

Protein S-S bridges reduction : a Raman and computational study of lysozyme interaction with TCEP

*Catalina David, Sarah Foley and Mironel Enescu**

University of Franche-Comte, Laboratoire de Chimie Physique et Rayonnement, UMR CEA
E4, 16 route de Gray, 25030 Besancon, France.

E-mail: mironel.enescu@univ-fcomte.fr

Electronic Supplementary Information

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1. Gaussian 03 input files and optimised structures (QM)

%Chk=modelQM_cys6_127

B3LYP/6-311+G(d,p) Opt(GDIIS) Test

model QM

O	1		
C	4.341014	2.974944	-0.431932
C	3.866260	1.714018	0.264043
O	3.649901	1.669149	1.460546
N	3.703638	0.615459	-0.557295
C	2.988445	-0.576633	-0.123390
C	1.728551	-0.840055	-0.957585
S	0.452089	0.480186	-0.857474
C	3.858852	-1.853969	-0.085690
O	3.346046	-2.956398	-0.004304
N	5.202563	-1.657054	-0.130211
C	-4.537710	2.823246	0.382861
C	-4.097945	1.514322	-0.238067
O	-4.362917	1.231528	-1.404102
N	-3.401814	0.668394	0.569135
C	-2.790364	-0.566790	0.078875
C	-1.595996	-0.981476	0.933774
S	-0.264335	0.277225	1.101156
C	-3.833719	-1.718450	0.054930
O	-3.823664	-2.617298	0.879335
N	-4.724934	-1.626181	-0.962833
H	4.803948	2.785740	-1.403012
H	5.048300	3.492472	0.215806
H	3.479087	3.631425	-0.579723
H	3.777646	0.771858	-1.552367
H	2.696605	-0.394605	0.916112
H	1.970660	-0.898092	-2.024808
H	1.300217	-1.796849	-0.666835
H	5.588671	-0.728386	-0.091250
H	5.802674	-2.453237	0.020426
H	-4.241500	2.933211	1.427442
H	-5.624056	2.900434	0.306922
H	-4.108236	3.642155	-0.197908
H	-3.177220	0.966211	1.505988
H	-2.462344	-0.377530	-0.946786
H	-1.907876	-1.186422	1.961953
H	-1.176188	-1.908356	0.545652
H	-4.778508	-0.771374	-1.507915
H	-5.491364	-2.282340	-0.978909

%Chk=modelQM_cys30_115

B3LYP/6-311+G(d,p) Opt(GDIIS) Test

model QM

O	1		
C	-6.270177	1.629034	-0.955724
C	-5.314324	0.460622	-0.797675
O	-5.619005	-0.676870	-1.102409
N	-4.076496	0.771104	-0.274717

c	-2.985338	-0.205250	-0.236446
c	-1.667772	0.552142	-0.507115
s	-0.180333	-0.468844	-0.856365
c	-2.939490	-1.031605	1.067228
o	-2.329613	-2.081155	1.115873
n	-3.568960	-0.479764	2.145832
c	4.795846	-2.587217	-0.613630
c	4.214300	-1.213704	-0.888001
o	4.092778	-0.766714	-2.013607
n	3.838636	-0.496256	0.230421
c	2.992758	0.686787	0.130549
c	1.847973	0.662321	1.150833
s	0.689384	-0.762477	1.023172
c	3.743248	2.031063	0.266982
o	3.124297	3.081978	0.273254
n	5.093349	1.956783	0.387440
h	-5.903027	2.560961	-0.520711
h	-7.223189	1.366479	-0.493917
h	-3.842835	1.746868	-0.163592
h	-3.160563	-0.932596	-1.030842
h	-1.801471	1.139880	-1.420075
h	-1.433358	1.242314	0.306691
h	-4.253545	0.245969	2.009628
h	-3.637228	-1.051557	2.974340
h	5.126529	-2.719855	0.418698
h	5.632503	-2.759123	-1.290770
h	4.029798	-3.336274	-0.831935
h	3.821965	-0.997455	1.106841
h	2.572452	0.699786	-0.879484
h	2.238550	0.586646	2.172835
h	1.299677	1.599399	1.078041
h	5.570370	1.081316	0.248255
h	5.617739	2.817581	0.358717
h	-6.454681	1.784668	-2.021340

%Chk=modelQM_cys64_80

B3LYP/6-311+G(d,p) Opt(GDIIS) Test

model QM

0	1		
c	5.653016	-1.460282	-0.327343
c	4.317089	-0.999876	-0.878829
o	3.878360	-1.411422	-1.946389
n	3.631095	-0.112937	-0.105858
c	2.397009	0.500093	-0.551006
c	1.199597	-0.465488	-0.472881
s	0.845038	-1.144166	1.209726
c	2.222168	1.811788	0.237599
o	3.031020	2.151491	1.088965
n	1.157377	2.572433	-0.114048
c	-3.060882	3.097679	-0.533430
c	-2.479917	1.709923	-0.712442
o	-1.438061	1.520302	-1.330160
n	-3.197590	0.692998	-0.146366
c	-2.712948	-0.679660	-0.030846
c	-2.232952	-1.017775	1.388141
s	-0.777951	-0.047097	1.960705
c	-3.758335	-1.715907	-0.508129

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o	-3.738137	-2.862339	-0.103793
n	-4.671526	-1.262742	-1.412472
h	5.908039	-1.004009	0.630669
h	6.430430	-1.225048	-1.057246
h	5.628441	-2.545815	-0.211821
h	4.055215	0.320255	0.704751
h	2.500331	0.760438	-1.612559
h	0.296497	-0.009405	-0.874972
h	1.444190	-1.336439	-1.083490
h	0.395247	2.231004	-0.688296
h	0.996663	3.400411	0.439023
h	-2.479353	3.622573	0.229595
h	-2.957728	3.647768	-1.468943
h	-4.108478	3.093628	-0.226332
h	-3.981906	0.951529	0.435553
h	-1.873446	-0.765961	-0.724899
h	-3.022369	-0.805681	2.116765
h	-1.999680	-2.078441	1.452065
h	-4.589897	-0.349053	-1.826760
h	-5.279605	-1.943011	-1.842787

%Chk=modelQM_cys76_90
B3LYP/6-311+G(d,p) Opt(GDIIS) Test

model QM

0	1		
c	-4.810125	-1.945824	1.981555
c	-4.213099	-0.616367	1.562997
o	-4.106159	0.324013	2.328538
n	-3.802450	-0.539847	0.247041
c	-2.970429	0.556811	-0.237023
c	-1.783597	0.046763	-1.061735
s	-0.661735	-0.976681	-0.008909
c	-3.724781	1.624120	-1.067184
o	-3.110746	2.526022	-1.609757
n	-5.071694	1.481780	-1.140540
c	4.662237	3.030155	0.963034
c	3.999079	1.671357	1.044643
o	3.856228	1.082730	2.110979
n	3.560101	1.143093	-0.135131
c	2.869024	-0.148310	-0.204255
c	1.952712	-0.190276	-1.421990
s	0.771613	-1.601482	-1.398291
c	3.908396	-1.298745	-0.245866
o	4.227136	-1.843921	-1.289185
n	4.426058	-1.609753	0.968355
h	-5.075356	-2.588544	1.139629
h	-5.694308	-1.759753	2.591748
h	-4.081109	-2.470310	2.604920
h	-3.784166	-1.399035	-0.283320
h	-2.609861	1.091984	0.647185
h	-2.122035	-0.562699	-1.903733
h	-1.242592	0.907105	-1.449498
h	-5.546648	0.786471	-0.589300
h	-5.603112	2.219455	-1.576464
h	4.729664	3.423915	-0.052707
h	5.664537	2.958584	1.389715
h	4.092093	3.729437	1.578143
h	3.807189	1.600810	-0.999564

h	2.278606	-0.227537	0.710658
h	1.389791	0.739264	-1.510502
h	2.538735	-0.350072	-2.330532
h	4.257117	-0.997404	1.758315
h	5.191127	-2.266818	1.002787

2. Gaussian 03 input files and optimised structures (QM/MM)

```
%chk=model_cys6_127
# ONIOM(B3LYP/6-311+G(d,p):Amber) Opt(GDIIS, Micro, CalcFC)
```

model

5	1	0	1	0	1			
N-N3-0.0966				-14.26055	1.85315	2.58761	L	
H-H-0.2165				-13.66858	1.98279	1.77272	L	
H-H-0.2165				-13.69612	2.08327	3.39669	L	
H-H-0.2165				-15.0479	2.48386	2.53114	L	
C-CT--0.0015				-14.70549	0.43346	2.68432	L	
H-HP-0.118				-15.35731	0.34339	3.55403	L	
C-CT-0.0212				-15.52058	-0.00703	1.44326	L	
H-HC-0.0283				-15.79783	-1.05571	1.55569	L	
H-HC-0.0283				-16.44995	0.56475	1.41497	L	
C-CT--0.0048				-14.79345	0.18808	0.09876	L	
H-HC-0.0121				-14.75998	1.25541	-0.12064	L	
H-HC-0.0121				-13.76946	-0.17158	0.17378	L	
C-CT--0.0608				-15.48249	-0.51387	-1.0832	L	
H-HC-0.0633				-16.55497	-0.30906	-1.06066	L	
H-HC-0.0633				-15.07837	-0.10036	-2.00953	L	
C-CT--0.0181				-15.23844	-2.03049	-1.0899	L	
H-HP-0.1171				-14.16455	-2.22241	-1.14209	L	
H-HP-0.1171				-15.6243	-2.47481	-0.17297	L	
N-N3--0.03764				-15.89166	-2.6778	-2.24132	L	
H-H-0.03382				-15.52864	-2.28862	-3.10001	L	
H-H-0.03382				-15.7081	-3.67114	-2.22077	L	
H-H-0.03382				-16.88882	-2.52119	-2.19837	L	
C-C-0.7214				-13.49952	-0.47082	2.97401	L	
O-O--0.6013				-12.43995	0.06226	3.27311	L	
N-N--0.4157				-13.63822	-1.79912	2.91678	L	
H-H-0.2719				-14.54259	-2.19579	2.71616	L	
C-CT--0.0875				-12.49289	-2.72908	2.83398	L	
H-H1-0.0969				-11.7459	-2.42224	3.56807	L	
C-CT-0.2985				-12.93974	-4.16477	3.19102	L	
H-HC--0.0297				-13.42969	-4.11602	4.16418	L	
C-CT--0.3192				-13.94788	-4.76068	2.19816	L	
H-HC-0.0791				-13.49553	-4.87439	1.21245	L	
H-HC-0.0791				-14.26098	-5.74545	2.54913	L	
H-HC-0.0791				-14.83253	-4.13144	2.12203	L	
C-CT--0.3192				-11.7526	-5.12235	3.33528	L	
H-HC-0.0791				-11.01943	-4.71037	4.02942	L	
H-HC-0.0791				-12.10244	-6.07512	3.73576	L	
H-HC-0.0791				-11.27982	-5.30905	2.37087	L	
C-C-0.5973				-11.8446	-2.65226	1.44137	L	
O-O--0.5679				-12.5422	-2.38655	0.46187	L	
N-N--0.4157				-10.53216	-2.87665	1.35162	L	
H-H-0.2719				-10.02834	-3.14407	2.1856	L	
C-CT--0.0014				-9.73487	-2.8423	0.11769	L	
H-H1-0.0876				-10.3922	-2.94134	-0.74748	L	

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C-CT--0.0152	-8.9865	-1.50102	0.01886	L	
H-HC-0.0295	-8.2731	-1.44017	0.84193	L	
H-HC-0.0295	-8.41017	-1.48272	-0.90624	L	
C-CA--0.0011	-9.88217	-0.27499	0.05231	L	
C-CA--0.1906	-9.93793	0.52118	1.21232	L	
H-HA-0.1699	-9.32297	0.27903	2.06909	L	
C-CA--0.2341	-10.81564	1.61855	1.2757	L	
H-HA-0.1656	-10.86128	2.21702	2.1731	L	
C-C-0.3226	-11.64272	1.9224	0.17698	L	
O-OH--0.5579	-12.56316	2.91821	0.28647	L	
H-HO-0.3992	-12.58105	3.42727	-0.53229	L	
C-CA--0.2341	-11.56391	1.15005	-1.00212	L	
H-HA-0.1656	-12.1924	1.38011	-1.84953	L	
C-CA--0.1906	-10.68559	0.0492	-1.05894	L	
H-HA-0.1699	-10.6418	-0.56639	-1.94732	L	
C-C-0.5973	-8.73903	-4.01132	0.10349	L	
O-O--0.5679	-8.27329	-4.43738	1.15991	L	
N-N--0.4157	-8.3984	-4.53386	-1.0777	L	
H-H-0.2719	-8.77553	-4.09281	-1.9099	L	
C-CT--0.0252	-7.42177	-5.6252	-1.20866	L	
H-H1-0.0698	-7.69496	-6.43485	-0.5304	L	
H-H1-0.0698	-7.44206	-6.0041	-2.23026	L	
C-C-0.5973	-5.99503	-5.15918	-0.88936	L	
O-O--0.5679	-5.64579	-4.02043	-1.2005	L	
N-N--0.3479	-5.14182	-6.0279	-0.31833	L	H-H1-0.0923
H-H-0.2747	-5.51376	-6.93729	-0.08182	L	
C-CT--0.2637	-3.78266	-5.65773	0.1788	H	
H-H1-0.156	-3.93452	-5.07539	1.09104	H	
C-CT--0.0007	-2.98947	-6.92594	0.55947	L	H-H1-0.0
H-HC-0.0327	-3.63263	-7.59916	1.12924	L	
H-HC-0.0327	-2.66777	-7.43883	-0.34815	L	
C-CT-0.039	-1.76297	-6.57577	1.42813	L	
H-HC-0.0285	-1.14459	-5.83114	0.92519	L	
H-HC-0.0285	-2.1194	-6.13798	2.36165	L	
C-CT-0.0486	-0.88423	-7.78733	1.77513	L	
H-H1-0.0687	-0.20524	-7.49756	2.57838	L	
H-H1-0.0687	-1.50473	-8.6058	2.14115	L	
N-N2--0.05295	-0.05917	-8.2216	0.63582	L	
H-H-0.03456	0.77199	-7.673	0.46421	L	
C-CA-0.08076	-0.28177	-9.26663	-0.18147	L	
N-N2--0.08627	-1.34614	-10.07022	-0.03487	L	
H-H-0.04478	-2.00759	-9.90656	0.71016	L	
H-H-0.04478	-1.47892	-10.84881	-0.66478	L	
N-N2--0.08627	0.58643	-9.50875	-1.17182	L	
H-H-0.04478	1.39184	-8.91148	-1.29257	L	
H-H-0.04478	0.43825	-10.28939	-1.7955	L	
C-C-0.7341	-2.9959	-4.73952	-0.77015	H	
O-O--0.5894	-2.54536	-3.66689	-0.40796	H	
N-N--0.4157	-2.85264	-5.1598	-2.07569	H	
H-H-0.2719	-3.07306	-6.11864	-2.30487	H	
C-CT-0.0429	-2.00652	-4.38638	-2.96652	H	
H-H1-0.0766	-1.21992	-3.9572	-2.34907	H	
C-CT--0.079	-1.34357	-5.23126	-4.04823	H	
H-H1-0.091	-2.07035	-5.76233	-4.67173	H	
H-H1-0.091	-0.75372	-4.57849	-4.69032	H	
S-S--0.1081	-0.26069	-6.59961	-3.39793	H	
C-C-0.5973	-2.69847	-3.14648	-3.58089	H	
O-O--0.5679	-2.02138	-2.22239	-3.98642	H	
N-N--0.4157	-4.06286	-3.1745	-3.62039	H	
H-H-0.2719	-4.54103	-3.85793	-3.04265	H	
C-CT-0.0145	-4.8571	-1.96676	-3.88344	L	H-H-0.0145

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H-H1-0.0779	-4.53514	-1.53423	-4.83279	L
C-CT--0.0071	-6.33244	-2.39086	-4.02191	L
H-HC-0.0256	-6.42774	-3.01515	-4.91199	L
H-HC-0.0256	-6.607	-3.00193	-3.16779	L
C-CT--0.0174	-7.35714	-1.25131	-4.11781	L
H-HC-0.043	-7.27232	-0.59401	-3.25302	L
H-HC-0.043	-7.17271	-0.67033	-5.0222	L
C-C-0.6801	-8.77937	-1.81093	-4.14423	L
O-O--0.5838	-9.17879	-2.55773	-3.25473	L
O-OH--0.6511	-9.56804	-1.46101	-5.17701	L
H-HO-0.4641	-10.35352	-2.00117	-5.08435	L
C-C-0.5973	-4.63624	-0.89402	-2.79808	L
O-O--0.5679	-4.34127	0.25789	-3.10974	L
N-N--0.4157	-4.76482	-1.2758	-1.52364	L
H-H-0.2719	-5.03139	-2.2391	-1.35087	L
C-CT--0.0518	-4.43635	-0.45009	-0.35721	L
H-H1-0.0922	-5.08166	0.42929	-0.37564	L
C-CT--0.1102	-4.77539	-1.27823	0.90202	L
H-HC-0.0457	-5.8249	-1.56399	0.82542	L
H-HC-0.0457	-4.20309	-2.2044	0.89067	L
C-CT-0.3531	-4.59655	-0.62198	2.28432	L
H-HC--0.0361	-5.15094	-1.23517	2.99527	L
C-CT--0.4121	-3.14281	-0.61475	2.75003	L
H-HC-0.1	-2.54899	0.08318	2.16446	L
H-HC-0.1	-3.09919	-0.30833	3.79524	L
H-HC-0.1	-2.71478	-1.61336	2.66685	L
C-CT--0.4121	-5.17296	0.79231	2.35284	L
H-HC-0.1	-6.20329	0.79023	1.99914	L
H-HC-0.1	-5.15637	1.13777	3.38642	L
H-HC-0.1	-4.57807	1.47636	1.74701	L
C-C-0.5973	-2.98456	0.06456	-0.42995	L
O-O--0.5679	-2.75086	1.26838	-0.33741	L
N-N--0.4157	-2.01841	-0.8313	-0.65041	L
H-H-0.2719	-2.28025	-1.80982	-0.6435	L
C-CT-0.0337	-0.60859	-0.50308	-0.86702	L
H-H1-0.0823	-0.22793	-0.06074	0.05438	L
C-CT--0.1825	0.16475	-1.80408	-1.11178	L
H-HC-0.0603	-0.07516	-2.1973	-2.09621	L
H-HC-0.0603	1.23491	-1.61635	-1.07052	L
H-HC-0.0603	-0.07949	-2.53951	-0.34435	L
C-C-0.5973	-0.39781	0.53706	-1.99146	L
O-O--0.5679	0.29379	1.52988	-1.7825	L
N-N--0.4157	-1.00628	0.3508	-3.16894	L
H-H-0.2719	-1.51991	-0.51046	-3.31315	L
C-CT-0.0337	-0.97004	1.30806	-4.27974	L
H-H1-0.0823	0.06655	1.4138	-4.60067	L
C-CT--0.1825	-1.76468	0.74511	-5.4639	L
H-HC-0.0603	-2.81187	0.61505	-5.19365	L
H-HC-0.0603	-1.69838	1.43355	-6.30722	L
H-HC-0.0603	-1.34788	-0.21722	-5.76403	L
C-C-0.5973	-1.44226	2.71685	-3.87165	L
O-O--0.5679	-0.75146	3.69655	-4.15004	L
N-N--0.4157	-2.57932	2.83708	-3.17639	L
H-H-0.2719	-3.109	1.99351	-2.98377	L
C-CT-0.0337	-3.009	4.10609	-2.57954	L
H-H1-0.0823	-3.13996	4.82734	-3.38694	L
C-CT--0.1825	-4.36745	3.9143	-1.89351	L
H-HC-0.0603	-4.28126	3.21373	-1.06354	L
H-HC-0.0603	-4.72044	4.87308	-1.51213	L
H-HC-0.0603	-5.09253	3.53005	-2.612	L
C-C-0.5973	-1.93812	4.68793	-1.63049	L

