H	14.72237400	8.83280700	28.78651600
H	13.17749000	10.55453600	29.72569000
H	10.72915300	10.07739800	29.86956500
IM2b^{triplet}-exo			
Co	9.37581500	6.26002100	4.68177500
C	6.94333800	7.62996800	2.81121900
O	8.93174300	10.13862000	6.28332700
N	9.38472000	8.21481500	5.24603600
P	7.05829900	6.54483100	4.29662500
N	9.64835000	6.04612900	2.71079200
O	9.69803900	6.64840600	0.56526000
C	5.84809800	8.50063500	2.70157200
H	5.09265700	8.51756300	3.48948300
C	5.69813600	9.34820800	1.59926500
H	4.83506100	10.01528700	1.54425000
C	6.65149100	9.33523500	0.57951600
H	6.54865800	9.99375200	-0.28530000
C	7.74581400	8.47534900	0.66746500
H	8.49187700	8.46624800	-0.12662200
C	7.91275700	7.61857100	1.77509800
C	9.09983400	6.74274200	1.74922200
C	10.73239700	5.22188500	2.10860200
H	11.63396100	5.29610800	2.72955500
C	10.94570600	5.92726600	0.75629600

H	11.75409300	6.67152000	0.78483000
H	11.07593500	5.24916400	-0.09389000
C	4.43893800	8.21323500	7.02385100
H	3.41209900	8.02826200	7.34693700
C	5.01374100	7.39457800	6.04519800
H	4.42204300	6.58773000	5.60950200
C	6.32865000	7.60276500	5.60513700
C	6.48454400	9.48924000	7.14520700
H	7.06289000	10.30470700	7.57892600
C	5.17447800	9.26656300	7.56997700
H	4.73430400	9.91585900	8.32948100
C	8.49732400	8.95908200	5.84725700
C	7.08634300	8.66283600	6.17483800
C	10.33052100	10.28225800	5.92287400
H	10.89239400	10.50857100	6.83728300
H	10.40452200	11.12251200	5.21970600
C	10.69943000	8.91936700	5.29521300
H	11.34593700	8.34513000	5.97575800
C	5.88203400	5.17587800	3.98835300
C	5.72534500	4.18360400	4.97788400
H	6.25048500	4.26542000	5.93214900
C	4.88231700	3.09233800	4.75231500
C	4.20179400	2.96754100	3.53446100
C	4.36366500	3.94189800	2.54406600
C	5.19811500	5.04341100	2.76645600
H	5.31137200	5.79618100	1.98430000
C	10.34126800	3.75813900	1.95736800
C	11.34733800	2.77900700	2.01932500
C	9.02100400	3.36114000	1.69226300
C	11.04021900	1.42915300	1.81929000
H	12.37856500	3.07738200	2.22819100
C	8.71328100	2.00957500	1.49580000
H	8.21861700	4.10140800	1.64885200
C	9.72065200	1.04007700	1.55830400
H	11.83328700	0.67894400	1.87308800
H	7.67981500	1.71533700	1.29570500
H	9.47828800	-0.01480400	1.40700500
C	11.39384800	9.02659200	3.95109900
C	12.68971300	8.51222300	3.78992500
C	10.78452300	9.69360000	2.87384800
C	13.36967100	8.66485500	2.57493400
H	13.17206200	7.99683000	4.62528900
C	11.46047300	9.84238900	1.65930300
H	9.77841900	10.10685400	2.98756000

C	12.75680000	9.33105800	1.50794000
H	14.38100300	8.26552800	2.46460500
H	10.97674500	10.36350600	0.82932400
H	13.28710000	9.45426200	0.56031200
C	9.28936900	6.53857900	8.11780100
C	9.01352200	5.63763600	6.96724800
C	10.02080300	4.95361700	6.27337900
H	11.06792800	5.17032600	6.51607100
C	9.72987600	4.19513300	5.12962700
H	8.72187500	3.80191800	4.96319700
H	10.54572700	3.72038600	4.58174100
H	8.56953800	7.36740800	8.17787000
H	7.97845600	5.30928800	6.82863600
H	3.83625900	3.85072900	1.59151800
H	3.54734000	2.11042200	3.35857600
H	4.76126500	2.33490200	5.53041300
H	9.15234600	5.94705300	9.04362300
H	10.31646400	6.92919500	8.10975100
IM3a^{CSS}-endo			
Co	9.42602400	5.66759900	5.06729900
C	7.46933000	7.57257000	3.15957700
O	10.17997000	9.61750700	6.26221400
N	10.01756600	7.59746700	5.29984400
P	7.43224400	6.52604800	4.67348500
N	9.56894500	5.37355800	3.07631500
O	9.72610900	5.79072200	0.87950400
C	6.60122900	8.67127000	3.07088000
H	5.94468100	8.91714200	3.90701200
C	6.55884400	9.45941600	1.91620300
H	5.87574000	10.31043300	1.87002100
C	7.38225100	9.15278700	0.82945500
H	7.35204000	9.76214500	-0.07619000
C	8.24993700	8.06325300	0.90319600
H	8.89737300	7.81857100	0.06155300
C	8.30756400	7.27028200	2.06449100
C	9.21835800	6.11887000	2.07268600
C	10.37286900	4.23841400	2.51706600
H	11.26420400	4.12322800	3.14005300
C	10.72942300	4.76772800	1.11832800
H	11.71453300	5.25537600	1.08582300
H	10.64935000	4.02150500	0.31959200
C	5.40773700	8.90711500	7.38884500
H	4.38510500	9.00532200	7.75954500
C	5.70832800	7.91176800	6.45082000

H	4.90820900	7.26473900	6.09067900
C	7.01207400	7.75715300	5.96057600
C	7.70815000	9.64260000	7.34072600
H	8.49234200	10.31731100	7.68355400
C	6.40854600	9.77259100	7.83371100
H	6.18131600	10.55351900	8.56226700
C	9.42524800	8.55899200	5.94529700
C	8.02841600	8.63828800	6.40957400
C	11.55451700	9.26563200	5.96285200
H	12.05185000	9.03188600	6.91576300
H	12.03252000	10.13191600	5.49128900
C	11.42829000	8.03252000	5.04692200
H	12.08888100	7.23520900	5.39514800
C	5.97633000	5.43778500	4.41779500
C	5.31344100	4.80971300	5.49214700
H	5.60413600	5.00919000	6.52486600
C	4.24853100	3.93667300	5.25207200
C	3.83477200	3.67028900	3.94209400
C	4.48689400	4.28828200	2.87036500
C	5.55021200	5.16648100	3.10318800
H	6.04051400	5.64306000	2.25304600
C	9.61104600	2.92350900	2.48027700
C	10.24424700	1.75420300	2.93174700
C	8.31752000	2.82773600	1.94001700
C	9.59772600	0.51515000	2.85263900
H	11.25101200	1.81856300	3.35366100
C	7.66769800	1.59107600	1.86420000
H	7.80645700	3.72254200	1.57576600
C	8.30566900	0.43067100	2.32117500
H	10.10378600	-0.38499400	3.21128800
H	6.65916000	1.53361900	1.44659800
H	7.79716100	-0.53506200	2.26223000
C	11.72610700	8.32667800	3.58675000
C	12.75150800	7.62714900	2.93092200
C	11.05699400	9.35390100	2.89817500
C	13.10441600	7.94738700	1.61390100
H	13.28524800	6.83281500	3.45916500
C	11.40943700	9.67556300	1.58369200
H	10.25855200	9.91620200	3.39090200
C	12.43411300	8.97246200	0.93708100
H	13.90815500	7.39645800	1.11872700
H	10.88274300	10.47899600	1.06263700
H	12.71100800	9.22636600	-0.08933100
O	11.30966500	5.04490000	5.02774500

C	12.41404700	4.77358300	5.61425100
O	13.29009000	4.01975400	5.19888500
O	12.58769300	5.45246200	6.80392500
C	13.80852700	5.19270100	7.50105200
H	14.67835400	5.49428600	6.89765000
H	13.76616900	5.79223600	8.42019300
H	13.90010700	4.12531500	7.75374300
H	3.74071800	3.46586000	6.09697200
H	3.00304400	2.98605700	3.75809400
H	4.16845500	4.09189200	1.84391300
C	9.51079600	5.33385200	7.25900000
C	8.56106800	4.55149900	6.59956100
H	7.50871300	4.73677300	6.83698100
C	8.88523100	3.75308300	5.47246700
H	8.06273000	3.28785900	4.92231900
H	9.84168500	3.22721900	5.43412100
H	10.56158500	5.04549800	7.21832800
C	9.16032300	6.26519100	8.37712500
H	9.40308100	5.76435200	9.33276400
H	9.76712100	7.18385900	8.35220400
H	8.09465100	6.53258700	8.39458900
IM3b ^{CSS} - <i>exo</i>			
Co	9.50508000	6.09845400	4.81787600
C	7.22154700	7.55106600	2.84294000
O	9.13799000	10.06960900	6.21431600
N	9.51932200	8.14529100	5.12195300
P	7.35383200	6.47256400	4.32820600
N	9.81942100	5.95342900	2.84443900
O	10.00527300	6.51069600	0.68331700
C	6.10539400	8.39191600	2.71351600
H	5.35173400	8.42187000	3.50233100
C	5.93461400	9.19055400	1.57793100
H	5.05660500	9.83553800	1.50025400
C	6.88165100	9.15682800	0.55123600
H	6.75491000	9.77663500	-0.33883500
C	7.99804300	8.32875000	0.66595400
H	8.74375600	8.30038000	-0.12815000
C	8.18192000	7.52503000	1.80713800
C	9.35635500	6.64498600	1.84597100
C	10.86784300	5.04691300	2.28338300
H	11.72673100	5.01442100	2.95742900
C	11.21704100	5.76398500	0.97135500
H	12.03588200	6.48897300	1.08852200
H	11.41475800	5.09570700	0.12619700

C	4.63689100	8.14491400	6.97246400
H	3.60164000	7.96626600	7.27136800
C	5.23189500	7.31152800	6.01706500
H	4.64616700	6.50290500	5.57848700
C	6.55843700	7.51520600	5.61431700
C	6.68218000	9.41981100	7.13261400
H	7.25359100	10.24207500	7.56309100
C	5.36250800	9.19871900	7.53092100
H	4.90448800	9.85223500	8.27624800
C	8.68461800	8.88154200	5.79565300
C	7.29421800	8.58582500	6.17914800
C	10.57005800	10.07665500	5.97698200
H	11.06433600	9.86066600	6.93599500
H	10.85201200	11.07541900	5.62489300
C	10.76963200	8.95783700	4.94347700
H	11.61490800	8.31727600	5.20703400
C	6.17486000	5.10455500	4.00149800
C	5.80157000	4.23296700	5.04617800
H	6.17351800	4.38924600	6.06120700
C	4.93810500	3.16334200	4.79487400
C	4.44594200	2.94296000	3.50269700
C	4.81763500	3.79911600	2.46135000
C	5.67798700	4.87571700	2.70570300
H	5.95254700	5.53783500	1.88266000
C	10.37175900	3.62524900	2.05374300
C	11.24211800	2.55526700	2.32193000
C	9.10583900	3.35050800	1.51099400
C	10.85665000	1.23761800	2.05200200
H	12.21998800	2.76044900	2.76374700
C	8.71828800	2.03208100	1.24476600
H	8.40649900	4.16249500	1.29777100
C	9.59223100	0.97172200	1.51333000
H	11.54379400	0.41600300	2.27052500
H	7.72790900	1.83371100	0.82686000
H	9.28733400	-0.05736900	1.30675000
C	10.95974300	9.46644800	3.52420600
C	12.09776800	9.07949800	2.79841600
C	10.06798200	10.38891700	2.94772200
C	12.34387400	9.60477100	1.52352000
H	12.79890700	8.36851300	3.24327300
C	10.31492900	10.91719500	1.67680700
H	9.17659500	10.70924500	3.49490900
C	11.45425700	10.52671900	0.96077800
H	13.23666200	9.29727900	0.97277500

H	9.61623500	11.63778900	1.24426100
H	11.64835600	10.94280800	-0.03114500
C	9.59410800	6.48500300	8.05262100
C	8.98451300	5.71557400	6.91627200
C	9.67756200	4.66493000	6.30179800
H	10.71524000	4.49738100	6.60091900
C	9.26462800	4.07092900	5.08867300
H	8.21541200	3.85231800	4.88176400
H	9.98954900	3.41962300	4.59800700
O	11.43236800	6.25952000	5.06292500
C	12.42873400	5.45559900	5.18326200
O	12.45403800	4.22902200	5.08880600
O	13.56949800	6.16559500	5.44457700
C	14.76386800	5.39481400	5.58415200
H	14.99848300	4.85020700	4.65602200
H	15.56315100	6.11523000	5.80324000
H	14.67668500	4.67162400	6.40987100
H	9.19912400	7.50998100	8.11720200
H	7.89009300	5.72354500	6.87576100
H	4.43605100	3.63527900	1.45078700
H	3.77247900	2.10459100	3.30912000
H	4.65053000	2.50029000	5.61410100
H	9.34254600	5.99224500	9.00975600
H	10.68980700	6.53052400	7.96707200
IM4 ^{triplet}			
Co	9.43840600	6.14356500	4.51703700
C	7.03175700	7.69646200	2.79906200
O	9.10196800	9.85843800	6.51180300
N	9.43326100	8.16494200	5.08276100
P	7.23640700	6.49119200	4.18497100
N	9.64129600	6.14584500	2.46745700
O	9.56845700	6.73842100	0.31288400
C	5.93780000	8.57412300	2.83265100
H	5.25186700	8.55524200	3.68101500
C	5.70314500	9.47798100	1.79064700
H	4.84647900	10.15326500	1.84642000
C	6.55844700	9.50873600	0.68710800
H	6.38264000	10.20992300	-0.13126400
C	7.64496700	8.63526300	0.63077200
H	8.31695200	8.65245000	-0.22747800
C	7.89706300	7.73027600	1.67875900
C	9.05719500	6.83590300	1.53937200
C	10.74807100	5.37639200	1.85242600
H	11.68321800	5.67777700	2.34234400

C	10.72827100	5.86524500	0.38058700
H	11.61032200	6.46180700	0.11365100
H	10.58170500	5.06085200	-0.35106900
C	4.62651500	7.81049200	7.10471600
H	3.60310800	7.58277400	7.41079000
C	5.19582800	7.11677000	6.03116600
H	4.59823400	6.36862500	5.50931000
C	6.50633300	7.38391000	5.60811500
C	6.66236100	9.08454900	7.35096800
H	7.23755900	9.85745700	7.86053200
C	5.36229700	8.79524000	7.76680900
H	4.92610000	9.34445400	8.60372100
C	8.63004100	8.76576400	5.90586500
C	7.25413900	8.38841100	6.27983600
C	10.45773400	10.08158100	6.04406900
H	11.11985100	10.07573700	6.91956000
H	10.48461100	11.06902600	5.56434400
C	10.72478100	8.90868400	5.06973500
H	11.48717500	8.22833500	5.46958900
C	6.10867100	5.11391500	3.73161900
C	5.67187500	4.17055600	4.68515600
H	5.91753400	4.28686600	5.74191800
C	4.88863900	3.08095500	4.29421300
C	4.53573400	2.90906800	2.95079400
C	4.96470500	3.83899500	1.99840900
C	5.74418200	4.93516100	2.38273500
H	6.06273400	5.65098700	1.62341700
C	10.58610400	3.87377900	2.00353000
C	11.73275700	3.06489200	2.06291100
C	9.32129300	3.26514900	2.02632100
C	11.61813900	1.67298400	2.13958600
H	12.72188700	3.53111100	2.05703900
C	9.20576900	1.87257100	2.11300800
H	8.42008700	3.88155600	1.98761900
C	10.35323500	1.07253500	2.16625700
H	12.51932400	1.05611300	2.18660200
H	8.21440300	1.41270600	2.13774800
H	10.26250400	-0.01466700	2.23291900
C	11.15900600	9.34109100	3.68034900
C	12.40064300	8.92009500	3.17843000
C	10.36335400	10.19631200	2.89821100
C	12.84364200	9.34920900	1.92107400
H	13.01904900	8.24672600	3.77675200
C	10.80313200	10.62249100	1.64052000

