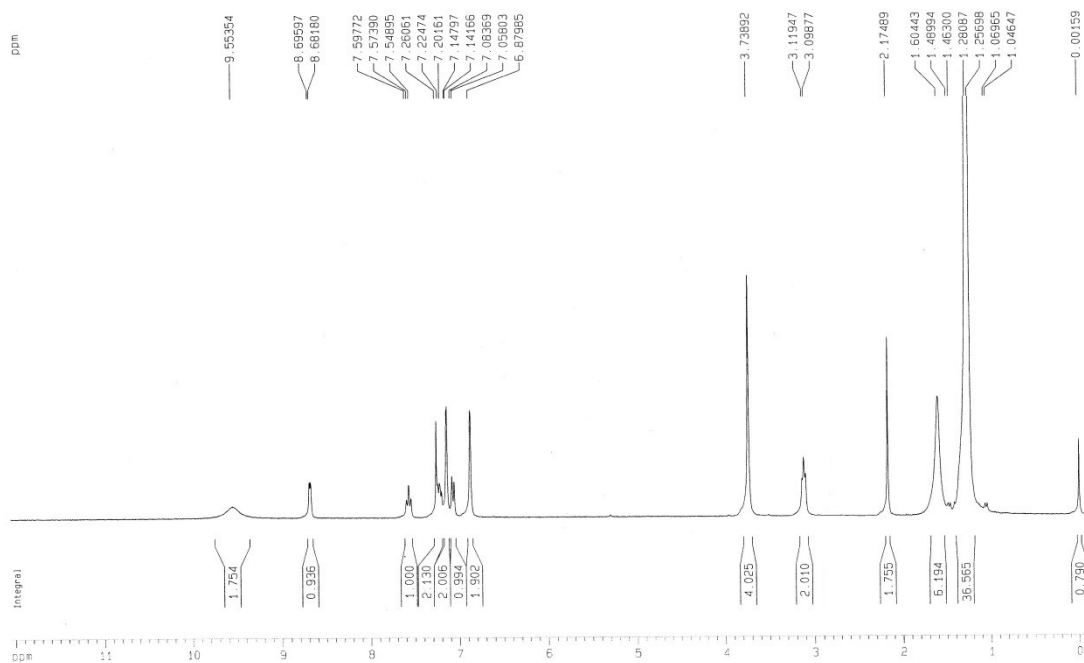


*Electronic Supplementary File for Dalton Transaction-2017*

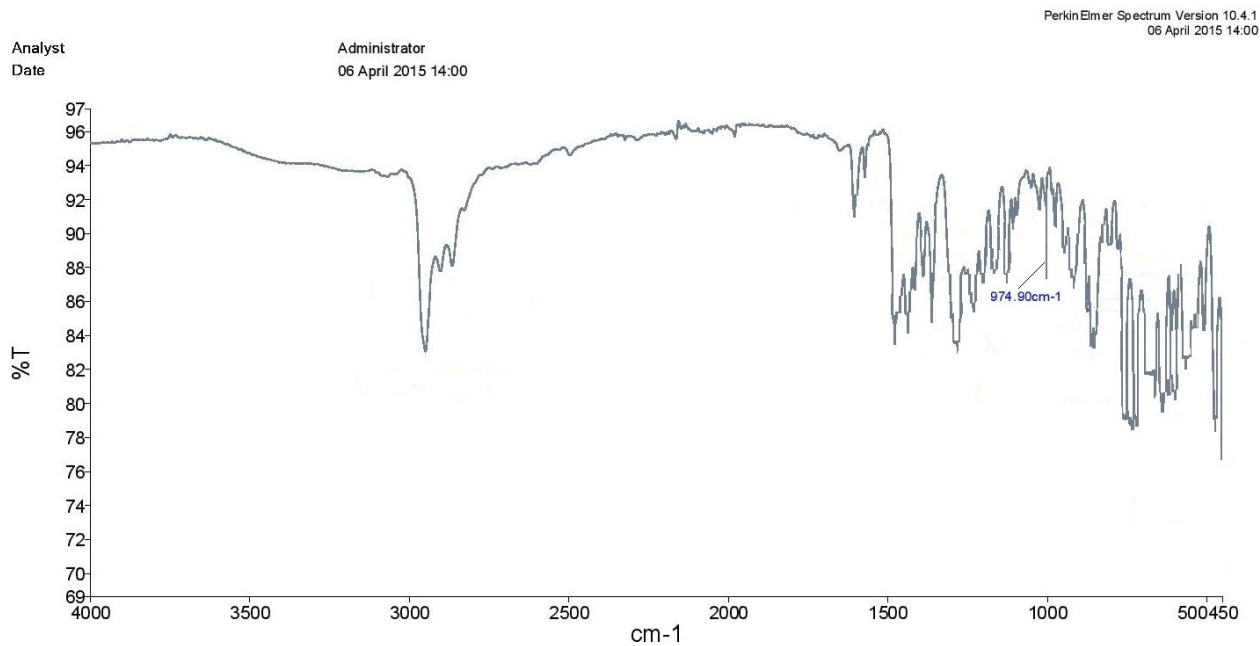
**Mono- and dinuclear oxidovanadium(V) complexes of an amine-bis(phenolate) ligand with bromo-peroxidase activities: synthesis, characterization, catalytic, kinetic and computational studies**

Mainak Debnath<sup>a</sup>, Malay Dolai<sup>a</sup>, Kaberi Pal<sup>a</sup>, Sourav Bhunya<sup>b</sup>, Akan Paul<sup>b</sup>, Hon Man Lee<sup>b</sup> and  
Mahammad Ali<sup>a,\*</sup>

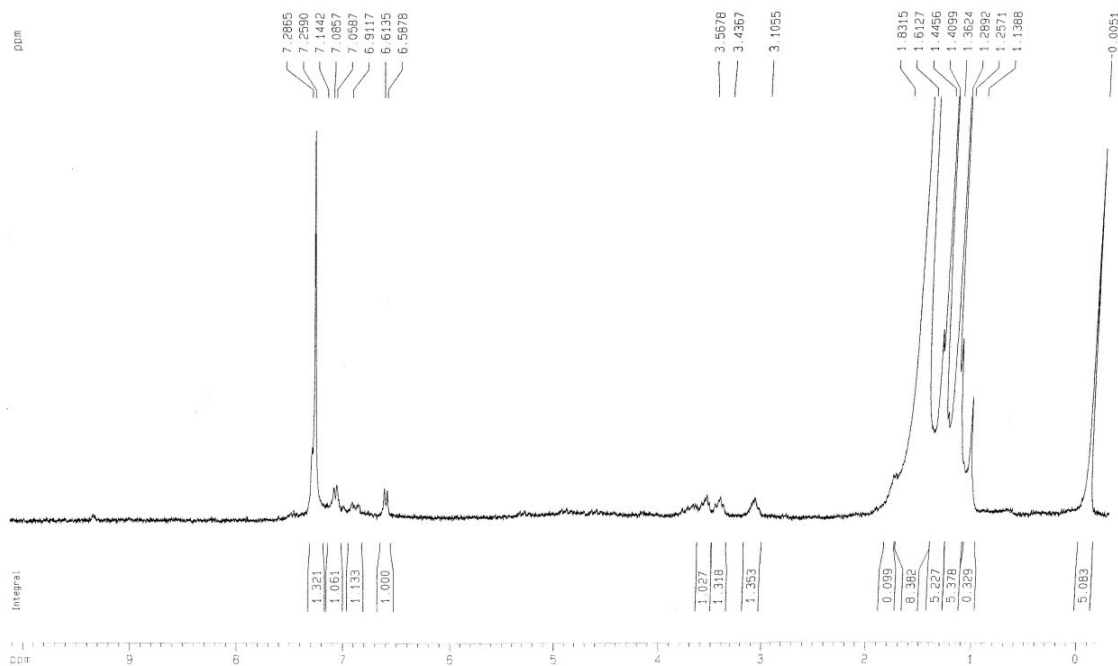
E-mail: [m\\_ali2062@yahoo.com](mailto:m_ali2062@yahoo.com)



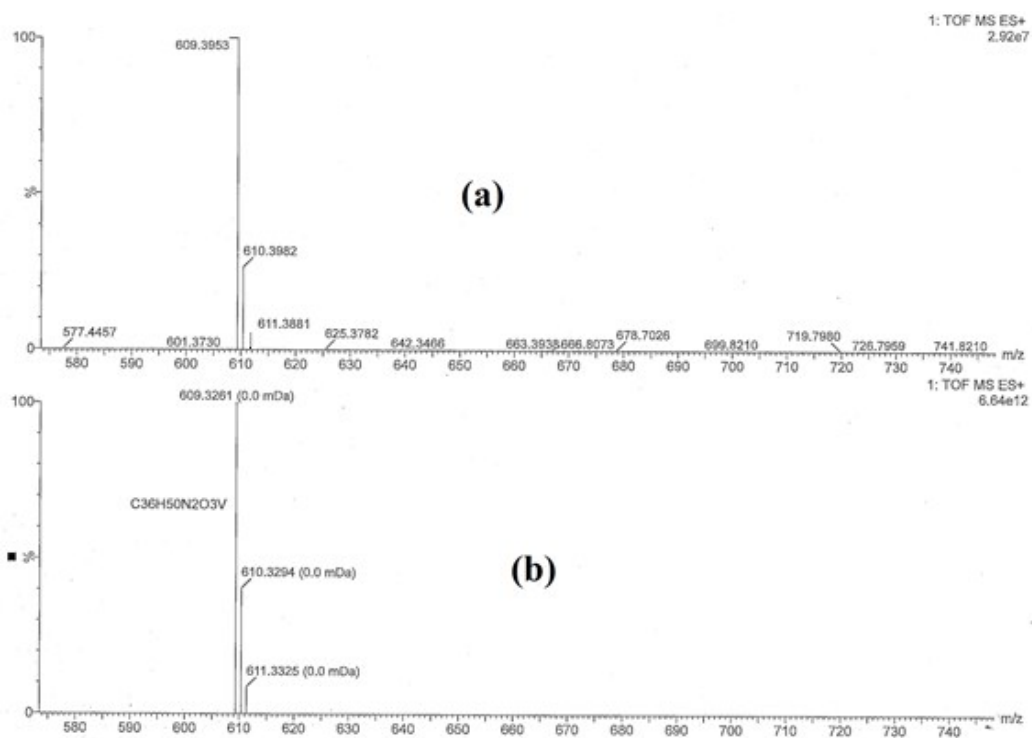
**Figure S1.** <sup>1</sup>H-NMR spectra of ligand.



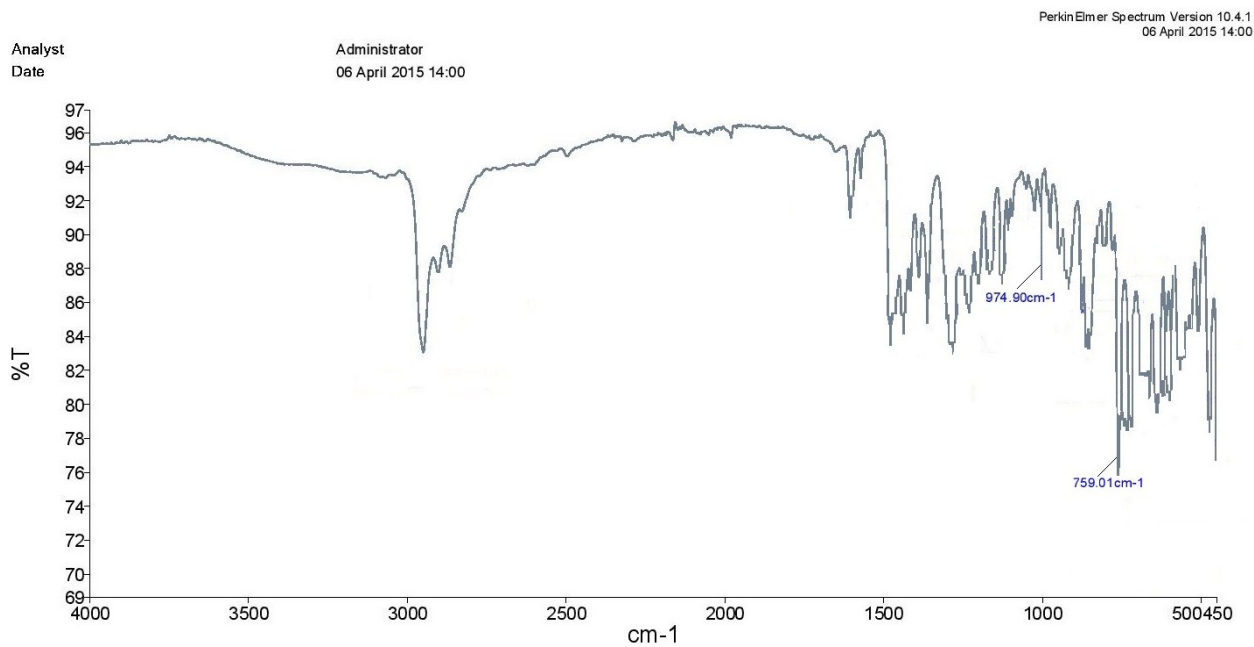
**Figure S2.** FT-IR spectra of complex -1.



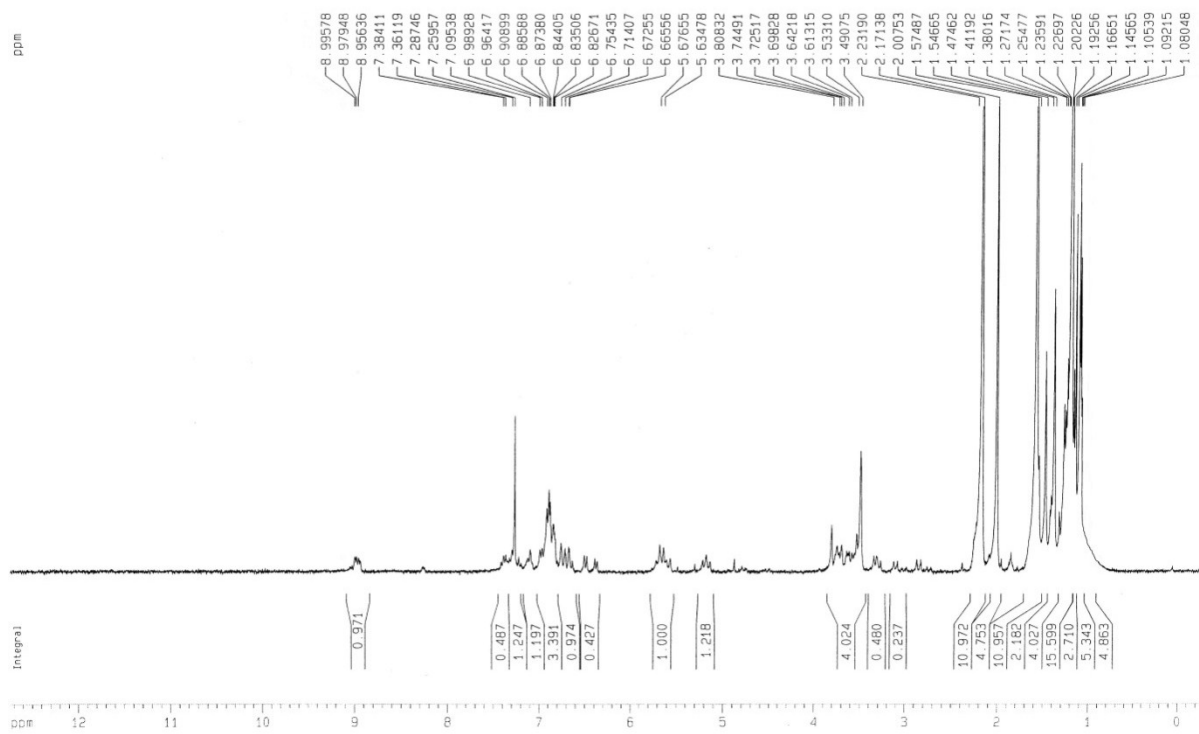
**Figure S3.** <sup>1</sup>H-NMR spectra of complex-1.



