

Electronic Supplementary Information: Liquid-Jet Photoemission Spectroscopy as a Structural Tool: Site-Specific Acid-Base Chemistry of Vitamin C

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1 Comparison of spectra measured at 400.88 eV and 850 eV photon energy

In Fig. S1, we compare liquid-jet photoemission spectra measured at 400.88 eV photon energy presented in the main text with additional measurements using 850 eV photon energy. The respective kinetic energies of emitted photoelectrons are approx. 105 eV and 455 eV (plus 64 eV from bias), translating into probing of 3–4 and 6 solution layers, respectively. The spectral shapes measured at two different photon energies are very similar, providing essentially identical fitted peak positions. The small discrepancies are attributed to experimental differences in the two measurement campaigns, such as alignment and settings.

2 Evaluation of the agreement between experimental and theoretical spectra using Kullback–Leibler (KL) divergence

We provide a quantitative evaluation of the agreement between our modeled and measured liquid-jet photoelectron spectra of vitamin C solutions at different pH values. We use Kullback–Leibler (KL) divergence, measuring how much is one probability distribution different from another. Specifically, we determine how well is the experimental spectrum represented by a calculated one. The lower the KL divergence value, the better represented the spectrum is, with the KL divergence of 0 corresponding to two identical spectra. The calculated values are presented in Tab. S1, confirming our assignment in the main text, *i.e.*, the calculated spectra shown in red in Fig. 3 having the best agreement with the experiment. However, in comparing the experimental spectrum at pH = 7 with modeled spectra for the deprotonation at C2–O[−] and C3–O[−], we got a lower KL divergence value for C2–O[−] (0.040 vs. 0.071). Nevertheless, we argue that C3–O[−] is the real deprotonation center based on examining the similarity in spectral features: the magnitude of separation between the main and the smaller peak and the appearance of the low-energy shoulder. We show in Tab. S1 in parentheses for those two cases how the results change in favor of C3–O[−] if we shift the experimental spectrum by −0.2 eV to match the position of the main peak with those two calculated spectra.

Table S1 KL divergence values for comparing the agreement between an experimental spectrum at the indicated pH value and the respective calculated spectrum. Values in parentheses are contained using an experimental spectrum at pH = 7 shifted by −0.2 eV.

Calculated spectrum	KL divergence
pH = 2	
A tautomer	0.014
B tautomer	0.059
pH = 7	
C2–O [−]	0.040 (0.073)
C3–O [−]	0.071 (0.016)
C5–O [−]	0.109
C6–O [−]	0.130
pH = 13	
C2–O [−] + C3–O [−]	0.070
C2–O [−] + C5–O [−]	0.161
C2–O [−] + C6–O [−]	0.119
C3–O [−] + C5–O [−]	0.108
C3–O [−] + C6–O [−]	0.094
C5–O [−] + C6–O [−]	0.123

3 Cartesian coordinates of optimized structures

3.1 Fully protonated molecule of vitamin C

A tautomer

C	1.833065	0.670477	0.707193
C	0.915838	-0.103747	-0.199674
C	-0.142393	-0.527446	0.501520
C	0.011848	-0.077940	1.874804
O	1.169465	0.625502	1.985642
O	1.133648	-0.317669	-1.502978
O	-1.200485	-1.257628	0.080709
O	-0.734449	-0.269994	2.812072
C	2.049954	2.135344	0.308542
C	3.016700	2.822966	1.261162
O	3.323867	4.099451	0.721887
O	0.817423	2.817154	0.193479
H	-1.796575	-1.407220	0.835359
H	2.797826	0.163969	0.817201
H	2.559015	2.918376	2.254106
H	3.923980	2.213324	1.356227
H	3.905842	4.568354	1.337646
H	2.492619	2.155374	-0.692935
H	0.440798	2.947805	1.078745
H	2.003936	0.002835	-1.789838

B tautomer

O	1.878940	0.590637	0.781638
C	0.991198	-0.124044	-0.118663
C	-0.166194	-0.573402	0.766009
C	0.152485	-0.135366	2.079718
C	1.337755	0.526879	2.007657

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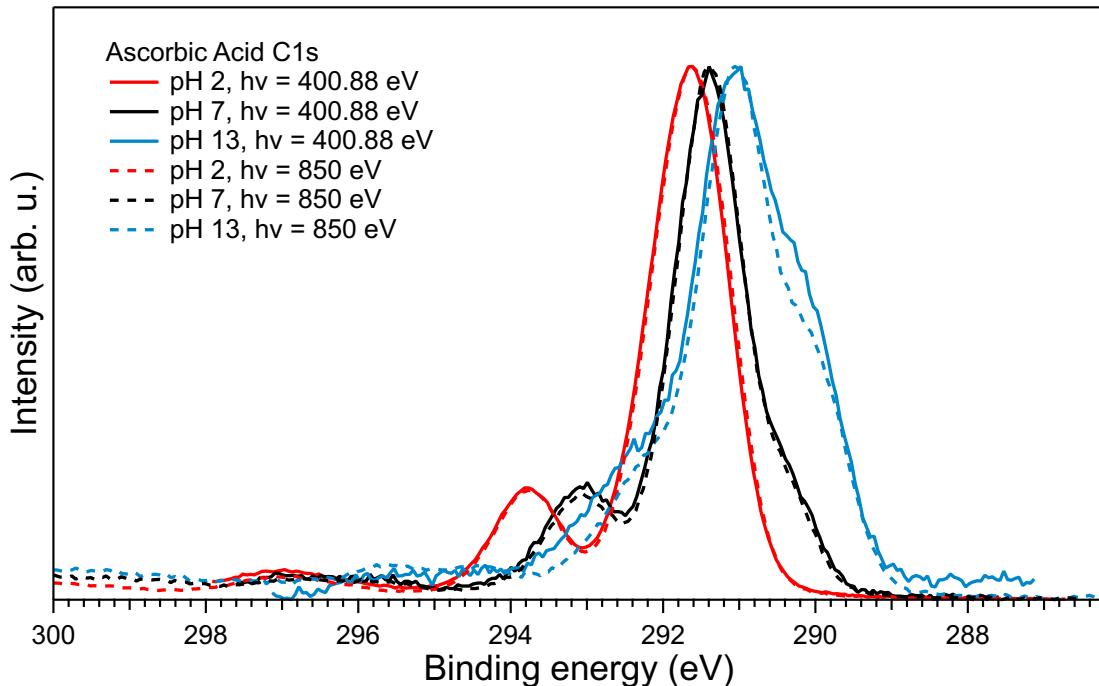


Fig. S1 Comparison of C 1s liquid-jet photoemission spectra of aqueous solutions of vitamin C (ascorbic acid) measured using two different photon energies, 400.88 eV and 850 eV. Results for solutions pH values of 2, 7, and 13 are shown.