H	9.39329900	10.53569900	3.27280900
C	12.04556700	10.20084600	1.14890100
H	13.81465400	9.01656600	1.54497300
H	10.17436700	11.28723100	1.04258600
H	12.39009400	10.53748200	0.16769500
C	9.21459500	6.64434100	9.51431800
C	8.66340400	6.02906400	8.26956900
C	9.40950600	5.54967900	7.24178000
H	10.50107400	5.61757200	7.31195900
C	8.86006800	4.92694100	6.04183500
H	7.80018100	4.67056600	6.12248800
H	9.47196800	4.10500100	5.63572500
O	11.34624900	5.98638900	4.80815800
C	12.10719000	4.99254500	5.13015700
O	11.78575500	3.89110700	5.56402600
O	13.41929600	5.32370000	4.93961400
C	14.37173300	4.32528500	5.30858800
H	14.23591200	3.40569600	4.71857200
H	15.35911600	4.75836300	5.10020700
H	14.29187800	4.07691100	6.37858200
H	8.82897400	7.67157400	9.64812400
H	7.57053600	5.94925800	8.20644500
H	4.69026300	3.71825200	0.94778700
H	3.92429200	2.05530000	2.64891200
H	4.55138900	2.36580000	5.04814800
H	8.89277900	6.08026500	10.40836100
H	10.31456400	6.68300100	9.50229400
IMS ^{triplet}			
Co	9.53469000	5.94416200	4.70037500
C	11.77216900	5.64525800	2.26655300
O	8.26681000	2.61593600	2.55890600
N	8.97134000	4.67114100	3.10540000
P	11.60002300	5.20974900	4.04676100
N	10.07829100	7.74158500	3.74222300
O	10.64371200	9.12927700	2.07511600
C	12.43737600	4.75432800	1.41238700
H	12.79982200	3.80021400	1.79972900
C	12.65944100	5.07634800	0.06842700
H	13.17882900	4.36481400	-0.57737700
C	12.22615200	6.30425500	-0.43598500
H	12.39986100	6.56548000	-1.48185400
C	11.56257300	7.20219300	0.40152600
H	11.21759000	8.16016100	0.01262900
C	11.32042500	6.88332300	1.75053900

C	10.64460700	7.89328100	2.58086800
C	9.73240000	9.10521400	4.23659300
H	8.70803600	9.11186100	4.61667700
C	9.81755100	9.94406300	2.94645400
H	8.83932500	10.06658000	2.45850800
H	10.30676800	10.91710800	3.06791600
C	12.61912200	1.23202500	4.51954200
H	13.49027600	0.67293700	4.86822700
C	12.66552500	2.63117300	4.48670800
H	13.57446500	3.14222300	4.80750600
C	11.56593600	3.37725700	4.04123800
C	10.36468200	1.28879300	3.65387200
H	9.46326900	0.77032300	3.32657400
C	11.46694900	0.56076300	4.10573200
H	11.42240700	-0.52999700	4.13161900
C	9.20509600	3.39391900	3.10229200
C	10.39478700	2.69427800	3.61559600
C	7.11792400	3.45958300	2.27810800
H	6.35890700	3.24331500	3.04076800
H	6.74579800	3.19868800	1.28019700
C	7.67779100	4.89260800	2.39442900
H	7.03716600	5.50983800	3.03426400
C	13.20633100	5.72492900	4.77777100
C	13.49249300	5.48409500	6.13772400
H	12.78280700	4.95606400	6.77527700
C	14.70579100	5.90213500	6.69082700
C	15.64862600	6.57286100	5.90303300
C	15.37121200	6.82229400	4.55550300
C	14.16013700	6.40312800	3.99391500
H	13.96839300	6.60691000	2.93972500
C	10.66169500	9.58533300	5.34039500
C	10.12585000	10.31927600	6.41118500
C	12.05099600	9.38695500	5.28026300
C	10.96082300	10.84759200	7.40262800
H	9.04602200	10.48256200	6.46529500
C	12.88608200	9.91105700	6.27328100
H	12.49113400	8.82042300	4.45606100
C	12.34383300	10.64312000	7.33696900
H	10.52827900	11.41644800	8.22964500
H	13.96505000	9.74816300	6.21414600
H	12.99755900	11.05219900	8.11146900
C	7.86366400	5.60572400	1.06391800
C	7.34353400	6.89674900	0.88168400
C	8.51057800	4.97600000	-0.01447900

C	7.46546300	7.54851500	-0.35223600
H	6.82918000	7.39154200	1.71027700
C	8.62765000	5.62252400	-1.24858100
H	8.92043600	3.96887900	0.10427800
C	8.10515400	6.91134300	-1.42097100
H	7.05195300	8.55237700	-0.47921200
H	9.12814000	5.11868000	-2.07927800
H	8.19511500	7.41514500	-2.38672900
C	9.08087900	7.76356100	9.18294000
C	9.01365000	6.69176300	8.14803100
C	10.07703200	6.21463200	7.44507900
H	11.06143000	6.66701100	7.61628700
C	10.01252300	5.09748000	6.51822700
H	9.08237000	4.51044400	6.50616400
H	10.89441100	4.45101100	6.51447900
O	5.60827800	5.29654900	6.12496600
C	6.69259100	4.99926100	5.65778700
O	7.31570000	3.97078900	5.41373600
O	7.55893100	6.23764900	5.24904700
C	6.97010900	7.52094300	5.45074100
H	6.86130900	8.03975600	4.48496800
H	5.97756600	7.37480900	5.89708900
H	7.59068100	8.11873900	6.13603500
H	8.03126100	6.23095400	7.98690300
H	8.37927200	8.58340200	8.94688900
H	8.76092700	7.36661700	10.16366800
H	10.09350800	8.18005000	9.28653900
H	14.91237200	5.69940800	7.74429000
H	16.59618600	6.89857400	6.33883600
H	16.09967200	7.34380200	3.93010600
TS2 ^{triplet}			
Co	9.54263800	5.99463000	4.66570100
C	11.78890900	5.61024700	2.22913200
O	8.28219800	2.59739100	2.55458400
N	8.96120000	4.65665000	3.12180400
P	11.59555600	5.22374000	4.01887200
N	10.10658500	7.74947100	3.64681900
O	10.73738500	9.11073900	1.98050600
C	12.44312600	4.69234700	1.39515600
H	12.78949300	3.74047600	1.80207700
C	12.67417900	4.98414600	0.04572000
H	13.18371600	4.25158100	-0.58427200
C	12.26342800	6.20907600	-0.48446400
H	12.44516300	6.44647100	-1.53467600

C	11.61385300	7.13499600	0.33331400
H	11.28779500	8.09176600	-0.07453800
C	11.36128300	6.84523300	1.68670100
C	10.69831000	7.87956000	2.49688800
C	9.76179700	9.12145700	4.11916100
H	8.71831700	9.14463600	4.44364500
C	9.92753400	9.95909600	2.83424900
H	8.97174900	10.13386300	2.31909400
H	10.46117000	10.90585600	2.97688100
C	12.62363300	1.25596200	4.57406900
H	13.49558700	0.70625800	4.93550800
C	12.66478900	2.65465300	4.51810600
H	13.57111900	3.17391500	4.83310200
C	11.56416400	3.38950200	4.05689200
C	10.37305400	1.28942400	3.69769700
H	9.47485700	0.76260800	3.37465500
C	11.47619000	0.57314200	4.16615200
H	11.43619000	-0.51726200	4.20929400
C	9.20787600	3.38309300	3.11151900
C	10.39827700	2.69412500	3.63775900
C	7.13463600	3.43329900	2.24566300
H	6.34506900	3.18921400	2.96822100
H	6.80488200	3.18706300	1.22914900
C	7.66771700	4.87311600	2.40953800
H	7.02451400	5.46252200	3.07356900
C	13.19808500	5.75065900	4.75173700
C	13.46787700	5.53746600	6.11953700
H	12.74982900	5.02117700	6.75736800
C	14.67384000	5.96807300	6.67910900
C	15.62517600	6.62483900	5.88958800
C	15.36410400	6.84641400	4.53394800
C	14.16064800	6.41355500	3.96597500
H	13.98173900	6.59459000	2.90527900
C	10.63886200	9.58204700	5.27257500
C	10.05440900	10.26666700	6.35045400
C	12.03296100	9.40815600	5.25400400
C	10.84589400	10.76932400	7.39013500
H	8.97102500	10.41195100	6.37261300
C	12.82444600	9.90648400	6.29446800
H	12.51078900	8.88212600	4.42389700
C	12.23336800	10.58852400	7.36567100
H	10.37542200	11.29980400	8.22190500
H	13.90746000	9.76326800	6.26693500
H	12.85293600	10.97766800	8.17763000

C	7.84402600	5.63202300	1.10339700
C	7.33908600	6.93605700	0.97771700
C	8.47202000	5.03781600	-0.00572900
C	7.45722400	7.63456600	-0.23060200
H	6.84110800	7.40396100	1.83151600
C	8.58453400	5.73082900	-1.21485100
H	8.87295900	4.02290800	0.06932100
C	8.07718500	7.03186100	-1.33071500
H	7.05573100	8.64788800	-0.31362000
H	9.07011500	5.25389300	-2.06997000
H	8.16336200	7.57204100	-2.27697300
C	9.07505000	7.70679700	9.24317800
C	8.99609200	6.66244700	8.17845400
C	10.04399100	6.22137700	7.43602100
H	11.02649400	6.68251600	7.59731800
C	9.97853800	5.13121900	6.46918300
H	9.05861900	4.53215500	6.48405800
H	10.86066200	4.48348600	6.46712500
O	5.58953900	5.31521000	6.19845100
C	6.56062000	4.82202800	5.71785000
O	7.18282700	3.84978100	5.40946900
O	7.66617400	6.28121300	5.16583100
C	7.14186400	7.53741600	5.51469600
H	6.94374300	8.15629400	4.61895600
H	6.18203500	7.39596500	6.03859500
H	7.81491100	8.09315000	6.19382000
H	8.01546600	6.19579500	8.02361700
H	8.37170500	8.53405900	9.03976200
H	8.77270600	7.28520800	10.21908700
H	10.08895600	8.12214900	9.34209700
H	14.86799700	5.78681800	7.73887000
H	16.56675600	6.96109600	6.33036700
H	16.09962700	7.35640200	3.90726100
IM6 ^{triplet}			
Co	9.74256000	5.74370800	4.45367300
C	7.46662100	7.57839300	2.80693500
O	9.44118200	9.23557100	6.81936100
N	9.72814100	7.72168200	5.19022700
P	7.54710700	6.22657100	4.06622600
N	9.97321800	5.88933400	2.41425000
O	10.02912600	6.67618500	0.32160600
C	6.43681100	8.52634700	2.89413900
H	5.72156500	8.47458800	3.71700000
C	6.30236400	9.53941300	1.93807900

H	5.49327200	10.26704300	2.03380700
C	7.19561900	9.61121100	0.86690400
H	7.09677600	10.39660900	0.11464100
C	8.22170600	8.67161800	0.75814700
H	8.92324300	8.72147200	-0.07495900
C	8.37422900	7.65739600	1.72161000
C	9.47652800	6.70041800	1.53557600
C	11.04435800	5.09960800	1.77034600
H	11.97590900	5.27710500	2.32437700
C	11.13159100	5.72969500	0.35472800
H	12.05985000	6.29323900	0.19159600
H	10.97827700	5.01164300	-0.46068500
C	4.86421700	7.31940400	7.02421800
H	3.82218500	7.09930600	7.26674800
C	5.44707600	6.73579000	5.89336300
H	4.84317100	6.07807100	5.26721600
C	6.78146700	6.99603500	5.54738700
C	6.93627800	8.46521400	7.49264600
H	7.52421200	9.14336200	8.11131200
C	5.61104700	8.18419700	7.82684100
H	5.16449100	8.64489300	8.71048200
C	8.93640400	8.24375300	6.07305900
C	7.53839400	7.88045400	6.36267500
C	10.85453500	9.33975300	6.49944000
H	11.41840800	8.95642000	7.36199600
H	11.08746000	10.40028400	6.34400900
C	11.02152800	8.45957100	5.24138200
H	11.80763500	7.70757100	5.37845100
C	6.35547900	4.98053000	3.42598100
C	5.88402400	3.93304500	4.24491900
H	6.14917600	3.88833100	5.30272900
C	5.04417700	2.94685200	3.71954000
C	4.66936400	2.98151000	2.37124600
C	5.13461200	4.01393200	1.55063500
C	5.97017600	5.00779600	2.07163600
H	6.31676100	5.80692600	1.41443000
C	10.75916100	3.60615000	1.76302400
C	11.83225400	2.70479700	1.65512200
C	9.45030100	3.10195600	1.80684800
C	11.59964300	1.32720800	1.58646800
H	12.85697500	3.08532300	1.62415500
C	9.21747900	1.72222300	1.74570800
H	8.60773000	3.79060200	1.89852900
C	10.29046500	0.83119500	1.63273800

H	12.44425800	0.63837600	1.50268800
H	8.19220300	1.34551800	1.78635800
H	10.10868600	-0.24548700	1.58432000
C	11.29378800	9.22604500	3.95757600
C	12.40849400	8.89370400	3.17166200
C	10.47064700	10.29122000	3.55068100
C	12.69841800	9.60893500	2.00286800
H	13.05793800	8.07144000	3.48321800
C	10.76015200	11.00863500	2.38551000
H	9.59683400	10.56920900	4.14741700
C	11.87520900	10.66908500	1.60772200
H	13.57255600	9.33993400	1.40406500
H	10.11311900	11.83617800	2.08356000
H	12.10162200	11.23161400	0.69830500
C	9.27893800	5.46965200	9.54693500
C	8.80068300	5.06519800	8.18760600
C	9.60190000	4.76576900	7.13714300
H	10.68741300	4.83157900	7.27581400
C	9.12358300	4.37106700	5.80825300
H	8.05717900	4.12343400	5.80015900
H	9.70750500	3.56651700	5.32728400
O	11.51939500	5.57174300	4.92135800
C	12.30813200	4.42845300	5.02633100
H	11.73012900	3.50071100	5.22511300
H	12.90105700	4.24270400	4.10607300
H	13.03359300	4.53673600	5.85858300
H	7.71239800	5.00520000	8.05186600
H	8.89083500	6.46719500	9.82335700
H	8.91006100	4.77324100	10.32168700
H	10.37833500	5.49903400	9.60231900
H	4.68062500	2.14896300	4.37149200
H	4.01320900	2.20852600	1.96383700
H	4.84469500	4.05418400	0.49793700
IM6 ^{triplet}			
C	11.48708600	7.10783900	28.01798900
O	8.61483400	1.69053900	26.90826200
N	9.61417300	3.40165800	25.86493100
P	10.92410100	5.50754100	27.31927000
N	11.80485900	5.61482600	24.51212400
O	13.96510900	5.32589700	23.99923600
C	12.84717900	7.46859800	27.99469700
H	13.59980000	6.76573000	27.63276700
C	13.25120900	8.73152800	28.44223100
C	9.09092500	4.57761300	30.91764300

H	9.08472700	4.98445500	31.93131000
C	9.88372000	5.18410100	29.93608200
H	10.48813900	6.05171200	30.20410900
C	9.91715700	4.69069400	28.62366800
C	10.54066300	8.03863800	28.49503500
H	9.48082200	7.77975700	28.53363500
C	10.95232400	9.29585500	28.94665200
C	12.30713000	9.64739300	28.91802200
C	8.32036900	3.45727200	30.60020200
H	7.69691100	2.98013200	31.35920000
C	8.35496400	2.93924100	29.30468200
H	7.76439300	2.05822900	29.05230100
C	9.14810800	2.91602700	26.97424000
C	9.14299100	3.54203700	28.30683600
C	8.57984000	1.30961900	25.50633300
H	7.53481400	1.37576500	25.17129200
H	8.93291300	0.27452900	25.42890900
C	9.48754500	2.34762000	24.81547500
H	8.98692800	2.78892300	23.94723400
C	12.46273500	4.48495800	27.25816600
C	12.86129600	3.77838200	28.40264800
H	12.24368400	3.80881100	29.30202200
C	14.04762700	3.03583000	28.41858700
H	14.33076300	2.49243800	29.32291100
C	14.86419100	2.99957200	27.28631100
H	15.79350400	2.42610600	27.29146600
C	14.48752200	3.70066800	26.13982000
H	15.11731100	3.67624000	25.25006600
C	13.28935100	4.43696100	26.10745500
C	12.95817500	5.15035600	24.86313800
C	13.40573200	5.93756500	22.80333900
H	13.44135500	5.18814800	22.00028700
H	14.03519800	6.79653100	22.54030300
C	11.96067500	6.31089400	23.20798300
H	11.22252400	5.88398900	22.51923600
C	8.70886300	6.98177100	25.75511200
H	9.35842500	7.72436000	26.23626700
H	8.40688000	7.31149400	24.75184300
C	7.60888800	6.50308400	26.59428500
H	7.83674800	6.34294500	27.65710600
C	6.34380000	6.23909700	26.18249200
O	9.24978500	5.24800600	23.55041100
C	7.90852400	5.12287700	23.19651000
H	7.32916900	4.45795500	23.87215200