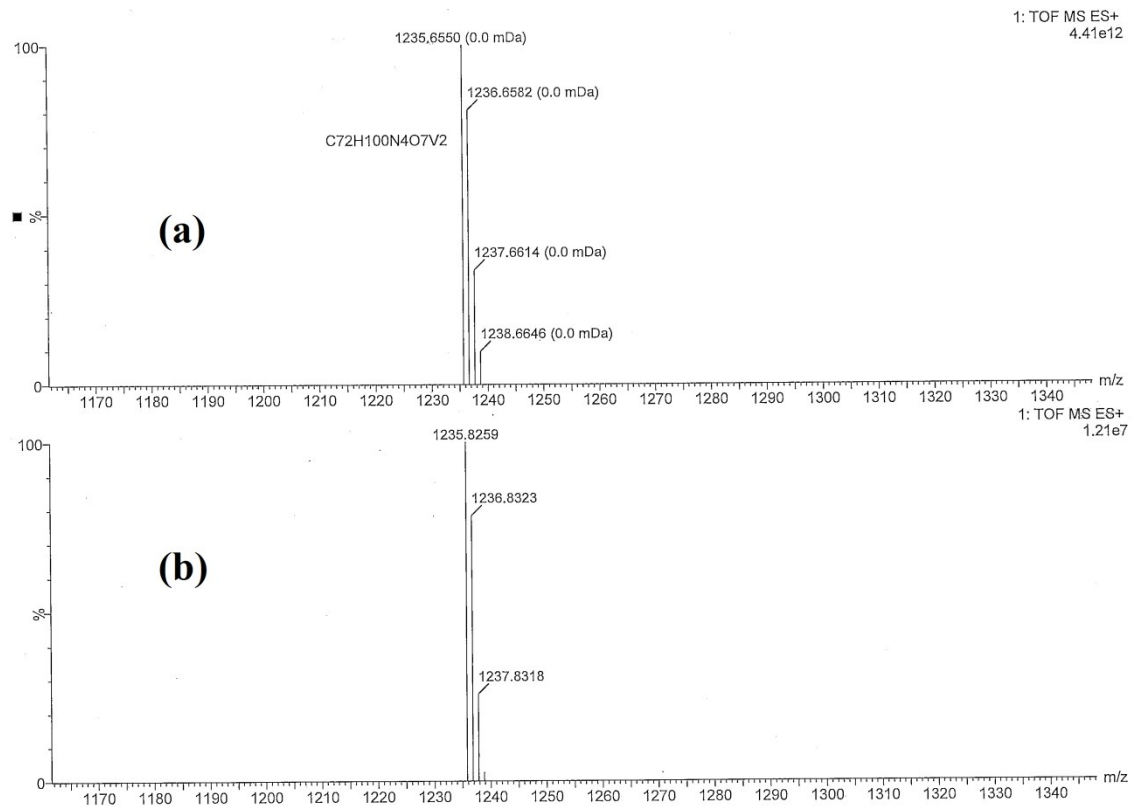
**Figure S4.** (a) Obtained HRMS of the complex 1( $[L^1VO]^+$ ); (b) simulated HRMS spectra.



**Figure S5.** FT-IR spectra of complex -2.



**Figure S6.** <sup>1</sup>H-NMR spectra of complex-2.



**Figure S7. (a)** Simulated HRMS of the complex **2** ( $[L^1VO(\mu_2-O)VOL^1]$ ); **(b)** Obtained HRMS.

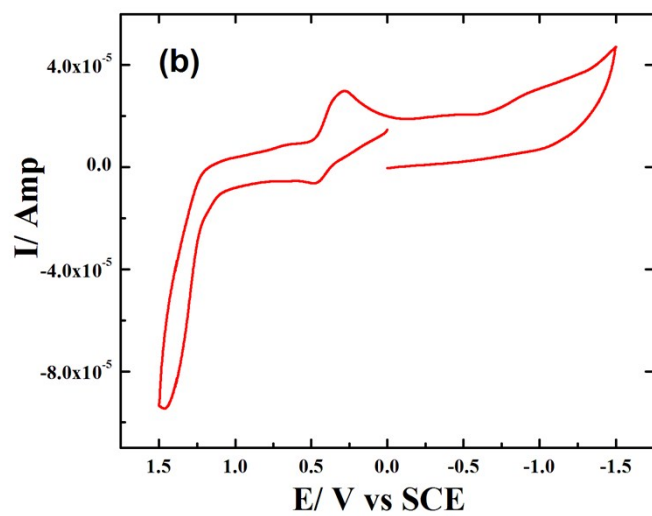
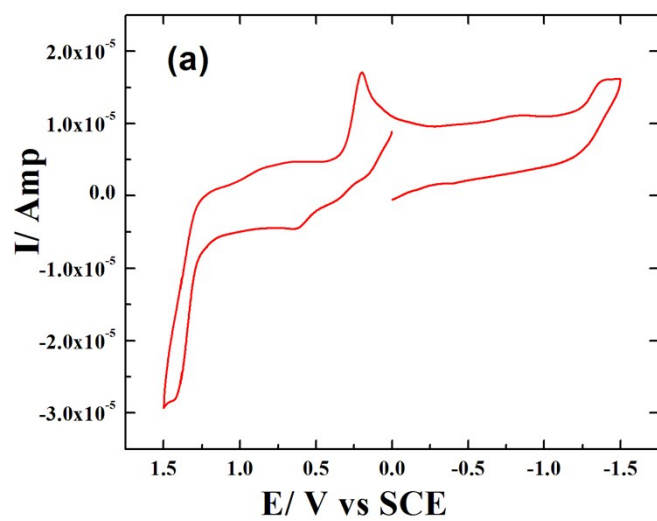
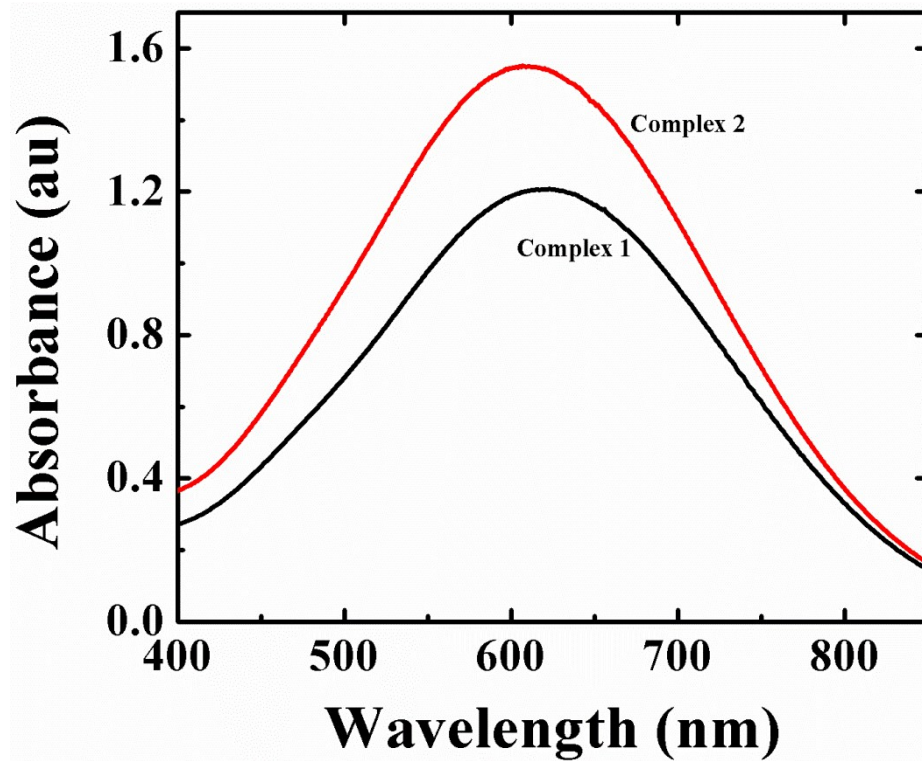


Figure S8. CV of (a) complex 1 and (b) complex 2 in presence of  $1.0 \times 10^{-3}$  M perchloric acid.



**Figure S9.** Electronic spectra of complexes 1 and 2 in MeCN at  $[C] = 0.50$  mM at 25 °C.

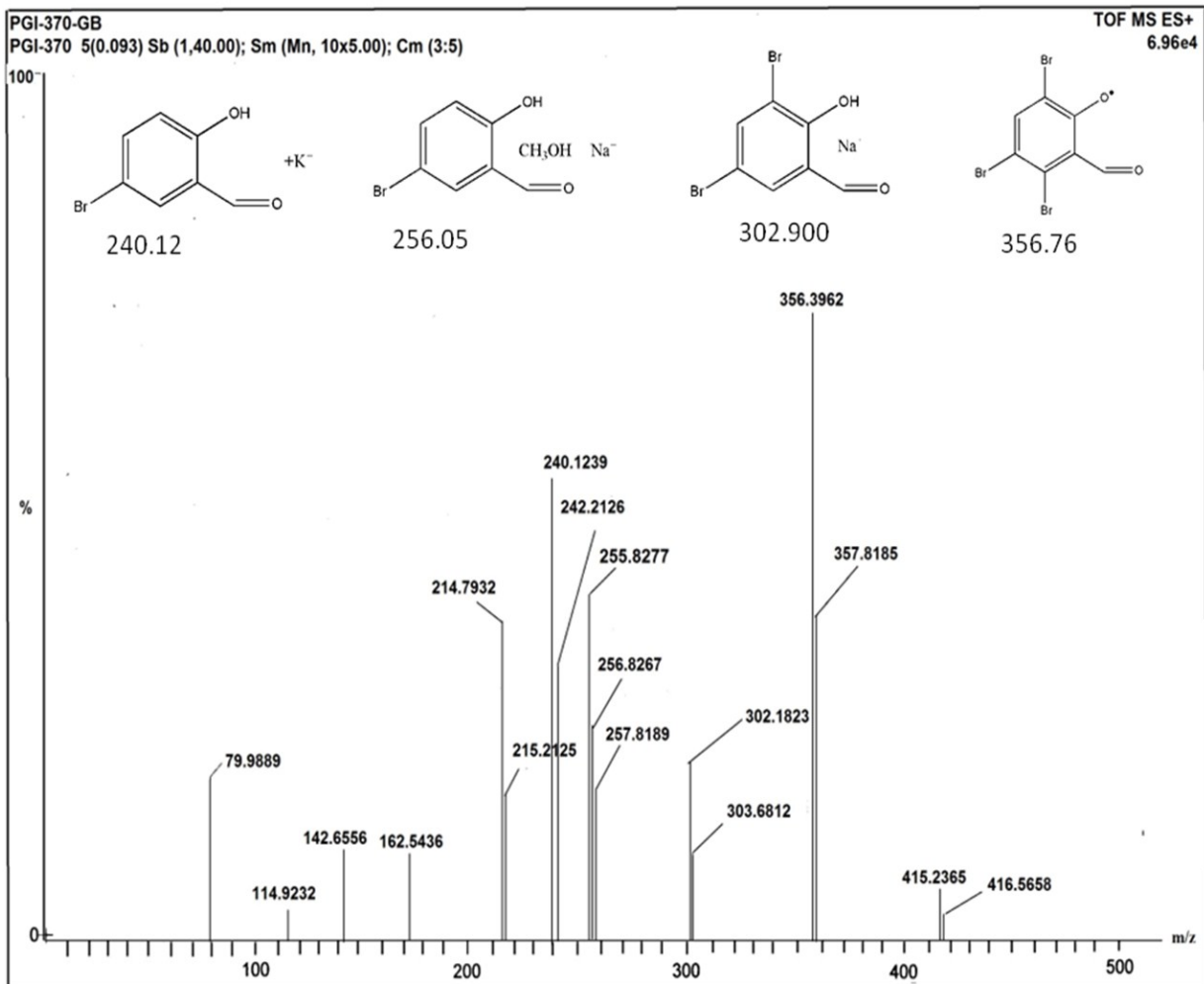


Figure S10. Products of bromoperoxidation of salicylaldehyde.