C	0.570195	0.794845	-1.260077
O	-0.099885	1.939160	-0.762650
O	-1.159107	-1.194055	0.383904
O	-0.592567	-0.321155	3.204582
O	1.995918	1.104385	2.990715
C	1.742088	1.147612	-2.162276
O	1.230366	1.836078	-3.293547
H	-1.387190	-0.824963	2.958354
H	1.539774	-0.993303	-0.490759
H	2.461053	1.774468	-1.618181
H	2.250879	0.224559	-2.466480
H	1.967822	2.085874	-3.869228
H	-0.173679	0.246519	-1.846717
H	0.544829	2.526232	-0.336017
H	2.822057	1.507285	2.666294

O	2.381108	-0.606555	2.728369
C	1.678086	1.264921	-1.977234
O	1.450613	2.467196	-2.696815
H	0.712700	-1.020642	-0.975242
H	2.666898	1.276107	-1.500518
H	1.627179	0.396862	-2.646150
H	2.152384	2.576963	-3.354938
H	-0.378969	1.239377	-1.412818
H	1.527971	2.207566	0.440169
H	-1.894942	-0.554158	-0.518592
H	-1.021795	0.618684	3.811167
O	-1.369803	1.507260	4.106930
H	-0.807525	1.793067	4.842445
H	-1.317423	2.610540	2.636084
O	-1.319656	3.188487	1.843665
H	-0.676932	2.792730	1.224081
H	-3.191315	1.150481	4.464638
O	-4.076216	0.732176	4.462953
H	-3.935938	-0.065010	3.906147
H	-2.250738	-1.255037	3.004375
O	-3.221526	-1.417435	2.877293
H	-3.350388	-1.229220	1.934195
H	-0.492588	-2.806939	3.452553
O	-0.171390	-3.636595	3.860302
H	0.469017	-3.290684	4.510836

3.2 Singly deprotonated molecule of vitamin C with six explicit water molecules

Deprotonated at C2-O⁻

O	1.844723	-0.286673	0.575607
C	0.650470	-0.226850	-0.221966
C	-0.443520	-0.482616	0.767605
C	0.051710	-0.642734	2.011771
C	1.514811	-0.521557	1.879217
C	0.593265	1.138796	-0.919843
O	0.649051	2.194543	0.026480
O	-1.757352	-0.509257	0.440683
O	-0.557426	-0.872713	3.165756

H 0.527703 -1.164366 4.583697
O 1.201657 -1.516986 5.212734
H 2.021383 -1.344843 4.719316

Deprotonated at C3-O⁻

C 1.330033 0.016732 1.892220
C 1.825876 -0.384786 0.685862
C 0.748788 -0.831888 -0.155158
O -0.436635 -0.702261 0.534031
C -0.173701 -0.146958 1.834593
O 3.134941 -0.409610 0.273260
O 0.751311 -1.275980 -1.290767
C -0.948766 1.163658 1.983968
O -0.639180 2.051953 0.912967
O 1.944364 0.476888 2.934476
C -2.444614 0.924009 2.090912
O -3.071984 2.163732 2.386960
O 3.742323 1.981881 1.345920
H 3.521150 0.481208 0.487891
H -0.512065 -0.868056 2.585802
H -2.827733 0.508790 1.149587
H -2.630183 0.195826 2.890344
H -4.030134 2.029203 2.424341
H -0.603790 1.668144 2.890358
H -0.941188 1.654903 0.078829
H 3.072914 2.613251 0.987808
H 3.312717 1.615795 2.147338
H 0.849755 3.031677 0.646629
O 1.662515 3.540252 0.425608
H 1.570567 4.396781 0.868638
H 1.521489 2.169516 3.672201
O 1.313237 3.020410 4.107978
H 1.176156 2.790239 5.051936
H 1.522594 -0.126800 4.531887
O 1.396545 -0.389112 5.477973
H 0.660180 -1.018491 5.492435
H 3.463497 -0.745743 3.095383
O 4.140513 -1.388722 2.803780
H 4.057529 -1.342476 1.833035
H 1.623006 2.200789 7.344756
O 0.925625 2.000622 6.703161
H 1.096598 1.079514 6.386603

Deprotonated at C5-O⁻

O 1.982086 0.978682 0.890931
C 1.405661 -0.113566 0.143700
C 0.399305 -0.696189 1.092453
C 0.361978 0.037959 2.208587
C 1.355584 1.095306 2.082788
C 0.787026 0.419471 -1.169244
O -0.168665 1.391465 -0.927966
O -0.398133 -1.742633 0.805471
O -0.413982 -0.112845 3.305206
O 1.624570 1.958924 2.894684
C 1.927782 0.874897 -2.082562
O 1.398317 1.242100 -3.363002
H -0.213517 0.607843 3.928022
H 2.214798 -0.820571 -0.069286

H 2.447342 1.735183 -1.646280
H 2.647683 0.059237 -2.204676
H 2.020532 0.969339 -4.052385
H 0.337638 -0.463994 -1.663343
H -0.070908 -2.250892 0.044332
H -1.135797 2.191761 0.539341
O -1.944540 2.412803 1.049735
H -2.493608 1.622711 0.877542
H 0.536415 2.883412 -0.675195
O 0.883064 3.824621 -0.617463
H 1.683663 3.782573 -0.074181
H 1.164896 3.074800 -3.513363
O 0.876990 4.003201 -3.378781
H 0.991425 4.136305 -2.409850
H -1.080519 2.167538 -2.197862
O -1.591874 2.764013 -2.807930
H -0.891389 3.342162 -3.178061
H -2.715152 3.663513 -0.107556
O -3.024062 4.180677 -0.881766
H -2.563702 3.746031 -1.636829
H -1.645921 0.502621 -0.688443
O -2.498869 0.067674 -0.412095
H -2.223957 -0.746249 0.039460