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O-O--0.5679	-1.54668	5.84946	-1.7635	L
N-N--0.4157	-1.42308	3.87645	-0.70137	L
H-H-0.2719	-1.79903	2.93346	-0.64999	L
C-CT--0.0237	-0.31938	4.23224	0.20177	L
H-H1-0.088	-0.60894	5.13154	0.74076	L
C-CT-0.0342	-0.10273	3.1332	1.25141	L
H-HC-0.0241	-0.07014	2.15387	0.77684	L
H-HC-0.0241	0.84819	3.30115	1.75579	L
C-CT-0.0018	-1.20864	3.16373	2.30911	L
H-H1-0.044	-1.24824	4.16542	2.73886	L
H-H1-0.044	-2.16775	2.95141	1.83611	L
S-S--0.2737	-0.94997	1.98492	3.65573	L
C-CT--0.0536	-2.287	2.48922	4.76824	L
H-H1-0.0684	-3.24548	2.38325	4.26199	L
H-H1-0.0684	-2.27375	1.85976	5.65814	L
H-H1-0.0684	-2.14827	3.52871	5.06382	L
C-C-0.5973	1.00345	4.5928	-0.49695	L
O-O--0.5679	1.84226	5.24459	0.12148	L
N-N--0.3479	1.23614	4.22876	-1.76756	L
H-H-0.2747	0.56931	3.59516	-2.19832	L
C-CT--0.24	2.42143	4.68439	-2.52274	L
H-H1-0.1426	3.30434	4.38908	-1.96246	L
C-CT--0.0094	2.49722	4.01431	-3.90631	L
H-HC-0.0362	2.41838	2.9332	-3.77585	L
H-HC-0.0362	1.66936	4.35206	-4.52919	L
C-CT-0.0187	3.82026	4.33879	-4.62267	L
H-HC-0.0103	3.8135	5.38867	-4.91923	L
H-HC-0.0103	4.65279	4.17302	-3.93701	L
C-CT--0.0479	4.02202	3.46309	-5.87052	L
H-HC-0.0621	4.23489	2.43956	-5.56022	L
H-HC-0.0621	3.10234	3.45862	-6.45695	L
C-CT--0.0143	5.16116	3.95679	-6.77617	L
H-HP-0.1135	5.23835	3.28896	-7.63536	L
H-HP-0.1135	4.92814	4.95949	-7.13535	L
N-N3--0.03854	6.46604	3.98491	-6.0914	L
H-H-0.034	6.68481	3.0593	-5.7476	L
H-H-0.034	7.18342	4.28271	-6.73712	L
H-H-0.034	6.4248	4.62615	-5.31251	L
C-C-0.7341	2.47696	6.21063	-2.57685	L
O-O--0.5894	3.52459	6.79127	-2.29173	L
N-N--0.3479	1.32974	6.83424	-2.86989	L
H-H-0.2747	0.5528	6.20918	-3.0453	L
C-CT--0.2637	1.05707	8.27044	-2.68874	L
H-H1-0.156	1.8918	8.85606	-3.08114	L
C-CT--0.0007	-0.23558	8.66501	-3.42476	L
H-HC-0.0327	-1.06322	8.10467	-2.99322	L
H-HC-0.0327	-0.42258	9.72689	-3.25317	L
C-CT-0.039	-0.19986	8.41437	-4.94167	L
H-HC-0.0285	0.59789	9.01533	-5.38011	L
H-HC-0.0285	0.00746	7.36255	-5.14331	L
C-CT-0.0486	-1.53018	8.79051	-5.61198	L
H-H1-0.0687	-1.76576	9.83359	-5.39731	L
H-H1-0.0687	-1.41295	8.69064	-6.69161	L
N-N2--0.05295	-2.63533	7.91058	-5.18659	L
H-H-0.03456	-2.67629	7.00722	-5.63665	L
C-CA-0.08076	-3.57034	8.17982	-4.25443	L
N-N2--0.08627	-3.60749	9.35114	-3.60021	L
H-H-0.04478	-2.92366	10.0666	-3.80087	L
H-H-0.04478	-4.32186	9.51837	-2.90597	L
N-N2--0.08627	-4.48919	7.24908	-3.96685	L
H-H-0.04478	-4.47788	6.36192	-4.44927	L

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H-H-0.04478	-5.1956	7.43638	-3.26974	L
C-C-0.7341	0.93301	8.64029	-1.20561	L
O-O--0.5894	1.59599	9.55887	-0.74625	L
N-N--0.4157	0.03454	7.96881	-0.48022	L
H-H-0.2719	-0.47113	7.23324	-0.95919	L
C-CT--0.0518	-0.37272	8.31648	0.88616	L
H-H1-0.0922	-0.27507	9.39539	1.01853	L
C-CT--0.1102	-1.86111	7.94555	1.07978	L
H-HC-0.0457	-1.96566	6.86411	0.9976	L
H-HC-0.0457	-2.15931	8.22809	2.09081	L
C-CT-0.3531	-2.836	8.59585	0.0771	L
H-HC--0.0361	-2.54775	8.33663	-0.94071	L
C-CT--0.4121	-4.24849	8.06041	0.31048	L
H-HC-0.1	-4.58255	8.31401	1.31716	L
H-HC-0.1	-4.93309	8.49744	-0.41617	L
H-HC-0.1	-4.25352	6.97732	0.19125	L
C-CT--0.4121	-2.87084	10.1196	0.20093	L
H-HC-0.1	-1.90036	10.54006	-0.06065	L
H-HC-0.1	-3.61467	10.52961	-0.48206	L
H-HC-0.1	-3.12648	10.40799	1.22093	L
C-C-0.5973	0.54952	7.6688	1.94028	L
O-O--0.5679	0.15545	6.69816	2.59587	L
O-OH-0.0	1.77842	8.24273	2.08604	L
H-HO-0.0	2.31694	7.81164	2.75369	L
H-H-0.0	0.24023	9.20649	3.98283	L
N-N--0.4157	0.56113	10.01439	4.49736	L
H-H-0.2719	0.11091	10.91662	4.39321	L
C-CT--0.0252	1.71382	9.88506	5.39107	L
H-H1-0.0698	2.54401	10.46571	4.98802	L
H-H1-0.0698	1.45869	10.28995	6.37027	L
C-C-0.5973	2.18986	8.44128	5.58089	L
O-O--0.5679	3.38624	8.19054	5.69458	L
N-N--0.4157	1.26158	7.48238	5.60227	L
H-H-0.2719	0.30596	7.78199	5.45536	L
C-CT--0.0389	1.46608	6.02936	5.78685	L
H-H1-0.1007	2.1103	5.86228	6.64984	L
C-CT-0.3654	0.09943	5.36684	6.06182	L
H-H1-0.0043	0.19059	4.28151	6.00441	L
C-CT--0.2438	-0.43105	5.71698	7.45086	L
H-HC-0.0642	-0.58319	6.7925	7.54092	L
H-HC-0.0642	-1.38388	5.21165	7.60888	L
H-HC-0.0642	0.27536	5.38436	8.2112	L
O-OH--0.6761	-0.86436	5.81628	5.12909	L
H-HO-0.4102	-0.46342	5.79008	4.24499	L
C-C-0.5973	2.1414	5.35287	4.57997	L
O-O--0.5679	1.63749	4.3686	4.03986	L
N-N--0.4157	3.27381	5.88417	4.11719	L
H-H-0.2719	3.65153	6.66896	4.63884	L
C-CT-0.0341	3.78656	5.5945	2.77942	L
H-H1-0.0864	2.95834	5.78775	2.10388	L
C-CT--0.0316	4.90991	6.56982	2.40954	L
H-HC-0.0488	4.64707	7.57704	2.73579	L
H-HC-0.0488	5.84024	6.27602	2.89641	L
C-C-0.6462	5.0926	6.5857	0.89669	L
O-O--0.5554	5.86566	5.79388	0.36176	L
O-OH--0.6376	4.32196	7.46005	0.2166	L
H-HO-0.4747	4.2703	7.23051	-0.72606	L
C-C-0.5973	4.21701	4.12892	2.58417	L
O-O--0.5679	4.95681	3.57447	3.39613	L
N-N--0.4157	3.79107	3.52585	1.46532	L
H-H-0.2719	3.18939	4.10177	0.88481	L

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C-CT--0.0875	3.82774	2.07759	1.16294	L
H-H1-0.0969	3.04058	1.6272	1.76102	L
C-CT-0.2985	3.47701	1.80362	-0.30976	L
H-HC--0.0297	2.60841	2.40536	-0.54697	L
C-CT--0.3192	4.60072	2.1719	-1.2869	L
H-HC-0.0791	5.4353	1.47451	-1.19784	L
H-HC-0.0791	4.23063	2.11108	-2.30911	L
H-HC-0.0791	4.95466	3.18269	-1.0949	L
C-CT--0.3192	3.07498	0.34824	-0.5379	L
H-HC-0.0791	2.30916	0.06394	0.18222	L
H-HC-0.0791	2.67527	0.24442	-1.54522	L
H-HC-0.0791	3.93349	-0.31421	-0.42901	L
C-C-0.5973	5.10858	1.33828	1.53702	L
O-O--0.5679	5.0427	0.17889	1.92379	L
N-N--0.3479	6.267	1.98777	1.40448	L
H-H-0.2747	6.17525	2.9476	1.11421	L
C-CT--0.1354	7.6087	1.42241	1.58838	L
H-H1-0.1212	7.7441	0.66145	0.82055	L
C-CT--0.0414	8.6551	2.51723	1.31346	L
H-HC-0.081	8.5251	3.34604	2.01189	L
H-HC-0.081	9.65549	2.1016	1.45472	L
C-CC--0.0012	8.53011	3.00759	-0.11291	L
N-NA--0.1513	7.91508	4.17403	-0.54251	L
H-H-0.3866	7.52993	4.92237	0.03489	L
C-CR--0.017	7.66249	4.04573	-1.86141	L
H-H5-0.2681	7.05633	4.71696	-2.46022	L
N-NA--0.1718	8.10905	2.84663	-2.27533	L
H-H-0.3911	7.78677	2.33375	-3.11641	L
C-CW--0.1141	8.67288	2.1937	-1.20011	L
H-H4-0.2317	8.97207	1.14986	-1.20376	L
C-C-0.7341	7.80894	0.66409	2.91099	L
O-O--0.5894	8.54923	-0.31165	2.92625	L
N-N--0.4157	7.12649	1.05714	3.98882	L
H-H-0.2719	6.50934	1.85308	3.8961	L
C-CT-0.0337	7.11595	0.32605	5.26138	L
H-H1-0.0823	8.14611	0.09098	5.53562	L
C-CT--0.1825	6.55422	1.27187	6.3285	L
H-HC-0.0603	5.54206	1.578	6.06493	L
H-HC-0.0603	6.53436	0.76492	7.29431	L
H-HC-0.0603	7.18486	2.15754	6.41085	L
C-C-0.5973	6.35133	-1.02528	5.23543	L
O-O--0.5679	6.55587	-1.86099	6.11193	L
N-N--0.4157	5.47249	-1.26148	4.2527	L
H-H-0.2719	5.34638	-0.52987	3.56459	L
C-CT--0.0275	4.47484	-2.34593	4.23525	L
H-H1-0.1123	4.5642	-2.92212	5.15677	L
C-CT--0.005	3.05205	-1.74716	4.19699	L
H-HC-0.0339	2.7594	-1.65482	3.14922	L
H-HC-0.0339	2.36728	-2.46345	4.65249	L
C-C*-0.1415	2.811	-0.40539	4.82616	L
C-CW--0.1638	2.21222	0.62787	4.19492	L
H-H4-0.2062	1.8268	0.59405	3.18601	L
N-NA--0.3418	2.16599	1.72426	5.02855	L
H-H-0.3412	1.78661	2.62363	4.73806	L
C-CN-0.138	2.68646	1.43559	6.27034	L
C-CA--0.2601	2.83968	2.1951	7.43951	L
H-HA-0.1572	2.51336	3.22202	7.46957	L
C-CA--0.1134	3.42514	1.59719	8.56849	L
H-HA-0.1417	3.55594	2.16373	9.48073	L
C-CA--0.1972	3.84662	0.25647	8.51157	L
H-HA-0.1447	4.3037	-0.19841	9.38028	L

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C-CA--0.2387	3.68961	-0.49549	7.33058	L	
H-HA-0.17	4.03378	-1.51897	7.29841	L	
C-CB-0.1243	3.10666	0.07303	6.17674	L	
C-C-0.5973	4.62612	-3.34038	3.06404	L	
O-O--0.5679	3.74405	-4.17508	2.86366	L	
N-N--0.4157	5.7087	-3.2739	2.27689	L	
H-H-0.2719	6.37955	-2.56154	2.53014	L	
C-CT--0.0597	5.89008	-3.94268	0.96175	L	
H-H1-0.0869	4.9976	-3.7338	0.37193	L	
C-CT-0.1303	7.08725	-3.31337	0.20323	L	
H-HC-0.0187	7.19978	-3.83384	-0.74675	L	
C-CT--0.3204	6.77497	-1.85127	-0.14007	L	
H-HC-0.0882	6.73476	-1.26441	0.77079	L	
H-HC-0.0882	7.53983	-1.44236	-0.79906	L	
H-HC-0.0882	5.81775	-1.7845	-0.65672	L	
C-CT--0.043	8.41486	-3.45029	0.98404	L	
H-HC-0.0236	8.38001	-2.84395	1.88942	L	
H-HC-0.0236	8.54669	-4.49069	1.28202	L	
C-CT--0.066	9.64864	-3.04458	0.16792	L	
H-HC-0.0186	9.63148	-1.9755	-0.04294	L	
H-HC-0.0186	10.54806	-3.26889	0.74196	L	
H-HC-0.0186	9.67684	-3.60296	-0.76839	L	
C-C-0.5973	6.0087	-5.48747	0.97769	L	
O-O--0.5679	6.56744	-6.08942	0.05939	L	
N-N--0.3479	5.44746	-6.17143	1.9807	L	
H-H-0.2747	4.90798	-5.60484	2.62654	L	
C-CT--0.2637	5.36841	-7.63728	2.06843	L	
H-H1-0.156	6.37422	-8.04013	1.93871	L	
C-CT--0.0007	4.86647	-8.02586	3.47098	L	
H-HC-0.0327	5.49623	-7.52594	4.2091	L	
H-HC-0.0327	3.84144	-7.67436	3.60514	L	
C-CT-0.039	4.92438	-9.5442	3.71391	L	
H-HC-0.0285	4.25643	-10.04511	3.01226	L	
H-HC-0.0285	5.94013	-9.90306	3.53983	L	
C-CT-0.0486	4.49748	-9.92261	5.13875	L	
H-H1-0.0687	3.50441	-9.51731	5.33709	L	
H-H1-0.0687	4.4512	-11.01002	5.21252	L	
N-N2--0.05295	5.44209	-9.42213	6.14982	L	
H-H-0.03456	6.24617	-8.91824	5.80358	L	
C-CA-0.08076	5.32313	-9.57552	7.48086	L	
N-N2--0.08627	4.28687	-10.23283	8.02401	L	
H-H-0.04478	3.57084	-10.63015	7.43337	L	
H-H-0.04478	4.22527	-10.33311	9.02736	L	
N-N2--0.08627	6.26244	-9.05932	8.28397	L	
H-H-0.04478	7.04857	-8.56235	7.89003	L	
H-H-0.04478	6.18602	-9.16793	9.28534	L	
C-C-0.7341	4.48832	-8.18481	0.93636	L	
O-O--0.5894	3.26014	-8.15212	1.0149	L	
N-N--0.4157	5.11738	-8.65097	-0.14277	L	H-H1-0.0
H-H-0.2719	6.11575	-8.49727	-0.17535	L	
C-CT--0.0252	4.43144	-9.06494	-1.37028	H	
H-H1-0.0698	5.02092	-9.83644	-1.86226	H	
H-H1-0.0698	3.45254	-9.47802	-1.11045	H	
C-C-0.5973	4.30717	-7.88675	-2.31878	H	
O-O--0.5679	4.88153	-7.8747	-3.40064	H	
N-N--0.4157	3.56574	-6.83019	-1.87751	H	
H-H-0.2719	2.99796	-6.94802	-1.04727	H	
C-CT-0.0429	3.27194	-5.6746	-2.72562	H	
H-H1-0.0766	3.06051	-6.0415	-3.73482	H	
C-CT--0.079	2.08403	-4.87	-2.19432	H	
H-H1-0.091	2.37902	-4.33221	-1.28905	H	

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H-H1-0.091	1.79827	-4.11723	-2.92752	H	
S-S--0.1081	0.60455	-5.81139	-1.66432	H	
C-C-0.5973	4.49192	-4.70168	-2.79266	H	
O-O--0.5679	4.50864	-3.66702	-2.14603	H	
N-N--0.3479	5.484	-5.11491	-3.6184	H	
H-H-0.2747	5.43164	-6.04484	-4.0256	H	
C-CT--0.2637	6.68307	-4.31592	-3.89876	L	H-H--0.0706
H-H1-0.156	7.11573	-3.99177	-2.95337	L	
C-CT--0.0007	7.70971	-5.21199	-4.619	L	
H-HC-0.0327	7.78966	-6.13999	-4.04916	L	
H-HC-0.0327	7.34057	-5.47714	-5.61161	L	
C-CT-0.039	9.13651	-4.64379	-4.73624	L	
H-HC-0.0285	9.47099	-4.27041	-3.76679	L	
H-HC-0.0285	9.78584	-5.47942	-5.00093	L	
C-CT-0.0486	9.33081	-3.56947	-5.8182	L	
H-H1-0.0687	10.32623	-3.69371	-6.24644	L	
H-H1-0.0687	8.59776	-3.70732	-6.61468	L	
N-N2--0.05295	9.23903	-2.20215	-5.28355	L	
H-H-0.03456	9.0407	-2.11036	-4.29725	L	
C-CA-0.08076	9.41741	-1.07704	-5.99915	L	
N-N2--0.08627	9.66709	-1.11414	-7.31701	L	
H-H-0.04478	9.72039	-2.00034	-7.79813	L	
H-H-0.04478	9.79839	-0.25368	-7.82923	L	
N-N2--0.08627	9.34854	0.1098	-5.38443	L	
H-H-0.04478	9.13864	0.15375	-4.39647	L	
H-H-0.04478	9.48047	0.96122	-5.91087	L	
C-C-0.7341	6.30134	-3.06248	-4.69656	L	
O-O--0.5894	6.05849	-3.13988	-5.89879	L	
N-N--0.3821	6.23809	-1.92611	-4.00377	L	
H-H-0.2681	6.51097	-1.96038	-3.03206	L	
C-CT--0.2847	5.79112	-0.59997	-4.45455	L	
H-H1-0.1346	5.94683	-0.49185	-5.52681	L	
C-CT--0.2469	4.29104	-0.46601	-4.10512	L	
H-HC-0.0974	4.17789	-0.72742	-3.05293	L	
H-HC-0.0974	3.99559	0.57558	-4.21697	L	
C-CT-0.3706	3.32922	-1.33645	-4.93098	L	
H-HC--0.0374	3.6289	-2.38223	-4.89389	L	
C-CT--0.4163	1.93516	-1.2291	-4.32304	L	
H-HC-0.1038	1.62646	-0.18683	-4.29859	L	
H-HC-0.1038	1.22562	-1.81187	-4.9096	L	
H-HC-0.1038	1.96904	-1.62238	-3.31057	L	
C-CT--0.4163	3.25537	-0.876	-6.38538	L	
H-HC-0.1038	4.22708	-1.01969	-6.85757	L	
H-HC-0.1038	2.52574	-1.47783	-6.92548	L	
H-HC-0.1038	2.97672	0.17498	-6.43688	L	
C-C-0.8326	6.62788	0.49751	-3.78642	L	
O-O2--0.8199	7.41218	0.1704	-2.87346	L	
O-O2--0.8199	6.50659	1.68121	-4.1703	L	

%chk=model_cys30_115

ONIOM(B3LYP/6-311+G(d,p):Amber) Opt(GDIIS, Micro)

model

3	1	0	1	0	1		
H-H-0.0			13.407		-3.883	33.705	L
N-N--0.4157	13.560			-3.919		34.702	L
H-H-0.2719	13.518			-4.794		35.215	L
C-CT--0.0252		13.796			-2.678	35.447	L
H-H1-0.0698	12.835			-2.210		35.660	L

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H-H1-0.0698	14.272	-2.926	36.396	L	
C-C-0.5973	14.674	-1.649	34.718	L	
O-O--0.5679	14.972	-1.791	33.530	L	
N-N--0.4157	15.090	-0.599	35.434	L	
H-H-0.2719	14.815	-0.551	36.403	L	
C-CT--0.0014	15.815	0.565	34.898	L	
H-H1-0.0876	15.386	0.809	33.929	L	
C-CT--0.0152	15.545	1.787	35.795	L	
H-HC-0.0295	15.678	1.518	36.844	L	
H-HC-0.0295	16.268	2.567	35.567	L	
C-CA--0.0011	14.167	2.387	35.580	L	
C-CA--0.1906	13.993	3.384	34.598	L	
H-HA-0.1699	14.845	3.750	34.042	L	
C-CA--0.2341	12.716	3.924	34.355	L	
H-HA-0.1656	12.578	4.687	33.604	L	
C-C-0.3226	11.609	3.477	35.107	L	
O-OH--0.5579	10.375	3.997	34.882	L	
H-HO-0.3992	10.403	4.679	34.207	L	
C-CA--0.2341	11.786	2.489	36.099	L	
H-HA-0.1656	10.928	2.173	36.674	L	
C-CA--0.1906	13.063	1.945	36.336	L	
H-HA-0.1699	13.190	1.203	37.110	L	
C-C-0.5973	17.320	0.310	34.645	L	
O-O--0.5679	18.191	1.030	35.129	L	
N-N--0.4157	17.636	-0.675	33.800	L	
H-H-0.2719	16.868	-1.232	33.445	L	
C-CT--0.0249	18.956	-0.833	33.166	L	
H-H1-0.0843	19.715	-0.844	33.949	L	
C-CT-0.2117	19.013	-2.171	32.416	L	
H-H1-0.0352	20.002	-2.309	31.976	L	
H-H1-0.0352	18.838	-2.980	33.127	L	
O-OH--0.6546	18.028	-2.233	31.399	L	
H-HO-0.4275	18.433	-1.977	30.550	L	
C-C-0.5973	19.274	0.328	32.208	L	
O-O--0.5679	18.361	1.023	31.758	L	
N-N--0.4157	20.554	0.500	31.851	L	
H-H-0.2719	21.225	-0.116	32.284	L	
C-CT--0.0518	21.127	1.579	31.022	L	
H-H1-0.0922	21.318	2.428	31.682	L	
C-CT--0.1102	22.500	1.105	30.504	L	
H-HC-0.0457	23.089	0.818	31.378	L	
H-HC-0.0457	22.379	0.211	29.890	L	
C-CT-0.3531	23.294	2.169	29.713	L	
H-HC--0.0361	22.998	3.166	30.039	L	
C-CT--0.4121	24.793	2.007	29.970	L	
H-HC-0.1	25.127	1.016	29.661	L	
H-HC-0.1	25.347	2.760	29.408	L	
H-HC-0.1	25.007	2.148	31.030	L	
C-CT--0.4121	23.081	2.043	28.203	L	
H-HC-0.1	22.039	2.200	27.939	L	
H-HC-0.1	23.674	2.798	27.687	L	
H-HC-0.1	23.394	1.058	27.854	L	
C-C-0.5973	20.199	2.112	29.912	L	
O-O--0.5679	19.902	3.305	29.883	L	
N-N--0.4157	19.709	1.236	29.030	L	
H-H-0.2719	19.980	0.267	29.120	L	
C-CT--0.0252	18.854	1.601	27.897	L	
H-H1-0.0698	19.446	2.196	27.207	L	
H-H1-0.0698	18.536	0.702	27.379	L	
C-C-0.5973	17.608	2.418	28.249	L	
O-O--0.5679	17.204	3.273	27.466	L	