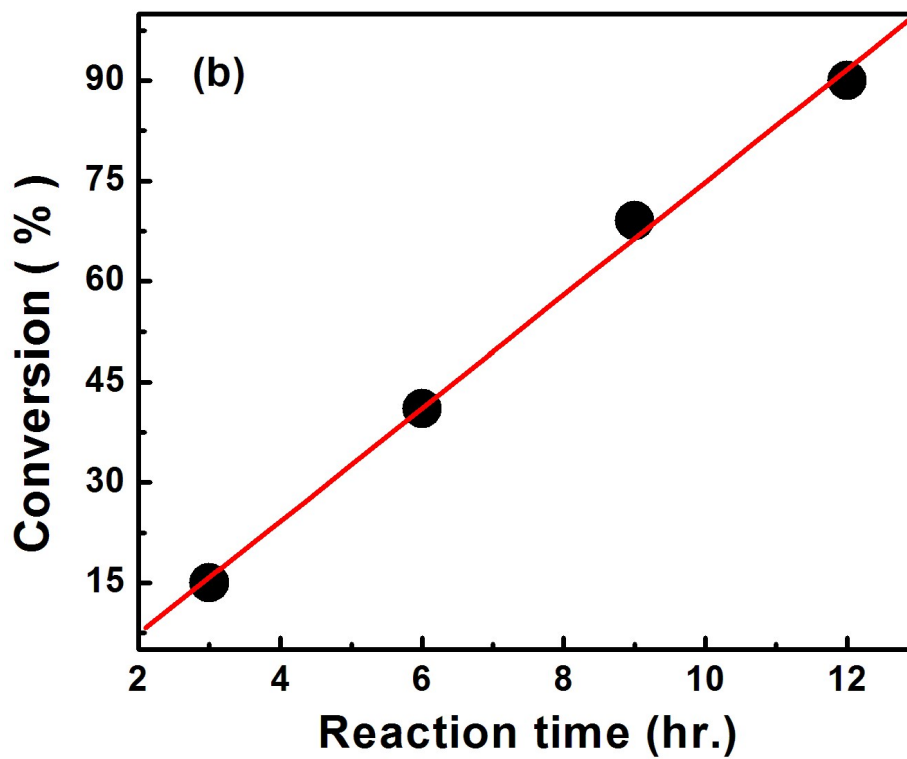
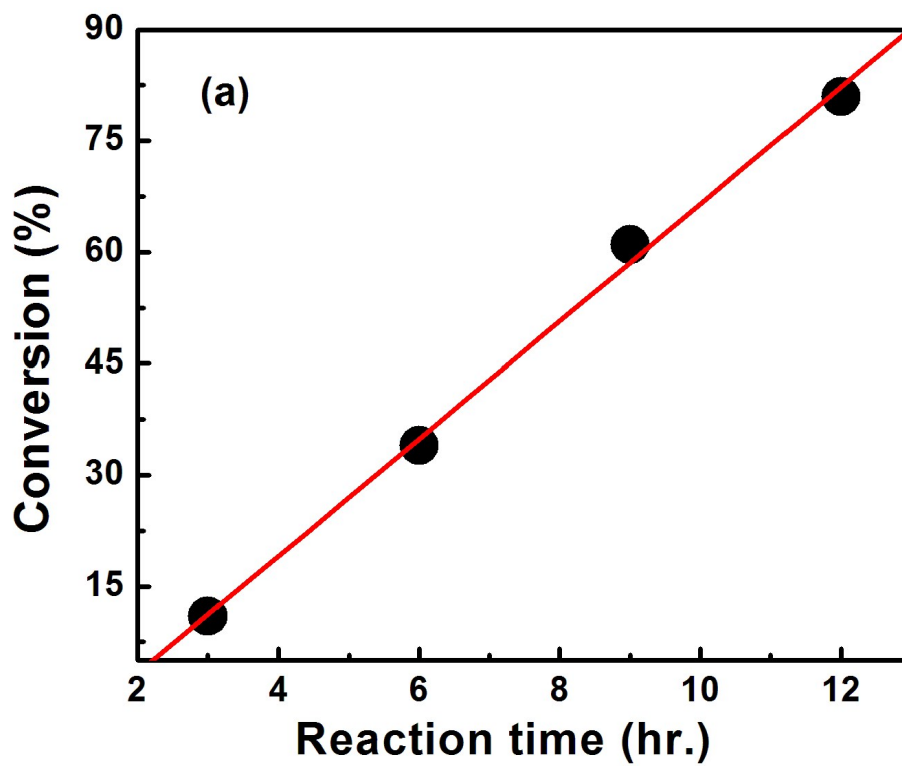
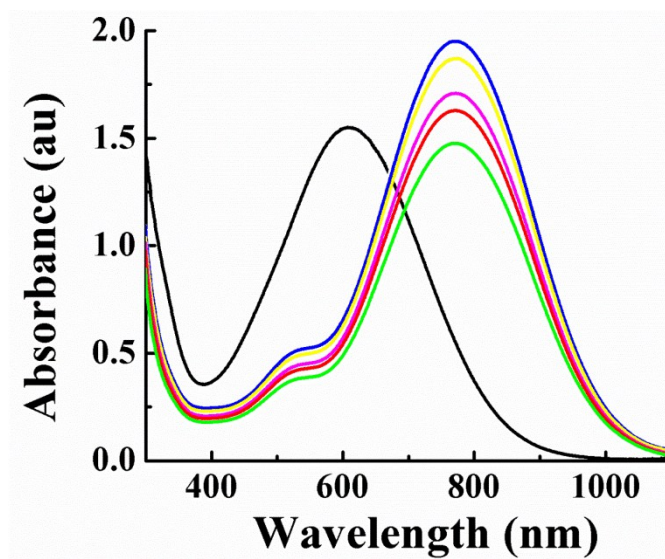
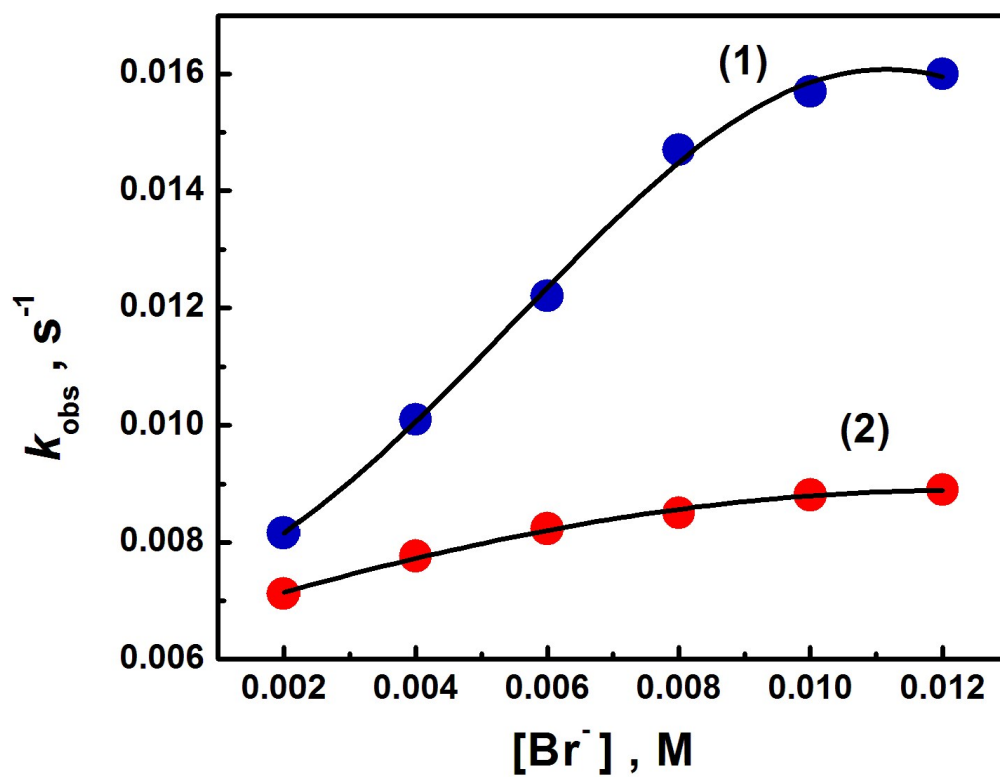


Figure S11. Plot of % conversion as a function of time for (a) complex 1 and (b) complex 2.



**Figure S12.** Shift in  $\lambda_{\text{max}}$  of complex 2 (0.50 mM at 25 °C) with addition of HClO<sub>4</sub> (blue line with 1 equiv acid, yellow with 2 equiv acid, magenta with 4 equiv acid, red with 6 equiv acid and green with 10 equiv acid).



**Figure S13.** Variation of rate ( $k_{\text{obs}}$ ) with  $[\text{Br}^-]$  in MeCN at  $[\text{C}] = 1 \times 10^{-4}$  M,  $[\text{Substrate}] = 2.5 \times 10^{-3}$  M,  $[\text{H}^+] = 0.025$  M and  $[\text{H}_2\text{O}_2] = 1.25 \times 10^{-3}$  M.

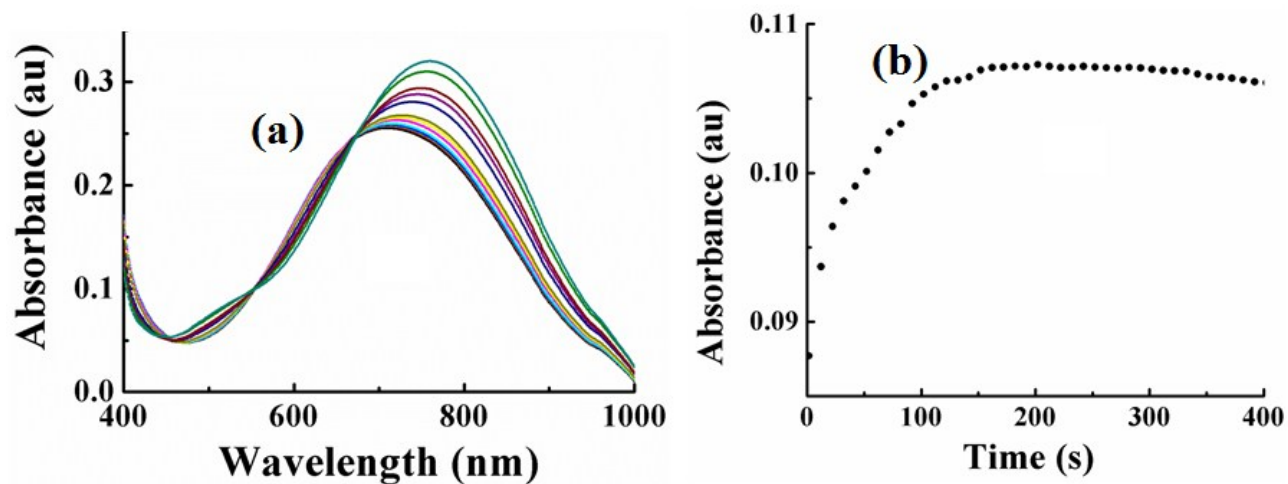


Figure S14. (a) Time resolved spectra for the protonation of **2** showing two clean isosbestic points at 550 and 670 nm; (b) time-dependent kinetic trace for the protonation of [L<sup>1</sup>(O)VOV(O)L<sup>1</sup>].

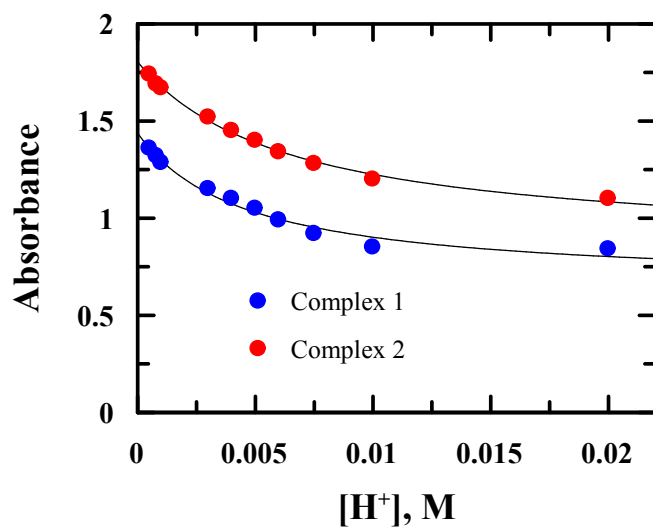
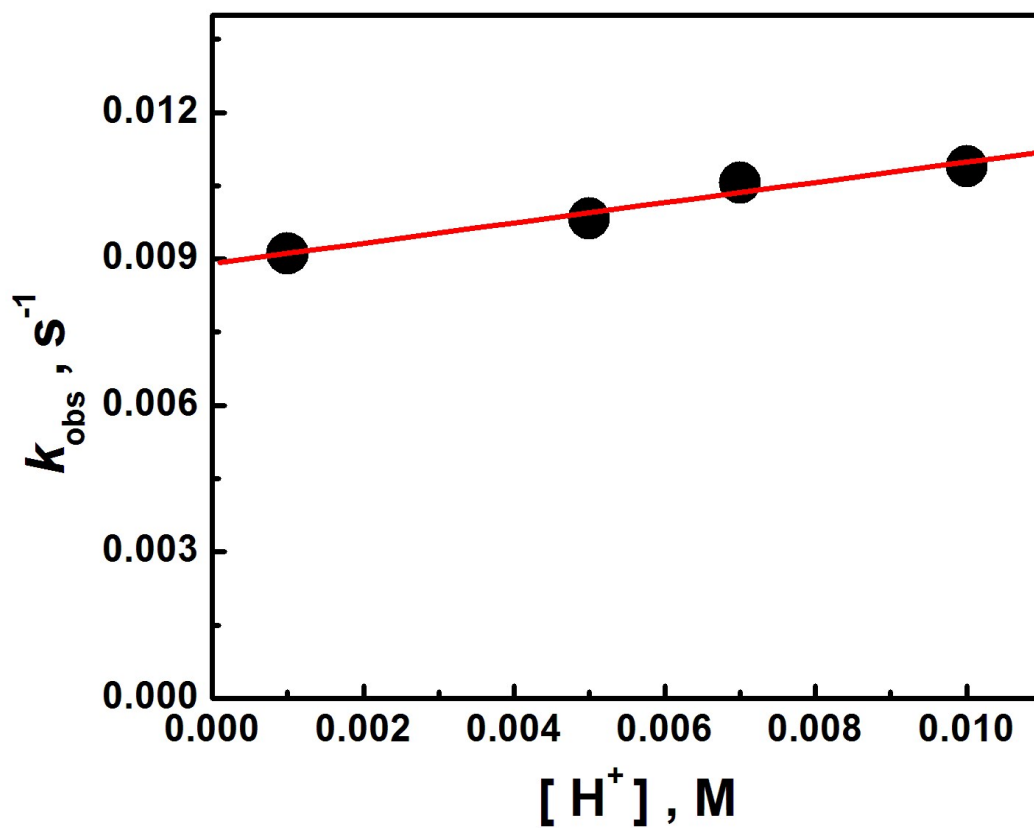
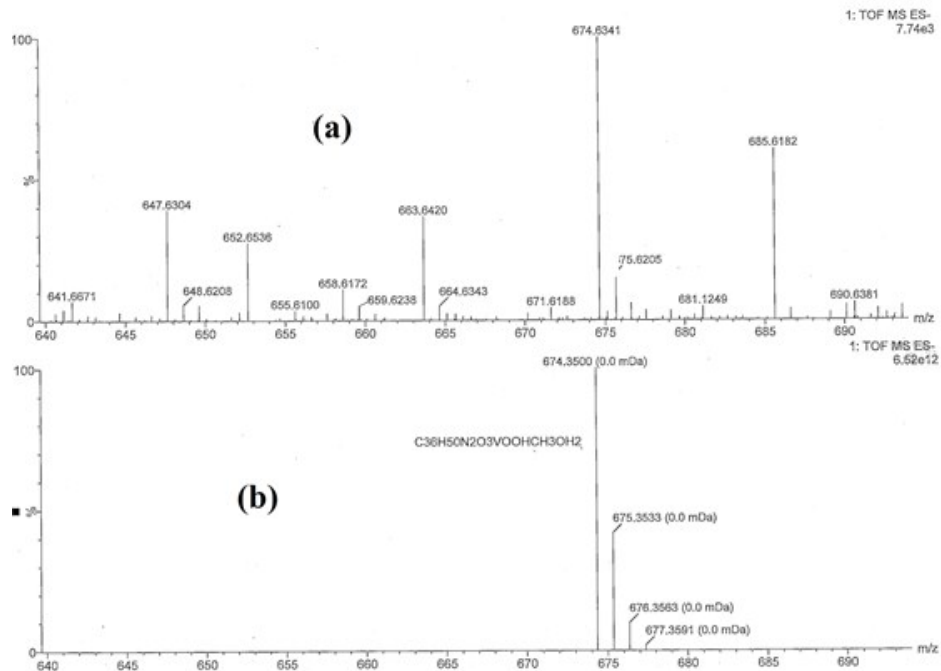


Figure S15. Plots of absorbance (at 685 nm for **1** and 600 nm for **2**) vs. [H<sup>+</sup>].



**Figure S16.** Variation of rate ( $k_{\text{obs}}$ ) with buffer concentration at pH 2.93 in MeCN at  $[C] = 1 \times 10^{-4}$  M,  $[\text{Substrate}] = 2.5 \times 10^{-3}$  M,  $[\text{Br}^-] = 1.25 \times 10^{-3}$  M and  $[\text{H}_2\text{O}_2] = 1.25 \times 10^{-3}$  M for complex 1.



