

Electronic Supplemental Information

**Mechanism of an asymmetric ring-opening reaction of
epoxide with amine catalyzed by a metal-organic framework:
insights from combined quantum mechanics and molecular
mechanics calculations**

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Table S1 QM/MM and QM energies of key species (in kcal/mol) in the four possible pathways, obtained from QM/MM calculations using B3LYP-D3/SV(P) as the QM method

	RC	TS1	Int1	Int2	Int3	Int3-2	TS3	PC
(R,R)-1								
QM/MM	0.0	20.6	-1.3	-	-	-	-	-
QM	0.0	20.1	-3.2	-	-	-	-	-
(R,R)-2								
QM/MM	3.1	19.8	-3.7	-2.5	4.7	7.3	5.7	-13.9
QM	1.9	18.8	-5.4	-4.4	2.7	6.0	3.3	-14.6
(S,S)-1								
QM/MM	0.4	21.5	-1.7	-	4.7	5.4	5.0	-14.1
QM	1.4	22.4	-1.2	-	5.9	6.0	6.4	-13.0
(S,S)-2								
QM/MM	5.6	-	-	-	-	-	-	-
QM	6.4	-	-	-	-	-	-	-

Table S2 QM/MM and QM energies of key species (in kcal/mol) in the four possible pathways, obtained from single-point QM/MM calculations using B3LYP-D3/TZVP as the QM method

	RC	TS1	Int1	Int2	Int3	Int3-2	TS3	PC
(R,R)-1								
QM/MM	0.0	17.4	-2.7	-	-	-	-	-
QM	0.0	17.0	-4.5	-	-	-	-	-
(R,R)-2								
QM/MM	2.3	16.6	-4.0	-2.1	4.2	5.8	5.8	-16.1
QM	1.2	15.6	-5.7	-4.1	2.2	4.4	3.4	-16.8
(S,S)-1								
QM/MM	0.9	17.9	-2.6	-	4.0	4.2	4.2	-16.1
QM	1.8	18.8	-2.0	-	5.2	4.7	5.7	-14.9
(S,S)-2								
QM/MM	3.6	-	-	-	-	-	-	-
QM	4.4	-	-	-	-	-	-	-

Table S3 Energy differences (in kcal/mol) between the triplet and open-shell singlet states of RCs ^a

spin state	(<i>R,R</i>)-1-RC	(<i>R,R</i>)-2-RC	(<i>S,S</i>)-1-RC	(<i>S,S</i>)-2-RC
triplet	0.0	0.0	0.0	0.0
open-shell singlet	-0.6	-0.6	-0.6	-0.6

^a The open-shell singlet state was described using a broken-symmetry approach.

Table S4 Relative energies (in kcal/mol) of (*R,R*)-2-TS1 and (*S,S*)-1-TS1 in the triplet and open-shell singlet states, with respect to (*R,R*)-2-TS1 in the triplet state ^a

	(<i>R,R</i>)-2-TS1	(<i>S,S</i>)-1-TS1
triplet	0.0	1.2
open-shell singlet	-0.2	1.0

^a The energies in the open-shell singlet state were calculated for the structures optimized in the triplet state. The open-shell singlet state was described using a broken-symmetry approach.

* The open-shell singlet state is more stable in both (*R,R*)-2-TS1 and (*S,S*)-1-TS1. Thus, the spin multiplicity hardly affects the energy difference between (*R,R*)-2-TS1 and (*S,S*)-1-TS1.

Table S5 Relative energies (kcal/mol) of (*R,R*)-2-TS1 and (*S,S*)-1-TS1 obtained with various methods.

(a) SV(P)^a

	(<i>R,R</i>)-2-TS1	(<i>S,S</i>)-1-TS1
E(QM/MM)	0.0	1.7
E(QM/MM)+ ZPE ^b	0.0	1.5
E(QM/MM)+ enthalpy correction ^c	0.0	1.6
E(QM/MM)+ free energy correction ^d	0.0	-0.2

(b) TZVP^e

	(<i>R,R</i>)-2-TS1	(<i>S,S</i>)-1-TS1
E(QM/MM)	0.0	1.3
E(QM/MM)+ ZPE ^b	0.0	1.1
E(QM/MM)+ enthalpy correction ^c	0.0	1.2
E(QM/MM)+ free energy correction ^d	0.0	-0.6

^a E(QM/MM) = E(B3LYP-D3/SV(P)/MM)

^b QM/MM energy with zero-point energy corrections for the QM atoms

^c QM/MM energy with enthalpy correction for the QM atoms

^d QM/MM energy with Gibbs free energy correction for the QM atoms

^e E(QM/MM) = E(B3LYP-D3/TZVP/MM//B3LYP-D3/SV(P)/MM)

* Thermal corrections were obtained for the QM atoms. For this purpose, geometry optimization and vibrational frequency calculations were performed for the QM atoms at the B3LYP-D3/SV(P) level using Gaussian 09. Here, B3LYP is as implemented in Gaussian 09; thus it is different from the B3LYP used in QM/MM calculations. During the geometry optimization, the hydroxy oxygen atoms of the four naphthol moieties were kept frozen.

Table S6 QM/MM energy and its components (QM(B3LYP-D3), D3 dispersion energy, and MM energy) in hartree for RC, TS1, and Int1 in the four pathways

method		RC	TS1	Int1
QM/MM	(<i>R,R</i>)-1	-6472.355942	-6472.323123	-6472.358091
	(<i>R,R</i>)-2	-6472.351039	-6472.324391	-6472.361856
	(<i>S,S</i>)-1	-6472.355276	-6472.321658	-6472.358638
	(<i>S,S</i>)-2	-6472.347003	-	-
QM(B3LYP-D3)	(<i>R,R</i>)-1	-6470.326788	-6470.294721	-6470.331889
	(<i>R,R</i>)-2	-6470.323692	-6470.2969	-6470.323692
	(<i>S,S</i>)-1	-6470.324601	-6470.291021	-6470.328642
	(<i>S,S</i>)-2	-6470.316654	-	-
D3	(<i>R,R</i>)-1	-0.1737586	-0.17846929	-0.18009431
	(<i>R,R</i>)-2	-0.16817506	-0.17797725	-0.18058663
	(<i>S,S</i>)-1	-0.17515605	-0.17114458	-0.1770756
	(<i>S,S</i>)-2	-0.15608726	-	-
MM	(<i>R,R</i>)-1	-2.029154413	-2.02840191	-2.026201676
	(<i>R,R</i>)-2	-2.027347289	-2.027490718	-2.026466773
	(<i>S,S</i>)-1	-2.03067541	-2.030637444	-2.029995895
	(<i>S,S</i>)-2	-2.030348904	-	-

Table S7 Relative QM/MM and QM energies (in kcal/mol) of key species in the ring-opening step, as obtained from single-point QM/MM calculations with M06-2X/TZVP used as the QM method

	RC	TS1	Int1
<i>(R,R)</i> -1			
QM/MM	0.0	24.0	-0.7
QM	0.0	23.5	-2.5
<i>(R,R)</i> -2			
QM/MM	3.5	22.3	-2.7
QM	2.3	21.3	-4.4
<i>(S,S)</i> -1			
QM/MM	2.3	22.1	-2.2
QM	3.2	23.1	-1.7
<i>(S,S)</i> -2			
QM/MM	3.5	-	-
QM	4.2	-	-

* With this method, the energy of *(R,R)*-2-TS1 was slightly higher than that of *(S,S)*-1-TS1.

Table S8 Relative QM/MM and QM energies (in kcal/mol) of TS1 species, as obtained from single-point QM/MM calculations with M06-2X-D3/TZVP used as the QM method

	<i>(R,R)</i> -2-TS1	<i>(R,R)</i> -1-TS1	<i>(S,S)</i> -1-TS1
QM/MM	0.0	2.0	0.1
QM	0.0	2.6	2.1

^a QM calculations were performed using Gaussian 09. Relative energies are with respect to *(R,R)*-2-TS1.

* *(R,R)*-2-TS1 was calculated as slightly more stable than *(S,S)*-1-TS1. These results also indicate that CH- π interactions affect the stability of TS1.

Table S9 Relative QM/MM and QM energies (in kcal/mol) of key species in the ring-opening step, as obtained from single-point QM/MM calculations with B3PW91/TZVP used as the QM method ^a

	RC	TS1	Int1
	<i>(R,R)</i> -1		
QM/MM	0.0	22.3	1.1
QM	0.0	21.9	-0.7
	<i>(R,R)</i> -2		
QM/MM	-0.3	21.7	0.3
QM	-1.4	20.6	-1.4
	<i>(S,S)</i> -1		
QM/MM	2.0	17.8	-1.5
QM	3.0	18.7	-1.0
	<i>(S,S)</i> -2		
QM/MM	-8.0	-	-
QM	-7.3	-	-

^a QM energies were calculated using Gaussian 09.

* With this method, the energy of *(R,R)*-2-TS1 was calculated as higher than that of *(S,S)*-1-TS1.

Table S10 Relative QM/MM and QM energies (in kcal/mol) of TS1 species, as obtained from single-point QM/MM calculations with B3PW91-D3/TZVP used as the QM method

	<i>(R,R)</i> -2-TS1	<i>(R,R)</i> -1-TS1	<i>(S,S)</i> -1-TS1
QM/MM	0.0	0.3	1.1
QM	0.0	0.9	3.1

^a QM calculations were performed using Gaussian 09. Relative energies are with respect to *(R,R)*-2-TS1.

* The energy of *(R,R)*-2-TS1 was lower than that of *(S,S)*-1-TS1 in the B3PW91-D3 results, whereas the energy of *(R,R)*-2-TS1 was higher in B3PW91 results. These results also indicate that CH- π interactions affect the stability of TS1.

Table S11 Effect of NH₂ substituents on the energy gap between (*R,R*)-2-TS1 and (*S,S*)-1-TS1.

	(<i>R,R</i>)-2-TS1	(<i>S,S</i>)-1-TS1
without NH ₂	0.0	2.3
with NH ₂	0.0	3.1

^a NH₂ substituents were attached at the C3 positions of naphthol groups. DFT calculations were performed for the QM region of the transition states. Relative energies (kcal/mol) are with respect to (*R,R*)-2-TS1.

* QM atoms were taken from the QM/MM optimized structures of (*R,R*)-2-TS1 and (*S,S*)-1-TS1. QM energies of (*R,R*)-2-TS1 and (*S,S*)-1-TS1 were calculated without point charges. NH₂ groups were attached at the C3 positions of the four ligands of the QM structures. After NH₂ groups had been introduced, the geometries of the four NH₂ groups were optimized, while the other atoms were kept frozen at the original positions.

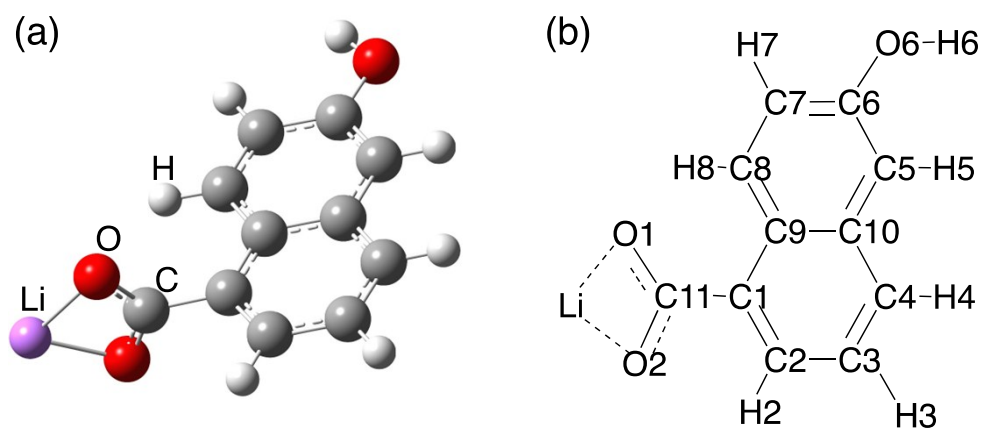


Fig. S1 (a) Optimized structure of lithium 6-hydroxy-1-naphthoate. (b) Atom labels .

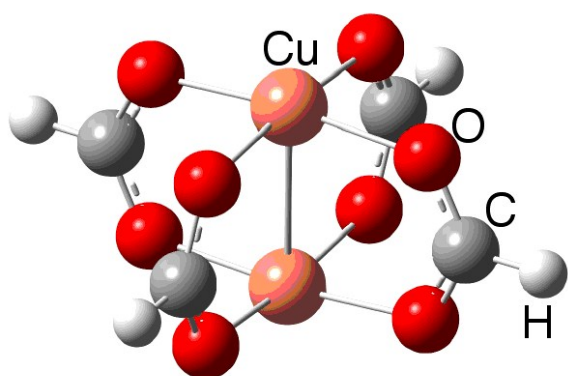


Fig. S2 Optimized structure of $\text{Cu}_2(\text{O}_2\text{CH})_4$.

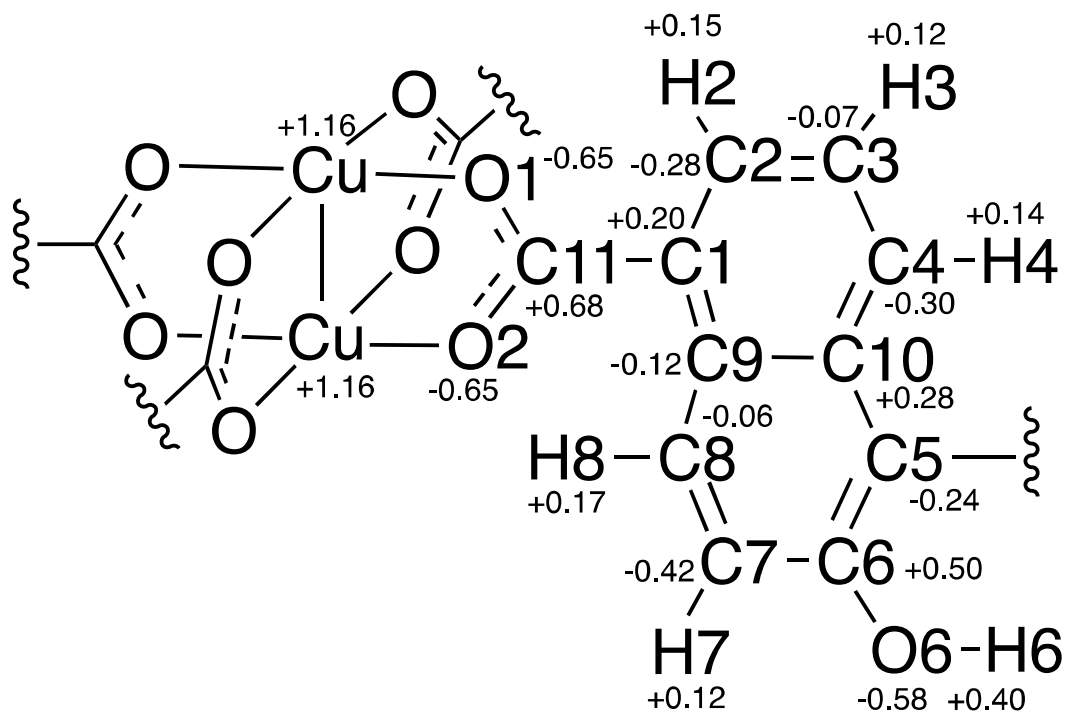


Fig. S3 Assigned atomic charges for the Cu-paddlewheel unit and the linker.

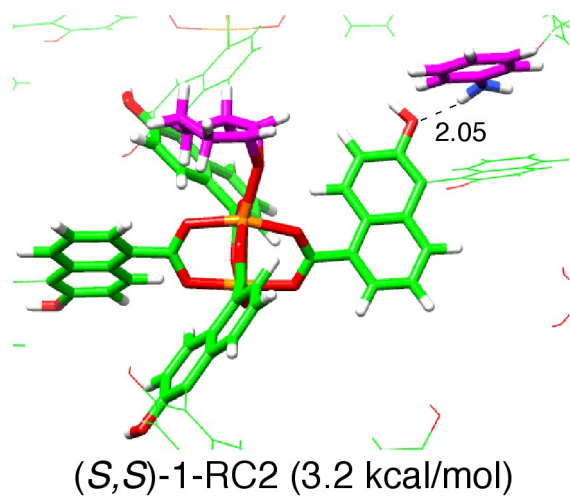


Fig. S4 One possible structure of RC. Cyclohexene oxide has conformation **A**. Relative energies shown in kcal/mol are with respect to (*R,R*)-1-RC. Interatomic distances are indicated in Å. Carbon atoms in the substrates and the MOF are colored magenta and light green, respectively.

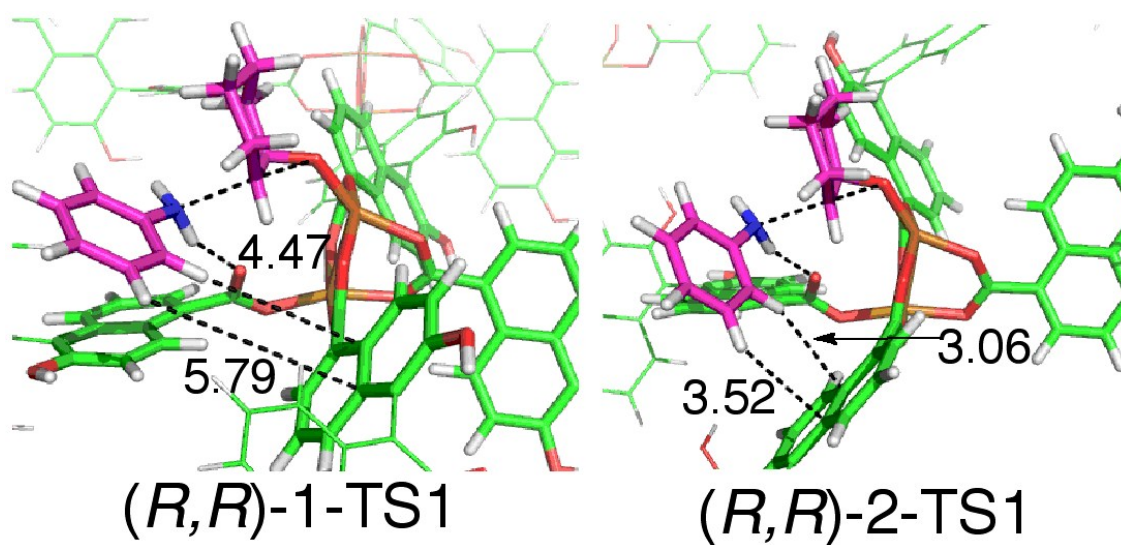


Fig. S5 QM/MM-optimized structures of *(R,R)*-1-TS1 and *(R,R)*-2-TS1 obtained using the B3LYP functional for the QM part. Interatomic distances are indicated in Å. Carbon atoms in the substrates and the MOF are colored magenta and light green, respectively.

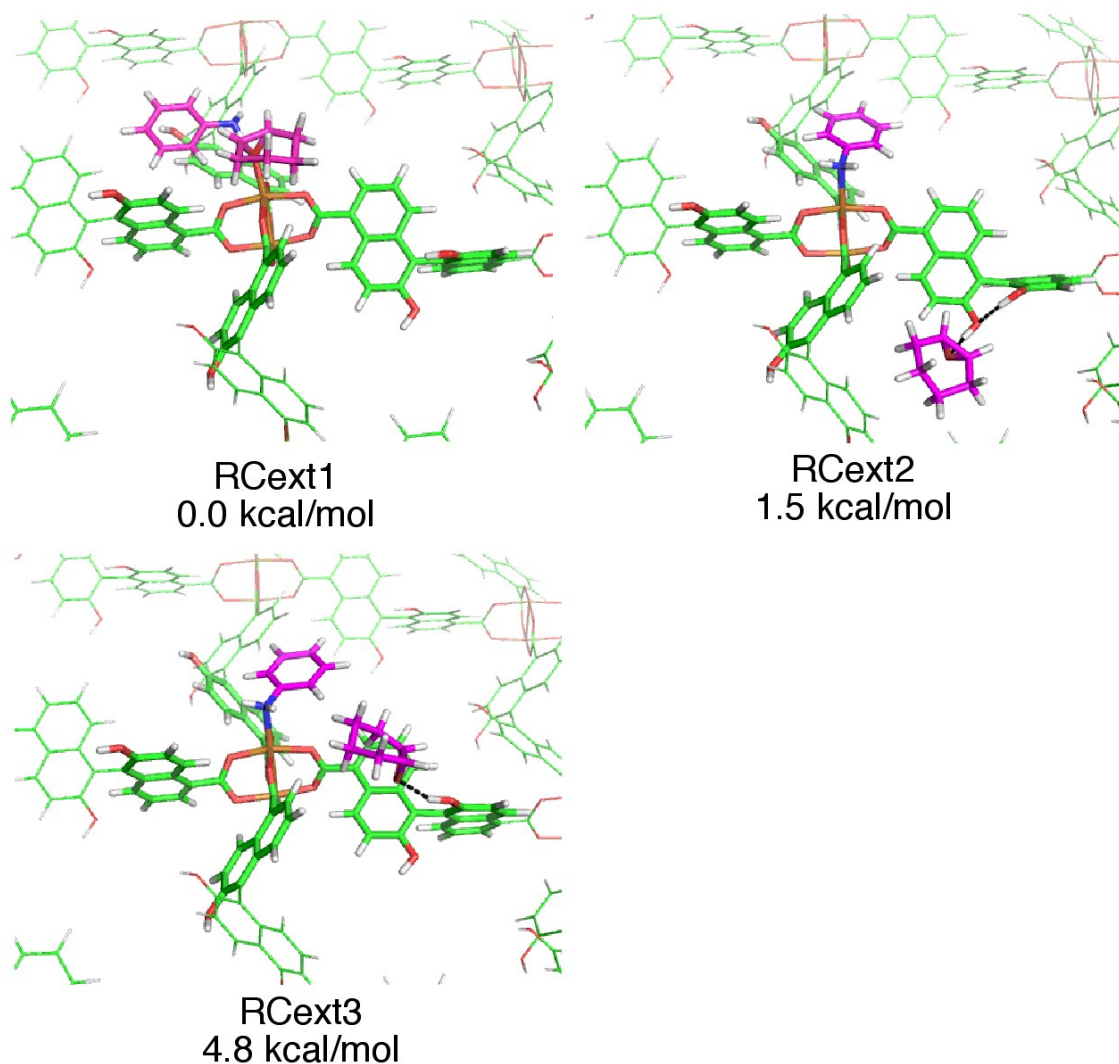


Fig. S6 Several RC species obtained using an extended QM region; RCext1 in which the epoxide coordinates to the Cu(II) ion; RCext2 and RCext3 in which aniline coordinates to the Cu(II) ion and the epoxide forms a hydrogen bond with the BINOL moiety. Relative energies shown in kcal/mol are with respect to RCext1. Carbon atoms in the substrates and the MOF are colored magenta and light green, respectively. QM atoms are shown in stick.

* Note that the epoxide forms a hydrogen bond with the BINOL moiety in both RCext2 and RCext3. One of the two OH groups of the BINOL moiety forms an intramolecular hydrogen bond with the other OH group in RCext2, but not in RCext3.

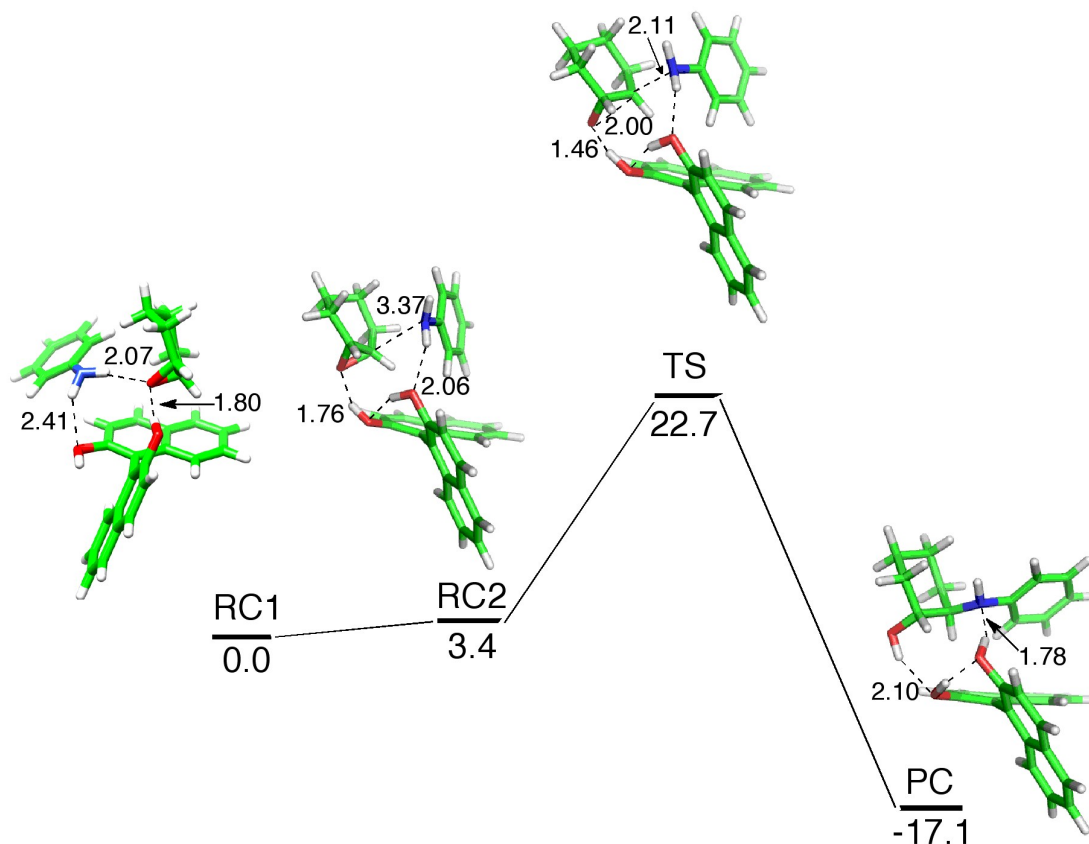


Fig. S7 Energy profile (in kcal/mol) and optimized structures of key species for the H-bond assisted ring-opening reaction obtained at the B3LYP-D3/6-311+G**// B3LYP-D3/6-31G* level. Interatomic distances are indicated in Å.

* We used DFT to calculate the activation energy for the H-bond assisted ring-opening reaction of epoxide catalyzed by *R*-BINOL alone. The barrier (22.7 kcal/mol) is somewhat higher than that obtained with QM/MM (18.4 kcal/mol), which suggests that the H-bond assisted ring-opening reaction might be enhanced in the MOF environment. However, the barrier obtained with QM/MM is still higher than the barriers obtained for the reactions in which Cu(II) acts as the Lewis acid site. These results suggest that cyclohexene oxide is activated preferentially by the copper center for the ring-opening reaction.

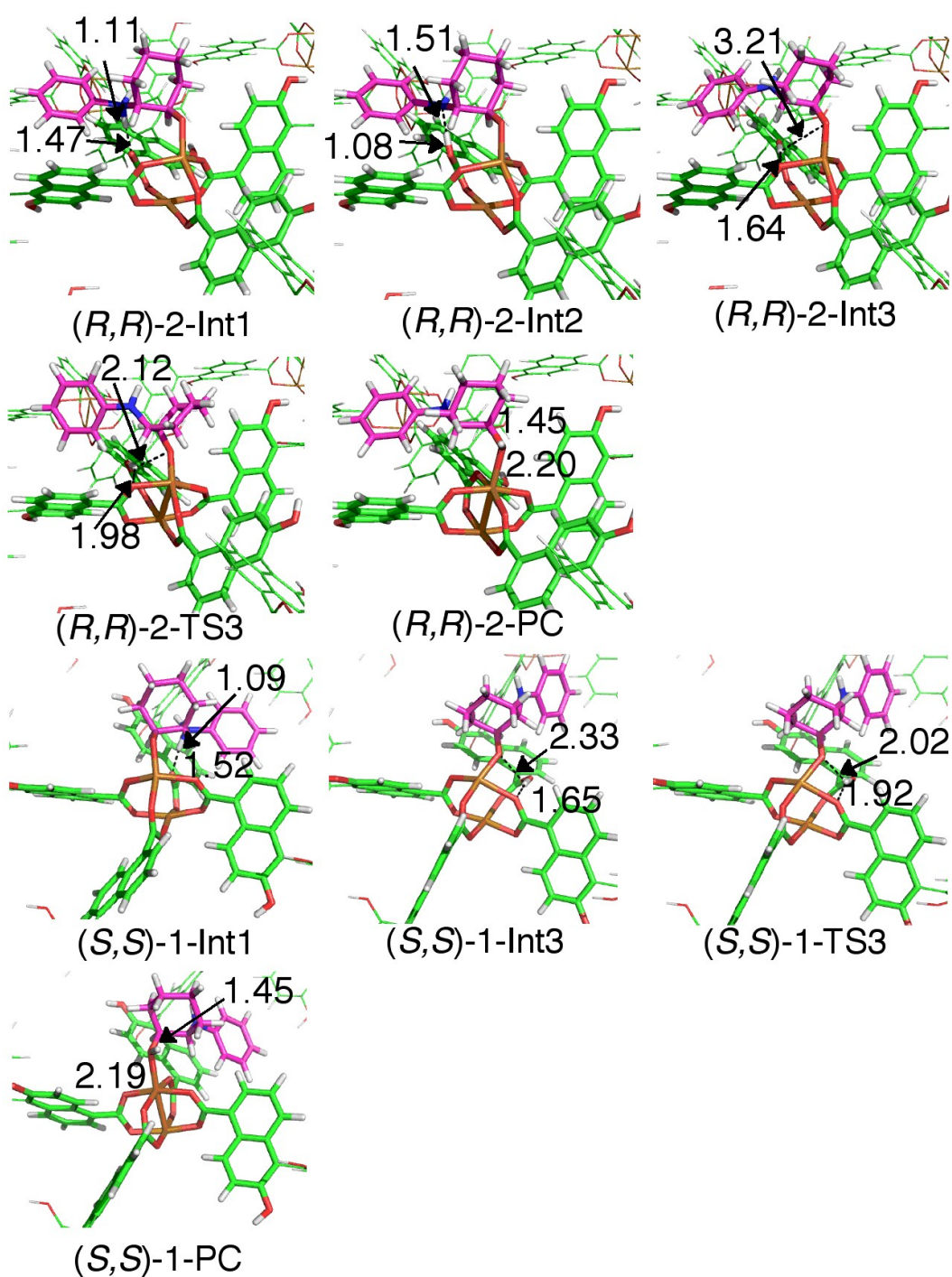


Fig. S8 QM/MM-optimized structures of species in the proton transfer step. Interatomic distances are indicated in Å. Carbon atoms in the substrates and the MOF are colored magenta and light green, respectively.