Deprotonated at C6-O⁻

O 1.841074 0.232596 0.874856
C 0.815771 -0.008675 -0.106698
C -0.393680 -0.385339 0.705990
C -0.077399 -0.303381 2.007029
C 1.313824 0.088286 2.114677
C 0.596217 1.219925 -0.985211
O 0.327148 2.320887 -0.137035
O -1.567036 -0.703819 0.170339
O -0.861265 -0.534011 3.092671
O 1.963190 0.260100 3.131067
C 1.746704 1.468046 -1.967853
O 1.336222 2.256150 -3.060682
H -0.323042 -0.398775 3.891838
H 1.147695 -0.846261 -0.728016
H 2.576104 1.943547 -1.421257
H 2.110214 0.489709 -2.324615
H -0.293827 0.996268 -1.587868
H 0.058626 3.082565 -0.699222
H -1.522782 -0.801714 -0.824186
H 0.001399 1.439246 -3.738816
O -0.660315 0.840267 -4.193852
H -0.157516 0.518364 -4.962938
H 0.418093 3.517531 -2.583766
O -0.116023 4.215188 -2.087339
H -0.998746 4.223764 -2.485779
H 2.498959 3.299937 -3.507289
O 3.240725 3.894387 -3.850195
H 2.955451 4.807250 -3.699259
H 3.219811 3.598745 -7.048803

O	3.619208	3.006956	-6.394592
H	3.514771	3.454687	-5.516209
H	1.848106	1.423430	-4.548479
O	1.980645	0.934037	-5.398118
H	2.535917	1.538311	-5.934331
H	-1.199246	-0.404688	-3.140745
O	-1.461500	-1.094616	-2.470973
H	-2.269884	-1.513119	-2.803224

H	3.746996	0.654433	-0.293554
H	5.245368	0.741502	0.167581
H	1.731503	-0.621248	-2.760213
H	3.225606	-0.902050	-3.223223
H	1.904244	-3.677788	-0.908156
H	2.914170	-4.797380	-0.478836
H	0.585684	-2.160690	-1.850893
H	1.531581	-2.738945	-2.891189
H	-1.320664	-0.598141	-2.133211
H	-2.070426	0.447293	-2.959012
H	0.004766	0.999462	-2.483428
H	0.346742	2.454656	-2.883671
H	2.737033	0.812045	-4.270153
O	3.303894	1.610907	-4.326936
H	2.929896	2.222154	-3.653667

3.3 Doubly deprotonated molecule of vitamin C with 12 explicit water molecules

Deprotonated at C2-O⁻ and C3-O⁻

O	0.041558	-0.353340	1.953593
C	1.066057	0.648626	1.825276
C	1.343638	0.735095	0.343174
C	0.538606	-0.159436	-0.305178
C	-0.256181	-0.838143	0.702603
C	0.569242	1.943351	2.471599
O	-0.643035	2.381104	1.877712
O	2.267640	1.543654	-0.114416
O	0.416585	-0.447573	-1.608254
O	-1.088974	-1.725119	0.577269
C	0.440041	1.792513	3.979256
O	0.171679	3.074597	4.535266
O	2.456388	-4.009308	-0.151691
O	2.289889	-0.914382	-3.527011
O	4.951939	-0.252658	-3.006235
O	0.930258	-3.034986	-2.181145
O	-2.189494	-0.437165	-2.574731
O	2.057777	3.057802	-2.298016
O	3.694566	3.278360	1.362109
O	-0.348455	1.776433	-2.988343
O	6.086072	2.024111	1.089442
O	4.182651	-2.205707	1.134163
O	4.611474	0.167693	-0.325311
H	1.953666	0.291133	2.360405
H	-0.369381	1.090923	4.218436
H	1.377942	1.389926	4.382761
H	0.047968	2.981637	5.490977
H	1.302308	2.727738	2.264594
H	-1.298589	1.670402	1.968983
H	4.642596	0.570126	-3.442988
H	4.936046	-0.065585	-2.036935
H	2.128910	2.494716	-1.473319
H	2.262686	3.967856	-2.037670
H	3.105894	2.668593	0.835987
H	3.626673	4.150774	0.946681
H	6.422723	1.729563	1.948563
H	5.282470	2.572683	1.277590
H	4.318947	-1.400897	0.589864
H	3.577642	-2.790735	0.629467

Deprotonated at C2-O⁻ and C5-O⁻

C	1.892663	0.317759	0.960959
O	1.079259	-0.192794	0.009766
C	-0.159899	-0.634723	0.610590
C	0.000602	-0.267906	2.057085
C	1.217508	0.276772	2.267349
C	-1.365735	-0.048673	-0.143482
C	-1.241389	-0.451076	-1.616071
O	-2.517149	-0.313098	-2.256648
O	-0.885877	-0.606321	3.014373
O	1.793491	0.711399	3.385841
O	3.012338	0.722173	0.689563
O	-1.550274	1.319215	0.037468
O	1.555039	4.442794	1.385381
O	2.461585	4.292349	5.015646
O	0.253442	2.619917	4.392008
O	1.558009	-1.180306	5.515172
O	4.029275	-0.657126	4.198463
O	3.321897	2.814288	2.726019
H	-0.185807	-1.726375	0.504172
H	-0.503900	0.191426	-2.109939
H	-0.912015	-1.494008	-1.695669
H	-2.463556	-0.716317	-3.135568
H	-2.231503	-0.614568	0.252880
H	-1.813267	-0.259502	2.867751
H	2.771042	2.026096	2.999959
H	3.847965	2.458547	1.990380
H	2.210070	3.889851	1.877985
H	2.044336	5.212671	1.059856
H	3.030421	3.957978	4.298381
H	1.623373	3.799590	4.887043
H	0.794160	1.830046	4.093892
H	-0.256983	2.323411	5.160964
H	1.347866	-0.519007	4.822998
H	2.510327	-1.324258	5.361017
H	3.310246	-0.129192	3.769707
H	4.407255	-1.212752	3.501270