**Figure S17.** (a) Obtained HRMS of the intermediate  $([L^1V(OH)(OOH)(MeO)(H)]^-)$ , proposed in the catalytic cycle; (b) simulated HRMS

## I. Coordinates of important optimized Intermediates and transition states:

*I*

V	-0.03687900	-1.46252200	-0.79782300
O	-1.83941200	-1.20519900	-0.59402900
O	1.78501700	-1.18317400	-0.83048600
O	-0.00382600	-3.00009700	-0.42226400
N	-0.07432000	0.99472900	-0.71246300
N	0.16085300	-0.88537700	1.31521300
C	0.33436700	-1.85474400	2.23640700
H	0.27370800	-2.86886500	1.85991900
C	0.58124000	-1.58148900	3.57474500
H	0.70994200	-2.39840700	4.27664600
C	0.66749500	-0.24807400	3.97859500
H	0.87151200	0.00730700	5.01451300
C	0.48696400	0.74999000	3.02885100
H	0.54246500	1.79944100	3.30263500
C	0.22292900	0.40043900	1.69971100
C	-0.08022800	1.47747300	0.68035200
H	0.62470600	2.30823300	0.81364200
H	-1.07806400	1.86721800	0.91316400
C	-5.05875000	0.28218300	0.17569500
H	-6.03172800	-0.00428400	0.55496100
C	-4.08778900	-0.71182800	0.03831100
C	-2.81333100	-0.30514400	-0.45963300
C	-4.38825400	-2.18571700	0.37983600
C	-4.20962100	-3.06171200	-0.88579300
H	-4.90239700	-2.74581100	-1.67491200
H	-3.19253900	-3.00443800	-1.27766000
H	-4.42773900	-4.10999900	-0.64608400
C	-3.44235100	-2.68527400	1.49920100
H	-2.40065200	-2.67073200	1.17696200
H	-3.54194500	-2.06667400	2.40007900
H	-3.70043900	-3.71680000	1.76948100
C	-5.83470800	-2.38150500	0.87910600
H	-6.03526600	-1.82399800	1.80196100
H	-6.57541900	-2.08400500	0.12791300
H	-5.99703300	-3.44313400	1.09558600
C	1.12079700	1.47544200	-1.45950200
C	2.44131100	1.09390400	-0.84853700
C	2.73252000	-0.26852500	-0.63008600
C	4.04034600	-0.66502600	-0.21808000
C	4.95958300	0.35780700	0.02501700
H	5.95476100	0.08122900	0.34995900
C	4.68207800	1.72852200	-0.13346600
C	5.77294800	2.77048600	0.17116700
C	7.00018700	2.52105000	-0.73849200
H	6.72762600	2.60953800	-1.79632400
C	5.28750700	4.21296300	-0.06951800

H	6.09313600	4.91786900	0.16528700
H	5.00010700	4.37770100	-1.11425100
H	4.43114800	4.46707100	0.56610200
C	6.20258200	2.65033600	1.65321300
H	6.59115100	1.65331100	1.88540400
H	6.99049200	3.37808100	1.88387800
H	5.35593200	2.84283900	2.32270200
C	4.43696900	-2.15104200	-0.10294700
C	3.54858400	-2.88427400	0.93006500
H	2.50588200	-2.90885900	0.61195000
H	3.89265000	-3.91988000	1.04420800
H	3.60899600	-2.40011000	1.91287700
C	5.90346400	-2.32665800	0.34314700
H	6.08894400	-1.90096500	1.33683000
H	6.13563400	-3.39603300	0.39643800
H	6.60906300	-1.87457100	-0.36334000
C	4.28304500	-2.82855800	-1.48820600
H	4.56543500	-3.88647400	-1.41934000
H	3.25443000	-2.77239400	-1.85044300
H	4.93781600	-2.35223700	-2.22763500
C	3.40617300	2.06940400	-0.58682700
H	3.14284400	3.10743000	-0.76510100
C	-2.59036700	1.03935100	-0.82524100
C	-4.85650600	1.63602000	-0.14904300
C	-3.60242500	1.98730200	-0.65247900
C	-1.28552700	1.44556700	-1.45738400
H	-1.26318200	2.54229000	-1.56682100
H	-1.20030200	1.01053800	-2.45796000
H	1.07027800	2.57235400	-1.55845300
H	1.03918100	1.04588900	-2.46344800
H	-3.39145500	3.01302700	-0.93829500
C	-5.99686900	2.65018700	0.04931000
C	-6.41458300	2.67488500	1.53942700
C	-5.58643900	4.07913900	-0.35522100
C	-7.21258500	2.23737600	-0.81540800
H	-6.75473800	1.69270000	1.88366300
H	-5.57634400	2.98037500	2.17656600
H	-7.23602400	3.38530700	1.69449600
H	-5.31348300	4.14154000	-1.41485600
H	-6.42522400	4.76485700	-0.19020700
H	-4.74057000	4.44440800	0.23896000
H	-8.03522400	2.95130000	-0.68388800
H	-6.94672800	2.21592400	-1.87835200
H	-7.58724100	1.24467500	-0.54503800
H	7.42529100	1.52354600	-0.58646300
H	7.78767300	3.25498200	-0.52686600
C1	-0.18078600	-1.42785700	-3.10375800

*1a*<sup>+</sup>

V	-0.04793600	-1.29290600	-0.55466000
O	-1.81539000	-1.06680200	-0.42858400
O	1.74009000	-1.03923100	-0.62213000
O	-0.01903300	-2.95721500	-0.14559900
N	-0.10003800	1.05441900	-0.71047500
N	0.10204900	-0.62804400	1.47076200
C	0.23817000	-1.53021700	2.46801500
H	0.19977100	-2.57031200	2.16952900
C	0.41760000	-1.15292300	3.79043300
H	0.51829800	-1.91333100	4.55700600
C	0.47019500	0.20810500	4.09818500
H	0.61814200	0.54041800	5.12117600
C	0.32708100	1.13365600	3.07074800
H	0.35633000	2.20020100	3.27152200
C	0.13442400	0.68523400	1.76103500
C	-0.10900100	1.67152700	0.64408400
H	0.63444500	2.47433400	0.70056700
H	-1.08834600	2.13186200	0.81486300
C	-5.10327800	0.35054600	0.14557600
H	-6.08046200	0.07048900	0.51570600
C	-4.11057000	-0.62906000	0.11321500
C	-2.83758200	-0.21065000	-0.37711900
C	-4.38485800	-2.08026100	0.55315700
C	-4.12244000	-3.04225000	-0.63373700
H	-4.77316800	-2.80076600	-1.48181700
H	-3.08510300	-3.00112700	-0.97394700
H	-4.34029000	-4.07184600	-0.32657100
C	-3.47911000	-2.46104100	1.74980200
H	-2.42171700	-2.44315100	1.47986000
H	-3.63834600	-1.78116800	2.59536800
H	-3.72178100	-3.47563100	2.08631000
C	-5.84836700	-2.27835400	0.99845400
H	-6.10515100	-1.66272300	1.86806300
H	-6.55823700	-2.05817600	0.19360400
H	-5.99526000	-3.32465700	1.28514100
C	1.09181200	1.51224200	-1.49694900
C	2.41702400	1.20099200	-0.86141100
C	2.71681500	-0.13261500	-0.50758800
C	4.02335800	-0.49700700	-0.06147400
C	4.93841900	0.54930600	0.06701300
H	5.93436300	0.31018900	0.41500800
C	4.66126600	1.89752500	-0.23294400
C	5.75426400	2.96224200	-0.05046900
C	6.96458300	2.61457200	-0.95232700
H	6.67541900	2.59229000	-2.00893400
C	5.26359100	4.37404400	-0.42514200
H	6.07213100	5.09557400	-0.26919300
H	4.96635100	4.44024200	-1.47804700
H	4.41722500	4.69279600	0.19483800
C	6.20571600	2.98351200	1.43076500



H	6.60884600	2.01759300	1.75208900
H	6.99164900	3.73387000	1.57252700
H	5.37121600	3.23839700	2.09438200
C	4.43131500	-1.95738900	0.21531200
C	3.53815400	-2.58497300	1.31158200
H	2.49675200	-2.65798100	0.99435000
H	3.89090500	-3.59759200	1.53888100
H	3.58199400	-1.99937800	2.23766800
C	5.89324700	-2.06946400	0.69599400
H	6.06261100	-1.53588500	1.63836200
H	6.12972300	-3.12415900	0.86985300
H	6.60518800	-1.69648600	-0.04826000
C	4.30672600	-2.77244000	-1.09614500
H	4.61278700	-3.81025000	-0.92106800
H	3.28186200	-2.78592700	-1.47207500
H	4.95529700	-2.35641700	-1.87533300
C	3.38014900	2.19590900	-0.71023700
H	3.12166400	3.21056000	-0.99403900
C	-2.62585900	1.10539700	-0.84303300
C	-4.92231900	1.68259500	-0.27677400
C	-3.66094000	2.03478300	-0.77354900
C	-1.31625700	1.47030600	-1.48688100
H	-1.28065600	2.55744700	-1.64552000
H	-1.22884900	0.99059400	-2.46658900
H	1.01119900	2.59634200	-1.65986500
H	1.01687500	1.02266700	-2.47302000
H	-3.47563700	3.04032900	-1.13549800
C	-6.09177000	2.67580700	-0.19353000
C	-6.55967500	2.79507700	1.27806900
C	-5.70356900	4.08127800	-0.69132700
C	-7.26340500	2.15923900	-1.06545500
H	-6.89483800	1.83493400	1.68362100
H	-5.75410000	3.16999700	1.91992200
H	-7.40019200	3.49476800	1.34710000
H	-5.40109300	4.07595800	-1.74484600
H	-6.56492000	4.75139400	-0.60367900
H	-4.89017500	4.51647100	-0.09874500
H	-8.10443500	2.85999500	-1.01441400
H	-6.96273600	2.06617600	-2.11496700
H	-7.62649400	1.18200800	-0.73091400
H	7.39812200	1.64110900	-0.70132200
H	7.75064600	3.36858400	-0.83157300
Cl	-0.13571200	-1.50200400	-2.86287000
H	0.57738400	-3.60721800	-0.67662400
O	1.21520700	-4.43461900	-1.84771300
H	0.68433500	-5.22312000	-2.05134500
H	1.06952300	-3.82257300	-2.59503700

*Ts1*

V	0.06822400	1.17424400	-0.28307500
O	1.81707900	0.91297800	-0.29221800
O	-1.67821400	0.90011200	-0.53281200
O	0.04841500	2.59503000	0.75293900
N	0.14633800	-1.24471200	-0.57651400
N	-0.22079700	0.22205500	1.74216300
C	-0.48830700	0.98553900	2.82040000
H	-0.38793700	2.05165300	2.66546700
C	-0.86292100	0.45733200	4.04868700
H	-1.05733000	1.12458200	4.88128500
C	-0.98845400	-0.92601400	4.17479500
H	-1.29586800	-1.37599800	5.11395300
C	-0.70083900	-1.71903500	3.07006300
H	-0.76611800	-2.80119800	3.12393700
C	-0.30294900	-1.11520600	1.87441300
C	0.18337700	-1.94741500	0.72832400
H	-0.37481300	-2.89025300	0.67422000
H	1.22562200	-2.20854500	0.94519300
C	5.15419700	-0.42402700	0.18670200
H	6.12999900	-0.12595500	0.54493800
C	4.13484700	0.52762800	0.19731200
C	2.86565900	0.08409000	-0.28703200
C	4.38417500	1.96943600	0.67950500
C	4.14937000	2.95488200	-0.49299400
H	4.81819800	2.72880100	-1.33123100
H	3.12051100	2.93289100	-0.85618600
H	4.36620300	3.97673200	-0.15952200
C	3.44530800	2.31609600	1.86193600
H	2.39457700	2.32390600	1.56743500
H	3.57743900	1.60696900	2.68843800
H	3.69291800	3.31518200	2.23937500
C	5.83404000	2.16632400	1.16983800
H	6.07713600	1.52023400	2.02125200
H	6.56815900	1.98957400	0.37610700
H	5.95813300	3.20255900	1.50018200
C	-1.04708200	-1.69197000	-1.36714400
C	-2.38923500	-1.33088800	-0.79323900
C	-2.68367000	0.01556700	-0.49318600
C	-4.00726000	0.43097300	-0.16550800
C	-4.96441200	-0.58077100	-0.08725600
H	-5.97879000	-0.30461900	0.16765700
C	-4.69990000	-1.94421800	-0.32583900
C	-5.83395400	-2.97436400	-0.20541700
C	-6.95405000	-2.62479700	-1.21656100
H	-6.57692800	-2.64350600	-2.24504300
C	-5.35350900	-4.40939400	-0.49531800
H	-6.19178400	-5.10494500	-0.38538700
H	-4.97278200	-4.51681600	-1.51734100
H	-4.57032600	-4.72866800	0.20238500
C	-6.40854800	-2.93755600	1.23237500

H	-6.80987900	-1.95227300	1.49156700
H	-7.22489300	-3.66233300	1.32793100
H	-5.64062100	-3.19413000	1.97142800
C	-4.37286000	1.91000600	0.07438000
C	-3.63671100	2.44409800	1.32663500
H	-2.55183200	2.41348000	1.21107600
H	-3.93277100	3.48332100	1.51839400
H	-3.90190400	1.85703200	2.21312400
C	-5.88513700	2.10120100	0.31388000
H	-6.22985800	1.58592300	1.21705600
H	-6.09616000	3.16748200	0.44888100
H	-6.48420700	1.75400600	-0.53471600
C	-3.99543300	2.75343500	-1.17069200
H	-4.26063500	3.80577000	-0.99480600
H	-2.93216800	2.68004500	-1.41448200
H	-4.55613700	2.42559600	-2.05267200
C	-3.39347800	-2.29107300	-0.68893700
H	-3.14535300	-3.32025800	-0.92454800
C	2.67326000	-1.23339800	-0.76182300
C	4.99995000	-1.75116600	-0.25963900
C	3.73443700	-2.13289200	-0.72499300
C	1.36057100	-1.64757800	-1.36767800
H	1.34753700	-2.74108100	-1.48376500
H	1.25190400	-1.19918800	-2.35632300
H	-0.98763700	-2.78293700	-1.48964600
H	-0.94613900	-1.23458000	-2.35439100
H	3.56588400	-3.14110200	-1.08692800
C	6.19771800	-2.71159100	-0.22613300
C	6.70473300	-2.84738700	1.23139400
C	5.83807800	-4.11699600	-0.74523900
C	7.33188200	-2.14164300	-1.11471800
H	7.02454800	-1.88707800	1.64860300
H	5.92559900	-3.25690500	1.88461700
H	7.56470700	-3.52565000	1.26492200
H	5.50467900	-4.09719400	-1.78912600
H	6.72196000	-4.76131500	-0.69798800
H	5.05642000	-4.59093200	-0.13986500
H	8.19334800	-2.81870500	-1.09771300
H	7.00359400	-2.03624300	-2.15465400
H	7.67419200	-1.16124200	-0.76804700
H	-7.38084700	-1.63334200	-1.03259600
H	-7.76773700	-3.35478200	-1.13999800
Cl	0.22380000	0.68271200	-3.34371100
H	-0.51812400	3.36537600	0.48688200
O	-1.29133100	4.84639400	-0.14898500
H	-2.08876000	4.61498000	-0.65494000
H	-1.52396900	5.60856300	0.40521700
O	-0.12423000	2.81121300	-1.69172000
H	0.08135300	2.33732400	-2.57545300
O	0.85760300	3.86626000	-1.60647800
H	0.28322000	4.56544100	-1.22344900

V	0.06846700	-1.33062500	-0.55464900
O	-1.72772100	-1.07866700	-0.61309900
O	1.84250100	-1.12946500	-0.44080800
O	-0.01448000	-2.99759000	0.01872200
N	0.14007100	1.00324600	-0.75970400
N	-0.07266100	-0.55340600	1.50180000
C	-0.22513100	-1.40317300	2.53899700
H	-0.19728500	-2.45660500	2.28745000
C	-0.40841300	-0.95959600	3.84152300
H	-0.52158600	-1.67853300	4.64562800
C	-0.44741900	0.41568800	4.08075200
H	-0.59768000	0.79983700	5.08523700
C	-0.28813400	1.28898400	3.01013400
H	-0.30741200	2.36443700	3.15830100
C	-0.09244800	0.77045100	1.72680900
C	0.17319900	1.69152800	0.55824600
H	1.16655900	2.13112100	0.69953000
H	-0.54620100	2.51790800	0.57385300
C	-4.88541900	0.58064800	0.11054800
H	-5.87752900	0.36507700	0.48466900
C	-3.99035500	-0.48286400	-0.02178700
C	-2.68926400	-0.15196400	-0.49982700
C	-4.41419900	-1.93431600	0.28046700
C	-4.33044500	-2.75826300	-1.02944600
H	-5.04009300	-2.38119500	-1.77413700
H	-3.32925900	-2.70782800	-1.46495900
H	-4.58252300	-3.80776400	-0.82805100
C	-3.50596400	-2.56792000	1.36082600
H	-2.47164900	-2.66068000	1.02535200
H	-3.51901400	-1.97033300	2.27964400
H	-3.87368700	-3.57033600	1.61162900
C	-5.86692700	-2.02409700	0.79151000
H	-6.00442900	-1.48535900	1.73570800
H	-6.58908200	-1.63882800	0.06370500
H	-6.11829200	-3.07422100	0.97452600
C	1.35038700	1.34987600	-1.57875100
C	2.66265800	1.01986500	-0.92234000
C	2.86973100	-0.27392600	-0.40107900
C	4.13307100	-0.66842200	0.12612700
C	5.12661000	0.31232400	0.12555600
H	6.09882900	0.04932700	0.52050300
C	4.95192900	1.62338000	-0.35894300
C	6.12150900	2.61966900	-0.30773100
C	7.30315300	2.06543300	-1.14157000
H	7.01559000	1.92799600	-2.18996600
C	5.73889300	4.00050800	-0.87416700
H	6.59996000	4.67389100	-0.81115500
H	5.44497200	3.94532500	-1.92869900
H	4.92064600	4.46334300	-0.30990900
C	6.57263600	2.80755900	1.16170400