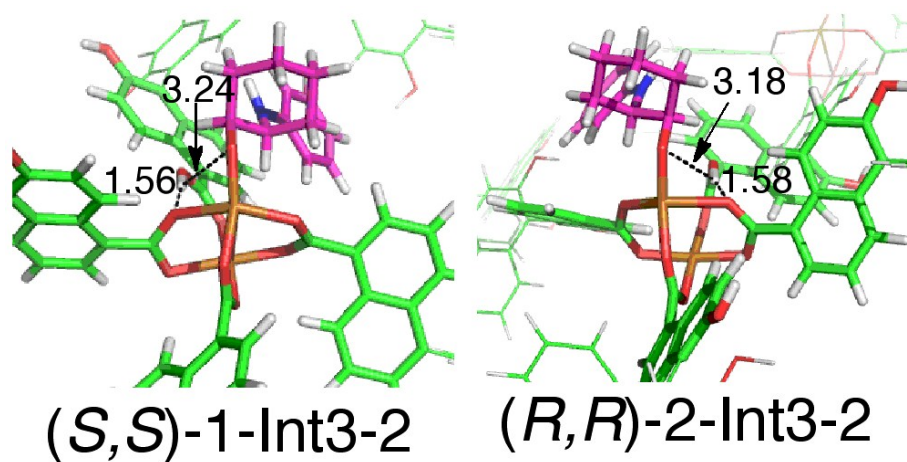


Fig. S9 QM/MM-optimized structures of (*S,S*)-1-Int3-2 and (*R,R*)-2-Int3-2. Interatomic distances are indicated in Å. Carbon atoms in the substrates and the MOF are colored magenta and light green, respectively.

XYZ coordinates of lithium 6-hydroxy-1-naphthoate and $\text{Cu}_2(\text{O}_2\text{CH})_4$

Lithium 6-hydroxy-1-naphthoate

C	0.243757	-2.497411	0.000000
C	0.843809	-1.114271	0.000000
O	-0.000578	-3.074003	1.111285
O	-0.000578	-3.074003	-1.111285
C	2.217532	-0.971168	0.000000
C	2.806105	0.317846	0.000000
C	2.019002	1.448614	0.000000
C	0.599267	1.343118	0.000000
C	-0.000578	0.038131	0.000000
H	2.856872	-1.853909	0.000000
H	3.892908	0.408783	0.000000
H	2.474239	2.439551	0.000000
C	-0.231836	2.495260	0.000000
C	-1.420164	-0.049455	0.000000
C	-1.604627	2.367486	0.000000
C	-2.206244	1.081842	0.000000
H	0.213613	3.489702	0.000000
O	-2.364490	3.511906	0.000000
H	-3.294969	0.994544	0.000000
H	-1.895660	-1.029435	0.000000
H	-3.300504	3.278566	0.000000
Li	-0.539155	-4.466317	0.000000

$\text{Cu}_2(\text{O}_2\text{CH})_4$			
Cu	0.000000	0.000000	1.259877
Cu	0.000000	0.000000	-1.259877
O	1.962887	0.000000	-1.135325
O	1.962887	0.000000	1.135325
O	-1.962887	0.000000	1.135325
O	0.000000	-1.962887	1.135325
O	0.000000	1.962887	1.135325
O	-1.962887	0.000000	-1.135325
O	0.000000	1.962887	-1.135325
O	0.000000	-1.962887	-1.135325
C	0.000000	2.520278	0.000000
C	-2.520278	0.000000	0.000000
C	0.000000	-2.520278	0.000000
C	2.520278	0.000000	0.000000
H	3.623712	0.000000	0.000000
H	-3.623712	0.000000	0.000000
H	0.000000	-3.623712	0.000000
H	0.000000	3.623712	0.000000

XYZ coordinates of optimized structures of key species for the H-bond assisted ring-opening reaction

RC1				H	1.386891	-2.511302	5.727052
C	6.370470	4.750159	-0.058854	H	-0.811890	-3.102040	4.747060
C	5.846636	3.334028	-0.021401	H	-1.490666	-2.129078	2.552618
C	4.999426	2.803268	-1.105543	H	3.522970	-1.289406	5.603215
C	4.576746	3.667027	-2.278290	H	5.031003	0.287976	4.408746
C	5.328247	5.010504	-2.352119	H	0.907613	2.458888	-2.526238
C	5.533876	5.657461	-0.973481	H	-0.064067	3.236978	-0.381866
O	4.414036	3.190256	0.171881	H	3.957258	-1.050190	0.533874
O	4.582393	1.438860	2.215796	H	2.497344	1.019022	-3.749205
C	3.678395	0.597146	2.763836	H	4.974152	-1.763077	-1.594097
C	2.449725	0.289843	2.181801	H	4.254787	-0.729092	-3.748465
C	1.565743	-0.623791	2.854073	H	0.908697	1.913737	2.713057
C	1.955639	-1.195182	4.110327	H	4.230167	1.913324	1.426928
C	3.224576	-0.852782	4.653018	H	4.723354	3.098153	-3.203542
C	4.062542	0.014312	4.002388	H	3.496262	3.828563	-2.184278
C	1.075729	-2.088402	4.774346	H	4.789327	5.695010	-3.018022
C	-0.145928	-2.417504	4.229276	H	6.315308	4.845193	-2.807001
C	-0.530130	-1.863023	2.985877	H	6.037507	6.624551	-1.084564
C	0.301060	-0.991168	2.315283	H	4.569678	5.861303	-0.495421
C	2.069212	0.880164	0.863623	H	6.405965	5.150106	0.962237
C	2.642509	0.416459	-0.364221	H	7.408096	4.705530	-0.420120
C	2.225033	1.002018	-1.605335	H	6.418115	2.623129	0.576408
C	1.229199	2.016625	-1.586722	H	4.978653	1.727072	-1.259446
C	0.682040	2.451506	-0.407135	H	1.745975	4.499875	1.761811
C	1.119448	1.892112	0.818403	N	2.159729	5.071850	1.032975
C	2.823612	0.565300	-2.815994	H	2.930512	4.574310	0.595973
C	3.801145	-0.406455	-2.815470	C	1.222447	5.608751	0.152453
C	4.208917	-0.991399	-1.592135	C	1.582071	5.992603	-1.153934
C	3.642380	-0.593976	-0.398927	C	0.638734	6.543664	-2.019170
O	0.561488	2.414832	1.951992	C	-0.684548	6.731662	-1.612710
H	-0.000919	-0.579829	1.357805	C	-1.047103	6.359156	-0.314911

C	-0.112230	5.806597	0.558076	H	33.434505	2.386920	53.674523
H	2.606380	5.856487	-1.486917	H	33.410811	1.787994	51.251419
H	0.944347	6.827193	-3.023822	H	31.718737	2.733410	49.749810
H	-1.416893	7.159944	-2.290754	H	29.719365	5.317896	54.253593
H	-2.071775	6.494543	0.023101	H	27.914505	6.174834	52.759139
H	-0.409626	5.504293	1.559456	H	33.804259	6.627774	48.551795
				H	31.913068	5.780729	49.857340
RC2				H	26.869233	3.323268	48.209519
C	32.157763	5.023275	46.056972	H	27.395700	5.030163	49.649111
C	33.141739	5.757994	46.678650	C	23.595892	5.255955	46.957594
C	31.040253	4.533489	46.784200	C	24.981009	5.045778	47.521614
C	29.991134	3.833373	46.134254	C	26.168543	5.225767	46.680925
C	28.876142	3.442992	46.829152	C	26.076186	5.612424	45.218604
C	31.719790	3.661171	53.520161	C	24.666907	6.083984	44.822606
C	32.677964	2.809680	53.019193	C	23.577222	5.182879	45.421767
C	32.666278	2.475306	51.644389	O	25.697594	3.877859	47.023184
C	31.717136	3.006640	50.798842	C	27.302140	8.190409	47.556574
C	30.721559	3.904404	51.277364	C	26.856379	9.004994	46.499281
C	30.721631	4.218789	52.677229	C	27.641174	9.177106	45.359649
C	29.711884	5.073427	53.194187	C	28.880169	8.540602	45.241155
C	28.720176	5.555024	52.378358	C	29.331840	7.737314	46.292946
C	28.716773	5.243006	50.997817	C	28.561166	7.568599	47.441667
C	29.727225	4.485784	50.414465	N	26.479498	7.936080	48.655536
O	27.667615	5.745374	50.266131	H	26.812039	6.399547	45.024680
C	33.039179	6.030479	48.063295	H	25.091906	5.197625	48.595520
C	31.977338	5.553085	48.800078	H	27.099748	5.481648	47.173355
C	30.945811	4.780508	48.194593	H	24.580408	6.121506	43.730311
C	28.770556	3.713645	48.217635	H	24.523945	7.110877	45.187621
C	29.805397	4.302705	48.933443	H	22.586926	5.477999	45.055528
O	27.600083	3.416399	48.876284	H	23.743040	4.145013	45.106617
H	33.987686	6.135824	46.111352	H	22.903780	4.526296	47.397210
H	30.069453	3.632015	45.068962	H	23.264725	6.251091	47.287185
H	28.051573	2.941801	46.331498	H	26.369901	4.738570	44.622261

H	25.885117	9.490472	46.572701	H	33.633522	6.013135	45.770878
H	27.275852	9.811175	44.555261	H	29.856280	3.262199	44.851404
H	29.485269	8.673876	44.349068	H	27.876895	2.511162	46.148885
H	30.294951	7.238725	46.228639	H	33.223688	3.020536	53.655958
H	28.922047	6.941887	48.251687	H	33.291129	2.137156	51.322000
H	25.861022	8.691902	48.920590	H	31.553320	2.759554	49.703370
H	26.935576	7.494794	49.448085	H	29.266328	5.672158	53.855901
H	32.211458	4.817606	44.990280	H	27.414384	6.175807	52.259100
H	31.706435	3.916552	54.577424	H	33.415995	6.614088	48.186986
				H	31.566288	5.743068	49.526638
TS				H	26.597473	2.966159	47.960648
C	31.860590	4.808375	45.773272	H	27.074153	4.550702	49.351203
C	32.806176	5.621733	46.356305	C	23.497925	4.727410	47.223420
C	30.771661	4.292448	46.523757	C	24.957576	4.465359	47.598719
C	29.764354	3.503280	45.907795	C	25.967117	5.206008	46.801861
C	28.676427	3.072906	46.620361	C	25.700398	5.511202	45.355069
C	31.414149	4.120621	53.337558	C	24.226943	5.843229	45.079303
C	32.447331	3.298958	52.948572	C	23.298484	4.791063	45.703475
C	32.487423	2.803716	51.623395	O	25.486781	3.285305	47.061018
C	31.514115	3.152247	50.713141	C	27.252737	7.812487	47.028360
C	30.441409	4.015578	51.073486	C	26.998277	8.797384	46.066434
C	30.387973	4.489725	52.426868	C	28.062337	9.378568	45.374782
C	29.299268	5.306904	52.832326	C	29.375285	8.975038	45.628519
C	28.281742	5.596367	51.958475	C	29.622949	7.987396	46.586187
C	28.335177	5.127947	50.625419	C	28.568796	7.407879	47.289448
C	29.421260	4.407075	50.137549	N	26.183104	7.123568	47.663383
O	27.249873	5.407788	49.823306	H	26.368821	6.316131	45.029597
C	32.684116	5.956154	47.725565	H	25.081952	4.566085	48.690448
C	31.643452	5.462128	48.483587	H	27.001337	5.070733	47.080728
C	30.658708	4.598677	47.921278	H	24.064864	5.918083	43.997626
C	28.545700	3.389557	48.002472	H	23.990550	6.833220	45.499323
C	29.542918	4.092496	48.680712	H	22.251563	5.016068	45.467408
O	27.404037	3.039692	48.654231	H	23.528651	3.806421	45.279593

H	22.888080	3.930337	47.664303	C	28.604041	3.340523	48.278986
H	23.176298	5.674728	47.684628	C	29.554153	4.204269	48.821746
H	25.994795	4.618496	44.791300	O	27.454198	2.977211	48.929193
H	25.974657	9.102693	45.859490	H	33.634224	5.692994	45.665582
H	27.860097	10.146534	44.633125	H	29.988543	2.646091	45.238771
H	30.199123	9.424269	45.081580	H	28.007805	2.086687	46.635627
H	30.635695	7.652339	46.788015	H	33.449015	3.645099	53.713374
H	28.759316	6.636916	48.027861	H	33.514171	2.675969	51.413379
H	25.302955	7.631636	47.664314	H	31.713258	3.126001	49.819842
H	26.422033	6.791836	48.602338	H	29.321161	6.006486	53.934619
H	31.926085	4.554949	44.717486	H	27.413006	6.356375	52.361337
H	31.360947	4.495434	54.357355	H	33.311377	6.767067	47.896689
				H	31.451818	6.101762	49.343180
PC				H	25.786552	2.964106	47.608787
C	31.908376	4.439430	45.865490	H	27.192680	3.717390	49.522182
C	32.803006	5.392633	46.297536	C	23.797333	5.464940	47.354577
C	30.817142	4.037106	46.681452	C	25.154369	4.788965	47.583122
C	29.861936	3.091197	46.222431	C	26.308078	5.481145	46.810402
C	28.772414	2.770796	46.990381	C	25.933064	5.716594	45.336230
C	31.564606	4.613776	53.400863	C	24.592815	6.444559	45.173174
C	32.640554	3.847321	53.016297	C	23.471092	5.661051	45.869020
C	32.679560	3.305319	51.710449	O	25.058390	3.432713	47.161188
C	31.667669	3.560631	50.810910	C	27.785148	7.504224	47.057061
C	30.553205	4.373810	51.162043	C	27.787888	8.878541	47.341235
C	30.497260	4.882294	52.502594	C	28.853896	9.680634	46.938328
C	29.358450	5.621738	52.918479	C	29.932299	9.128823	46.242208
C	28.309482	5.824556	52.059790	C	29.927510	7.763417	45.953657
C	28.368666	5.338123	50.731969	C	28.864634	6.953441	46.352388
C	29.478160	4.659613	50.242511	N	26.732354	6.690853	47.557198
O	27.208940	5.479473	49.996140	H	26.738639	6.258637	44.829937
C	32.624312	5.993061	47.566068	H	25.375216	4.833081	48.656552
C	31.580541	5.617775	48.382468	H	27.156376	4.796447	46.841782
C	30.651202	4.617235	47.982103	H	24.369023	6.578976	44.107939

H	24.662087	7.455634	45.603938	H	30.763324	9.754727	45.930276
H	22.508975	6.176762	45.759954	H	30.761002	7.307889	45.428096
H	23.367055	4.676923	45.394868	H	28.888036	5.895133	46.125023
H	23.032439	4.858482	47.851997	H	25.931805	7.263286	47.812635
H	23.800322	6.443817	47.859080	H	27.298255	5.956627	49.119182
H	25.862173	4.726831	44.868045	H	32.018799	3.981202	44.885265
H	26.953532	9.315680	47.886874	H	31.507104	5.019462	54.408353
H	28.837677	10.742676	47.169036				

XYZ coordinates of the QM region of QM/MM-optimized structures (QM(B3LYP)/MM stands for the QM/MM-optimized structures obtained with the B3LYP functional and open-shell singlet stands for the QM/MM-optimized structure in the open-shell singlet state.)

(<i>R,R</i>)-1-RC				C	31.9009352	4.8404895	35.5735360
C	26.8403266	7.2835157	42.0444136	C	31.8949961	5.1482945	36.9814444
C	25.9841073	6.4056462	41.4116358	C	31.1584596	6.2847574	37.4273570
C	26.4558496	5.2151553	40.7700254	C	30.4730465	7.0699735	36.5363194
C	27.8703512	4.9427789	40.8398246	C	30.4910742	6.7894896	35.1430230
C	27.5324024	2.9495470	39.4873574	C	31.2022954	5.6986533	34.6505323
C	26.1341013	3.1950616	39.4333957	O	29.7756658	7.6891681	34.4051797
C	25.5871966	4.3099166	40.0630002	O	32.9796704	5.7442620	39.6977016
O	25.4499417	2.2477121	38.7254039	O	32.3868693	3.6194351	40.1472755
Cu	33.0066963	6.3417500	41.5791104	C	32.6452793	4.5711905	39.3531884
Cu	32.4141618	3.8650797	42.1138601	C	28.7291114	5.8612019	41.5301639
C	36.6082742	3.9683968	41.8709074	C	28.2260934	7.0221822	42.0932986
C	37.1581110	3.2577243	42.9218702	C	28.3738853	3.7901365	40.1687057
C	38.5460610	2.9883492	42.9343037	O	30.9969913	6.5411340	41.4704182
C	39.3606853	3.4337905	41.9128636	O	30.5294051	4.4206354	42.0523717
C	38.8360156	4.1512737	40.7892270	C	30.1935252	5.5891568	41.6874980
C	37.4132499	4.3772383	40.7607387	C	32.3641106	5.9666395	45.7704955
C	36.8410389	4.9646378	39.6004945	C	33.2494784	6.8477225	46.3657160
C	37.6308345	5.3973106	38.5678458	C	31.2611204	5.4197949	46.5056982
C	39.0462057	5.3135483	38.6498100	C	30.2709646	4.5949028	45.8975908
C	39.6556639	4.6537467	39.7183459	C	29.2180114	4.1010512	46.6289699
O	39.7945670	5.8762151	37.6627731	O	32.9019806	6.5500229	43.5535356
O	34.8654014	5.5622263	41.7437594	O	32.4659089	4.3908437	44.0093196
O	34.3276595	3.4174991	42.1585849	C	32.5921821	5.6063348	44.3365468
C	35.1578871	4.3401079	41.9250989	C	33.1109695	7.1748477	47.7322327
C	32.5803167	4.2769897	37.8894017	C	32.0841089	6.6368867	48.4782302
C	33.2185796	3.1327263	37.4431788	C	31.1166461	5.7508538	47.9008082
C	33.2429379	2.8369415	36.0645091	C	29.0946688	4.3790669	48.0165541
C	32.6083564	3.6642317	35.1615105	C	30.0249544	5.1988337	48.6525246

O	28.0597040	3.8487894	48.7247210	C	37.7272019	8.6102212	38.7523720
H	26.4414256	8.1889930	42.5127406	C	37.6695119	8.7611615	37.3634281
H	24.9155819	6.6443547	41.3978604	C	36.4909667	8.4792533	36.6586544
H	27.9149052	2.0719366	38.9596575	C	35.3608742	8.0591687	37.3754952
H	24.4992618	2.4314126	38.6698497	C	35.4064420	7.9120108	38.7617926
H	36.5176849	2.9270753	43.7441620	N	36.6464456	7.9753480	40.8500924
H	38.9799016	2.4303093	43.7701714	H	33.4249481	11.3730525	39.8511546
H	40.4334871	3.2231292	41.9668464	H	34.9736179	9.8864650	40.9582436
H	35.7612393	5.1028256	39.5277217	H	34.3850947	9.2036054	43.2989390
H	37.1717827	5.8634220	37.6908069	H	30.8726245	11.2682459	40.3736958
H	33.7113838	2.4763471	38.1649408	H	31.9146153	11.9276958	41.6478623
H	33.7659630	1.9435280	35.7092328	H	30.2251430	10.3071058	42.5744645
H	32.6448911	3.3922812	34.1017551	H	30.9121563	9.0111512	41.5732745
H	31.1272713	6.5293258	38.4901830	H	32.3252981	10.5561606	43.8371253
H	29.8899973	7.9315203	36.8724435	H	31.9096920	8.8223468	43.8138926
H	28.9071290	7.7191957	42.5886699	H	32.6278963	9.8299101	39.5123069
H	29.4424585	3.5742734	40.1883924	H	38.6659143	8.8019120	39.2835340
H	34.0632141	7.2705788	45.7706512	H	38.5621477	9.1034034	36.8265519
H	30.3389717	4.3541636	44.8363854	H	36.4508683	8.5918724	35.5709288
H	28.4626764	3.4749994	46.1392198	H	34.4271419	7.8248834	36.8524325
H	29.7275046	7.4502503	33.4666508	H	34.5291207	7.5412212	39.2951252
H	39.2222160	6.4517936	37.1250811	H	35.9796916	7.2932093	41.2189103
H	33.8265016	7.8568185	48.2025435	H	37.5778538	7.8365214	41.2338652
H	32.0074548	6.9082787	49.5358056	H	24.5176790	4.5092042	39.9960437
H	27.5173926	3.2887268	48.1459531	H	40.7378413	4.5235264	39.7193925
C	33.5653826	9.3651925	42.5850217	H	31.2464659	5.4982783	33.5800346
C	33.9103671	9.7831657	41.2058463	H	29.9288363	5.3729848	49.7242051
C	32.9131844	10.5187467	40.3290837				
C	31.6656304	10.9999181	41.0940995		(R,R)-1-TS1		
C	31.1557616	9.9536229	42.0948471	C	26.4817298	7.4936254	42.4161287
C	32.2092225	9.6729152	43.1781829	C	25.7549016	6.4925917	41.8065631
O	33.5749022	8.4139759	41.5121954	C	26.3815484	5.3396092	41.2321525
C	36.5997349	8.1649429	39.4742113	C	27.8152757	5.2335539	41.3533629

C	27.7368959	3.1220700	40.1470361	C	32.5541963	5.8891046	39.5469170
C	26.3255619	3.2224668	40.0128920	C	28.5414160	6.2989337	41.9812559
C	25.6437713	4.3151981	40.5382860	C	27.8867579	7.4129437	42.4811172
O	25.7697133	2.1729176	39.3373501	C	28.4613497	4.0962299	40.7852540
Cu	32.4941388	7.8530863	41.7525606	O	30.6105236	7.3822467	41.7801654
Cu	32.5688988	4.9329758	42.2543577	O	30.6283921	5.2441776	42.4497162
C	36.5584525	3.8499093	41.6475418	C	30.0342809	6.2960062	42.0750374
C	37.0120226	3.3891573	42.8698567	C	32.3475867	6.9764505	45.9125328
C	38.3620754	2.9902221	43.0176695	C	32.9963398	7.9831123	46.6027287
C	39.2478536	3.0930125	41.9647935	C	31.3964514	6.1258270	46.5700477
C	38.8258165	3.5485231	40.6733569	C	30.6342945	5.1466422	45.8691314
C	37.4291228	3.8549934	40.5089512	C	29.7018848	4.3754343	46.5204970
C	36.9517373	4.1486127	39.2029553	O	32.6449379	7.8359481	43.7327647
C	37.8148330	4.2602210	38.1429623	O	32.8898555	5.6209696	44.0625413
C	39.2159553	4.1435579	38.3341337	C	32.6476855	6.7973169	44.4552663
C	39.7282871	3.7423406	39.5687541	C	32.7799239	8.1422352	47.9895672
O	40.0482624	4.4247593	37.2928427	C	31.8975889	7.3211103	48.6589272
O	35.1161363	5.6160695	40.9874629	C	31.1571511	6.2979010	47.9805122
O	34.2511552	3.9612712	42.2098177	C	29.4800354	4.5161511	47.9161745
C	35.2102205	4.5213850	41.5830912	C	30.1946361	5.4635332	48.6459158
C	32.6787092	5.5597470	38.0878009	O	28.5606538	3.7271495	48.5396778
C	33.2573735	4.3351547	37.7887562	H	25.9663876	8.3618243	42.8390032
C	33.4313213	3.9375968	36.4490046	H	24.6665635	6.6025397	41.7627838
C	32.9698864	4.7351948	35.4224765	H	28.2270369	2.2500892	39.7054456
C	32.3250187	5.9898397	35.6692888	H	24.8074997	2.2553476	39.2467473
C	32.2177175	6.4268472	37.0415807	H	36.3279395	3.3768495	43.7225965
C	31.6042832	7.6879277	37.3007249	H	38.7144035	2.6282495	43.9889639
C	31.1263698	8.4646883	36.2768943	H	40.2955125	2.8187009	42.1245643
C	31.2015311	8.0301554	34.9266665	H	35.8865953	4.3171712	39.0396456
C	31.7837608	6.8057855	34.6136963	H	37.4311814	4.5088638	37.1486760
O	30.6568798	8.9173136	34.0428296	H	33.5734652	3.6866876	38.6082393
O	32.7129868	7.0932499	39.9148272	H	33.9194707	2.9842573	36.2238178
O	32.3258018	4.9067468	40.3052628	H	33.1039644	4.3823076	34.3949081

H	31.5156094	8.0346524	38.3289272	H	37.1445832	9.0946929	42.6812611
H	30.6538539	9.4311854	36.4725390	H	35.7482345	9.6574689	43.6325054
H	28.4708679	8.2210686	42.9281451	H	34.7111778	10.5712353	39.5346263
H	29.5457599	4.0034175	40.8503350	H	39.2580050	7.8208305	38.4126239
H	33.6862971	8.6402558	46.0665719	H	39.5315901	7.6498455	35.9539898
H	30.7715107	5.0093713	44.7973671	H	37.5897177	6.9924922	34.5085407
H	29.1189560	3.6383194	45.9552761	H	35.3588053	6.5522940	35.5808869
H	30.7073661	8.6121097	33.1234906	H	35.0869645	6.7476440	38.0154942
H	39.5427065	4.8838939	36.5996137	H	36.4309618	6.5936684	40.1890766
H	33.3166484	8.9237226	48.5367866	H	37.8436148	7.5188641	40.2963905
H	31.7562367	7.4717888	49.7338169	H	24.5717260	4.4342535	40.3814067
H	28.1609468	3.1202980	47.8954149	H	40.8069163	3.6299862	39.6783078
C	35.2389588	8.6269313	41.8293390	H	31.7858181	6.4422482	33.5861250
C	35.2580984	8.7153981	40.3606962	H	30.0248747	5.5459070	49.7194437
C	35.6405420	9.9880538	39.6689775				
C	36.6743672	10.8016476	40.4602124		(R,R)-1-Int1		
C	36.2671257	10.9450372	41.9347261	C	26.2331868	7.3581398	42.4612969
C	36.1460415	9.5693690	42.6056754	C	25.5643531	6.3347341	41.8232135
O	33.9317108	9.1383519	41.6161942	C	26.2563292	5.2377679	41.2139667
C	37.1525079	7.3081924	38.3856640	C	27.6946167	5.2173360	41.3285305
C	38.3955639	7.5696046	37.7861122	C	27.7422249	3.1416566	40.0595041
C	38.5502908	7.4551752	36.4000503	C	26.3270711	3.1588092	39.9299426
C	37.4662800	7.0887816	35.5918295	C	25.5799374	4.1901329	40.4892401
C	36.2187572	6.8523996	36.1864720	O	25.8352428	2.0971563	39.2228289
C	36.0575486	6.9694875	37.5667135	Cu	32.2504319	8.0577737	41.8007059
N	36.9760481	7.3783187	39.7800747	Cu	32.4335932	5.0701634	42.2563121
H	35.9975134	9.7443595	38.6531852	C	36.4788177	4.0150361	41.6801626
H	34.6741780	7.9682517	39.8295235	C	36.9033351	3.5777469	42.9211369
H	35.2493193	7.6034487	42.2355124	C	38.2510994	3.1895519	43.1098599
H	36.8042799	11.7929922	39.9910740	C	39.1618175	3.2755478	42.0770499
H	37.6558190	10.2913118	40.4007675	C	38.7704763	3.7056950	40.7671020
H	37.0019373	11.5655091	42.4781788	C	37.3783408	4.0110800	40.5636083
H	35.2925914	11.4624602	41.9979006	C	36.9312234	4.2743109	39.2397370

C	37.8185075	4.3559260	38.1971648	O	32.7318768	5.6435992	44.0904491
C	39.2129053	4.2273731	38.4196957	C	32.4521283	6.8102016	44.5040088
C	39.6962111	3.8596760	39.6766927	C	32.6361525	8.0418215	48.0787283
O	40.0720385	4.4599739	37.3870704	C	31.7718180	7.1932357	48.7373276
O	34.9977399	5.6841065	40.8617744	C	31.0253863	6.1883377	48.0386097
O	34.1690221	4.1301087	42.2218743	C	29.3660641	4.3920588	47.9441721
C	35.1166486	4.6429287	41.5614322	C	30.0786944	5.3263302	48.6918255
C	32.6000303	5.6323693	38.1146651	O	28.4660820	3.5715259	48.5571658
C	33.2295669	4.4296249	37.8295492	H	25.6678140	8.1794174	42.9131932
C	33.4700869	4.0478503	36.4947040	H	24.4714211	6.3841576	41.7854421
C	33.0233517	4.8365222	35.4540954	H	28.2832802	2.3150326	39.5910295
C	32.3295813	6.0679261	35.6834725	H	24.8691513	2.1215761	39.1408123
C	32.1576015	6.4917804	37.0543124	H	36.1947795	3.5721109	43.7536868
C	31.5032620	7.7356883	37.2983960	H	38.5803691	2.8464200	44.0958066
C	31.0500786	8.5094856	36.2613134	H	40.2054344	3.0056072	42.2673925
C	31.1845993	8.0843450	34.9122716	H	35.8698286	4.4273211	39.0449218
C	31.8020020	6.8732935	34.6122669	H	37.4535207	4.5741913	37.1888545
O	30.6504529	8.9636785	34.0144419	H	33.5321736	3.7855094	38.6573659
O	32.5403978	7.1554815	39.9562556	H	33.9973039	3.1119051	36.2837297
O	32.2048633	4.9581106	40.3188584	H	33.2057161	4.4957627	34.4297030
C	32.4235775	5.9587925	39.5748279	H	31.3644249	8.0688803	38.3257447
C	28.3592906	6.3061654	41.9836768	H	30.5460879	9.4624316	36.4440216
C	27.6410962	7.3620002	42.5191066	H	28.1782207	8.1909085	42.9868703
C	28.4075279	4.1394163	40.7249952	H	29.4960006	4.1123213	40.7848073
O	30.3705710	7.5039764	41.7902639	H	33.5024375	8.6101377	46.1559873
O	30.4929426	5.3610223	42.4444573	H	30.5946121	5.0065457	44.8191978
C	29.8527838	6.3913019	42.0739070	H	28.9775468	3.5749111	45.9632320
C	32.1738184	6.9419359	45.9726918	H	30.7600233	8.6759797	33.0945277
C	32.8276361	7.9304650	46.6833486	H	39.5693049	4.7946309	36.6259805
C	31.2417199	6.0641219	46.6195912	H	33.1788952	8.8080352	48.6416589
C	30.4759939	5.1023387	45.8984227	H	31.6516174	7.3054146	49.8195373
C	29.5649393	4.2986475	46.5409016	H	28.0693732	2.9765835	47.9002429
O	32.4006639	7.8538356	43.8052797	C	34.9150888	8.7553755	41.6175572