H	7.38279300	6.10112900	23.17013400
H	7.83324600	4.69353500	22.17709900
H	6.08632900	6.41051300	25.13004200
Co	9.87600700	5.37802500	25.26868300
C	10.84727400	1.82889900	24.37582800
C	11.32275400	2.12949400	23.09002500
C	11.63794600	1.03524800	25.22572200
C	12.56185900	1.64285000	22.65561800
H	10.71392900	2.74837200	22.42628700
C	12.87416500	0.54566400	24.79181300
H	11.28785600	0.78939300	26.23245900
C	13.33926400	0.84775300	23.50510800
H	12.91672300	1.88145000	21.64958700
H	13.47643200	-0.07454900	25.46048800
H	14.30427300	0.46215000	23.16641000
C	11.69109100	7.80125100	23.34015800
C	10.63317700	8.38695200	22.62784800
C	12.48879600	8.61501600	24.16371700
C	10.37735700	9.75991100	22.73148400
H	10.00401500	7.75848200	21.99275600
C	12.23218100	9.98559500	24.27188300
H	13.31862200	8.17958200	24.72781100
C	11.17531100	10.56202100	23.55488400
H	9.55105900	10.20247100	22.16904100
H	12.85932100	10.60572200	24.91757500
H	10.97556600	11.63341100	23.63867800
C	5.24124000	5.74556400	27.06602700
H	4.38724100	6.44705600	27.06482000
H	4.84326300	4.78053600	26.70220100
H	5.57751800	5.61003200	28.10578100
H	14.31147000	8.99488900	28.42103200
H	12.62572900	10.63179400	29.26945400
H	10.20832100	10.00237500	29.32236600
IM7a^{CSS}-exo			
Co	10.19166500	6.06262700	5.04594700
C	7.42503100	7.61603100	3.83061800
O	9.77451800	9.43506700	7.51146800
N	10.02993900	7.97518100	5.82732600
P	7.93779300	6.26308600	4.97263200
N	10.18723300	6.51769100	3.07463500
O	9.94823600	7.63934000	1.14893100
C	6.20761400	8.27459800	4.06300500
H	5.59847400	8.00120000	4.92637700
C	5.75180400	9.27659600	3.20060400

H	4.80028000	9.77270200	3.40467900
C	6.51272700	9.63385900	2.08456600
H	6.16550600	10.41453500	1.40446400
C	7.72649000	8.99199400	1.84068500
H	8.32843900	9.27048900	0.97610400
C	8.19747600	7.98495100	2.70590800
C	9.47454900	7.34068500	2.36808700
C	11.28688700	6.03504600	2.19614400
H	12.21888700	6.06766800	2.76597300
C	11.28817500	7.09006200	1.07722500
H	11.99755100	7.90956300	1.26486200
H	11.43618900	6.68291900	0.07059800
C	5.57568100	6.91056300	8.32228000
H	4.62000900	6.54492000	8.70451300
C	6.06177000	6.42521800	7.10158900
H	5.47261200	5.69433000	6.54648100
C	7.28427100	6.87248400	6.58366200
C	7.52455100	8.32075400	8.53412400
H	8.10088400	9.06329400	9.08626700
C	6.30780000	7.85864500	9.03927500
H	5.93500600	8.24161200	9.99152400
C	9.30619600	8.38021900	6.82757900
C	8.02670300	7.83646600	7.31242400
C	11.13388800	9.65377000	7.03791900
H	11.81454900	9.17590600	7.75912900
H	11.31233000	10.73448000	7.00642400
C	11.14143200	8.96433000	5.66800200
H	12.05334800	8.38205500	5.49283600
C	6.84904900	4.85920300	4.49528100
C	6.73663700	3.73389800	5.33913700
H	7.23861200	3.71388500	6.30869000
C	5.96938400	2.63253000	4.94976600
C	5.31640900	2.63002300	3.71133100
C	5.43200800	3.73675600	2.86415200
C	6.19285900	4.84626600	3.25085500
H	6.26752500	5.70276900	2.57838300
C	11.05247600	4.62984000	1.66083500
C	12.16404000	3.81151200	1.39736700
C	9.77022700	4.15012400	1.34922600
C	11.99851200	2.54002700	0.83676700
H	13.16780300	4.17424600	1.63562200
C	9.60303000	2.87687600	0.79220700
H	8.88960400	4.76280600	1.55663900
C	10.71585300	2.06768300	0.53357100

H	12.87403400	1.91538500	0.64115500
H	8.59713500	2.51557600	0.56280100
H	10.58379800	1.07277300	0.10072600
C	10.91289800	9.92887600	4.51392700
C	11.87879700	10.04307700	3.50114300
C	9.79224700	10.77914200	4.47659100
C	11.73229500	10.98468400	2.47429100
H	12.75807300	9.39387200	3.52403400
C	9.64661700	11.72280600	3.45525700
H	9.02678800	10.71625400	5.25479800
C	10.61652600	11.82842300	2.44969000
H	12.49533400	11.06076800	1.69512700
H	8.77268800	12.37917700	3.44474700
H	10.50289400	12.56698800	1.65197200
C	10.74007600	5.67397500	8.21606100
C	10.03255900	5.13604700	7.00348400
C	10.72297300	4.36320400	6.05867300
H	11.79907300	4.25651500	6.20465000
C	10.19616400	4.02919600	4.78989700
H	9.15669000	3.71945600	4.65993800
H	10.89283700	3.60318000	4.06353000
O	12.06872100	6.42843300	4.99334000
C	13.17626700	5.59390700	4.99413700
H	13.07263900	4.68575200	4.35910800
H	14.04573000	6.15349000	4.58727700
H	13.48672700	5.24238100	6.00553300
H	8.95261000	4.99913600	7.11900000
H	10.25051700	6.57532600	8.61455100
H	4.92521600	3.74414200	1.89615600
H	4.71876800	1.76681800	3.40848100
H	5.88455100	1.77273200	5.61857700
H	10.71599900	4.92254100	9.02671500
H	11.79203000	5.91050000	7.99868500
IM7b^{CSS}-endo			
C	11.08284200	7.10246800	28.13040500
O	8.84991200	1.37551200	27.13442400
N	9.56614800	3.20896100	26.05774400
P	10.62758000	5.44591800	27.47235000
N	11.29713400	5.40895900	24.63246400
O	13.38465100	4.98774400	23.93490300
C	12.40506700	7.56573300	27.98625900
H	13.17286000	6.91987800	27.55700800
C	12.75490900	8.85597400	28.39895100
C	9.10277000	4.28484900	31.14888300

H	9.06049700	4.69430800	32.16062500
C	9.71671700	5.02392500	30.13003600
H	10.15767900	5.99217500	30.36973900
C	9.78295800	4.52973700	28.82033100
C	10.12154200	7.96266100	28.70022100
H	9.09197800	7.63140800	28.84806100
C	10.47832400	9.24953500	29.11405800
C	11.79383400	9.70190300	28.96139000
C	8.56007900	3.02924700	30.86995200
H	8.08330900	2.44427100	31.65923900
C	8.62769700	2.51752000	29.57261100
H	8.20437600	1.53832000	29.34898100
C	9.24497500	2.65679200	27.18889100
C	9.22834700	3.25486200	28.53614100
C	8.66353700	1.06059900	25.72739100
H	7.58525600	1.12222100	25.51548100
H	9.02175500	0.03876900	25.55784100
C	9.47369300	2.14809500	25.00652100
H	8.92917200	2.59709600	24.16832600
C	12.24352600	4.55906800	27.40208800
C	12.79740200	4.05350800	28.58809800
H	12.26068300	4.16868200	29.53136700
C	14.03758300	3.40706900	28.58658600
H	14.44628700	3.02233500	29.52358500
C	14.74665500	3.26032400	27.39134900
H	15.71564400	2.75685400	27.38107600
C	14.21250500	3.76030500	26.20404700
H	14.75889700	3.64991300	25.26757200
C	12.96149600	4.40685500	26.19464900
C	12.47521000	4.94664600	24.91853400
C	12.67464200	5.36736400	22.72678700
H	12.49307600	4.45247600	22.14450200
H	13.31141800	6.05675200	22.16076100
C	11.37784200	5.99706500	23.26546100
H	10.50893200	5.65161800	22.69940500
C	8.90757300	7.09544900	25.23915300
H	9.54529500	7.93093000	25.54344300
H	8.57088100	7.13568700	24.20168000
C	8.08179000	6.51364900	26.24389000
H	8.17066100	6.87347500	27.27434400
C	7.38170000	5.32094500	26.05388800
H	7.09983300	5.02401500	25.04400000
Co	9.52394900	5.20810700	25.54212300
C	10.83247900	1.66900800	24.52142800

C	11.16920800	1.79934600	23.16472600
C	11.73558500	1.01936800	25.38277300
C	12.37989100	1.29279100	22.67546100
H	10.47096400	2.29621900	22.48658600
C	12.94435900	0.51157400	24.89596000
H	11.49318900	0.89734600	26.44243200
C	13.27055100	0.64682600	23.53999000
H	12.62435000	1.39958000	21.61532100
H	13.63352200	0.00641800	25.57756400
H	14.21419400	0.24715700	23.15981800
C	11.42604800	7.51805300	23.27184800
C	10.72258800	8.23246000	22.28846400
C	12.22348800	8.23056100	24.18302400
C	10.80546800	9.62814600	22.22071400
H	10.10289200	7.68947500	21.56961100
C	12.30600600	9.62589700	24.11862000
H	12.78255700	7.69929400	24.95694300
C	11.59617200	10.32984900	23.13783300
H	10.24809300	10.16772600	21.45054300
H	12.92701300	10.16489500	24.83884300
H	11.65963000	11.41993900	23.08922700
H	9.72125200	9.89835800	29.56088600
H	12.06898000	10.70881600	29.28445800
H	13.78669500	9.19571300	28.28123000
C	6.61208300	4.65406600	27.15268000
H	5.54331800	4.91284900	27.03584400
H	6.66779700	3.55607400	27.09100200
H	6.93207800	4.97652700	28.15355100
O	8.87499900	4.61403900	23.81732400
C	8.05257500	5.22614300	22.88683900
H	8.51115100	6.10117600	22.36913800
H	7.80263200	4.49395200	22.09007000
H	7.07338200	5.58376200	23.28541000
(R)-TS4^{CSS}			
C	11.92827200	7.71857700	27.67541400
O	8.78610000	2.32978200	27.85835800
N	9.79444200	3.75246100	26.43877200
P	11.25456100	6.03700500	27.33096200
N	11.79807000	5.29985100	24.54495500
O	13.84055500	4.58057600	23.94504400
C	13.30853200	7.97557900	27.57217300
H	14.00645400	7.16345700	27.36019600
C	13.80588000	9.27284800	27.74393400
C	9.69394600	5.91902600	31.17913200

H	9.76111400	6.52976000	32.08242100
C	10.39376400	6.30580600	30.02957400
H	11.00550300	7.20860200	30.06091500
C	10.32761900	5.55066500	28.84965300
C	11.05802600	8.79454700	27.94957100
H	9.98236100	8.62950000	28.04135800
C	11.56045300	10.08724500	28.12566800
C	12.93520000	10.33156700	28.02147000
C	8.92246800	4.75506700	31.16706900
H	8.37510200	4.44362800	32.05941700
C	8.85163000	3.98483700	30.00529400
H	8.25183400	3.07465400	29.98783900
C	9.40752200	3.50825300	27.65131500
C	9.54025500	4.36828900	28.83863700
C	8.53875200	1.76172500	26.54452200
H	7.48090900	1.94043500	26.29703400
H	8.73274200	0.68378200	26.59836300
C	9.50032800	2.53764700	25.62702500
H	9.01809900	2.89409700	24.70795200
C	12.74832800	4.96087700	27.44069300
C	13.27149600	4.61762800	28.69750400
H	12.77861000	4.97344200	29.60420100
C	14.42182300	3.83101700	28.81240300
H	14.80724700	3.57728500	29.80260100
C	15.07337100	3.37848100	27.66113800
H	15.97263500	2.76361000	27.73985100
C	14.57011600	3.71184500	26.40415700
H	15.07065700	3.35814600	25.50287100
C	13.40595800	4.49634600	26.27691200
C	12.94380400	4.81800400	24.91953000
C	13.13996800	4.74499600	22.68867800
H	12.89168500	3.74337300	22.30694000
H	13.80863400	5.25959600	21.98883900
C	11.88883800	5.55363500	23.08658500
H	10.99438000	5.13863600	22.61227000
C	9.48074300	7.38923200	25.11910700
H	10.12239300	8.22594300	25.42272500
H	9.10534300	7.50332800	24.09543400
C	8.57857800	6.86728400	26.13270200
H	8.68790100	7.23205900	27.16156200
C	7.32948900	6.22948100	25.87423300
H	7.21959600	5.75720600	24.89794800
Co	10.08105900	5.58849500	25.51821400
C	10.75799300	1.76133900	25.26987100

C	11.05531900	1.49562600	23.92363500
C	11.60602900	1.24063300	26.26407200
C	12.17236500	0.72544100	23.57506200
H	10.40156200	1.89338400	23.14295100
C	12.72082900	0.46988100	25.91859200
H	11.39473000	1.43110600	27.32014600
C	13.00811400	0.21012900	24.57202200
H	12.38728000	0.52639300	22.52179000
H	13.36797000	0.07038400	26.70371500
H	13.87894500	-0.39305900	24.30257300
C	12.01483800	7.03147600	22.74219600
C	11.62822600	7.46170300	21.46030700
C	12.58153100	7.96426200	23.62416000
C	11.80418100	8.79364800	21.06970000
H	11.18859000	6.74482400	20.76105600
C	12.75384300	9.29876600	23.23637200
H	12.87890700	7.65342900	24.62828500
C	12.36710900	9.71815400	21.95826000
H	11.49684000	9.11046700	20.06953700
H	13.19162100	10.01264500	23.93911000
H	12.50179600	10.76001500	21.65631000
N	6.01703300	7.67421300	25.34911600
H	6.37653200	7.91974400	24.42344600
C	5.94662800	8.78752500	26.22267700
C	5.01453100	8.80707100	27.27463400
C	6.86481000	9.84182000	26.08107100
C	5.00195100	9.87983700	28.17059300
H	4.29776100	7.98876200	27.37799500
C	6.84385700	10.90879000	26.98463600
H	7.58123600	9.82778700	25.25647900
C	5.91625000	10.93257000	28.03320400
H	4.26861500	9.89285800	28.98087500
H	7.55674100	11.72836800	26.86334800
H	5.90087900	11.76927500	28.73565200
H	5.12447400	7.18385400	25.24649600
H	10.87098000	10.90635600	28.34469600
H	13.32529400	11.34314400	28.15828900
H	14.88105700	9.45124600	27.66352400
C	6.56457500	5.57492400	26.98779400
H	6.58698200	6.17159900	27.91230500
H	5.52060700	5.37671500	26.70419000
H	7.02726400	4.59913000	27.20726000
O	9.13792600	4.82594800	24.00722900
C	8.57338200	5.42476200	22.89870100