H	6.90590200	1.86789700	1.61421800
H	7.41006600	3.51286300	1.20920500
H	5.75823700	3.20765400	1.77670500
C	4.39900600	-2.09633500	0.64158800
C	3.47009700	-2.41617300	1.83810200
H	2.41769500	-2.40198000	1.54929700
H	3.69888000	-3.41625500	2.22451600
H	3.62107200	-1.69927500	2.65406800
C	5.85389600	-2.27304000	1.12254200
H	6.09654900	-1.61195200	1.96227800
H	5.99308800	-3.30277200	1.46756900
H	6.57891300	-2.09698900	0.32018100
C	4.15679400	-3.11693400	-0.49950200
H	4.37400300	-4.12946100	-0.13952500
H	3.12319000	-3.09693500	-0.85248400
H	4.81772600	-2.91450000	-1.35010100
C	3.69622200	1.95355700	-0.88293000
H	3.51247600	2.94312500	-1.28737600
C	-2.37561000	1.16591100	-0.88645000
C	-4.58977600	1.91849300	-0.21664900
C	-3.31672200	2.18292300	-0.73114600
C	-1.05792000	1.42638800	-1.55732100
H	-0.96771600	2.49799000	-1.78528500
H	-1.00636500	0.87817300	-2.50358100
H	1.32263000	2.42234000	-1.81765000
H	1.24492100	0.79667800	-2.51732200
H	-3.04538300	3.18711800	-1.03945100
C	-5.65708000	3.00806900	-0.02216600
C	-6.07362400	3.05753500	1.46839300
C	-5.14575900	4.40460500	-0.42560200
C	-6.89532500	2.67642800	-0.89089300
H	-6.49419000	2.10586100	1.80976400
H	-5.21743200	3.29674400	2.10981500
H	-6.83632300	3.82968100	1.62056100
H	-4.87169300	4.45169000	-1.48581400
H	-5.93470400	5.14554400	-0.25992000
H	-4.27805000	4.71190900	0.17015600
H	-7.66423900	3.44630800	-0.75951000
H	-6.63192900	2.63803100	-1.95382300
H	-7.34088000	1.71381600	-0.61948000
H	7.65973000	1.10249500	-0.76144500
H	8.14515100	2.76629900	-1.11002500
H	-0.55712100	-3.59077700	-0.55644200
O	-1.29988100	-4.22666500	-2.12988700
H	-0.71105200	-4.83039500	-2.61372400
H	-2.16598900	-4.66516000	-2.09140900
O	0.21611700	-1.44565100	-2.35571100
O	-0.93841100	-1.60792300	-3.17555100
H	-1.24274700	-2.50595700	-2.90305500

V	0.07052200	-1.31485100	-0.60663800
O	-1.75471300	-1.09379000	-0.68519900
O	1.83842900	-1.10897900	-0.43066000
O	-0.05335300	-2.91739500	0.21080100
N	0.13970500	1.02173600	-0.79037700
N	-0.15701300	-0.55132200	1.43781700
C	-0.35963700	-1.39834000	2.46901900
H	-0.31412000	-2.44947100	2.21744500
C	-0.61585000	-0.95529600	3.75973200
H	-0.76510900	-1.67889000	4.55371500
C	-0.68374100	0.41732200	4.00010500
H	-0.89508400	0.79960300	4.99422000
C	-0.47075100	1.28969800	2.93889600
H	-0.50503600	2.36533900	3.08166000
C	-0.19638500	0.77283300	1.67035900
C	0.16105600	1.69205400	0.53541600
H	1.17548600	2.06283800	0.71793800
H	-0.50316400	2.56381200	0.53401700
C	-4.90380500	0.58222600	0.03861900
H	-5.90066500	0.36328800	0.39849800
C	-4.01159700	-0.48115200	-0.10837200
C	-2.70236700	-0.15434000	-0.57137600
C	-4.44688200	-1.93798400	0.14932700
C	-4.37771000	-2.71449300	-1.19076300
H	-5.11553400	-2.33515400	-1.90624200
H	-3.39250700	-2.60843900	-1.65580700
H	-4.59669200	-3.77811200	-1.02329800
C	-3.53991400	-2.61777200	1.20221800
H	-2.50545400	-2.70364000	0.86480200
H	-3.54944700	-2.05290000	2.14153100
H	-3.91680300	-3.62500500	1.41915500
C	-5.89863300	-2.03503500	0.66182100
H	-6.02751900	-1.52589900	1.62341000
H	-6.62137200	-1.62125700	-0.04950800
H	-6.15720100	-3.08867700	0.81227000
C	1.36128600	1.40899600	-1.57780800
C	2.66553800	1.04794900	-0.91652200
C	2.86050300	-0.24735900	-0.39306500
C	4.11551200	-0.64392800	0.15399400
C	5.11530700	0.32991700	0.16423900
H	6.08114300	0.06178500	0.57119400
C	4.95232500	1.64123300	-0.32237800
C	6.12548500	2.63247100	-0.25725600
C	7.31306800	2.07376900	-1.07963000
H	7.03559400	1.93887700	-2.13108800
C	5.75523600	4.01584300	-0.82577800
H	6.61852300	4.68533800	-0.75223400
H	5.47274200	3.96355300	-1.88359000
H	4.93289400	4.48147200	-0.26982100
C	6.56238600	2.81649000	1.21689900

H	6.88609600	1.87470600	1.67186900
H	7.40293900	3.51738500	1.27382900
H	5.74372700	3.22009300	1.82389000
C	4.36858000	-2.07582700	0.66534000
C	3.39434000	-2.42205900	1.81818600
H	2.35611900	-2.44217200	1.48239400
H	3.63760100	-3.41397100	2.21684400
H	3.48720300	-1.70102400	2.63935600
C	5.80399000	-2.24948400	1.20297300
H	6.00890600	-1.59258600	2.05606300
H	5.93391600	-3.28096300	1.54639800
H	6.56107100	-2.06565100	0.43259800
C	4.18086500	-3.07967500	-0.50099700
H	4.36953900	-4.09916200	-0.14436800
H	3.16880500	-3.04385100	-0.91108100
H	4.88863600	-2.87188100	-1.31168600
C	3.70371700	1.97658200	-0.85960500
H	3.52831300	2.96929300	-1.26024200
C	-2.38132100	1.17166600	-0.92862800
C	-4.59718500	1.92519700	-0.25446100
C	-3.31858400	2.19053100	-0.75249200
C	-1.05838500	1.46261800	-1.58071500
H	-0.97258300	2.54298900	-1.76363600
H	-0.99164300	0.95934500	-2.54958500
H	1.33211400	2.49383600	-1.75158300
H	1.27429000	0.91467900	-2.54786800
H	-3.03783600	3.20051600	-1.03272000
C	-5.65770200	3.01826300	-0.04222100
C	-6.08179500	3.03873200	1.44670600
C	-5.13416100	4.41939300	-0.41279200
C	-6.89374500	2.71564700	-0.92437400
H	-6.50806900	2.08189600	1.76584100
H	-5.22753100	3.26017900	2.09705900
H	-6.84168500	3.81105600	1.61174700
H	-4.85385300	4.48688900	-1.47028900
H	-5.91857000	5.16253200	-0.23558900
H	-4.26753900	4.70768000	0.19396500
H	-7.65765100	3.48822300	-0.78013500
H	-6.62501400	2.69873800	-1.98659000
H	-7.34820300	1.75067400	-0.67694000
H	7.66079400	1.10859300	-0.69702000
H	8.15813800	2.77045300	-1.03860500
H	-0.24609800	-3.67440600	-0.37691500
O	-1.36226100	-4.34452300	-2.00098300
H	-1.30679800	-5.15292100	-2.53615900
H	-2.29912500	-4.23422000	-1.76622300
O	0.12443200	-1.02322600	-2.48161800
O	0.38999200	-2.40981900	-2.34379600
H	-0.46200400	-2.89501200	-2.52835000

**Ts2**

V	0.07287100	-1.24142300	-0.72049300
O	-1.72453100	-1.07973200	-0.75760800
O	1.82529700	-1.08554700	-0.43329900
O	-0.07770000	-3.04319600	0.06111200
N	0.14814800	1.02289300	-0.78294900
N	-0.21346300	-0.60378900	1.39416600
C	-0.48124600	-1.48091400	2.38187400
H	-0.45201500	-2.52237300	2.08928100
C	-0.78750600	-1.07775500	3.67562300
H	-0.98782100	-1.82385900	4.43692500
C	-0.84274700	0.28721100	3.95952400
H	-1.09220800	0.63896500	4.95606300
C	-0.57294300	1.19286800	2.93890200
H	-0.60271000	2.26336200	3.11682000
C	-0.25049300	0.71151700	1.66799600
C	0.16564300	1.64956200	0.57149100
H	1.19049200	1.97344800	0.78110800
H	-0.46354700	2.54659200	0.57712700
C	-4.89287000	0.55541200	0.03255500
H	-5.88863200	0.32534000	0.38696800
C	-4.00441400	-0.50867100	-0.14829600
C	-2.70002400	-0.16155700	-0.60226000
C	-4.45981700	-1.96725700	0.06255800
C	-4.40508200	-2.70381300	-1.29912400
H	-5.07050200	-2.22387500	-2.02569800
H	-3.39598700	-2.72079500	-1.71520900
H	-4.73579900	-3.74208500	-1.17576900
C	-3.56309700	-2.69015400	1.09364100
H	-2.52742900	-2.76063200	0.75978800
H	-3.58230800	-2.17045300	2.05902700
H	-3.93666400	-3.70818400	1.25618500
C	-5.91124200	-2.05538200	0.57935700
H	-6.03642000	-1.56305600	1.55063100
H	-6.63168900	-1.62521700	-0.12467900
H	-6.17738400	-3.10944500	0.70972400
C	1.37861100	1.45075800	-1.54149100
C	2.67797500	1.06730600	-0.87888000
C	2.86382100	-0.23286300	-0.36990900
C	4.10917500	-0.64383500	0.17818800
C	5.11868300	0.32088500	0.20090500
H	6.08098100	0.03935700	0.60760700
C	4.96858400	1.63791600	-0.27236800
C	6.14965600	2.61956900	-0.19247100
C	7.33461100	2.06228100	-1.01910300
H	7.05816600	1.94176700	-2.07257500
C	5.79028900	4.01227500	-0.74505200
H	6.65767800	4.67513700	-0.66068500
H	5.51073500	3.97501700	-1.80428600
H	4.96942300	4.47647600	-0.18569800
C	6.58450900	2.78305900	1.28445100



H	6.89990600	1.83349200	1.72920300
H	7.43049200	3.47639900	1.35188200
H	5.76768900	3.18595400	1.89440100
C	4.34491700	-2.08112900	0.68506500
C	3.39380400	-2.39740400	1.86503000
H	2.34195700	-2.32491100	1.57854500
H	3.58007100	-3.41425800	2.23075400
H	3.56338200	-1.70734700	2.69965400
C	5.78703200	-2.28707100	1.19297000
H	6.02269800	-1.63722800	2.04301700
H	5.90396700	-3.32206000	1.53098600
H	6.52987800	-2.11464400	0.40668400
C	4.11616600	-3.08716800	-0.47183100
H	4.27541600	-4.11082800	-0.11197400
H	3.10770400	-3.01815100	-0.88938000
H	4.82439400	-2.90710300	-1.28822400
C	3.72482100	1.98750400	-0.80849700
H	3.55736700	2.98589700	-1.19836700
C	-2.37553500	1.17547900	-0.91564000
C	-4.59009600	1.90570400	-0.22026700
C	-3.31239600	2.18836400	-0.71059300
C	-1.05259600	1.49463400	-1.55767900
H	-0.96602100	2.58109200	-1.69146400
H	-0.98375300	1.03183700	-2.54559300
H	1.34212900	2.54179400	-1.66257900
H	1.30379900	1.00088200	-2.53356700
H	-3.03223300	3.20616100	-0.96121000
C	-5.65241300	2.98976500	0.02619200
C	-6.06949300	2.96783200	1.51701400
C	-5.13399100	4.40174700	-0.30831600
C	-6.89142100	2.70789800	-0.85864700
H	-6.48893100	2.00041600	1.81208300
H	-5.21340900	3.17662600	2.16926600
H	-6.83267900	3.73131400	1.70606100
H	-4.85822700	4.49845300	-1.36473600
H	-5.91981500	5.13752000	-0.10820500
H	-4.26601900	4.67642500	0.30290500
H	-7.65636500	3.47425300	-0.68924600
H	-6.62765700	2.72117100	-1.92211800
H	-7.34234400	1.73526400	-0.63636500
H	7.67457700	1.09005100	-0.64721100
H	8.18497200	2.75181900	-0.96844100
H	0.81558400	-3.42446000	0.13097100
O	-1.21353900	-3.98579100	-1.94335100
H	-0.89129200	-4.84016100	-2.28328500
O	0.17135300	-0.91706600	-2.56614000
O	0.38424600	-2.27989200	-2.34962500
H	-0.59450800	-3.10526700	-2.39553400
H	-0.83220000	-3.81455200	-0.96492000

V	0.06872200	-1.16444300	-0.90579100
O	-1.73690200	-1.08052800	-0.95269200
O	1.81912500	-1.11947700	-0.47743000
N	0.13308000	1.00106400	-0.67122100
N	-0.31942700	-0.89691400	1.28861400
C	-0.67066900	-1.87513700	2.14559300
H	-0.62059200	-2.88439300	1.75965500
C	-1.07963200	-1.61820200	3.44860400
H	-1.34192800	-2.44306600	4.10205500
C	-1.15373300	-0.29337000	3.87991800
H	-1.48357400	-0.05404800	4.88627700
C	-0.79640000	0.71933900	2.99520700
H	-0.83689400	1.76259000	3.29192900
C	-0.37077800	0.37978400	1.70947600
C	0.16448800	1.41755900	0.76673900
H	1.21070300	1.60032800	1.03323300
H	-0.37173100	2.36548600	0.88442300
C	-4.96166000	0.37742100	-0.08438900
H	-5.97325800	0.08426500	0.16297900
C	-4.04640100	-0.63269500	-0.39598300
C	-2.72691600	-0.20343200	-0.69882000
C	-4.47197300	-2.11416200	-0.47507000
C	-4.20879000	-2.64273600	-1.90828500
H	-4.79100100	-2.07730800	-2.64433400
H	-3.15335800	-2.57070300	-2.18477200
H	-4.51169100	-3.69426300	-1.97892800
C	-3.69231600	-2.97207900	0.54853500
H	-2.62308500	-2.99030800	0.32860400
H	-3.82931200	-2.59221600	1.56767700
H	-4.05994100	-4.00471400	0.52357300
C	-5.97480500	-2.29926000	-0.18011400
H	-6.23919700	-1.99131200	0.83797800
H	-6.60501300	-1.74652500	-0.88510700
H	-6.23060900	-3.35951200	-0.27728000
C	1.36360200	1.54516000	-1.35826900
C	2.67139200	1.07321200	-0.76854600
C	2.85987900	-0.26659600	-0.37442400
C	4.11445800	-0.71851700	0.11580000
C	5.13486000	0.23264700	0.18161500
H	6.10386900	-0.08553100	0.54315600
C	4.98595400	1.58151200	-0.19013100
C	6.17934700	2.54513400	-0.07364700
C	7.33816400	2.03339100	-0.96416100
H	7.03377600	1.98105700	-2.01552200
C	5.82212100	3.97465700	-0.52387900
H	6.69903000	4.62186900	-0.41886400
H	5.51464100	4.00950100	-1.57543800
H	5.02147700	4.40922400	0.08635300
C	6.65077900	2.60550300	1.39964100
H	6.96064200	1.62392900	1.77324800