C	35.2620023	8.6630561	40.1062878	H	29.9078176	5.3898355	49.7664579
C	35.5648026	10.0315545	39.4999759				
C	36.6096154	10.8266141	40.2960267	(<i>R,R</i>)-2-RC			
C	36.1794415	10.9727853	41.7631419	C	26.6847521	7.0688011	42.3128167
C	35.9450229	9.5983571	42.3981089	C	25.8672926	6.2899802	41.5197053
O	33.6491021	9.2950626	41.7073501	C	26.3759370	5.1973682	40.7433415
C	36.8063036	7.4761676	38.4963319	C	27.7896365	4.9341495	40.8260662
C	38.1390664	7.6759422	38.1380494	C	27.5353415	3.1202339	39.2286024
C	38.5281203	7.4929236	36.8054378	C	26.1359574	3.3577374	39.1515706
C	37.5815214	7.1187046	35.8448995	C	25.5473450	4.3751145	39.8990604
C	36.2464990	6.9154715	36.2207446	O	25.4931707	2.4948816	38.3105245
C	35.8530439	7.0954021	37.5482004	Cu	32.8768731	6.2713307	41.5442875
N	36.3853818	7.6472766	39.8855351	Cu	32.3284553	3.7960750	42.1764530
H	35.8512942	9.9355379	38.4378637	C	36.5086659	4.0255013	41.8076006
H	34.3881799	8.2072183	39.6266321	C	37.0051961	3.1532212	42.7595631
H	34.9480801	7.7283150	42.0397173	C	38.3820169	2.8422389	42.7860557
H	36.7564594	11.8174510	39.8293738	C	39.2392778	3.3827329	41.8518936
H	37.5965788	10.3188899	40.2464218	C	38.7719397	4.2600498	40.8196068
H	36.9371532	11.5391797	42.3350293	C	37.3665208	4.5834105	40.8018315
H	35.2369329	11.5473457	41.8088398	C	36.8772108	5.4160929	39.7545323
H	36.9101009	9.0486066	42.4583347	C	37.7245482	5.9149751	38.7942492
H	35.5692283	9.6927563	43.4311783	C	39.1163538	5.6321084	38.8250169
H	34.6045122	10.5742071	39.5273559	C	39.6440111	4.8106649	39.8195311
H	38.8813653	7.9559038	38.8925278	O	39.9356883	6.1630603	37.8751592
H	39.5752203	7.6434833	36.5265078	O	34.7308555	5.5811336	41.7112926
H	37.8816247	6.9846926	34.8006544	O	34.2519335	3.4193799	42.1225423
H	35.4983078	6.5995861	35.4886706	C	35.0532436	4.3707695	41.8793706
H	34.8160568	6.9192614	37.8396216	C	32.3627346	3.9449901	37.9617557
H	35.9755377	6.7120725	40.2861120	C	32.9939692	2.7896266	37.5364981
H	37.1961268	7.8957259	40.4639073	C	33.0570176	2.4932952	36.1580690
H	24.5044975	4.2584713	40.3254558	C	32.4783521	3.3375373	35.2330488
H	40.7697139	3.7180876	39.8016365	C	31.7748618	4.5235742	35.6233005
H	31.8069637	6.4977533	33.5890312	C	31.7108577	4.8184169	37.0314995

C	30.9568598	5.9506715	37.4561383	H	38.7701775	2.1682321	43.5561091
C	30.3327650	6.7628883	36.5450852	H	40.3011597	3.1222852	41.9024538
C	30.4274887	6.5075840	35.1500941	H	35.8152848	5.6591831	39.7084409
C	31.1361887	5.4050669	34.6802447	H	37.3257686	6.5520140	37.9959018
O	29.7735385	7.4347828	34.3891328	H	33.4606964	2.1309627	38.2735899
O	32.7864132	5.4631528	39.7117755	H	33.5758950	1.5905882	35.8204841
O	32.1819023	3.3641677	40.2497064	H	32.5569629	3.0741664	34.1732905
C	32.4392991	4.2829499	39.4170246	H	30.8680896	6.1714169	38.5205363
C	28.6066786	5.7624726	41.6598369	H	29.7411774	7.6252057	36.8642306
C	28.0717017	6.8152011	42.3808399	H	28.7141634	7.4305144	43.0164414
C	28.3375984	3.8767883	40.0426584	H	29.4061097	3.6578299	40.0894376
O	30.8585589	6.4551184	41.4743827	H	33.9419575	7.4018882	45.7081442
O	30.4339544	4.3546281	42.1573501	H	30.2691571	4.3985144	44.8390243
C	30.0742754	5.5028268	41.7716401	H	28.4035590	3.5245235	46.1602406
C	32.2717325	6.0614392	45.7387827	H	29.7947107	7.2262210	33.4421597
C	33.1371883	6.9754667	46.3124484	H	39.4183552	6.7162610	37.2678254
C	31.1759690	5.5136520	46.4852395	H	33.6851181	8.0455845	48.1226449
C	30.1984574	4.6615148	45.8949970	H	31.8898152	7.0847819	49.4806704
C	29.1520887	4.1687385	46.6370280	H	27.4706462	3.3525042	48.1714031
O	32.7914535	6.5880088	43.4997875	C	32.7661182	8.5853562	39.3318734
O	32.4372191	4.4304887	44.0350639	C	33.2081452	9.5562596	40.3572276
C	32.5167060	5.6617981	44.3179960	C	34.5318620	10.2894628	40.2243165
C	32.9870905	7.3346074	47.6699041	C	35.1716294	10.1363744	38.8310857
C	31.9733262	6.7904637	48.4296849	C	35.0641358	8.7006454	38.2980756
C	31.0260524	5.8700051	47.8740087	C	33.5959223	8.2928552	38.1048877
C	29.0289952	4.4667835	48.0207460	O	33.3290078	8.1327806	40.5733718
C	29.9496993	5.3085830	48.6419286	C	30.0382582	9.8797270	42.6315630
O	28.0051784	3.9297265	48.7404119	C	29.3360991	11.0548478	42.9709654
H	26.2591328	7.8930668	42.8936316	C	29.4236425	11.5887699	44.2596564
H	24.7993392	6.5287517	41.4903960	C	30.2034290	10.9670521	45.2421551
H	27.9479859	2.3139545	38.6165932	C	30.9022607	9.7994640	44.9098146
H	24.5471954	2.6890384	38.2231188	C	30.8290359	9.2605553	43.6238369
H	36.3220563	2.7242324	43.4969355	N	29.9972139	9.3532944	41.3400102

H	34.3768741	11.3575846	40.4594662	C	36.5972677	3.6608130	41.5530020
H	32.4282768	10.0090331	40.9821021	C	37.0720968	2.6755618	42.3987052
H	31.6886806	8.3919582	39.2520767	C	38.4293723	2.2875792	42.3380751
H	36.2275633	10.4582798	38.8728282	C	39.2891719	2.8865367	41.4424266
H	34.6623102	10.8165827	38.1197432	C	38.8377569	3.8813130	40.5143766
H	35.6016855	8.6073661	37.3368586	C	37.4460224	4.2492732	40.5558596
H	35.5472240	8.0061680	39.0089797	C	36.9599847	5.1666640	39.5799348
H	33.1501880	8.8461938	37.2555444	C	37.8016308	5.7124345	38.6409003
H	33.5035149	7.2176824	37.8749814	C	39.1904211	5.4132135	38.6409968
H	35.2092461	9.8904167	41.0024104	C	39.7130902	4.5105192	39.5647614
H	28.7199756	11.5518468	42.2128132	O	40.0124018	6.0117135	37.7346386
H	28.8697119	12.5038326	44.4980836	O	35.0565220	5.4195713	41.7120376
H	30.2642969	11.3849597	46.2518355	O	34.2886688	3.3398293	42.0293859
H	31.5140494	9.2877112	45.6605624	C	35.2061591	4.1648393	41.7721711
H	31.3916797	8.3556774	43.3823223	C	32.4463682	4.6163708	38.0423780
H	30.2183641	8.3566386	41.2726567	C	32.8275791	3.3380114	37.6665217
H	29.1803917	9.6086066	40.7910236	C	32.8355333	2.9730885	36.3047616
H	24.4736721	4.5553775	39.8461604	C	32.4297541	3.8699545	35.3392466
H	40.7181219	4.6259988	39.8353654	C	31.9808365	5.1883611	35.6725820
H	31.2022880	5.2017000	33.6114420	C	32.0032766	5.5653312	37.0635551
H	29.8665600	5.4802336	49.7150970	C	31.5364430	6.8632731	37.4182572
				C	31.0795753	7.7374363	36.4657508
				C	31.0651275	7.3800219	35.0908417
(R,R)-2-TS1				C	31.5125845	6.1264787	34.6855730
C	26.4613101	6.3389260	43.3334521	O	30.5918735	8.3731626	34.2790057
C	25.7402047	5.7841093	42.2965831	O	33.0028331	6.0733604	39.8418090
C	26.3564068	4.9679786	41.2917030	O	32.2117078	4.0138742	40.2977274
C	27.7823582	4.7680935	41.3905565	C	32.5517529	4.9370945	39.5049809
C	27.7203566	3.4171535	39.3719087	C	28.5071699	5.3892973	42.4574603
C	26.3127300	3.5907095	39.2736275	C	27.8563990	6.1508796	43.4138057
C	25.6222340	4.3605149	40.2079568	C	28.4361762	3.9867572	40.3919486
O	25.7700573	2.9296966	38.2088113	O	30.6423092	6.3964472	42.6040055
Cu	33.6184973	6.7124343	41.6309355	O	30.5480398	4.1667740	42.5058467
Cu	32.4705927	4.0574028	42.2550177				

C	30.0086955	5.3246452	42.5248413	H	28.8574593	3.8704459	46.0127345
C	32.7841703	6.3394108	45.7963639	H	30.5488862	8.1060397	33.3475828
C	33.6345022	7.2319621	46.4243983	H	39.5043302	6.6374029	37.1934065
C	31.6583337	5.7856099	46.4984932	H	34.1393101	8.2437197	48.2804527
C	30.7002779	4.9425748	45.8661647	H	32.2708573	7.2964068	49.5470094
C	29.5880238	4.4976634	46.5372167	H	27.7675835	3.7800899	47.9541547
O	33.4571090	6.9194144	43.6052633	C	31.7509211	8.7559905	40.9101238
O	32.8937803	4.7770113	44.0352812	C	31.7436915	9.1998830	42.3122502
C	33.0640887	5.9829946	44.3637880	C	32.0612628	10.6135009	42.6841994
C	33.4450392	7.5571590	47.7857113	C	31.6542049	11.6206180	41.6002292
C	32.3920977	7.0190872	48.4950572	C	32.1327719	11.1697421	40.2124454
C	31.4450885	6.1366683	47.8806465	C	31.5219182	9.8123464	39.8374587
C	29.3811788	4.8208304	47.9035714	O	33.1179848	8.5368991	41.2095568
C	30.3016723	5.6185137	48.5808477	C	29.3644634	9.4454023	44.1770277
O	28.2839349	4.3429163	48.5540023	C	28.6535925	10.6153829	44.4960747
H	25.9514476	6.9427839	44.0912204	C	28.5592793	11.0421263	45.8243998
H	24.6651849	5.9844846	42.2599208	C	29.1805724	10.3207283	46.8503542
H	28.2121250	2.8164203	38.6021914	C	29.8974555	9.1606783	46.5313972
H	24.8122084	3.0584653	38.1342652	C	29.9852321	8.7180323	45.2106094
H	36.3950997	2.2302864	43.1324273	N	29.5491005	9.0409405	42.8446201
H	38.8037436	1.5188852	43.0215116	H	31.5818978	10.8351913	43.6544872
H	40.3398195	2.5796318	41.4376896	H	31.8283447	8.4250248	43.0697182
H	35.9050067	5.4418454	39.5657484	H	31.1942274	7.8267645	40.7104787
H	37.4026451	6.4058292	37.8906724	H	32.0547129	12.6188113	41.8507367
H	33.1354308	2.6267100	38.4364414	H	30.5500609	11.7152864	41.5931160
H	33.1634072	1.9701229	36.0135907	H	31.8695582	11.9238873	39.4495465
H	32.4478686	3.5466614	34.2934374	H	33.2346650	11.0806503	40.2145199
H	31.5465152	7.1601060	38.4649801	H	30.4284402	9.9157721	39.6885092
H	30.7136169	8.7318070	36.7361904	H	31.9436250	9.4377012	38.8888780
H	28.4245279	6.6042037	44.2304009	H	33.1507516	10.6568266	42.8677204
H	29.5153189	3.8313434	40.4431660	H	28.1708813	11.1892062	43.6972093
H	34.4596102	7.6684774	45.8561459	H	27.9949231	11.9513503	46.0566826
H	30.8481051	4.6343324	44.8354150	H	29.1098849	10.6568029	47.8889976

H	30.4107556	8.5927975	47.3122901	C	35.1417076	4.1237869	41.5547209
H	30.5432126	7.8092585	44.9736370	C	32.0271328	4.2776223	38.0991318
H	29.6632100	8.0233209	42.7093242	C	32.1369788	2.9553152	37.6886684
H	28.8983890	9.4507740	42.1766192	C	32.1182131	2.6215355	36.3216825
H	24.5517319	4.5379256	40.1049165	C	31.9608549	3.6047274	35.3690780
H	40.7924009	4.3635562	39.6042162	C	31.8052606	4.9830358	35.7221642
H	31.5259215	5.8577742	33.6293124	C	31.8620039	5.3262942	37.1252356
H	30.1725613	5.7711684	49.6523389	C	31.7355211	6.7026423	37.4797013
				C	31.5292778	7.6641262	36.5237881
(R,R)-2-Int1				C	31.4511161	7.3323015	35.1462467
C	26.3371055	6.2854466	43.3624219	C	31.6076125	6.0126308	34.7328977
C	25.6605264	5.7820186	42.2709325	O	31.2344084	8.4168112	34.3394197
C	26.3004564	4.9539765	41.2909141	O	32.3874987	5.6620989	40.0343946
C	27.7120784	4.6982384	41.4607480	O	31.9466737	3.4997089	40.3275735
C	27.7036134	3.4064421	39.4022399	C	32.1253017	4.5141764	39.5808015
C	26.3074940	3.6215431	39.2427263	C	28.3940858	5.2607492	42.5890732
C	25.5961581	4.3829995	40.1680848	C	27.7116732	6.0265039	43.5242788
O	25.7970617	2.9972319	38.1423831	C	28.3864353	3.9182061	40.4742275
Cu	33.5044111	6.6393497	41.4648025	O	30.4917533	6.1599696	43.1887246
Cu	32.3883946	3.8790822	42.2033242	O	30.4443048	4.0270631	42.5588892
C	36.5446368	3.6147373	41.4018602	C	29.8785215	5.1360902	42.7857132
C	36.9870545	2.6710907	42.3110555	C	32.7758813	6.1463784	45.7099279
C	38.3450834	2.2808447	42.3248089	C	33.5582184	7.1309012	46.2890518
C	39.2415129	2.8333907	41.4354412	C	31.7112063	5.5327374	46.4585272
C	38.8278272	3.7809352	40.4429823	C	30.8304961	4.5682180	45.8904018
C	37.4361943	4.1537306	40.4143201	C	29.7692629	4.0622878	46.5990064
C	36.9935063	5.0273970	39.3801846	O	33.3896478	6.7326837	43.5018758
C	37.8715770	5.5267743	38.4488086	O	32.9119873	4.5755893	43.9506357
C	39.2567617	5.2199667	38.5123467	C	33.0445094	5.7919628	44.2689680
C	39.7402145	4.3589308	39.4957678	C	33.3544636	7.5076968	47.6353079
O	40.1140776	5.7706323	37.6077542	C	32.3508018	6.9264274	48.3819499
O	34.9724622	5.3654638	41.3963468	C	31.4776113	5.9382083	47.8233662
O	34.2423980	3.2962250	41.8687960	C	29.5416189	4.4446117	47.9461897

C	27.6862181	4.6922282	41.3765918	O	31.9320410	3.3372498	40.3174725
C	27.6772676	3.3522654	39.3505923	C	32.0272919	4.3915055	39.6041373
C	26.2820970	3.5651085	39.1828022	C	28.3618335	5.2848989	42.4961087
C	25.5714265	4.3469885	40.0914112	C	27.6786939	6.0764451	43.4111029
O	25.7725373	2.9178046	38.0973659	C	28.3596950	3.8870324	40.4120557
Cu	33.4646075	6.6276294	41.3711609	O	30.4786928	6.1275019	43.1927455
Cu	32.3961392	3.8393353	42.1529019	O	30.4044080	4.0361902	42.5022603
C	36.5488305	3.6497827	41.2967767	C	29.8215278	5.1124516	42.7214389
C	36.9924636	2.7198153	42.2203360	C	32.7626178	6.1141134	45.6446987
C	38.3527327	2.3405878	42.2511981	C	33.5413384	7.1137570	46.2021113
C	39.2527596	2.8922408	41.3653168	C	31.7129844	5.4992198	46.4153262
C	38.8415279	3.8286743	40.3613630	C	30.8339960	4.5171832	45.8754694
C	37.4465383	4.1889837	40.3134930	C	29.7941103	4.0027342	46.6096687
C	37.0108428	5.0505553	39.2663208	O	33.3805796	6.6624563	43.4228560
C	37.8974455	5.5539413	38.3450399	O	32.8680961	4.5228286	43.9011839
C	39.2843048	5.2606203	38.4284612	C	33.0258232	5.7430626	44.2074355
C	39.7613125	4.4069440	39.4214321	C	33.3484521	7.5080418	47.5449071
O	40.1487574	5.8140090	37.5328271	C	32.3634266	6.9233977	48.3129713
O	34.9329886	5.3652618	41.2094699	C	31.4969839	5.9155716	47.7806222
O	34.2631828	3.3104969	41.8152519	C	29.5849197	4.3968035	47.9561679
C	35.1380128	4.1401327	41.4373846	C	30.4340664	5.3283677	48.5507865
C	31.9659573	4.2034480	38.1164108	O	28.5587768	3.8529887	48.6688810
C	31.9991882	2.8851471	37.6763516	H	25.7787440	6.9652928	43.9561010
C	31.9795721	2.5809142	36.3039732	H	24.5768365	6.0524670	42.0439867
C	31.8992004	3.5923736	35.3713776	H	28.1909516	2.7402335	38.6046386
C	31.8339064	4.9706761	35.7505847	H	24.8356145	3.1139250	37.9441591
C	31.8976135	5.2827363	37.1623247	H	36.2824369	2.3114422	42.9435857
C	31.8893394	6.6594073	37.5394191	H	38.6961356	1.6169801	42.9973430
C	31.7728520	7.6489011	36.5961665	H	40.3043268	2.5951972	41.4300334
C	31.6681544	7.3484898	35.2130067	H	35.9566904	5.3132812	39.1879561
C	31.7225526	6.0280064	34.7759709	H	37.5361416	6.2066652	37.5411053
O	31.5370133	8.4604752	34.4266282	H	32.0528953	2.0879234	38.4189964
O	32.1689640	5.5289501	40.1338756	H	32.0285116	1.5374607	35.9770937

H	31.8880079	3.3124051	34.3133434	H	32.3084476	10.9051750	40.1689012
H	31.9945174	6.9269401	38.5886971	H	29.6404559	9.3753432	40.2682908
H	31.7607551	8.7033491	36.8857732	H	30.9769625	9.0491163	39.1540782
H	28.1973511	6.4900820	44.2789659	H	32.7054271	10.4342242	42.6531191
H	29.4228808	3.6744410	40.5204460	H	27.4361463	9.6085133	43.7424481
H	34.3086039	7.5903299	45.5871607	H	26.6288433	10.1527071	46.0294156
H	30.9933459	4.1597702	44.8642909	H	28.1389788	9.8359302	48.0053035
H	29.1263451	3.2602125	46.1561399	H	30.4572349	8.9606558	47.6463086
H	31.4324763	8.2455765	33.4866241	H	31.2458668	8.3893064	45.3835794
H	39.6664689	6.4065266	36.9338205	H	30.0223679	7.0990897	43.1315781
H	33.9845637	8.2870783	47.9770480	H	29.1301558	8.8653218	42.4019504
H	32.2356561	7.2545284	49.3486215	H	24.4981103	4.5024216	39.9823270
H	28.0917488	3.1998849	48.1229177	H	40.8370097	4.2512894	39.5033693
C	31.3794948	8.4393259	41.1814514	H	31.6948759	5.7983687	33.7108104
C	31.2082515	8.9316436	42.6464003	H	30.3067938	5.5300949	49.6143533
C	31.6121951	10.4015454	42.8087789				
C	30.9372559	11.3318414	41.7935866				
C	31.2206639	10.8598910	40.3603977	(R,R)-2-Int3			
C	30.7454175	9.4170673	40.1673215	C	26.3407492	6.8752554	42.5796749
O	32.7263616	8.2642785	40.9192917	C	25.6381349	6.0153345	41.7619377
C	29.3970794	8.9749385	44.4065314	C	26.2692404	4.9374726	41.0577290
C	28.0980311	9.4682902	44.6043948	C	27.6902980	4.7665528	41.2406138
C	27.6458169	9.7710656	45.8920911	C	27.6383343	2.9070059	39.6743643
C	28.4878820	9.5980392	46.9961910	C	26.2367764	3.0560981	39.4976915
C	29.7841926	9.1085864	46.7965935	C	25.5447154	4.0527425	40.1796556
C	30.2390187	8.7894585	45.5143143	O	25.7010482	2.1430641	38.6373321
N	29.8242060	8.5924860	43.0987231	Cu	33.5659395	6.6584322	41.2005268
H	31.4229554	10.7342899	43.8446970	Cu	32.4078962	3.9354250	42.1258925
H	31.8867052	8.3118453	43.2466882	C	36.5382768	3.5777362	41.3802196
H	30.8367022	7.4755529	41.0684132	C	36.9868802	2.6418249	42.2952149
H	31.2910803	12.3684385	41.9424664	C	38.3504012	2.2725438	42.3224867
H	29.8416016	11.3506447	41.9683354	C	39.2469790	2.8413510	41.4436944
H	30.7313155	11.5255899	39.6255469	C	38.8297633	3.7823726	40.4462845
				C	37.4318275	4.1306884	40.3993638

C	36.9900400	4.9920258	39.3546337	O	32.9168364	6.5813556	43.3134591
C	37.8726917	5.5085260	38.4369306	O	32.7898595	4.4475724	43.9708987
C	39.2620121	5.2281602	38.5207983	C	32.7884293	5.6860963	44.2121404
C	39.7450403	4.3737173	39.5106300	C	33.1238728	7.5715229	47.4704572
O	40.1222144	5.7910438	37.6284020	C	32.1736955	6.9698349	48.2689977
O	34.9370008	5.3015344	41.3117851	C	31.3161275	5.9361560	47.7710468
O	34.2385924	3.2515715	41.8836684	C	29.4303117	4.3933819	47.9935789
C	35.1313177	4.0713187	41.5227558	C	30.2843461	5.3338638	48.5681742
C	31.9578451	4.3102918	38.0536428	O	28.4440103	3.8246961	48.7390453
C	32.1948675	3.0050562	37.6384433	H	25.8270399	7.6885905	43.1004194
C	32.2093948	2.6769406	36.2708566	H	24.5625040	6.1859909	41.6526232
C	31.9686721	3.6475335	35.3223714	H	28.1406187	2.1188808	39.1074643
C	31.6873495	5.0046253	35.6795302	H	24.7571301	2.2922503	38.4725546
C	31.6922041	5.3434338	37.0850102	H	36.2806175	2.2228304	43.0163736
C	31.4131459	6.6951033	37.4447645	H	38.6995639	1.5443155	43.0612895
C	31.1425032	7.6408489	36.4887344	H	40.3012365	2.5539392	41.5078287
C	31.1346056	7.3152347	35.1070074	H	35.9336615	5.2436526	39.2706254
C	31.4124346	6.0165391	34.6912052	H	37.5054515	6.1595963	37.6345348
O	30.8453405	8.3812909	34.3015569	H	32.3884609	2.2403605	38.3924731
O	32.2081941	5.7116430	40.0005323	H	32.4178670	1.6483042	35.9604965
O	31.9863513	3.5177944	40.2780540	H	31.9959017	3.3527745	34.2684703
C	32.0499267	4.5497805	39.5297383	H	31.4277796	6.9785687	38.4946482
C	28.3921216	5.6860363	42.0944315	H	30.9254797	8.6759359	36.7667529
C	27.7289657	6.7237487	42.7395201	H	28.2815789	7.4173870	43.3754464
C	28.3448095	3.7282063	40.5163808	H	29.4193821	3.5797638	40.6195675
O	30.4097762	6.7694928	42.5160675	H	34.0544984	7.6352118	45.4973347
O	30.4752956	4.5279113	42.3694164	H	30.6960840	4.2331546	44.8323729
C	29.8490287	5.6010105	42.3241458	H	28.8928018	3.3021801	46.1882305
C	32.5389511	6.1252116	45.6184438	H	30.8190278	8.1459416	33.3609179
C	33.3037634	7.1572475	46.1322346	H	39.6383998	6.3868014	37.0337878
C	31.5012695	5.5163383	46.4043328	H	33.7441261	8.3766193	47.8758868
C	30.5988256	4.5542273	45.8677690	H	32.0616939	7.3131182	49.3021740
C	29.5862401	4.0268528	46.6311505	H	27.9544818	3.1800007	48.2029200

C	32.0116173	9.0508109	40.8657792	H	31.4304843	5.7699087	33.6296431
C	31.8630909	9.6122367	42.3056070	H	30.1825986	5.5407644	49.6334939
C	32.9026409	10.7230928	42.5556234				
C	32.8075712	11.8381160	41.5047048		(R,R)-2-Int3-2		
C	32.9661238	11.2738702	40.0832037	C	26.4971768	6.4767202	42.9809171
C	31.9364876	10.1700742	39.8062250	C	25.7283602	5.7159066	42.1263646
O	33.2230765	8.3861228	40.7404654	C	26.3026823	4.7467739	41.2382063
C	29.7634983	9.7657907	43.6991761	C	27.7307408	4.5770456	41.2910227
C	28.4028715	10.1574333	43.7624129	C	27.5891509	2.8702314	39.5677905
C	27.6227232	9.8777499	44.8835993	C	26.1818692	3.0471362	39.4831764
C	28.1611919	9.1994761	45.9859380	C	25.5322148	3.9699431	40.3004279
C	29.5068608	8.8177134	45.9367809	O	25.5974168	2.2339682	38.5559443
C	30.3019536	9.0951496	44.8230965	Cu	33.9400618	6.9736067	41.6425051
N	30.4973315	10.0338663	42.5658484	Cu	32.6560788	4.0948080	42.2314274
H	32.7659327	11.1268957	43.5753640	C	36.7804823	3.7654949	41.5222932
H	32.0918478	8.7747950	42.9747158	C	37.2885287	2.8526667	42.4284934
H	31.1727269	8.3451116	40.6838166	C	38.6413022	2.4538496	42.3470085
H	33.5729426	12.6119082	41.6988297	C	39.4660676	2.9765337	41.3743036
H	31.8237338	12.3411827	41.5948190	C	38.9800343	3.8982403	40.3895784
H	32.8729399	12.0809981	39.3328642	C	37.5895737	4.2645723	40.4464503
H	33.9781464	10.8426006	39.9742930	C	37.0691246	5.0948329	39.4119369
H	30.9143323	10.5998629	39.7974431	C	37.8778794	5.5715813	38.4088752
H	32.0991526	9.7122959	38.8143290	C	39.2706566	5.2924456	38.3997503
H	33.9056456	10.2610717	42.5089715	C	39.8240342	4.4649285	39.3740645
H	27.9596240	10.6789869	42.9062351	O	40.0658339	5.8356963	37.4368235
H	26.5743867	10.1964298	44.8943253	O	35.2256898	5.5274214	41.5526279
H	27.5468383	8.9885649	46.8664218	O	34.5148655	3.4895222	42.1634008
H	29.9688469	8.2949624	46.7806294	C	35.4015476	4.2951965	41.7562116
H	31.3456030	8.7786197	44.8333133	C	32.7429788	4.5610823	38.1436994
H	31.3777136	6.7110672	42.7676371	C	33.4515327	3.4329945	37.7522794
H	30.0119541	10.5183970	41.8212862	C	33.6046339	3.1294622	36.3860443
H	24.4702186	4.1820355	40.0500162	C	33.0032978	3.9183890	35.4273716
H	40.8218475	4.2222540	39.5855413	C	32.2373446	5.0790705	35.7685889