H	-2.198477	2.265982	-1.387154	H	-3.752140	-1.352265	0.949975
O	-2.671994	2.510433	-2.217999	H	-3.827628	-1.748781	2.472861
H	-2.878986	1.618621	-2.553186	H	1.162237	0.728509	4.730975
H	-3.235739	1.305935	0.275128	O	0.964408	0.698690	5.703125
O	-4.187790	1.126350	0.535663	H	0.151396	1.232051	5.757875
H	-4.640140	1.981646	0.502698	H	3.015119	2.964331	5.327600
H	-3.780152	0.606285	2.206447	O	3.219540	2.298717	6.024924
O	-3.264290	0.580132	3.046407	H	2.391625	1.771383	6.106470
H	-2.807470	1.458278	3.020869	H	3.233909	0.886295	3.418461
H	-1.516450	2.205984	1.568618	O	4.134119	0.811511	3.823084
O	-1.742913	2.731695	2.381903	H	3.994819	1.191905	4.719957
H	-0.965891	2.721220	2.980475	H	4.983385	2.160603	3.075883
H	-0.259565	2.381381	-0.419027	O	5.226137	3.048130	2.704670
O	0.369026	3.086059	-0.735012	H	5.997223	3.351621	3.205903
H	0.777022	3.507880	0.053130	H	2.215607	2.951604	3.315609
H	1.478717	2.615895	-1.963907	O	2.675449	3.749791	3.674594
O	2.113078	2.368348	-2.685129	H	3.574945	3.712370	3.282603
H	1.850036	2.894248	-3.453604	H	0.025875	2.285274	3.793321
Deprotonated at C2–O[−] and C6–O[−]				O	-0.845837	2.455960	4.216753
C	1.744470	0.670955	0.760540	H	-1.398449	1.759906	3.818214
O	0.989772	0.050420	-0.188838	Deprotonated at C3–O[−] and C5–O[−]			
C	-0.305677	-0.248282	0.354819	C	1.756268	0.380589	2.296165
C	-0.211961	0.212331	1.776427	C	2.248465	0.158201	0.883385
C	0.991186	0.775386	2.020441	C	1.412511	-0.747417	0.301999
C	-1.412284	0.430862	-0.448787	C	0.411201	-1.151243	1.255080
C	-1.623412	-0.199260	-1.830186	O	0.599002	-0.468390	2.422123
O	-2.912274	0.064699	-2.336636	O	3.315575	0.742330	0.427789
O	-1.243063	0.100788	2.640130	O	1.460398	-1.361280	-0.922829
O	1.491998	1.332024	3.115889	O	-0.487188	-1.973844	1.149450
O	2.879407	1.036611	0.512083	C	1.418535	1.830164	2.670675
O	-1.139212	1.820371	-0.502115	C	1.042236	1.890647	4.150064
O	-4.576157	-1.586278	-5.700791	O	1.145911	3.249187	4.605421
O	-4.095844	-2.333752	-3.019269	O	0.446943	2.402829	1.853320
O	-3.205494	-1.526443	1.764091	O	2.950717	2.266119	-1.733381
O	-3.399485	2.605091	-1.888065	O	3.986307	4.979670	1.730154
O	-2.906776	0.420988	-4.941362	O	5.127509	2.408114	1.739997
O	-4.592285	-0.987966	-0.508478	O	3.506320	-3.340540	-0.644593
H	-0.444108	-1.333526	0.293215	O	4.951981	-0.917756	-0.925224
H	-0.843626	0.180128	-2.509053	O	3.034617	-0.255519	-2.831732
H	-1.472851	-1.288018	-1.738116	H	1.985798	-0.843241	-1.589347
H	-2.335411	0.263274	0.122028	H	2.512419	0.000994	2.994217
H	-1.914552	2.268329	-0.907818	H	0.017289	1.528739	4.288211
H	-1.975404	-0.473905	2.286266	H	1.724029	1.269580	4.742466
H	-3.999675	-0.489084	-1.143711	H	1.013782	3.260184	5.565087
H	-4.837415	-1.773534	-1.029435	H	2.379564	2.368241	2.575965
H	-3.334595	1.623082	-2.112603	H	3.012180	0.717406	-2.697097
H	-4.203049	2.715573	-1.358877	H	3.882372	-0.533090	-2.423280
H	-2.886594	0.333061	-3.933892	H	3.162606	1.783060	-0.886381
H	-3.140198	1.340724	-5.133937	H	3.609620	2.969234	-1.835923
H	-5.466157	-1.261295	-5.900792	H	4.370777	5.562669	1.059258
H	-4.020383	-0.783072	-5.529420	H	3.013676	4.950854	1.543078
H	-3.607848	-1.488610	-2.853801	H	4.458546	1.813608	1.335080
H	-4.393919	-2.254968	-3.949822	H	4.728464	3.304646	1.724188

H	2.664934	-2.851610	-0.740660
H	4.175950	-2.628952	-0.697220
H	4.444927	-0.286291	-0.344887
H	5.894287	-0.726060	-0.808002
H	-0.930122	3.219438	2.579441
O	-1.783991	3.658683	2.830252
H	-1.491105	4.531704	3.157650
H	0.451203	4.886339	4.040729
O	0.045748	5.676664	3.625690
H	0.442657	5.674476	2.729036
H	0.977871	3.890989	1.563081
O	1.293656	4.820721	1.299166
H	1.066950	4.855387	0.353511
H	0.490623	2.625024	0.096111
O	0.420233	3.004377	-0.818880
H	1.273104	2.793736	-1.255313
H	-1.085848	2.159231	-1.435026
O	-1.936670	1.669757	-1.480814
H	-2.106988	1.461918	-0.535525
H	-1.077818	1.480525	1.496541
O	-2.031492	1.295504	1.295336
H	-2.481440	2.060572	1.694766

Deprotonated at C3–O[−] and C6–O[−]