H	8.30147900	4.64629400	22.15149100
H	7.62560300	5.98748400	23.09495700
H	9.23414000	6.14448300	22.36347100
(S)-TS4 ^{CSS}			
Co	10.04443000	6.12026100	4.76794200
C	7.43170800	7.35766000	3.13383300
O	9.16767400	9.77804600	6.73280100
N	9.71331700	8.11024400	5.32488300
P	7.84081400	6.15315000	4.47951000
N	10.20570800	6.16028600	2.78817400
O	10.07872600	6.80065600	0.63961800
C	6.23063000	8.08225700	3.18201900
H	5.55406000	7.95446300	4.02893900
C	5.87275900	8.96166100	2.15417600
H	4.93144200	9.51234300	2.21848600
C	6.71473400	9.12633300	1.05070500
H	6.44218500	9.80934600	0.24322500
C	7.91165900	8.41384300	0.98349200
H	8.57763600	8.53763500	0.12937700
C	8.28425300	7.53396200	2.01819600
C	9.54761100	6.80223900	1.87436200
C	11.35450700	5.49865500	2.12260700
H	12.25352700	5.71743700	2.70635600
C	11.40059800	6.21762000	0.75777500
H	12.13372300	7.03760700	0.73726100
H	11.55743300	5.55185800	-0.09898400
C	5.05820500	7.06056900	7.42664400
H	4.09643400	6.66680000	7.76336900
C	5.72287300	6.44354600	6.35989600
H	5.26155300	5.58464200	5.87024500
C	6.96004200	6.92027700	5.90352400
C	6.84942400	8.67122900	7.60147900
H	7.29651900	9.54111000	8.08300900
C	5.62034100	8.18048500	8.04432300
H	5.10558900	8.67296600	8.87213100
C	8.84168500	8.60814900	6.14638600
C	7.53723200	8.05049600	6.54103000
C	10.56457800	10.01575700	6.41355100
H	11.16101600	9.71662500	7.28950000
H	10.69327700	11.08776600	6.22252000
C	10.81432000	9.11283700	5.19768500
H	11.75111100	8.54731400	5.26864300
C	6.83998600	4.67887400	4.00193000
C	6.71779200	3.59147000	4.88991600

H	7.15288900	3.64420100	5.88875400
C	6.02167400	2.43855600	4.51461900
C	5.44817900	2.34463300	3.24096800
C	5.57057400	3.41427700	2.34825300
C	6.25904000	4.57391000	2.72388400
H	6.33841400	5.39745300	2.01211300
C	11.18668600	3.99174900	1.99124800
C	12.33354900	3.17936700	1.97111100
C	9.93071400	3.39079100	1.81295200
C	12.22800200	1.79703500	1.77966600
H	13.31845500	3.63507800	2.10679000
C	9.82295000	2.00755600	1.62536300
H	9.02486900	4.00085300	1.83472300
C	10.97055100	1.20584900	1.60772500
H	13.13071200	1.18046700	1.76965900
H	8.83614300	1.55564600	1.49440800
H	10.88534700	0.12581000	1.46252500
C	10.76472300	9.83712700	3.86121600
C	11.78139600	9.62941100	2.91569100
C	9.73885100	10.75238500	3.56102000
C	11.77951400	10.32363600	1.69885800
H	12.57867100	8.91713400	3.14182100
C	9.73588000	11.44768000	2.34773000
H	8.93715000	10.93302400	4.28272800
C	10.75787500	11.23637500	1.41280800
H	12.58168800	10.15424500	0.97558000
H	8.93401700	12.15853200	2.13193600
H	10.75766900	11.78292100	0.46617700
C	9.39412000	5.89179300	8.68353100
C	9.31031600	4.98767700	7.49030700
C	10.32700600	5.01442100	6.49336000
H	11.30141500	5.34298800	6.86863900
C	10.30150900	4.26187200	5.25030200
H	9.45532800	3.58406700	5.07435200
H	11.25227500	3.84066200	4.90193400
O	11.92192400	6.54403000	4.83972500
C	13.01286600	5.73677200	5.09114700
H	13.22169400	4.97685900	4.29959000
H	13.92912300	6.36373000	5.15705000
H	12.97108400	5.16847200	6.05102200
H	8.29924900	4.70850900	7.18208100
H	9.08504900	6.90692900	8.38761100
N	9.55383600	3.18961000	8.41933600
H	9.65895900	2.59219200	7.59564400

C	8.53861500	2.74788500	9.30347400
C	8.62713100	3.02308600	10.67934700
C	7.40590600	2.08902400	8.79378900
C	7.58860100	2.63915700	11.53285600
H	9.51369800	3.52507100	11.07469000
C	6.37470500	1.70935200	9.65667000
H	7.34587100	1.86697400	7.72547400
C	6.45835700	1.98425300	11.02790000
H	7.66796800	2.85058300	12.60217500
H	5.50108200	1.19128200	9.25316500
H	5.65021400	1.68469000	11.69926600
H	10.46500300	3.30213900	8.87157700
H	5.12578700	3.35281900	1.35194200
H	4.90694900	1.44189100	2.94720400
H	5.92910100	1.61050900	5.22174400
H	8.71820000	5.57095400	9.48931200
H	10.42369800	5.95375700	9.06803800
<i>E-TS3a</i> ^{triplet}			
Co	9.83217500	6.27024300	4.59871800
C	7.27519700	7.73432800	2.80459100
O	9.26427800	10.20069900	6.33299700
N	9.55029200	8.48154700	4.90563600
P	7.44962300	6.62066700	4.27086600
N	9.78302100	5.95605500	2.51999400
O	9.85769900	6.64480000	0.38556300
C	6.22617800	8.66678300	2.77338300
H	5.54098400	8.73253300	3.62083200
C	6.02838600	9.50954100	1.67483600
H	5.20060900	10.22261200	1.68150200
C	6.88674500	9.42925800	0.57591700
H	6.74457700	10.08080800	-0.28900800
C	7.93631500	8.51076600	0.58639400
H	8.61192800	8.44815400	-0.26631000
C	8.14912700	7.65854100	1.68965200
C	9.28022700	6.71593500	1.59728300
C	10.85212300	5.14172200	1.89652500
H	11.75717400	5.23647800	2.50815200
C	11.04617800	5.82820000	0.52465400
H	11.91956100	6.49604900	0.50405200
H	11.08373500	5.13639700	-0.32537800
C	4.86992200	8.07065200	7.18340700
H	3.86305800	7.83500300	7.53627700
C	5.41325100	7.34864100	6.11631400
H	4.81428900	6.56344400	5.65336500

C	6.69940400	7.62396400	5.62177500
C	6.88537600	9.38966200	7.30518500
H	7.46752100	10.18937600	7.76324600
C	5.61046200	9.09215700	7.78462000
H	5.19687700	9.66019000	8.62080700
C	8.78759500	9.07079400	5.77208900
C	7.44624000	8.67155500	6.22932300
C	10.64050700	10.33749000	5.89564600
H	11.28726100	10.07186100	6.74561400
H	10.80753500	11.38617000	5.61957600
C	10.75956400	9.33789500	4.73157400
H	11.61666200	8.65942700	4.84415100
C	6.19539600	5.31314700	3.91887800
C	5.90175300	4.35859800	4.91577500
H	6.35834300	4.43933600	5.90545400
C	5.01137900	3.31171100	4.65922800
C	4.41607100	3.18342900	3.39769400
C	4.71180600	4.11507500	2.39766200
C	5.59043200	5.17487600	2.65556200
H	5.79891300	5.89738800	1.86410200
C	10.47440000	3.67358300	1.78043200
C	11.47181700	2.69174200	1.90173400
C	9.15810400	3.27181300	1.50100300
C	11.15977800	1.33537200	1.75274700
H	12.50030900	2.99240000	2.12060600
C	8.84395100	1.91583200	1.35495700
H	8.36691500	4.02019400	1.41086000
C	9.84319600	0.94287500	1.48141500
H	11.94670200	0.58328900	1.85380500
H	7.81318900	1.61907300	1.14387200
H	9.59713300	-0.11617400	1.36907000
C	10.80826400	9.95943400	3.34470900
C	11.72072300	9.45930500	2.40125700
C	9.97825400	11.03437200	2.97932800
C	11.81291900	10.02558000	1.12388700
H	12.35420500	8.61401100	2.68226500
C	10.06755700	11.60074500	1.70306200
H	9.25841800	11.44086600	3.69573000
C	10.98756400	11.09996200	0.77235400
H	12.53311000	9.62890600	0.40316800
H	9.41851500	12.43858600	1.43503200
H	11.06022500	11.54711700	-0.22250000
C	10.23805400	6.19577600	7.51042400
C	9.51703300	5.40911800	6.44090800

C	10.17369200	4.36871900	5.71676700
H	11.26086700	4.28482900	5.79479100
C	9.48636400	3.30611200	5.07428100
H	8.41401900	3.41939000	4.89793600
H	10.01512200	2.74425200	4.30160500
O	11.73783100	6.68293400	4.62125500
C	12.86873000	5.93253200	4.86124900
H	13.79111800	6.48294200	4.56345800
H	13.01370400	5.66786000	5.93773500
H	12.90677000	4.96338800	4.30637800
H	9.74362400	7.15854400	7.71277200
H	8.44211800	5.28086000	6.61856800
H	4.25237100	4.02607900	1.40993500
H	3.72423200	2.36154300	3.19753300
H	4.78272600	2.59225500	5.44932500
H	10.24225600	5.63236100	8.46322200
H	11.28163400	6.39518300	7.22608700
N	9.33110500	1.74280600	6.21029800
H	8.79784600	1.08235000	5.63633400
C	8.75657700	1.94850000	7.49321500
C	9.56513000	2.38032500	8.55678700
C	7.37328900	1.78984700	7.67617100
C	8.98507000	2.64539900	9.80195400
H	10.64159100	2.49357900	8.40833500
C	6.80544800	2.05785700	8.92422100
H	6.75376600	1.44845600	6.84330700
C	7.60669900	2.48827400	9.99046500
H	9.61819800	2.97382800	10.62992500
H	5.72994000	1.92462700	9.06502000
H	7.15856600	2.69444700	10.96530800
H	10.30244700	1.42314400	6.26290900
<i>E-TS3b</i> ^{triplet}			
C	11.82885900	7.61832700	27.93576800
O	9.02574800	2.04427900	28.23708700
N	9.68839700	3.55631500	26.71320100
P	11.11322600	5.96496200	27.53636100
N	11.68956400	5.71928100	24.64288300
O	13.73996200	5.12097900	23.94212500
C	13.21338300	7.84262600	28.05570000
H	13.91441100	7.00934600	27.97923400
C	13.70920300	9.13341900	28.27711400
C	9.74327500	5.76016900	31.45144900
H	9.80087400	6.38652600	32.34490500
C	10.37456900	6.17620700	30.27392300

H	10.92188900	7.12051800	30.27105100
C	10.32893300	5.40028000	29.10481900
C	10.95553000	8.72111200	28.04091000
H	9.87683300	8.57608700	27.95021900
C	11.45303000	10.00634100	28.27540100
C	12.83289100	10.21782900	28.39024400
C	9.05569800	4.54406500	31.48292500
H	8.56424900	4.20735800	32.39834200
C	8.99555100	3.75734000	30.33234600
H	8.45486700	2.81070700	30.34595000
C	9.46857400	3.28866300	27.96311000
C	9.61230400	4.17095100	29.13486600
C	8.71501400	1.42534600	26.96275500
H	7.62569300	1.48131300	26.81852700
H	9.02840900	0.37590500	27.00594200
C	9.48047300	2.28806700	25.94871300
H	8.86424700	2.52090200	25.07386500
C	12.61855100	4.89245500	27.45791500
C	13.13601900	4.31499300	28.62880600
H	12.63452500	4.49244800	29.58216800
C	14.29290500	3.52893800	28.60664000
H	14.67157000	3.09721900	29.53617500
C	14.96181900	3.31065100	27.39985500
H	15.86837300	2.70221100	27.36981000
C	14.46324100	3.87216400	26.22422000
H	14.97532300	3.69945800	25.27776000
C	13.29186700	4.65545000	26.23177900
C	12.83602700	5.19970600	24.93801500
C	13.06048700	5.51234200	22.72299200
H	12.89168900	4.60391100	22.12599700
H	13.71570900	6.20129600	22.17557500
C	11.74342700	6.14805600	23.22595400
H	10.86716900	5.70112400	22.73645800
C	8.67331800	7.70290700	24.82502400
H	9.45696400	8.45634700	24.92994500
H	8.64580300	7.19287700	23.85855200
C	8.30684900	6.94752900	25.97288100
H	8.45153800	7.40591900	26.95616500
C	7.63664900	5.69848500	25.89715000
H	7.23027200	5.41548300	24.92232500
Co	9.70774900	5.33699900	25.56200100
C	10.80296300	1.70203800	25.46778600
C	11.23975200	1.97043100	24.15977600
C	11.59502500	0.88474500	26.29386000

C	12.43076000	1.41395100	23.67818000
H	10.64083500	2.64474100	23.54101800
C	12.78795000	0.33242600	25.81389200
H	11.28442300	0.66911300	27.31974800
C	13.20576900	0.58912300	24.50219400
H	12.75326100	1.62284000	22.65454100
H	13.39038000	-0.30465000	26.46669300
H	14.13297800	0.14921400	24.12573400
C	11.70076200	7.65866700	23.06284200
C	11.01568700	8.21133200	21.96757300
C	12.37435400	8.52166400	23.94329700
C	11.00362600	9.59481600	21.75436700
H	10.48494800	7.54966000	21.27688100
C	12.36087300	9.90584800	23.73401600
H	12.90711800	8.11367300	24.80602700
C	11.67570600	10.44723000	22.63907500
H	10.46566700	10.00767700	20.89679300
H	12.88769900	10.56367500	24.43034400
H	11.66562200	11.52804000	22.47615300
N	7.33110800	9.04581200	24.34783300
H	7.38899400	9.71055000	25.12422200
C	6.01780600	8.54698100	24.14861500
C	5.62492000	8.08813400	22.88029100
C	5.14068800	8.44197800	25.23987400
C	4.35206400	7.53757900	22.70855400
H	6.31396200	8.17172100	22.03594300
C	3.86953800	7.88857600	25.05561400
H	5.45220100	8.80550000	26.22212900
C	3.47039400	7.43406100	23.79285200
H	4.04676500	7.18994500	21.71849900
H	3.18676200	7.81701100	25.90589800
H	2.47553300	7.00495500	23.65243900
H	7.72927900	9.47756700	23.50838000
C	6.89343700	5.13176900	27.07481900
H	5.85953300	5.52706400	27.08840900
H	6.80971000	4.03511600	27.02350400
H	7.36083600	5.40371000	28.03283700
H	14.78765000	9.28723600	28.36691000
H	13.22209200	11.22370600	28.56660000
H	10.75900100	10.84614500	28.36290100
O	9.33119300	4.62957400	23.77852700
C	8.19102000	4.19453900	23.13365300
H	8.43498900	3.71656200	22.15756600
H	7.59967300	3.43441400	23.70122000

H	7.46964000	5.01296700	22.89172600
(R)-IM9 ^{CSS}			
C	11.94954800	7.76552400	27.69057700
O	8.74290100	2.41596400	27.83950100
N	9.78024600	3.83550500	26.43403800
P	11.29957600	6.07573700	27.33594700
N	11.84325000	5.26662400	24.54954100
O	13.87128100	4.48893700	23.95689700
C	13.31454100	8.06444100	27.52106400
H	14.02298500	7.27413400	27.26472900
C	13.78190400	9.37433800	27.68261500
C	9.80201900	5.91593100	31.21248600
H	9.89839600	6.50796800	32.12560800
C	10.48813400	6.30939400	30.05712900
H	11.11744400	7.20002500	30.09337600
C	10.38647000	5.57912900	28.86345100
C	11.06314900	8.81267100	28.01837500
H	9.99855400	8.61115600	28.15813000
C	11.53539400	10.11796300	28.18546300
C	12.89578800	10.40383200	28.01656400
C	9.00610400	4.76815500	31.19288100
H	8.46874900	4.45084800	32.08934700
C	8.89774000	4.02280200	30.01831800
H	8.27862200	3.12576100	29.99458700
C	9.40016600	3.58042700	27.64668800
C	9.57319100	4.41387600	28.84542400
C	8.45915000	1.88636500	26.51867300
H	7.40661400	2.11101800	26.28511200
H	8.61128000	0.80065500	26.54685900
C	9.44108100	2.64463000	25.60701100
H	8.96589700	3.02960200	24.69545000
C	12.81536600	5.02574300	27.45201600
C	13.36058000	4.73183100	28.71295300
H	12.87430300	5.11225400	29.61331800
C	14.52114400	3.96378600	28.84286200
H	14.92217700	3.75159700	29.83668600
C	15.16167600	3.47451000	27.69994300
H	16.06794900	2.87120500	27.78856500
C	14.63791800	3.75673600	26.43953000
H	15.12946400	3.37431600	25.54508700
C	13.46498300	4.52767100	26.29642800
C	12.98795500	4.79000700	24.93177700
C	13.14930800	4.58529600	22.70751700
H	12.87442900	3.56652700	22.39513800