C	32.1385721	5.4243613	37.1675999	H	36.6414833	2.4746439	43.2241935
C	31.3951936	6.5865672	37.5240596	H	39.0410690	1.7412918	43.0753585
C	30.7842895	7.3539022	36.5658533	H	40.5153778	2.6657255	41.3529357
C	30.8581301	7.0109155	35.1895305	H	36.0116584	5.3568930	39.4047926
C	31.5700538	5.8863276	34.7798853	H	37.4508204	6.1982105	37.6168675
O	30.1815515	7.8806449	34.3828040	H	33.8859078	2.7858834	38.5175196
O	32.5964466	5.9334556	40.1283554	H	34.1861660	2.2523317	36.0856904
O	32.4942209	3.7163688	40.3183197	H	33.1217347	3.6323320	34.3773965
C	32.5989330	4.7673271	39.6154541	H	31.3138772	6.8695729	38.5719994
C	28.4964940	5.4278113	42.1513185	H	30.2125478	8.2456771	36.8362278
C	27.9040951	6.3627084	42.9761130	H	28.5103915	7.0163754	43.6046983
C	28.3430209	3.6154201	40.4364301	H	29.4238993	3.4612142	40.4673274
O	30.4696968	6.4811623	41.4655770	H	34.1964573	7.7770621	45.7897361
O	30.6578991	4.4196517	42.3346397	H	30.6846322	4.6211481	44.7885302
C	29.9752760	5.4036450	42.0111680	H	28.7988089	3.6932674	46.0236597
C	32.5972195	6.3549451	45.7548432	H	30.2376788	7.6461620	33.4433635
C	33.3969294	7.3049300	46.3659954	H	39.5444775	6.4341053	36.8775964
C	31.5032269	5.7515184	46.4664067	H	33.8437896	8.3750753	48.2036729
C	30.5708028	4.8762810	45.8398672	H	32.0615314	7.3100216	49.5006982
C	29.5130385	4.3472886	46.5376824	H	27.8059018	3.4632367	47.9989795
O	33.3058246	6.8863736	43.5564348	C	32.2970275	9.2655642	41.0390206
O	32.7997596	4.7489207	44.0415735	C	31.8326956	9.5126680	42.5042650
C	32.9251963	5.9741180	44.3413172	C	32.7599517	10.5323134	43.1926239
C	33.1932506	7.6378013	47.7231864	C	32.8318324	11.8496814	42.4089335
C	32.1874180	7.0352230	48.4487890	C	33.2995135	11.6100373	40.9642531
C	31.2957246	6.0846016	47.8544413	C	32.4042896	10.5887172	40.2506562
C	29.3353548	4.6225275	47.9192137	O	33.5440411	8.6616147	41.0686601
C	30.2119564	5.4807282	48.5822419	C	29.5951154	9.5520010	43.6150519
O	28.3034468	4.0464323	48.5951790	C	28.2287479	9.9255698	43.5778031
H	26.0277866	7.2048521	43.6475140	C	27.3632430	9.5894358	44.6171499
H	24.6464651	5.8781666	42.1344832	C	27.8155018	8.8632807	45.7285501
H	28.0497210	2.1330367	38.9052417	C	29.1644707	8.4954336	45.7771189
H	24.6404475	2.3721747	38.4837159	C	30.0478274	8.8351832	44.7504869

O	30.5538192	4.5359143	42.2163655	H	30.6394455	4.2993163	44.8402801
C	29.8295355	5.5093686	42.4677817	H	28.6908400	3.5279118	46.0996695
C	32.6167783	5.9890475	45.7451050	H	30.9482186	8.1964608	33.5507751
C	33.4855588	6.8914840	46.3311457	H	39.4407431	6.6997131	37.1967414
C	31.4981567	5.4609309	46.4737801	H	34.0165157	7.9635091	48.1433337
C	30.5235487	4.6114224	45.8766899	H	32.1679823	7.0566389	49.4659329
C	29.4351915	4.1679338	46.5883057	H	27.6689631	3.4493994	48.0790904
O	33.0894460	6.5739194	43.5085344	C	31.8865686	8.8584768	41.3801041
O	32.7330001	4.4103756	43.9821569	C	33.0596831	9.5179262	42.1803806
C	32.8448168	5.6234596	44.3162038	C	34.2669240	9.8122555	41.2725712
C	33.3178310	7.2584887	47.6833869	C	33.9019288	10.6130677	40.0148218
C	32.2735666	6.7455232	48.4220303	C	32.7751045	9.9206736	39.2362177
C	31.3165386	5.8445072	47.8509733	C	31.5510505	9.6991820	40.1320338
C	29.2685946	4.5085301	47.9570567	O	32.1552373	7.5482632	40.9828968
C	30.1983140	5.3306233	48.5915377	C	31.8056571	10.6618309	44.0148566
O	28.2006665	4.0272596	48.6502992	C	31.1733664	11.8405730	44.4745660
H	25.7069821	7.2149104	43.6133315	C	30.3849478	11.8310319	45.6251016
H	24.4950147	5.8203628	42.0404301	C	30.1954166	10.6514231	46.3578505
H	28.1898776	2.1941035	39.0369350	C	30.8119543	9.4795046	45.9067666
H	24.7856756	2.2382477	38.5111633	C	31.6008278	9.4740829	44.7542406
H	36.5170352	2.1987723	43.1591962	N	32.6239801	10.7075531	42.8925368
H	38.9333003	1.5236114	42.9956719	H	35.0464975	10.3242484	41.8645541
H	40.4243373	2.6188442	41.3935139	H	33.3874245	8.7964025	42.9407946
H	35.9025877	5.4038355	39.6136362	H	31.0024385	8.8776498	42.0500861
H	37.3545428	6.4175383	37.9252355	H	34.7976933	10.7381125	39.3791946
H	32.8523124	2.0994351	38.2177369	H	33.5835870	11.6384692	40.2950796
H	32.6694515	1.5868082	35.7625840	H	32.4978012	10.5139839	38.3451529
H	32.1549273	3.3551108	34.1647541	H	33.1332052	8.9416504	38.8706711
H	31.9316865	6.8180241	38.5726702	H	31.1441169	10.6763781	40.4610970
H	31.2929817	8.5803474	36.9635376	H	30.7458992	9.1844871	39.5790922
H	28.1947887	7.0690562	43.7851600	H	34.6961183	8.8424664	40.9518577
H	29.4436847	3.5968215	40.6169599	H	31.3124657	12.7743374	43.9170308
H	34.3016570	7.3123112	45.7387594	H	29.9115466	12.7627437	45.9542008

H	29.5803286	10.6479718	47.2628719	O	34.3595365	3.4020787	42.0830452
H	30.6901696	8.5409646	46.4587900	C	35.1537742	4.3568233	41.8361288
H	32.0548210	8.5373217	44.4340139	C	32.1978227	3.8439753	38.0441597
H	31.2722040	6.7476870	42.7365717	C	32.4766369	2.5502887	37.6334444
H	32.5360761	11.5493156	42.3336637	C	32.4290670	2.2178439	36.2643566
H	24.4653310	4.0370365	40.1864455	C	32.0926019	3.1717866	35.3266297
H	40.8151366	4.4310572	39.5702493	C	31.7457702	4.5111896	35.6964146
H	31.6272335	5.8252734	33.6601585	C	31.7887462	4.8456235	37.0983349
H	30.0923779	5.5159222	49.6604196	C	31.3844883	6.1558208	37.4918707
				C	30.9919328	7.0824839	36.5609729
				C	30.9903845	6.7765172	35.1742317
(R,R)-2-PC				C	31.3642579	5.5108450	34.7324153
C	26.7911815	6.8741670	42.5383229	O	30.6021081	7.8277330	34.3899896
C	25.9526815	6.1351415	41.7283684	O	32.8465515	5.3073477	39.7821584
C	26.4315188	5.0435287	40.9315977	O	32.1429681	3.2471951	40.3367029
C	27.8348021	4.7300119	41.0214330	C	32.4010643	4.1589566	39.4923706
C	27.5410339	2.9663586	39.3780786	C	28.6727827	5.5193194	41.8699457
C	26.1524503	3.2566717	39.2878451	C	28.1695123	6.5789870	42.6011705
C	25.5859699	4.2722051	40.0555788	C	28.3580744	3.6733028	40.2214089
O	25.4943986	2.4398090	38.4112264	O	30.9211041	6.1745210	41.6396193
Cu	32.9321788	6.1273114	41.5851645	O	30.4963168	4.0888539	42.3589306
Cu	32.4202829	3.6658140	42.2525211	C	30.1367874	5.2370767	41.9610330
C	36.6078212	4.0130747	41.7410413	C	32.4227466	5.9831270	45.7911830
C	37.1285293	3.1709976	42.7068559	C	33.2933827	6.8771134	46.3871976
C	38.5079701	2.8705729	42.7143384	C	31.2919404	5.4663486	46.5053282
C	39.3425497	3.3938400	41.7503744	C	30.3066198	4.6480646	45.8814212
C	38.8481702	4.2389283	40.7036087	C	29.2159010	4.1992864	46.5849605
C	37.4397236	4.5457860	40.7016938	O	32.9342683	6.5112967	43.5492452
C	36.9182974	5.3330909	39.6349727	O	32.6156567	4.3506200	44.0953297
C	37.7412710	5.8093446	38.6423318	C	32.6783283	5.5826086	44.3717299
C	39.1386872	5.5512058	38.6608344	C	33.1153043	7.2392352	47.7406112
C	39.6955786	4.7715099	39.6727496	C	32.0668758	6.7214316	48.4712640
O	39.9353049	6.0633108	37.6813963	C	31.1099225	5.8285493	47.8877344
O	34.8306593	5.5712202	41.6873028				

C	29.0568914	4.5031622	47.9636315	O	32.9950757	8.1904272	40.8366363
C	29.9876388	5.3078935	48.6185037	C	29.5532356	9.5581123	43.9529426
O	27.9879633	4.0073637	48.6463224	C	28.2777520	10.1397033	44.1396116
H	26.3967142	7.7041354	43.1329807	C	27.6184028	10.0446460	45.3646455
H	24.8928757	6.4080036	41.6965633	C	28.2030518	9.3700331	46.4452126
H	27.9334322	2.1627320	38.7494116	C	29.4609604	8.7861872	46.2663659
H	24.5609080	2.6779036	38.3037128	C	30.1331455	8.8714266	45.0435990
H	36.4631212	2.7577108	43.4690682	N	30.1676702	9.6375807	42.7112704
H	38.9164222	2.2186049	43.4929344	H	32.3403054	10.5207135	44.0626540
H	40.4069364	3.1419055	41.7869608	H	31.7171451	8.3047993	42.9985341
H	35.8502341	5.5522484	39.5947876	H	30.9934088	8.2902536	40.6363696
H	37.3188594	6.4031142	37.8225233	H	33.2931312	12.3054493	42.5444414
H	32.7584132	1.8053892	38.3813042	H	31.5645076	12.0644988	42.2472038
H	32.6733165	1.2003423	35.9433571	H	32.7891259	12.1918745	40.0687501
H	32.0846605	2.8781671	34.2720626	H	33.8720440	10.8924416	40.5702467
H	31.3840891	6.4246277	38.5469007	H	30.8313006	10.6742545	40.0856805
H	30.6707254	8.0840762	36.8602711	H	32.0994330	9.9415674	39.0894615
H	28.8326800	7.1761599	43.2292774	H	33.5794798	9.8505628	42.9986836
H	29.4193000	3.4202404	40.2754449	H	27.8036437	10.6649007	43.3024324
H	34.1248961	7.2840595	45.8057123	H	26.6326719	10.5093596	45.4765929
H	30.4037099	4.3755213	44.8303026	H	27.6883346	9.3106271	47.4090649
H	28.4597623	3.5865115	46.0800073	H	29.9481616	8.2525868	47.0886304
H	30.5498593	7.5953620	33.4497334	H	31.1089245	8.3923127	44.9483203
H	39.4003336	6.5847431	37.0613266	H	33.7667981	8.6982181	41.1397016
H	33.8174242	7.9331232	48.2133173	H	29.7581774	10.3029175	42.0657830
H	31.9601525	7.0207674	49.5185779	H	24.5192698	4.4872174	39.9924365
H	27.4512004	3.4517896	48.0579358	H	40.7736755	4.6115927	39.6868898
C	31.7842087	8.9657301	40.9863749	H	31.3964674	5.2893155	33.6656662
C	31.5492972	9.2577039	42.4825294	H	29.8835475	5.4744170	49.6906517
C	32.5657507	10.2995550	43.0051291				
C	32.5561049	11.5794795	42.1567022	(S,S)-1-RC			
C	32.8345663	11.2704997	40.6764363	C	26.8892028	7.4717016	41.8392651
C	31.8450861	10.2303062	40.1248224	C	26.0228685	6.5741744	41.2486693

C	26.4772071	5.3383869	40.6844234	O	32.9741239	5.5065291	39.6674439
C	27.8840843	5.0430459	40.7865306	O	32.2561557	3.4447731	40.2162542
C	27.5271495	2.9855621	39.5410873	C	32.5700046	4.3407361	39.3800405
C	26.1335208	3.2508487	39.4615321	C	28.7504036	5.9819046	41.4356540
C	25.6002101	4.4073666	40.0241094	C	28.2681252	7.1850385	41.9223243
O	25.4389765	2.2762060	38.8026576	C	28.3756820	3.8464157	40.1871625
Cu	32.9935269	6.3132708	41.4978099	O	31.0248902	6.6053242	41.3230490
Cu	32.3679342	3.8678376	42.1534048	O	30.5167605	4.5492318	42.0817317
C	36.5313029	3.8924339	41.8999168	C	30.2043133	5.6890856	41.6219974
C	37.0668747	3.0907836	42.8889373	C	32.3590146	6.2000939	45.6846188
C	38.4592774	2.8596987	42.9315368	C	33.2232122	7.1080048	46.2696767
C	39.2895524	3.4062068	41.9769273	C	31.2899955	5.6083127	46.4379909
C	38.7809670	4.2132242	40.9071792	C	30.3123682	4.7635397	45.8382793
C	37.3612630	4.4575477	40.8745050	C	29.2908385	4.2266504	46.5839266
C	36.8308231	5.2308109	39.8016236	O	32.8421352	6.7490148	43.4308126
C	37.6548760	5.7581872	38.8352445	O	32.5260400	4.5863636	43.9765958
C	39.0598998	5.5445680	38.8728708	C	32.5877234	5.8208938	44.2547262
C	39.6257064	4.7718116	39.8863705	C	33.1053920	7.4072305	47.6456014
O	39.8535691	6.0878691	37.9080329	C	32.1191490	6.8201114	48.4096598
O	34.7643088	5.4317990	41.8215409	C	31.1655642	5.9131445	47.8416265
O	34.2508951	3.2774433	42.1728687	C	29.1878333	4.4809655	47.9775726
C	35.0736975	4.2144314	41.9656206	C	30.1063964	5.3183181	48.6090669
C	32.4918048	3.9987896	37.9252158	O	28.1793189	3.9119645	48.6951168
C	33.1600534	2.8701558	37.4870959	H	26.5045056	8.4116145	42.2478525
C	33.2013052	2.5758062	36.1068768	H	24.9598758	6.8327756	41.2065677
C	32.5646852	3.3933622	35.1954939	H	27.8994240	2.0740604	39.0663564
C	31.8241993	4.5514864	35.6008869	H	24.4922687	2.4730162	38.7275099
C	31.7854041	4.8447081	37.0106649	H	36.4067226	2.6699777	43.6515249
C	30.9984698	5.9442541	37.4580540	H	38.8817444	2.2516341	43.7372713
C	30.3036145	6.7189401	36.5662556	H	40.3643066	3.2129541	42.0453960
C	30.3682532	6.4661336	35.1693876	H	35.7570866	5.4148337	39.7391652
C	31.1233794	5.4049721	34.6747396	H	37.2250607	6.3475278	38.0157088
O	29.6461988	7.3612562	34.4321706	H	33.6686489	2.2289892	38.2122379

H	33.7460749	1.6929998	35.7573622	H	32.5692526	11.0506116	39.1480700
H	32.6232813	3.1284763	34.1350232	H	31.1441613	10.5997630	40.1048801
H	30.9355488	6.1710486	38.5230393	H	32.4991077	9.5511040	41.8394576
H	29.6800943	7.5509749	36.9036192	H	33.2773572	11.1028345	41.4756578
H	28.9603771	7.8926020	42.3863503	H	33.7375208	9.1887569	37.6416113
H	29.4395891	3.6111600	40.2332321	H	39.3536365	7.9940126	43.1994712
H	34.0128072	7.5661980	45.6702432	H	40.0402915	7.4713769	45.5238824
H	30.3606435	4.5438630	44.7712085	H	38.4000243	6.4816339	47.1387865
H	28.5424237	3.5880064	46.0995799	H	36.0587675	6.0184068	46.3642295
H	29.6218503	7.1396927	33.4886053	H	35.3899318	6.5140578	44.0227728
H	39.3080465	6.5615184	37.2594765	H	37.6753747	7.5284510	41.4462225
H	33.8122530	8.1041390	48.1067265	H	36.0950158	7.0860985	41.8249855
H	32.0632022	7.0667031	49.4746192	H	24.5307217	4.6076749	39.9597851
H	27.6403143	3.3507590	48.1144117	H	40.7030995	4.6066878	39.8814126
C	34.3295412	9.3631188	40.7752518	H	31.1853330	5.2205756	33.6022536
C	34.5066728	8.5808033	39.5271434	H	30.0077764	5.4888274	49.6811056
C	33.4279804	8.5220266	38.4704150				
C	32.0545594	8.9507962	39.0096501	(S,S)-1-TS1			
C	32.1502914	10.2597069	39.8023780	C	26.5351180	7.0539030	42.4035600
C	33.0374851	10.1118917	41.0515373	C	25.7709540	6.1132140	41.7453290
O	34.2141952	7.9282418	40.7692984	C	26.3518720	4.9620490	41.1206130
C	37.3268281	7.2727062	43.4406111	C	27.7800950	4.7956690	41.2353810
C	38.6358204	7.5411922	43.8910863	C	27.6253080	2.7511440	39.9265180
C	39.0148987	7.2548835	45.2041992	C	26.2184450	2.9084500	39.8021730
C	38.1005985	6.7031902	46.1096170	C	25.5760990	3.9966640	40.3843770
C	36.7939951	6.4457625	45.6735617	O	25.6252260	1.9105740	39.0822140
C	36.4076642	6.7225537	44.3608205	Cu	32.5509130	7.2609340	41.6643020
N	36.9331921	7.5777835	42.1400363	Cu	32.5229670	4.3408400	42.2460910
H	33.3790025	7.4947662	38.0699672	C	36.5423870	3.6327070	41.7664510
H	35.5336626	8.3809623	39.1859027	C	37.0417010	2.7632190	42.7161680
H	35.2319359	9.6809154	41.3146318	C	38.4153170	2.4250830	42.7133700
H	31.6422833	8.1589088	39.6578646	C	39.2708250	2.9651500	41.7774540
H	31.3554277	9.0590191	38.1631368	C	38.7973540	3.8425810	40.7472830

C	37.3891800	4.1399730	40.7250590	C	29.4323190	4.4242160	46.5504700
C	36.8799770	4.9323670	39.6562470	O	32.7943300	7.2863610	43.6368300
C	37.7165110	5.4582970	38.7001680	O	32.7562970	5.0663260	44.0552520
C	39.1193340	5.2340710	38.7585720	C	32.6870960	6.2795660	44.3966600
C	39.6613930	4.4268910	39.7591420	C	33.1111650	7.6612470	47.8966740
O	39.9342480	5.8028070	37.8273590	C	32.1072960	7.0226360	48.5935570
O	34.9887240	5.4097120	41.8232210	C	31.1978860	6.1211190	47.9490560
O	34.2187320	3.3584950	42.2276140	C	29.2562770	4.6312030	47.9446400
C	35.1490970	4.1733870	41.9358000	C	30.1235050	5.4678200	48.6444530
C	32.7143320	4.9623860	38.0443440	O	28.2335180	4.0105440	48.5965540
C	33.4589700	3.8475080	37.6954910	H	26.0533000	7.9218290	42.8647260
C	33.5900720	3.4844350	36.3396130	H	24.6888040	6.2722990	41.7018730
C	32.9412250	4.2058900	35.3588630	H	28.0832830	1.8846560	39.4420280
C	32.1323070	5.3483180	35.6649770	H	24.6695930	2.0408880	38.9805450
C	32.0388880	5.7417520	37.0494310	H	36.3717060	2.3764450	43.4887120
C	31.2298550	6.8673690	37.3833020	H	38.8069320	1.7490120	43.4799460
C	30.5591830	7.5639950	36.4120440	H	40.3338900	2.7096380	41.8249090
C	30.6450170	7.1863970	35.0453630	H	35.8080430	5.1224210	39.5861930
C	31.4174690	6.0936840	34.6607430	H	37.2992510	6.0563490	37.8810420
O	29.9187420	7.9977540	34.2197000	H	33.9365570	3.2578170	38.4822380
O	32.7663540	6.4944400	39.8533300	H	34.1968130	2.6154070	36.0657750
O	32.4436660	4.2999500	40.2749820	H	33.0511690	3.8771200	34.3205650
C	32.6242420	5.2847720	39.5051800	H	31.1420590	7.1766100	38.4245640
C	28.5453860	5.7996420	41.9146250	H	29.9322020	8.4240900	36.6620420
C	27.9354260	6.9131040	42.4687260	H	28.5504240	7.6737850	42.9558500
C	28.3842660	3.6640520	40.6126120	H	29.4639060	3.5255600	40.6757130
O	30.6606410	6.8006200	41.7669360	H	34.0713220	7.9469890	45.9562930
O	30.5817030	4.6373980	42.3398060	H	30.5790950	4.8194780	44.8059260
C	30.0361590	5.7296730	42.0101930	H	28.7337640	3.7736460	46.0107120
C	32.4554900	6.5435510	45.8539710	H	29.9514270	7.7175440	33.2920710
C	33.2807600	7.4351030	46.5120930	H	39.4034860	6.2932920	37.1786970
C	31.3856500	5.8799020	46.5414440	H	33.7814390	8.3508260	48.4196880
C	30.4684510	5.0184090	45.8719030	H	32.0031500	7.2238810	49.6644090

H	27.7379790	3.4552240	47.9726930	H	40.7408887	4.2787234	39.7874598
C	35.4501540	8.3604300	42.1719310	H	31.4672203	5.7932192	33.6141714
C	35.0595710	8.3002370	40.7554650	H	29.9914841	5.5875478	49.7197679
C	35.6600530	9.3364530	39.8171470				
C	35.8393940	10.7024140	40.4935750	(S,S)-1-Int1			
C	36.6276570	10.5635950	41.8046540	C	26.4178722	7.0579246	42.5101417
C	35.9097300	9.6395590	42.7988980	C	25.6914319	6.1360490	41.7857489
O	33.8170370	8.6863760	41.3129520	C	26.3178123	5.0533342	41.0867167
C	37.8968300	7.0669700	43.4363330	C	27.7520905	4.9376420	41.1970147
C	38.9927950	7.8742510	43.7863640	C	27.6843493	2.9812126	39.7540359
C	39.5094640	7.8370310	45.0838100	C	26.2737159	3.0965785	39.6229940
C	38.9307110	7.0111630	46.0542810	C	25.5826986	4.1115058	40.2785853
C	37.8236330	6.2244590	45.7115930	O	25.7276033	2.1335909	38.8218024
C	37.3048810	6.2470320	44.4153910	Cu	32.4096055	7.5423492	41.5471815
N	37.3309830	7.1439220	42.1557530	Cu	32.5103944	4.4760183	42.2545684
H	35.0076530	9.4096800	38.9288030	C	36.5008556	3.5718086	41.8742375
H	35.0386690	7.2961810	40.3084660	C	37.0031441	2.6968766	42.8171279
H	35.1008140	7.5526080	42.8113910	C	38.3831827	2.3865503	42.8297901
H	34.8429880	11.1304150	40.7075230	C	39.2408592	2.9532936	41.9114431
H	36.3536730	11.3993170	39.8078620	C	38.7658571	3.8329117	40.8833044
H	37.6307790	10.1462340	41.5841260	C	37.3535772	4.1157994	40.8534143
H	36.7937660	11.5513500	42.2698040	C	36.8478898	4.9159108	39.7874100
H	35.0114230	10.1333930	43.2118590	C	37.6881453	5.4606845	38.8446670
H	36.5518780	9.3958620	43.6640130	C	39.0907632	5.2383431	38.9031355
H	36.6401520	8.9511050	39.4704560	C	39.6304718	4.4240873	39.8996299
H	39.4334410	8.5345850	43.0310780	O	39.9063579	5.8123875	37.9782714
H	40.3701590	8.4642800	45.3389080	O	34.9064621	5.3148984	41.8738498
H	39.3366800	6.9845090	47.0700430	O	34.1606909	3.2889682	42.3374184
H	37.3562830	5.5781050	46.4614280	C	35.0931867	4.0704086	42.0268930
H	36.4436310	5.6283850	44.1478240	C	32.6843146	4.8562343	38.0765613
H	37.9675250	7.4098730	41.4065890	C	33.4620082	3.7620948	37.7346781
H	36.7374470	6.3471000	41.8937370	C	33.6033215	3.3911190	36.3811642
H	24.5051370	4.1512104	40.2531432	C	32.9318935	4.0823226	35.3938218

C	32.0869802	5.2004087	35.6916901	H	24.7739003	2.2523823	38.6933002
C	31.9832297	5.6021453	37.0735680	H	36.3287081	2.2849481	43.5725655
C	31.1393160	6.7041672	37.3993926	H	38.7769687	1.7066964	43.5918793
C	30.4382993	7.3648772	36.4249360	H	40.3073123	2.7139733	41.9689865
C	30.5314078	6.9768277	35.0619389	H	35.7755571	5.0964867	39.7023437
C	31.3464453	5.9132626	34.6820637	H	37.2696786	6.0621269	38.0291236
O	29.7674797	7.7513118	34.2336770	H	33.9571683	3.1921681	38.5251679
O	32.6941357	6.4134777	39.8701643	H	34.2374852	2.5393077	36.1144586
O	32.4515634	4.2185618	40.3215870	H	33.0503834	3.7482404	34.3579558
C	32.5920518	5.2057734	39.5350984	H	31.0493536	7.0236127	38.4371233
C	28.4783675	5.9286233	41.9347154	H	29.7819269	8.2041580	36.6695547
C	27.8234897	6.9738522	42.5637673	H	28.4075622	7.7300784	43.0941624
C	28.4034380	3.8718173	40.5089531	H	29.4871669	3.7666626	40.5768443
O	30.5360304	7.0352998	41.7467554	H	34.0790477	8.0964374	45.8935640
O	30.5753038	4.8644965	42.3127089	H	30.5496622	5.0012543	44.7901128
C	29.9765871	5.9351838	41.9971893	H	28.7061423	3.9747516	46.0179690
C	32.4520635	6.7035993	45.8127344	H	29.7924270	7.4550787	33.3109502
C	33.2918839	7.5900440	46.4596335	H	39.3789138	6.3159161	37.3366388
C	31.3856996	6.0526300	46.5168354	H	33.8216426	8.5086440	48.3588908
C	30.4530529	5.1999649	45.8578810	H	32.0528516	7.3946007	49.6305060
C	29.4189148	4.6169154	46.5489900	H	27.7284346	3.6705226	47.9893674
O	32.7765052	7.3954428	43.5684535	C	35.6431230	8.2212798	42.2967872
O	32.7673341	5.1894672	44.0529640	C	34.9623143	8.2844464	40.8999742
C	32.6763085	6.4178393	44.3545446	C	35.7908210	9.0992644	39.8853752
C	33.1408303	7.8212828	47.8463307	C	36.2178222	10.4683498	40.4215677
C	32.1423279	7.1909350	48.5586335	C	37.0015625	10.3123062	41.7328829
C	31.2178384	6.2957754	47.9269344	C	36.1575092	9.5731453	42.7804421
C	29.2624482	4.8251495	47.9454824	O	33.7017145	8.8097283	41.0787796
C	30.1474170	5.6512319	48.6363554	C	37.3414984	6.8284821	43.5503808
O	28.2412305	4.2147559	48.6090320	C	38.6575426	7.2269125	43.7848531
H	25.9012184	7.8717144	43.0289998	C	39.2542214	6.9346628	45.0153779
H	24.6045223	6.2591006	41.7472161	C	38.5273283	6.2617006	46.0028598
H	28.1780194	2.1681329	39.2152649	C	37.2024001	5.8790698	45.7589326

C	36.6009321	6.1565787	44.5288483	Cu	32.6689823	6.9425462	41.4465686
N	36.6989845	7.1223977	42.2750952	Cu	32.4268891	3.7768152	42.3255305
H	35.1780337	9.1945061	38.9726891	C	36.6488736	3.4796579	41.8212559
H	34.9039623	7.2535714	40.4962573	C	37.1722155	2.3892566	42.4912969
H	34.8871502	7.8370823	42.9937301	C	38.5374626	2.0620889	42.3335376
H	35.3135332	11.0758758	40.6080958	C	39.3484368	2.8205938	41.5165578
H	36.8240654	11.0059843	39.6695666	C	38.8359681	3.9169522	40.7466471
H	37.9446389	9.7571067	41.5375061	C	37.4389773	4.2307456	40.8884155
H	37.3066618	11.2975625	42.1288604	C	36.8815027	5.2502579	40.0662931
H	35.2500073	10.1659372	42.9912358	C	37.6661201	5.9414936	39.1743349
H	36.6984066	9.4646394	43.7381469	C	39.0593458	5.6829400	39.0703917
H	36.6938027	8.5137346	39.6045454	C	39.6502904	4.6890916	39.8499017
H	39.2111735	7.7712159	43.0136957	O	39.8197770	6.4077209	38.2051292
H	40.2890518	7.2379970	45.2013462	O	35.2271785	5.2205052	42.4231201
H	38.9939337	6.0368324	46.9668838	O	34.3465661	3.1562524	42.3991111
H	36.6270780	5.3561158	46.5284758	C	35.2958949	3.9408597	42.2216457
H	35.5708320	5.8482988	44.3280930	C	32.8744226	4.1577862	38.1958917
H	37.3967441	7.2951520	41.5430821	C	33.3303055	2.9132772	37.7901146
H	36.0955749	6.2575264	41.9842378	C	33.4062406	2.5997479	36.4180533
H	24.5081895	4.2366842	40.1450673	C	32.9756279	3.5060280	35.4716644
H	40.7089313	4.2671270	39.9184677	C	32.4451751	4.7856129	35.8334809
H	31.4077396	5.6136038	33.6358734	C	32.4259077	5.1257729	37.2355180
H	30.0267551	5.7705100	49.7130541	C	31.9070358	6.3987736	37.6125079
				C	31.4358732	7.2777416	36.6716550
(S,S)-1-Int3				C	31.4416315	6.9471751	35.2902117
C	26.6610525	6.9078490	42.3215065	C	31.9363633	5.7183871	34.8623079
C	25.8535582	6.0221594	41.6389393	O	30.9265339	7.9346460	34.4981646
C	26.3823703	4.8696693	40.9720080	O	33.2333755	5.5426870	40.1109321
C	27.8034615	4.6408665	41.0710146	O	32.4565592	3.4619034	40.4020597
C	27.5569350	2.6584059	39.6822765	C	32.8447165	4.4238409	39.6693047
C	26.1562680	2.8734089	39.5798717	C	28.6144012	5.5836593	41.7858047
C	25.5615130	3.9616001	40.2113361	C	28.0544068	6.7035198	42.3778949
O	25.5199752	1.9251993	38.8295676	C	28.3562959	3.5106357	40.3994886