C	0.441723	0.520084	1.215997
C	1.397631	0.347345	0.057986
C	0.649508	0.252864	-1.076702
C	-0.743994	0.383847	-0.734310
O	-0.866838	0.554455	0.621827
O	2.687867	0.299819	0.246573
O	1.009899	0.080308	-2.380750
O	-1.735732	0.366343	-1.446336
C	0.683074	1.789299	2.027759
C	-0.049847	1.819847	3.371899
O	0.524933	2.756172	4.240345
O	0.420864	2.950747	1.244382
O	4.980921	1.808014	-2.969366
O	3.912376	2.703361	-0.662793
O	4.323171	0.918710	2.532813
O	3.277863	-2.301885	1.134948
O	5.687102	2.961811	1.431261
O	3.648237	-0.498819	-2.225700
H	1.975940	-0.141822	-2.435254
H	0.488855	-0.352153	1.877244
H	-1.116937	2.036644	3.190544
H	-0.002413	0.807163	3.807416
H	1.755102	1.826515	2.235929
H	-0.514858	2.934144	0.985814
H	4.166731	0.247706	-2.608909
H	3.545407	-0.278281	-1.271056
H	4.608500	2.275967	-3.731234
H	4.624487	2.261458	-2.159515
H	3.432490	1.909621	-0.336923
H	4.595832	2.888289	0.024709

H	3.658589	0.692304	1.846729
H	3.839270	1.232105	3.337784
H	3.083004	-1.390865	0.822369
H	3.066002	-2.880817	0.388402
H	6.595889	2.695681	1.227991
H	5.271753	2.197607	1.914332
H	1.431196	3.940482	3.446788
O	1.961261	4.678990	3.027604
H	1.607884	4.716579	2.125054
H	-0.396797	4.007938	4.811231
O	-0.769326	4.760903	5.365405
H	-1.421902	5.221802	4.818550
H	0.421261	2.469125	5.906706
O	0.434591	2.488238	6.907128
H	-0.219647	3.169067	7.130829
H	2.637678	4.576873	6.350648
O	2.933413	3.753469	6.804788
H	2.088045	3.298559	7.023538
H	2.076587	2.113529	4.554628
O	2.990845	1.779765	4.776274
H	3.297093	2.434015	5.440609
H	0.829210	5.674122	5.562804
O	1.771180	5.941195	5.461886
H	1.954238	5.717480	4.522175

Deprotonated at C5–O[−] and C6–O[−]

C	2.251020	-0.322709	0.109142
O	1.306723	-0.699275	-0.780486
C	0.095485	-1.054721	-0.076507
C	0.458903	-0.901894	1.372098
C	1.722383	-0.458118	1.451151
C	-1.079354	-0.145044	-0.472036
C	-1.449654	-0.334361	-1.952173
O	-2.778608	0.057013	-2.230161
O	-0.371632	-1.117728	2.387776
O	2.402738	-0.042438	2.556921
O	3.360044	0.062202	-0.220140
O	-0.883181	1.174309	-0.092053
O	-4.628065	-1.118464	-3.799848
O	-4.150643	-1.562344	-0.443584
O	-3.064908	-1.234565	2.015916
O	-2.770618	2.772185	-2.740671
O	-2.584030	0.930111	-4.831723
O	-5.518697	0.707894	-1.845977
H	3.324317	0.139338	2.301900
H	-0.127384	-2.096322	-0.329422
H	-0.736280	0.240488	-2.563529
H	-1.312671	-1.397851	-2.215162
H	-1.921835	-0.579941	0.087561
H	-1.320381	-1.248739	2.123012
H	-4.546467	0.747988	-1.735540
H	-5.605135	0.122267	-2.626566
H	-2.750821	1.856427	-2.346930
H	-2.753571	2.567401	-3.696771
H	-2.637655	0.505528	-3.934987

```

H -3.342188 0.566710 -5.314189 $basis
H -3.840574 -0.899222 -3.230987 H 0
H -4.817724 -2.058137 -3.663305 aug-cc-pVTZ
H -3.620455 -0.996002 -1.071393 ****
H -5.040906 -1.174681 -0.486321 C 0
H -3.523558 -1.459945 1.160702 aug-cc-pCVTZ
H -3.529663 -1.702908 2.726565 ****
H 0.040584 1.836662 1.134254 O 0
O 0.504303 2.415174 1.817858 aug-cc-pCVTZ
H 1.179103 1.861441 2.243255 ****
H 0.599325 4.193809 -0.635332 $end
O 1.026032 4.628973 0.140233
H 0.953523 3.945288 0.838050 $pcm
H -0.361329 2.277264 -1.184108 THEORY IEFPCM
O -0.136013 3.044643 -1.797223 RADII UFF
H -0.994509 3.212007 -2.236606 vdwScale 1.1
H -4.509102 3.411592 -2.480372 NonEquilibrium
O -5.477707 3.490315 -2.343649 $end
H -5.740555 2.560504 -2.183699
H -2.244131 1.528937 0.793324 $solvent
O -3.043358 1.626033 1.399757 Dielectric 78.39
H -3.181828 0.731905 1.764533 OpticalDielectric 1.78
H -0.869673 2.986237 2.932726 $end
O -1.755029 3.160292 3.316191
H -2.343135 2.650477 2.711664 $end

```

4 Sample input for calculating core-level ionization energies using the maximum overlap method within the Q-Chem 6.0 software

```

$molecule
0 1
C 1.825823 0.674620 0.709209 $basis
C 0.912154 -0.096275 -0.194739 H 0
C -0.136831 -0.526982 0.504213 aug-cc-pVTZ
C 0.016518 -0.081475 1.875330 ****
O 1.168415 0.623924 1.985358 C 0
O 1.134066 -0.303772 -1.493924 aug-cc-pCVTZ
O -1.191973 -1.256956 0.089733 ****
O -0.721961 -0.279053 2.806705 O 0
C 2.048409 2.132593 0.306830 aug-cc-pCVTZ
C 3.010325 2.815911 1.258550 ****
O 3.344138 4.080424 0.714940 $end
O 0.825702 2.823450 0.179275
H -1.773955 -1.411373 0.845365
H 2.789155 0.171351 0.809316
H 2.541475 2.923753 2.240192
H 3.902363 2.194827 1.372274
H 3.894457 4.554854 1.343548
H 2.499691 2.140598 -0.686906
H 0.445142 2.959890 1.053561
H 1.988809 0.038980 -1.777962
$end

$rem
METHOD CAM-B3LYP $pcm
BASIS General THEORY IEFPCM
MAX_SCF_CYCLES 129 RADII UFF
solvent_method pcm vdwScale 1.1
PCM_PRINT 1 StateSpecific Marcus
MEM_TOTAL 16000 $end
$end

$solvent