H	13.81106600	5.04186800	21.96198200
C	11.92061200	5.43873400	23.07972200
H	11.00820000	5.02135000	22.64165800
C	9.50301400	7.47760100	25.19197000
H	10.13535100	8.30618100	25.53877900
H	9.14074300	7.63868500	24.16768600
C	8.62819500	6.83766500	26.15827300
H	8.70258000	7.18417800	27.19998500
C	7.22936200	6.40920900	25.82114800
H	7.23767300	5.79103900	24.91632200
Co	10.11851600	5.66383600	25.54015300
C	10.66539100	1.82455100	25.23161900
C	10.86641100	1.45177100	23.89260200
C	11.56953600	1.36029200	26.20359800
C	11.94366300	0.63332100	23.52973500
H	10.16866000	1.80389400	23.12803500
C	12.64615700	0.54251500	25.84377300
H	11.43459500	1.63395100	27.25365300
C	12.83720100	0.17650200	24.50505300
H	12.08370500	0.35269600	22.48241600
H	13.33885300	0.18956400	26.61217600
H	13.67848100	-0.46259800	24.22467800
C	12.07385600	6.89523800	22.65906800
C	11.75793300	7.25633100	21.33641300
C	12.58925400	7.87621300	23.51970000
C	11.95378800	8.56618900	20.88644600
H	11.35608200	6.50284400	20.65288600
C	12.78187000	9.18933900	23.07186500
H	12.82699000	7.61862600	24.55403300
C	12.46623900	9.53916200	21.75428900
H	11.70111800	8.82872300	19.85567700
H	13.17973800	9.94062200	23.75929500
H	12.61606200	10.56404600	21.40502900
N	6.36797000	7.65155200	25.35198300
H	6.87917100	8.06282700	24.55773400
C	6.07509500	8.69568800	26.33485800
C	4.89014300	8.62889500	27.07357200
C	6.99293200	9.73263200	26.52413800
C	4.62817100	9.61772000	28.02781700
H	4.17733600	7.82010000	26.89849700
C	6.71992800	10.71469300	27.48232300
H	7.90344300	9.77825300	25.92413100
C	5.54240600	10.65711300	28.23638700
H	3.70229100	9.57471200	28.60573200

H	7.43097400	11.53032300	27.63253600
H	5.33248400	11.42770300	28.98179400
H	5.48577700	7.28929800	24.96173000
H	10.83471000	10.91452000	28.44830400
H	13.26298600	11.42491300	28.14634500
H	14.84603800	9.58584200	27.55078100
C	6.47987900	5.70305300	26.93692900
H	6.47479100	6.29074700	27.86786900
H	5.44029100	5.47861500	26.65018700
H	6.98162300	4.74834800	27.14349700
O	9.11316300	4.95919900	24.03070700
C	8.62112100	5.59648700	22.91012300
H	8.31849200	4.84327800	22.14767500
H	7.70497100	6.21757700	23.08368500
H	9.34084500	6.27630000	22.40027000
(S)-IM9^{CSS}			
Co	9.99524300	6.07374500	4.78669800
C	7.43004900	7.34261900	3.08606600
O	9.14264500	9.72961300	6.73967100
N	9.68996600	8.05412600	5.33733600
P	7.82094500	6.13529600	4.44114800
N	10.20637300	6.16614900	2.77314400
O	10.12253100	6.81490600	0.62050500
C	6.22948300	8.06993800	3.12336700
H	5.54639100	7.94380700	3.96539200
C	5.87834100	8.94936000	2.09332600
H	4.93665900	9.50028900	2.15126500
C	6.72793300	9.11316200	0.99532500
H	6.46143900	9.79589800	0.18546400
C	7.92527700	8.40091700	0.93850000
H	8.59934400	8.52561500	0.09078000
C	8.29160800	7.52083500	1.97590200
C	9.56324100	6.80153100	1.84702200
C	11.37724800	5.52445700	2.13152900
H	12.25602900	5.74685400	2.74562700
C	11.44945300	6.25264700	0.77182300
H	12.17019400	7.08412700	0.77781500
H	11.64214800	5.59583700	-0.08481900
C	4.98181400	7.05943800	7.33640400
H	4.00841800	6.67620900	7.65149800
C	5.66027500	6.44094500	6.27903200
H	5.19839600	5.59041900	5.77499500
C	6.91240700	6.90406500	5.84921300
C	6.79004800	8.64549800	7.55793600

H	7.23918000	9.50623200	8.05398500
C	5.54618000	8.16817000	7.97284500
H	5.02138500	8.66177600	8.79378600
C	8.80871400	8.56444200	6.14083400
C	7.49101700	8.02304600	6.50647700
C	10.55140400	9.93597600	6.45584100
H	11.12161200	9.60984600	7.34000300
H	10.71188100	11.00672600	6.28211100
C	10.80559500	9.04232800	5.23415900
H	11.73384800	8.46264000	5.30864400
C	6.81056400	4.67010900	3.94676100
C	6.68192700	3.57888600	4.82940600
H	7.11584700	3.62825700	5.82908400
C	5.98541700	2.42825200	4.44758500
C	5.41701700	2.33996800	3.17111800
C	5.54641900	3.41245700	2.28272300
C	6.23580100	4.56944700	2.66568200
H	6.32071600	5.39520800	1.95697900
C	11.22720300	4.01631100	1.98472400
C	12.38293200	3.21684500	1.94612100
C	9.97709100	3.40177400	1.81129900
C	12.29171400	1.83546800	1.74054500
H	13.36385500	3.68225700	2.07806600
C	9.88338800	2.01940600	1.60943600
H	9.06518000	4.00182800	1.84925900
C	11.03981700	1.23122000	1.57266000
H	13.20143900	1.22962700	1.71621600
H	8.90059200	1.55758700	1.48244000
H	10.96599200	0.15191800	1.41600700
C	10.77684100	9.78500500	3.90699700
C	11.82188200	9.61484200	2.98510200
C	9.74069400	10.68463500	3.59428900
C	11.83601300	10.32767800	1.77901500
H	12.62999200	8.91760600	3.21987300
C	9.75378000	11.39893100	2.39226700
H	8.91789300	10.83819100	4.29814100
C	10.80264200	11.22270300	1.47999300
H	12.65947700	10.18569600	1.07397000
H	8.94286700	12.09650200	2.16708700
H	10.81425600	11.78290600	0.54143500
C	9.25998500	5.84338500	8.74086200
C	9.14525000	4.85611600	7.59087300
C	10.15177500	5.06662900	6.49160300
H	11.12066700	5.35429600	6.92293100

C	10.20773300	4.21663400	5.31467600
H	9.36708700	3.53486900	5.11736900
H	11.17106900	3.78099100	5.01802000
O	11.89022400	6.45651600	4.88589600
C	12.94333900	5.62746000	5.20574400
H	13.17937000	4.85698100	4.43026300
H	13.87345100	6.22745600	5.32603200
H	12.82973200	5.06478100	6.16418200
H	8.11149200	4.78964700	7.22679300
H	9.10200500	6.85849100	8.35502600
N	9.40206800	3.41159100	8.16693900
H	9.36782300	2.77481500	7.35683100
C	8.51514000	2.92403800	9.22520700
C	8.96717100	2.92068100	10.54704100
C	7.22895800	2.49105000	8.89138500
C	8.10819500	2.47373000	11.55656500
H	9.97972600	3.25716100	10.78141300
C	6.37978700	2.04669400	9.90952100
H	6.89798900	2.49362300	7.85112100
C	6.81614900	2.03905700	11.24004800
H	8.45462700	2.46374700	12.59233000
H	5.37435900	1.70158000	9.65840600
H	6.14883300	1.68924500	12.03109400
H	10.37941700	3.38663800	8.49393700
H	5.10632900	3.35517200	1.28399300
H	4.87538800	1.43933000	2.87151500
H	5.88961300	1.59704000	5.15070800
H	8.51401800	5.65923500	9.52814100
H	10.26720000	5.80550100	9.18672000
<i>E-IM8a</i>^{CSS}			
Co	9.58276400	6.22986000	4.52805500
C	7.25525200	7.82345500	2.73945100
O	9.57551500	10.02255400	6.29528100
N	9.66156000	8.27448400	4.87845100
P	7.44435400	6.68763100	4.19454400
N	9.81876300	6.18246200	2.50251400
O	9.83519300	6.74006300	0.32173000
C	6.18009500	8.72667100	2.71251700
H	5.49418500	8.77393200	3.56035100
C	5.95781400	9.56579300	1.61647600
H	5.11160200	10.25682400	1.62662700
C	6.81521800	9.51063900	0.51372000
H	6.65144700	10.15993500	-0.34924200
C	7.88994000	8.62270000	0.51996800

H	8.56802700	8.57782100	-0.33237900
C	8.12810700	7.77748300	1.62375700
C	9.27777200	6.86670000	1.54562500
C	10.88065800	5.34595600	1.89406400
H	11.78191700	5.44760000	2.50715500
C	11.06708800	6.00254000	0.50994100
H	11.89973600	6.72216300	0.49466600
H	11.17128400	5.29227700	-0.31898500
C	4.94285100	8.41125600	7.05657200
H	3.90149300	8.30324300	7.36894800
C	5.43111700	7.62906800	6.00231900
H	4.75049500	6.93498400	5.50873900
C	6.76217700	7.72973800	5.56904500
C	7.10261200	9.46297500	7.26437200
H	7.76289500	10.18806800	7.74086200
C	5.78353900	9.32416100	7.69678000
H	5.41355400	9.93509200	8.52319000
C	8.97662000	8.94002500	5.75396100
C	7.60403400	8.68161500	6.20514900
C	10.95910600	9.97502000	5.85592100
H	11.55732800	9.55768600	6.68109700
H	11.28337300	11.00013300	5.64019100
C	10.91695800	9.04579900	4.63455000
H	11.72724900	8.30565300	4.63676700
C	6.10523300	5.45348600	3.85645800
C	5.56359100	4.66311900	4.89188400
H	5.87909100	4.81745400	5.92645300
C	4.60535500	3.68270500	4.61454900
C	4.18555600	3.45735800	3.29818000
C	4.72625300	4.22450000	2.26152100
C	5.67429500	5.21704100	2.53739500
H	6.07142800	5.81377800	1.71405600
C	10.48546100	3.87870600	1.80074600
C	11.45898100	2.88423500	1.99381500
C	9.18472100	3.48680800	1.44089600
C	11.14145300	1.52983500	1.83386800
H	12.47678000	3.17433400	2.26870000
C	8.86483200	2.13390700	1.28107800
H	8.40838900	4.24068200	1.28977700
C	9.84225900	1.14999300	1.47631000
H	11.91223600	0.77021300	1.98922600
H	7.84639400	1.84797400	1.00517500
H	9.59191400	0.09325500	1.35214600
C	10.88662900	9.77982500	3.30303600

C	11.84123400	9.47811400	2.31847300
C	9.95197900	10.80000000	3.04461400
C	11.86569900	10.17611900	1.10391500
H	12.57398000	8.68982700	2.50974900
C	9.97620500	11.50061400	1.83450000
H	9.20141700	11.05941100	3.79649500
C	10.93371600	11.19063400	0.85940000
H	12.61754200	9.92803300	0.34993400
H	9.24531900	12.29267300	1.65189800
H	10.95292200	11.73945800	-0.08572900
C	10.19507000	6.04607400	7.46230600
C	9.28682800	5.54460900	6.35947400
C	9.64581200	4.47932300	5.44069000
H	10.68945000	4.14335800	5.47070600
C	8.73993300	3.32528700	5.15869600
H	7.67957700	3.58599600	5.08628800
H	9.03463600	2.74607000	4.27426800
O	11.51899200	6.34290200	4.64639200
C	12.49986500	5.42708000	4.95447400
H	13.50219100	5.89201900	4.81310600
H	12.49252300	5.06052200	6.01095400
H	12.50349600	4.50780200	4.31920800
H	9.85087900	7.02267300	7.84485100
H	8.22788400	5.54681000	6.66965800
H	4.40543200	4.05963800	1.22984200
H	3.43858900	2.68921100	3.08337000
H	4.18614700	3.09230800	5.43293500
H	10.21315200	5.35678000	8.33055300
H	11.22563100	6.17527500	7.10457700
N	8.81441100	2.30320400	6.32575000
H	9.81095200	2.09687300	6.48984200
C	8.07711600	1.05157300	6.13394300
C	6.78009000	0.93913900	6.63802300
C	8.68156600	0.01317900	5.42100700
C	6.07239600	-0.24815800	6.42188800
H	6.33442000	1.76391600	7.19871000
C	7.96318200	-1.16791000	5.21121600
H	9.70007700	0.12543100	5.04232700
C	6.66083600	-1.29905500	5.70880700
H	5.05902100	-0.34993200	6.81662200
H	8.42708600	-1.98910500	4.66034800
H	6.10473900	-2.22479100	5.54385800
H	8.48620900	2.77888900	7.17891600

E-IM8b^{CSS}

C	11.45608500	7.50188600	28.21170800
O	8.93969300	1.82381700	27.64201200
N	9.72193100	3.55766100	26.43642200
P	10.91975000	5.83217900	27.62188600
N	11.47251600	5.59713400	24.74666900
O	13.51933200	5.10173300	23.95332300
C	12.78969100	7.92583900	28.05302500
H	13.54292900	7.23962700	27.66195400
C	13.17172700	9.22859500	28.39532900
C	9.63670100	4.91617000	31.47250600
H	9.70285300	5.36985500	32.46419800
C	10.23151200	5.55499900	30.37768700
H	10.75951300	6.49687900	30.53580200
C	10.16447600	5.00475500	29.08965700
C	10.51606300	8.42225200	28.71933800
H	9.47467800	8.12686700	28.85573300
C	10.90241500	9.72051700	29.06742800
C	12.23096300	10.12992600	28.90364500
C	8.96890200	3.70194400	31.29279800
H	8.50143000	3.19613600	32.14056400
C	8.90177200	3.13149700	30.02116500
H	8.38704900	2.18167100	29.87389200
C	9.39683400	3.09528600	27.60614500
C	9.48832200	3.76814800	28.90974100
C	8.74213900	1.43136500	26.25920900
H	7.67580800	1.56668500	26.01862900
H	9.01861200	0.37512500	26.16096400
C	9.64411700	2.40486600	25.48805700
H	9.18623400	2.76149100	24.56204500
C	12.54362400	4.94055100	27.51715000
C	13.15613700	4.49748900	28.70087300
H	12.65244000	4.64916900	29.65742600
C	14.40665000	3.87198700	28.68630400
H	14.85688500	3.54033800	29.62488000
C	15.07320900	3.67935000	27.47259300
H	16.05093400	3.19298300	27.44827100
C	14.48130200	4.10772800	26.28522100
H	14.98991500	3.95473500	25.33334100
C	13.21850700	4.73499600	26.28880000
C	12.66718600	5.16655700	24.99886500
C	12.71602900	5.32568000	22.76765900
H	12.49463200	4.34540100	22.31831500
H	13.30062400	5.93511000	22.06844500
C	11.45949300	6.01904500	23.32578400