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N-N--0.4157	17.003	2.195	29.421	L	
H-H-0.2719	17.445	1.536	30.048	L	
C-CT-0.0143	15.855	2.979	29.884	L	
H-H1-0.1048	15.052	2.867	29.159	L	
C-CT--0.2041	15.364	2.489	31.255	L	
H-HC-0.0797	16.163	2.577	31.991	L	
H-HC-0.0797	14.545	3.132	31.578	L	
C-C-0.713	14.841	1.067	31.249	L	
O-O--0.5931	13.664	0.803	31.099	L	
N-N--0.9191	15.692	0.098	31.464	L	
H-H-0.4196	15.253	-0.763	31.753	L	
H-H-0.4196	16.665	0.312	31.643	L	
C-C-0.5973	16.181	4.475	29.921	L	
O-O--0.5679	15.434	5.275	29.366	L	
N-N--0.4157	17.297	4.828	30.560	L	
H-H-0.2719	17.859	4.086	30.950	L	
C-CT--0.0275	17.839	6.182	30.685	L	
H-H1-0.1123	17.071	6.825	31.118	L	
C-CT--0.005	19.031	6.146	31.652	L	
H-HC-0.0339	19.876	5.656	31.168	L	
H-HC-0.0339	19.331	7.171	31.873	L	
C-C*--0.1415	18.751	5.439	32.948	L	
C-CW--0.1638	18.987	4.130	33.193	L	
H-H4-0.2062	19.432	3.441	32.490	L	
N-NA--0.3418	18.561	3.811	34.468	L	
H-H-0.3412	18.625	2.880	34.879	L	
C-CN-0.138	18.028	4.908	35.111	L	
C-CA--0.2601	17.470	5.089	36.384	L	
H-HA-0.1572	17.410	4.264	37.078	L	
C-CA--0.1134	17.003	6.363	36.749	L	
H-HA-0.1417	16.577	6.526	37.731	L	
C-CA--0.1972	17.104	7.433	35.842	L	
H-HA-0.1447	16.756	8.414	36.136	L	
C-CA--0.2387	17.664	7.238	34.563	L	
H-HA-0.17	17.744	8.069	33.879	L	
C-CB-0.1243	18.139	5.970	34.164	L	
C-C-0.5973	18.218	6.774	29.321	L	
O-O--0.5679	17.835	7.900	29.015	L	
N-N--0.4157	18.916	6.006	28.475	L	H-H1--0.2272
H-H-0.2719	19.212	5.099	28.818	L	
C-CT--0.0875	19.226	6.389	27.068	H	
H-H1-0.0969	19.865	7.271	27.098	H	
C-CT-0.2985	20.015	5.252	26.376	L	H-H1-0.2985
H-HC--0.0297	19.441	4.330	26.434	L	
C-CT--0.3192	20.283	5.556	24.896	L	
H-HC-0.0791	20.835	6.491	24.798	L	
H-HC-0.0791	20.872	4.750	24.457	L	
H-HC-0.0791	19.347	5.628	24.343	L	
C-CT--0.3192	21.374	5.034	27.051	L	
H-HC-0.0791	21.244	4.737	28.090	L	
H-HC-0.0791	21.914	4.242	26.532	L	
H-HC-0.0791	21.965	5.950	27.013	L	
C-C-0.5973	17.957	6.794	26.287	H	
O-O--0.5679	17.811	7.867	25.720	H	
N-N--0.4157	16.957	5.854	26.285	H	
H-H-0.2719	17.158	4.974	26.751	H	
C-CT-0.0429	15.704	6.050	25.577	H	
H-H1-0.0766	15.915	6.298	24.536	H	
C-CT--0.079	14.901	4.735	25.633	H	
H-H1-0.091	15.591	3.910	25.425	H	
H-H1-0.091	14.467	4.566	26.620	H	

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S-S--0.1081	13.612	4.571	24.331	H	
C-C-0.5973	14.925	7.258	26.135	H	
O-O--0.5679	14.251	7.962	25.404	H	
N-N--0.4157	15.007	7.433	27.487	H	
H-H-0.2719	15.662	6.890	28.042	H	
C-CT-0.0337	14.418	8.588	28.157	L	H-H-0.0337
H-H1-0.0823	13.359	8.626	27.905	L	
C-CT--0.1825	14.523	8.440	29.679	L	
H-HC-0.0603	15.562	8.427	30.001	L	
H-HC-0.0603	14.019	9.278	30.162	L	
H-HC-0.0603	14.040	7.515	29.995	L	
C-C-0.5973	15.023	9.896	27.642	L	
O-O--0.5679	14.293	10.714	27.094	L	
N-N--0.4157	16.340	10.074	27.761	L	
H-H-0.2719	16.878	9.340	28.211	L	
C-CT-0.0337	17.066	11.221	27.219	L	
H-H1-0.0823	16.755	12.114	27.766	L	
C-CT--0.1825	18.559	11.005	27.479	L	
H-HC-0.0603	18.906	10.113	26.957	L	
H-HC-0.0603	19.118	11.872	27.133	L	
H-HC-0.0603	18.733	10.881	28.549	L	
C-C-0.5973	16.740	11.474	25.731	L	
O-O--0.5679	16.407	12.598	25.358	L	
N-N--0.3479	16.777	10.431	24.887	L	
H-H-0.2747	17.106	9.550	25.273	L	
C-CT--0.24	16.369	10.472	23.471	L	
H-H1-0.1426	17.074	11.121	22.952	L	
C-CT--0.0094	16.483	9.064	22.850	L	
H-HC-0.0362	17.412	8.617	23.205	L	
H-HC-0.0362	15.667	8.430	23.197	L	
C-CT-0.0187	16.544	9.020	21.310	L	
H-HC-0.0103	17.340	9.677	20.958	L	
H-HC-0.0103	16.826	8.002	21.036	L	
C-CT--0.0479	15.230	9.342	20.574	L	
H-HC-0.0621	15.077	8.598	19.791	L	
H-HC-0.0621	14.389	9.270	21.263	L	
C-CT--0.0143	15.258	10.728	19.914	L	
H-HP-0.1135	15.544	11.487	20.641	L	
H-HP-0.1135	16.007	10.744	19.120	L	
N-N3--0.03854	13.947	11.086	19.348	L	
H-H-0.034	13.255	11.100	20.084	L	
H-H-0.034	14.003	12.001	18.923	L	
H-H-0.034	13.682	10.406	18.650	L	
C-C-0.7341	14.982	11.104	23.297	L	
O-O--0.5894	14.867	12.135	22.646	L	
N-N--0.4157	13.919	10.504	23.829	L	
H-H-0.2719	14.066	9.662	24.376	L	
C-CT--0.0024	12.554	10.977	23.555	L	
H-H1-0.0978	12.527	11.334	22.524	L	
C-CT--0.0343	11.569	9.806	23.630	L	
H-HC-0.0295	11.720	9.253	24.559	L	
H-HC-0.0295	10.552	10.196	23.637	L	
C-CA-0.0118	11.698	8.883	22.433	L	
C-CA--0.1256	11.253	9.309	21.165	L	
H-HA-0.133	10.801	10.284	21.051	L	
C-CA--0.1704	11.400	8.471	20.045	L	
H-HA-0.143	11.060	8.802	19.073	L	
C-CA--0.1072	11.987	7.202	20.189	L	
H-HA-0.1297	12.092	6.551	19.332	L	
C-CA--0.1704	12.437	6.778	21.451	L	
H-HA-0.143	12.889	5.804	21.572	L	

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C-CA--0.1256	12.302	7.623	22.566	L
H-HA-0.133	12.672	7.304	23.527	L
C-C-0.5973	12.106	12.193	24.380	L
O-O--0.5679	11.265	12.948	23.905	L
N-N--0.4157	12.629	12.402	25.592	L
H-H-0.2719	13.319	11.742	25.935	L
C-CT-0.0145	12.309	13.571	26.425	L
H-H1-0.0779	11.233	13.746	26.370	L
C-CT--0.0071	12.679	13.316	27.898	L
H-HC-0.0256	13.734	13.048	27.962	L
H-HC-0.0256	12.552	14.245	28.456	L
C-CT--0.0174	11.828	12.223	28.574	L
H-HC-0.043	11.880	11.299	27.999	L
H-HC-0.043	12.238	12.026	29.564	L
C-C-0.6801	10.365	12.627	28.739	L
O-O--0.5838	9.465	11.982	28.209	L
O-OH--0.6511	10.099	13.699	29.513	L
H-HO-0.4641	9.223	13.996	29.265	L
C-C-0.5973	12.973	14.869	25.933	L
O-O--0.5679	12.324	15.910	25.962	L
N-N--0.4157	14.254	14.838	25.538	L
H-H-0.2719	14.771	13.972	25.623	L
C-CT--0.0249	15.042	16.051	25.236	L
H-H1-0.0843	14.365	16.872	24.996	L
C-CT-0.2117	15.832	16.457	26.490	L
H-H1-0.0352	16.372	17.386	26.300	L
H-H1-0.0352	15.134	16.628	27.310	L
O-OH--0.6546	16.751	15.445	26.868	L
H-HO-0.4275	17.651	15.807	26.756	L
C-C-0.5973	16.002	15.925	24.044	L
O-O--0.5679	16.806	16.824	23.814	L
N-N--0.4157	15.959	14.814	23.299	L
H-H-0.2719	15.238	14.140	23.517	L
C-CT-0.0143	17.016	14.355	22.389	L
H-H1-0.1048	16.928	13.274	22.313	L
C-CT--0.2041	16.776	14.901	20.973	L
H-HC-0.0797	15.716	14.830	20.733	L
H-HC-0.0797	17.073	15.949	20.921	L
C-C-0.713	17.536	14.089	19.940	L
O-O--0.5931	17.045	13.109	19.405	L
N-N--0.9191	18.771	14.428	19.668	L
H-H-0.4196	19.255	13.890	18.975	L
H-H-0.4196	19.211	15.130	20.251	L
C-C-0.5973	18.426	14.590	22.967	L
O-O--0.5679	19.301	15.188	22.341	L
N-N--0.4157	18.633	14.062	24.175	L
H-H-0.2719	17.820	13.632	24.604	L
C-CT--0.0024	19.810	14.260	25.021	L
H-H1-0.0978	19.602	13.758	25.964	L
C-CT--0.0343	21.046	13.559	24.421	L
H-HC-0.0295	21.378	14.093	23.530	L
H-HC-0.0295	21.860	13.605	25.146	L
C-CA-0.0118	20.801	12.104	24.049	L
C-CA--0.1256	20.950	11.090	25.013	L
H-HA-0.133	21.279	11.338	26.012	L
C-CA--0.1704	20.665	9.753	24.683	L
H-HA-0.143	20.775	8.978	25.428	L
C-CA--0.1072	20.240	9.422	23.385	L
H-HA-0.1297	20.025	8.394	23.132	L
C-CA--0.1704	20.106	10.430	22.414	L
H-HA-0.143	19.795	10.179	21.409	L

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C-CA--0.1256	20.387	11.767	22.745	L
H-HA-0.133	20.283	12.540	21.996	L
C-C-0.5973	19.991	15.743	25.390	L
O-O--0.5679	19.353	16.164	26.360	L
O-OH-0.0	20.840	16.497	24.630	L
H-HO-0.0	20.897	17.408	24.925	L
H-H-0.0	6.076	9.372	33.897	L
N-N--0.4157	5.961	10.063	34.624	L
H-H-0.2719	5.641	9.804	35.549	L
C-CT-0.0337	6.257	11.464	34.334	L
H-H1-0.0823	5.336	12.040	34.431	L
C-CT--0.1825	7.260	11.979	35.374	L
H-HC-0.0603	8.190	11.413	35.317	L
H-HC-0.0603	7.471	13.033	35.187	L
H-HC-0.0603	6.840	11.879	36.376	L
C-C-0.5973	6.770	11.665	32.897	L
O-O--0.5679	6.340	12.579	32.195	L
N-N--0.4157	7.702	10.820	32.447	L
H-H-0.2719	8.002	10.097	33.085	L
C-CT--0.0275	8.288	10.884	31.105	L
H-H1-0.1123	8.548	11.919	30.890	L
C-CT--0.005	9.582	10.058	31.065	L
H-HC-0.0339	9.332	9.015	31.265	L
H-HC-0.0339	9.981	10.120	30.056	L
C-C*-0.1415	10.707	10.436	31.977	L
C-CW--0.1638	10.963	11.664	32.488	L
H-H4-0.2062	10.366	12.553	32.317	L
N-NA--0.3418	12.113	11.610	33.253	L
H-H-0.3412	12.507	12.404	33.740	L
C-CN-0.138	12.668	10.347	33.254	L
C-CA--0.2601	13.816	9.803	33.849	L
H-HA-0.1572	14.458	10.418	34.461	L
C-CA--0.1134	14.118	8.446	33.636	L
H-HA-0.1417	14.996	8.007	34.088	L
C-CA--0.1972	13.276	7.657	32.833	L
H-HA-0.1447	13.525	6.621	32.659	L
C-CA--0.2387	12.122	8.213	32.248	L
H-HA-0.17	11.484	7.600	31.630	L
C-CB-0.1243	11.788	9.572	32.444	L
C-C-0.5973	7.294	10.429	30.017	L
O-O--0.5679	7.355	9.304	29.521	L
N-N--0.4157	6.375	11.316	29.626	L
H-H-0.2719	6.319	12.159	30.188	L
C-CT--0.0875	5.329	11.069	28.614	L
H-H1-0.0969	4.715	10.245	28.978	L
C-CT-0.2985	4.389	12.282	28.441	L
H-HC--0.0297	3.702	12.064	27.623	L
C-CT--0.3192	3.548	12.490	29.705	L
H-HC-0.0791	4.181	12.749	30.553	L
H-HC-0.0791	2.833	13.297	29.542	L
H-HC-0.0791	2.994	11.581	29.934	L
C-CT--0.3192	5.112	13.599	28.121	L
H-HC-0.0791	5.656	13.519	27.181	L
H-HC-0.0791	4.377	14.397	28.013	L
H-HC-0.0791	5.799	13.869	28.923	L
C-C-0.5973	5.871	10.601	27.259	L
O-O--0.5679	5.331	9.663	26.678	L
N-N--0.4157	6.938	11.215	26.742	L
H-H-0.2719	7.401	11.925	27.293	L
C-CT-0.0337	7.539	10.827	25.467	L
H-H1-0.0823	6.744	10.761	24.723	L

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C-CT--0.1825	8.509	11.920	25.011	L
H-HC-0.0603	9.388	11.949	25.653	L
H-HC-0.0603	8.823	11.720	23.987	L
H-HC-0.0603	8.017	12.893	25.032	L
C-C-0.5973	8.194	9.437	25.554	L
O-O--0.5679	7.930	8.582	24.712	L
N-N--0.4157	8.995	9.182	26.599	L
H-H-0.2719	9.139	9.950	27.244	L
C-CT--0.0275	9.539	7.853	26.927	L
H-H1-0.1123	10.249	7.563	26.153	L
C-CT--0.005	10.276	7.919	28.267	L
H-HC-0.0339	11.053	8.682	28.204	L
H-HC-0.0339	9.566	8.232	29.023	L
C-C*-0.1415	10.896	6.651	28.767	L
C-CW--0.1638	12.062	6.139	28.330	L
H-H4-0.2062	12.655	6.573	27.542	L
N-NA--0.3418	12.397	5.025	29.068	L
H-H-0.3412	13.304	4.580	29.000	L
C-CN-0.138	11.407	4.707	29.972	L
C-CA--0.2601	11.259	3.666	30.900	L
H-HA-0.1572	12.010	2.895	30.987	L
C-CA--0.1134	10.106	3.629	31.702	L
H-HA-0.1417	9.968	2.823	32.412	L
C-CA--0.1972	9.135	4.640	31.584	L
H-HA-0.1447	8.253	4.607	32.210	L
C-CA--0.2387	9.297	5.684	30.651	L
H-HA-0.17	8.543	6.453	30.565	L
C-CB-0.1243	10.433	5.740	29.813	L
C-C-0.5973	8.441	6.781	26.965	L
O-O--0.5679	8.491	5.815	26.206	L
N-N--0.3479	7.418	6.976	27.807	L
H-H-0.2747	7.466	7.821	28.371	L
C-CT--0.2637	6.213	6.138	27.924	L
H-H1-0.156	6.484	5.191	28.391	L
C-CT--0.0007	5.210	6.880	28.824	L
H-HC-0.0327	5.701	7.111	29.771	L
H-HC-0.0327	4.948	7.823	28.348	L
C-CT-0.039	3.912	6.113	29.122	L
H-HC-0.0285	3.517	5.672	28.207	L
H-HC-0.0285	4.119	5.313	29.834	L
C-CT-0.0486	2.838	7.052	29.691	L
H-H1-0.0687	2.555	7.764	28.914	L
H-H1-0.0687	1.958	6.466	29.960	L
N-N2--0.05295	3.312	7.788	30.875	L
H-H-0.03456	4.179	7.469	31.283	L
C-CA-0.08076	2.733	8.878	31.409	L
N-N2--0.08627	1.571	9.357	30.939	L
H-H-0.04478	1.108	8.899	30.168	L
H-H-0.04478	1.157	10.177	31.360	L
N-N2--0.08627	3.331	9.500	32.433	L
H-H-0.04478	4.207	9.152	32.797	L
H-H-0.04478	2.906	10.320	32.842	L
C-C-0.7341	5.619	5.799	26.554	L
O-O--0.5894	5.393	4.630	26.253	L
N-N--0.4157	5.369	6.817	25.736	L
H-H-0.2719	5.547	7.748	26.097	L
C-CT-0.0143	4.649	6.698	24.469	L
H-H1-0.1048	3.881	5.929	24.577	L
C-CT--0.2041	3.929	8.034	24.196	L
H-HC-0.0797	4.659	8.843	24.181	L
H-HC-0.0797	3.457	7.979	23.216	L

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C-C-0.713	2.840	8.370	25.211	L	
O-O--0.5931	2.617	7.704	26.211	L	
N-N--0.9191	2.094	9.422	24.970	L	
H-H-0.4196	1.376	9.588	25.652	L	
H-H-0.4196	2.230	9.995	24.159	L	
C-C-0.5973	5.525	6.253	23.276	L	
O-O--0.5679	4.984	6.031	22.194	L	
N-N--0.3479	6.853	6.110	23.434	L	H-H1-0.2769
H-H-0.2747	7.225	6.423	24.325	L	
C-CT--0.2637		7.798	5.734 22.337	H	
H-H1-0.156	7.212	5.421	21.472	H	
C-CT--0.0007		8.621	6.970 21.931	L	H-H1--0.0007
H-HC-0.0327	9.176	7.323	22.800	L	
H-HC-0.0327	9.357	6.673	21.184	L	
C-CT-0.039	7.789	8.140	21.368	L	
H-HC-0.0285	7.026	8.427	22.090	L	
H-HC-0.0285	8.445	9.000	21.234	L	
C-CT-0.0486	7.108	7.834	20.025	L	
H-H1-0.0687	6.462	6.962	20.122	L	
H-H1-0.0687	6.475	8.682	19.763	L	
N-N2--0.05295		8.087	7.646 18.940	L	
H-H-0.03456	8.494	8.491	18.566	L	
C-CA-0.08076		8.501	6.477 18.414	L	
N-N2--0.08627		8.022	5.297 18.834	L	
H-H-0.04478	7.327	5.262	19.565	L	
H-H-0.04478	8.360	4.439	18.421	L	
N-N2--0.08627		9.423	6.494 17.443	L	
H-H-0.04478	9.793	7.373	17.112	L	
H-H-0.04478	9.744	5.627	17.038	L	
C-C-0.7341	8.742	4.549	22.603	H	
O-O--0.5894	9.143	3.827	21.705	H	
N-N--0.4157	9.111	4.341	23.906	H	
H-H-0.2719	8.842	5.048	24.583	H	
C-CT-0.0429	10.028		3.290 24.301	H	
H-H1-0.0766	10.675		3.075 23.448	H	
C-CT--0.079	10.880		3.718 25.503	H	
H-H1-0.091	10.246		3.950 26.366	H	
H-H1-0.091	11.553		2.912 25.779	H	
S-S--0.1081	11.847		5.258 25.210	H	
C-C-0.5973	9.294	1.963	24.606	H	
O-O--0.5679	9.875	0.893	24.565	H	
N-N--0.3479	7.977	2.100	24.942	H	
H-H-0.2747	7.544	2.999	24.756	H	
C-CT--0.24	7.040	0.969	24.979	L	H-H--0.24
H-H1-0.1426	7.320	0.318	25.807	L	
C-CT--0.0094		5.643	1.561 25.248	L	
H-HC-0.0362	5.675	2.063	26.216	L	
H-HC-0.0362	5.429	2.311	24.483	L	
C-CT-0.0187	4.484	0.553	25.273	L	
H-HC-0.0103	4.391	0.076	24.297	L	
H-HC-0.0103	4.678	-0.208	26.031	L	
C-CT--0.0479		3.168	1.276 25.596	L	
H-HC-0.0621	3.236	1.728	26.588	L	
H-HC-0.0621	3.002	2.068	24.862	L	
C-CT--0.0143		1.987	0.300 25.556	L	
H-HP-0.1135	1.920	-0.144	24.562	L	
H-HP-0.1135	2.149	-0.495	26.286	L	
N-N3--0.03854		0.716	0.979 25.862	L	
H-H-0.034	0.551	1.709	25.183	L	
H-H-0.034	-0.042		0.312 25.826	L	
H-H-0.034	0.761	1.385	26.786	L	