O	30.8041390	6.4545538	41.7425500	H	33.7603995	7.5136264	45.7326270
O	30.5386247	4.2715155	42.2084806	H	30.2326950	4.3211515	44.8788280
C	30.0988657	5.4234286	41.9099377	H	28.3701534	3.4286957	46.1907242
C	32.1793451	6.0674682	45.7686290	H	30.9194655	7.6991591	33.5572145
C	32.9467432	7.0831307	46.3178494	H	39.2655148	7.0594538	37.7456673
C	31.0686339	5.5193549	46.5015451	H	33.3360888	8.3187976	48.0606932
C	30.1337236	4.6124713	45.9241893	H	31.5844429	7.2878380	49.4290042
C	29.0896497	4.1083456	46.6629352	H	27.4353604	3.2445855	48.2057564
O	33.2636876	6.2592458	43.6479593	C	35.3812190	8.9402013	43.0668589
O	32.3831258	4.2921759	44.2108317	C	35.1987112	8.3622390	41.6152661
C	32.6197075	5.5133816	44.4539305	C	35.9695862	9.2060293	40.5861378
C	32.7114979	7.5270792	47.6359520	C	35.5163983	10.6725279	40.6280386
C	31.7218197	6.9455160	48.3983468	C	35.6633469	11.2663143	42.0383648
C	30.8600396	5.9310565	47.8675157	C	34.9346113	10.4104573	43.0890395
C	28.9367788	4.4326240	48.0375453	O	33.8515740	8.3241325	41.3019463
C	29.8090953	5.3337945	48.6443354	C	37.3069857	7.6003788	43.9780531
O	27.9331847	3.8656015	48.7619266	C	38.6883498	7.3625963	43.7955690
H	26.2189118	7.7797443	42.8139563	C	39.2801058	6.1779533	44.2354442
H	24.7784537	6.2262043	41.6094970	C	38.5154001	5.1893811	44.8656252
H	27.9764695	1.7953775	39.1585443	C	37.1502123	5.4214018	45.0628193
H	24.5690147	2.0933860	38.7407078	C	36.5519047	6.6052774	44.6333181
H	36.5389627	1.8270580	43.1825360	N	36.7440581	8.8007383	43.5536212
H	38.9594665	1.2168347	42.8857898	H	35.7966538	8.7717016	39.5847746
H	40.4085985	2.5580883	41.4468584	H	35.6182568	7.3379577	41.6396962
H	35.8153612	5.4794788	40.1151296	H	34.7086960	8.3548790	43.7097109
H	37.2145933	6.7158851	38.5432832	H	34.4526768	10.7112565	40.3304773
H	33.6382905	2.1859368	38.5451532	H	36.0829076	11.2766035	39.8954434
H	33.7989105	1.6278339	36.1027843	H	36.7393381	11.3517155	42.2961958
H	33.0415230	3.2224607	34.4161498	H	35.2698960	12.2991770	42.0631820
H	31.8782255	6.6784796	38.6645580	H	33.8521020	10.4228184	42.8700971
H	31.0309381	8.2516249	36.9591052	H	35.0802649	10.8237477	44.1035927
H	28.7022154	7.4167541	42.8936176	H	37.0567799	9.1299865	40.7864161
H	29.4289368	3.3220620	40.4501142	H	39.2954477	8.1210591	43.2878279

H	40.3505060	6.0177437	44.0721829	O	34.9046836	5.5684278	40.0726549
H	38.9751549	4.2516593	45.1904769	O	34.2399618	4.4148709	41.8740422
H	36.5294255	4.6633631	45.5535502	C	35.1123477	4.7076435	41.0343893
H	35.4828863	6.7454107	44.7849255	C	31.7907511	4.7790419	38.0552739
H	37.4089476	9.4223238	43.1054792	C	31.8676909	3.4311793	37.7214623
H	34.3732022	5.5672648	42.8920594	C	31.8154373	3.0239274	36.3768412
H	24.4934655	4.1513909	40.1049382	C	31.6765775	3.9611564	35.3749949
H	40.7315291	4.5561798	39.8135160	C	31.5530599	5.3599845	35.6518387
H	31.9132491	5.4569590	33.8043913	C	31.6076531	5.7763693	37.0341336
H	29.7329490	5.5033115	49.7183616	C	31.4501294	7.1631614	37.3238069
				C	31.2532899	8.0750954	36.3183658
(S,S)-1-Int3-2				C	31.2201189	7.6772585	34.9554851
C	26.0457990	7.0538801	42.2920286	C	31.3822725	6.3383847	34.6096864
C	25.4018276	6.0160968	41.6517091	O	31.0314344	8.7194857	34.0931381
C	26.1158987	4.9176346	41.0689858	O	32.4421201	6.2418241	39.8660203
C	27.5498731	4.9133646	41.2142300	O	31.8296839	4.1735723	40.3438026
C	27.6544209	2.8315442	39.9625522	C	31.9951152	5.0987482	39.4937565
C	26.2432347	2.8368836	39.7901387	C	28.1868443	6.0248270	41.8533092
C	25.4704111	3.8563706	40.3359165	C	27.4521431	7.0795648	42.3664667
O	25.7817774	1.7719173	39.0704892	C	28.2906977	3.8352216	40.6468426
Cu	31.9691762	7.8625176	41.3840851	O	30.1394382	7.2253230	41.4030918
Cu	32.3001427	4.9353908	42.1089266	O	30.3630087	5.2148160	42.3845549
C	36.4748286	4.1287232	41.1035250	C	29.6751553	6.1585504	41.8840558
C	36.8246658	3.5630895	42.3212072	C	32.1425868	7.0992716	45.6558520
C	38.1375140	3.1115128	42.5537067	C	32.8331111	8.1292232	46.2661884
C	39.1015230	3.2558646	41.5812642	C	31.2725421	6.2451347	46.4118889
C	38.8044968	3.8181822	40.2978695	C	30.4813651	5.2358287	45.7941522
C	37.4422784	4.2177194	40.0343726	C	29.6174852	4.4649506	46.5345901
C	37.1298971	4.6581461	38.7169366	O	32.1000649	7.8435646	43.4048581
C	38.0999405	4.7700209	37.7495358	O	32.6987322	5.7189180	43.8307510
C	39.4568576	4.4768313	38.0334417	C	32.3178809	6.8813505	44.1820005
C	39.8153403	3.9893814	39.2904212	C	32.7350830	8.3100131	47.6650171
O	40.4055818	4.6607828	37.0749141	C	31.9258354	7.4926412	48.4253588

C	31.1452702	6.4461115	47.8336818	C	34.9904189	9.2951013	43.2077197
C	29.4934898	4.6447726	47.9380255	O	33.2684134	9.0165970	40.8242087
C	30.2463534	5.6199830	48.5918141	C	37.0986167	6.9711016	43.0351321
O	28.6264389	3.8672529	48.6445109	C	38.5082243	6.8697644	43.0382062
H	25.4621410	7.8748541	42.7204543	C	39.1781232	6.1558512	44.0289987
H	24.3104647	6.0619379	41.5871997	C	38.4671101	5.5324920	45.0628246
H	28.2166971	2.0086919	39.5131772	C	37.0715890	5.6333531	45.0727342
H	24.8244115	1.8125513	38.9207621	C	36.3865864	6.3347109	44.0775011
H	36.0791079	3.5174036	43.1154147	N	36.4630383	7.6520680	42.0091610
H	38.3978505	2.6870467	43.5264682	H	34.9399552	10.4136933	39.4242890
H	40.1227014	2.9311031	41.8036205	H	34.8539320	7.9815669	39.9849133
H	36.1051621	4.9065581	38.4565781	H	34.4482060	7.3647830	42.3854269
H	37.8242634	5.1078961	36.7432353	H	34.2021741	11.4111371	41.5639808
H	31.9965626	2.6962000	38.5180742	H	35.8326805	12.0148257	41.1827371
H	31.8957850	1.9618357	36.1256382	H	36.8363400	10.3492768	42.7632642
H	31.6543973	3.6042060	34.3406361	H	35.6305685	11.3331784	43.6106274
H	31.4907602	7.5050774	38.3558167	H	33.9181525	9.5206313	43.3260464
H	31.1215363	9.1376584	36.5391528	H	35.3569860	8.9020705	44.1722949
H	27.9713110	7.9295621	42.8169328	H	36.4338334	9.8155462	40.1682584
H	29.3767822	3.8086573	40.7477023	H	39.0730199	7.3695215	42.2440319
H	33.4683007	8.7841022	45.6653065	H	40.2708864	6.0901980	43.9923944
H	30.5375220	5.0770121	44.7169695	H	38.9927246	4.9809744	45.8481816
H	29.0070286	3.7031034	46.0353389	H	36.4920470	5.1506744	45.8671970
H	30.9641182	8.4363593	33.1677459	H	35.2955971	6.3579930	44.0995072
H	40.0009608	5.0315543	36.2740947	H	37.0854626	8.1489991	41.3820749
H	33.3078048	9.1080190	48.1477556	H	33.9612015	5.9419056	40.0563998
H	31.8747423	7.6615453	49.5056031	H	24.3929000	3.9023323	40.1780436
H	28.1724210	3.2540405	48.0438316	H	40.8732301	3.8149586	39.4866667
C	35.1199879	8.2013728	42.1286745	H	31.4126462	6.0401633	33.5617323
C	34.6270346	8.7473484	40.7540980	H	30.1178180	5.7474480	49.6666619
C	35.3685744	10.0472294	40.3735121				
C	35.2613419	11.1126458	41.4707193				
C	35.7514133	10.5693019	42.8208146				
				(S,S)-1-TS3			
				C	27.0500771	7.6142467	41.4221955

C	26.1497503	6.6484435	41.0245033	O	30.4709335	7.7038164	34.5875204
C	26.5656926	5.3303198	40.6518062	O	33.6421820	5.9975150	40.0665510
C	27.9741585	5.0263705	40.7427069	O	32.9742190	3.8765050	40.3789030
C	27.5123006	2.7883326	39.9032627	C	33.3465590	4.8420050	39.6488520
C	26.1221604	3.0709977	39.8337411	C	28.8845214	6.0448654	41.1905385
C	25.6386715	4.3243790	40.1991248	C	28.4253573	7.3178787	41.4948520
O	25.3809169	2.0141612	39.3825918	C	28.4084124	3.7290409	40.3415373
Cu	33.0159430	6.8557910	41.7684560	O	31.1325370	6.7783650	41.2452450
Cu	32.5541730	4.1415050	42.2547120	O	30.7029780	4.6471410	41.8064650
C	36.8267728	4.0699694	43.2507190	C	30.3457310	5.7994140	41.4148920
C	37.5257930	3.6480354	44.3640168	C	31.6627751	5.6723996	45.9449078
C	38.8773049	3.2576698	44.2282862	C	32.3101635	6.7335064	46.5582377
C	39.5194561	3.3607469	43.0132511	C	30.6918691	4.8931890	46.6623456
C	38.8498612	3.8451011	41.8424157	C	29.9234444	3.8618612	46.0498894
C	37.4537514	4.1703134	41.9654940	C	29.0062226	3.1370750	46.7738398
C	36.7627808	4.6540341	40.8192932	O	32.5278130	6.3160870	43.8333000
C	37.4049023	4.8012514	39.6151393	O	32.0552210	4.1652840	44.1358260
C	38.7881517	4.5021738	39.4861683	C	32.0819990	5.3705690	44.5432370
C	39.5134095	4.0361466	40.5827146	C	32.0639260	7.0330286	47.9134455
O	39.4077946	4.6844657	38.2891299	C	31.1742346	6.2741846	48.6417996
O	35.2313480	5.5115570	44.2057780	C	30.4535935	5.1830131	48.0542574
O	34.5287690	3.9948270	42.6876800	C	28.8122678	3.3727654	48.1616687
C	35.4123470	4.5147780	43.3745380	C	29.5195525	4.3864275	48.8024671
C	33.4412722	4.5635865	38.1812928	O	27.9295214	2.6100936	48.8652232
C	34.1745810	3.4641828	37.7703117	H	26.6951113	8.6142590	41.6905547
C	34.2591692	3.1544340	36.3961982	H	25.0884466	6.9147705	40.9933230
C	33.5713274	3.9067356	35.4657402	H	27.8437367	1.7954183	39.5873537
C	32.7657001	5.0298002	35.8420141	H	24.4336590	2.2143552	39.3252753
C	32.7291050	5.3769619	37.2415803	H	37.0322846	3.6102503	45.3391030
C	31.9314215	6.4857786	37.6509979	H	39.4232469	2.8900615	45.1025315
C	31.2176531	7.2106521	36.7325650	H	40.5734216	3.0731757	42.9532074
C	31.2415253	6.8748640	35.3517848	H	35.7136464	4.9360892	40.8862186
C	31.9969243	5.7967195	34.8963724	H	36.8458372	5.1752880	38.7493867

H	34.6824535	2.8452788	38.5150057	H	35.0438389	10.0834882	39.5463559
H	34.8591296	2.2993431	36.0685017	H	36.4814385	11.1075703	41.2890467
H	33.6455672	3.6191610	34.4121192	H	34.8184721	11.6585509	41.5255426
H	31.8766420	6.7607087	38.7054979	H	34.4447237	9.9692139	43.3107524
H	30.5973297	8.0572403	37.0386943	H	35.8464091	10.9843948	43.7278003
H	29.1413028	8.0776534	41.8154580	H	36.8863042	8.6186083	40.4432548
H	29.4684261	3.4833570	40.3801719	H	40.1152665	10.2330747	43.5737665
H	33.0268072	7.3203269	45.9795962	H	41.9060399	9.1655567	44.9048161
H	30.0603216	3.6497510	44.9900824	H	41.5662993	6.8864068	45.8953725
H	28.4201066	2.3534210	46.2786023	H	39.3822838	5.7159937	45.5170020
H	30.4789459	7.4673489	33.6470249	H	37.5994834	6.7576143	44.1993283
H	38.7803312	5.0537533	37.6460039	H	37.9731096	10.1356118	42.6950744
H	32.5898103	7.8656492	48.3904868	H	34.4268520	6.0636090	43.9638350
H	31.0153159	6.5282294	49.6943536	H	24.5741737	4.5457375	40.1222398
H	27.5407875	1.9361512	48.2840752	H	40.5916898	3.9058135	40.4911095
C	36.3130028	8.9363017	43.1664676	H	31.9717673	5.5133661	33.8441631
C	35.7995740	7.8654640	42.1431020	H	29.4122117	4.5247726	49.8782947
C	35.8315753	8.4152007	40.7086813				
C	34.9971960	9.6961118	40.5802820		(S,S)-1-PC		
C	35.4669199	10.7648335	41.5783697	C	27.0179093	7.6003048	41.6907634
C	35.4779055	10.2205511	43.0174441	C	26.1217925	6.6758930	41.1943980
O	34.5273500	7.5205700	42.5740630	C	26.5386955	5.3851366	40.7346883
C	38.7178490	8.5834844	43.7784532	C	27.9398370	5.0644036	40.8426594
C	39.9558909	9.2332028	43.9947235	C	27.5090806	2.9112252	39.7971092
C	40.9621728	8.6310995	44.7498114	C	26.1214505	3.2052383	39.7124834
C	40.7739837	7.3606907	45.3082283	C	25.6269847	4.4216346	40.1755299
C	39.5531633	6.7121790	45.0982459	O	25.3917408	2.1957793	39.1493654
C	38.5331843	7.3035117	44.3485193	Cu	33.0829104	6.2774051	41.4850027
N	37.7321817	9.2099704	43.0308414	Cu	32.4070034	3.8758760	42.1962857
H	35.4562624	7.6365810	40.0232230	C	36.5850700	3.8686409	41.9058098
H	36.4859889	6.9957277	42.2051488	C	37.1235876	3.1053521	42.9226202
H	36.1298495	8.5145168	44.1705096	C	38.5156878	2.8726243	42.9669847
H	33.9349426	9.4553102	40.7782913	C	39.3413556	3.3792899	41.9874348

C	38.8262310	4.1354863	40.8839512	C	30.2938668	4.9389439	45.8423327
C	37.4076630	4.3778447	40.8478065	C	29.2245674	4.4867627	46.5770520
C	36.8655038	5.0776692	39.7323833	O	32.8988283	6.7288804	43.4383042
C	37.6792115	5.5415886	38.7254832	O	32.5708713	4.5802079	44.0281640
C	39.0852552	5.3423710	38.7714054	C	32.6464309	5.8179168	44.2809872
C	39.6605846	4.6401552	39.8289955	C	33.2391941	7.3988444	47.6657397
O	39.8720751	5.8298869	37.7703168	C	32.2027120	6.8927975	48.4209457
O	34.8573734	5.4507816	41.8335827	C	31.1962366	6.0481424	47.8483628
O	34.2957805	3.3057979	42.1944605	C	29.1211275	4.7611575	47.9673661
C	35.1364727	4.2246910	41.9771701	C	30.0891881	5.5347443	48.6063895
C	32.4807001	3.9403653	37.9765687	O	28.0660943	4.2705663	48.6751147
C	32.9464897	2.7109733	37.5443582	H	26.6613904	8.5810088	42.0212384
C	32.9363727	2.4049281	36.1666716	H	25.0643775	6.9556825	41.1459738
C	32.4441447	3.3132549	35.2517716	H	27.8498456	1.9504314	39.4024363
C	31.9049134	4.5788775	35.6522862	H	24.4496884	2.4116260	39.0671272
C	31.9224739	4.8892319	37.0582726	H	36.4703425	2.7240240	43.7109582
C	31.3396414	6.1158529	37.4940899	H	38.9422966	2.3013373	43.7967450
C	30.7921417	6.9916476	36.5926145	H	40.4168176	3.1908784	42.0607162
C	30.8033869	6.7133313	35.1994475	H	35.7882914	5.2381979	39.6584550
C	31.3523458	5.5273198	34.7209615	H	37.2401948	6.0707205	37.8709549
O	30.2440812	7.7078233	34.4464646	H	33.3420198	1.9991858	38.2738894
O	33.1220324	5.4051286	39.7018201	H	33.3266607	1.4424211	35.8209731
O	32.2455872	3.4133214	40.2755830	H	32.4615429	3.0401785	34.1914622
C	32.6188618	4.2761927	39.4258329	H	31.3168870	6.3637101	38.5561283
C	28.8391009	6.0361443	41.3934405	H	30.3316457	7.9271188	36.9209457
C	28.3906208	7.2882972	41.7784009	H	29.1064975	8.0162896	42.1685796
C	28.3905980	3.8050652	40.3477840	H	29.4492842	3.5483157	40.3966231
O	31.1288217	6.6079591	41.2497411	H	34.1869602	7.4670029	45.7052594
O	30.5749466	4.6117106	42.1283146	H	30.3444760	4.7012643	44.7785090
C	30.2880113	5.7284169	41.5971758	H	28.4392760	3.8977173	46.0882331
C	32.4355417	6.2261123	45.7065681	H	30.2142786	7.4910914	33.5015901
C	33.3551957	7.0746034	46.2952795	H	39.3185610	6.2581557	37.0973744
C	31.3180859	5.7206940	46.4500655	H	33.9852559	8.0505708	48.1310106

H	32.1480059	7.1567116	49.4818450	H	24.5621073	4.6438441	40.1067876
H	27.5030248	3.7331372	48.0946018	H	40.7396047	4.4862005	39.8379513
C	35.7090876	8.2691424	42.6218601	H	31.3807549	5.3237223	33.6505375
C	35.3485130	8.3384886	41.1230262	H	30.0044047	5.7007357	49.6803192
C	35.8815373	9.5964677	40.4345791				
C	35.4953034	10.8818743	41.1841901		(S,S)-2-RC		
C	35.9242146	10.8163654	42.6590148	C	26.9386991	7.1243402	41.7121512
C	35.3339548	9.5787657	43.3504392	C	26.0457856	6.1838240	41.2389237
O	33.9151667	8.2324678	40.9582965	C	26.4736861	4.9023961	40.7600382
C	37.5522460	7.0585008	43.8109143	C	27.8824488	4.6028432	40.8392044
C	38.9345253	7.0067931	44.1001116	C	27.4549550	2.4362775	39.8202015
C	39.4345749	6.1631765	45.0904577	C	26.0638430	2.7176115	39.7467726
C	38.5742100	5.3514010	45.8402784	C	25.5668261	3.9346067	40.2036500
C	37.2036001	5.4010138	45.5676325	O	25.3358099	1.7002095	39.2044510
C	36.6933492	6.2327573	44.5694989	Cu	33.0526000	6.0107390	41.4984387
N	37.0974959	7.8848030	42.7912266	Cu	32.4276708	3.5584065	42.0470740
H	35.5163020	9.6146864	39.3927783	C	36.6000099	3.6920591	41.7508430
H	35.7392157	7.4356851	40.6391127	C	37.1229790	2.7375834	42.6034793
H	35.0982567	7.4621099	43.0302174	C	38.5025207	2.4378745	42.5642659
H	34.3975885	11.0296104	41.1285372	C	39.3330303	3.0786112	41.6695112
H	35.9426242	11.7596655	40.6846076	C	38.8332197	4.0441710	40.7355226
H	37.0304324	10.7751834	42.7139284	C	37.4245709	4.3436514	40.7747786
H	35.6234496	11.7363765	43.1915205	C	36.8939534	5.2466540	39.8086458
H	34.2287449	9.6631354	43.3853084	C	37.7112032	5.8428143	38.8786392
H	35.6642298	9.5083312	44.4017972	C	39.1104096	5.5972230	38.8665900
H	36.9849449	9.5176512	40.3830115	C	39.6735188	4.7044630	39.7760506
H	39.6197762	7.6435404	43.5305306	O	39.9022090	6.2333398	37.9584556
H	40.5135289	6.1458039	45.2790710	O	34.8535070	5.2701064	41.8789711
H	38.9645335	4.6939342	46.6227957	O	34.3306016	3.0830539	41.9876927
H	36.5054047	4.7755795	46.1345178	C	35.1523489	4.0418675	41.8808344
H	35.6239417	6.2116450	44.3600497	C	32.6164379	3.9143436	37.8352214
H	37.7916269	8.5212298	42.4152138	C	33.1891279	2.7552635	37.3448664
H	33.4612463	8.9445178	41.4412031	C	33.1663356	2.4975311	35.9575502

C	32.5463163	3.3759075	35.0933736	H	27.7974909	1.4726614	39.4343862
C	31.9042002	4.5708783	35.5560898	H	24.3944958	1.9167440	39.1120358
C	31.9531822	4.8416202	36.9690393	H	36.4621731	2.2366373	43.3157983
C	31.2987630	6.0071382	37.4658377	H	38.9150302	1.6945645	43.2537827
C	30.6235279	6.8482821	36.6177193	H	40.3983822	2.8275218	41.6715336
C	30.5646930	6.5863018	35.2221783	H	35.8251419	5.4632705	39.7910751
C	31.2152304	5.4832885	34.6793349	H	37.2813372	6.5258931	38.1361893
O	29.8358801	7.5157255	34.5321413	H	33.6686645	2.0566590	38.0357137
O	33.1902871	5.3029085	39.6497219	H	33.6398837	1.5920273	35.5650030
O	32.3057616	3.2780990	40.0879560	H	32.5416403	3.1316828	34.0262965
C	32.7096662	4.1849848	39.3020626	H	31.3214272	6.2311213	38.5338991
C	28.7797437	5.5914513	41.3635382	H	30.1010522	7.7306012	36.9945827
C	28.3194154	6.8371370	41.7580340	H	29.0326136	7.5790600	42.1250344
C	28.3378325	3.3455827	40.3428794	H	29.4006523	3.1048347	40.3708917
O	31.0562778	6.2161285	41.1973747	H	33.9384046	7.1182092	45.6182870
O	30.5584914	4.1912551	42.0385412	H	30.4516625	3.8865608	44.8290232
C	30.2405843	5.3113376	41.5367253	H	28.6958549	2.8636776	46.2000375
C	32.3455265	5.6888836	45.6801005	H	29.6839046	7.2633862	33.6080099
C	33.1800042	6.6380272	46.2422823	H	39.3613467	6.8235499	37.4092641
C	31.3165714	5.0584843	46.4551271	H	33.7483240	7.6868645	48.0585191
C	30.3888056	4.1381303	45.8881705	H	32.0421576	6.6220642	49.4520283
C	29.4020613	3.5677569	46.6561713	H	27.7925731	2.6687800	48.2243032
O	32.7337751	6.3066933	43.4399442	C	32.4953878	8.9981536	40.5853968
O	32.5612534	4.1151613	43.9296374	C	33.0735028	9.0902007	41.9430104
C	32.5591551	5.3422907	44.2406554	C	34.1267159	10.1223627	42.2742294
C	33.0651102	6.9571246	47.6127951	C	34.8410350	10.6421788	41.0163984
C	32.1021051	6.3533141	48.3928018	C	33.8214062	11.0905878	39.9590824
C	31.1823127	5.3977345	47.8498315	C	32.9306094	9.9317691	39.4706870
C	29.2786949	3.8735178	48.0380132	O	33.5133462	8.0647109	41.0285283
C	30.1484351	4.7842757	48.6349375	C	26.5367101	7.4625656	37.3947392
O	28.3008771	3.2823544	48.7790039	C	25.3972975	7.9761563	38.0543064
H	26.5738083	8.0991361	42.0500131	C	24.2836787	8.4041715	37.3288156
H	24.9834107	6.4451355	41.2202856	C	24.2700400	8.3407936	35.9288746

C	28.3120627	3.6538095	40.1485564	H	29.3735892	3.4157313	40.2064802
O	30.9048455	6.4395772	41.5937181	H	34.1344009	7.0599143	45.8349979
O	30.5049706	4.2634407	41.9820829	H	30.3073272	4.2868089	44.8517722
C	30.1309394	5.4473520	41.7164141	H	28.3766490	3.4908213	46.1215851
C	32.3686280	5.8464990	45.7941078	H	29.5095252	7.2887552	33.4017050
C	33.2948176	6.6664006	46.4137539	H	39.4218662	6.0193300	36.7766283
C	31.2410395	5.3341268	46.5222061	H	33.9158361	7.6069894	48.2705850
C	30.2277141	4.5434796	45.9073696	H	32.0363864	6.7500105	49.5760066
C	29.1451695	4.0921273	46.6226833	H	27.3826571	3.3664418	48.1041162
O	32.9303362	6.4698739	43.5820208	C	33.2961504	9.4141259	42.6380613
O	32.4022147	4.3225205	43.9830047	C	33.7347246	9.8134689	41.2827009
C	32.5805348	5.5222711	44.3441080	C	32.9439161	10.8188191	40.4629470
C	33.1665763	6.9738502	47.7853864	C	31.8608111	11.5541585	41.2750548
C	32.1052515	6.4858424	48.5161333	C	31.1052322	10.6197878	42.2308156
C	31.0976294	5.6589681	47.9198118	C	32.0577158	10.0081393	43.2696615
C	29.0113207	4.3802779	48.0059274	O	33.0694617	8.5476326	41.5171097
C	29.9702146	5.1555036	48.6558830	C	36.6874229	8.4446958	39.2187743
O	27.9402041	3.8983254	48.6954171	C	37.8381346	9.0292401	38.6499642
H	26.3600216	8.0005734	42.5761540	C	37.8827000	9.3439873	37.2897211
H	24.8533238	6.5168845	41.3631347	C	36.7846025	9.0861673	36.4595929
H	27.8700008	1.9714767	38.8864044	C	35.6363718	8.5094663	37.0185919
H	24.4788209	2.4221718	38.4532223	C	35.5807202	8.1934823	38.3776702
H	36.5050868	3.2057288	43.6867003	N	36.6261003	8.1577468	40.5799075
H	38.9377713	2.6148189	43.7620818	H	33.6483778	11.5448775	40.0185653
H	40.4223545	3.1935836	41.9079834	H	34.7956753	9.6813834	41.0351544
H	35.8778276	5.2518613	39.3693713	H	34.0522120	9.0285286	43.3349482
H	37.3269711	5.7997045	37.4840784	H	31.1575517	12.0544498	40.5851754
H	33.6378994	2.4875512	38.1510009	H	32.3366071	12.3585198	41.8705464
H	33.6499125	1.8896388	35.7151066	H	30.3038589	11.1750556	42.7505767
H	32.4936915	3.2876553	34.0879525	H	30.6159605	9.8099889	41.6593343
H	31.0196752	6.5265040	38.4158170	H	32.3882678	10.7853913	43.9871332
H	29.7310146	7.8649264	36.7884396	H	31.5527741	9.2228016	43.8608074
H	28.8187553	7.5172326	42.6823545	H	32.4876539	10.2745866	39.6153931