H	10.53317900	5.62832600	22.88372300
C	8.39341700	7.81186500	24.46884800
H	9.15573200	8.47412400	24.04286600
H	8.15172600	7.01711700	23.75500600
C	8.76074900	7.25360800	25.80443600
H	9.19578300	8.00485400	26.47899400
C	7.96029600	6.20271900	26.40742100
H	7.19955800	5.77460700	25.74148400
Co	9.71757200	5.51409100	25.80190900
C	11.01477100	1.82739600	25.16403700
C	11.45326900	1.78249200	23.83110100
C	11.83299000	1.26729900	26.16259200
C	12.68086400	1.19478700	23.49895700
H	10.82164900	2.20589100	23.04556900
C	13.05711900	0.67697000	25.83285700
H	11.51053200	1.27912500	27.20714000
C	13.48606200	0.64000700	24.49940200
H	13.00533400	1.16838400	22.45536800
H	13.67853600	0.24303500	26.62043000
H	14.44282600	0.17788900	24.24278900
C	11.51381900	7.53091000	23.15569700
C	11.05300000	8.08946000	21.95014100
C	12.05983100	8.38300300	24.12801600
C	11.13566300	9.46697900	21.72179700
H	10.62155000	7.43672600	21.18557800
C	12.13757300	9.76350900	23.90403100
H	12.41599200	7.97088700	25.07462100
C	11.67696800	10.31064900	22.70101600
H	10.77153000	9.88410500	20.77904700
H	12.55960700	10.41258400	24.67597300
H	11.73786400	11.38801900	22.52659500
N	7.11008500	8.69581300	24.51247200
H	6.79386700	8.83687300	23.54210200
C	7.24869600	9.99742600	25.16897400
C	6.93095200	10.12069600	26.52291000
C	7.72923900	11.07990400	24.42705500
C	7.09880100	11.36226700	27.14654900
H	6.55018500	9.26156000	27.07901000
C	7.89109800	12.31545000	25.06151500
H	7.96876900	10.95863500	23.36806000
C	7.57854100	12.45730800	26.41916600
H	6.84864900	11.47073900	28.20429300
H	8.25996900	13.16971300	24.48942500
H	7.70546600	13.42513000	26.90977600

H	6.36788200	8.14986800	24.97387300
C	7.43337200	6.26589000	27.82657100
H	6.49699100	6.85712600	27.87105300
H	7.18810500	5.26350400	28.21631100
H	8.13920600	6.72511300	28.53405800
H	14.21291000	9.53459300	28.26573900
H	12.53066400	11.14577400	29.17295800
H	10.15820200	10.41418200	29.46670300
O	8.96409800	4.94394100	24.10424100
C	7.67768100	4.51283700	23.85425400
H	7.64222700	3.95536800	22.89091100
H	7.25833000	3.82119900	24.62411000
H	6.92208200	5.33235800	23.74571600
IM10 ^{triplet}			
Co	9.37583700	5.45504300	4.82427600
C	7.66748200	7.43368700	2.55931700
O	9.08207300	9.42850200	6.54721500
N	9.51412500	7.59837800	5.31536000
P	7.35117900	6.23236400	3.90758100
N	10.04624500	5.43152200	2.87877800
O	10.39989200	5.85988100	0.70822100
C	6.79937400	8.51360700	2.34143800
H	5.93953900	8.65588300	2.99939100
C	7.01136900	9.40667100	1.28535800
H	6.32275600	10.24135600	1.13563200
C	8.09471100	9.22012900	0.42336100
H	8.26535500	9.90795900	-0.40747200
C	8.96952600	8.15173400	0.62725200
H	9.82105800	8.00954000	-0.03804300
C	8.77762700	7.25773500	1.69825600
C	9.74606200	6.15082700	1.83578100
C	11.00320200	4.37660500	2.43370900
H	11.88505200	4.39524000	3.08351200
C	11.39113800	4.84814700	1.01671300
H	12.37908600	5.32873000	0.98525900
H	11.32673800	4.06726700	0.24956900
C	4.39696400	7.81476000	6.33406800
H	3.31751500	7.69026600	6.44665600
C	5.07762600	7.08715000	5.35033400
H	4.51759900	6.40710100	4.70617500
C	6.46214100	7.22242800	5.17554100
C	6.47637400	8.84505700	7.00034500
H	7.02939400	9.53054500	7.64289300
C	5.09738000	8.69635600	7.15954800

H	4.57541100	9.26897400	7.92909600
C	8.63184800	8.32955200	5.92103800
C	7.17504500	8.11296900	6.02227400
C	10.53036700	9.37233100	6.50666000
H	10.88059300	9.06732700	7.50374400
H	10.90418100	10.37559500	6.27045100
C	10.82425300	8.30982500	5.42926000
H	11.57708400	7.60129900	5.79114400
C	6.10265200	5.07107200	3.23538000
C	5.79989100	3.92709000	4.00081400
H	6.28387700	3.77563500	4.96847600
C	4.87960500	2.98756800	3.52843000
C	4.26606300	3.16868000	2.28190800
C	4.57296400	4.29580300	1.51183100
C	5.48542100	5.24661200	1.98424800
H	5.71065800	6.12397000	1.37473900
C	10.39225900	2.98581500	2.48964100
C	11.12879900	1.92817600	3.04757000
C	9.12240400	2.71851900	1.94932100
C	10.60796500	0.62874500	3.06913900
H	12.11968400	2.12442800	3.46627800
C	8.59915800	1.42128400	1.97471600
H	8.53271600	3.52323300	1.50239500
C	9.33957800	0.37304800	2.53596100
H	11.19362700	-0.18343300	3.50733000
H	7.60836100	1.22944300	1.55518700
H	8.92885300	-0.63958400	2.55607600
C	11.30669900	8.87213700	4.10042700
C	12.44225100	8.32197200	3.48493300
C	10.67306500	9.97160400	3.49418400
C	12.93783500	8.85511200	2.28861600
H	12.95023000	7.47496500	3.95415600
C	11.17193700	10.51112700	2.30407100
H	9.78813600	10.41974800	3.95494100
C	12.30549900	9.95412600	1.69730300
H	13.82515400	8.41643300	1.82478700
H	10.67336000	11.37028800	1.84834900
H	12.69483000	10.37853100	0.76836300
C	11.98569100	4.35858200	9.31764300
C	11.71960700	4.13782900	7.85917400
C	11.46065600	5.11254200	6.95783000
H	11.44923500	6.14859700	7.32476500
C	11.20081900	4.91340700	5.52595200
H	11.33448400	3.86689900	5.21144700

H	11.80207800	5.58837000	4.89324700
H	11.24357400	3.82879800	9.94263000
N	8.47230300	4.93937400	6.36329200
C	8.36148300	3.72483100	6.99297800
C	7.76867800	3.61412100	8.28072000
C	8.80981400	2.52957400	6.37106200
C	7.63821300	2.37421600	8.90675000
H	7.41313500	4.52205200	8.77721500
C	8.67601900	1.29624700	7.00927400
H	9.25328800	2.59112100	5.37460100
C	8.09152800	1.20245500	8.28176900
H	7.17790100	2.32180300	9.89768900
H	9.02813000	0.39302800	6.50261500
H	7.98702500	0.23335700	8.77551000
H	7.98295600	5.67673500	6.87635800
H	11.74656700	3.09601200	7.51206700
H	4.09892700	4.44131400	0.53797600
H	3.55144400	2.42978200	1.91092300
H	4.64746900	2.10753500	4.13322300
H	12.97405300	3.95995100	9.61052400
H	11.95415900	5.42776900	9.58116300
IM10 ^{triplet}			
Co	9.50533900	5.53259900	5.02513300
C	9.02498500	8.40084100	3.15585000
O	12.77747300	5.75614600	2.20444000
N	10.81110000	5.59090600	3.27788300
P	9.74557800	7.86146000	4.75282400
N	7.63377000	5.80575500	4.21672900
O	5.87978000	6.53889900	3.03161600
C	9.59510100	9.45478200	2.42694400
H	10.49618900	9.94525800	2.80099600
C	9.02005800	9.89693600	1.23031800
H	9.48295600	10.71807700	0.67830200
C	7.85366400	9.29351600	0.75415800
H	7.39394000	9.63494800	-0.17568000
C	7.27334700	8.24305000	1.46717700
H	6.36889100	7.76383900	1.09272100
C	7.85329000	7.77648700	2.66248900
C	7.16913100	6.66467200	3.35476000
C	6.48866400	4.96605700	4.67285300
H	6.74987400	3.90865300	4.55371300
C	5.37431600	5.34191400	3.67416000
H	5.22942400	4.58118700	2.89424200
H	4.41505900	5.58998500	4.14370400

C	13.43695800	9.68023300	5.17316000
H	13.83016800	10.55729900	5.69230500
C	12.07087400	9.38418100	5.25459700
H	11.41654500	10.03674500	5.83518900
C	11.53070400	8.26836300	4.59976600
C	13.76645800	7.74394900	3.76865800
H	14.42414000	7.09768100	3.18687900
C	14.28599000	8.85947200	4.42835400
H	15.35266500	9.08297700	4.35897700
C	11.92664100	6.23242800	3.12637600
C	12.39719700	7.42971100	3.84911300
C	12.23673100	4.49057300	1.74497900
H	12.82992800	3.68755400	2.20668000
H	12.34113400	4.45230600	0.65428000
C	10.77967500	4.51002800	2.24915900
H	10.54004700	3.56818300	2.75373400
C	9.09011500	9.03762000	5.99705600
C	9.29612000	8.72092700	7.35462100
H	9.84136500	7.81333100	7.62355000
C	8.80840200	9.56430900	8.35635600
C	8.09441200	10.72045800	8.01553100
C	7.87306100	11.03158200	6.66921700
C	8.36918000	10.19705300	5.66051800
H	8.19358000	10.45495100	4.61415100
C	6.13136200	5.21129600	6.12999100
C	5.83560200	4.11600700	6.95801700
C	6.03277300	6.50962100	6.65850000
C	5.44644800	4.31119500	8.28830100
H	5.90904300	3.10217500	6.55506900
C	5.64681400	6.70536700	7.98936700
H	6.25896900	7.37709200	6.03300500
C	5.35267200	5.60752300	8.80771800
H	5.21950700	3.44828500	8.91960500
H	5.57534200	7.72043200	8.38803600
H	5.05224300	5.76280500	9.84703200
C	9.73794300	4.75963800	1.16973600
C	8.60498500	3.93430100	1.09097200
C	9.90594200	5.77273200	0.20861800
C	7.65728800	4.11369200	0.07566100
H	8.46854400	3.13689100	1.82640000
C	8.96513100	5.94769800	-0.81137800
H	10.78093600	6.42783000	0.24667000
C	7.83767600	5.11876000	-0.88080400
H	6.78271700	3.45969600	0.02743200

H	9.11341400	6.73408200	-1.55573300
H	7.10468300	5.25534600	-1.68000000
N	10.85371300	5.56074600	6.31294800
C	9.22180100	3.53278600	5.16869400
H	8.52413200	3.54452400	6.02241100
H	8.69576200	3.26190500	4.23931000
C	10.39572700	2.68663300	5.42056500
H	10.89573700	2.81974100	6.38827400
C	10.89585200	1.74796800	4.58343100
H	10.39536600	1.57418900	3.62068100
H	7.31294800	11.93001000	6.39827400
H	7.70733800	11.37604600	8.79957300
H	8.97942100	9.31232400	9.40581300
C	12.08891400	0.88677500	4.86974700
H	12.87549300	1.02667600	4.10560400
H	12.52546900	1.11033200	5.85594100
H	11.82434500	-0.18591900	4.84384800
C	10.89868700	5.17681200	7.63106800
C	9.72407400	4.80918100	8.33977300
C	12.12946100	5.15498300	8.34401900
C	9.78660500	4.42814200	9.68077200
H	8.76259600	4.84332300	7.82277000
C	12.17723200	4.77474900	9.68499800
H	13.04569800	5.44222700	7.81911100
C	11.00907500	4.40411700	10.36869700
H	8.86350900	4.15275600	10.19909700
H	13.14006800	4.76687600	10.20408400
H	11.05032500	4.10675500	11.41924600
H	11.75863300	5.92328300	6.00276400
IM11 triplet			
Co	10.43058500	5.28369300	5.25545200
C	8.21586600	8.05567500	5.46338500
O	7.27483100	4.25438900	7.83689600
N	9.08268200	5.06385300	6.79110700
P	8.66192200	6.66009400	4.33224600
N	11.13762500	7.19206900	5.99748000
O	11.36256700	9.17359500	7.02448700
C	6.89412300	8.53298300	5.45072500
H	6.16105000	8.06773800	4.78869700
C	6.49413100	9.60005900	6.26042800
H	5.45921100	9.94789400	6.22532100
C	7.42195900	10.21557100	7.10445700
H	7.12397500	11.05136500	7.74119200
C	8.73806700	9.75644200	7.13371000

H	9.46536300	10.23073500	7.79217700
C	9.15060400	8.67546400	6.32766100
C	10.56581500	8.27430800	6.42286200
C	12.59928300	7.38319100	6.17755200
H	13.04769700	6.46781600	6.58509100
C	12.64487500	8.52333800	7.21247900
H	12.68667800	8.15630500	8.24827400
H	13.43236600	9.26492700	7.03763000
C	5.01867000	4.87263900	3.47777600
H	4.30459200	4.87526600	2.65089400
C	6.18178100	5.64601200	3.39041800
H	6.35646900	6.25075700	2.49863700
C	7.12066600	5.66485800	4.43112400
C	5.69369600	4.12114800	5.67117000
H	5.50630000	3.52296900	6.56288700
C	4.77194500	4.11253900	4.62321300
H	3.86528700	3.50931800	4.70425600
C	7.81361800	4.77795200	6.73241800
C	6.87942800	4.87873500	5.59004100
C	8.33244500	4.04866600	8.80446100
H	8.42551500	2.96817900	8.97703900
H	8.03640400	4.55077100	9.73410000
C	9.58567800	4.66728500	8.13754700
H	10.34762300	3.89123800	7.97413000
C	8.67352100	7.42863600	2.66367400
C	8.96169300	6.60136800	1.55801800
H	9.09894400	5.52697600	1.69957500
C	9.06429800	7.14444500	0.27416900
C	8.90479900	8.52204900	0.07703200
C	8.63588200	9.35192900	1.17043800
C	8.51769600	8.81174800	2.45688500
H	8.30349300	9.47579200	3.29644000
C	13.31914600	7.76958200	4.89112300
C	14.68296000	7.45887000	4.76015800
C	12.69590900	8.51771400	3.87986300
C	15.40996000	7.88772500	3.64380600
H	15.18095000	6.87702100	5.54078100
C	13.42055700	8.94256700	2.75999600
H	11.63307800	8.76046700	3.95314800
C	14.78048600	8.63142900	2.63859200
H	16.46985900	7.63440500	3.55741400
H	12.91768700	9.51829300	1.97840600
H	15.34511700	8.96361200	1.76362600
C	10.20376300	5.77154600	8.97594900

C	11.48284100	5.58120200	9.52245200
C	9.47758700	6.92131100	9.33105800
C	12.02767300	6.51776400	10.41017700
H	12.05043400	4.68357700	9.26147800
C	10.02436500	7.86260700	10.20865600
H	8.47277900	7.07845400	8.93000100
C	11.29915300	7.66155700	10.75492500
H	13.02153100	6.35099900	10.83331300
H	9.44900100	8.75264300	10.47580600
H	11.72001200	8.39338800	11.44904500
C	9.48693500	3.11883100	3.41095200
C	10.19341000	3.22596600	4.75340800
C	9.58697400	2.38810100	5.80144800
H	8.49030700	2.33083500	5.81795100
C	10.27301000	1.64007400	6.69166900
H	11.36875000	1.63136100	6.70930400
H	9.76120400	1.00397200	7.42033900
H	11.26609400	3.00468600	4.67014600
H	9.99454600	3.71020200	2.63663500
N	11.67690400	5.34497500	3.88322600
H	11.39601600	5.93058300	3.09348300
C	12.83005100	4.65444000	3.61386300
C	13.41642300	4.67248700	2.31785300
C	13.50727200	3.92153600	4.62743100
C	14.60776300	3.99623800	2.05715700
H	12.91642400	5.23397200	1.52305600
C	14.69520000	3.24236500	4.35124200
H	13.09499500	3.91258500	5.63962000
C	15.25844600	3.27032900	3.06705300
H	15.03374400	4.03226800	1.05030600
H	15.19351700	2.69078000	5.15365200
H	16.19003400	2.73931400	2.85725500
H	8.51233100	10.42816400	1.02594100
H	8.99366900	8.94640600	-0.92606600
H	9.27755800	6.48871100	-0.57366500
H	9.47565200	2.06418000	3.07274300
H	8.43651200	3.44520800	3.46916700
IM13 ^{triplet} - <i>exo</i>			
Co	9.15321900	5.63365200	5.62522800
C	7.61794400	8.70260300	5.04900200
O	10.13191200	7.43269700	9.41005400
N	9.91472800	6.80236800	7.26830800
P	7.25582300	7.03285200	5.77418800
N	7.31351100	6.67117900	2.81652000