```

Dielectric	78.39	H	-1.177277458294119	-1.6188882045294117	-1.3261760555294118
OpticalDielectric	1.78	H	0.29290603147058825	-1.8568991045294116	-2.1440689555294115
\$end		H	-1.2508337735294119	-3.7217844045294122	-0.89572518552941183
		H	1.364326314705880	-1.9482711045294119	0.26207672447058822
		H	8.0600231470588257E-002	-1.3755826045294115	2.016129344705883
		H	1.8690693314705882	1.0363397354705883	2.664882444705883
\$occupied		C	0.78058292982352961	7.9318864117647048E-002	-0.12746648405882346
1:46		C	1.1014151298235295	0.98591657411764699	1.0242491959411764
1:6 8:46		C	0.18424712982352931	1.986336641176470	0.97304057594117654
\$end		C	-0.81909626017647064	1.7089933641176469	-5.408536505882348E-002
		O	-0.38759958017647056	0.63062646411764711	-0.76649163405882337
		O	2.14339622982352956	0.68060480411764712	1.7600544959411766
		O	6.9831298235294437E-003	2.9713161641176473	1.8952759959411765
		O	-1.8144461801764706	2.3684504641176471	-0.3138145105882349
		C	0.45971342982352947	-1.430456385823531	0.161929809594117654
		C	-0.18721177017647062	-2.0098970358823527	-1.1663659040588235
		O	-0.24261807017647063	-3.4615343358823529	-1.0125060405882345
		O	-0.59206645017647064	-1.4074428358823530	1.1886532959411764
		H	-0.32655213017647056	3.7902654641176472	1.4762790959411765
		H	1.61830902982352959	0.2215994211764705	-0.75258908405882341
		H	-1.2349894071764707	-1.5943265358823531	-1.2561124040588236
		H	0.45304192982352931	-1.7287704358823530	-2.1161791040588236
		H	-1.14318069701764705	-3.7909944358823531	-0.91612736405882345
		C	1.35895712982352959	-1.9805829358823528	0.43573231594117651
		H	-0.38125618017647056	-0.97781403588235311	1.9114545959411764
		H	2.088532998235296	1.1333170041176470	2.5837204959411766
		C	0.91452563929411745	0.13421282411764701	-0.23194648911764706
		C	1.094305294117647059	0.978492111764703	1.03183264088223530
	7.0955757647058748E-002	C	0.30341725847058827	1.84000367017647058	1.15437321594117651
		C	0.11274803929411759	1.89377032411764649	0.43573231594117651
		O	-0.70181134070588258	1.7580566241176472	-0.14074598411764708
		C	-0.19742125070588257	0.79968446411764704	-0.90028348911764700
		O	2.1070901329941175	0.57885844411764709	1.79413634088223530
		O	-0.14216986070588256	2.8474078241176470	2.0348067408823529
		O	-1.642593867058825	2.411854421176472	-0.4666542911764712
		C	0.47031513929411739	-1.279323758823530	9.432279088235920E-002
		H	0.16140822576470588	-1.3589571298235295	-1.0829481091176472
		H	-0.1266506423529412	-1.9444826758823530	-0.73391251911764710
		H	-1.617165152941177	-3.3140110758823531	-1.18599754088223529
		H	-0.45286405764705884	-3.63507447070588250	3.3063837241176470
		H	-1.927770629352941	-0.93721782070588255	1.78649374088223529
		H	-1.0927678723529413	-1.0436887492352942	-0.90410308911764700
		H	-1.4429387576470589	0.33872569076470593	-1.192653591176470
	8.080357647057224E-003	H	-1.81562131529411779	1.773040239941174	-2.0605802591176472
		H	-0.99088341529411772	-1.4148616758823529	-1.3292485591176471
		H	2.0868538707647059	-3.6236330758823532	2.4565160408823528
		H	2.197245576470590	1.2921216647058822	1.2697278541176469
		C	0.88214317505882356	0.17377727352941175	-0.23194648911764706
		C	0.11184879750588235	0.10434523235294118	0.9609843702941177
		C	0.10618187505882348	1.9701581835294117	1.0605659702941175
		C	-0.72027704494117650	0.1596687835294117	0.2114610970588237
		O	-0.17044442494117651	-0.94732792970588231	0.83111574176470571
		O	0.75699184352941173	1.7917824702941176	0.10663871417647055
	-8.2585524941176463E-002	C	0.28365564835294119	0.20792905702941176	0.10207044176470581
		O	-0.15769318049411765	-0.534644644970588232	-0.714618438323529425
		C	0.43990497505882353	-1.3274668164705883	5.0243985294117645E-002
		C	-0.257477042494117641	-2.0753571164705882	-0.20883673823529425
		O	-0.29518242494117641	-3.4905279164705885	0.20498012417647056
		O	-0.53210322494117646	-1.3269045164705882	-0.11728125823529423
		H	-0.74509815494117648	1.8918322072941175	0.1465643592941176475
		H	1.7739962750588236	-0.80709572970588228	-0.228972028323529428
		H	-1.322650909411764	-1.7024893164705881	-0.228972028323529434
		H	-0.2692398750588236	-2.187028164705882	-0.339671870588235
		H	-1.0059060049411765	-3.7651588164705885	-0.788887294117648
		H	1.3501432750588234	-1.936872164705874	1.8117228125823529423
		H	-0.32403540494117644	-0.89688281647058821	-1.25931075882352942
		H	2.1172837750588234	1.2529332235294117	0.22711404176470573
		C	0.76646123147058831	0.10113704547058833	-0.70955041823529426
		C	1.0400114314705882	0.90740785547058833	-0.39654688823529427
		C	0.19764123147058821	1.9667360954705884	-1.3704917015882351
		C	-0.67508914852941182	1.8822859954705882	-1.3704917015882351
		O	-0.36108366852941187	0.81206989547058828	0.79991060120000013
		O	2.0207937314705884	0.5395448024705884	6.0371284882352994E-002
		O	0.19524303147058819	2.9659288954705882	0.10882917012000002
		O	-1.613878895294119	2.6265205954705881	0.85814900488235302
		C	0.45512123147058814	-1.3789583045294118	0.2185807012000006
		C	-0.21774226852941192	-2.0479463045294120	1.9082146648823530
		O	-0.33042276852941188	-3.4559775045294119	1.9284905941176466
		O	-0.44002125852941187	-1.5269543045294118	-1.2622420705882353
		H	-0.45823720852941185	3.6343889954705881	-1.1489340965882353
		H	1.5564085314705880	0.17138795547058833	-2.0251347965882354
		H	-1.0133391555294116	-3.8990135705882354	-1.2990552965882352
		C	0.78058292982352961	7.9318864117647048E-002	-0.2274799431176475
		C	1.1014151298235295	0.98591657411764699	1.9215442034117647
		C	0.18424712982352931	1.986336641176470	1.0803533259941176
		C	-0.81909626017647064	1.7089933641176469	-0.13655068900588235
		O	-0.38759958017647056	0.63062646411764711	-0.93555264400588245
		O	2.14339622982352956	0.68060480411764712	1.9851942259941175
		O	6.9831298235294437E-003	2.9713161641176473	-0.17138145105882349
		O	-1.8144461801764706	2.3684504641176471	1.8952759959411765
		C	0.45971342982352947	-1.430456385823531	0.161929809594117654
		C	-0.18721177017647062	-2.0098970358823527	-1.1663659040588235
		O	-0.24261807017647063	-3.4615343358823529	-1.0125060405882345
		O	-0.59206645017647064	-1.4074428358823530	1.1886532959411764
		H	-0.32655213017647056	3.7902654641176472	1.4762790959411765
		H	1.61830902982352959	0.2215994211764705	-0.75258908405882341
		H	-1.2349894071764707	-1.5943265358823531	-1.2561124040588236
		H	0.45304192982352931	-1.7287704358823530	-2.1161791040588236
		H	-1.14318069701764705	-3.7909944358823531	-0.91612736405882345
		C	1.35895712982352959	-1.9805829358823528	0.43573231594117651
		H	-0.38125618017647056	-0.97781403588235311	1.9114545959411764
		H	2.088532998235296	1.1333170041176470	2.5837204959411766
		C	0.91452563929411745	0.13421282411764701	-0.23194648911764706
		C	1.094305294117647059	0.978492111764703	1.03183264088223530
		C	0.11274803929411759	1.89377032411764649	1.15437321594117651
		O	-0.70181134070588258	1.7580566241176472	-0.14074598411764708
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		O	2.1070901329941175	0.57885844411764709	1.79413634088223530
		O	-0.14216986070588256	2.8474078241176470	2.03480674088223529
		O	-1.642593867058825	2.411854421176472	-0.4666542911764712
		C	0.47031513929411739	-1.279323758823530	9.432279088235920E-002
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		H	-0.1266506423529412	-1.9444826758823530	-0.73391251911764710
		H	-1.617165152941177	-3.3140110758823531	-1.18599754088223529
		H	-0.45286405764705884	-3.63507447070588250	3.3063837241176470
		H	-1.927770629352941	-0.93721782070588255	1.78649374088223529
		H	-1.0927678723529413	-1.0436887492352942	-0.90410308911764700
		H	-1.4429387576470589	0.33872569076470593	-1.192653591176470
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		H	-0.99088341529411772	-1.4148616758823529	-1.3292485591176471
		H	2.0868538707647059	-3.6236330758823532	2.4565160408823528
		H	2.197245576470590	1.2921216647058822	1.2697278541176469
		C	0.88214317505882356	0.17377727352941175	-0.23194648911764706
		C	0.11184879750588235	0.10434523235294118	0.9609843702941177
		C	0.10618187505882348	1.9701581835294117	1.0605659702941175