H	38.7091846	9.2271325	39.2842506	O	40.1215428	4.1371660	37.2671234
H	38.7917328	9.7947951	36.8758916	O	35.1799989	5.7610189	41.0181755
H	36.8207938	9.3374958	35.3954763	O	34.2600474	4.0404610	42.1130246
H	34.7657961	8.2946484	36.3890669	C	35.2418209	4.6384093	41.5600283
H	34.6800812	7.7281041	38.7908403	C	32.5493864	5.5941603	37.8905230
H	35.9992583	7.3988386	40.8584210	C	33.1495498	4.3914909	37.5443325
H	37.5256445	8.0914379	41.0497226	C	33.2180547	3.9875503	36.1975373
H	24.4736222	4.4164735	39.9087844	C	32.6546319	4.7658683	35.2092889
H	40.7988970	4.3606296	39.6074910	C	32.0005992	6.0066278	35.5010456
H	31.1188872	5.4038683	33.5338128	C	31.9646370	6.4323109	36.8808878
H	29.8719419	5.3236750	49.7283228	C	31.2978607	7.6542163	37.1892252
				C	30.7076069	8.4060566	36.2060290
				C	30.7407646	7.9979990	34.8460599
				C	31.3805185	6.8172222	34.4819318
				O	30.1142548	8.8735773	34.0053839
				O	32.5983916	7.1068753	39.7548145
				O	32.3921396	4.8937615	40.1141066
				C	32.5034307	5.9034638	39.3633382
				C	28.4018231	6.0392425	41.7034864
				C	27.7321458	7.1648056	42.1587070
				C	28.3320098	3.7878371	40.5913222
				O	30.4506897	7.1800460	41.6096803
				O	30.5190405	5.0091546	42.1450398
				C	29.8964643	6.0614324	41.8247465
				C	32.1488397	6.7945410	45.8249736
				C	32.8067116	7.8210110	46.4783200
				C	31.2324442	5.9439285	46.5340190
				C	30.4683871	4.9310109	45.8850551
				C	29.5687196	4.1614272	46.5831659
				O	32.4532726	7.6398456	43.6345994
				O	32.6003482	5.4182554	43.9591435
				C	32.4154846	6.6018184	44.3587346
				C	32.6330544	8.0068695	47.8672934
<i>(R,R)</i> -1-TS1 (QM(B3LYP)/MM)							
C	26.3291175	7.2408806	42.0701901				
C	25.6133484	6.2192658	41.4841841				
C	26.2502314	5.0463039	40.9626362				
C	27.6829911	4.9491476	41.1046674				
C	27.6179297	2.7913291	39.9759151				
C	26.2093443	2.8843286	39.8187853				
C	25.5221534	3.9913722	40.3030215				
O	25.6606287	1.8104323	39.1768635				
Cu	32.3194963	7.7277947	41.6431447				
Cu	32.5020919	4.8743076	42.0728546				
C	36.5834296	3.9485945	41.6421447				
C	37.0067399	3.4598755	42.8645966				
C	38.3383603	3.0092915	43.0263628				
C	39.2349428	3.0696262	41.9806506				
C	38.8399971	3.5359317	40.6844136				
C	37.4662072	3.9282859	40.5119881				
C	37.0197359	4.2678171	39.2039022				
C	37.8861406	4.2815053	38.1380437				
C	39.2692856	4.0210184	38.3241839				
C	39.7512455	3.6429562	39.5767762				

C	31.7806651	7.1924606	48.5809179	C	35.6086742	11.3060058	42.0517288
C	31.0325775	6.1463182	47.9475323	C	35.6273388	9.9520470	42.7747992
C	29.3809838	4.3386246	47.9786624	O	33.6387970	9.1412253	41.5862334
C	30.1010386	5.3163335	48.6614185	C	37.8745485	7.9346931	39.0773440
O	28.4905701	3.5529749	48.6466815	C	39.1980471	8.4071298	39.1231829
H	25.8062175	8.1220961	42.4551833	C	39.9276865	8.5934048	37.9464526
H	24.5263134	6.3313954	41.4184691	C	39.3461038	8.3243246	36.7026255
H	28.1154126	1.9032813	39.5763428	C	38.0226273	7.8691162	36.6510629
H	24.7047926	1.9067334	39.0425350	C	37.2894055	7.6736398	37.8242205
H	36.3127891	3.4573971	43.7094392	N	37.1205380	7.7652330	40.2593070
H	38.6654653	2.6309104	44.0003209	H	35.9914374	9.9449440	38.8436023
H	40.2664777	2.7428188	42.1466117	H	34.7629936	8.0305078	39.9432526
H	35.9699299	4.5180812	39.0426619	H	35.0864250	7.8572849	42.4278749
H	37.5185051	4.5314300	37.1365970	H	36.2063780	12.1635687	40.1320642
H	33.5540401	3.7557499	38.3342816	H	37.2712618	10.8787333	40.7242220
H	33.7036103	3.0416620	35.9367655	H	36.1663085	12.0554090	42.6417690
H	32.7092605	4.4005867	34.1788354	H	34.5652152	11.6630517	41.9802726
H	31.2567171	7.9880286	38.2249251	H	36.6729242	9.6502174	42.9884810
H	30.1870867	9.3382490	36.4425183	H	35.1067145	10.0132384	43.7472464
H	28.3049008	7.9894140	42.5886915	H	34.4699291	10.5632993	39.4781863
H	29.4132785	3.6947942	40.6867559	H	39.6665102	8.6078499	40.0929866
H	33.4727813	8.4758246	45.9106974	H	40.9637022	8.9413792	38.0049416
H	30.5871880	4.7634651	44.8152611	H	39.9200241	8.4706288	35.7825424
H	28.9865418	3.3957268	46.0562342	H	37.5499520	7.6626605	35.6847697
H	30.0827509	8.5556619	33.0898716	H	36.2585256	7.3098077	37.7741577
H	39.6578510	4.5501064	36.5204783	H	36.5896943	6.8789145	40.3499240
H	33.1788504	8.8048965	48.3807084	H	37.6757907	7.9024264	41.1044473
H	31.6712276	7.3656486	49.6560944	H	24.4450526	4.0898909	40.1680602
H	28.0817135	2.9268044	48.0268867	H	40.8268188	3.5236211	39.7070367
C	34.9675609	8.8467202	41.9561628	H	31.4155089	6.4984617	33.4401862
C	35.1854959	8.8675149	40.4954946	H	29.9573342	5.4244233	49.7364683
C	35.4531011	10.1598853	39.7839171				
C	36.2096971	11.1846098	40.6435047				

(*R,R*)-1-Int1 (QM(B3LYP)/MM)

C	26.2686907	7.3881558	42.3894496	C	31.6610312	6.8675141	34.5635496
C	25.5865155	6.3679348	41.7618713	O	30.6229364	9.0125444	33.9587314
C	26.2651536	5.2491192	41.1775743	O	32.5502060	7.1732140	39.9005494
C	27.7014043	5.2039237	41.3073248	O	32.2801009	4.9762702	40.2978282
C	27.7195170	3.1027730	40.0748641	C	32.4264136	5.9727024	39.5297875
C	26.3084982	3.1496297	39.9215874	C	28.3834585	6.2944488	41.9451664
C	25.5785952	4.2020407	40.4624752	C	27.6756098	7.3689113	42.4578193
O	25.8008385	2.0921160	39.2192241	C	28.3951089	4.0970248	40.7355472
Cu	32.2938230	8.0115091	41.7919523	O	30.4026423	7.4878576	41.7765262
Cu	32.4914356	5.0904731	42.2327453	O	30.5245141	5.3352826	42.3867040
C	36.5571463	3.9998736	41.6946669	C	29.8807195	6.3700975	42.0379709
C	36.9793527	3.5936504	42.9471757	C	32.1609094	6.8936799	45.9812533
C	38.3144204	3.1650503	43.1400102	C	32.8068127	7.8959217	46.6809966
C	39.2190615	3.1846140	42.0990582	C	31.2224777	6.0279788	46.6403506
C	38.8294561	3.5807162	40.7777399	C	30.4703179	5.0411655	45.9391493
C	37.4471044	3.9227920	40.5723907	C	29.5488819	4.2537582	46.5873707
C	36.9996197	4.1571068	39.2422532	O	32.4484263	7.7829857	43.8049524
C	37.8781161	4.1567041	38.1871091	O	32.7065951	5.5688340	44.1073464
C	39.2683549	3.9773925	38.4033659	C	32.4563769	6.7439673	44.5144192
C	39.7505113	3.6684429	39.6762218	C	32.5996007	8.0385688	48.0708320
O	40.1271607	4.1065418	37.3521549	C	31.7261919	7.2065866	48.7374979
O	35.1293508	5.7093868	40.8569716	C	30.9875474	6.1864400	48.0528013
O	34.2493511	4.1841737	42.2229166	C	29.3267680	4.3872318	47.9824702
C	35.2128151	4.6704248	41.5627800	C	30.0314490	5.3400507	48.7132763
C	32.4962323	5.6232482	38.0617792	O	28.4168954	3.5828312	48.6022039
C	33.0170354	4.3703524	37.7680595	H	25.7155797	8.2272490	42.8228825
C	33.1421858	3.9373088	36.4344397	H	24.4948127	6.4370650	41.7154052
C	32.7204500	4.7432682	35.3993555	H	28.2498904	2.2573979	39.6281510
C	32.1457995	6.0337444	35.6330237	H	24.8415214	2.1592941	39.0927089
C	32.0479396	6.4859500	37.0025956	H	36.2806273	3.6426244	43.7866538
C	31.4586392	7.7627435	37.2443596	H	38.6384310	2.8432978	44.1350336
C	31.0133477	8.5454733	36.2090463	H	40.2545331	2.8840003	42.2889636
C	31.1117231	8.1101908	34.8603716	H	35.9411929	4.3402448	39.0538959

C	39.2723852	3.3348363	41.8217267	C	31.2140003	5.4222819	46.4780902
C	38.8120673	4.2078732	40.7830202	C	30.2200094	4.5774942	45.9056572
C	37.4091147	4.5432713	40.7619875	C	29.1700282	4.1054223	46.6560884
C	36.9337317	5.3762584	39.7090352	O	32.8030510	6.5252491	43.4693307
C	37.7850935	5.8549951	38.7416526	O	32.3898780	4.3698728	43.9626100
C	39.1721075	5.5571777	38.7732949	C	32.5124690	5.5911392	44.2742717
C	39.6893050	4.7436281	39.7792338	C	33.0819151	7.1906222	47.6535455
O	39.9960908	6.0698532	37.8174441	C	32.0629254	6.6692332	48.4211502
O	34.7279259	5.5242942	41.6051620	C	31.0849115	5.7789669	47.8693977
O	34.2902928	3.3805314	42.1204138	C	29.0552985	4.4213189	48.0349512
C	35.0777569	4.3298619	41.8289198	C	29.9978987	5.2475324	48.6439559
C	32.3505648	3.9015664	37.8777601	O	28.0201756	3.9150727	48.7606750
C	32.9814864	2.7471691	37.4452761	H	26.2272588	7.7876945	42.8872984
C	33.0195962	2.4374907	36.0692457	H	24.7642731	6.4344859	41.4841211
C	32.4171840	3.2679673	35.1478956	H	27.8844635	2.1979318	38.6116472
C	31.7135124	4.4525274	35.5421483	H	24.4954540	2.6401241	38.1716061
C	31.6741995	4.7613745	36.9483928	H	36.3515535	2.7080802	43.4680995
C	30.9187696	5.8947433	37.3687879	H	38.7919934	2.1395763	43.5357235
C	30.2644643	6.6881613	36.4618610	H	40.3314768	3.0632712	41.8727847
C	30.3370896	6.4204445	35.0697005	H	35.8768915	5.6382283	39.6682808
C	31.0528015	5.3223721	34.6034212	H	37.3934624	6.4900675	37.9380463
O	29.6647609	7.3346826	34.3087925	H	33.4662459	2.0943851	38.1754520
O	32.6998857	5.4375531	39.6461978	H	33.5369543	1.5342782	35.7304073
O	32.2860192	3.2918818	40.1665228	H	32.4758357	2.9936314	34.0895279
C	32.4427248	4.2373469	39.3370823	H	30.8523761	6.1311350	38.4303318
C	28.5823292	5.6770780	41.6190113	H	29.6702785	7.5476251	36.7837930
C	28.0408450	6.7230146	42.3473306	H	28.6821039	7.3441588	42.9774132
C	28.2853636	3.7686318	40.0246982	H	29.3488590	3.5357149	40.0793724
O	30.8280614	6.4338611	41.4954627	H	34.0058872	7.2651674	45.6803184
O	30.4513610	4.2774300	42.0037107	H	30.2851963	4.2995421	44.8542199
C	30.0617374	5.4438105	41.7106629	H	28.4118211	3.4659098	46.1881144
C	32.3046637	5.9619665	45.7137049	H	29.6653574	7.1118208	33.3648370
C	33.1996773	6.8473374	46.2885843	H	39.4825020	6.6207805	37.2047124

C	32.7684400	3.1297090	36.1152490	H	24.5216020	5.8848570	42.0571710
C	32.3206640	4.0303000	35.1731700	H	28.1419470	2.5315290	38.6472790
C	31.8412470	5.3301590	35.5374360	H	24.7422750	2.7142810	38.1281010
C	31.8719790	5.6830150	36.9351270	H	36.3031820	2.2523710	43.0483220
C	31.3696240	6.9606500	37.3155990	H	38.7016150	1.5123730	43.0226590
C	30.8670650	7.8336620	36.3845430	H	40.2961290	2.5165550	41.4592270
C	30.8454950	7.5008280	35.0043280	H	35.9618790	5.4067280	39.4127560
C	31.3333630	6.2723260	34.5727290	H	37.5149500	6.3105160	37.7538850
O	30.3315870	8.4912810	34.2148010	H	33.1117570	2.7532700	38.2317170
O	32.8318730	6.1662630	39.7479320	H	33.1188110	2.1413180	35.8013580
O	32.2242540	4.0354280	40.1299720	H	32.3280480	3.7219900	34.1227180
C	32.4686400	5.0120800	39.3655770	H	31.3879250	7.2415020	38.3673340
C	28.3826290	5.3909300	42.3114110	H	30.4705570	8.8099680	36.6771520
C	27.6963910	6.1899280	43.2130020	H	28.2449520	6.7053420	44.0050840
C	28.3357720	3.8343840	40.3461150	H	29.4144100	3.6989870	40.4166220
O	30.4718630	6.4687510	42.6374610	H	34.3767310	7.5775210	45.7637450
O	30.4839940	4.2593320	42.2893890	H	30.8267630	4.4303640	44.8274190
C	29.8903250	5.3868100	42.4201390	H	28.9485740	3.5227120	46.0901990
C	32.7309320	6.2101450	45.7318220	H	30.2605550	8.2262920	33.2844890
C	33.5719720	7.1225340	46.3461770	H	39.6320500	6.4858770	37.1019660
C	31.6419100	5.6155520	46.4642570	H	34.0884370	8.1526660	48.1886740
C	30.7066800	4.7200510	45.8679050	H	32.2755260	7.1570920	49.4962150
C	29.6550890	4.2010110	46.5836760	H	27.9367180	3.3757860	48.0629790
O	33.4172530	6.8115980	43.5437180	C	31.7533760	8.9075260	41.0070370
O	32.7788570	4.6864610	43.9265960	C	31.8115830	9.2876480	42.4306640
C	32.9920750	5.8765040	44.2874700	C	32.2682900	10.6531240	42.8464040
C	33.4020650	7.4472010	47.7096690	C	31.9589050	11.7458480	41.8115790
C	32.3789290	6.8832190	48.4413710	C	32.3365840	11.3076260	40.3892820
C	31.4520990	5.9621810	47.8524720	C	31.5816980	10.0321370	39.9904460
C	29.4752550	4.5184600	47.9537340	O	33.1028910	8.5617550	41.2405030
C	30.3603350	5.3868450	48.5895480	C	29.3647850	9.7769490	44.3046000
O	28.4366800	3.9716140	48.6447030	C	28.6939140	11.0052270	44.4457230
H	25.7682200	6.9729460	43.8345840	C	28.4927680	11.5599660	45.7124870

C	27.6580292	6.2941954	43.1810979	H	28.1912351	6.7932109	43.9939249
C	28.3523236	3.9546977	40.3109780	H	29.4290557	3.8134741	40.4002901
O	30.4350309	6.5098063	42.8403574	H	34.3751358	7.6569002	45.7780109
O	30.4694893	4.3523278	42.2949479	H	30.8101330	4.5327586	44.8591189
C	29.8594141	5.4477397	42.4825951	H	28.8873562	3.6866431	46.1052513
C	32.7146438	6.3082350	45.7501827	H	30.1124315	7.7804575	33.3064317
C	33.5593392	7.2206328	46.3597494	H	39.6259571	5.9946980	36.9453490
C	31.6129506	5.7380722	46.4826007	H	34.0715294	8.2707281	48.1930181
C	30.6723085	4.8456313	45.8898373	H	32.2370053	7.3123223	49.4997755
C	29.5993565	4.3605573	46.5969025	H	27.8496086	3.5875372	48.0640260
O	33.4322816	6.8552908	43.5535284	C	31.8642986	8.8289833	41.1518526
O	32.7590790	4.7492373	43.9803234	C	31.5144691	9.3454043	42.5809729
C	32.9880559	5.9487635	44.3097662	C	31.9434817	10.7941492	42.8186257
C	33.3807427	7.5668763	47.7176000	C	31.5448770	11.7636383	41.6966375
C	32.3460155	7.0237982	48.4492507	C	32.0429580	11.2555181	40.3367681
C	31.4140816	6.1058337	47.8635471	C	31.4914317	9.8550449	40.0555615
C	29.4079036	4.7021592	47.9594700	O	33.2051558	8.5242090	41.1225373
C	30.3069655	5.5544503	48.5967509	C	29.4463091	9.5811466	44.0777736
O	28.3452249	4.1906986	48.6419079	C	28.3487466	10.4434082	44.0204676
H	25.7224385	7.0958773	43.7543223	C	27.7867579	10.9258835	45.2073698
H	24.5102524	6.0107312	41.9512529	C	28.3284897	10.5539729	46.4415764
H	28.1871649	2.6748089	38.5932188	C	29.4298718	9.6909788	46.4865714
H	24.7957366	2.8460051	38.0259418	C	29.9909298	9.1936521	45.3064573
H	36.3534567	2.3598542	43.2995829	N	30.0277393	9.0675185	42.8379540
H	38.7458435	1.5979809	43.3132149	H	31.5919813	11.1501417	43.8030743
H	40.3298939	2.4386274	41.6440277	H	32.0347209	8.6804296	43.2824229
H	35.9822814	5.1390459	39.3818784	H	31.2465037	7.9241427	40.9617191
H	37.5157480	5.8673054	37.6193472	H	31.9539457	12.7664492	41.9167612
H	33.2645968	2.5910682	38.3711615	H	30.4416210	11.8863707	41.6659959
H	33.3445647	1.9415268	35.9511354	H	31.7523635	11.9540515	39.5306901
H	32.4727259	3.4408519	34.2351756	H	33.1473908	11.2097483	40.3439937
H	31.3233411	6.9885089	38.4052529	H	30.3842661	9.9097436	39.9582322
H	30.3189404	8.4659416	36.6808123	H	31.8680129	9.4591676	39.0972260

H	33.0458693	10.7561678	42.8751747	C	39.7047934	4.6134721	39.7423465
H	27.9265525	10.7365709	43.0531241	O	39.9848944	5.9589711	37.7901049
H	26.9236649	11.5970115	45.1617304	O	34.8548708	5.4672854	41.7308999
H	27.8940902	10.9355249	47.3705933	O	34.3135777	3.3283147	42.1497576
H	29.8627296	9.4010174	47.4487059	C	35.1462370	4.2413078	41.8875070
H	30.8440702	8.5114965	45.3471100	C	32.5414350	3.9752821	37.8672324
H	29.9911048	7.9643200	42.8201800	C	33.1642069	2.8188146	37.4302818
H	29.4739016	9.4065739	42.0427828	C	33.1598520	2.4939763	36.0573377
H	24.4649996	4.3994461	39.9328040	C	32.5166307	3.3071483	35.1477652
H	40.8439548	4.0135787	39.6280020	C	31.8153926	4.4900857	35.5515106
H	31.3568987	5.6670621	33.5763684	C	31.8307793	4.8208405	36.9529649
H	30.1892848	5.7236891	49.6670668	C	31.0864985	5.9551226	37.3899297
				C	30.3702288	6.7160172	36.5020262
				C	30.3750371	6.4190022	35.1136338
(S,S)-1-RC (QM(B3LYP)/MM)				C	31.1002744	5.3348626	34.6292102
C	26.9000866	7.3549740	41.7288054	O	29.6397221	7.2987406	34.3705079
C	26.0148986	6.4677343	41.1529237	O	32.9999010	5.4890891	39.6338179
C	26.4433174	5.2134307	40.6094267	O	32.3812116	3.3885779	40.1494397
C	27.8435034	4.8875746	40.7165243	C	32.6416986	4.3136727	39.3243227
C	27.4267292	2.8055561	39.5242178	C	28.7348537	5.8219961	41.3439231
C	26.0421774	3.1062993	39.4336754	C	28.2721528	7.0412109	41.8122351
C	25.5434645	4.2894367	39.9697946	C	28.2973046	3.6606422	40.1490831
O	25.3190256	2.1366678	38.7978671	O	31.0119567	6.4604164	41.3175624
Cu	32.9945222	6.2194662	41.5076267	O	30.5070123	4.3589361	41.9330614
Cu	32.3906794	3.7803110	42.0909761	C	30.1906255	5.5221392	41.5378555
C	36.5905004	3.8517761	41.7752895	C	32.2378677	5.9965959	45.6979380
C	37.0956489	2.9749478	42.7183450	C	33.0738147	6.9495383	46.2552667
C	38.4676757	2.6413723	42.7163031	C	31.1753773	5.4146377	46.4716187
C	39.3164168	3.1749407	41.7716009	C	30.2238710	4.5125666	45.9146997
C	38.8414770	4.0585106	40.7479996	C	29.2023010	3.9969581	46.6759991
C	37.4377695	4.3861596	40.7449466	O	32.8238542	6.5234061	43.4690646
C	36.9396749	5.1994886	39.6863602	O	32.3738037	4.3773634	43.9666272
C	37.7766145	5.6899165	38.7108561	C	32.4903233	5.6027071	44.2717018
C	39.1709682	5.4237433	38.7422247				

C	32.9340219	7.3148224	47.6117096	C	31.9440223	9.6124583	39.0720811
C	31.9518659	6.7444886	48.3916109	C	32.1409402	10.8508598	39.9562673
C	31.0284117	5.7877836	47.8571843	C	32.9095319	10.5306701	41.2531864
C	29.0773847	4.3230535	48.0516157	O	33.7359968	8.1849599	40.9089586
C	29.9758474	5.2076067	48.6443363	C	37.5055461	7.4581681	43.6285141
O	28.0748952	3.7703694	48.7898057	C	38.8018945	7.9222410	43.9325781
H	26.5359407	8.3079533	42.1257049	C	39.3508347	7.7293985	45.2019905
H	24.9577539	6.7493161	41.1091182	C	38.6268680	7.0742308	46.2048627
H	27.7749163	1.8704690	39.0776748	C	37.3366517	6.6147418	45.9118749
H	24.3805394	2.3653899	38.7092395	C	36.7801889	6.8006718	44.6455871
H	36.4265734	2.5632576	43.4779539	N	36.9356559	7.6724994	42.3760948
H	38.8605481	1.9625037	43.4795157	H	33.1616904	8.0766759	38.1000372
H	40.3763672	2.9045377	41.8063917	H	35.2765907	8.5311608	39.4968906
H	35.8754457	5.4322143	39.6366123	H	34.9600319	9.7160365	41.6831346
H	37.3666953	6.2998514	37.8963616	H	31.3886056	8.8367014	39.6305104
H	33.6688119	2.1723359	38.1530097	H	31.3346773	9.8654121	38.1861816
H	33.6695570	1.5884945	35.7128175	H	32.7005908	11.6141093	39.3794657
H	32.5353489	3.0162200	34.0924091	H	31.1661090	11.3051152	40.2086972
H	31.0708427	6.2162756	38.4483379	H	32.2331864	10.0724128	41.9989935
H	29.7773747	7.5708856	36.8378898	H	33.2898593	11.4618776	41.7102868
H	28.9770321	7.7432705	42.2642288	H	33.7700365	9.7344387	37.8828190
H	29.3527947	3.3974554	40.2080587	H	39.3768721	8.4418837	43.1577752
H	33.8544574	7.4038631	45.6409370	H	40.3621925	8.0964014	45.4097253
H	30.2976151	4.2308130	44.8649609	H	39.0608981	6.9237815	47.1981941
H	28.4751862	3.3142895	46.2195592	H	36.7503036	6.0974435	46.6794842
H	29.5461031	7.0198913	33.4464239	H	35.7736021	6.4338267	44.4231275
H	39.4614166	6.4995163	37.1765572	H	37.6014559	7.8038896	41.6186584
H	33.6148187	8.0543851	48.0447443	H	36.1855014	7.0261361	42.1196710
H	31.8744705	7.0468985	49.4408440	H	24.4769018	4.5087493	39.9206784
H	27.5573719	3.1647717	48.2345430	H	40.7834235	4.4589459	39.7696478
C	34.0758906	9.5783587	41.0458472	H	31.1670513	5.1473524	33.5575539
C	34.2604245	8.8591446	39.7620949	H	29.8956168	5.3985661	49.7144596
C	33.2969728	9.0466896	38.6116994				

(S,S)-1-TS1 (QM(B3LYP)/MM)	C	30.5957133	7.4079780	34.9954753	
C 26.5537114	7.0780462	41.9998745	C 31.3021626	6.2879138	34.5687792
C 25.7653874	6.1035676	41.4267129	O 29.8826662	8.2664166	34.2071169
C 26.3185816	4.8918699	40.8991188	O 32.8324908	6.5600834	39.7327654
C 27.7437664	4.7013488	41.0217361	O 32.6234332	4.3524607	40.1219319
C 27.5231030	2.5533372	39.8938529	C 32.7076695	5.3550350	39.3574086
C 26.1212294	2.7362646	39.7603472	C 28.5391485	5.7408657	41.6137080
C 25.5144097	3.8855249	40.2540175	C 27.9493991	6.9088865	42.0736279
O 25.4945582	1.6988634	39.1296425	C 28.3087614	3.5009541	40.4990657
Cu 32.5533625	7.2404022	41.5824697	O 30.6607142	6.7477838	41.5725713
Cu 32.5546585	4.3801704	42.0949331	O 30.5839603	4.5588546	42.0162606
C 36.6343927	3.6432668	41.8110193	C 30.0317811	5.6614904	41.7369008
C 37.1074313	2.7528608	42.7556989	C 32.2542934	6.4939192	45.7787239
C 38.4526632	2.3152009	42.7064221	C 33.0172662	7.4628031	46.4054511
C 39.3084794	2.7752442	41.7288190	C 31.2540121	5.7651959	46.5093568
C 38.8570513	3.6651655	40.6995633	C 30.3905888	4.8161408	45.8891610
C 37.4759320	4.0660250	40.7278878	C 29.4162124	4.1648347	46.6066356
C 36.9805982	4.8601187	39.6536979	O 32.6691813	7.2431862	43.5728220
C 37.8021680	5.2700763	38.6299678	O 32.5420136	5.0245667	43.9545827
C 39.1876319	4.9570695	38.6442685	C 32.5025438	6.2333935	44.3187043
C 39.7180335	4.1690898	39.6649432	C 32.8628722	7.7074656	47.7875524
O 39.9984231	5.4376238	37.6604429	C 31.9283301	7.0095517	48.5212789
O 35.1921612	5.5145240	41.9368697	C 31.0767754	6.0282794	47.9159684
O 34.2910598	3.4870443	42.1997013	C 29.2497667	4.4001532	47.9962156
C 35.2725534	4.2682796	41.9883266	C 30.0672545	5.3180826	48.6518547
C 32.6923894	5.0511831	37.8853876	O 28.2867834	3.7270062	48.6856134
C 33.3453543	3.8946800	37.4867699	H 26.0950324	7.9929066	42.3882906
C 33.3729152	3.5268213	36.1274311	H 24.6866270	6.2833116	41.3757575
C 32.7228799	4.2949757	35.1851541	H 27.9564700	1.6356770	39.4867263
C 32.0088773	5.4864829	35.5373172	H 24.5435861	1.8523436	39.0153521
C 32.0047737	5.8714227	36.9280008	H 36.4431015	2.4158636	43.5564321
C 31.2671369	7.0327874	37.3024035	H 38.8222557	1.6197792	43.4670116
C 30.5833225	7.7681324	36.3689503	H 40.3501304	2.4391868	41.7360130

H	35.9251603	5.1354947	39.6305898	H	35.1357452	7.6736494	42.8520962
H	37.3905292	5.8586842	37.8010984	H	34.5383227	11.2864544	40.8676087
H	33.8323618	3.2718783	38.2405527	H	36.0304097	11.7515987	40.0232322
H	33.9015490	2.6188584	35.8196088	H	37.4081024	10.6307557	41.7865773
H	32.7542181	3.9605596	34.1431961	H	36.3637026	11.8636174	42.5102880
H	31.2424756	7.3352455	38.3482863	H	34.7998899	10.1847177	43.3677648
H	30.0070513	8.6518193	36.6565022	H	36.4161819	9.6289414	43.7974312
H	28.5803723	7.6931305	42.4971547	H	36.6016799	9.3697573	39.6110374
H	29.3825639	3.3375917	40.5810664	H	39.4419665	9.1041052	42.8198077
H	33.7506204	8.0255146	45.8226055	H	40.6546701	9.2365220	44.9841156
H	30.4984206	4.5988392	44.8272196	H	40.0409574	7.7108420	46.8695535
H	28.7595951	3.4462968	46.1013748	H	38.1974234	6.0493804	46.5537057
H	29.8319198	7.9721163	33.2846753	H	36.9911283	5.9089340	44.3836235
H	39.4750947	5.9572779	37.0286828	H	37.9373342	7.7462451	41.4325047
H	33.4893684	8.4586283	48.2791476	H	36.8868743	6.5828225	42.0776392
H	31.8344104	7.2259676	49.5900988	H	24.4420191	4.0451205	40.1418830
H	27.8200862	3.1227613	48.0853281	H	40.7987847	4.0363741	39.7142361
C	35.4505450	8.5255390	42.2542060	H	31.3424064	6.0214830	33.5126251
C	35.0638109	8.4915323	40.8283785	H	29.9473510	5.4569862	49.7262827
C	35.5754081	9.6254188	39.9446665				
C	35.5809784	10.9776425	40.6711616				
C	36.3503003	10.8854535	41.9973650	(S,S)-1-Int1 (QM(B3LYP)/MM)			
C	35.7526153	9.8255410	42.9361086	C	26.4548537	7.1382903	42.2566994
O	33.7763960	8.7276300	41.3465300	C	25.7037795	6.1840549	41.6045973
C	38.1371746	7.4946193	43.4585238	C	26.3034520	5.0444490	40.9762656
C	39.1693000	8.4326580	43.6415660	C	27.7352794	4.9026576	41.0843821
C	39.8498609	8.5044585	44.8599893	C	27.6022167	2.8465593	39.7852529
C	39.5079793	7.6520559	45.9157405	C	26.1950169	2.9877256	39.6561697
C	38.4748026	6.7244112	45.7376568	C	25.5410499	4.0655500	40.2425586
C	37.7912982	6.6416769	44.5223678	O	25.6123829	1.9858063	38.9314618
N	37.4074940	7.4564460	42.2540360	Cu	32.4592861	7.5098715	41.5445641
H	34.9446317	9.6621392	39.0386961	Cu	32.5432752	4.5252810	42.1558834
H	35.1629620	7.5108612	40.3363019	C	36.5764947	3.5240515	41.8352687
				C	37.0302079	2.5795793	42.7357656