O	8.14434400	8.21377600	1.38999400
C	7.72709800	9.80291800	5.91715200
H	7.53440500	9.67261300	6.98229400
C	8.07421600	11.07773600	5.45576000
H	8.14426100	11.90542800	6.16541100
C	8.32597100	11.28095300	4.09875200
H	8.59940900	12.26983200	3.72414100
C	8.21994900	10.20583400	3.21585800
H	8.40646600	10.35324900	2.15188400
C	7.86831700	8.91798000	3.66295800
C	7.75432300	7.86153300	2.63975500
C	7.35630000	5.98226400	1.51154200
H	8.06343500	5.14289400	1.59110100
C	7.91004200	7.06563100	0.54210300
H	8.86355200	6.78136600	0.07714600
H	7.19453800	7.35886300	-0.23951500
C	5.22996600	7.99601400	9.27362400
H	4.18575700	8.20206200	9.51980100
C	5.58118800	7.71203900	7.94952800
H	4.79214300	7.70620300	7.19857200
C	6.90589400	7.44051200	7.56644900
C	7.53407500	7.74755800	9.91444800
H	8.30876000	7.75583800	10.68064900
C	6.21123800	8.01284300	10.26430900
H	5.95439100	8.22863900	11.30357400
C	9.33430500	7.20815800	8.35056500
C	7.90105400	7.46143200	8.58368700
C	11.44724500	6.93625300	9.06086900
H	11.58942800	5.97074300	9.56900900
H	12.19073500	7.65988400	9.41498700
C	11.37851900	6.79354100	7.52399800
H	11.79363900	5.82755000	7.20873000
C	5.55690600	6.61947700	5.18638900
C	5.10362100	5.29367000	5.27791800
H	5.77050800	4.50922500	5.63748300
C	3.79482900	4.96527400	4.90642400
C	2.92602800	5.95729200	4.43880300
C	3.37407600	7.28025200	4.33956800
C	4.68140000	7.61198300	4.71007500
H	5.01561600	8.64919600	4.63276800
C	6.00684500	5.41144100	1.10443900
C	5.86684100	4.03646800	0.85911000
C	4.88625700	6.24485300	0.93989900
C	4.63734900	3.50255300	0.45242800

H	6.73174800	3.37845800	0.98398300
C	3.65773200	5.71465600	0.53327800
H	4.97307000	7.31833800	1.13064800
C	3.52958900	4.34102900	0.28721200
H	4.54698600	2.42972800	0.26272700
H	2.79610600	6.37585100	0.40892100
H	2.56943500	3.92772200	-0.03236800
C	12.11904000	7.90062700	6.78892700
C	13.37044600	7.63039600	6.21169400
C	11.61848200	9.21300500	6.74172800
C	14.11077900	8.65075300	5.60365300
H	13.76659700	6.61145300	6.23989000
C	12.35513600	10.23268100	6.12839000
H	10.64654600	9.44575300	7.18397400
C	13.60480000	9.95535100	5.55997400
H	15.08308300	8.42413900	5.15860700
H	11.95153000	11.24796800	6.09662300
H	14.18027000	10.75258600	5.08273000
C	7.51901200	4.07810000	8.11667000
C	8.24920200	4.03301600	6.80630000
C	9.64347900	3.88815600	6.71788100
H	10.25358200	4.03222200	7.61680000
C	10.25356000	3.88410800	5.45246300
H	9.70029800	3.46662600	4.60299800
H	11.34122700	3.91835700	5.35337000
H	7.67276900	3.67527300	5.94094200
H	8.13265900	4.52492900	8.91269900
N	10.19004100	6.64114100	4.45488600
C	10.84751200	6.48224700	3.25955100
C	10.74212000	5.29571000	2.48555400
C	11.66569300	7.52830300	2.74553200
C	11.43534700	5.16061100	1.28253800
H	10.10288500	4.48568300	2.83613100
C	12.35101200	7.38280200	1.54082100
H	11.75053800	8.45617900	3.31781400
C	12.24893900	6.19630200	0.79815600
H	11.33651800	4.23298400	0.71185000
H	12.97460800	8.20419400	1.17692500
H	12.79057100	6.08258400	-0.14387200
H	10.38445300	7.56768500	4.84484800
H	6.56973800	4.62858700	8.04829300
H	7.27051600	3.04584500	8.42579300
H	2.70327600	8.06113200	3.97230700
H	1.90436100	5.70056400	4.14815300

H	3.45644000	3.92892300	4.98222900
(R)-TSS ^{triplet}			
Co	9.72857800	5.40504100	4.77791400
C	7.80474100	7.24976800	2.79639500
O	9.53731000	9.27124500	6.63467900
N	9.85397000	7.50285900	5.27842300
P	7.62165300	6.01456800	4.15726300
N	10.28163700	5.38250600	2.86903900
O	10.39158400	5.77485000	0.66082900
C	6.87242900	8.29066900	2.66665400
H	6.07557400	8.39497700	3.40605000
C	6.93143900	9.18877500	1.59553800
H	6.19316900	9.99059100	1.52034000
C	7.92391800	9.04685900	0.62186600
H	7.97355000	9.73713200	-0.22301400
C	8.86069100	8.01949100	0.73365800
H	9.64202200	7.90833800	-0.01844700
C	8.82427900	7.12349100	1.82050000
C	9.84739600	6.06554600	1.85191600
C	11.21201700	4.34311200	2.33848200
H	12.14763600	4.36718400	2.90716800
C	11.46175500	4.82748400	0.89517300
H	12.41592400	5.36481000	0.79274000
H	11.39098100	4.03902000	0.13637800
C	4.87697900	7.57812000	6.84826200
H	3.81464300	7.43750000	7.06095200
C	5.47365800	6.85674600	5.80784400
H	4.86076500	6.17002300	5.22236500
C	6.83459700	7.00614200	5.49945300
C	6.98941400	8.64934000	7.30526400
H	7.58921000	9.35263600	7.88345600
C	5.63686200	8.47653500	7.60072900
H	5.18068700	9.04507600	8.41395600
C	9.03467300	8.18389600	6.01655300
C	7.60608700	7.92465600	6.26643800
C	10.97136700	9.23617200	6.42645100
H	11.43677200	8.85825700	7.34941600
H	11.31315200	10.25861900	6.22717900
C	11.13898800	8.26368600	5.24350700
H	11.96752300	7.57035900	5.42385100
C	6.28494100	4.91403900	3.52009300
C	5.80284200	3.87974700	4.34836500
H	6.17717100	3.77723900	5.36904900
C	4.83963000	2.98326300	3.87695800

C	4.35639500	3.09100100	2.56681500
C	4.83829000	4.10555700	1.73329000
C	5.79358400	5.01427600	2.20496600
H	6.15128500	5.80237000	1.53992800
C	10.61822900	2.94686200	2.44371700
C	11.39015200	1.89967700	2.97247400
C	9.32285500	2.66475800	1.97573600
C	10.87981100	0.59719900	3.03594700
H	12.40119300	2.10635400	3.33407500
C	8.81087300	1.36467300	2.04061500
H	8.70414400	3.46031500	1.55235600
C	9.58763900	0.32680500	2.57193200
H	11.49373800	-0.20636300	3.45078800
H	7.80113100	1.16195500	1.67468800
H	9.18653200	-0.68863400	2.62266400
C	11.37907300	8.94874700	3.90653100
C	12.44672600	8.53927900	3.09237500
C	10.58783300	10.03505800	3.49107400
C	12.72259300	9.19961000	1.88818700
H	13.07432300	7.70235900	3.41105400
C	10.86587000	10.69974700	2.29279000
H	9.75291500	10.37524000	4.10993400
C	11.93483600	10.28428400	1.48766700
H	13.56034900	8.87049900	1.26786800
H	10.24642700	11.54655300	1.98664400
H	12.15295600	10.80652200	0.55258000
C	10.80042300	5.02040900	9.15895500
C	10.98088000	4.53146900	7.75721900
C	11.71614700	5.21516300	6.77947300
H	12.08934700	6.21596700	7.02879300
C	11.71633400	4.79848200	5.43415000
H	11.58960200	3.72675500	5.23170500
H	12.38830600	5.31901200	4.74123200
H	9.80951400	4.74031400	9.55503000
N	9.12045300	4.86782900	6.59776300
C	8.33918600	3.75274400	6.88985800
C	7.37832400	3.76202500	7.93059400
C	8.54162100	2.54493900	6.17806200
C	6.64360100	2.61271000	8.23451300
H	7.20803900	4.68825500	8.48690200
C	7.80745600	1.40122000	6.49318400
H	9.28155500	2.52389100	5.37397300
C	6.85174900	1.42432000	7.52089400
H	5.90069000	2.64636300	9.03634700

H	7.97955200	0.48072400	5.92870400
H	6.27719200	0.52666800	7.76194900
H	8.81186100	5.66115100	7.16946500
H	10.80388800	3.46346400	7.59572500
H	4.46806100	4.19812000	0.70917800
H	3.60794400	2.38541400	2.19761200
H	4.47052300	2.19387300	4.53642300
H	11.54414200	4.55248300	9.83167500
H	10.91560900	6.11295300	9.23290000
(S)-TS^{triplet}			
Co	9.39034700	5.35558300	4.81122000
C	9.13088500	8.33292200	3.29788800
O	12.64280100	5.64430600	1.90414900
N	10.69868500	5.45053700	3.02532700
P	9.83604100	7.61136400	4.84244700
N	7.55418600	5.75754500	4.07431000
O	5.83490500	6.75396100	3.02825100
C	9.77829400	9.40506800	2.66294600
H	10.71979000	9.78060300	3.06880500
C	9.23179900	10.01527100	1.52906600
H	9.75796900	10.84723200	1.05530900
C	8.01117500	9.56608000	1.01768700
H	7.57174700	10.03913300	0.13683600
C	7.35287500	8.50245500	1.63418600
H	6.40653600	8.14041900	1.23260500
C	7.90476600	7.86614300	2.76419800
C	7.13981300	6.74357000	3.33487300
C	6.35985700	4.94985700	4.44527300
H	6.54074400	3.90051700	4.18588000
C	5.25825200	5.52418500	3.52675900
H	5.04925000	4.87550000	2.66426400
H	4.32447100	5.77188200	4.04594700
C	13.66518800	9.14094800	5.25480600
H	14.14247900	9.92193900	5.85128800
C	12.28983900	8.91674300	5.38356100
H	11.71331500	9.53381900	6.07454800
C	11.63802000	7.92398400	4.63601900
C	13.78576100	7.38626700	3.60284800
H	14.36603200	6.78435500	2.90342600
C	14.41542400	8.37452400	4.36026200
H	15.48871300	8.54294500	4.24880000
C	11.83766000	6.05624700	2.90031600
C	12.40455000	7.13900000	3.73050500
C	12.02095900	4.49192200	1.29110400

H	12.62719400	3.60851800	1.53723600
H	12.01571400	4.64500800	0.20466600
C	10.61260700	4.44252800	1.92776700
H	10.44532300	3.45634000	2.38072100
C	9.29107300	8.79450300	6.14551000
C	9.58123500	8.47860400	7.48829700
H	10.14493700	7.57417900	7.72805800
C	9.15758700	9.31915000	8.52166800
C	8.42131700	10.47495200	8.23207300
C	8.11728700	10.78864600	6.90306100
C	8.55076500	9.95709400	5.86338200
H	8.30954000	10.22117400	4.83212900
C	6.04281200	5.04217600	5.92923900
C	5.60057000	3.89964300	6.61614100
C	6.12492900	6.26200200	6.62164000
C	5.24487200	3.97322100	7.96801300
H	5.53250600	2.94554600	6.08585100
C	5.77189900	6.33603400	7.97369000
H	6.46856600	7.16295800	6.10725600
C	5.33045600	5.19235200	8.65071100
H	4.90347800	3.07500500	8.48901200
H	5.84332500	7.29127200	8.49997900
H	5.05576500	5.25121400	9.70697300
C	9.47288000	4.71346100	0.96010100
C	8.39935100	3.81285000	0.87281400
C	9.49372800	5.82982700	0.10614200
C	7.36651700	4.01953500	-0.05028800
H	8.37933200	2.93713600	1.52785500
C	8.46506700	6.03606700	-0.81844700
H	10.32164100	6.54326200	0.15511100
C	7.39810500	5.13147300	-0.89927100
H	6.54031900	3.30624900	-0.10991100
H	8.49653800	6.90588500	-1.47940600
H	6.59672400	5.29157800	-1.62508700
N	10.98016000	4.95467700	5.91845100
C	9.01806500	3.13215900	4.93173000
H	7.98251600	2.89339200	5.18684200
H	9.18609400	3.39124100	3.87442700
C	10.03658300	2.50713700	5.65732600
H	9.77377300	1.96717500	6.57501000
C	11.38465900	2.84126100	5.45179500
H	11.66821200	3.21301500	4.46228800
H	7.54151600	11.68753800	6.66854500
H	8.08316300	11.12730600	9.04107000

H	9.39763800	9.06417600	9.55685400
C	12.49877000	2.31230700	6.29754100
H	13.31692400	3.04467600	6.39280700
H	12.15431300	2.03549700	7.30582500
H	12.93985600	1.41078200	5.83096200
C	10.93695600	5.03747100	7.31147600
C	9.72772900	4.77475200	7.99914700
C	12.08873900	5.33492400	8.08025100
C	9.68016500	4.80186200	9.39472800
H	8.82616600	4.57074500	7.41671700
C	12.02932400	5.36890300	9.47576800
H	13.02873900	5.55236600	7.56460500
C	10.82719000	5.09875300	10.14510500
H	8.73306600	4.60034900	9.90290200
H	12.93045600	5.61175100	10.04599000
H	10.78240100	5.12921300	11.23656400
H	11.86577500	5.35558700	5.59014500
<i>E-TS6</i> ^{triplet}			
Co	9.15964700	5.76065900	5.89602900
C	7.29706100	8.91728500	5.53949000
O	10.14901100	8.29689900	9.17196800
N	9.96346400	7.22980700	7.20389700
P	7.19773100	7.10575100	5.96069600
N	7.64993100	7.26423900	3.04962500
O	8.46516900	9.10248700	2.01644600
C	7.01518100	9.86492000	6.54023700
H	6.71543800	9.53172800	7.53399700
C	7.10094000	11.24089900	6.30151100
H	6.86694600	11.94083600	7.10706200
C	7.47980700	11.70773600	5.04195400
H	7.55231800	12.77921200	4.84276800
C	7.76121100	10.78890600	4.03089800
H	8.05214000	11.13750700	3.03962800
C	7.66921900	9.40245600	4.25624300
C	7.92993100	8.51451000	3.11216200
C	7.95688200	6.81776800	1.67859400
H	8.64575300	5.96298300	1.72116400
C	8.66962000	8.04795400	1.04625600
H	9.75296400	7.89420000	0.93356200
H	8.23941800	8.37295000	0.08972900
C	5.40072600	6.99207100	9.71285000
H	4.39082700	6.81449900	10.09003500
C	5.63432200	6.97411600	8.33244900
H	4.79432700	6.78936300	7.66171900

C	6.91412000	7.18772300	7.79721300
C	7.73280800	7.46741000	10.08800200
H	8.56190200	7.66350800	10.76858600
C	6.45203200	7.24283700	10.59544700
H	6.28167000	7.26383500	11.67398600
C	9.38463600	7.64318600	8.28499400
C	7.98411100	7.42939000	8.70325400
C	11.50317900	8.31367500	8.65710400
H	12.14170000	7.76498900	9.36255400
H	11.82689700	9.36095200	8.59865700
C	11.39236800	7.62247400	7.27150400
H	11.99587600	6.70240400	7.25726100
C	5.56847200	6.56640700	5.30351500
C	5.40507800	5.21000500	4.97308600
H	6.24383700	4.51966000	5.08761900
C	4.17894000	4.74371000	4.48746300
C	3.10858000	5.63003600	4.31856800
C	3.26804900	6.98435600	4.63681800
C	4.49176600	7.45357000	5.12776100
H	4.60432400	8.51137800	5.37737900
C	6.70880900	6.38017400	0.92475700
C	6.79189300	5.33408200	-0.00956700
C	5.47826400	7.03467900	1.09946400
C	5.67192500	4.95293900	-0.75770200
H	7.74380200	4.81491100	-0.15235200
C	4.35646800	6.65244400	0.35470900
H	5.39332500	7.84480300	1.82817400
C	4.44961200	5.61122300	-0.57714300
H	5.75385300	4.13623000	-1.47988300
H	3.40472100	7.16896500	0.50532100
H	3.57275900	5.31248400	-1.15747100
C	11.84570200	8.50391700	6.11994100
C	13.07654600	8.24838700	5.49353900
C	11.09441600	9.61885800	5.71247300
C	13.54731200	9.08575200	4.47453700
H	13.67198800	7.38685100	5.80989400
C	11.56314000	10.45474700	4.69327900
H	10.13686200	9.83655600	6.19280100
C	12.79003300	10.19081600	4.07106600
H	14.50692500	8.87279000	3.99646600
H	10.96851500	11.31815000	4.38489300
H	13.15379500	10.84583300	3.27529700
C	7.38530200	3.93305000	8.08521700
C	8.40538400	4.01181300	6.98887000