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C-C-0.7341	7.087	0.138	23.688	L	
O-O--0.5894	7.344	0.665	22.610	L	
N-N--0.4157	6.865	-1.173	23.795	L	
H-H-0.2719	6.706	-1.548	24.715	L	
C-CT--0.0252	6.958	-2.106	22.665	L	
H-H1-0.0698	6.367	-2.997	22.879	L	
H-H1-0.0698	6.564	-1.644	21.759	L	
C-C-0.5973	8.402	-2.539	22.403	L	
O-O--0.5679	8.702	-3.729	22.409	L	
N-N--0.4157	9.305	-1.576	22.202	L	
H-H-0.2719	8.964	-0.621	22.204	L	
C-CT--0.0389	10.752	-1.836	22.113	L	
H-H1-0.1007	10.904	-2.541	21.296	L	
C-CT-0.3654	11.569	-0.565	21.792	L	
H-H1-0.0043	12.498	-0.887	21.322	L	
C-CT--0.2438	10.870	0.400	20.834	L	
H-HC-0.0642	10.013	0.874	21.314	L	
H-HC-0.0642	11.568	1.178	20.531	L	
H-HC-0.0642	10.539	-0.136	19.944	L	
O-OH--0.6761	11.922	0.163	22.950	L	
H-HO-0.4102	11.105	0.351	23.452	L	
C-C-0.5973	11.282	-2.483	23.401	L	
O-O--0.5679	10.744	-2.256	24.489	L	
N-N--0.4157	12.384	-3.239	23.330	L	
H-H-0.2719	12.797	-3.416	22.427	L	
C-CT-0.0341	13.077	-3.681	24.547	L	
H-H1-0.0864	12.318	-3.975	25.274	L	
C-CT--0.0316	13.937	-4.927	24.284	L	
H-HC-0.0488	13.320	-5.696	23.819	L	
H-HC-0.0488	14.750	-4.677	23.601	L	
C-C-0.6462	14.525	-5.508	25.574	L	
O-O--0.5554	14.021	-5.279	26.676	L	
O-OH--0.6376	15.616	-6.289	25.438	L	
H-HO-0.4747	15.754	-6.758	26.261	L	
C-C-0.5973	13.879	-2.522	25.172	L	
O-O--0.5679	15.111	-2.510	25.160	L	
N-N--0.4157	13.157	-1.571	25.775	L	
H-H-0.2719	12.152	-1.654	25.630	L	
C-CT--0.0875	13.631	-0.331	26.420	L	
H-H1-0.0969	13.872	0.370	25.622	L	
C-CT-0.2985	12.479	0.317	27.215	L	
H-HC--0.0297	11.668	0.508	26.514	L	
C-CT--0.3192	11.920	-0.574	28.334	L	
H-HC-0.0791	12.679	-0.766	29.091	L	
H-HC-0.0791	11.084	-0.061	28.812	L	
H-HC-0.0791	11.551	-1.514	27.925	L	
C-CT--0.3192	12.890	1.661	27.810	L	
H-HC-0.0791	13.368	2.281	27.051	L	
H-HC-0.0791	12.010	2.176	28.196	L	
H-HC-0.0791	13.582	1.490	28.628	L	
C-C-0.5973	14.920	-0.513	27.233	L	
O-O--0.5679	15.835	0.298	27.135	L	
N-N--0.3479	15.039	-1.640	27.946	L	
H-H-0.2747	14.217	-2.221	27.924	L	
C-CT--0.1354	16.226	-2.128	28.665	L	
H-H1-0.1212	16.261	-1.613	29.623	L	
C-CT--0.0414	16.084	-3.637	28.929	L	
H-HC-0.081	15.995	-4.165	27.979	L	
H-HC-0.081	16.992	-3.999	29.417	L	
C-CC--0.0012	14.919	-3.979	29.816	L	
N-NA--0.1513	13.741	-4.592	29.433	L	

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H-H-0.3866	13.553	-4.941	28.488	L
C-CR--0.017	12.961	-4.679	30.535	L
H-H5-0.2681	11.968	-5.119	30.572	L
N-NA--0.1718	13.623	-4.148	31.590	L
H-H-0.3911	13.304	-4.054	32.556	L
C-CW--0.1141	14.861	-3.720	31.153	L
H-H4-0.2317	15.646	-3.263	31.746	L
C-C-0.7341	17.585	-1.872	27.999	L
O-O--0.5894	18.550	-1.620	28.726	L
N-N--0.4157	17.673	-2.021	26.674	L
H-H-0.2719	16.810	-2.193	26.169	L
C-CT-0.0337	18.921	-2.215	25.933	L
H-H1-0.0823	19.769	-2.083	26.607	L
C-CT--0.1825	18.936	-3.676	25.459	L
H-HC-0.0603	18.125	-3.849	24.750	L
H-HC-0.0603	19.885	-3.894	24.965	L
H-HC-0.0603	18.826	-4.350	26.309	L
C-C-0.5973	19.146	-1.218	24.771	L
O-O--0.5679	19.964	-1.476	23.894	L
N-N--0.4157	18.487	-0.053	24.774	L
H-H-0.2719	17.815	0.122	25.506	L
C-CT--0.0275	18.841	1.053	23.869	L
H-H1-0.1123	18.734	0.714	22.837	L
C-CT--0.005	17.894	2.241	24.083	L
H-HC-0.0339	17.705	2.367	25.147	L
H-HC-0.0339	18.396	3.147	23.742	L
C-C*-0.1415	16.584	2.165	23.362	L
C-CW--0.1638	15.597	1.270	23.596	L
H-H4-0.2062	15.647	0.485	24.339	L
N-NA--0.3418	14.533	1.522	22.749	L
H-H-0.3412	13.648	1.017	22.763	L
C-CN-0.138	14.803	2.573	21.897	L
C-CA--0.2601	14.073	3.189	20.870	L
H-HA-0.1572	13.085	2.840	20.616	L
C-CA--0.1134	14.644	4.268	20.173	L
H-HA-0.1417	14.100	4.743	19.368	L
C-CA--0.1972	15.922	4.733	20.528	L
H-HA-0.1447	16.356	5.564	19.988	L
C-CA--0.2387	16.642	4.117	21.569	L
H-HA-0.17	17.626	4.479	21.825	L
C-CB-0.1243	16.105	3.016	22.275	L
C-C-0.5973	20.307	1.489	24.059	L
O-O--0.5679	20.676	1.885	25.167	L
O-OH-0.0	21.107	1.414	22.957	L
H-HO-0.0	22.008	1.700	23.126	L

%chk=model_64_80

ONIOM(B3LYP/6-311+G(d,p):Amber) Opt(GDIIS, Micro)

model

3	1	0	1	0	1
H-H-0.0			11.46	13.46	30.95 L
N-N--0.4157	11.55	12.68	31.58		L
H-H-0.2719	11.67	11.74	31.22		L
C-CT--0.0518		11.48	12.91	33.02	L
H-H1-0.0922	11.29	11.96	33.53		L
C-CT--0.1102		12.82	13.49	33.52	L
H-HC-0.0457	13.00	14.43	33.01		L

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H-HC-0.0457 12.72 13.70 34.59 L
C-CT-0.3531 14.05 12.59 33.33 L
H-HC--0.0361 14.14 12.30 32.28 L
C-CT--0.4121 15.30 13.37 33.72 L
H-HC-0.1 15.24 13.64 34.77 L
H-HC-0.1 16.19 12.76 33.55 L
H-HC-0.1 15.38 14.27 33.12 L
C-CT--0.4121 13.98 11.32 34.18 L
H-HC-0.1 13.12 10.72 33.90 L
H-HC-0.1 14.87 10.72 34.04 L
H-HC-0.1 13.89 11.59 35.24 L
C-C-0.5973 10.33 13.85 33.40 L
O-O--0.5679 9.64 13.61 34.39 L
N-N--0.4157 10.16 14.93 32.64 L
H-H-0.2719 10.74 14.97 31.81 L
C-CT--0.0031 9.16 16.00 32.83 L
H-H1-0.085 9.54 16.89 32.32 L
C-CT--0.0036 7.83 15.61 32.15 L
H-HC-0.0171 7.37 14.80 32.73 L
H-HC-0.0171 7.16 16.47 32.18 L
C-CT--0.0645 7.95 15.13 30.69 L
H-HC-0.0352 8.50 14.19 30.66 L
H-HC-0.0352 6.95 14.93 30.31 L
C-C-0.6951 8.66 16.13 29.78 L
O-O--0.6086 9.85 16.37 29.88 L
N-N--0.9407 7.97 16.75 28.86 L
H-H-0.4251 8.53 17.37 28.29 L
H-H-0.4251 6.99 16.59 28.70 L
C-C-0.5973 9.00 16.41 34.31 L
O-O--0.5679 7.90 16.38 34.87 L
N-N--0.4157 10.13 16.80 34.93 L
H-H-0.2719 10.97 16.77 34.38 L
C-CT--0.0597 10.27 17.05 36.38 L
H-H1-0.0869 9.95 16.14 36.89 L
C-CT-0.1303 11.75 17.29 36.78 L
H-HC-0.0187 12.08 18.25 36.36 L
C-CT--0.3204 11.84 17.37 38.31 L
H-HC-0.0882 11.54 16.41 38.75 L
H-HC-0.0882 12.86 17.58 38.62 L
H-HC-0.0882 11.21 18.16 38.70 L
C-CT--0.043 12.69 16.18 36.24 L
H-HC-0.0236 12.36 15.22 36.62 L
H-HC-0.0236 12.61 16.16 35.15 L
C-CT--0.066 14.17 16.38 36.57 L
H-HC-0.0186 14.35 16.21 37.63 L
H-HC-0.0186 14.76 15.66 36.00 L
H-HC-0.0186 14.49 17.39 36.30 L
C-C-0.5973 9.35 18.20 36.82 L
O-O--0.5679 9.69 19.38 36.77 L
N-N--0.4157 8.15 17.83 37.26 L
H-H-0.2719 7.94 16.85 37.17 L
C-CT-0.0143 7.07 18.75 37.58 L
H-H1-0.1048 7.10 19.56 36.85 L
C-CT--0.2041 5.69 18.07 37.39 L
H-HC-0.0797 4.93 18.63 37.94 L
H-HC-0.0797 5.43 18.12 36.34 L
C-C-0.713 5.59 16.61 37.81 L
O-O--0.5931 5.02 16.26 38.82 L
N-N--0.9191 6.12 15.70 37.02 L
H-H-0.4196 6.00 14.74 37.30 L
H-H-0.4196 6.57 15.93 36.14 L

C-C-0.5973	7.32	19.41	38.95	L
O-O--0.5679	6.93	18.91	40.00	L
N-N--0.4157	7.97	20.57	38.91	L
H-H-0.2719	8.31	20.85	38.00	L
C-CT--0.0249		8.50	21.35	40.05 L
H-H1-0.0843	9.14	20.70	40.64	L
C-CT-0.2117	9.38	22.48	39.49	L
H-H1-0.0352	9.80	23.06	40.31	L
H-H1-0.0352	10.20	22.02	38.93	L
O-OH--0.6546		8.65	23.32	38.62 L
H-HO-0.4275	9.29	23.89	38.18	L
C-C-0.5973	7.46	21.94	41.02	L
O-O--0.5679	7.82	22.69	41.93	L
N-N--0.3479	6.19	21.56	40.90	L
H-H-0.2747	6.00	20.91	40.15	L
C-CT--0.2637		5.22	21.66	42.01 L
H-H1-0.156	5.30	22.66	42.44	L
C-CT--0.0007		3.78	21.44	41.53 L
H-HC-0.0327	3.61	21.98	40.60	L
H-HC-0.0327	3.60	20.38	41.36	L
C-CT-0.039	2.80	21.97	42.59	L
H-HC-0.0285	2.93	21.43	43.53	L
H-HC-0.0285	3.02	23.03	42.77	L
C-CT-0.0486	1.34	21.83	42.15	L
H-H1-0.0687	1.20	22.37	41.21	L
H-H1-0.0687	1.12	20.78	42.01	L
N-N2--0.05295		0.44	22.40	43.17 L
H-H-0.03456	0.86	23.05	43.82	L
C-CA-0.08076		-0.87	22.15	43.29 L
N-N2--0.08627		-1.51	21.31	42.45 L
H-H-0.04478	-1.01	20.85	41.71	L
H-H-0.04478	-2.50	21.15	42.57	L
N-N2--0.08627		-1.56	22.75	44.26 L
H-H-0.04478	-1.09	23.39	44.89	L
H-H-0.04478	-2.55	22.58	44.37	L
C-C-0.7341	5.59	20.69	43.13	L
O-O--0.5894	5.41	21.01	44.29	L
N-N--0.4157	6.12	19.51	42.79	L
H-H-0.2719	6.22	19.31	41.81	L
C-CT--0.0275		6.46	18.47	43.76 L
H-H1-0.1123	6.12	18.77	44.75	L
C-CT--0.005	5.72	17.17	43.40	L
H-HC-0.0339	6.22	16.71	42.55	L
H-HC-0.0339	5.81	16.48	44.24	L
C-C*--0.1415		4.26	17.30	43.05 L
C-CW--0.1638		3.69	16.74	41.96 L
H-H4-0.2062	4.21	16.14	41.23	L
N-NA--0.3418		2.34	17.04	41.94 L
H-H-0.3412	1.71	16.69	41.23	L
C-CN-0.138	1.98	17.83	43.00	L
C-CA--0.2601		0.75	18.38	43.40 L
H-HA-0.1572	-0.15	18.19	42.83	L
C-CA--0.1134		0.70	19.17	44.56 L
H-HA-0.1417	-0.23	19.61	44.89	L
C-CA--0.1972		1.88	19.41	45.30 L
H-HA-0.1447	1.85	20.04	46.17	L
C-CA--0.2387		3.10	18.83	44.89 L
H-HA-0.17	3.99	19.03	45.46	L
C-CB-0.1243	3.19	18.02	43.74	L
C-C-0.5973	7.98	18.28	43.87	L
O-O--0.5679	8.55	18.53	44.93	L

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N-N--0.4157	8.61	17.83	42.79	L	H-H1-0.0203
H-H-0.2719	8.03	17.67	41.98	L	
C-CT--0.0275		9.92	17.16	42.77	H
H-H1-0.1123	9.92	16.44	43.59	H	
C-CT--0.005	9.98	16.34	41.47	L	H-H1--0.005
H-HC-0.0339	10.07	17.02	40.62	L	
H-HC-0.0339	10.86	15.69	41.48	L	
C-C*--0.1415		8.77	15.48	41.28	L
C-CW--0.1638		7.83	15.67	40.33	L
H-H4-0.2062	7.87	16.44	39.57	L	
N-NA--0.3418		6.78	14.80	40.54	L
H-H-0.3412	5.94	14.84	39.98	L	
C-CN-0.138	7.00	14.00	41.65	L	
C-CA--0.2601		6.22	13.02	42.28	L
H-HA-0.1572	5.25	12.75	41.89	L	
C-CA--0.1134		6.73	12.40	43.43	L
H-HA-0.1417	6.15	11.63	43.94	L	
C-CA--0.1972		8.00	12.76	43.93	L
H-HA-0.1447	8.39	12.26	44.81	L	
C-CA--0.2387		8.76	13.75	43.29	L
H-HA-0.17	9.74	14.00	43.67	L	
C-CB-0.1243	8.28	14.40	42.13	L	
C-C-0.5973	11.10	18.09	43.06	H	
O-O--0.5679	11.52	18.24	44.20	H	
N-N--0.4157	11.68	18.73	42.00	H	
H-H-0.2719	11.20	18.73	41.11	H	
C-CT-0.0429	12.69	19.73	42.23	H	
H-H1-0.0766	13.28	19.38	43.08	H	
C-CT--0.079	13.66	19.87	41.05	H	
H-H1-0.091	14.50	20.50	41.34	H	
H-H1-0.091	14.05	18.88	40.81	H	
S-S--0.1081	12.98	20.49	39.45	H	
C-C-0.5973	12.02	21.06	42.64	H	
O-O--0.5679	10.96	21.43	42.17	H	
N-N--0.4157	12.69	21.75	43.60	H	
H-H-0.2719	13.63	21.48	43.88	H	
C-CT-0.0143	12.24	23.05	44.08	L	H-H-0.0143
H-H1-0.1048	11.17	23.00	44.26	L	
C-CT--0.2041		12.96	23.33	45.41	L
H-HC-0.0797	12.91	22.43	46.01	L	
H-HC-0.0797	14.01	23.57	45.22	L	
C-C-0.713	12.34	24.46	46.21	L	
O-O--0.5931	11.73	25.39	45.69	L	
N-N--0.9191	12.49	24.43	47.51	L	
H-H-0.4196	12.05	25.16	48.03	L	
H-H-0.4196	12.97	23.64	47.94	L	
C-C-0.5973	12.52	24.16	43.04	L	
O-O--0.5679	13.60	24.22	42.46	L	
N-N--0.4157	11.57	25.07	42.84	L	
H-H-0.2719	10.68	24.92	43.32	L	
C-CT-0.0341	11.83	26.36	42.19	L	
H-H1-0.0864	12.89	26.57	42.27	L	
C-CT--0.0316		11.48	26.27	40.69	L
H-HC-0.0488	11.90	27.14	40.19	L	
H-HC-0.0488	11.96	25.39	40.27	L	
C-C-0.6462	9.99	26.21	40.38	L	
O-O--0.5554	9.14	26.30	41.25	L	
O-OH--0.6376		9.64	26.10	39.08	L
H-HO-0.4747	8.67	26.06	39.14	L	
C-C-0.5973	11.13	27.56	42.86	L	
O-O--0.5679	11.23	28.67	42.34	L	

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N-N--0.4157	10.39	27.36	43.96	L
H-H-0.2719	10.47	26.45	44.42	L
C-CT--0.0252		9.52	28.36	44.60 L
H-H1-0.0698	9.17	27.96	45.55	L
H-H1-0.0698	10.10	29.26	44.81	L
C-C-0.5973	8.30	28.74	43.76	L
O-O--0.5679	7.16	28.52	44.17	L
N-N--0.3479	8.54	29.36	42.59	L
H-H-0.2747	9.53	29.44	42.39	L
C-CT--0.2637		7.57	29.97	41.67 L
H-H1-0.156	7.07	30.78	42.21	L
C-CT--0.0007		8.31	30.62	40.48 L
H-HC-0.0327	7.58	31.15	39.86	L
H-HC-0.0327	9.02	31.35	40.87	L
C-CT-0.039	9.07	29.61	39.60	L
H-HC-0.0285	9.81	29.09	40.21	L
H-HC-0.0285	8.37	28.89	39.19	L
C-CT-0.0486	9.80	30.31	38.45	L
H-H1-0.0687	9.07	30.79	37.79	L
H-H1-0.0687	10.46	31.08	38.85	L
N-N2--0.05295		10.61	29.35	37.68 L
H-H-0.03456	11.60	29.36	37.87	L
C-CA-0.08076		10.16	28.48	36.76 L
N-N2--0.08627		8.87	28.39	36.43 L
H-H-0.04478	8.19	29.00	36.88	L
H-H-0.04478	8.56	27.72	35.74	L
N-N2--0.08627		11.04	27.66	36.16 L
H-H-0.04478	12.02	27.71	36.39	L
H-H-0.04478	10.72	27.00	35.47	L
C-C-0.7341	6.43	29.07	41.19	L
O-O--0.5894	5.33	29.57	40.96	L
N-N--0.4157	6.66	27.77	41.00	L
H-H-0.2719	7.56	27.40	41.26	L
C-CT--0.0389		5.57	26.83	40.68 L
H-H1-0.1007	5.01	27.23	39.84	L
C-CT-0.3654	6.10	25.44	40.28	L
H-H1-0.0043	6.59	24.96	41.12	L
C-CT--0.2438		4.96	24.56	39.76 L
H-HC-0.0642	4.44	25.05	38.94	L
H-HC-0.0642	5.37	23.61	39.40	L
H-HC-0.0642	4.26	24.35	40.57	L
O-OH--0.6761		7.01	25.54	39.20 L
H-HO-0.4102	7.26	24.62	38.98	L
C-C-0.5973	4.68	26.71	41.92	L
O-O--0.5679	5.19	26.32	42.97	L
N-N--0.2548	3.37	27.05	41.85	L
C-CT-0.0192	2.60	27.32	40.65	L
H-H1-0.0391	2.78	26.57	39.88	L
H-H1-0.0391	2.85	28.32	40.28	L
C-CT-0.0189	1.14	27.28	41.10	L
H-HC-0.0213	0.79	26.25	41.11	L
H-HC-0.0213	0.50	27.89	40.46	L
C-CT--0.007	1.20	27.82	42.53	L
H-HC-0.0253	0.38	27.45	43.13	L
H-HC-0.0253	1.19	28.91	42.50	L
C-CT--0.0266		2.57	27.35	43.04 L
H-H1-0.0641	3.04	28.18	43.57	L
C-C-0.5896	2.49	26.16	44.01	L
O-O--0.5748	1.85	25.15	43.72	L
N-N--0.4157	3.17	26.30	45.15	L
H-H-0.2719	3.70	27.15	45.25	L