H	7.50931800	3.28032100	1.49244600
H	5.85478200	2.97917000	2.05415500
C	4.34649300	-2.18639100	0.53131100
C	3.41992700	-2.55710100	1.71571300
H	2.36233100	-2.42710900	1.47152900
H	3.58264400	-3.60168000	2.00732600
H	3.63698300	-1.93141300	2.58905100
C	5.79683500	-2.43724500	0.99481900
H	6.05833500	-1.83951400	1.87483300
H	5.90931500	-3.49105300	1.27090700
H	6.52417000	-2.22753100	0.20326600
C	4.08764200	-3.12600800	-0.67356600
H	4.22988300	-4.17092000	-0.37242000
H	3.07973000	-3.01240200	-1.08514100
H	4.78963800	-2.91649300	-1.48806000
C	3.73048400	1.97825000	-0.65688300
H	3.55998900	3.00595800	-0.95984800
C	-2.40563300	1.16729500	-0.77700800
C	-4.66401800	1.75268100	-0.08472600
C	-3.36890700	2.12506800	-0.45838600
C	-1.07778400	1.58803000	-1.35181000
H	-0.98835600	2.68099100	-1.30810900
H	-1.00799600	1.28716700	-2.40087000
H	1.31910600	2.64080700	-1.30354400
H	1.28228700	1.26333600	-2.41004900
H	-3.09898100	3.17330600	-0.53164600
C	-5.75506500	2.77357000	0.28112800
C	-6.26781900	2.48707400	1.71351600
C	-5.23573000	4.22356600	0.23643800
C	-6.93075600	2.65039500	-0.71917500
H	-6.69881400	1.48445400	1.80312900
H	-5.45804900	2.57245300	2.44757700
H	-7.04767500	3.20750800	1.98525600
H	-4.89836000	4.50814100	-0.76690000
H	-6.04113000	4.91075800	0.51556500
H	-4.40908300	4.38543500	0.93861600
H	-7.71776200	3.36973700	-0.46543200
H	-6.59997300	2.85698300	-1.74319800
H	-7.37857200	1.65136000	-0.70546800
H	7.67957300	1.03752200	-0.66283000
H	8.19556400	2.71229800	-0.89270300
O	0.11413100	-3.27775400	-0.30007300
H	1.06317400	-3.50834100	-0.29406100
O	0.30072400	-0.68719700	-2.67920000
O	0.25310000	-2.05025000	-2.49210100
H	-0.28245500	-3.80071600	-1.02153800

V	0.03927100	-1.17815200	-1.00150700
O	-1.76456500	-1.14544700	-0.93324200
O	1.80091400	-1.18138300	-0.66365300
N	0.07531500	0.93340500	-0.71641800
N	-0.16381500	-1.08969900	1.14433400
C	-0.33047900	-2.16452100	1.93692500
H	-0.28112700	-3.13657600	1.45499400
C	-0.55675500	-2.04831700	3.30150800
H	-0.67967400	-2.93858400	3.90804500
C	-0.62710200	-0.76842000	3.85720500
H	-0.81258200	-0.63787200	4.91888100
C	-0.45446900	0.34040000	3.03353600
H	-0.49860900	1.34747500	3.43611300
C	-0.21283500	0.14360200	1.67221100
C	0.08592700	1.29463300	0.74781700
H	1.08455700	1.67240800	0.98851600
H	-0.62555400	2.10853200	0.91714200
C	-4.97991000	0.28737200	0.01638800
H	-5.97782700	-0.01340900	0.30596800
C	-4.05906200	-0.71897400	-0.29141800
C	-2.75905400	-0.27884800	-0.65413200
C	-4.46013200	-2.20898900	-0.30213700
C	-4.24596100	-2.78453700	-1.72541700
H	-4.86459900	-2.25272400	-2.45680800
H	-3.20310500	-2.71420000	-2.04554100
H	-4.53703000	-3.84112800	-1.74525800
C	-3.62168100	-3.01515200	0.71722600
H	-2.56340000	-3.02376600	0.44856100
H	-3.72259500	-2.60287200	1.72818000
H	-3.96756000	-4.05478500	0.74175200
C	-5.94550800	-2.40828000	0.06437000
H	-6.17293800	-2.06400100	1.07984700
H	-6.61550400	-1.89627300	-0.63472100
H	-6.18453500	-3.47583700	0.02034800
C	1.31257100	1.49467100	-1.38397500
C	2.61404300	1.03089000	-0.77710700
C	2.83222100	-0.33035000	-0.47573200
C	4.09335300	-0.79138800	-0.01592700
C	5.08124200	0.18363300	0.14808700
H	6.05487500	-0.13658900	0.49455200
C	4.89838300	1.55461700	-0.10937500
C	6.05963400	2.53864500	0.11370000
C	7.24765500	2.14248300	-0.79706200
H	6.96231900	2.17577700	-1.85447300
C	5.66476900	3.99130700	-0.21406600
H	6.51861700	4.65245400	-0.03371600
H	5.37570800	4.11171300	-1.26454600
H	4.83979300	4.34489400	0.41591800
C	6.50482700	2.48045000	1.59530000
H	6.84188000	1.47960700	1.88444300

H	7.33824400	3.17145800	1.76481300
H	5.68626100	2.76722100	2.26572000
C	4.37380100	-2.28445200	0.25149900
C	3.45968000	-2.80487100	1.38694000
H	2.40216200	-2.72385500	1.12612600
H	3.67878100	-3.86017900	1.58636500
H	3.62939000	-2.24535900	2.31451600
C	5.83286500	-2.52867600	0.68928100
H	6.07698600	-2.01863400	1.62812300
H	5.98184000	-3.60099500	0.85292200
H	6.55092300	-2.21335200	-0.07549000
C	4.13497200	-3.10171600	-1.04332700
H	4.33736700	-4.16234400	-0.85445100
H	3.10918700	-3.01206200	-1.40935300
H	4.80899700	-2.76949100	-1.84074100
C	3.64217100	1.95452500	-0.57411200
H	3.45122400	2.99677300	-0.80682400
C	-2.45985600	1.09420100	-0.78056500
C	-4.70609000	1.66649200	-0.03911300
C	-3.42805200	2.04720500	-0.46050300
C	-1.14679100	1.52299000	-1.38324600
H	-1.05579000	2.61492500	-1.33292400
H	-1.08694600	1.22817200	-2.43506700
H	1.25281500	2.58868600	-1.32709700
H	1.24324800	1.21091100	-2.43746000
H	-3.17703500	3.09698200	-0.56994100
C	-5.80333500	2.68145800	0.32452100
C	-6.27251700	2.43353800	1.77899900
C	-5.30940700	4.13715100	0.21918100
C	-7.00296500	2.50665500	-0.63908400
H	-6.68328400	1.42748400	1.91353400
H	-5.44549600	2.55783100	2.48783800
H	-7.05770800	3.14923700	2.04751800
H	-5.00296300	4.39414100	-0.80138000
H	-6.11888000	4.82005800	0.49669700
H	-4.46835700	4.33529300	0.89447700
H	-7.79435400	3.22166200	-0.38715800
H	-6.70357000	2.68451700	-1.67803000
H	-7.43374800	1.50180400	-0.58048100
H	7.61437300	1.13397900	-0.57929200
H	8.08237000	2.83704900	-0.64910800
O	0.18247400	-0.77109700	-2.80625400
O	0.13020000	-2.12471700	-2.52349900

**Ts3**

V	0.04232800	-1.42610000	-0.17846100
O	-1.73981200	-1.15968500	-0.48307200
O	1.81535000	-1.08137400	-0.04797200
N	0.10437700	0.94078300	-0.72525600
N	-0.33056900	-0.31330600	1.72791100
C	-0.64543500	-0.98396100	2.84928300
H	-0.56260600	-2.06323600	2.77701400
C	-1.05596700	-0.34623900	4.01378500
H	-1.29356900	-0.93311200	4.89449700
C	-1.16540500	1.04446400	4.00916800
H	-1.49990100	1.57870500	4.89388200
C	-0.83615400	1.73860600	2.84980300
H	-0.90067500	2.82156300	2.80773300
C	-0.40595400	1.03005000	1.72405100
C	0.10884000	1.75738400	0.50869900
H	1.14678900	2.03730900	0.72235900
H	-0.45118700	2.69068400	0.36379400
C	-4.93572700	0.49283700	0.03823500
H	-5.93812900	0.27919100	0.38778500
C	-4.02032200	-0.56326200	-0.00698100
C	-2.70846400	-0.23888200	-0.45106700
C	-4.42569500	-2.00917100	0.34222000
C	-4.21850700	-2.90952400	-0.90227400
H	-4.83287400	-2.56048900	-1.74093800
H	-3.17353800	-2.92242400	-1.21998400
H	-4.51760200	-3.93926600	-0.67033000
C	-3.58093300	-2.55707400	1.51722100
H	-2.52776800	-2.65702000	1.24863600
H	-3.66451700	-1.90528700	2.39608500
H	-3.94831900	-3.55099200	1.80216000
C	-5.90992800	-2.10765400	0.75104000
H	-6.13089000	-1.52639800	1.65455400
H	-6.58296400	-1.77430700	-0.04735900
H	-6.15209900	-3.15390000	0.96705400
C	1.32633100	1.22370200	-1.54622400
C	2.62498400	0.99852500	-0.82257600
C	2.81933800	-0.20295800	-0.11848700
C	4.07007900	-0.49409700	0.49404000
C	5.06109600	0.48452400	0.38084900
H	6.02195500	0.28936600	0.84030000
C	4.89338900	1.70866500	-0.29285100
C	6.05495700	2.71728900	-0.35231700
C	7.26549900	2.06988600	-1.06736500
H	7.00725800	1.78392400	-2.09333500
C	5.67618200	3.99900100	-1.11904900
H	6.52969900	4.68612900	-1.13423800
H	5.40548800	3.78666200	-2.15963700
H	4.83787000	4.52453000	-0.64672400
C	6.46588300	3.12120700	1.08407000
H	6.79385300	2.25800300	1.67241300

H	7.29430700	3.83982500	1.05651200
H	5.62817600	3.58874300	1.61472000
C	4.32105000	-1.83184300	1.21799200
C	3.33061000	-2.00320900	2.39663000
H	2.29941100	-2.08579100	2.04896300
H	3.57181400	-2.91884500	2.95090900
H	3.40389500	-1.15970600	3.09506700
C	5.74879300	-1.91318200	1.79675100
H	5.94057400	-1.13163000	2.54193800
H	5.87792100	-2.88024400	2.29496500
H	6.51605100	-1.84295900	1.01695900
C	4.15141400	-3.00537000	0.22019300
H	4.34677100	-3.95657700	0.73070500
H	3.14257700	-3.04449700	-0.19524900
H	4.86420800	-2.91468900	-0.60814000
C	3.65306400	1.94186300	-0.89095200
H	3.46648500	2.86150700	-1.43649400
C	-2.40750000	1.05448500	-0.91102000
C	-4.64697200	1.81500900	-0.34951400
C	-3.36556300	2.06761700	-0.84447200
C	-1.07868100	1.26946600	-1.57604000
H	-0.99650600	2.31634100	-1.90887200
H	-0.99969900	0.62613800	-2.45892100
H	1.28433000	2.26439100	-1.90463000
H	1.25944200	0.56576200	-2.41797700
H	-3.09496200	3.05466500	-1.20652100
C	-5.73489300	2.89921600	-0.24586800
C	-6.20531800	3.02287900	1.22343700
C	-5.22694100	4.28094500	-0.70130800
C	-6.94019500	2.51307200	-1.13679300
H	-6.61995400	2.08185300	1.59967200
H	-5.37336800	3.30698500	1.87855800
H	-6.98497200	3.78954300	1.31209600
H	-4.91405300	4.27594300	-1.75175800
H	-6.02874300	5.02112200	-0.60090100
H	-4.38160400	4.62527800	-0.09373400
H	-7.72592500	3.27585400	-1.06983800
H	-6.63817300	2.42630500	-2.18665900
H	-7.37841200	1.55605400	-0.83553400
H	7.61144000	1.17048800	-0.54760400
H	8.10526400	2.77447300	-1.11100300
O	0.14250900	-3.02790800	-0.87263300
O	-0.04029000	-2.78831200	0.88685800
Br	0.33724100	-2.02501100	-2.93703500

V	0.08471500	-1.43278300	-0.06000800
O	-1.74951500	-1.15093400	-0.19612200
O	1.90271100	-1.15736200	0.06131800
N	0.18589400	0.88993300	-0.83620000
N	-0.10638500	-0.11023200	1.73273700
C	-0.33135400	-0.67305600	2.93578000
H	-0.30893600	-1.75638300	2.95228500
C	-0.58069600	0.07665400	4.07812200
H	-0.75177900	-0.42273900	5.02580100
C	-0.61376600	1.46779500	3.96744700
H	-0.81742800	2.08931200	4.83485500
C	-0.38142000	2.04687500	2.72528200
H	-0.39615000	3.12544600	2.59910200
C	-0.11868900	1.22811800	1.62143600
C	0.24601500	1.84294500	0.28541500
H	1.27316100	2.21528900	0.37225500
H	-0.39460000	2.71547100	0.10091500
C	-4.82277500	0.75059100	0.19648000
H	-5.81166700	0.64897700	0.62605200
C	-3.95735900	-0.34324400	0.27654000
C	-2.65512000	-0.17538100	-0.28209200
C	-4.41226300	-1.68655600	0.88424000
C	-4.36788600	-2.77885300	-0.21367000
H	-5.05713800	-2.53433200	-1.03114300
H	-3.36406900	-2.88781000	-0.62947200
H	-4.67326200	-3.74524700	0.20717600
C	-3.50009500	-2.10470500	2.06165300
H	-2.48169000	-2.30264300	1.72560700
H	-3.47477600	-1.32456100	2.83273300
H	-3.88987800	-3.02049900	2.52374600
C	-5.85751600	-1.62117900	1.42015200
H	-5.96756500	-0.88775100	2.22823100
H	-6.58117600	-1.37886000	0.63342000
H	-6.13316000	-2.60086900	1.82600200
C	1.38708200	0.96778100	-1.71696600
C	2.69614400	0.81512500	-0.99207900
C	2.89443600	-0.29101200	-0.13909200
C	4.16178400	-0.49738800	0.48389300
C	5.15257600	0.45273700	0.22822500
H	6.12125800	0.31542400	0.69201700
C	4.97744600	1.57820900	-0.59815300
C	6.14219100	2.56189400	-0.80805400
C	7.34008400	1.81650700	-1.44484500
H	7.06399800	1.39126000	-2.41646300
C	5.76060800	3.73160900	-1.73542700
H	6.61661300	4.40614800	-1.85004200
H	5.47843000	3.38425800	-2.73591000
H	4.92919200	4.31944000	-1.32918000
C	6.57503900	3.15315900	0.55533800
H	6.89185500	2.37409300	1.25663100



H	7.41687300	3.84409400	0.42292500
H	5.75150900	3.70689600	1.02130300
C	4.43428700	-1.72829800	1.37248900
C	3.47910700	-1.73631000	2.59076200
H	2.43656000	-1.80894700	2.27913600
H	3.70441500	-2.59694500	3.23284600
H	3.60541200	-0.82653900	3.19099800
C	5.87704400	-1.74128900	1.91861000
H	6.08856300	-0.87200100	2.55277500
H	6.01899700	-2.63756000	2.53262800
H	6.62329300	-1.77315600	1.11637800
C	4.23632200	-3.02393200	0.54581800
H	4.43586200	-3.90046600	1.17498700
H	3.21843500	-3.10393200	0.16005400
H	4.93182600	-3.05279700	-0.30167500
C	3.72782200	1.73453200	-1.20076900
H	3.53487200	2.57520100	-1.86010900
C	-2.32451700	1.02183800	-0.94904900
C	-4.50002800	1.97678400	-0.41394800
C	-3.23592100	2.07969400	-0.99688800
C	-1.01594700	1.10808600	-1.68491100
H	-0.93932000	2.09166900	-2.17758700
H	-0.97439300	0.34261100	-2.46721900
H	1.38507800	1.92394600	-2.26557000
H	1.26386500	0.16176700	-2.44936500
H	-2.93967400	2.98470300	-1.51852100
C	-5.53286200	3.11781500	-0.43460700
C	-5.90054000	3.51023800	1.01660000
C	-5.00039100	4.37497200	-1.14859100
C	-6.80940500	2.65200000	-1.17570600
H	-6.31780800	2.66489600	1.57364700
H	-5.01803800	3.86598000	1.56126700
H	-6.64822400	4.31322400	1.01856000
H	-4.75557600	4.17503500	-2.19804800
H	-5.76361800	5.16132900	-1.13223400
H	-4.10474900	4.77409700	-0.65811300
H	-7.55531700	3.45640700	-1.19589500
H	-6.58049800	2.37349200	-2.21066200
H	-7.26938800	1.78437600	-0.69115500
H	7.69414200	0.99702700	-0.81086100
H	8.18020700	2.50489500	-1.60013000
O	0.29780800	-1.92963000	-1.83869500
O	-0.00429700	-2.75940400	0.81125200
Br	-0.87970900	-3.07904300	-2.67769100