C	38.3749504	2.1409984	42.6864333	C	33.0760520	7.6147788	46.4284353
C	39.2508128	2.6555164	41.7549126	C	31.2586702	5.9784543	46.5267100
C	38.8203749	3.6003798	40.7661067	C	30.3658956	5.0605562	45.9012657
C	37.4381308	4.0015423	40.7886668	C	29.3548504	4.4568133	46.6093347
C	36.9641744	4.8447163	39.7420036	O	32.7499064	7.3572093	43.5764931
C	37.8073755	5.3073045	38.7581277	O	32.5819002	5.1522052	44.0119728
C	39.1915269	4.9907920	38.7821044	C	32.5527194	6.3759182	44.3425562
C	39.6995217	4.1491258	39.7713340	C	32.9142814	7.8760616	47.8072566
O	40.0226855	5.5158973	37.8407753	C	31.9526836	7.2124548	48.5380315
O	35.1501223	5.4102788	41.9954927	C	31.0762486	6.2552295	47.9304678
O	34.2226139	3.4188735	42.2730679	C	29.1847508	4.7029602	47.9967343
C	35.2212139	4.1483084	42.0403717	C	30.0360061	5.5837966	48.6606463
C	32.6136965	4.9586180	37.9570977	O	28.1873928	4.0724584	48.6775761
C	33.2859057	3.7988066	37.6017542	H	25.9609272	7.9973129	42.7221464
C	33.3279149	3.3813359	36.2568936	H	24.6186773	6.3245802	41.5695783
C	32.6674329	4.0998098	35.2834123	H	28.0726566	1.9837090	39.3060974
C	31.9256446	5.2859874	35.5911424	H	24.6585665	2.1178953	38.8154655
C	31.9160296	5.7283447	36.9653587	H	36.3510463	2.2040440	43.5060603
C	31.1651254	6.8960967	37.2903709	H	38.7281642	1.4016644	43.4123674
C	30.4530548	7.5693761	36.3314824	H	40.2916466	2.3167229	41.7638357
C	30.4537944	7.1398862	34.9783588	H	35.9074582	5.1128844	39.7004510
C	31.1952328	6.0272778	34.5935272	H	37.4108573	5.9339336	37.9502884
O	29.6985574	7.9324588	34.1592596	H	33.7753295	3.2102120	38.3808822
O	32.6889702	6.5316131	39.7620299	H	33.8747962	2.4721832	35.9867399
O	32.6068657	4.3296514	40.2142393	H	32.7081396	3.7294170	34.2536865
C	32.6260998	5.3207947	39.4200146	H	31.1545608	7.2517262	38.3193788
C	28.4909856	5.9251979	41.7508079	H	29.8631117	8.4551142	36.5828420
C	27.8574610	7.0249360	42.3079010	H	28.4595965	7.8007509	42.7857624
C	28.3486011	3.7716216	40.4693374	H	29.4282736	3.6446923	40.5423360
O	30.5667636	7.0212047	41.6893863	H	33.8291981	8.1552292	45.8493434
O	30.5835227	4.8159292	42.0770702	H	30.4793960	4.8315832	44.8421989
C	29.9903580	5.9096993	41.8378597	H	28.6732211	3.7655408	46.0992798
C	32.2917249	6.6639855	45.7997642	H	29.5971011	7.5587143	33.2703672

H	39.5135483	6.0563040	37.2146608	H	37.4971058	7.5390040	41.6505864
H	33.5561088	8.6145154	48.2985405	H	36.2944829	6.4112110	42.1457483
H	31.8530147	7.4413258	49.6038308	H	24.4665700	4.2034486	40.1219633
H	27.7000407	3.4890469	48.0731335	H	40.7783330	4.0017335	39.8214142
C	35.7134118	8.3687861	42.4339696	H	31.2612589	5.7394081	33.5443189
C	35.0474658	8.4089448	41.0226395	H	29.9274793	5.7074017	49.7381481
C	35.8277316	9.3147679	40.0410539				
C	36.1270599	10.7038747	40.6116265				
C	36.9175243	10.5835054	41.9216973	(S,S)-2-RC (QM(B3LYP)/MM)			
C	36.1387473	9.7450516	42.9463408	C	27.0581687	7.1913249	41.6241301
O	33.7465716	8.8251883	41.1767168	C	26.1420135	6.2552485	41.1887208
C	37.5694552	7.1122913	43.6568638	C	26.5308395	4.9257424	40.8204879
C	38.8810536	7.5705245	43.7904297	C	27.9265879	4.5798429	40.9540359
C	39.5698153	7.3488234	44.9873820	C	27.4222627	2.3560958	40.0959010
C	38.9421440	6.6817164	46.0440010	C	26.0459745	2.6832870	39.9746265
C	37.6244164	6.2321332	45.9002525	C	25.5929804	3.9505047	40.3288170
C	36.9312672	6.4411806	44.7049021	O	25.2857884	1.6556916	39.4974428
N	36.8392376	7.3277262	42.4094420	Cu	33.1221293	6.0035982	41.6019400
H	35.2319097	9.3770807	39.1144040	Cu	32.5508261	3.5444242	42.0855400
H	35.0866335	7.3828427	40.6004335	C	36.7339717	3.7284814	41.7208151
H	34.9726564	7.9307232	43.1159225	C	37.2908843	2.8227803	42.6055674
H	35.1719394	11.2250984	40.8068800	C	38.6709466	2.5293885	42.5434433
H	36.6847791	11.3120445	39.8759073	C	39.4722559	3.1268674	41.5945342
H	37.9089652	10.1254893	41.7161211	C	38.9406787	4.0423372	40.6282611
H	37.1303187	11.5805702	42.3478059	C	37.5313988	4.3351491	40.6913361
H	35.1934991	10.2661878	43.1801536	C	36.9751545	5.1895955	39.6961076
H	36.6899079	9.6555775	43.9000603	C	37.7603377	5.7350163	38.7089763
H	36.7853851	8.8187741	39.7668770	C	39.1589021	5.4953911	38.6706109
H	39.3606448	8.1020501	42.9623071	C	39.7518962	4.6613317	39.6156153
H	40.6006625	7.7001884	45.0932693	O	39.9198275	6.0841080	37.7055126
H	39.4810949	6.5110266	46.9811111	O	34.9656742	5.2921765	41.8106213
H	37.1278632	5.7068705	46.7214985	O	34.4747928	3.1139611	42.0776046
H	35.9074081	6.0776033	44.5834977	C	35.2822272	4.0701911	41.8783939
				C	32.6592228	3.9456196	37.8683391

C	33.2330368	2.7817418	37.3868083	H	26.7243466	8.1995180	41.8890455
C	33.2270514	2.5146854	36.0016910	H	25.0905044	6.5538002	41.1260511
C	32.6239784	3.3894841	35.1226373	H	27.7342637	1.3529546	39.7932911
C	31.9722793	4.5851869	35.5696756	H	24.3561672	1.9016547	39.3678546
C	32.0003299	4.8629762	36.9830646	H	36.6572305	2.3525065	43.3618878
C	31.3173143	6.0199017	37.4592626	H	39.1074041	1.8241886	43.2579240
C	30.6328558	6.8414061	36.5995132	H	40.5380850	2.8784247	41.5776894
C	30.6063548	6.5798675	35.2034295	H	35.9087482	5.4133498	39.7062764
C	31.2874076	5.4872363	34.6767209	H	37.3053252	6.3775717	37.9453484
O	29.8784994	7.4999732	34.4990399	H	33.7014599	2.0839183	38.0855190
O	33.1305078	5.3660350	39.7040752	H	33.7018726	1.6040609	35.6227254
O	32.4828632	3.2538033	40.1234377	H	32.6360924	3.1383974	34.0571849
C	32.7583385	4.2119238	39.3412263	H	31.3287384	6.2506614	38.5246126
C	28.8539900	5.5715252	41.4290630	H	30.0890551	7.7171667	36.9655157
C	28.4223706	6.8541878	41.7323747	H	29.1500674	7.5932713	42.0739182
C	28.3313944	3.2682825	40.5658173	H	29.3803288	2.9889982	40.6404879
O	31.1247785	6.2367865	41.4067646	H	34.0453788	6.9410458	45.8169103
O	30.6551693	4.1297256	42.0187790	H	30.4748006	3.8369574	44.8725727
C	30.3161809	5.2868934	41.6262181	H	28.6242105	2.8838492	46.1626210
C	32.3983140	5.5709480	45.7953905	H	29.7882005	7.2707795	33.5608897
C	33.2456672	6.4812097	46.4029040	H	39.3590372	6.6469263	37.1473427
C	31.3198866	4.9712348	46.5318728	H	33.7776584	7.5015060	48.2463054
C	30.3782056	4.0893564	45.9280756	H	31.9823843	6.4943899	49.5651478
C	29.3405576	3.5542513	46.6529022	H	27.6459747	2.7013002	48.1444542
O	32.9131736	6.2200464	43.5824427	C	32.6911856	9.0677218	40.7361687
O	32.5777391	4.0353546	43.9946399	C	33.3087655	9.1605090	42.0766086
C	32.6446133	5.2498364	44.3489976	C	34.4199985	10.1482951	42.3537438
C	33.0891842	6.7961812	47.7701235	C	35.1222290	10.6218849	41.0708061
C	32.0763975	6.2238051	48.5088135	C	34.0997940	11.0778537	40.0200383
C	31.1475184	5.3016205	47.9255439	C	33.1544640	9.9421972	39.5840066
C	29.1813774	3.8488020	48.0325280	O	33.6537206	8.0834608	41.1849501
C	30.0675456	4.7143787	48.6709862	C	26.0019305	7.8234426	37.1159962
O	28.1541357	3.2873228	48.7287633	C	24.8052323	8.2019768	37.7671634

C	28.7289579	5.8612805	41.5302017	H	29.8900124	7.9315599	36.8724647
C	28.2262134	7.0221463	42.0932531	H	28.9071796	7.7191669	42.5886545
C	28.3739136	3.7900864	40.1687100	H	29.4424917	3.5742052	40.1883914
O	30.9969182	6.5410871	41.4703408	H	34.0632293	7.2705389	45.7706547
O	30.5292943	4.4205335	42.0523201	H	30.3389655	4.3541239	44.8363599
C	30.1940834	5.5890868	41.6876184	H	28.4626224	3.4749842	46.1391730
C	32.3641707	5.9666906	45.7706337	H	29.7275094	7.4502690	33.4666939
C	33.2494502	6.8477024	46.3656443	H	39.2222144	6.4517485	37.1250579
C	31.2611033	5.4197663	46.5056217	H	33.8264797	7.8568153	48.2025261
C	30.2709372	4.5948683	45.8975724	H	32.0074503	6.9082421	49.5358063
C	29.2179913	4.1010327	46.6289413	H	27.5173688	3.2887203	48.1459258
O	32.9018185	6.5500628	43.5536540	C	33.5654264	9.3652166	42.5849870
O	32.4657678	4.3908008	44.0094388	C	33.9103507	9.7831522	41.2058053
C	32.5923551	5.6062284	44.3360724	C	32.9131673	10.5186889	40.3290337
C	33.1109335	7.1748023	47.7322533	C	31.6656414	10.9998589	41.0940714
C	32.0841091	6.6368535	48.4782163	C	31.1557868	9.9535782	42.0948152
C	31.1166287	5.7508686	47.9008362	C	32.2092744	9.6729468	43.1781364
C	29.0946585	4.3790755	48.0165734	O	33.5750100	8.4139757	41.5121982
C	30.0249322	5.1988158	48.6525498	C	36.5996835	8.1649715	39.4741950
O	28.0596974	3.8487872	48.7246853	C	37.7271566	8.6102365	38.7523833
H	26.4414796	8.1890064	42.5127541	C	37.6695015	8.7611891	37.3634448
H	24.9156258	6.6443604	41.3978506	C	36.4909681	8.4792990	36.6586416
H	27.9149024	2.0718868	38.9596698	C	35.3608859	8.0591938	37.3754537
H	24.4992817	2.4314232	38.6698692	C	35.4064211	7.9120264	38.7617625
H	36.5176844	2.9270945	43.7441756	N	36.6464193	7.9753683	40.8500827
H	38.9799012	2.4303704	43.7702056	H	33.4249124	11.3729758	39.8510469
H	40.4334788	3.2231556	41.9668526	H	34.9735871	9.8865192	40.9582473
H	35.7612201	5.1028465	39.5276819	H	34.3851508	9.2037222	43.2989243
H	37.1717907	5.8634550	37.6907705	H	30.8726234	11.2681781	40.3737052
H	33.7113704	2.4763300	38.1649572	H	31.9146208	11.9276447	41.6477970
H	33.7659643	1.9434894	35.7092552	H	30.2251398	10.3070077	42.5744220
H	32.6449088	3.3922874	34.1017738	H	30.9121955	9.0111035	41.5732555
H	31.1272958	6.5293441	38.4902082	H	32.3252960	10.5561529	43.8371364

H	31.9097483	8.8224231	43.8138506	C	39.0599213	5.5445709	38.8729117
H	32.6278521	9.8298128	39.5123142	C	39.6257624	4.7718291	39.8863783
H	38.6658517	8.8018993	39.2835670	O	39.8535415	6.0878891	37.9080688
H	38.5621504	9.1034235	36.8265951	O	34.7642925	5.4319621	41.8213974
H	36.4508969	8.5919098	35.5709068	O	34.2511127	3.2775118	42.1727712
H	34.4271738	7.8248864	36.8523759	C	35.0732444	4.2142862	41.9657697
H	34.5291029	7.5412101	39.2950494	C	32.4918614	3.9986624	37.9250133
H	35.9796301	7.2933042	41.2189464	C	33.1599919	2.8701744	37.4871678
H	37.5778373	7.8365047	41.2337976	C	33.2012697	2.5758444	36.1067983
H	24.5176623	4.5091947	39.9960500	C	32.5647089	3.3933524	35.1954698
H	40.7378829	4.5234995	39.7193827	C	31.8242086	4.5514559	35.6008555
H	31.2464955	5.4983020	33.5800144	C	31.7854376	4.8447047	37.0107304
H	29.9288094	5.3729950	49.7242253	C	30.9984703	5.9442757	37.4580695
				C	30.3036489	6.7189452	36.5662637
				C	30.3682975	6.4661247	35.1693547
(<i>S,S</i>)-1-RC (open-shell singlet)				C	31.1233904	5.4049935	34.6746952
C	26.8891526	7.4716274	41.8392391	O	29.6462298	7.3612854	34.4321586
C	26.0228645	6.5741577	41.2486777	O	32.9740812	5.5065680	39.6673081
C	26.4771861	5.3383914	40.6844074	O	32.2560975	3.4447532	40.2161020
C	27.8841621	5.0430183	40.7865420	C	32.5700853	4.3407810	39.3805531
C	27.5271458	2.9855298	39.5411097	C	28.7502298	5.9819942	41.4356688
C	26.1334780	3.2508435	39.4615505	C	28.2682111	7.1849831	41.9222717
C	25.6001664	4.4073377	40.0241089	C	28.3756987	3.8463604	40.1871474
O	25.4389500	2.2761818	38.8026703	O	31.0247929	6.6053060	41.3229516
Cu	32.9937053	6.3133474	41.4978457	O	30.5166429	4.5491545	42.0816239
Cu	32.3680083	3.8677810	42.1535351	C	30.2048483	5.6890299	41.6220875
C	36.5314758	3.8923953	41.9000022	C	32.3590848	6.2001355	45.6848111
C	37.0668388	3.0907515	42.8889039	C	33.2231731	7.1079768	46.2696120
C	38.4593298	2.8596861	42.9314868	C	31.2900100	5.6082685	46.4379383
C	39.2895767	3.4062039	41.9769341	C	30.3123517	4.7635019	45.8382921
C	38.7810219	4.2132068	40.9072066	C	29.2908367	4.2266176	46.5839224
C	37.3612396	4.4575700	40.8745329	O	32.8419840	6.7489757	43.4309943
C	36.8308458	5.2308088	39.8016293	O	32.5258461	4.5862472	43.9766700
C	37.6548691	5.7581874	38.8352582				

C	32.5879294	5.8208659	44.2541968	C	33.4279802	8.5220725	38.4704369
C	33.1053373	7.4071868	47.6456414	C	32.0545564	8.9508358	39.0096717
C	32.1191400	6.8200989	48.4096590	C	32.1502806	10.2597469	39.8024000
C	31.1655606	5.9131567	47.8416604	C	33.0374926	10.1119529	41.0515502
C	29.1878529	4.4809592	47.9775963	O	34.2141511	7.9282804	40.7693332
C	30.1063840	5.3182949	48.6091110	C	37.3268345	7.2727250	43.4406084
O	28.1793398	3.9119472	48.6951081	C	38.6358301	7.5412044	43.8910844
H	26.5044958	8.4115790	42.2478493	C	39.0149187	7.2548821	45.2041813
H	24.9598571	6.8327494	41.2065493	C	38.1005925	6.7031713	46.1095602
H	27.8994162	2.0740003	39.0663655	C	36.7939749	6.4457692	45.6735442
H	24.4922551	2.4730337	38.7275081	C	36.4076607	6.7225864	44.3608117
H	36.4067765	2.6699046	43.6515045	N	36.9331935	7.5778058	42.1400393
H	38.8817844	2.2515604	43.7372089	H	33.3790047	7.4948234	38.0699735
H	40.3643412	3.2129613	42.0453761	H	35.5336553	8.3809657	39.1859426
H	35.7571108	5.4148099	39.7391732	H	35.2319350	9.6809477	41.3146578
H	37.2250392	6.3475120	38.0156821	H	31.6422977	8.1589596	39.6578979
H	33.6686223	2.2289516	38.2122128	H	31.3554118	9.0590514	38.1631684
H	33.7460527	1.6929888	35.7573342	H	32.5692408	11.0506392	39.1480864
H	32.6232839	3.1284836	34.1349796	H	31.1441496	10.5998128	40.1049047
H	30.9355578	6.1710515	38.5230630	H	32.4991147	9.5511669	41.8394649
H	29.6801087	7.5510013	36.9036336	H	33.2773486	11.1028962	41.4756795
H	28.9603684	7.8925878	42.3863369	H	33.7375082	9.1888250	37.6416476
H	29.4396128	3.6111066	40.2332272	H	39.3536346	7.9940004	43.1994576
H	34.0127871	7.5662035	45.6702763	H	40.0403228	7.4713612	45.5238639
H	30.3606320	4.5438317	44.7712217	H	38.4000064	6.4816195	47.1387161
H	28.5423926	3.5879657	46.0995712	H	36.0587375	6.0184035	46.3641991
H	29.6218851	7.1396878	33.4886051	H	35.3899481	6.5140823	44.0227351
H	39.3080425	6.5615250	37.2594749	H	37.6753688	7.5284910	41.4462108
H	33.8122048	8.1041380	48.1067517	H	36.0950641	7.0860854	41.8249549
H	32.0631559	7.0666774	49.4746237	H	24.5306784	4.6076511	39.9597946
H	27.6402836	3.3507556	48.1144334	H	40.7031527	4.6066874	39.8814073
C	34.3295411	9.3631652	40.7752762	H	31.1853557	5.2205882	33.6022114
C	34.5066624	8.5808240	39.5271721	H	30.0077568	5.4888275	49.6811454

(*R,R*)-2-RC (open-shell singlet)

C	26.6847029	7.0687800	42.3127996	C	30.3327837	6.7628889	36.5450812
C	25.8673109	6.2899983	41.5197242	C	30.4275122	6.5075613	35.1500619
C	26.3759236	5.1974034	40.7433580	C	31.1362201	5.4050607	34.6802086
C	27.7896967	4.9341423	40.8260954	O	29.7735513	7.4347600	34.3891226
C	27.5353532	3.1202490	39.2286218	O	32.7863712	5.4632146	39.7117060
C	26.1359299	3.3577764	39.1516046	O	32.1819070	3.3641617	40.2495012
C	25.5473149	4.3751153	39.8990745	C	32.4393306	4.2828963	39.4175549
O	25.4931736	2.4948991	38.3105447	C	28.6064808	5.7625742	41.6598961
Cu	32.8770064	6.2714774	41.5442945	C	28.0717853	6.8151655	42.3808172
Cu	32.3285087	3.7959894	42.1765546	C	28.3376176	3.8767840	40.0426606
C	36.5088386	4.0254183	41.8076663	O	30.8584879	6.4551448	41.4743548
C	37.0051485	3.1532026	42.7595284	O	30.4338323	4.3546442	42.1572785
C	38.3820763	2.8422524	42.7860322	C	30.0747353	5.5027458	41.7717286
C	39.2392674	3.3827281	41.8519071	C	32.2718058	6.0615347	45.7389479
C	38.7719696	4.2600281	40.8196148	C	33.1371601	6.9754606	46.3123863
C	37.3664619	4.5834370	40.8018375	C	31.1759727	5.5136304	46.4851681
C	36.8771952	5.4161209	39.7545410	C	30.1984555	4.6615121	45.8949675
C	37.7245460	5.9149910	38.7942718	C	29.1521072	4.1687419	46.6370075
C	39.1163730	5.6321127	38.8250253	O	32.7913462	6.5880742	43.4998617
C	39.6440492	4.8106779	39.8195408	O	32.4370711	4.4305161	44.0351822
O	39.9356728	6.1630529	37.8751614	C	32.5168921	5.6616321	44.3175020
O	34.7309445	5.5811808	41.7111922	C	32.9870783	7.3345958	47.6699405
O	34.2521103	3.4193564	42.1224745	C	31.9733452	6.7904592	48.4296617
C	35.0526940	4.3707890	41.8794944	C	31.0260660	5.8700342	47.8740227
C	32.3627680	3.9448993	37.9615826	C	29.0290121	4.4667866	48.0207569
C	32.9939267	2.7896514	37.5365655	C	29.9497152	5.3085616	48.6419570
C	33.0570047	2.4933220	36.1580206	O	28.0051903	3.9297277	48.7403848
C	32.4783650	3.3375244	35.2330686	H	26.2591204	7.8930939	42.8936335
C	31.7748708	4.5235497	35.6232840	H	24.7993686	6.5287492	41.4904028
C	31.7108750	4.8184335	37.0315529	H	27.9480280	2.3139517	38.6165981
C	30.9568684	5.9506914	37.4561508	H	24.5472237	2.6890647	38.2231389
				H	36.3220887	2.7242047	43.4969023
				H	38.7701919	2.1681940	43.5561213

H	40.3011448	3.1223013	41.9024444	H	32.4282801	10.0090485	40.9821055
H	35.8152590	5.6592026	39.7084693	H	31.6886776	8.3919852	39.2520761
H	37.3257461	6.5520435	37.9959202	H	36.2275697	10.4582617	38.8728541
H	33.4606735	2.1309378	38.2735529	H	34.6623184	10.8165720	38.1197444
H	33.5758822	1.5905623	35.8204753	H	35.6017015	8.6073366	37.3368987
H	32.5569709	3.0741790	34.1733200	H	35.5471910	8.0061509	39.0090308
H	30.8681058	6.1714259	38.5205503	H	33.1502153	8.8461865	37.2555530
H	29.7411804	7.6252284	36.8642511	H	33.5034993	7.2176899	37.8750019
H	28.7141249	7.4305296	43.0164531	H	35.2092262	9.8904354	41.0024403
H	29.4061438	3.6578444	40.0894527	H	28.7199653	11.5517590	42.2127763
H	33.9419421	7.4018992	45.7081596	H	28.8696738	12.5037551	44.4980426
H	30.2691675	4.3985289	44.8389777	H	30.2642759	11.3849191	46.2518033
H	28.4035596	3.5245272	46.1601975	H	31.5140738	9.2876932	45.6605423
H	29.7947197	7.2261886	33.4421731	H	31.3917306	8.3556584	43.3823007
H	39.4183637	6.7162637	37.2677968	H	30.2184338	8.3565928	41.2726441
H	33.6851408	8.0456252	48.1226486	H	29.1804010	9.6085013	40.7910083
H	31.8898187	7.0847618	49.4806366	H	24.4736423	4.5553818	39.8461832
H	27.4706235	3.3525018	48.1713943	H	40.7181556	4.6259844	39.8353635
C	32.7661149	8.5853554	39.3318892	H	31.2023174	5.2016945	33.6114056
C	33.2081440	9.5562507	40.3572490	H	29.8665703	5.4802361	49.7151211
C	34.5318545	10.2894597	40.2243280				
C	35.1716334	10.1363655	38.8310974		(S,S)-2-RC (open-shell singlet)		
C	35.0641342	8.7006314	38.2981097	C	26.9386888	7.1242977	41.7121897
C	33.5959262	8.2928532	38.1049101	C	26.0457978	6.1838344	41.2389740
O	33.3289835	8.1327837	40.5733902	C	26.4736586	4.9024402	40.7600254
C	30.0382885	9.8796878	42.6315353	C	27.8825112	4.6028587	40.8392097
C	29.3361027	11.0547782	42.9709297	C	27.4550030	2.4362731	39.8201738
C	29.4236205	11.5887076	44.2596184	C	26.0638463	2.7176459	39.7467595
C	30.2034261	10.9670099	45.2421200	C	25.5667964	3.9346162	40.2036483
C	30.9022899	9.7994402	44.9097889	O	25.3358824	1.7002185	39.2044153
C	30.8290880	9.2605282	43.6238032	Cu	33.0527143	6.0109656	41.4985541
N	29.9972412	9.3532273	41.3399832	Cu	32.4277136	3.5582454	42.0472308
H	34.3768802	11.3575851	40.4594692	C	36.6001762	3.6919331	41.7509065

C	37.1229257	2.7376059	42.6034401	C	32.3455788	5.6889833	45.6802565
C	38.5025896	2.4379204	42.5642622	C	33.1799877	6.6380076	46.2422384
C	39.3330224	3.0786125	41.6695200	C	31.3165907	5.0584719	46.4550517
C	38.8332392	4.0441439	40.7355340	C	30.3887773	4.1381365	45.8881565
C	37.4244827	4.3436644	40.7747755	C	29.4020312	3.5677744	46.6561326
C	36.8939477	5.2466734	39.8086100	O	32.7338052	6.3067316	43.4400138
C	37.7111817	5.8428374	38.8786239	O	32.5610874	4.1151736	43.9297048
C	39.1104199	5.5972147	38.8666054	C	32.5593272	5.3422495	44.2401399
C	39.6735536	4.7045026	39.7760640	C	33.0650804	6.9571256	47.6128565
O	39.9021651	6.2332787	37.9583951	C	32.1020937	6.3533592	48.3927995
O	34.8535639	5.2701670	41.8787890	C	31.1823267	5.3977778	47.8498494
O	34.3307237	3.0830654	41.9876261	C	29.2787255	3.8735193	48.0380200
C	35.1517584	4.0418340	41.8810051	C	30.1484531	4.7842550	48.6349748
C	32.6164222	3.9141936	37.8350214	O	28.3008707	3.2823481	48.7789383
C	33.1889805	2.7552431	37.3450057	H	26.5738219	8.0991212	42.0500600
C	33.1662719	2.4975611	35.9575304	H	24.9834180	6.4451424	41.2202294
C	32.5463786	3.3759157	35.0933850	H	27.7975648	1.4726521	39.4342702
C	31.9042045	4.5708343	35.5560572	H	24.3945626	1.9167249	39.1119618
C	31.9531806	4.8416008	36.9691170	H	36.4622082	2.2366380	43.3157824
C	31.2987181	6.0071571	37.4658494	H	38.9150743	1.6945710	43.2538088
C	30.6235197	6.8483037	36.6177442	H	40.3983894	2.8275640	41.6715143
C	30.5647166	6.5862763	35.2221532	H	35.8251393	5.4632972	39.7910641
C	31.2152419	5.4833197	34.6792949	H	37.2813065	6.5259531	38.1361707
O	29.8358705	7.5157562	34.5321738	H	33.6685874	2.0565948	38.0357572
O	33.1901406	5.3028889	39.6496936	H	33.6398329	1.5920062	35.5650419
O	32.3057159	3.2779913	40.0877612	H	32.5416522	3.1317058	34.0262978
C	32.7096985	4.1849629	39.3026569	H	31.3214095	6.2311271	38.5339127
C	28.7796234	5.5915319	41.3635862	H	30.1010216	7.7306562	36.9946112
C	28.3195133	6.8371315	41.7580406	H	29.0326312	7.5790666	42.1251367
C	28.3378562	3.3455894	40.3428416	H	29.4006697	3.1048363	40.3709016
O	31.0561807	6.2161308	41.1974301	H	33.9384140	7.1182069	45.6183443
O	30.5584537	4.1911504	42.0384161	H	30.4516699	3.8865719	44.8290121
C	30.2410349	5.3112468	41.5368597	H	28.6958033	2.8636936	46.1999622