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C-CT--0.0252	3.32	25.26	46.17	L
H-H1-0.0698	3.51	25.72	47.13	L
H-H1-0.0698	2.38	24.69	46.25	L
C-C-0.5973	4.45	24.26	45.89	L
O-O--0.5679	4.26	23.07	46.12	L
N-N--0.4157	5.62	24.73	45.42	L
H-H-0.2719	5.63	25.71	45.15	L
C-CT--0.0249		6.82	23.94	45.13 L
H-H1-0.0843	6.56	23.22	44.36	L
C-CT-0.2117	7.92	24.85	44.55	L
H-H1-0.0352	7.47	25.51	43.80	L
H-H1-0.0352	8.35	25.47	45.34	L
O-OH--0.6546		8.94	24.10	43.92 L
H-HO-0.4275	8.54	23.59	43.18	L
C-C-0.5973	7.33	23.15	46.36	L
O-O--0.5679	8.12	23.63	47.17	L
N-N--0.3479	6.84	21.91	46.51	L
H-H-0.2747	6.14	21.67	45.81	L
C-CT--0.24	6.85	21.07	47.72	L
H-H1-0.1426	6.63	21.72	48.57	L
C-CT--0.0094		5.70	20.06	47.58 L
H-HC-0.0362	4.84	20.57	47.15	L
H-HC-0.0362	6.01	19.27	46.90	L
C-CT-0.0187	5.24	19.43	48.91	L
H-HC-0.0103	6.02	18.80	49.32	L
H-HC-0.0103	5.00	20.22	49.62	L
C-CT--0.0479		3.99	18.56	48.68 L
H-HC-0.0621	3.16	19.18	48.34	L
H-HC-0.0621	4.21	17.82	47.91	L
C-CT--0.0143		3.58	17.81	49.96 L
H-HP-0.1135	2.79	17.10	49.71	L
H-HP-0.1135	4.44	17.25	50.34	L
N-N3--0.03854		3.09	18.72	51.01 L
H-H-0.034	2.28	19.22	50.67	L
H-H-0.034	2.83	18.18	51.83	L
H-H-0.034	3.82	19.37	51.25	L
C-C-0.7341	8.20	20.41	48.04	L
O-O--0.5894	8.30	19.70	49.04	L
N-N--0.4157	9.25	20.67	47.25	L
H-H-0.2719	9.05	21.28	46.48	L
C-CT-0.0143	10.65	20.36	47.58	L
H-H1-0.1048	11.26	20.62	46.72	L
C-CT--0.2041		11.03	21.31	48.74 L
H-HC-0.0797	10.75	22.33	48.47	L
H-HC-0.0797	10.47	21.04	49.63	L
C-C-0.713	12.51	21.34	49.11	L
O-O--0.5931	13.34	21.83	48.37	L
N-N--0.9191	12.87	20.87	50.28	L
H-H-0.4196	13.85	20.84	50.50	L
H-H-0.4196	12.23	20.31	50.82	L
C-C-0.5973	10.93	18.86	47.87	L
O-O--0.5679	11.83	18.55	48.64	L
N-N--0.4157	10.24	17.91	47.22	L
H-H-0.2719	9.56	18.22	46.53	L
C-CT--0.0518		10.40	16.47	47.47 L
H-H1-0.0922	10.17	16.28	48.51	L
C-CT--0.1102		9.43	15.64	46.59 L
H-HC-0.0457	9.30	16.14	45.64	L
H-HC-0.0457	9.91	14.68	46.37	L
C-CT-0.3531	8.05	15.32	47.18	L
H-HC--0.0361		7.49	14.79	46.41 L

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C-CT--0.4121	8.13	14.41	48.41	L
H-HC-0.1	8.60	14.93	49.24	L
H-HC-0.1	7.13	14.10	48.70	L
H-HC-0.1	8.71	13.52	48.16	L
C-CT--0.4121	7.24	16.57	47.55	L
H-HC-0.1	7.15	17.21	46.67	L
H-HC-0.1	6.25	16.27	47.88	L
H-HC-0.1	7.74	17.12	48.35	L
C-C-0.5973	11.85	15.99	47.28	L
O-O--0.5679	12.42	15.35	48.16	L
N-N--0.4157	12.48	16.33	46.15	L
H-H-0.2719	11.97	16.90	45.48	L
C-CT-0.0429	13.89	16.02	45.88	L
H-H1-0.0766	14.07	14.97	46.12	L
C-CT--0.079	14.17	16.22	44.38	L
H-H1-0.091	14.03	17.27	44.14	L
H-H1-0.091	15.21	15.97	44.19	L
S-S--0.1081	13.15	15.25	43.24	L
C-C-0.5973	14.89	16.85	46.72	L
O-O--0.5679	16.09	16.67	46.56	L
N-N--0.4157	14.41	17.78	47.57	L
H-H-0.2719	13.40	17.81	47.70	L
C-CT-0.0143	15.18	18.68	48.43	L
H-H1-0.1048	14.52	19.48	48.74	L
C-CT--0.2041	15.58	17.91	49.71	L
H-HC-0.0797	16.01	16.94	49.46	L
H-HC-0.0797	16.33	18.47	50.26	L
C-C-0.713	14.40	17.72	50.66	L
O-O--0.5931	14.18	18.52	51.55	L
N-N--0.9191	13.60	16.70	50.50	L
H-H-0.4196	12.82	16.71	51.12	L
H-H-0.4196	13.63	16.08	49.70	L
C-C-0.5973	16.35	19.40	47.73	L
O-O--0.5679	17.41	19.63	48.31	L
N-N--0.4157	16.15	19.81	46.47	L
H-H-0.2719	15.25	19.61	46.06	L
C-CT--0.0597	17.20	20.34	45.59	L
H-H1-0.0869	17.89	20.89	46.21	L
C-CT-0.1303	17.95	19.13	44.97	L
H-HC-0.0187	18.12	18.40	45.76	L
C-CT--0.3204	17.11	18.42	43.89	L
H-HC-0.0882	17.01	19.04	43.01	L
H-HC-0.0882	17.58	17.47	43.63	L
H-HC-0.0882	16.12	18.21	44.29	L
C-CT--0.043	19.35	19.47	44.40	L
H-HC-0.0236	19.72	18.60	43.86	L
H-HC-0.0236	19.27	20.29	43.69	L
C-CT--0.066	20.38	19.79	45.49	L
H-HC-0.0186	20.51	18.92	46.14	L
H-HC-0.0186	21.34	20.01	45.02	L
H-HC-0.0186	20.07	20.64	46.09	L
C-C-0.5973	16.60	21.30	44.53	L
O-O--0.5679	15.49	21.04	44.03	L
N-N--0.2548	17.26	22.42	44.19	L
C-CT-0.0192	18.48	22.94	44.79	L
H-H1-0.0391	19.29	22.22	44.76	L
H-H1-0.0391	18.28	23.24	45.83	L
C-CT-0.0189	18.87	24.17	43.98	L
H-HC-0.0213	19.49	23.87	43.13	L
H-HC-0.0213	19.38	24.92	44.59	L
C-CT--0.007	17.52	24.67	43.47	L

H-H1-0.1234

H-H1--0.007

H-HC-0.0253	17.62	25.28	42.57	L	
H-HC-0.0253	17.03	25.24	44.26	L	
C-CT--0.0266		16.73	23.38	43.21	H
H-H1-0.0641	15.69	23.58	43.45	H	
C-C-0.5896	16.90	22.91	41.76	H	
O-O--0.5748	17.93	22.44	41.29	H	
N-N--0.4157	15.82	23.18	40.96	H	
H-H-0.2719	14.94	23.41	41.41	H	
C-CT-0.0429	15.78	22.72	39.58	H	
H-H1-0.0766	15.90	21.64	39.53	H	
C-CT--0.079	14.47	23.12	38.89	H	
H-H1-0.091	14.36	24.21	38.87	H	
H-H1-0.091	14.49	22.76	37.86	H	
S-S--0.1081	12.90	22.56	39.69	H	
C-C-0.5973	16.93	23.29	38.73	H	
O-O--0.5679	17.38	22.65	37.80	H	
N-N--0.4157	17.31	24.56	39.04	H	
H-H-0.2719	17.06	24.97	39.93	H	
C-CT--0.0249		18.45	25.23	38.41	L
H-H1-0.0843	18.22	25.36	37.35	L	H-H--0.0249
C-CT-0.2117	18.65	26.62	39.01	L	
H-H1-0.0352	19.58	27.05	38.65	L	
H-H1-0.0352	17.82	27.27	38.69	L	
O-OH--0.6546		18.65	26.55	40.43	L
H-HO-0.4275	19.02	27.38	40.77	L	
C-C-0.5973	19.78	24.46	38.45	L	
O-O--0.5679	20.58	24.60	37.54	L	
N-N--0.4157	20.03	23.66	39.50	L	
H-H-0.2719	19.33	23.59	40.22	L	
C-CT-0.0337	21.15	22.72	39.51	L	
H-H1-0.0823	22.06	23.24	39.19	L	
C-CT--0.1825		21.37	22.22	40.95	L
H-HC-0.0603	20.48	21.71	41.32	L	
H-HC-0.0603	22.21	21.52	40.96	L	
H-HC-0.0603	21.60	23.06	41.60	L	
C-C-0.5973	20.90	21.57	38.52	L	
O-O--0.5679	21.67	21.36	37.60	L	
N-N--0.4157	19.80	20.84	38.73	L	
H-H-0.2719	19.23	21.13	39.51	L	
C-CT--0.0518		19.41	19.61	38.03	L
H-H1-0.0922	20.16	18.84	38.24	L	
C-CT--0.1102		18.05	19.14	38.59	L
H-HC-0.0457	17.44	20.00	38.86	L	
H-HC-0.0457	17.52	18.59	37.81	L	
C-CT-0.3531	18.18	18.19	39.79	L	
H-HC--0.0361		18.67	17.28	39.45	L
C-CT--0.4121		18.97	18.78	40.95	L
H-HC-0.1	18.53	19.72	41.27	L	
H-HC-0.1	18.97	18.06	41.77	L	
H-HC-0.1	20.01	18.94	40.66	L	
C-CT--0.4121		16.78	17.83	40.29	L
H-HC-0.1	16.19	17.42	39.47	L	
H-HC-0.1	16.86	17.09	41.08	L	
H-HC-0.1	16.29	18.72	40.68	L	
C-C-0.5973	19.35	19.74	36.51	L	
O-O--0.5679	19.91	18.89	35.80	L	
N-N--0.4157	18.62	20.73	35.99	L	
H-H-0.2719	18.22	21.39	36.65	L	
C-CT--0.0518		18.37	20.95	34.56	L
H-H1-0.0922	18.22	19.98	34.08	L	
C-CT--0.1102		17.07	21.77	34.40	L

H-HC-0.0457	17.08	22.60	35.11	L
H-HC-0.0457	17.08	22.21	33.39	L
C-CT-0.3531	15.75	20.98	34.52	L
H-HC--0.0361		15.72	20.23	33.73 L
C-CT--0.4121		15.54	20.27	35.86 L
H-HC-0.1	15.68	20.97	36.68	L
H-HC-0.1	14.53	19.86	35.91	L
H-HC-0.1	16.25	19.45	35.95	L
C-CT--0.4121		14.58	21.94	34.32 L
H-HC-0.1	14.67	22.43	33.35	L
H-HC-0.1	13.64	21.39	34.34	L
H-HC-0.1	14.57	22.69	35.11	L
C-C-0.5973	19.60	21.60	33.90	L
O-O--0.5679	19.56	22.74	33.43	L
N-N--0.4157	20.70	20.86	33.87	L
H-H-0.2719	20.63	19.93	34.28	L
C-CT--0.0249		22.01	21.25	33.33 L
H-H1-0.0843	21.86	21.84	32.43	L
C-CT-0.2117	22.73	22.11	34.38	L
H-H1-0.0352	23.58	22.61	33.90	L
H-H1-0.0352	22.06	22.89	34.76	L
O-OH--0.6546		23.21	21.32	35.45 L
H-HO-0.4275	22.58	21.41	36.20	L
C-C-0.5973	22.83	19.99	32.97	L
O-O--0.5679	22.27	18.90	32.82	L
N-N--0.4157	24.16	20.10	32.91	L
H-H-0.2719	24.57	21.02	32.98	L
C-CT--0.0249		25.09	18.97	32.93 L
H-H1-0.0843	24.95	18.40	32.02	L
C-CT-0.2117	26.54	19.48	32.96	L
H-H1-0.0352	26.76	19.91	33.93	L
H-H1-0.0352	27.22	18.64	32.79	L
O-OH--0.6546		26.74	20.46	31.96 L
H-HO-0.4275	27.68	20.64	31.88	L
C-C-0.5973	24.88	18.01	34.12	L
O-O--0.5679	25.35	16.87	34.07	L
N-N--0.4157	24.19	18.43	35.19	L
H-H-0.2719	23.84	19.39	35.14	L
C-CT-0.0341	23.81	17.64	36.36	L
H-H1-0.0864	24.70	17.11	36.71	L
C-CT--0.0316		23.36	18.63	37.45 L
H-HC-0.0488	24.07	19.46	37.50	L
H-HC-0.0488	22.39	19.02	37.17	L
C-C-0.6462	23.25	18.05	38.86	L
O-O--0.5554	22.58	18.61	39.71	L
O-OH--0.6376		23.95	16.93	39.16 L
H-HO-0.4747	23.78	16.87	40.10	L
C-C-0.5973	22.72	16.57	36.07	L
O-O--0.5679	21.81	16.33	36.88	L
N-N--0.4157	22.82	15.89	34.92	L
H-H-0.2719	23.61	16.13	34.34	L
C-CT--0.0597		21.84	14.92	34.40 L
H-H1-0.0869	20.91	15.46	34.26	L
C-CT-0.1303	22.26	14.39	33.01	L
H-HC-0.0187	21.49	13.69	32.69	L
C-CT--0.3204		22.27	15.56	32.00 L
H-HC-0.0882	23.11	16.23	32.19	L
H-HC-0.0882	22.34	15.18	30.98	L
H-HC-0.0882	21.35	16.13	32.08	L
C-CT--0.043	23.62	13.65	33.02	L
H-HC-0.0236	24.42	14.33	33.30	L

H-HC-0.0236	23.58	12.85	33.76	L
C-CT--0.066	23.98	12.99	31.68	L
H-HC-0.0186	24.17	13.75	30.92	L
H-HC-0.0186	24.89	12.40	31.80	L
H-HC-0.0186	23.17	12.34	31.35	L
C-C-0.5973	21.53	13.79	35.38	L
O-O--0.5679	20.38	13.38	35.48	L
N-N--0.4157	22.52	13.33	36.15	L
H-H-0.2719	23.46	13.67	35.96	L
C-CT--0.0389		22.38	12.35	37.23 L
H-H1-0.1007	22.11	11.39	36.79	L
C-CT-0.3654	23.72	12.15	37.97	L
H-H1-0.0043	23.93	13.01	38.61	L
C-CT--0.2438		23.73	10.88	38.82 L
H-HC-0.0642	23.55	10.01	38.19	L
H-HC-0.0642	24.69	10.78	39.32	L
H-HC-0.0642	22.95	10.93	39.58	L
O-OH--0.6761		24.76	12.03	37.03 L
H-HO-0.4102	25.54	11.70	37.49	L
C-C-0.5973	21.29	12.75	38.22	L
O-O--0.5679	20.32	12.02	38.41	L
N-N--0.4157	21.40	13.94	38.82	L
H-H-0.2719	22.15	14.55	38.54	L
C-CT-0.0337	20.40	14.45	39.75	L
H-H1-0.0823	20.28	13.73	40.56	L
C-CT--0.1825		20.91	15.76	40.37 L
H-HC-0.0603	20.98	16.52	39.59	L
H-HC-0.0603	20.22	16.08	41.14	L
H-HC-0.0603	21.89	15.60	40.82	L
C-C-0.5973	19.01	14.62	39.09	L
O-O--0.5679	18.00	14.35	39.73	L
N-N--0.4157	18.96	15.04	37.82	L
H-H-0.2719	19.83	15.28	37.37	L
C-CT--0.0249		17.71	15.04	37.04 L
H-H1-0.0843	16.99	15.68	37.55	L
C-CT-0.2117	17.91	15.62	35.63	L
H-H1-0.0352	18.84	15.28	35.19	L
H-H1-0.0352	17.08	15.30	35.00	L
O-OH--0.6546		17.89	17.03	35.68 L
H-HO-0.4275	18.79	17.39	35.68	L
C-C-0.5973	17.07	13.65	36.97	L
O-O--0.5679	15.91	13.52	37.36	L
N-N--0.4157	17.77	12.61	36.51	L
H-H-0.2719	18.73	12.77	36.22	L
C-CT--0.0875		17.22	11.23	36.46 L
H-H1-0.0969	16.26	11.30	35.95	L
C-CT-0.2985	18.07	10.23	35.64	L
H-HC--0.0297		17.54	9.27	35.65 L
C-CT--0.3192		18.20	10.66	34.18 L
H-HC-0.0791	18.69	11.63	34.10	L
H-HC-0.0791	18.78	9.92	33.63	L
H-HC-0.0791	17.21	10.72	33.72	L
C-CT--0.3192		19.48	9.98	36.18 L
H-HC-0.0791	19.44	9.68	37.23	L
H-HC-0.0791	19.95	9.18	35.61	L
H-HC-0.0791	20.07	10.88	36.09	L
C-C-0.5973	16.89	10.66	37.84	L
O-O--0.5679	15.94	9.90	37.96	L
N-N--0.4157	17.63	11.02	38.89	L
H-H-0.2719	18.46	11.59	38.71	L
C-CT-0.0143	17.27	10.72	40.28	L

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H-H1-0.1048 17.12 9.64 40.37 L
C-CT--0.2041      18.40 11.14 41.25 L
H-HC-0.0797 18.54 12.22 41.18 L
H-HC-0.0797 18.10 10.91 42.27 L
C-C-0.713    19.75 10.48 41.02 L
O-O--0.5931 20.80 11.07 41.24 L
N-N--0.9191 19.81 9.23 40.63 L
H-H-0.4196  20.74 8.88 40.52 L
H-H-0.4196  18.98 8.70 40.43 L
C-C-0.5973  15.94 11.37 40.69 L
O-O--0.5679 15.11 10.74 41.34 L
N-N--0.4157 15.73 12.64 40.33 L
H-H-0.2719  16.48 13.10 39.82 L
C-CT-0.0429 14.50 13.39 40.55 L
H-H1-0.0766 14.03 13.04 41.47 L
C-CT--0.079 14.93 14.86 40.77 L
H-H1-0.091  15.76 14.87 41.47 L
H-H1-0.091  15.29 15.25 39.82 L
S-S--0.1081 13.67 15.99 41.41 L
C-C-0.5973  13.48 13.21 39.40 L
O-O--0.5679 12.62 14.08 39.19 L
O-OH-0.0     13.55 12.06 38.67 L
H-HO-0.0     12.89 12.00 37.99 L
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%chk=model_76_94