V	0.07081100	-1.24711500	0.19147800
O	-1.71103700	-1.01872600	-0.03447500
O	1.88345400	-1.02145200	0.10828900
N	0.13321600	0.97059600	-0.77368500
N	-0.05532400	0.03537100	1.85415400
C	-0.21482200	-0.48706300	3.09207300
H	-0.19699000	-1.56810600	3.15072900
C	-0.39631900	0.30408700	4.21562200
H	-0.51690800	-0.16227600	5.18713700
C	-0.42650800	1.69128700	4.05935500
H	-0.57537900	2.34316200	4.91480600
C	-0.26194400	2.22594300	2.78680600
H	-0.27505800	3.29972400	2.62723700
C	-0.06906700	1.37512900	1.69463700
C	0.20335100	1.96003500	0.32442100
H	1.21051300	2.39071000	0.34936700
H	-0.49016800	2.79078500	0.14659900
C	-4.88887600	0.72198000	0.24148100
H	-5.87652200	0.59589100	0.66437900
C	-3.97777300	-0.32681600	0.38240900
C	-2.68237500	-0.10677500	-0.17169000
C	-4.37374500	-1.65168500	1.06504600
C	-4.24400600	-2.81111100	0.04553300
H	-4.91002300	-2.65264400	-0.81052700
H	-3.22186100	-2.91173400	-0.32616100
H	-4.52865300	-3.75698900	0.52105900
C	-3.47012400	-1.93453200	2.28946000
H	-2.43325000	-2.10469300	1.99510000
H	-3.50472200	-1.10345300	3.00444700
H	-3.82367400	-2.83439900	2.80609600
C	-5.83396100	-1.62960000	1.56280500
H	-6.00302800	-0.85658700	2.32136500
H	-6.54768100	-1.47686800	0.74581600
H	-6.06861300	-2.59516000	2.02254200
C	1.31996100	1.05376700	-1.68182900
C	2.64618600	0.93148700	-0.98559100
C	2.88270400	-0.16371900	-0.12696900
C	4.16734400	-0.36146100	0.46416000
C	5.13671600	0.60027100	0.17510200
H	6.11769300	0.48167800	0.61545300
C	4.92687500	1.71791600	-0.65599500
C	6.07269000	2.71185700	-0.90490500
C	7.25694100	1.96993900	-1.57264400
H	6.95953500	1.53858000	-2.53505400
C	5.65043900	3.87301500	-1.82540900
H	6.49545400	4.55493800	-1.96540300
H	5.34731500	3.52115100	-2.81820100
H	4.82664200	4.45636600	-1.39760300
C	6.53711900	3.30964900	0.44626200
H	6.89098900	2.53859900	1.13850900

H	7.36334300	4.01062700	0.28239300
H	5.72311900	3.85536500	0.93729900
C	4.48408500	-1.57434700	1.36259300
C	3.55373300	-1.59404400	2.59972500
H	2.50692600	-1.71756500	2.31779900
H	3.82949100	-2.42765900	3.25628000
H	3.65506600	-0.66745400	3.17683400
C	5.93778100	-1.55281000	1.87881200
H	6.14073300	-0.67487000	2.50218100
H	6.11082200	-2.43923300	2.49794300
H	6.66919000	-1.57661000	1.06362800
C	4.30331900	-2.87993600	0.54819600
H	4.52175200	-3.74805900	1.18141800
H	3.27921300	-2.96886500	0.17681800
H	4.98799300	-2.90489000	-0.30742600
C	3.65885000	1.85809300	-1.23039300
H	3.44595600	2.68983600	-1.89358100
C	-2.38933300	1.07315500	-0.88650200
C	-4.61548400	1.93442900	-0.42164400
C	-3.34755700	2.07982300	-0.99465300
C	-1.08095100	1.17707000	-1.61771100
H	-1.01536800	2.15800600	-2.11234200
H	-1.03786700	0.41551000	-2.40606500
H	1.29011900	1.99985200	-2.24278500
H	1.19957900	0.24059100	-2.40712100
H	-3.09496000	2.97562700	-1.55203500
C	-5.70156100	3.01921900	-0.50627800
C	-6.11327500	3.44474900	0.92442300
C	-5.21839700	4.27289900	-1.26075700
C	-6.93703700	2.45420700	-1.24969500
H	-6.51308200	2.60637600	1.50407600
H	-5.25971700	3.85821900	1.47420400
H	-6.89086900	4.21563300	0.87753300
H	-4.94870700	4.04896300	-2.29926200
H	-6.02081500	5.01746200	-1.28592400
H	-4.35496200	4.73954400	-0.77177000
H	-7.71891700	3.21954900	-1.31369000
H	-6.67788300	2.14855200	-2.26958200
H	-7.36485300	1.58646100	-0.73688900
H	7.64080400	1.15955000	-0.94448400
H	8.08229300	2.66774100	-1.75421400
O	0.30620400	-2.11120000	-1.74740500
O	0.05761200	-2.60414500	1.02885200
Br	-1.13428200	-2.58665600	-2.86686700
H	0.76373300	-3.01052400	-1.55401800
O	1.24088100	-4.38371400	-0.95883300
H	0.94636500	-4.30013700	-0.03180300
H	2.20507100	-4.49417900	-0.91902200

*Ts4*

V	0.00904700	0.95209100	0.74022400
O	1.74944800	0.90243000	0.26257900
O	-1.77063600	0.70701100	0.62292600
N	-0.08068800	-0.98935400	-0.75903800
N	0.35662500	-0.70859100	1.98627900
C	0.67087500	-0.50597300	3.28688500
H	0.63168900	0.52281000	3.62101800
C	1.02354900	-1.54125300	4.13838200
H	1.26278000	-1.32450800	5.17358100
C	1.06885200	-2.84104000	3.63136000
H	1.35145100	-3.67589900	4.26542700
C	0.74186600	-3.04840400	2.29647100
H	0.75627700	-4.04492000	1.86641100
C	0.37700100	-1.96572000	1.49199000
C	-0.10501100	-2.20144800	0.08140500
H	-1.13992800	-2.55560200	0.15301200
H	0.47560900	-3.01462300	-0.37331100
C	5.01616600	-0.67052200	-0.03777400
H	6.03085000	-0.56438600	0.32181800
C	4.07691100	0.28299000	0.35970700
C	2.74875100	0.09481400	-0.12589600
C	4.47864800	1.48179400	1.24360000
C	4.20971000	2.79837600	0.47306400
H	4.80985500	2.83953400	-0.44381500
H	3.15470500	2.89153400	0.20411400
H	4.48610700	3.65737200	1.09611300
C	3.68264000	1.48417900	2.57071400
H	2.61682300	1.65339900	2.40805900
H	3.81193000	0.53517900	3.10470100
H	4.05430200	2.28478400	3.22120400
C	5.97843400	1.45840200	1.60610700
H	6.24779300	0.57419700	2.19476600
H	6.62110400	1.49470300	0.71973000
H	6.21217900	2.33822700	2.21453000
C	-1.30059500	-0.89910700	-1.62163700
C	-2.60832800	-0.91193200	-0.87840000
C	-2.80217800	-0.05111500	0.22140400
C	-4.06004800	0.02377200	0.88823700
C	-5.06789000	-0.80579700	0.39279100
H	-6.03598800	-0.77439600	0.87413400
C	-4.90953600	-1.68668600	-0.69439400
C	-6.09325200	-2.55158600	-1.15689700
C	-7.26095000	-1.62962400	-1.58769000
H	-6.96326100	-0.97598200	-2.41529700
C	-5.72632000	-3.45511500	-2.34975000
H	-6.59814300	-4.05031900	-2.64032700
H	-5.42067400	-2.87388500	-3.22731300
H	-4.92073600	-4.15579600	-2.10054300
C	-6.55618700	-3.45625200	0.01155400
H	-6.88383400	-2.87392000	0.87898900

H	-7.40075900	-4.07760100	-0.30715900
H	-5.74995800	-4.12347200	0.33754000
C	-4.30439300	0.95233400	2.09626400
C	-3.37643500	0.54958900	3.26901900
H	-2.32150200	0.66437500	3.01083300
H	-3.58103800	1.18459400	4.13901100
H	-3.55398000	-0.49079800	3.56581900
C	-5.75879800	0.86793100	2.60466700
H	-6.01769000	-0.13827000	2.95213300
H	-5.87991900	1.54647600	3.45527900
H	-6.48347500	1.16875100	1.83991100
C	-4.04211000	2.42758400	1.70389600
H	-4.29161500	3.08727700	2.54248800
H	-2.98969900	2.58873300	1.45812600
H	-4.65852700	2.72345900	0.84724500
C	-3.65438700	-1.72468700	-1.31235500
H	-3.47906400	-2.38059000	-2.15817800
C	2.44256300	-0.95696800	-1.01516600
C	4.73459300	-1.76361800	-0.88072800
C	3.42827400	-1.87673200	-1.36781000
C	1.09534700	-0.99130500	-1.67992900
H	1.03464500	-1.87394400	-2.33465300
H	0.99039900	-0.09898100	-2.30369100
H	-1.29337800	-1.72363500	-2.35042700
H	-1.20349700	0.03059600	-2.19069200
H	3.16427500	-2.67541600	-2.05251100
C	5.85018200	-2.75625900	-1.24640800
C	6.40751900	-3.40009000	0.04708200
C	5.34939000	-3.88379000	-2.16943500
C	6.98942600	-2.00247200	-1.97640400
H	6.82788700	-2.65414000	0.72941700
H	5.62440200	-3.94656700	0.58532500
H	7.20542800	-4.10916300	-0.20095400
H	4.97543200	-3.49716400	-3.12433200
H	6.17498400	-4.56667200	-2.39510600
H	4.55431000	-4.47508100	-1.70003300
H	7.79185700	-2.70070300	-2.24016100
H	6.62650100	-1.53803500	-2.90009100
H	7.42673700	-1.21583100	-1.35308200
H	-7.60865200	-0.99497800	-0.76600600
H	-8.11159900	-2.23403200	-1.92244300
O	0.37024200	1.99697200	-2.07168800
O	0.11314500	1.92199300	2.00905800
Br	-0.90389700	2.56379700	-3.31160600
H	0.84891500	2.85282000	-1.83851900
O	1.52957000	4.30091900	-1.40472100
H	2.48610400	4.36125800	-1.26439500
H	1.10665200	4.57241500	-0.56530700
O	-0.80895900	3.40977100	-0.03612000
O	-0.19130300	4.35544000	0.87183500
H	-1.75711200	3.52060300	0.17062500
H	0.08108000	3.73892100	1.59283200

V	0.03197900	-1.43476700	-0.55640000
O	-1.74636100	-1.13356200	-0.77628600
O	1.81001900	-1.14696400	-0.60984800
N	0.06561300	1.01797000	-0.64631400
N	-0.12688600	-0.83972800	1.44844800
C	-0.27280000	-1.78353500	2.40864900
H	-0.22576200	-2.80995700	2.06665400
C	-0.47472000	-1.46465000	3.74177100
H	-0.58242500	-2.25829400	4.47275500
C	-0.54189600	-0.11815900	4.10528400
H	-0.70822200	0.17079300	5.13858800
C	-0.39056900	0.84920400	3.11889700
H	-0.43154200	1.90608300	3.36399500
C	-0.17441200	0.46458800	1.79247900
C	0.08264300	1.52505300	0.74179800
H	1.06926200	1.95352200	0.95183500
H	-0.64573200	2.33478800	0.87033100
C	-4.98878600	0.32980600	-0.02045500
H	-5.98781400	0.03858000	0.27536100
C	-4.04753100	-0.67989300	-0.23330200
C	-2.74144900	-0.24848300	-0.60394700
C	-4.41842600	-2.17117500	-0.10187500
C	-4.18726100	-2.88402300	-1.45807700
H	-4.79943200	-2.43317500	-2.24746400
H	-3.13841100	-2.83672600	-1.76332800
H	-4.46668600	-3.94055800	-1.37670700
C	-3.56759400	-2.85142800	0.99745000
H	-2.50644800	-2.85719200	0.74318700
H	-3.69769100	-2.34465700	1.96116800
H	-3.88864200	-3.89228700	1.12155300
C	-5.90229700	-2.36678600	0.27348300
H	-6.14341100	-1.92808800	1.24836700
H	-6.57961600	-1.94179100	-0.47556100
H	-6.11710300	-3.43860200	0.33674400
C	1.26958200	1.46546500	-1.41344900
C	2.58967700	1.07083900	-0.81151900
C	2.82381700	-0.27975100	-0.48203700
C	4.10411700	-0.71908300	-0.03654500
C	5.07783900	0.27281200	0.10115700
H	6.05900600	-0.02326900	0.44792200
C	4.87130200	1.63665400	-0.18266400
C	6.01966800	2.64008600	0.01405300
C	7.21254400	2.23844600	-0.88823900
H	6.92601400	2.24365300	-1.94593900
C	5.60681800	4.08014400	-0.34584800
H	6.45300400	4.75531800	-0.18169900
H	5.31426200	4.17334400	-1.39811000
H	4.77841400	4.43747100	0.27716400
C	6.46691800	2.62108300	1.49648500
H	6.81558600	1.63111700	1.80798300

H	7.29213100	3.32593200	1.64877400
H	5.64538400	2.91341000	2.16069700
C	4.40927900	-2.20022000	0.26450400
C	3.50644400	-2.71520300	1.41248700
H	2.45207700	-2.71495400	1.13101000
H	3.78460200	-3.74496700	1.66507700
H	3.63257000	-2.10387400	2.31421000
C	5.87462100	-2.40912700	0.69957400
H	6.11258300	-1.87714400	1.62781400
H	6.04306800	-3.47517100	0.88331500
H	6.58515300	-2.09531900	-0.07324100
C	4.17593800	-3.05094000	-1.00951500
H	4.41381000	-4.10057500	-0.80196600
H	3.13852600	-3.00133300	-1.34802500
H	4.82684500	-2.71559700	-1.82552700
C	3.60525000	2.01172200	-0.64733500
H	3.39812400	3.04496300	-0.90502000
C	-2.45905200	1.11556600	-0.81292500
C	-4.72990300	1.70616600	-0.17149000
C	-3.44514600	2.07474400	-0.58366700
C	-1.13051200	1.50410700	-1.39740200
H	-1.07983400	2.59971400	-1.49124800
H	-1.03940500	1.08790000	-2.40769300
H	1.24026600	2.55815000	-1.54215500
H	1.16563300	1.02074200	-2.41013400
H	-3.19992200	3.11782200	-0.75385500
C	-5.84803800	2.72765000	0.09568500
C	-6.32535200	2.59208100	1.56245700
C	-5.37901600	4.17861100	-0.12540800
C	-7.03578300	2.45332200	-0.85923500
H	-6.71328000	1.59119400	1.77829000
H	-5.50712800	2.79449000	2.26337800
H	-7.12878400	3.30952700	1.76451100
H	-5.06179200	4.35444600	-1.15974200
H	-6.20499500	4.86640800	0.08336800
H	-4.55183200	4.44888400	0.54159000
H	-7.83969500	3.17519300	-0.67548500
H	-6.72919800	2.54724100	-1.90710900
H	-7.45315800	1.45075200	-0.71973400
H	7.59307300	1.24048500	-0.64741700
H	8.03769600	2.94774500	-0.75727900
O	-0.00093600	-2.98096200	-0.20433200
O	0.09239800	-2.03536300	-2.71655800
O	0.03296500	-0.92684700	-3.65043500
H	-0.75288500	-2.49486000	-2.89857700
H	0.77698900	-1.16391000	-4.23836800