C	9.76648700	4.26347600	7.21731700
H	10.09046800	4.66128000	8.18482700
C	10.72897200	4.12592000	6.16460600
H	10.54807600	3.35711200	5.40782700
H	11.78012800	4.29105100	6.41044300
H	8.15521300	3.45820900	6.07135400
H	7.65563700	4.55608500	8.95005000
N	10.73405700	5.57481700	4.66672700
C	10.87104700	4.89038100	3.47123000
C	9.84818300	4.02685700	3.00669100
C	12.03828900	5.02247400	2.67721700
C	9.98969200	3.33524100	1.80122300
H	8.94010700	3.91030100	3.60469500
C	12.15819400	4.34359500	1.46301500
H	12.84469300	5.67506900	3.02414100
C	11.13983300	3.49001900	1.01397900
H	9.18634700	2.67146500	1.46949900
H	13.06501300	4.47488000	0.86569000
H	11.24316700	2.95093400	0.06928500
H	11.60049500	6.05762800	4.90809000
H	6.38409100	4.22462900	7.73616800
H	7.30942400	2.88587500	8.43368000
H	2.43649600	7.68093000	4.50344600
H	2.15207700	5.26679100	3.93448300
H	4.06324100	3.68721100	4.23296200
(R)-IM12 ^{triplet}			
Co	10.10869600	5.56311600	4.23293200
C	9.55240300	6.03848700	0.94862600
O	7.77262600	2.14299800	3.20905100
N	8.67010100	4.13218500	3.74390100
P	10.81904100	5.29591700	2.07645500
N	9.27371200	7.33734900	3.75069700
O	8.46409800	9.12171100	2.66446300
C	9.35237400	5.48252300	-0.32546700
H	9.91461300	4.59268900	-0.61626700
C	8.45845300	6.04958200	-1.23892500
H	8.32425900	5.59134100	-2.22155600
C	7.75285500	7.20523700	-0.89328000
H	7.05678500	7.66249400	-1.59986500
C	7.93525100	7.77489200	0.36644900
H	7.37814500	8.66977900	0.64495100
C	8.81638300	7.19904300	1.30463100
C	8.89235500	7.85157800	2.62494000
C	9.09490900	8.35414400	4.81355000

H	8.31220700	7.99264100	5.49749700
C	8.59343900	9.59424200	4.02945500
H	7.60894200	9.94677100	4.36233600
H	9.30919400	10.42773200	4.02760800
C	11.79828900	1.65021500	0.35739800
H	12.55906300	1.28658200	-0.33729500
C	11.76954000	3.00571500	0.70413500
H	12.50719100	3.67956300	0.26528800
C	10.81199700	3.51569600	1.59474600
C	9.88243200	1.26224400	1.77139800
H	9.13837900	0.58452300	2.19044000
C	10.85222300	0.77492200	0.89467700
H	10.86421700	-0.28525800	0.63267800
C	8.77289000	3.03465000	3.06314800
C	9.84620900	2.62225600	2.13878400
C	6.92181000	2.63154700	4.27478800
H	7.12033800	2.02532200	5.17075400
H	5.87803200	2.50402800	3.96298300
C	7.35736400	4.10290700	4.44736200
H	7.52767400	4.34336700	5.50434100
C	12.39866900	5.97937200	1.41895200
C	13.61789900	5.49333100	1.93656500
H	13.62163800	4.65894200	2.64207000
C	14.83326500	6.05938000	1.54203700
C	14.85291300	7.13065000	0.63953500
C	13.64891300	7.62714300	0.13011800
C	12.42902800	7.05585900	0.51314800
H	11.50076400	7.45560500	0.10013900
C	10.36115100	8.58438500	5.61719800
C	10.28110900	8.77086900	7.00631000
C	11.61802800	8.64850500	4.99147600
C	11.43563100	9.01599500	7.75967900
H	9.30687600	8.72261400	7.50098900
C	12.77291300	8.88572200	5.74504000
H	11.69639800	8.50552300	3.91041000
C	12.68495800	9.07105700	7.13085400
H	11.35821500	9.16016400	8.84040500
H	13.74514800	8.92723300	5.24723500
H	13.58774700	9.25755800	7.71798500
C	6.37570000	5.11320900	3.87407500
C	5.79913100	6.08218200	4.70997300
C	5.98824900	5.06545600	2.52310700
C	4.85852900	6.99105300	4.20854200
H	6.08373400	6.12072300	5.76477200

C	5.04566200	5.96908300	2.02200400
H	6.42010500	4.31600000	1.85366700
C	4.47985800	6.93670200	2.86284000
H	4.41849800	7.73905600	4.87321300
H	4.75210500	5.91783900	0.97049800
H	3.74379700	7.64253400	2.46955300
C	10.92090200	3.46281900	8.07050900
C	10.06914900	4.09382500	6.95094700
C	10.95452500	4.89246200	6.01592700
H	11.36530200	5.81021800	6.46484700
C	11.65475400	4.33343200	4.94616600
H	11.50305000	3.28528600	4.66271000
H	12.60356500	4.77663700	4.63042000
H	10.29187900	2.90356300	8.78130000
N	9.01782900	4.97131600	7.47815000
C	7.97958900	4.52760100	8.28319400
C	7.27952300	5.45409600	9.09554600
C	7.54100900	3.18182400	8.28595300
C	6.18611100	5.05231900	9.86302600
H	7.61000000	6.49694400	9.11376600
C	6.44357700	2.79412300	9.06238500
H	8.05782300	2.43514100	7.68030400
C	5.75303200	3.71789800	9.85577400
H	5.66842500	5.79269100	10.47966000
H	6.12867700	1.74673500	9.04440000
H	4.89848600	3.40558600	10.46058200
H	9.35371200	5.90372800	7.71631900
H	9.58769500	3.28581200	6.37652000
H	13.65317000	8.46268500	-0.57452300
H	15.80364100	7.57595700	0.33605800
H	15.76871900	5.66321200	1.94505000
H	11.66065500	2.76756100	7.64363200
H	11.46089300	4.24567200	8.62825200
(S)-IM12^{triplet}			
Co	9.23000300	5.67959200	4.65949600
C	6.62166200	7.31748400	3.31034100
O	9.66371100	9.55329000	6.34040200
N	9.55150300	7.68684500	5.09452500
P	7.01596800	6.22360400	4.75156400
N	9.08656100	5.56352600	2.61635000
O	8.45161100	5.82133500	0.48348200
C	5.65455000	8.32626100	3.44879800
H	5.16411000	8.47003900	4.41355800
C	5.29334300	9.14585400	2.37454800

H	4.53820700	9.92258700	2.51615600
C	5.89256000	8.95984800	1.12607200
H	5.61592000	9.59005800	0.27806200
C	6.85506900	7.96364000	0.96493100
H	7.33378100	7.82010300	-0.00399200
C	7.24051500	7.14388300	2.04491700
C	8.29082000	6.14487100	1.77439300
C	9.91161500	4.59482000	1.86133600
H	10.97021300	4.76290400	2.10653300
C	9.63884100	4.99319900	0.39225800
H	10.44339800	5.60688300	-0.03737800
H	9.41258300	4.15019600	-0.27118200
C	5.22278600	8.07859500	7.99888900
H	4.26978300	7.99106400	8.52585600
C	5.48099200	7.25768700	6.89530300
H	4.71802100	6.54604200	6.57497100
C	6.69133400	7.33619300	6.18851800
C	7.38828900	9.10597200	7.72367700
H	8.14018000	9.82746500	8.04369700
C	6.17970900	9.00711600	8.41372500
H	5.98992300	9.65478000	9.27240100
C	8.97787100	8.45740000	5.96336800
C	7.66756600	8.27981000	6.61668000
C	10.97325200	9.47644600	5.72678500
H	11.70768000	9.27593800	6.52008300
H	11.18680700	10.44570100	5.25895700
C	10.84978000	8.30571200	4.72105900
H	11.64220700	7.56336100	4.89105200
C	5.62155500	5.01939400	4.76193300
C	5.60403400	4.04244800	5.78003000
H	6.36046100	4.05807900	6.56860400
C	4.61626900	3.05424100	5.79895100
C	3.64434900	3.01042500	4.79048500
C	3.66319400	3.96529800	3.76898800
C	4.64205200	4.96725900	3.75384400
H	4.63593100	5.70718500	2.95069900
C	9.56392700	3.14525600	2.18462700
C	10.28107900	2.11905900	1.54226100
C	8.55840500	2.79736500	3.09804600
C	9.99001600	0.77650900	1.80087100
H	11.07511400	2.37335400	0.83416700
C	8.26974400	1.45093100	3.36138800
H	7.99990800	3.58294100	3.61367500
C	8.98129100	0.43704700	2.71275500

H	10.55536000	-0.00809100	1.29130700
H	7.48098500	1.19910200	4.07508500
H	8.75375100	-0.61257500	2.91551700
C	10.89512500	8.72620900	3.26112800
C	11.91131700	8.24226900	2.42301400
C	9.95835900	9.63431700	2.73716100
C	11.99445200	8.65570700	1.08731400
H	12.64568400	7.53675400	2.82128800
C	10.03989900	10.04865100	1.40393700
H	9.15795600	10.02471100	3.37219700
C	11.05813700	9.56007500	0.57438600
H	12.79344100	8.27041400	0.44853800
H	9.30530100	10.75587200	1.01052200
H	11.12114700	9.88560100	-0.46708500
N	12.49391200	4.57410000	4.88288300
C	13.47223700	3.83985000	4.22722600
C	14.63066200	4.49703300	3.74261900
C	13.34352000	2.45382500	3.97223800
C	15.60376600	3.80152100	3.02493100
H	14.75538500	5.56567200	3.94218200
C	14.32834500	1.76987500	3.25117700
H	12.47081900	1.90830600	4.33504000
C	15.46503500	2.42922600	2.76847300
H	16.48594100	4.33950500	2.66607300
H	14.19961600	0.69895300	3.06914200
H	16.23040000	1.88599100	2.20923200
H	12.81498100	5.49220200	5.18866700
C	9.18072900	4.73896400	6.52609400
H	8.62356500	5.35545000	7.23778200
H	8.80382200	3.71837300	6.38829100
C	10.50483400	5.03809400	6.20708600
H	10.95784800	5.93884800	6.64521100
C	11.50853500	3.97806500	5.79349200
H	10.97668700	3.18191100	5.24887500
H	2.91007300	3.93732200	2.97732700
H	2.87670800	2.23257400	4.80144700
H	4.60977000	2.31196900	6.60120400
C	12.16879500	3.36248400	7.04349300
H	12.92364300	2.61022200	6.76374000
H	12.66549500	4.14600100	7.63933000
H	11.41214000	2.87253200	7.67618100
<i>E-IM14</i> ^{triplet}			
Co	9.09042000	6.03492000	5.85578700
C	7.19372500	9.04634400	5.66900500

O	10.02037400	8.45149900	9.20158200
N	9.86516000	7.35206300	7.24852600
P	7.10059700	7.21965300	6.02463300
N	7.67802300	7.42314800	3.19210800
O	8.32579600	9.31239000	2.13405200
C	6.91648000	9.96953000	6.69306600
H	6.61328200	9.60964000	7.67706900
C	7.00861800	11.35080600	6.48806800
H	6.77986100	12.03277000	7.31049300
C	7.38498500	11.84727200	5.23867300
H	7.46074300	12.92316400	5.06610100
C	7.66070800	10.95351000	4.20372200
H	7.95044100	11.32665100	3.22083400
C	7.56835900	9.56189600	4.39676000
C	7.85620600	8.69311900	3.24335000
C	8.01255000	6.98459500	1.82070900
H	8.79767900	6.21710900	1.87346100
C	8.55980100	8.27606700	1.14974000
H	9.64108700	8.22746500	0.95621400
H	8.03383900	8.55578200	0.22685500
C	5.35155700	6.85955600	9.78950200
H	4.36020600	6.61033200	10.17542800
C	5.56165600	6.90716200	8.40576400
H	4.72236600	6.70348500	7.73931700
C	6.81875600	7.21300100	7.86102200
C	7.66050700	7.45224600	10.14956500
H	8.48882700	7.66861800	10.82538500
C	6.40112100	7.14086800	10.66558900
H	6.24604700	7.11695700	11.74641900
C	9.27335100	7.75592300	8.32742200
C	7.89066500	7.47147400	8.76114500
C	11.30652100	8.68134000	8.57387700
H	12.09338900	8.45927600	9.30452600
H	11.35195200	9.74097100	8.28148300
C	11.29662100	7.72644300	7.35983900
H	11.85151500	6.80397000	7.59718000
C	5.46318500	6.74492700	5.32652000
C	5.31080000	5.44869200	4.80488500
H	6.16375700	4.76620300	4.79797400
C	4.08202000	5.03605800	4.27852800
C	2.99634100	5.91956500	4.25658100
C	3.14426600	7.21766200	4.76014800
C	4.37099200	7.63074400	5.29253400
H	4.47338000	8.64624800	5.68305400

C	6.80433700	6.37653500	1.12350500
C	6.85176100	5.05892300	0.64307300
C	5.62540100	7.12165200	0.94226700
C	5.74655200	4.49331000	-0.00582100
H	7.76412400	4.47106500	0.77780700
C	4.52076600	6.55914300	0.29517500
H	5.56562700	8.14953800	1.31183700
C	4.57801400	5.24211200	-0.18109600
H	5.80051200	3.46538100	-0.37391700
H	3.61060200	7.14997000	0.16267900
H	3.71383500	4.80316400	-0.68641800
C	11.88961900	8.32579900	6.10120800
C	13.19168900	7.97284100	5.70901200
C	11.18121800	9.26953100	5.33899700
C	13.77667600	8.55295500	4.57639000
H	13.75223600	7.24057000	6.29713300
C	11.76114800	9.84182300	4.20183700
H	10.16796500	9.55235800	5.63397700
C	13.06132500	9.48699400	3.81848500
H	14.79151700	8.27063700	4.28498800
H	11.19517200	10.56707400	3.61186100
H	13.51414300	9.93737600	2.93158400
C	7.41838500	3.74272800	7.36388800
C	8.55356200	4.04385700	6.41726400
C	9.83134800	4.35961000	6.87410600
H	9.98168400	4.49859400	7.95153900
C	11.07961900	4.24729300	6.02403700
H	11.25278100	3.22478500	5.64916000
H	11.96353700	4.52976000	6.61198700
H	8.44590500	3.62834500	5.40457000
H	7.58071200	4.20865700	8.34799300
N	10.97081300	5.18893700	4.87351700
C	10.98191000	4.69831200	3.54284300
C	10.42135900	3.45503000	3.19548800
C	11.55226600	5.49221100	2.52731300
C	10.44015300	3.02154800	1.86463600
H	9.97021400	2.81895200	3.95872000
C	11.56211900	5.05205300	1.20164700
H	11.99737800	6.45612800	2.78889700
C	11.00767700	3.81165600	0.85843600
H	10.00332500	2.05033300	1.61737000
H	12.01662100	5.68270600	0.43290200
H	11.02063600	3.46559800	-0.17766300
H	11.65268900	5.94514100	4.96150700

H	6.44301800	4.07808800	6.98082500
H	7.34149900	2.65051600	7.52310600
H	2.30190000	7.91385500	4.73907100
H	2.03759700	5.59946700	3.84074900
H	3.97662800	4.02590600	3.87500300