ONIOM(B3LYP/6-311+G(d,p):Amber) Opt(GDIIS, Micro)

model

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4      1      0      1      0      1
H-H-0.0      12.54 16.28 43.26 L
N-N--0.4157 12.06 17.07 42.85 L
H-H-0.2719 11.17 16.96 42.38 L
C-CT-0.0429 12.62 18.41 42.96 L
H-H1-0.0766 13.36 18.40 43.76 L
C-CT--0.079 13.34 18.73 41.64 L
H-H1-0.091 13.91 19.66 41.76 L
H-H1-0.091 14.05 17.93 41.45 L
S-S--0.1081 12.28 18.89 40.17 L
C-C-0.5973 11.56 19.46 43.33 L
O-O--0.5679 10.36 19.18 43.32 L
N-N--0.4157 11.99 20.69 43.63 L
H-H-0.2719 12.99 20.83 43.64 L
C-CT-0.0143 11.13 21.82 44.00 L
H-H1-0.1048 10.12 21.45 44.19 L
C-CT--0.2041      11.65 22.43 45.31 L
H-HC-0.0797 11.95 21.64 46.00 L
H-HC-0.0797 12.53 23.05 45.12 L
C-C-0.713    10.60 23.30 45.98 L
O-O--0.5931 9.75 23.90 45.35 L
N-N--0.9191 10.59 23.39 47.29 L
H-H-0.4196 9.90 24.01 47.67 L
H-H-0.4196 11.27 22.89 47.86 L
C-C-0.5973 11.05 22.89 42.90 L
O-O--0.5679 12.05 23.51 42.53 L
N-N--0.4157 9.84 23.15 42.41 L
H-H-0.2719 9.12 22.46 42.60 L
C-CT-0.0341 9.43 24.43 41.82 L
H-H1-0.0864 10.04 25.22 42.26 L
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C-CT--0.0316	9.70	24.42	40.30	L
H-HC-0.0488	9.48	25.41	39.89	L
H-HC-0.0488	10.75	24.21	40.13	L
C-C-0.6462	8.86	23.40	39.53	L
O-O--0.5554	7.69	23.19	39.84	L
O-OH--0.6376		9.43	22.78	38.48 L
H-HO-0.4747	8.72	22.21	38.14	L
C-C-0.5973	7.96	24.80	42.14	L
O-O--0.5679	7.47	25.81	41.64	L
N-N--0.4157	7.24	23.98	42.92	L
H-H-0.2719	7.71	23.20	43.35	L
C-CT--0.0252		5.80	24.11	43.14 L
H-H1-0.0698	5.51	23.46	43.98	L
H-H1-0.0698	5.56	25.14	43.41	L
C-C-0.5973	4.96	23.71	41.92	L
O-O--0.5679	4.24	22.71	41.96	L
N-N--0.3479	5.05	24.49	40.84	L
H-H-0.2747	5.74	25.23	40.93	L
C-CT--0.2637		4.36	24.32	39.54 L
H-H1-0.156	3.31	24.14	39.73	L
C-CT--0.0007		4.47	25.65	38.76 L
H-HC-0.0327	3.99	25.52	37.79	L
H-HC-0.0327	3.92	26.43	39.29	L
C-CT-0.039	5.93	26.12	38.56	L
H-HC-0.0285	6.21	26.79	39.37	L
H-HC-0.0285	6.60	25.26	38.60	L
C-CT-0.0486	6.14	26.82	37.22	L
H-H1-0.0687	5.76	26.19	36.41	L
H-H1-0.0687	5.59	27.76	37.21	L
N-N2--0.05295		7.56	27.10	36.98 L
H-H-0.03456	7.87	28.04	37.15	L
C-CA-0.08076		8.48	26.20	36.56 L
N-N2--0.08627		8.16	24.93	36.30 L
H-H-0.04478	7.20	24.61	36.41	L
H-H-0.04478	8.87	24.28	35.99	L
N-N2--0.08627		9.75	26.59	36.42 L
H-H-0.04478	10.01	27.55	36.61	L
H-H-0.04478	10.45	25.93	36.10	L
C-C-0.7341	4.86	23.12	38.71	L
O-O--0.5894	5.28	23.26	37.56	L
N-N--0.4157	4.82	21.91	39.27	L
H-H-0.2719	4.51	21.89	40.24	L
C-CT--0.0389		5.18	20.63	38.63 L
H-H1-0.1007	4.79	20.63	37.61	L
C-CT-0.3654	6.71	20.48	38.58	L
H-H1-0.0043	7.12	20.75	39.55	L
C-CT--0.2438		7.25	19.10	38.20 L
H-HC-0.0642	6.93	18.84	37.19	L
H-HC-0.0642	8.34	19.13	38.22	L
H-HC-0.0642	6.91	18.35	38.91	L
O-OH--0.6761		7.24	21.37	37.61 L
H-HO-0.4102	6.58	22.08	37.50	L
C-C-0.5973	4.54	19.49	39.43	L
O-O--0.5679	4.57	19.53	40.67	L
N-N--0.2548	3.94	18.46	38.79	L
C-CT-0.0192	3.86	18.24	37.36	L
H-H1-0.0391	4.79	18.49	36.84	L
H-H1-0.0391	3.04	18.83	36.94	L
C-CT-0.0189	3.55	16.75	37.20	L
H-HC-0.0213	4.48	16.18	37.24	L
H-HC-0.0213	3.02	16.55	36.27	L

C-CT--0.007	2.71	16.44	38.43	L
H-HC-0.0253	2.78	15.39	38.71	L
H-HC-0.0253	1.67	16.71	38.23	L
C-CT--0.0266		3.27	17.38	39.51 L
H-H1-0.0641	2.43	17.79	40.08	L
C-C-0.5896	4.22	16.67	40.48	L
O-O--0.5748	5.32	16.27	40.11	L
N-N--0.4157	3.82	16.57	41.75	L
H-H-0.2719	2.91	16.95	41.97	L
C-CT--0.0252		4.61	15.95	42.82 L
H-H1-0.0698	3.94	15.62	43.61	L
H-H1-0.0698	5.12	15.07	42.42	L
C-C-0.5973	5.68	16.86	43.46	L
O-O--0.5679	6.30	16.44	44.43	L
N-N--0.4157	5.90	18.09	42.97	L
H-H-0.2719	5.33	18.37	42.18	L
C-CT--0.0249		7.03	18.97	43.33 L
H-H1-0.0843	7.93	18.35	43.34	L
C-CT-0.2117	7.19	20.01	42.22	L
H-H1-0.0352	7.13	19.49	41.27	L
H-H1-0.0352	6.38	20.74	42.28	L
O-OH--0.6546		8.43	20.67	42.27 L
H-HO-0.4275	9.11	20.01	42.54	L
C-C-0.5973	6.94	19.62	44.73	L
O-O--0.5679	7.43	20.73	44.97	L
N-N--0.3479	6.38	18.92	45.72	L
H-H-0.2747	6.09	17.98	45.46	L
C-CT--0.24	6.38	19.28	47.15	L
H-H1-0.1426	6.22	20.36	47.24	L
C-CT--0.0094		5.22	18.56	47.85 L
H-HC-0.0362	4.31	18.72	47.27	L
H-HC-0.0362	5.42	17.48	47.88	L
C-CT-0.0187	4.97	19.08	49.28	L
H-HC-0.0103	5.86	18.94	49.88	L
H-HC-0.0103	4.74	20.14	49.23	L
C-CT--0.0479		3.80	18.32	49.94 L
H-HC-0.0621	2.89	18.49	49.37	L
H-HC-0.0621	4.03	17.26	49.93	L
C-CT--0.0143		3.58	18.76	51.39 L
H-HP-0.1135	2.84	18.10	51.85	L
H-HP-0.1135	4.52	18.66	51.95	L
N-N3--0.03854		3.09	20.15	51.50 L
H-H-0.034	2.22	20.24	51.01	L
H-H-0.034	2.96	20.39	52.47	L
H-H-0.034	3.77	20.77	51.09	L
C-C-0.7341	7.76	18.96	47.75	L
O-O--0.5894	7.91	18.04	48.55	L
N-N--0.4157	8.78	19.72	47.33	L
H-H-0.2719	8.51	20.40	46.63	L
C-CT-0.0143	10.21	19.54	47.60	L
H-H1-0.1048	10.69	20.35	47.07	L
C-CT--0.2041		10.52	19.76	49.10 L
H-HC-0.0797	9.75	20.40	49.54	L
H-HC-0.0797	10.51	18.81	49.63	L
C-C-0.713	11.84	20.47	49.32	L
O-O--0.5931	12.09	21.54	48.78	L
N-N--0.9191	12.73	19.94	50.12	L
H-H-0.4196	13.55	20.50	50.29	L
H-H-0.4196	12.64	18.99	50.47	L
C-C-0.5973	10.84	18.26	47.01	L
O-O--0.5679	11.86	18.34	46.33	L

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N-N--0.4157	10.22	17.10	47.24	L	H-H1-0.1699
H-H-0.2719	9.41	17.17	47.85	L	
C-CT--0.0518		10.45	15.76	46.65	H
H-H1-0.0922	9.93	15.06	47.31	H	
C-CT--0.1102		9.72	15.73	45.29	L H-H1--0.1102
H-HC-0.0457	8.67	15.96	45.46	L	
H-HC-0.0457	10.13	16.51	44.66	L	
C-CT-0.3531	9.81	14.39	44.52	L	
H-HC--0.0361		10.85	14.13	44.34	L
C-CT--0.4121		9.14	13.25	45.29	L
H-HC-0.1	8.10	13.49	45.50	L	
H-HC-0.1	9.17	12.33	44.69	L	
H-HC-0.1	9.67	13.06	46.22	L	
C-CT--0.4121		9.10	14.54	43.17	L
H-HC-0.1	9.58	15.32	42.59	L	
H-HC-0.1	9.17	13.60	42.62	L	
H-HC-0.1	8.05	14.78	43.32	L	
C-C-0.5973	11.90	15.25	46.64	H	
O-O--0.5679	12.30	14.43	47.46	H	
N-N--0.4157	12.73	15.71	45.65	H	
H-H-0.2719	12.36	16.43	45.03	H	
C-CT-0.0429	14.14	15.37	45.60	H	
H-H1-0.0766	14.23	14.41	46.11	H	
C-CT--0.079	14.65	15.25	44.16	H	
H-H1-0.091	14.38	16.12	43.56	H	
H-H1-0.091	15.74	15.18	44.19	H	
S-S--0.1081	13.94	13.74	43.38	H	
C-C-0.5973	15.06	16.31	46.42	H	
O-O--0.5679	16.26	16.14	46.41	H	
N-N--0.4157	14.41	17.24	47.17	H	
H-H-0.2719	13.40	17.35	47.07	H	
C-CT-0.0143	15.04	18.18	48.09	L H-H-0.0143	
H-H1-0.1048	14.28	18.90	48.39	L	
C-CT--0.2041		15.48	17.44	49.37	L
H-HC-0.0797	16.28	16.75	49.13	L	
H-HC-0.0797	15.86	18.16	50.09	L	
C-C-0.713	14.33	16.68	50.03	L	
O-O--0.5931	13.24	17.20	50.22	L	
N-N--0.9191	14.54	15.44	50.40	L	
H-H-0.4196	13.74	15.00	50.83	L	
H-H-0.4196	15.43	15.00	50.28	L	
C-C-0.5973	16.15	19.03	47.44	L	
O-O--0.5679	17.18	19.32	48.03	L	
N-N--0.4157	15.88	19.47	46.20	L	
H-H-0.2719	14.98	19.20	45.82	L	
C-CT--0.0597		16.75	20.25	45.32	L
H-H1-0.0869	17.34	20.92	45.94	L	
C-CT-0.1303	17.69	19.27	44.57	L	
H-HC-0.0187	18.15	18.62	45.31	L	
C-CT--0.3204		16.93	18.36	43.59	L
H-HC-0.0882	16.53	18.95	42.77	L	
H-HC-0.0882	17.61	17.61	43.18	L	
H-HC-0.0882	16.12	17.85	44.10	L	
C-CT--0.043	18.84	19.97	43.80	L	
H-HC-0.0236	19.30	19.26	43.12	L	
H-HC-0.0236	18.44	20.79	43.21	L	
C-CT--0.066	19.94	20.48	44.73	L	
H-HC-0.0186	20.41	19.64	45.25	L	
H-HC-0.0186	20.70	20.99	44.14	L	
H-HC-0.0186	19.55	21.18	45.47	L	
C-C-0.5973	15.84	21.07	44.38	L	

O-O--0.5679 14.80 20.55 43.97 L
 N-N--0.2548 16.14 22.34 44.04 L
 C-CT-0.0192 17.25 23.16 44.51 L
 H-H1-0.0391 18.20 22.63 44.48 L
 H-H1-0.0391 17.05 23.49 45.53 L
 C-CT-0.0189 17.30 24.36 43.57 L
 H-HC-0.0213 17.90 24.11 42.69 L
 H-HC-0.0213 17.69 25.25 44.06 L
 C-CT--0.007 15.84 24.53 43.16 L
 H-HC-0.0253 15.74 25.04 42.20 L
 H-HC-0.0253 15.31 25.08 43.93 L
 C-CT--0.0266 15.31 23.10 43.11 L
 H-H1-0.0641 14.28 23.09 43.45 L
 C-C-0.5896 15.37 22.49 41.70 L
 O-O--0.5748 16.43 22.08 41.23 L
 N-N--0.4157 14.23 22.43 41.00 L
 H-H-0.2719 13.39 22.79 41.44 L
 C-CT-0.0429 14.13 21.81 39.67 L
 H-H1-0.0766 14.47 20.78 39.75 L
 C-CT--0.079 12.67 21.77 39.20 L
 H-H1-0.091 12.29 22.79 39.14 L
 H-H1-0.091 12.64 21.36 38.19 L
 S-S--0.1081 11.54 20.79 40.23 L
 C-C-0.5973 15.05 22.45 38.61 L
 O-O--0.5679 15.47 21.78 37.68 L
 N-N--0.4157 15.41 23.73 38.76 L
 H-H-0.2719 15.08 24.23 39.58 L
 C-CT--0.0249 16.45 24.41 37.97 L
 H-H1-0.0843 16.11 24.45 36.93 L
 C-CT-0.2117 16.64 25.85 38.45 L
 H-H1-0.0352 17.51 26.28 37.96 L
 H-H1-0.0352 15.76 26.43 38.19 L
 O-OH--0.6546 16.82 25.88 39.86 L
 H-HO-0.4275 17.10 26.77 40.10 L
 C-C-0.5973 17.79 23.67 37.96 L
 O-O--0.5679 18.45 23.64 36.92 L
 N-N--0.4157 18.21 23.04 39.06 L
 H-H-0.2719 17.61 23.08 39.88 L
 C-CT-0.0337 19.40 22.19 39.10 L
 H-H1-0.0823 20.26 22.80 38.81 L
 C-CT--0.1825 19.63 21.70 40.54 L
 H-HC-0.0603 18.82 21.05 40.84 L
 H-HC-0.0603 20.57 21.14 40.58 L
 H-HC-0.0603 19.69 22.55 41.22 L
 C-C-0.5973 19.30 21.02 38.11 L
 O-O--0.5679 20.24 20.78 37.35 L
 N-N--0.4157 18.17 20.31 38.10 L
 H-H-0.2719 17.43 20.64 38.70 L
 C-CT--0.0518 17.89 19.21 37.17 L
 H-H1-0.0922 18.70 18.48 37.26 L
 C-CT--0.1102 16.55 18.53 37.49 L
 H-HC-0.0457 15.76 19.27 37.62 L
 H-HC-0.0457 16.28 17.93 36.62 L
 C-CT-0.3531 16.57 17.58 38.70 L
 H-HC--0.0361 17.44 16.93 38.64 L
 C-CT--0.4121 16.60 18.31 40.04 L
 H-HC-0.1 15.78 19.01 40.11 L
 H-HC-0.1 16.52 17.58 40.85 L
 H-HC-0.1 17.54 18.84 40.16 L
 C-CT--0.4121 15.32 16.71 38.68 L
 H-HC-0.1 15.31 16.11 37.77 L

H-HC-0.1	15.31	16.04	39.53	L
H-HC-0.1	14.43	17.33	38.70	L
C-C-0.5973	17.89	19.68	35.71	L
O-O--0.5679	18.49	19.04	34.85	L
N-N--0.4157	17.19	20.78	35.42	L
H-H-0.2719	16.72	21.23	36.20	L
C-CT--0.0518		17.12	21.43	34.11 L
H-H1-0.0922	17.13	20.66	33.33	L
C-CT--0.1102		15.77	22.19	34.01 L
H-HC-0.0457	15.60	22.75	34.93	L
H-HC-0.0457	15.86	22.92	33.20	L
C-CT-0.3531	14.54	21.32	33.68	L
H-HC--0.0361		14.72	20.81	32.73 L
C-CT--0.4121		14.18	20.28	34.74 L
H-HC-0.1	14.06	20.76	35.71	L
H-HC-0.1	13.25	19.78	34.47	L
H-HC-0.1	14.96	19.52	34.79	L
C-CT--0.4121		13.32	22.23	33.51 L
H-HC-0.1	13.52	22.97	32.73	L
H-HC-0.1	12.46	21.64	33.21	L
H-HC-0.1	13.11	22.75	34.44	L
C-C-0.5973	18.35	22.33	33.87	L
O-O--0.5679	18.24	23.50	33.50	L
N-N--0.4157	19.55	21.77	34.05	L
H-H-0.2719	19.58	20.79	34.30	L
C-CT--0.0249		20.83	22.44	33.79 L
H-H1-0.0843	20.73	23.07	32.91	L
C-CT-0.2117	21.21	23.33	34.99	L
H-H1-0.0352	21.96	24.06	34.66	L
H-H1-0.0352	20.34	23.89	35.32	L
O-OH--0.6546		21.76	22.58	36.06 L
H-HO-0.4275	21.06	21.99	36.40	L
C-C-0.5973	21.96	21.43	33.52	L
O-O--0.5679	21.75	20.22	33.56	L
N-N--0.4157	23.19	21.93	33.34	L
H-H-0.2719	23.30	22.93	33.22	L
C-CT--0.0249		24.42	21.13	33.31 L
H-H1-0.0843	24.39	20.50	32.43	L
C-CT-0.2117	25.64	22.05	33.19	L
H-H1-0.0352	25.81	22.56	34.14	L
H-H1-0.0352	26.52	21.45	32.95	L
O-OH--0.6546		25.43	23.02	32.18 L
H-HO-0.4275	26.27	23.44	31.97	L
C-C-0.5973	24.60	20.22	34.54	L
O-O--0.5679	25.28	19.21	34.44	L
N-N--0.4157	24.00	20.55	35.69	L
H-H-0.2719	23.39	21.36	35.69	L
C-CT-0.0341	24.05	19.72	36.91	L
H-H1-0.0864	25.06	19.33	37.00	L
C-CT--0.0316		23.78	20.61	38.14 L
H-HC-0.0488	24.41	21.49	38.09	L
H-HC-0.0488	22.74	20.93	38.13	L
C-C-0.6462	24.08	19.89	39.46	L
O-O--0.5554	24.95	19.04	39.54	L
O-OH--0.6376		23.36	20.26	40.54 L
H-HO-0.4747	23.79	19.78	41.25	L
C-C-0.5973	23.10	18.49	36.84	L
O-O--0.5679	22.39	18.17	37.79	L
N-N--0.4157	23.18	17.73	35.74	L
H-H-0.2719	23.80	18.07	35.01	L
C-CT--0.0597		22.46	16.47	35.51 L

H-H1-0.0869 21.40 16.70 35.55 L
C-CT-0.1303 22.76 15.90 34.10 L
H-HC-0.0187 22.17 14.98 34.00 L
C-CT--0.3204 22.26 16.89 33.03 L
H-HC-0.0882 22.91 17.77 32.99 L
H-HC-0.0882 22.26 16.41 32.05 L
H-HC-0.0882 21.25 17.21 33.25 L
C-CT--0.043 24.25 15.54 33.91 L
H-HC-0.0236 24.85 16.45 33.92 L
H-HC-0.0236 24.58 14.91 34.73 L
C-CT--0.066 24.53 14.78 32.61 L
H-HC-0.0186 24.33 15.41 31.74 L
H-HC-0.0186 25.58 14.48 32.59 L
H-HC-0.0186 23.91 13.88 32.56 L
C-C-0.5973 22.71 15.42 36.60 L
O-O--0.5679 21.89 14.51 36.78 L
N-N--0.4157 23.78 15.57 37.38 L
H-H-0.2719 24.43 16.30 37.12 L
C-CT--0.0389 24.07 14.96 38.69 L
H-H1-0.1007 24.46 13.96 38.51 L
C-CT-0.3654 25.11 15.79 39.46 L
H-H1-0.0043 24.60 16.49 40.12 L
C-CT--0.2438 26.03 14.91 40.30 L
H-HC-0.0642 26.59 14.23 39.66 L
H-HC-0.0642 26.73 15.53 40.85 L
H-HC-0.0642 25.44 14.33 41.01 L
O-OH--0.6761 25.93 16.55 38.59 L
H-HO-0.4102 25.96 17.44 38.95 L
C-C-0.5973 22.82 14.84 39.57 L
O-O--0.5679 22.59 13.79 40.17 L
N-N--0.4157 22.03 15.91 39.66 L
H-H-0.2719 22.27 16.73 39.11 L
C-CT-0.0337 20.73 15.91 40.32 L
H-H1-0.0823 20.86 15.56 41.34 L
C-CT--0.1825 20.21 17.36 40.38 L
H-HC-0.0603 20.05 17.75 39.37 L
H-HC-0.0603 19.27 17.38 40.93 L
H-HC-0.0603 20.93 17.99 40.90 L
C-C-0.5973 19.75 14.95 39.62 L
O-O--0.5679 19.27 14.00 40.23 L
N-N--0.4157 19.47 15.19 38.33 L
H-H-0.2719 19.90 15.99 37.90 L
C-CT--0.0249 18.55 14.42 37.48 L
H-H1-0.0843 17.53 14.62 37.82 L
C-CT-0.2117 18.64 14.92 36.03 L
H-H1-0.0352 19.61 14.66 35.60 L
H-H1-0.0352 17.85 14.46 35.43 L
O-OH--0.6546 18.48 16.32 36.04 L
H-HO-0.4275 18.59 16.70 35.15 L
C-C-0.5973 18.75 12.91 37.56 L
O-O--0.5679 17.83 12.18 37.94 L
N-N--0.4157 19.96 12.42 37.27 L
H-H-0.2719 20.68 13.09 37.02 L
C-CT--0.0875 20.31 10.98 37.25 L
H-H1-0.0969 19.61 10.48 36.58 L
C-CT-0.2985 21.72 10.72 36.67 L
H-HC--0.0297 21.86 9.64 36.59 L
C-CT--0.3192 21.86 11.29 35.26 L
H-HC-0.0791 21.82 12.38 35.27 L
H-HC-0.0791 22.82 10.99 34.83 L
H-HC-0.0791 21.06 10.91 34.62 L