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O	-1.3323371762000000	2.7994317648823528	-0.48497940400588235	C	0.73795154582352995	0.1297688270000003	-0.21453671117647061
C	0.3223633012000001	-1.3641225351176471	0.10076850599411766	C	0.97360174582352976	0.7859009670000012	1.1282452788235293
C	-0.2844939879999993	-1.9783666351176472	-1.1381663340058823	C	8.936504582352976E-002	1.2882830170000001	1.2799731988235294
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H	-0.18512693782352962	-1.1026488711764708	1.9674470647647060	O	-0.1729957700000022	-3.4442971299999998	-0.96609102258823520
H	1.895804621764702	0.63753561882352927	2.7635034647647059	O	-0.4109291200000015	-1.3583068300000001	1.359454874117646
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C	0.35095310664705874	1.9149647740758824	1.0702571820764706	H	9.501572999999854E-002	-1.740808130000002	-2.0040315425882351
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C	0.64573598576470603	8.1653425294117649E-002	-0.29756749558823531	H	1.2315010970000000	-4.3152667647058829E-002	-1.2593069125882352
C	1.3215721857647060	1.0099090352941176	0.68685106441176469	H	-1.3577665420000000	-1.5767078276470587	-1.1795270125882353
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C	-0.74589437423529392	1.8348472352941176	9.8639104411764683E-002	H	-1.1202431830000001	-3.9983279276470589	-1.0055440125882353
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O	2.478729857647061	0.61199641529411763	1.1295834644117646	H	-0.14249390300000009	-0.83524562764705879	2.0285966874117647
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O	-1.7183957542352939	2.6374743352941179	7.539167441176498E-002				
C	0.283588756470614	-1.3047921647058822	0.19711314941176469	C	0.60434515047058834	7.5588339764705956E-002	-0.37707662029411770
C	-0.20424131423529400	-2.1052214647058825	-0.99018891558823530	C	1.25949665404705882	0.97733952876470598	0.6600922590758823
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O	-0.64220742423529398	-1.22651690647058823	1.2265743044117647	C	-0.6885095952941166	1.9333379587647059	3.4408227705882297E-002
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H	2.7889932857647057	1.3047884352941177	1.7723510844117647	O	-0.79092376952941157	-1.1511336412352939	1.2110183497058822
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C	1.1787250659999999	0.99211066117647051	0.80892902135294120	H	-1.2862673495294117	-1.6286288412352941	-1.1696616502941177
C	0.3209171659999964	1.9528818511764705	1.0828589013529413	H	0.37984635047058846	2.0557590587647061	0.91722950970588235
C	-0.8348583040000027	1.7495285511764704	0.17032384835294123	H	-1.31539226752941166	-3.894468412352936	-1.0045813502941179
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C	0.70406860823529449	0.15090290882352939	-0.39958032300000002	H	1.1342157900588234	0.12950324237058833	-1.3232922002941176
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C	-0.724081971676470557	1.8832358688235293	-3.33709229999997E-002	H	-1.409801990411765	-3.8146865616294114	-0.66115380029411763
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O	-0.72463706176470566	-3.4802098311764706	-0.52145388300000006	C	0.3		