V	0.05302800	-1.36126000	-0.36246100
O	-1.71827700	-1.06472700	-0.61029900
O	1.84209200	-1.10973500	-0.32896400
N	0.13459900	1.04539400	-0.69626200
N	-0.17074900	-0.56588900	1.57523300
C	-0.40526700	-1.39466000	2.61805100
H	-0.36954500	-2.45320700	2.39238700
C	-0.67900000	-0.92690200	3.89415400
H	-0.85568000	-1.63242000	4.69846100
C	-0.72847100	0.45229400	4.10471300
H	-0.95190200	0.85624800	5.08746200
C	-0.48366700	1.30283600	3.03258700
H	-0.50561300	2.38070500	3.15960900
C	-0.19445500	0.76875000	1.77405800
C	0.19614000	1.68559400	0.63535700
H	1.22771400	2.00539000	0.82119400
H	-0.42549300	2.58917400	0.66730000
C	-4.93384200	0.51117100	0.00675700
H	-5.93902100	0.26250400	0.32060100
C	-4.01323400	-0.52983700	-0.12860900
C	-2.69569400	-0.15344100	-0.52283300
C	-4.41762800	-1.99997000	0.10058500
C	-4.20397200	-2.80162600	-1.20824400
H	-4.81209400	-2.38855400	-2.02109300
H	-3.15945800	-2.79651400	-1.52819300
H	-4.50933400	-3.84419800	-1.05974800
C	-3.58292800	-2.62779000	1.24244200
H	-2.52311600	-2.68129800	0.98742900
H	-3.69261600	-2.05254500	2.16967900
H	-3.93515900	-3.64741800	1.43912500
C	-5.90468700	-2.13608800	0.48905200
H	-6.13589200	-1.62811600	1.43244300
H	-6.57297600	-1.74795800	-0.28747900
H	-6.14271800	-3.19643400	0.62277600
C	1.33685700	1.36497500	-1.52766700
C	2.65618900	1.03595000	-0.88527800
C	2.86387000	-0.24683000	-0.33698700
C	4.13706900	-0.62645400	0.18047000
C	5.13200300	0.35254100	0.14754000
H	6.10759100	0.09873800	0.54025800
C	4.95319400	1.65227900	-0.36427800
C	6.12204200	2.65109300	-0.34325800
C	7.30104100	2.08003400	-1.16902400
H	7.00998100	1.91962700	-2.21328800
C	5.73402500	4.01745800	-0.94009200
H	6.59495600	4.69283700	-0.90060700
H	5.43143000	3.93585900	-1.99050000
H	4.91978100	4.49338100	-0.38100600
C	6.57990100	2.87456400	1.11912700
H	6.91757700	1.94627500	1.59150700



H	7.41555400	3.58308100	1.14696800
H	5.76707500	3.28623900	1.72855200
C	4.40874900	-2.03862100	0.73715100
C	3.49939100	-2.31757700	1.95926400
H	2.44208900	-2.31070700	1.68793300
H	3.73431000	-3.30401300	2.37612400
H	3.66510800	-1.57346100	2.74754200
C	5.87057000	-2.20507800	1.20134700
H	6.12737200	-1.52077700	2.01790500
H	6.01307600	-3.22472700	1.57409300
H	6.58416400	-2.05368400	0.38377900
C	4.14837400	-3.09646100	-0.36494900
H	4.36796900	-4.09740500	0.02494700
H	3.10997900	-3.08246500	-0.70312700
H	4.79860800	-2.92442900	-1.23059200
C	3.69230600	1.96941400	-0.88158500
H	3.50321000	2.95032700	-1.30447800
C	-2.38853400	1.18621000	-0.83708800
C	-4.64695800	1.86755100	-0.24421600
C	-3.35583100	2.17832800	-0.68303100
C	-1.06082800	1.50137900	-1.46515400
H	-0.98582100	2.58594500	-1.63794800
H	-0.99863200	1.00528600	-2.43977400
H	1.32382500	2.43039700	-1.80311700
H	1.21204400	0.79403800	-2.45607500
H	-3.09081700	3.20012200	-0.93385400
C	-5.74358500	2.92825000	-0.05365100
C	-6.22641800	2.90622300	1.41740100
C	-5.24377100	4.35016200	-0.37411000
C	-6.93487000	2.61203900	-0.99109400
H	-6.63374700	1.93058300	1.70189900
H	-5.40582000	3.14198700	2.10509300
H	-7.01640900	3.65124800	1.56564800
H	-4.92434900	4.44784700	-1.41804200
H	-6.05437100	5.06837200	-0.21270100
H	-4.40971300	4.64742200	0.27256200
H	-7.72269100	3.36336000	-0.86415000
H	-6.62294000	2.62197300	-2.04151000
H	-7.37501100	1.63185400	-0.78076700
H	7.65970300	1.12574500	-0.76947900
H	8.14281400	2.78176800	-1.15597400
O	-0.00734900	-2.88486600	0.11509000
O	0.26643700	-1.96980400	-2.44515800
O	-0.53869300	-1.20767900	-3.37990000
H	-0.14648900	-2.90375200	-2.48404400
H	0.06747000	-1.18469900	-4.14532300
O	-0.72477300	-4.35252900	-2.19121100
H	-0.12543300	-5.08462000	-2.41070800
H	-0.75111300	-4.31432300	-1.21579500

**Ts5**

V	-0.03590500	-1.35831500	-0.49456800
O	-1.81119700	-1.11115500	-0.41613100
O	1.78382600	-1.12154200	-0.62145900
N	-0.06382800	1.01869000	-0.74076500
N	0.12659800	-0.57546200	1.50984600
C	0.25799200	-1.43106900	2.54763500
H	0.21461000	-2.48341800	2.29457000
C	0.43719900	-0.99614100	3.85249500
H	0.53409400	-1.72082900	4.65347600
C	0.49197100	0.37750900	4.09813100
H	0.63803500	0.75571400	5.10544300
C	0.35330700	1.25596200	3.02951300
H	0.38498700	2.33047400	3.18236600
C	0.16298100	0.74957600	1.74034200
C	-0.06854100	1.69307800	0.57979300
H	0.68559900	2.48794600	0.60807200
H	-1.04133400	2.17381300	0.73138500
C	-5.05820200	0.39160600	0.18014100
H	-6.03366700	0.14338700	0.57667100
C	-4.08950900	-0.61274700	0.14785300
C	-2.81599300	-0.23520900	-0.37147000
C	-4.39070200	-2.04952600	0.61661100
C	-4.20500700	-3.02731000	-0.57173400
H	-4.89849600	-2.78539800	-1.38537600
H	-3.18802900	-3.00082500	-0.96889500
H	-4.41819500	-4.05124900	-0.24302000
C	-3.45009600	-2.45078800	1.77944400
H	-2.40636200	-2.48698600	1.46286100
H	-3.54128800	-1.74997200	2.61817500
H	-3.72455000	-3.44697300	2.14542300
C	-5.84056300	-2.19827900	1.12157200
H	-6.04415200	-1.56356300	1.99168700
H	-6.57603500	-1.96741500	0.34296600
H	-6.00670500	-3.23611400	1.42812700
C	1.12674300	1.41754100	-1.55182700
C	2.45240900	1.12545900	-0.90831000
C	2.75025200	-0.19953700	-0.53065800
C	4.05928100	-0.54947200	-0.08440600
C	4.97607600	0.49728600	0.02908800
H	5.97261900	0.26478900	0.38108200
C	4.69521200	1.84042400	-0.28928400
C	5.78428700	2.91220800	-0.11710300
C	6.99949300	2.56038000	-1.00998300
H	6.71420700	2.52512500	-2.06741600
C	5.28823600	4.31698200	-0.51069600
H	6.09273100	5.04468100	-0.36199000
H	4.99272600	4.36830000	-1.56498300
H	4.43847100	4.63885000	0.10292300
C	6.23098500	2.95509900	1.36485700
H	6.63891100	1.99547800	1.69916900

H	7.01171200	3.71205100	1.50116600
H	5.39231700	3.21184800	2.02243300
C	4.46096500	-2.00717900	0.22150400
C	3.58017200	-2.60088600	1.34671500
H	2.53163200	-2.66921900	1.05197000
H	3.93029000	-3.60890800	1.59980400
H	3.64559000	-1.98882700	2.25364500
C	5.93055000	-2.12596900	0.67619500
H	6.11614900	-1.58260600	1.60931200
H	6.16560700	-3.17967400	0.85981400
H	6.63184500	-1.76216900	-0.08252500
C	4.31252400	-2.85459500	-1.06767100
H	4.54943700	-3.90539400	-0.86068100
H	3.29260700	-2.78626900	-1.46036300
H	4.99245600	-2.50349700	-1.85147600
C	3.41510600	2.12591900	-0.77348200
H	3.15364600	3.13525500	-1.07382800
C	-2.58648500	1.06464900	-0.87017200
C	-4.85550000	1.70949900	-0.27529300
C	-3.59770500	2.02073100	-0.80668000
C	-1.27866600	1.36704100	-1.54504400
H	-1.24372000	2.43237900	-1.81656200
H	-1.20107800	0.78695100	-2.47132900
H	1.06133400	2.49094000	-1.78410300
H	1.04213600	0.86942100	-2.49681000
H	-3.39605700	3.01247900	-1.19716000
C	-6.00037400	2.73168300	-0.19088800
C	-6.43295300	2.89781200	1.28678800
C	-5.59089700	4.11539000	-0.73092500
C	-7.20294900	2.22376300	-1.02447800
H	-6.78275700	1.95626900	1.72246400
H	-5.60388700	3.26646400	1.90180400
H	-7.25389200	3.62035500	1.35751300
H	-5.31047800	4.07721300	-1.78991500
H	-6.43464000	4.80756700	-0.64259300
H	-4.75525300	4.54552800	-0.16629100
H	-8.02702400	2.94437900	-0.97121100
H	-6.92795100	2.10055400	-2.07803200
H	-7.58012600	1.26247300	-0.66055200
H	7.43553800	1.59119600	-0.74654500
H	7.78301700	3.31812100	-0.89529500
O	0.01932200	-2.94631000	-0.03080900
O	0.03741400	-1.60086800	-2.40600300
O	-1.25596400	-1.82773000	-3.04099300
H	0.62113300	-3.08665600	-2.46112200
H	-1.05081800	-1.52684300	-3.94597200
O	0.85437400	-4.00476600	-2.04282300
H	1.82928500	-4.07676600	-2.02039900
H	0.50841000	-3.72816900	-1.01409400

*Ald*

C	-2.05350100	-1.02040700	0.00005800
C	-2.30309800	0.36377000	0.00005600
C	-0.74217000	-1.46634700	-0.00028300
C	-1.26578100	1.28710400	-0.00038200
H	-3.32939100	0.72183000	0.00111200
C	0.33233200	-0.55462700	-0.00019400
H	-0.52115300	-2.53179200	0.00018900
C	0.06582200	0.84209700	-0.00036400
H	-1.45411900	2.35579100	0.00039100
H	-2.87821700	-1.72603900	0.00120400
O	1.05138400	1.75101000	0.00032900
H	1.90856000	1.25227600	-0.00046700
C	1.70411000	-1.03453700	0.00002600
O	2.70033500	-0.30597400	0.00013200
H	1.83428600	-2.13467100	0.00038200

*Ald\_(H<sub>2</sub>O<sub>3</sub>Br)<sup>+</sup>*

O	3.47623300	-1.08593700	-0.77190100
H	3.97385200	-1.65718100	-0.16309800
Br	1.45095500	-0.46848500	0.39131400
H	4.02639400	-0.26387400	-0.88879600
O	4.94644400	1.15449600	-1.18621800
H	5.04370200	1.33604600	-2.13471300
H	5.84282500	1.22730000	-0.82203800
C	-0.29461800	0.06349600	1.49957000
C	-0.49586400	1.48483400	1.21355700
C	-1.26938000	-0.85866600	0.93740800
C	-1.48061900	1.92164300	0.38140200
H	0.18696400	2.19334000	1.67242800
C	-2.25814100	-0.43562300	0.08744700
H	-1.18280800	-1.91327300	1.18821200
C	-2.37617900	0.97752100	-0.20494900
H	-1.61973500	2.97077000	0.14403400
H	0.04921300	-0.17159800	2.50577000
O	-3.30047200	1.42133800	-1.00289400
H	-3.85324700	0.64154600	-1.32835300
C	-3.21049400	-1.38010100	-0.52537200
O	-4.10323100	-1.00947600	-1.27974800
H	-3.09063000	-2.44808900	-0.27773400

*Ald\_(H<sub>2</sub>O<sub>3</sub>Br)<sup>+</sup>\_1*

O	-2.05659300	1.23263300	2.23842500
H	-2.87168500	0.96595200	2.69151300
Br	-1.92831800	-0.98794400	-0.85306500
H	-2.32445100	1.86238400	1.53323600
O	-2.28880900	2.72163200	-0.10231100

H	-2.33157300	3.69072800	-0.05153600
H	-3.00701700	2.46934500	-0.70521300
C	-0.53061200	-0.42958900	0.46030800
C	0.17107200	-1.62051000	0.97454500
C	0.31101700	0.60254600	-0.16155500
C	1.52499800	-1.72070600	0.96899900
H	-0.43751900	-2.41682000	1.39221100
C	1.67147700	0.50829000	-0.17683500
H	-0.19868500	1.47721400	-0.56265300
C	2.30543000	-0.66947000	0.39382300
H	2.04950600	-2.57955700	1.37424700
H	-1.15316100	0.06988700	1.26343000
O	3.59324500	-0.79577400	0.39142600
H	4.00556800	0.01856700	-0.04658200
C	2.51936200	1.56706600	-0.76295900
O	3.74185300	1.48529800	-0.77998100
H	2.00611700	2.44426900	-1.18981500

*Ald\_(H<sub>2</sub>O<sub>3</sub>Br)<sup>+</sup>\_2*

O	-0.24474700	2.66913700	-0.72480900
H	0.00142900	3.61063600	-0.75312600
Br	-2.36212100	-1.02325600	0.12926700
H	-1.47624700	2.33785600	-0.91188900
O	-2.52422500	1.94689400	-1.15459000
H	-3.24985600	2.48598400	-0.78539900
H	-2.63767000	0.99917900	-0.84947200
C	-0.52057000	-0.52814500	0.39794400
C	-0.19405100	0.34434900	1.44618600
C	0.45614000	-1.01449700	-0.45743100
C	1.12170400	0.77680800	1.60466900
H	-0.95899000	0.67555600	2.14193700
C	1.79018100	-0.61085400	-0.29409500
H	0.20079000	-1.70352600	-1.25742300
C	2.13527300	0.30249400	0.74113300
H	1.40350700	1.42538600	2.42868300
H	0.19828200	2.23971100	0.04237500
O	3.37664000	0.73107300	0.93370000
H	3.96277300	0.29253000	0.25985000
C	2.83597900	-1.12619400	-1.18966400
O	4.01311500	-0.79342500	-1.09988000
H	2.51599900	-1.84254900	-1.96772400

*Ald\_Br*

Br	-2.69387600	-0.26737300	0.00003700
C	-0.83595500	0.17350200	-0.00006400
C	-0.44395900	1.52203700	0.00000800
C	0.11650800	-0.82848200	-0.00013000
C	0.90053100	1.86472800	0.00001500

H	-1.20059800	2.29937900	0.00020900
C	1.48600500	-0.49934000	-0.00022300
H	-0.18115400	-1.87291700	-0.00023100
C	1.88618700	0.86382500	-0.00015700
H	1.21370800	2.90352600	0.00024700
O	3.17491200	1.22658900	-0.00001000
H	3.71415400	0.39401500	0.00026700
C	2.48903700	-1.55492600	-0.00000100
O	3.70555600	-1.35414900	0.00021800
H	2.10568200	-2.59351800	-0.00014500