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C-CT--0.3192	22.85	11.26	37.56	L	
H-HC-0.0791	22.85	10.74	38.52	L	
H-HC-0.0791	23.81	11.08	37.07	L	
H-HC-0.0791	22.73	12.32	37.73	L	
C-C-0.5973	20.16	10.27	38.61	L	
O-O--0.5679	20.17	9.04	38.66	L	
N-N--0.4157	20.01	11.02	39.71	L	H-H1-0.1557
H-H-0.2719	20.02	12.02	39.59	L	
C-CT-0.0143	19.72	10.47	41.04	H	
H-H1-0.1048	19.82	9.38	41.01	H	
C-CT--0.2041	20.80	10.97	42.02	L	H-H1--0.2041
H-HC-0.0797	20.83	12.07	42.00	L	
H-HC-0.0797	20.55	10.65	43.03	L	
C-C-0.713	22.16	10.41	41.67	L	
O-O--0.5931	22.39	9.21	41.73	L	
N-N--0.9191	23.10	11.23	41.27	L	
H-H-0.4196	24.01	10.84	41.08	L	
H-H-0.4196	22.89	12.21	41.09	L	
C-C-0.5973	18.29	10.71	41.53	H	
O-O--0.5679	17.67	9.85	42.15	H	
N-N--0.4157	17.71	11.90	41.21	H	
H-H-0.2719	18.23	12.56	40.65	H	
C-CT-0.0429	16.29	12.14	41.44	H	
H-H1-0.0766	16.07	12.02	42.50	H	
C-CT--0.079	15.96	13.58	41.03	H	
H-H1-0.091	16.65	14.27	41.52	H	
H-H1-0.091	16.08	13.72	39.94	H	
S-S--0.1081	14.22	14.10	41.34	H	
C-C-0.5973	15.42	11.09	40.74	H	
O-O--0.5679	14.49	10.58	41.33	H	
N-N--0.4157	15.81	10.74	39.47	H	
H-H-0.2719	16.59	11.20	39.02	H	
C-CT-0.0337	15.23	9.63	38.72	L	H-H-0.0337
H-H1-0.0823	14.22	9.91	38.41	L	
C-CT--0.1825	16.06	9.42	37.45	L	
H-HC-0.0603	17.10	9.17	37.71	L	
H-HC-0.0603	15.64	8.60	36.87	L	
H-HC-0.0603	16.05	10.32	36.84	L	
C-C-0.5973	15.10	8.34	39.56	L	
O-O--0.5679	14.02	7.77	39.67	L	
N-N--0.3479	16.20	7.91	40.19	L	
H-H-0.2747	17.03	8.47	40.07	L	
C-CT--0.24	16.25	6.75	41.11	L	
H-H1-0.1426	15.95	5.86	40.55	L	
C-CT--0.0094	17.67	6.53	41.66	L	
H-HC-0.0362	17.94	7.36	42.30	L	
H-HC-0.0362	17.66	5.63	42.28	L	
C-CT-0.0187	18.74	6.35	40.57	L	
H-HC-0.0103	18.56	5.42	40.03	L	
H-HC-0.0103	18.68	7.18	39.87	L	
C-CT--0.0479	20.14	6.34	41.19	L	
H-HC-0.0621	20.27	7.25	41.78	L	
H-HC-0.0621	20.25	5.47	41.83	L	
C-CT--0.0143	21.20	6.31	40.08	L	
H-HP-0.1135	21.20	5.32	39.61	L	
H-HP-0.1135	20.93	7.04	39.32	L	
N-N3--0.3854	22.55	6.63	40.61	L	
H-H-0.34	22.83	5.98	41.32	L	
H-H-0.34	23.23	6.65	39.87	L	
H-H-0.34	22.53	7.57	41.03	L	
C-C-0.7341	15.24	6.90	42.25	L	

O-O--0.5894	14.48	5.97	42.50	L
N-N--0.3479	15.23	8.06	42.93	L
H-H-0.2747	15.89	8.76	42.63	L
C-CT--0.24	14.27	8.36	44.02	L
H-H1-0.1426	14.41	7.61	44.80	L
C-CT--0.0094	14.55	9.75	44.63	L
H-HC-0.0362	15.61	9.84	44.87	L
H-HC-0.0362	14.29	10.53	43.92	L
C-CT-0.0187	13.72	9.93	45.92	L
H-HC-0.0103	12.67	9.74	45.71	L
H-HC-0.0103	14.06	9.21	46.66	L
C-CT--0.0479	13.85	11.35	46.50	L
H-HC-0.0621	14.90	11.57	46.67	L
H-HC-0.0621	13.44	12.07	45.79	L
C-CT--0.0143	13.10	11.48	47.84	L
H-HP-0.1135	13.47	10.72	48.54	L
H-HP-0.1135	13.29	12.47	48.26	L
N-N3--0.03854	11.64	11.31	47.69	L
H-H-0.034	11.44	10.40	47.30	L
H-H-0.034	11.20	11.41	48.59	L
H-H-0.034	11.29	12.03	47.07	L
C-C-0.7341	12.82	8.22	43.56	L
O-O--0.5894	12.08	7.45	44.17	L
N-N--0.4157	12.40	8.95	42.52	L
H-H-0.2719	13.07	9.55	42.07	L
C-CT--0.0597	11.01	8.89	42.03	L
H-H1-0.0869	10.37	9.09	42.89	L
C-CT-0.1303	10.68	10.00	41.00	L
H-HC-0.0187	9.61	9.93	40.78	L
C-CT--0.3204	10.92	11.38	41.65	L
H-HC-0.0882	11.99	11.57	41.77	L
H-HC-0.0882	10.49	12.16	41.04	L
H-HC-0.0882	10.44	11.41	42.63	L
C-CT--0.043	11.45	9.87	39.67	L
H-HC-0.0236	12.51	9.93	39.86	L
H-HC-0.0236	11.24	8.89	39.23	L
C-CT--0.066	11.07	10.91	38.61	L
H-HC-0.0186	11.40	11.91	38.93	L
H-HC-0.0186	11.57	10.67	37.67	L
H-HC-0.0186	10.00	10.92	38.45	L
C-C-0.5973	10.61	7.48	41.57	L
O-O--0.5679	9.56	7.01	41.96	L
N-N--0.4157	11.48	6.78	40.82	L
H-H-0.2719	12.33	7.23	40.51	L
C-CT-0.0337	11.27	5.38	40.45	L
H-H1-0.0823	10.38	5.32	39.83	L
C-CT--0.1825	12.46	4.91	39.60	L
H-HC-0.0603	13.38	4.97	40.18	L
H-HC-0.0603	12.30	3.88	39.29	L
H-HC-0.0603	12.55	5.54	38.71	L
C-C-0.5973	11.05	4.47	41.67	L
O-O--0.5679	10.12	3.65	41.68	L
N-N--0.4157	11.85	4.63	42.73	L
H-H-0.2719	12.58	5.33	42.64	L
C-CT--0.0249	11.74	3.90	44.00	L
H-H1-0.0843	11.83	2.84	43.79	L
C-CT-0.2117	12.86	4.28	44.97	L
H-H1-0.0352	12.75	5.32	45.28	L
H-H1-0.0352	12.79	3.65	45.86	L
O-OH--0.6546	14.14	4.09	44.39	L
H-HO-0.4275	14.22	4.71	43.64	L

C-C-0.5973	10.39	4.09	44.72	L
O-O--0.5679	10.04	3.28	45.58	L
N-N--0.4157	9.61	5.13	44.38	L
H-H-0.2719	9.97	5.76	43.68	L
C-CT--0.0252		8.22	5.32	44.81 L
H-H1-0.0698	7.88	4.47	45.39	L
H-H1-0.0698	8.17	6.21	45.44	L
C-C-0.5973	7.25	5.50	43.63	L
O-O--0.5679	6.27	6.23	43.76	L
N-N--0.4157	7.52	4.85	42.50	L
H-H-0.2719	8.39	4.32	42.47	L
C-CT--0.0252		6.79	5.03	41.25 L
H-H1-0.0698	5.78	4.63	41.36	L
H-H1-0.0698	6.70	6.10	41.04	L
C-C-0.5973	7.47	4.36	40.05	L
O-O--0.5679	7.92	5.06	39.14	L
O-OH-0.0	7.51	3.00	40.08	L
H-HO-0.0	7.95	2.62	39.31	L

3. EPS derived charges of TCEP

Cartesian structure

P	0.234861	-0.332439	-0.752969
C	1.783224	-0.968509	0.083149
C	3.053169	-0.255344	-0.383118
C	4.326669	-0.935651	0.108694
O	5.478183	-0.247477	-0.129093
O	4.369627	-2.003027	0.650352
C	-1.017105	-1.389993	0.162311
C	-2.378803	-1.456875	-0.533127
C	-3.375550	-2.350535	0.196771
O	-3.164411	-2.914256	1.232229
O	-4.587519	-2.481312	-0.413139
C	0.065690	1.310968	0.131333
C	-1.185834	2.098855	-0.258019
C	-1.134071	3.545800	0.187188
O	-0.153905	4.139799	0.558488
O	-2.353292	4.131113	0.096102
H	1.692525	-0.904668	1.171841
H	1.863837	-2.030034	-0.163038
H	3.065846	0.788823	-0.050577
H	-1.134185	-1.049698	1.194779
H	-0.601346	-2.399467	0.217404
H	-2.831752	-0.462303	-0.624330
H	-2.265390	-1.829721	-1.558133
H	0.099081	1.164284	1.216185
H	0.942809	1.906879	-0.133936
H	-2.098367	1.657049	0.150413
H	-1.317916	2.114224	-1.347181
H	5.290980	0.598088	-0.554940
H	-2.251662	5.056776	0.365509

H -4.610835 -1.984861 -1.240451
H 3.099668 -0.229791 -1.479616

Charges (in |e|)

1 P -0.501367
2 C 0.103303
3 C -0.082355
4 C 0.637108
5 O -0.557239
6 O -0.538341
7 C 0.405453
8 C -0.371787
9 C 0.764568
10 O -0.568282
11 O -0.597400
12 C -0.024201
13 C -0.097477
14 C 0.667652
15 O -0.587030
16 O -0.637441
17 H -0.008772
18 H 0.073453
19 H 0.044184
20 H -0.034255
21 H -0.019073
22 H 0.083093
23 H 0.104419
24 H 0.068561
25 H 0.101948
26 H 0.091912
27 H 0.093060
28 H 0.411506
29 H 0.478841
30 H 0.433005
31 H 0.062954

4. Example of input file for a MD calculation with amber

```
input for sander for md
&cntrl
  nmropt = 1,          cut      = 10.0,      nsnb    = 9999,
  ntx     = 5,          irest    = 1,
  ntb     = 2, ntf = 2, ntt = 3, gamma_ln = 1.0, ntp = 1,
  imin = 0, ntwr = 100, ntwx = 100, ntwv = 100, ntc = 2,
  tempi = 300.0, temp0 = 300.0,
  nstlim = 1000000, dt = 0.002,
  scee=1.2, ntpv    = 100,
/
&ewald
  diptol = 1.d-6, indmeth=1, scaldip=0, chngmask=0, frameon=0,
/
```

&wt type = 'END'
/

5. QM frequencies (unscaled) and Raman intensities

cys6-cys127 model system

frequency (cm⁻¹); Raman intensity; Depolarisation factor

13.304";"0.3067";"0.7276
17.9533";"0.1367";"0.7493
23.3131";"0.5551";"0.7492
31.4251";"0.4296";"0.5502
35.4838";"2.0889";"0.7348
45.5087";"0.9237";"0.6699
54.5685";"1.6066";"0.6996
56.6513";"1.9004";"0.7164
64.1248";"0.7177";"0.5359
68.7565";"0.7201";"0.6576
83.1047";"1.508";"0.735
94.4528";"0.4311";"0.7342
110.1644";"0.7022";"0.7406
139.6258";"1.1347";"0.193
150.158";"0.496";"0.7406
181.1818";"0.3471";"0.6864
188.0602";"0.555";"0.6389
216.2628";"1.3953";"0.2598
242.3225";"0.8161";"0.7101
286.3188";"0.505";"0.3194
305.455";"1.6297";"0.7467
312.2472";"1.8656";"0.1666
327.6559";"2.6768";"0.2286
334.0674";"0.5529";"0.2326
339.0336";"2.7684";"0.4306
367.8778";"1.9545";"0.7302
413.0918";"0.3334";"0.6873
416.2993";"0.1859";"0.6549
421.0165";"1.1047";"0.3102
467.4882";"10.6855";"0.1062
485.4113";"1.8316";"0.6955
499.6637";"1.3265";"0.3717
507.8297";"0.2111";"0.5988
534.3224";"2.0959";"0.5645
574.0123";"0.2383";"0.2484
586.8506";"2.4606";"0.6414
601.5399";"3.947";"0.1359
615.0999";"7.4271";"0.0793
623.0127";"2.7107";"0.1486
635.0799";"1.433";"0.2574

637.1499";"7.9137";"0.142
674.1576";"1.2365";"0.6985
689.3077";"5.6351";"0.4278
729.7931";"5.7896";"0.5892
745.0269";"1.4978";"0.6841
770.3823";"4.9658";"0.2728
828.0176";"5.8713";"0.0776
841.9625";"2.2455";"0.1217
899.5389";"5.6349";"0.539
904.3966";"8.1945";"0.3854
966.4372";"8.9432";"0.0339
971.4064";"7.5538";"0.0345
996.7648";"3.1514";"0.1893
1006.2276";"2.8181";"0.4123
1043.4792";"3.3139";"0.6205
1053.0182";"0.5306";"0.5189
1056.3024";"0.2853";"0.6818
1064.2141";"2.5569";"0.7457
1086.7846";"4.1563";"0.3504
1114.9957";"0.7002";"0.5808
1128.155";"5.7257";"0.1712
1137.9191";"4.5472";"0.1844
1200.015";"5.6526";"0.229
1200.6367";"3.6275";"0.1587
1251.13";"4.1114";"0.4616
1267.2642";"1.3844";"0.2914
1272.5749";"4.4691";"0.5463
1286.5384";"12.1183";"0.503
1311.3661";"2.6453";"0.7036
1331.99";"4.6872";"0.7465
1343.4067";"12.0749";"0.6421
1359.2966";"5.6625";"0.6872
1366.4571";"6.3";"0.75
1389.1402";"6.8644";"0.4695
1398.4582";"1.995";"0.7394
1403.3524";"3.9253";"0.6489
1457.6891";"11.7571";"0.6266
1458.3665";"5.8811";"0.725
1470.719";"4.8657";"0.75
1471.0326";"6.2262";"0.749
1486.9241";"4.9903";"0.7464
1489.2517";"5.7572";"0.7466
1518.7557";"1.5875";"0.619
1532.6263";"0.8015";"0.4455
1599.3573";"3.4643";"0.7215
1624.3359";"5.1275";"0.6119
1712.7036";"10.7662";"0.2377
1755.8947";"6.8322";"0.3503
1759.4027";"8.0852";"0.3908
1760.2092";"9.2456";"0.1937

3035.2989";"147.1032";"0.1167
3041.0513";"157.2121";"0.0091
3046.2903";"174.7135";"0.0186
3058.6521";"114.395";"0.0982
3058.8511";"51.974";"0.0384
3067.6773";"15.4434";"0.2363
3105.1888";"44.19";"0.7495
3117.415";"67.7892";"0.7398
3122.556";"53.1996";"0.631
3125.5468";"39.2446";"0.5561
3134.2849";"79.7578";"0.5828
3138.361";"39.6086";"0.35
3490.0057";"136.9281";"0.1055
3588.221";"209.362";"0.1361
3603.1947";"45.4954";"0.156
3628.2599";"48.7775";"0.0851
3662.9446";"129.8644";"0.3772
3719.6547";"51.8565";"0.6828

cys30-cys115 model system

frequency (cm^{-1}); Raman intensity; Depolarisation factor

2.0053";"0.2424";"0.7324
15.0499";"0.2138";"0.6632
17.66";"0.3254";"0.7422
23.3666";"0.6473";"0.5306
35.9819";"0.9449";"0.6776
45.1065";"1.3981";"0.7435
55.3832";"1.7224";"0.7474
61.6125";"0.8536";"0.7309
64.4665";"0.2642";"0.7103
65.7833";"1.1993";"0.5349
79.1285";"1.6682";"0.7293
90.5674";"0.7902";"0.6831
98.3119";"0.7696";"0.7274
127.229";"2.1755";"0.3615
141.3189";"0.9755";"0.2989
158.5872";"0.9259";"0.4592
171.556";"0.6552";"0.5835
215.5516";"2.2724";"0.1397
246.5261";"0.9208";"0.5831
294.0355";"1.3314";"0.3635
304.2035";"1.348";"0.552
322.7984";"0.3534";"0.7368
323.7189";"2.8765";"0.1759
342.2142";"0.5913";"0.1504
349.7405";"0.8348";"0.3137
369.9607";"1.605";"0.7219

377.1648";"2.0158";"0.5279
399.389";"0.6258";"0.7096
407.6774";"0.5884";"0.7497
473.6451";"8.6375";"0.1338
479.7075";"1.4746";"0.5888
488.8113";"1.2498";"0.7499
513.81";"2.9459";"0.3828
531.1722";"2.8753";"0.5765
548.6143";"3.4104";"0.223
561.0602";"0.4177";"0.2961
588.8184";"0.937";"0.071
596.9855";"4.2675";"0.1802
633.4308";"8.6829";"0.1192
636.175";"0.7244";"0.2499
643.0779";"0.7417";"0.3443
661.8291";"1.2758";"0.374
685.5389";"6.2616";"0.4404
716.0161";"12.7397";"0.188
735.6168";"0.6703";"0.7314
751.0264";"1.1855";"0.7016
784.3877";"3.3342";"0.662
841.9601";"2.7362";"0.0776
904.261";"4.8748";"0.5305
937.8946";"9.4711";"0.2756
957.2143";"0.7437";"0.3541
958.8073";"13.7609";"0.0322
996.8487";"3.8981";"0.4194
999.2294";"2.0753";"0.4394
1048.8217";"2.5475";"0.7444
1051.0912";"2.7245";"0.181
1054.4451";"1.1442";"0.4802
1055.3605";"1.7458";"0.2268
1091.2451";"7.7787";"0.2309
1091.5427";"4.0972";"0.6259
1108.3405";"0.4794";"0.6048
1126.8967";"5.201";"0.0996
1190.2054";"5.3067";"0.3627
1198.0044";"6.2357";"0.2937
1248.7619";"6.6176";"0.2871
1257.4473";"4.8097";"0.4209
1274.7271";"2.9214";"0.7172
1281.2801";"2.282";"0.6948
1318.8967";"12.9867";"0.7377
1325.346";"9.3093";"0.4572
1352.9105";"6.3633";"0.7487
1355.4769";"6.8971";"0.6934
1365.7551";"4.9491";"0.7307
1374.0378";"6.4887";"0.4941
1398.7304";"2.4883";"0.7354
1400.0013";"3.0219";"0.5843

1455.3585";"13.1677";"0.4402
1458.6341";"7.0258";"0.6969
1470.486";"5.4318";"0.7489
1471.4823";"6.1155";"0.7497
1487.5579";"4.6288";"0.736
1488.592";"5.5384";"0.7494
1508.0374";"2.6402";"0.7278
1516.9258";"1.2477";"0.6052
1599.3134";"3.1938";"0.7127
1602.0529";"2.5062";"0.738
1752.5399";"8.9551";"0.2356
1758.6495";"10.0444";"0.6424
1759.483";"11.9959";"0.1274
1773.3386";"10.2542";"0.2109
3027.6566";"146.5459";"0.1334
3038.8662";"107.8808";"0.0641
3041.9336";"159.1658";"0.0093
3042.6723";"196.235";"0.0201
3064.0656";"28.0579";"0.0736
3087.0807";"45.1869";"0.5282
3102.0574";"30.5578";"0.13
3106.6881";"44.5764";"0.749
3111.742";"64.4876";"0.6917
3123.4553";"74.8145";"0.6177
3132.2189";"34.9049";"0.3414
3132.8135";"85.8731";"0.5688
3582.8722";"144.5437";"0.1034
3587.9771";"202.8726";"0.1298
3606.2349";"44.4173";"0.1137
3607.7961";"64.8853";"0.1097
3708.693";"38.2938";"0.7495
3717.8991";"51.8463";"0.6849

cys64-cys80 model system

frequency (cm⁻¹); Raman intensity; Depolarisation fact

23.1987";"0.5579";"0.744
29.6579";"0.8451";"0.7479
39.802";"1.2823";"0.706
43.1184";"1.2417";"0.7036
53.6301";"0.3668";"0.6851
56.7352";"1.5879";"0.6183
63.9162";"0.7915";"0.6819
66.5455";"0.6399";"0.7498
74.4588";"1.2746";"0.66
88.7925";"0.7809";"0.6497
96.272";"0.3215";"0.7442
100.8697";"0.3077";"0.427

130.0233";"1.484";"0.6736
134.315";"1.2978";"0.75
150.0779";"0.1826";"0.7208
172.3163";"1.0065";"0.0371
187.6003";"0.9374";"0.3855
199.0444";"1.4517";"0.69
233.1074";"1.9272";"0.3192
278.8908";"1.3683";"0.6832
291.9183";"0.7199";"0.2278
326.3998";"2.6717";"0.2534
335.6731";"0.7787";"0.3044
348.2531";"3.1434";"0.1474
357.6059";"1.2049";"0.5018
368.299";"2.0852";"0.742
423.0436";"0.2417";"0.4282
448.0128";"2.7864";"0.2101
467.5329";"10.6397";"0.1228
483.9196";"2.0616";"0.6075
494.3159";"0.798";"0.4225
515.5206";"0.943";"0.6138
537.749";"1.3553";"0.5938
557.3235";"0.5281";"0.7282
569.9538";"1.3721";"0.126
586.1006";"0.1988";"0.749
601.9359";"1.0014";"0.4479
612.5409";"3.6289";"0.4923
615.6305";"9.5744";"0.0205
634.279";"9.7276";"0.2362
646.4179";"6.0169";"0.1558
656.2483";"1.4131";"0.5011
666.6156";"3.3247";"0.2756
690.9736";"5.2388";"0.4811
743.1178";"1.4288";"0.6873
755.0307";"2.3029";"0.1292
833.9721";"1.6576";"0.3298
839.8861";"1.5091";"0.2758
897.1095";"4.899";"0.6025
914.3158";"0.6826";"0.5865
962.8061";"2.987";"0.2444
987.6148";"10.4506";"0.074
1000.5813";"3.7758";"0.2091
1012.0065";"4.2";"0.3053
1016.3403";"4.7943";"0.2382
1033.5412";"3.2175";"0.4479
1053.5742";"0.2626";"0.6167
1057.1471";"0.2461";"0.2937
1083.6448";"3.514";"0.3419
1111.9591";"6.3377";"0.1569
1125.5784";"5.3421";"0.2516
1162.2247";"7.5708";"0.2707