H	29.6839229	7.2634387	33.6080400	H	27.4180401	7.0730571	35.4503148
H	39.3613508	6.8235624	37.4092327	H	28.2603215	6.3786305	37.6533533
H	33.7482871	7.6869340	48.0585606	H	27.5034961	6.8461862	39.0954242
H	32.0420929	6.6220767	49.4520397	H	24.5057951	4.1672335	40.1129195
H	27.7925444	2.6687721	48.2242484	H	40.7535569	4.5574114	39.7712217
C	32.4953853	8.9981203	40.5854095	H	31.2430367	5.3249778	33.6012310
C	33.0735102	9.0901739	41.9430149	H	30.0362972	4.9994483	49.6976034
C	34.1266788	10.1223666	42.2742162				
C	34.8409852	10.6421789	41.0163951	RCext1			
C	33.8213619	11.0905679	39.9590791	C	27.1164496	7.4277875	41.6356270
C	32.9305943	9.9317242	39.4707004	C	26.2012760	6.5062191	41.1695765
O	33.5133271	8.0646831	41.0285576	C	26.5898806	5.1897635	40.7613574
C	26.5367026	7.4625645	37.3947624	C	27.9855728	4.8438371	40.8813919
C	25.3972883	7.9761743	38.0543373	C	27.5057495	2.6670896	39.9082948
C	24.2836737	8.4041740	37.3288231	C	26.1225088	2.9825299	39.8245483
C	24.2700129	8.3407508	35.9288761	C	25.6540615	4.2265829	40.2398178
C	25.4070447	7.8532267	35.2684960	O	25.3710003	1.9642227	39.3075551
C	26.5268035	7.4227162	35.9815755	Cu	33.1700484	6.0581304	41.6506438
N	27.6473272	7.0483948	38.1101958	Cu	32.4485015	3.6274648	42.1993203
H	34.8479394	9.6764997	42.9842579	C	36.6480858	3.6345715	41.9899442
H	32.4966424	8.6855825	42.7847821	C	37.2057102	2.9135852	43.0267200
H	31.5178230	8.5109717	40.4809651	C	38.5990002	2.6725868	43.0424931
H	35.4830244	9.8424922	40.6034767	C	39.4053867	3.1368970	42.0253778
H	35.5049513	11.4813627	41.2891896	C	38.8674855	3.8534469	40.9060625
H	33.1816093	11.8796247	40.4019207	C	37.4479202	4.0898164	40.8921241
H	34.3338899	11.5526340	39.0965908	C	36.8760421	4.7432958	39.7639532
H	33.4649184	9.3184548	38.7211886	C	37.6639648	5.1688495	38.7207101
H	32.0314401	10.3273503	38.9657418	C	39.0733113	4.9844191	38.7461834
H	33.6289451	10.9579933	42.8041119	C	39.6774402	4.3308250	39.8193777
H	25.3908595	8.0170045	39.1472575	O	39.8346572	5.4430874	37.7140989
H	23.4109919	8.7883087	37.8689496	O	34.9486248	5.2408385	41.9879522
H	23.3962814	8.6785467	35.3629887	O	34.3473153	3.0797020	42.1883701
H	25.4257477	7.8127989	34.1734276	C	35.1989323	4.0052481	42.0594711

C	32.6100903	3.8983514	37.9909584	C	30.5481807	4.9040177	52.4634045
C	33.0252742	2.6649609	37.5204283	C	29.5978822	5.8887838	52.8834224
C	33.0316125	2.4103255	36.1327136	C	28.8690536	6.6127591	51.9751683
C	32.5946936	3.3711295	35.2442453	C	29.0481783	6.4222548	50.5799818
C	32.1060372	4.6452476	35.6818140	C	29.9323102	5.4551556	50.1126152
C	32.1212969	4.9081932	37.0979526	O	28.3103322	7.2178923	49.7773735
C	31.6005912	6.1515849	37.5654725	C	33.4438020	6.6775937	47.8771426
C	31.1193089	7.0867727	36.6852338	C	32.3358936	6.2551986	48.5826508
C	31.1237990	6.8480591	35.2840880	C	31.2462316	5.6065767	47.9300165
C	31.6036969	5.6450597	34.7756016	C	29.0149292	4.6336104	47.9523383
O	30.6237381	7.8917770	34.5574480	C	30.0634706	5.2317866	48.6457527
O	33.2604220	5.2577277	39.8038138	O	27.8980548	4.3001753	48.6476344
O	32.3069532	3.2719215	40.2536477	H	26.7820974	8.4288991	41.9260007
C	32.7264901	4.1619272	39.4570793	H	25.1505997	6.8077978	41.1067648
C	28.9055120	5.8122056	41.4075573	H	27.8249186	1.6868919	39.5439415
C	28.4799410	7.0859111	41.7467711	H	24.4274842	2.1815778	39.2497002
C	28.4086898	3.5615611	40.4223985	H	36.5699137	2.5600519	43.8431916
O	31.2065283	6.3665898	41.3438021	H	39.0429002	2.1233920	43.8787065
O	30.6130042	4.3549148	42.1544194	H	40.4808655	2.9414965	42.0779662
C	30.3469006	5.4859676	41.6432556	H	35.7976477	4.9094540	39.7179937
C	32.5305236	5.7624279	45.8317810	H	37.2047075	5.6625032	37.8557344
C	33.5358555	6.4525427	46.4841648	H	33.3671500	1.9075586	38.2305312
C	31.3514421	5.3392976	46.5238229	H	33.3874138	1.4448312	35.7590439
C	30.2591783	4.7040940	45.8644869	H	32.6191685	3.1346127	34.1754143
C	29.1195151	4.3739529	46.5601414	H	31.5671461	6.3586188	38.6362643
O	32.9380974	6.3977560	43.5932304	H	30.7065135	8.0365689	37.0362908
O	32.5960269	4.2187963	44.0659989	H	29.2086507	7.8086983	42.1211999
C	32.7018327	5.4406125	44.3814259	H	29.4631802	3.2885675	40.4697772
C	31.3406746	4.1056965	53.3500137	H	34.4056597	6.7998684	45.9189928
C	32.1505989	3.0824344	52.8913770	H	30.3178542	4.4798534	44.7972696
C	32.2357870	2.8346773	51.5013360	H	28.2797093	3.8982466	46.0399224
C	31.5318421	3.6119161	50.6068579	H	30.5918635	7.7060749	33.6058633
C	30.6748927	4.6616063	51.0490635	H	39.2680648	5.8626339	37.0464305

H	32.7397202	2.4669018	53.5798075	H	36.5114751	7.2733113	40.5298636
H	32.8714918	2.0209971	51.1392532	H	38.4154725	8.0640328	41.8999367
H	31.6193565	3.4168436	49.5357673	H	38.0371605	9.6828426	43.7753369
H	29.4251867	6.0805052	53.9461951	H	35.7160256	10.4911958	44.2474738
H	28.1428187	7.3621948	52.3005542	H	33.8067351	9.6897785	42.8700343
H	34.2561779	7.1947914	48.3977442	H	34.1902054	7.6663480	39.8881730
H	32.2742711	6.4257717	49.6596918	H	33.1487368	8.6001040	40.7929015
H	27.2307641	3.9254684	48.0494762	H	24.5945804	4.4690724	40.1575666
H	28.6563682	7.2557793	48.8552751	H	40.7609839	4.2127638	39.8271983
C	28.9998300	11.0855523	47.7111262	H	31.5963319	5.4538607	33.7025428
C	29.2663525	9.8038513	48.4698021	H	31.3359034	4.3011934	54.4223125
C	30.5659713	9.1141311	48.3577497				
C	31.6773627	9.6456738	47.4663258	RCext2			
C	31.4176982	11.0821148	46.9783440	C	26.8985670	7.1413500	42.5026840
C	29.9637269	11.2806339	46.5307715	C	26.0378840	6.3429930	41.7772270
O	29.3990049	8.6091862	47.6785761	C	26.4988280	5.2064340	41.0378220
C	35.0433444	8.4621817	41.5871809	C	27.9048140	4.8994750	41.1066590
C	36.3409391	7.9996438	41.3280873	C	27.5587240	3.0327780	39.5874130
C	37.4090318	8.4387915	42.1124628	C	26.1685490	3.3193950	39.5204610
C	37.1975167	9.3389776	43.1633199	C	25.6307600	4.3851730	40.2366550
C	35.8991301	9.7904122	43.4262685	O	25.4821230	2.4589120	38.7115390
C	34.8243009	9.3527891	42.6470029	Cu	33.0479980	6.0849930	41.9312830
N	33.9409953	7.9569426	40.8362188	Cu	32.3816740	3.6129850	42.4111720
H	32.6339229	9.5917240	48.0145464	C	36.5446410	3.6037700	42.1445120
H	28.6800947	9.6499756	49.3867098	C	37.0879750	2.7815610	43.1127980
H	30.8776419	8.4749520	49.1941943	C	38.4743310	2.5068530	43.1070640
H	32.1141815	11.3297456	46.1568620	C	39.2901140	3.0364510	42.1300850
H	31.6352851	11.7946900	47.7990318	C	38.7679470	3.8560120	41.0759330
H	29.8247119	12.2889344	46.1010350	C	37.3541590	4.1323970	41.0853760
H	29.7197703	10.5533288	45.7352334	C	36.8020600	4.8875150	40.0121350
H	27.9477700	11.0948755	47.3687710	C	37.5995570	5.3586950	38.9972520
H	29.1099802	11.9244787	48.4270900	C	39.0021500	5.1359620	39.0053280
H	31.7768564	8.9573807	46.6071763	C	39.5900980	4.3911430	40.0265050

O	39.7750740	5.6541260	38.0092730	C	32.0097930	3.2470740	52.8270510
O	34.8196230	5.1963040	42.1463070	C	32.0031290	2.9554640	51.4439790
O	34.2601210	3.0392800	42.4412720	C	31.1628010	3.6383070	50.5920650
C	35.0973130	3.9702410	42.2493090	C	30.2672640	4.6398020	51.0672690
C	32.6580950	4.0639140	38.1864260	C	30.2484850	4.9363140	52.4779290
C	33.1707220	2.8399120	37.7896510	C	29.2704430	5.8709610	52.9452840
C	33.2435980	2.5166910	36.4190710	C	28.3441320	6.4151460	52.0910010
C	32.7694840	3.3965240	35.4681350	C	28.3690640	6.1297880	50.7008700
C	32.1869600	4.6554860	35.8229780	C	29.3712160	5.3198350	50.1653350
C	32.1464420	4.9961810	37.2238310	O	27.3979260	6.6964790	49.9424530
C	31.5461740	6.2321350	37.6040400	C	32.9862670	6.6535360	48.1875890
C	31.0371550	7.0871270	36.6604450	C	31.8108460	6.2584740	48.7928170
C	31.0868050	6.7678060	35.2764790	C	30.7928200	5.5729420	48.0657790
C	31.6464700	5.5671150	34.8481120	C	28.5342810	4.7012150	47.8718100
O	30.5410580	7.7367850	34.4815860	C	29.5522460	5.1851680	48.6887960
O	33.0592220	5.5148540	40.0208070	O	27.3143050	4.4695400	48.4393390
O	32.3425800	3.4214180	40.4324360	H	26.5089120	8.0074690	43.0476070
C	32.6785600	4.3622430	39.6541650	H	24.9741500	6.6018720	41.7692110
C	28.7667380	5.7410590	41.8803170	H	27.9335650	2.1923430	38.9971610
C	28.2788240	6.8521720	42.5450040	H	24.5419920	2.6834320	38.6330090
C	28.4007530	3.7927540	40.3564220	H	36.4407560	2.3694660	43.8915630
O	31.0482690	6.3630110	41.7942180	H	38.9028140	1.8731380	43.8902640
O	30.5225860	4.2471650	42.3555830	H	40.3606470	2.8105690	42.1611010
C	30.2250660	5.4314870	42.0102440	H	35.7335570	5.1048820	39.9906050
C	32.2684090	5.6852560	46.0882160	H	37.1533170	5.9330110	38.1758720
C	33.2207770	6.3661250	46.8242120	H	33.5287480	2.1401620	38.5487430
C	31.0158980	5.3044370	46.6718900	H	33.6751100	1.5596150	36.1092890
C	29.9594500	4.7285420	45.9070630	H	32.8405770	3.1075040	34.4146170
C	28.7389880	4.4697110	46.4867290	H	31.4827810	6.4962220	38.6600330
O	32.8896040	6.3255500	43.9033560	H	30.5666660	8.0320170	36.9461820
O	32.4415050	4.1533750	44.3074330	H	28.9661430	7.4853830	43.1120590
C	32.5589350	5.3636260	44.6551030	H	29.4629940	3.5464850	40.3876720
C	31.1652740	4.2253830	53.3195670	H	34.1557850	6.6691560	46.3437420

H	30.1061230	4.5030030	44.8489700	H	22.7829580	3.7734790	45.7428220
H	27.9187530	4.0596770	45.8886750	H	22.6322650	4.2561020	48.1598510
H	30.5685200	7.5101530	33.5389040	H	22.3760880	5.9859550	47.8501950
H	39.2143530	6.1195700	37.3676910	H	24.8158070	5.0606990	44.3126640
H	32.6836600	2.6885400	53.4859210	H	35.8667130	7.9974010	39.9219890
H	32.6620460	2.1743350	51.0522670	H	38.2589060	7.9289460	40.5831920
H	31.1608580	3.3894880	49.5293510	H	38.9034500	8.0909730	42.9956920
H	29.2170860	6.1415370	54.0039800	H	37.1159410	8.3096390	44.7324740
H	27.5596030	7.0824640	52.4568780	H	34.7160720	8.3321430	44.0629940
H	33.7400330	7.1972940	48.7662090	H	33.6011670	8.3579390	40.5989050
H	31.6413110	6.4932140	49.8446300	H	33.1683580	8.7306870	42.1666620
H	26.6225490	4.2127130	47.7716870	H	24.5670492	4.6130283	40.1683345
H	27.1680400	6.0496060	49.2382480	H	40.6701700	4.2446809	40.0187652
C	22.8846480	5.0797980	47.4668220	H	31.6547454	5.3111318	33.7886449
C	24.3739920	5.3362930	47.5252380	H	31.1981198	4.4107399	54.3931733
C	25.1243930	5.7233950	46.3144040				
C	24.4424610	5.8693820	44.9660940				
C	22.9061880	5.8294650	45.0524130	RCext3			
C	22.4052080	4.7675590	46.0403840	C	26.9815540	7.4357870	42.1244300
O	25.1987200	4.3732720	46.8347280	C	26.1004920	6.5520620	41.5350960
C	35.1477090	8.2150330	41.9492040	C	26.5378530	5.3173690	40.9547190
C	36.1457520	8.0932210	40.9764030	C	27.9408930	5.0009230	41.0499090
C	37.4907140	8.0479940	41.3532700	C	27.5474160	2.9502010	39.8044250
C	37.8504640	8.1322770	42.7012220	C	26.1585150	3.2406330	39.7244470
C	36.8486350	8.2551310	43.6721390	C	25.6457970	4.4060950	40.2877610
C	35.5028740	8.2901570	43.3038830	O	25.4468250	2.2817810	39.0601900
N	33.7683510	8.1439810	41.5834960	Cu	33.0816040	6.1273830	41.7486970
H	24.7759370	6.8105970	44.4983350	Cu	32.3695930	3.6942070	42.3071930
H	24.7759280	5.6327730	48.5064580	C	36.5419130	3.6407510	41.8911780
H	26.0659510	6.2764360	46.4471660	C	37.0582690	2.7277810	42.7908770
H	22.4884960	5.6558860	44.0454690	C	38.4376490	2.4212660	42.7708380
H	22.5322860	6.8187160	45.3824810	C	39.2749540	3.0169120	41.8518310
H	21.3018580	4.7138490	46.0242930	C	38.7814500	3.9374510	40.8698500
				C	37.3728570	4.2368450	40.8860670

C	36.8471520	5.0856730	39.8707080	O	32.9286350	6.3988860	43.7230360
C	37.6684020	5.6381730	38.9166710	O	32.6132510	4.2129450	44.1823900
C	39.0690660	5.3978810	38.9281350	C	32.7322500	5.4291660	44.5069320
C	39.6273860	4.5523490	39.8851870	C	31.0900690	4.1769010	53.3429740
O	39.8658550	5.9886360	37.9944390	C	31.6715650	3.0156560	52.8608770
O	34.8568110	5.2749130	41.9901100	C	31.6539910	2.7476150	51.4728020
O	34.2509970	3.1151430	42.1794750	C	31.0792650	3.6439160	50.5996930
C	35.1052490	4.0359790	42.0252010	C	30.4569210	4.8378800	51.0646510
C	32.4372070	3.9486000	38.1005430	C	30.4242440	5.1089070	52.4782500
C	32.8318820	2.6823160	37.7024630	C	29.6819020	6.2594730	52.9035870
C	32.8372180	2.3462730	36.3329020	C	29.0781690	7.1004220	52.0015190
C	32.4247760	3.2624600	35.3877230	C	29.1869910	6.8757580	50.6040330
C	31.9587140	4.5678330	35.7483330	C	29.8579440	5.7517030	50.1386080
C	31.9685480	4.9112290	37.1475520	O	28.6170250	7.7922310	49.7963220
C	31.4601280	6.1843770	37.5393300	C	33.5062480	6.6344070	48.0135750
C	30.9937020	7.0728600	36.6046730	C	32.3282520	6.3570880	48.6786410
C	31.0110280	6.7574530	35.2190340	C	31.2152800	5.7779250	48.0001930
C	31.4847870	5.5238070	34.7822460	C	28.9001830	5.0298600	47.9503930
O	30.5307110	7.7656150	34.4305650	C	29.9808870	5.5174890	48.6752810
O	33.0525360	5.3883250	39.8790460	O	27.7301330	4.8224760	48.6084450
O	32.1437610	3.3896810	40.3713920	H	26.6121160	8.3751800	42.5485670
C	32.5452260	4.2729740	39.5559420	H	25.0392330	6.8195250	41.5073920
C	28.8231560	5.9281570	41.6941810	H	27.9028890	2.0323730	39.3286010
C	28.3580100	7.1340560	42.1876630	H	24.5015380	2.4896930	38.9966510
C	28.4124140	3.7969200	40.4480730	H	36.3946090	2.2698970	43.5291000
O	31.1158440	6.5052870	41.5714410	H	38.8451320	1.7121790	43.4985240
O	30.5542240	4.4725160	42.3573650	H	40.3401990	2.7661640	41.8724990
C	30.2729710	5.6139610	41.8796090	H	35.7771350	5.2960660	39.8391420
C	32.5894400	5.7467110	45.9595680	H	37.2423740	6.2792690	38.1350650
C	33.6392110	6.3377920	46.6370540	H	33.1553440	1.9609480	38.4569820
C	31.3462760	5.4697310	46.6071700	H	33.1727370	1.3529100	36.0185570
C	30.2168380	4.9506570	45.9108410	H	32.4491560	2.9640010	34.3348370
C	29.0223600	4.7580710	46.5630430	H	31.4264010	6.4496180	38.5967460

H	30.5878650	8.0447450	36.8983460	H	30.7552930	9.1226620	48.4646250
H	29.0614660	7.8319760	42.6450120	H	31.6083500	9.7010110	44.2281080
H	29.4732950	3.5452760	40.4884820	H	31.1180190	11.0748460	45.2392250
H	34.5626690	6.5731820	46.0997830	H	29.2163830	10.2251240	43.8050460
H	30.2901620	4.7058900	44.8493700	H	29.3306110	8.6496010	44.6229980
H	28.1525870	4.3798660	46.0140310	H	27.5308090	9.9701910	45.6919200
H	30.5072970	7.5282010	33.4903630	H	28.6335660	11.3401580	45.9559650
H	39.3272700	6.5371830	37.4014920	H	31.6754110	8.1751080	46.0657500
H	32.1578640	2.2982870	53.5308090	H	36.3289130	7.8492760	40.4566080
H	32.1046170	1.8250850	51.0940010	H	38.3610290	8.2561660	41.8128040
H	31.0781290	3.4364610	49.5273690	H	38.1602130	9.0817530	44.1699320
H	29.5617650	6.4926910	53.9645020	H	35.8872730	9.4754970	45.1428610
H	28.5083860	7.9714970	52.3355180	H	33.8522350	9.0346200	43.7842430
H	34.3434290	7.0903880	48.5521040	H	33.9449180	8.1700670	40.2535190
H	32.2293450	6.5897270	49.7414940	H	32.9978510	8.7683610	41.4863130
H	27.0607010	4.4700650	47.9988880	H	24.5825349	4.6326588	40.2089638
H	28.8061420	7.6200760	48.8400100	H	40.7064327	4.3983464	39.8879804
C	28.5869460	10.2355890	45.8871290	H	31.5077637	5.2863307	33.7186937
C	29.0039480	9.6606620	47.2234830	H	31.1576135	4.3563453	54.4159623
C	30.3780550	9.1639540	47.4332100				
C	31.4251720	9.2136840	46.3351790	RC _{BINOL}			
C	30.9708430	9.9876120	45.0837600	C	32.1498739	5.5173470	46.1074779
C	29.4942860	9.7333350	44.7543510	C	33.0895520	6.2381857	46.8190598
O	29.2806070	8.2501230	47.2178120	C	30.8994434	5.1172876	46.6921639
C	34.9632700	8.4675490	42.0182010	C	29.8202745	4.5165932	45.9692292
C	36.2330890	8.2334470	41.4760900	C	28.6230786	4.2306176	46.5768115
C	37.3761540	8.4535900	42.2481290	C	31.1896364	4.1533062	53.3464409
C	37.2640080	8.9093950	43.5660970	C	32.0628960	3.2021222	52.8538673
C	35.9923570	9.1319620	44.1084690	C	32.0407890	2.8872599	51.4761852
C	34.8450670	8.9071810	43.3440770	C	31.1646963	3.5312089	50.6304205
N	33.7900510	8.1622770	41.2634500	C	30.2423384	4.5057958	51.1098770
H	32.3509910	9.6540420	46.7454430	C	30.2281198	4.8129154	52.5161449
H	28.4332010	9.9892720	48.1047960	C	29.2105915	5.6966068	52.9971119

C	28.2463975	6.1917889	52.1552608	C	29.1788982	8.4522712	46.0606720
C	28.2829390	5.9115782	50.7670396	C	28.2864497	8.1232488	47.0823687
C	29.3095925	5.1461957	50.2174273	N	26.0663805	8.2610219	48.0739632
O	27.2805090	6.4349142	50.0050988	H	24.9290834	6.5539397	44.4943719
C	32.8419388	6.5569829	48.1748667	H	24.7908480	5.5119690	48.5072829
C	31.6845418	6.1375666	48.7928305	H	26.1431501	6.0335229	46.4824508
C	30.6867468	5.4021110	48.0887254	H	22.5977318	5.5012527	44.0203043
C	28.4423673	4.4686725	47.9615807	H	22.6797793	6.6756316	45.3458356
C	29.4677510	4.9909981	48.7418398	H	21.3449931	4.6189169	45.9843260
O	27.2434200	4.2078191	48.5532688	H	22.8033841	3.6298644	45.7568634
H	34.0246911	6.5680071	46.3550537	H	22.6123878	4.1760094	48.1647172
H	29.9085027	4.2935505	44.9034357	H	22.4229104	5.9063797	47.7999535
H	27.8007517	3.7968413	46.0001450	H	24.8916607	4.7899935	44.3448377
H	32.7685049	2.6801886	53.5089524	H	25.5404409	9.8213243	45.9569862
H	32.7154494	2.1194202	51.0853161	H	27.1397929	10.4063427	44.1531779
H	31.1540428	3.2706411	49.5709371	H	29.4922359	9.5492668	44.2111235
H	29.1560465	5.9617174	54.0568976	H	30.1982837	8.0535238	46.0990798
H	27.4264689	6.8088480	52.5317834	H	28.6088425	7.4808780	47.9060803
H	33.5782922	7.1418416	48.7346038	H	25.2582821	8.8663101	48.1815199
H	31.5124940	6.3943354	49.8390185	H	26.4762171	7.9559514	48.9574377
H	26.5350717	3.9773058	47.8825935	H	32.3645462	5.2947745	45.0622776
H	27.0349172	5.7458793	49.3404214	H	31.2218428	4.3514764	54.4177755
C	22.9065076	4.9714852	47.4541651				
C	24.4009018	5.1825108	47.5338235		TS _{BINOL}		
C	25.1936574	5.5023751	46.3358530	C	32.1297379	4.9772959	46.0026662
C	24.5478979	5.6347663	44.9695591	C	33.0182828	5.7832470	46.6931833
C	23.0099839	5.6661914	45.0302449	C	30.9700255	4.4092758	46.6354201
C	22.4487794	4.6410048	46.0250552	C	29.9366707	3.6857059	45.9557578
O	25.2068299	4.1591881	46.9035877	C	28.8042333	3.2668483	46.6074983
C	26.9640871	8.6184782	47.0699291	C	31.3178150	3.7936258	53.4221657
C	26.5658241	9.4339638	45.9895518	C	32.2732272	2.8807619	53.0146369
C	27.4698774	9.7616253	44.9750015	C	32.3189607	2.4766930	51.6605629
C	28.7847832	9.2821567	45.0025675	C	31.4137423	2.9839041	50.7548521

C	30.4066418	3.9127216	51.1468819	C	27.0774557	8.7136731	45.7965093
C	30.3406478	4.3300623	52.5243616	C	28.1315954	9.1804189	45.0042379
C	29.2699464	5.1966056	52.9108810	C	29.4375454	8.7258160	45.2216698
C	28.2948362	5.5622641	52.0134980	C	29.6863827	7.8049913	46.2474110
C	28.3671026	5.1497576	50.6609758	C	28.6421528	7.3410882	47.0492610
C	29.4466751	4.4025444	50.1939084	N	26.2667350	7.2028968	47.5518240
O	27.3367515	5.4885144	49.8254648	H	26.3014653	6.2861444	44.9288082
C	32.8023537	6.0408149	48.0657417	H	25.1443410	4.6781971	48.6924615
C	31.7215519	5.4910860	48.7188443	H	27.0141400	5.1102017	46.9874570
C	30.7802053	4.6576929	48.0444744	H	23.9805287	5.7368616	43.9362993
C	28.6146836	3.5102321	47.9972820	H	23.9161301	6.7770577	45.3745230
C	29.6184680	4.1491024	48.7321129	H	22.2057508	4.9329571	45.5184516
O	27.4489067	3.1919392	48.5847989	H	23.5054801	3.7246701	45.3825365
H	33.8843156	6.2348088	46.1978523	H	22.9113494	3.9966574	47.7711662
H	29.9996460	3.4716597	44.8866992	H	23.2041692	5.7516008	47.6765130
H	28.0105731	2.7491324	46.0620271	H	25.9709769	4.5723966	44.7345000
H	32.9945483	2.4544617	53.7206675	H	26.0534016	9.0574851	45.6127542
H	33.0673932	1.7459860	51.3389850	H	27.9257331	9.8999179	44.2052048
H	31.4452999	2.6513258	49.7156890	H	30.2586764	9.0816426	44.5925812
H	29.1883444	5.5532088	53.9421575	H	30.6995414	7.4334172	46.4250895
H	27.4393012	6.1685557	52.3217261	H	28.8368107	6.6159559	47.8435685
H	33.4948719	6.6911939	48.6088477	H	25.4037710	7.7462443	47.5616181
H	31.5652812	5.7214849	49.7729070	H	26.5314372	6.8889732	48.4946615
H	26.5878470	3.0895351	47.8735253	H	32.3134522	4.8382783	44.9373073
H	27.1563382	4.6438502	49.3145572	H	31.3049032	4.0499931	54.4814936
C	23.5106214	4.7704013	47.2592421				
C	24.9802680	4.5345888	47.6049181	PC _{BINOL}			
C	25.9628962	5.2210292	46.7337746	C	31.7964786	5.5635190	45.9988796
C	25.6510767	5.4720562	45.2901472	C	32.4542760	6.6197564	46.6116701
C	24.1660359	5.7545308	45.0241352	C	30.7441788	4.8481312	46.6752513
C	23.2694255	4.7389899	45.7454669	C	29.9462643	3.7898284	46.1222628
O	25.5077505	3.3367365	47.1002310	C	28.9605831	3.1649630	46.8481947
C	27.3306028	7.7914496	46.8241538	C	31.1554031	4.0257844	53.3704045

C	32.0782522	3.1126353	52.8917628	C	25.4824273	5.3429846	45.2650110
C	32.0836669	2.7861118	51.5177229	C	24.0291357	5.8312763	45.3128076
C	31.1701761	3.3639054	50.6623322	C	23.1954239	4.9672680	46.2691708
C	30.1908031	4.2851889	51.1325029	O	25.2650030	3.0844203	47.3020285
C	30.1715497	4.6294369	52.5274154	C	27.4349760	7.4390635	46.7356438
C	29.1415319	5.5221623	52.9700713	C	27.4806038	8.7556917	47.2382431
C	28.2085525	6.0285390	52.1028862	C	28.4524092	9.6539388	46.7990147
C	28.2473801	5.7224562	50.7102578	C	29.4039463	9.2642362	45.8482915
C	29.2339952	4.8663356	50.2247557	C	29.3625148	7.9607670	45.3466845
O	27.3014698	6.3218446	49.9656225	C	28.3891778	7.0532659	45.7770720
C	32.1172233	7.0079404	47.9267711	N	26.4964621	6.5419978	47.2801442
C	31.1278559	6.3430869	48.6127242	H	26.0879225	5.9794669	44.5988537
C	30.4234317	5.2607205	48.0184926	H	25.6992978	4.5900085	48.6624826
C	28.6987315	3.5456272	48.1853903	H	27.0824264	4.7007786	46.5520983
C	29.4010223	4.5845412	48.7696737	H	23.5979022	5.8115877	44.2955256
O	27.7305667	2.8488927	48.8475028	H	23.9983599	6.8875878	45.6495905
H	33.2394712	7.1796985	46.0926554	H	22.1511562	5.3268393	46.3138035
H	30.0714362	3.4478054	45.0946043	H	23.1646125	3.9292313	45.8947349
H	28.3610520	2.3659885	46.4052861	H	23.2411865	4.3032314	48.3548198
H	32.8117555	2.6400123	53.5534253	H	23.7838165	5.9755012	48.1034528
H	32.8159132	2.0691571	51.1333670	H	25.5019831	4.3235927	44.8388335
H	31.1857292	3.1019417	49.6027822	H	26.7545064	9.0628012	47.9992078
H	29.0792544	5.8166628	54.0219129	H	28.4680576	10.6689089	47.2100482
H	27.4189157	6.6995777	52.4500671	H	30.1716328	9.9647925	45.5065602
H	32.6395412	7.8490956	48.3916753	H	30.1083505	7.6382588	44.6137452
H	30.8607236	6.6507851	49.6256253	H	28.3869305	6.0394401	45.3751564
H	26.0510444	2.6875392	47.7209880	H	25.6952739	7.0243808	47.6821300
H	27.6775828	3.1702253	49.7707131	H	27.3435349	6.1653507	48.9860910
C	23.8150572	4.9542275	47.6724523	H	32.0618105	5.3619717	44.9610722
C	25.2660237	4.4570903	47.6527501	H	31.1882454	4.2451400	54.4375835
C	26.1440325	5.2607104	46.6558702				