1201.9417";"2.4925";"0.1119
1217.3726";"9.1328";"0.7177
1251.5564";"7.4509";"0.3113
1258.3993";"5.5651";"0.5152
1267.2171";"5.2653";"0.4481
1279.7178";"1.8287";"0.1069
1301.4492";"4.0133";"0.5613
1319.1332";"4.7934";"0.6607
1344.7238";"9.2807";"0.724
1350.759";"3.2664";"0.7016
1362.0437";"4.0782";"0.4901
1396.4163";"0.6858";"0.6036
1401.3353";"2.5387";"0.6828
1405.8954";"6.3624";"0.5279
1452.5178";"7.3479";"0.7351
1467.3681";"4.9125";"0.5754
1471.252";"5.774";"0.7496
1473.1361";"5.9788";"0.7453
1486.2223";"4.579";"0.7238
1490.7206";"5.2644";"0.714
1523.8109";"2.1729";"0.7298
1537.0715";"0.8689";"0.6652
1605.7159";"3.7937";"0.7434
1651.3497";"1.8328";"0.7099
1720.9556";"8.1134";"0.6879
1723.2415";"18.8595";"0.0717
1751.4279";"8.3764";"0.3142
1765.7586";"9.1726";"0.268
3012.9179";"79.1204";"0.1556
3042.1371";"157.4815";"0.1759
3043.0295";"172.8305";"0.0116
3045.1542";"194.5291";"0.0234
3075.6174";"115.8968";"0.0709
3085.1698";"32.429";"0.0719
3107.5647";"45.5079";"0.7035
3114.8445";"76.4373";"0.7421
3122.3003";"56.1848";"0.6592
3133.776";"66.0605";"0.6422
3137.8055";"52.5021";"0.6096
3142.2205";"47.9653";"0.3791
3516.3819";"169.0773";"0.1216
3574.51";"48.8762";"0.0901
3585.6784";"207.96";"0.1425
3603.9399";"56.1168";"0.184
3669.6741";"64.3562";"0.5936
3716.2387";"50.3669";"0.6863

cys76-cys94 model system

frequency (cm⁻¹); Raman intensity; Depolarisation fact

13.5159";"0.314";"0.6525
13.711";"0.9007";"0.7071
18.4218";"0.9528";"0.744
25.1663";"0.351";"0.7462
38.4564";"1.8789";"0.7261
52.2121";"1.4887";"0.7467
55.0115";"2.0911";"0.7368
61.921";"1.5239";"0.701
72.578";"0.2257";"0.7499
78.3018";"1.3486";"0.5575
81.6955";"1.267";"0.6577
89.6995";"0.37";"0.5233
108.7598";"0.2873";"0.7486
125.2639";"0.4682";"0.6196
125.79";"0.971";"0.4359
167.5688";"1.3363";"0.1481
182.9901";"0.735";"0.333
224.0857";"2.9612";"0.1389
239.6164";"0.4257";"0.6639
266.8841";"1.1529";"0.2598
290.5526";"0.8593";"0.5437
305.4285";"2.1758";"0.5661
315.3522";"2.035";"0.6056
321.4477";"1.3024";"0.1205
342.2282";"0.7694";"0.1802
365.217";"2.2483";"0.6734
409.241";"1.04";"0.2746
431.7853";"0.3118";"0.2378
450.0503";"1.225";"0.6507
474.4269";"6.2323";"0.0894
484.2105";"6.3479";"0.2543
498.7523";"1.0307";"0.5829
502.8857";"2.3546";"0.5904
532.4486";"2.829";"0.3555
567.0023";"0.5714";"0.1433
577.3035";"3.4368";"0.3052
599.5186";"1.3167";"0.1838
624.3187";"5.1165";"0.1624
636.6492";"0.4627";"0.7364
638.8979";"1.2617";"0.5446
643.6773";"7.7451";"0.126
653.5548";"2.2415";"0.2725
698.6472";"6.0235";"0.3256
718.8061";"11.0398";"0.2712
750.8869";"6.2031";"0.1939
756.1066";"2.4504";"0.4006
802.9136";"1.7674";"0.2844
861.0895";"2.3599";"0.1406

907.7398";"10.1812";"0.4064
946.3614";"4.5658";"0.6202
962.8473";"14.5959";"0.015
963.7027";"6.5536";"0.076
998.3907";"2.8128";"0.3556
1003.2871";"2.3925";"0.3533
1045.3313";"3.5596";"0.3551
1053.597";"0.3356";"0.438
1056.3713";"0.1061";"0.446
1088.8055";"4.0311";"0.4169
1093.8851";"1.7226";"0.6687
1102.9596";"1.495";"0.7243
1121.8145";"6.8332";"0.1334
1128.0829";"4.0083";"0.1731
1193.7598";"2.559";"0.5358
1205.4299";"5.7269";"0.2894
1254.9764";"3.4442";"0.4879
1257.8708";"8.3653";"0.2105
1266.7356";"1.5655";"0.7497
1282.2708";"6.465";"0.7198
1314.1495";"1.9496";"0.747
1324.943";"4.1186";"0.5958
1353.1998";"6.3286";"0.7462
1363.2473";"7.5554";"0.6728
1367.8121";"7.9878";"0.527
1399.6547";"2.6493";"0.6897
1400.8759";"7.6216";"0.7466
1403.4597";"4.0351";"0.6
1444.1836";"9.2991";"0.5461
1469.852";"5.1371";"0.7117
1471.7012";"6.2636";"0.7483
1479.2011";"11.3498";"0.5067
1486.7147";"4.2819";"0.7425
1488.2026";"7.2044";"0.7361
1517.7615";"0.9341";"0.7272
1524.161";"1.6244";"0.6024
1600.1984";"3.4245";"0.75
1627.877";"4.0711";"0.611
1717.7314";"8.6344";"0.2965
1757.1704";"10.3749";"0.1803
1758.282";"9.5089";"0.4643
1763.6412";"4.4418";"0.4591
3042.9348";"163.5609";"0.0101
3045.8768";"177.9545";"0.0185
3049.666";"107.6796";"0.0612
3059.9824";"143.8123";"0.0622
3062.6477";"1.7037";"0.6359
3082.0448";"27.6612";"0.1941
3108.8244";"45.7787";"0.75
3117.811";"65.9065";"0.75

3120.1613";"34.3497";"0.7417
3121.8342";"60.1565";"0.6326
3130.6773";"81.2165";"0.5892
3139.7371";"34.3315";"0.3864
3514.7837";"125.9222";"0.0978
3590.148";"200.4868";"0.1313
3607.1555";"43.3188";"0.1245
3623.0063";"56.4891";"0.1333
3668.835";"96.4352";"0.4154
3720.3178";"49.4433";"0.6969

6. QM/MM frequencies (unscaled) and Raman intensities

cys6-cys127 model system

frequency (cm^{-1}); Raman intensity

4.1776";"0.0133
4.7941";"0.0041
5.8226";"0.0052
7.5136";"0.0058
7.9543";"0.0016
9.3368";"0.0373
11.6394";"0.0023
12.9046";"0.0142
13.2215";"0.0101
14.7271";"0.0028
16.0874";"0.0024
16.4991";"0.0325
18.1817";"0.0134
18.5694";"0.0039
19.7719";"0.0035
20.5743";"0.0017
21.2347";"0.0159
21.8353";"0.0301
22.9568";"0.0055
23.3228";"0.0272
24.4503";"0.0187
25.1096";"0.0217
25.3626";"0.0387
26.3578";"0.0425
27.2236";"0.038
28.0727";"0.0269
28.6437";"0.0268
29.4037";"0.0142
29.757";"0.0479
30.7287";"0.0719
31.0805";"0.0309
32.4778";"0.0383

33.0821";"0.0671
33.9039";"0.0057
34.5604";"0.0042
35.7917";"0.0295
37.3175";"0.0793
38.2518";"0.0526
39.2995";"0.0325
39.6773";"0.0071
39.9494";"0.0357
40.9404";"0.0088
41.7665";"0.0508
42.4439";"0.0179
43.2632";"0.0203
44.3094";"0.0134
45.6372";"0.0713
46.0308";"0.066
47.5439";"0.0165
48.422";"0.072
48.9517";"0.004
49.5477";"0.0085
50.0015";"0.0187
50.7852";"0.0091
53.1316";"0.0249
53.415";"0.0564
54.0904";"0.0055
55.6862";"0.0029
56.5913";"0.0144
58.0369";"0.0128
59.2894";"0.0416
59.7422";"0.0132
60.2983";"0.0188
61.55";"0.0094
61.8683";"0.0405
63.971";"0.0077
64.6606";"0.0112
65.0139";"0.0178
66.3406";"0.0745
66.671";"0.0178
66.9319";"0.0092
68.0763";"0.0057
68.5814";"0.0111
69.9801";"0.0064
70.6742";"0.0734
71.4616";"0.0537
71.9044";"0.1164
73.9523";"0.0238
74.0308";"0.0085
76.1127";"0.0543
77.1005";"0.0788
77.6595";"0.2695

78.4472";"0.0836
81.0214";"0.4959
82.8324";"0.0201
83.3265";"0.0393
83.9505";"0.0932
84.309";"0.1787
84.9859";"0.0646
86.1366";"0.0414
87.0376";"0.057
88.8079";"0.117
89.7981";"0.0484
92.025";"0.1522
92.3793";"0.2971
93.6355";"0.1338
94.1586";"0.0388
95.179";"0.0063
95.8198";"0.0619
96.1995";"0.113
96.7825";"0.0405
97.3621";"0.0867
97.8122";"0.0601
100.6603";"0.0773
101.8856";"0.1224
103.3321";"0.0571
104.2243";"0.0426
104.7871";"0.0431
107.2109";"0.0818
108.5252";"0.073
109.9944";"0.0276
110.4819";"0.0277
111.2199";"0.2391
111.9661";"0.0477
112.6618";"0.0123
114.0274";"0.0157
114.5431";"0.0467
115.8259";"0.0334
116.3981";"0.0541
117.1819";"0.0304
117.9615";"0.0518
119.1191";"0.1046
119.647";"0.3248
120.8016";"0.2217
122.6688";"0.0741
124.1723";"0.0643
124.824";"0.0905
126.7003";"0.1132
127.7125";"0.0857
128.2917";"0.1034
128.4838";"0.0312
131.798";"0.0126

133.496";"0.0154
134.3834";"0.1383
135.3492";"0.0685
136.5505";"0.0189
138.3272";"0.1404
139.02";"0.0492
140.7911";"0.0759
141.6551";"0.1926
143.4305";"0.1337
143.7862";"0.1913
146.5915";"0.0333
147.5767";"0.1148
150.7385";"0.2828
151.0254";"0.1753
152.4961";"0.0466
152.8159";"0.0678
153.8367";"0.0198
154.3778";"0.2267
155.0388";"0.0464
158.614";"0.1316
159.5101";"0.0862
159.8121";"0.0156
161.4032";"0.0418
162.8366";"0.118
163.841";"0.0668
165.0777";"0.0665
165.422";"0.1008
166.4843";"0.0617
166.6939";"0.0025
167.9851";"0.008
169.1096";"0.0793
169.5855";"0.0676
171.9774";"0.0356
174.0284";"0.2449
175.5909";"0.2411
176.5115";"0.4796
179.994";"0.0284
180.7009";"0.0037
183.6287";"0.0194
185.2484";"0.0052
186.7486";"0.0296
187.8435";"0.066
190.1208";"0.1611
190.5224";"0.2084
193.5497";"0.0684
194.0993";"0.2096
195.244";"0.0458
195.8944";"0.1175
197.6378";"0.0203
197.9344";"0.0523

200.1851";"0.1052
200.4088";"0.0137
201.899";"0.0543
202.6714";"0.1434
203.5726";"0.0155
204.0228";"0.0776
205.1321";"0.0449
205.9768";"0.1115
206.8695";"0.1766
210.1714";"0.2206
212.1006";"0.0521
214.6065";"0.3149
216.4923";"0.0157
220.868";"0.1012
222.6344";"0.0599
223.8041";"0.0589
224.6179";"0.0268
225.9581";"0.0567
228.1276";"0.0117
231.0525";"0.0025
231.2155";"0.0045
234.8728";"0.2859
235.4398";"0.265
237.1395";"0.0037
239.8998";"0.0064
240.9244";"0.0163
241.0045";"0.0784
242.2713";"0.1636
245.5263";"0.1353
246.2302";"0.0433
247.1532";"0.0241
248.4574";"0.3548
249.5532";"0.1336
249.796";"0.2952
252.1209";"0.0482
253.0297";"0.082
254.0725";"0.0629
255.9824";"0.008
257.1323";"0.0049
258.5868";"0.1887
260.1379";"0.0125
260.2471";"0.0797
260.3659";"0.0415
261.1326";"0.0364
263.7144";"0.2935
267.3746";"0.1118
267.8719";"0.1109
268.7467";"0.199
271.2561";"0.072
272.1115";"0.4099

273.9307";"0.0112
276.1499";"0.0055
279.2939";"0.1709
279.9458";"0.13
281.3111";"0.0366
282.4419";"0.1099
283.7287";"0.2731
284.327";"0.3084
288.3223";"0.3028
291.5";"0.0034
292.1844";"0.0005
292.7693";"0.2129
294.6614";"0.1952
295.3821";"0.1746
296.3829";"0.0652
298.0114";"0.0583
300.5715";"0.0263
300.7191";"0.2111
301.9572";"0.0263
305.0881";"0.199
305.8941";"0.0014
306.2409";"0.4401
307.5775";"0.0962
311.4253";"0.0942
311.9744";"0.0518
316.1712";"0.0142
321.8005";"0.0028
322.3962";"0.7501
324.2455";"0.17
324.5016";"0.0016
325.6562";"0.035
327.3373";"0.3828
328.475";"0.034
328.8511";"0.2224
330.0089";"0.023
330.6101";"0.0376
333.9809";"0.0005
336.1574";"0.213
337.0675";"0.0406
339.9791";"0.0065
341.863";"0.0068
342.6902";"0.0267
344.0536";"0.1126
346.5424";"0.0342
348.0602";"0.0179
349.5976";"0.0313
350.3936";"0.0117
351.0345";"0.0237
353.306";"0.0241
354.2371";"0.0066

354.5741";"0.0266
357.0312";"0.0317
357.8388";"0.009
358.7052";"0.0064
364.2936";"0.1645
364.9817";"0.128
366.6448";"0.0175
369.4975";"0.5838
370.1815";"0.0677
370.8957";"0.0044
372.4026";"0.0008
375.1546";"0.0025
376.2889";"0.0029
378.0346";"0.0656
378.9151";"0.0261
379.367";"0.0216
380.3584";"0.0054
381.9031";"0.0039
383.936";"0.01
385.1139";"0.4099
386.1303";"0.2198
386.9321";"0.0489
387.8006";"0.0381
391.5997";"0.0052
392.399";"0.0807
396.2909";"0.0055
397.3164";"0.1033
398.2752";"0.0542
400.206";"0.0594
401.822";"0.3357
402.5823";"0.008
409.193";"0.0774
410.1295";"0.0019
412.7309";"0.5841
414.1401";"0.0009
415.4538";"0.0897
416.8774";"0.2298
418.0966";"0.0353
418.1504";"0.0077
420.4285";"0.0008
421.6322";"0.5951
422.4102";"0.7756
428.0129";"0.0235
430.3742";"0.3394
430.6532";"0.36
432.5016";"0.0074
433.4797";"0.0022
436.0936";"0.0699
439.3512";"0.0197
439.6679";"0.0002

441.1511";"0.034
443.5271";"0.0468
446.561";"0.525
451.6978";"0.0016
454.5886";"0.6017
457.1185";"0.3098
460.0045";"1.4597
461.7648";"0.6642
462.2751";"0.0294
464.9925";"3.2455
466.7633";"0.6414
468.5436";"1.2036
470.0728";"0.0784
473.286";"0.0807
474.3763";"4.5988
478.8308";"0.0225
481.2857";"0.1427
482.3143";"0.0134
486.0534";"0.0679
486.8034";"0.0543
488.8288";"0.0249
490.6063";"0.0215
490.9153";"0.8568
492.4153";"0.4946
493.6877";"0.0185
495.5665";"0.0288
500.2909";"0.0023
502.5308";"0.3409
503.0654";"0.0066
505.7443";"0.0719
507.4488";"0.167
509.2102";"0.6107
510.7765";"0.1388
513.6396";"0.0962
516.9337";"0.1239
519.1058";"0.0102
519.7999";"0.0324
522.4142";"0.017
524.0217";"0.0888
528.1146";"0.1687
528.6408";"0.0652
529.0201";"0.268
529.8943";"0.0773
532.9006";"0.0073
536.6097";"0.0058
537.7022";"0.5019
538.2849";"0.0064
541.5085";"0.5198
542.032";"0.0021
542.2509";"0.0009

542.6967";"0.0748
543.4196";"0.0044
543.543";"0.0001
543.6017";"0.0069
543.9702";"0.0059
546.7806";"0.1581
548.8598";"0.0062
549.3089";"0.9792
551.2761";"0.0105
552.2852";"0.2059
552.3387";"0.0111
553.7743";"0.005
557.8109";"0.0124
558.0391";"0.0041
559.4336";"0.5903
559.9829";"0.0184
563.5716";"0.0001
564.7447";"0.001
569.2385";"0.0317
572.2173";"1.2354
574.5566";"0.0002
580.8812";"0.0002
581.7158";"0.
583.3457";"0.
583.6649";"0.0033
590.7702";"0.
596.1051";"0.6009
597.7311";"0.069
600.2125";"0.7611

cys30-cys115 model system

frequency (cm^{-1}); Raman intensity

5.3959";"0.002
7.5387";"0.0076
8.4982";"0.0076
10.0258";"0.0026
12.6049";"0.0071
12.9863";"0.0039
13.4274";"0.0256
14.4441";"0.0049
14.8945";"0.0319
16.1847";"0.005
17.2465";"0.0297
17.5373";"0.0225
18.3827";"0.0087
18.8487";"0.0128
19.7566";"0.0149

20.334";"0.0201
20.7509";"0.0203
21.1875";"0.0206
21.9292";"0.0051
23.1025";"0.0067
23.7203";"0.0319
24.8591";"0.0187
25.6264";"0.0099
26.1364";"0.0297
26.8123";"0.007
27.805";"0.0154
27.9986";"0.0019
29.2822";"0.0099
29.7626";"0.0071
30.0678";"0.0113
31.1142";"0.0425
31.4633";"0.0949
32.1563";"0.0159
33.001";"0.0152
33.5855";"0.0024
34.5251";"0.042
34.6203";"0.0153
35.5263";"0.0085
36.1041";"0.0275
36.4071";"0.0148
37.0066";"0.0091
38.2927";"0.0185
38.6472";"0.0242
39.4563";"0.0138
40.6893";"0.0363
40.879";"0.0026
41.2426";"0.0464
41.979";"0.0212
42.4665";"0.0566
43.6759";"0.0831
44.1255";"0.0123
45.457";"0.0111
45.683";"0.0099
46.3198";"0.0105
46.9248";"0.0717
47.7071";"0.0173
48.9694";"0.0118
49.2484";"0.0059
49.5706";"0.048
50.1926";"0.002
50.7432";"0.0275
51.3718";"0.0255
52.0873";"0.0265
52.2604";"0.006
53.3026";"0.1077

54.501";"0.0064
55.3614";"0.061
56.76";"0.0287
57.3684";"0.0274
57.8156";"0.0497
58.3552";"0.0387
58.6066";"0.0497
59.7354";"0.0316
59.8325";"0.0161
61.431";"0.032
62.4138";"0.0675
62.6336";"0.0487
63.3738";"0.0571
64.4777";"0.0146
64.7577";"0.0542
65.8795";"0.0204
66.5212";"0.0077
66.8556";"0.0253
68.6843";"0.1083
69.0008";"0.0889
70.065";"0.0422
71.0727";"0.0525
71.5535";"0.0201
72.0881";"0.0503
73.8486";"0.0445
74.2305";"0.0776
75.0548";"0.0597
75.2588";"0.1255
75.8018";"0.0602
77.1031";"0.0317
77.5507";"0.0691
78.2144";"0.0123
78.6895";"0.0825
79.7859";"0.0773
80.5651";"0.0204
81.2721";"0.0491
81.5369";"0.0364
83.4653";"0.0824
83.6287";"0.0556
84.9911";"0.0349
85.4687";"0.0239
86.3982";"0.0581
88.338";"0.0563
88.8624";"0.0511
89.3443";"0.0319
89.6896";"0.0407
90.8565";"0.0159
91.4835";"0.0294
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cys64-cys80 model system

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cys76-cys94 model system

frequency (cm⁻¹); Raman intensity

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593.6533";"0.0091
595.1302";"0.0029
599.7642";"0.0088