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C	0.23830676235294113	1.8157599218823530	1.1600759423529412	H	0.10055843254117692	-1.9174945467058824	-2.02054943320058826
C	-0.84412097746705896	1.6715465218823529	0.26860477235294117	H	-1.3914693306588231	-3.6511782467058822	-0.70549437300588225
O	-0.49662903764705901	0.80489852188235278	-0.79450378764705876	H	1.0704087325411769	-1.820501467058824	0.12119736699411765
O	0.23898803623529412	0.67200152188235285	1.26682647223529411	H	-0.18267386745882308	-1.5389314467058823	1.8207128069941176
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H	-8.6454537647058904E-002	3.4753378218823525	1.9288368223529411	O	-0.6350121079999974	0.96695656988235290	-0.69332982999999992
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O	-0.4930490499999977	0.89008396034705894	-0.79445023035294127	H	1.2712091294117649	-1.7644200801764705	0.25018767605882347
O	2.3398700700000004	0.47368044444705887	1.3654530696470588	H	-0.37035337058823514	-1.52655938017647057	1.7794580360588235
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O	-1.895766799999996	2.2849989103470589	0.3815097364705879	C	0.73409682941176491	0.20150160982352941	-0.45163180394117652
C	0.4297997000000036	-1.2941456896529411	-1.0266236035294124	C	1.0627577082352939	0.1021658842352941	0.6974096730000001
C	-0.1450738299999963	-1.9700501896529410	-1.340831303529411	C	7.0753308235294021E-002	1.88149154952352941	1.1195406300000000
O	-0.5164613099999973	-3.3056195896529412	-1.0110817303529411	C	-1.0581514817647060	1.6482198523529412	0.2391901659999999
O	-0.5083606399999970	-1.4089792896529412	0.8844840694705877	O	-0.70516440176470596	0.79459894235294101	-0.7352817469999993
H	-0.4627900199999969	3.3168661103470591	1.9755392696470588	O	2.2267719082352939	0.79964858235294112	1.2459428530000001
H	1.5317266700000003	0.29941612034705889	-1.2054329303529412	O	0.14961570823529402	2.7632670523529410	2.1492081530000000
H	-0.9663996499999972	-1.3817622896529411	-1.6298013303529413	O	-2.1380373303529414	2.1851898523529409	0.2908241489999998
H	0.5453822700000017	-2.1359084896529410	-2.1083073303529414	H	0.3523101823529396	-1.2874503476470589	3.4650713000000000E-002
H	-1.4531986399999977	-3.2194967896529412	-0.66307845035294122	C	0.13348870823529402	-2.0166012476470589	-1.2187742470000000
H	1.3976136700000001	-1.7133721896529410	0.19935197764705878	O	-0.25739929176470588	-3.333097476470590	-1.0284651469999999
H	1.1743970000000031E-002	-1.6155078896529411	1.6949101696470588	O	-0.77771564176470598	-1.4816291476470589	0.8047590030000003
H	2.7869147000000007	1.0372610203470589	2.0384895696470586	H	2.2283173082352938	1.3560183423529411	2.0153696530000000
C	0.77526596235294121	0.22397636317647063	-0.4024225500000005	H	1.2634463082352938	0.21802755235294108	-1.2119068470000001
C	1.2327168623529412	0.93478168317647059	0.8502384399999999	H	-0.54616508176470602	-1.4562330476470589	-1.8369844469999999
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O	2.409479623529409	0.51221789217647063	1.3762572199999999	H	-0.569563111764		

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C	1.1467195792941176	0.90590334147058837	0.89443291035294115	H	1.1051194276470588	0.55426171941176472	-1.4787484982352941
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C	-0.89322265070588247	1.6771756514705882	0.32691455435294114	H	0.29739502764705872	-1.6778400505882356	-2.376890282352942
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O	2.3506642792941177	0.62162147647058830	1.4136311303529412	H	0.11565482764705881	-2.2206199505882354	1.3348378517647059
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O	-1.9748714707058825	2.1906078514705882	0.53664533035294115				
C	0.28905157929411751	-1.2920975485294117	-7.594934964705880E-002	C	0.61405907323529396	0.27224000294117634	-0.51535538897647060
C	-0.11966672070588236	-2.0880821485294114	-1.3436108696470588	C	1.3149803732352940	0.97129461294117636	0.69689912102352936
O	-0.43086728070588243	-3.4324957485294116	-0.96950726964705880	C	0.43774677323529394	1.8568236629411763	1.1889848410235295
O	-0.82569837070588237	-1.3452897485294115	0.8184635035294111	C	0.84774460676470609	1.7238583629411763	0.4023167036325945
H	-0.23717131070588238	3.6907124514705885	1.6540371303529411	O	-0.71717751676470609	0.83544643294117638	-0.61242565897647072
H	1.273432792941174	0.37870228147058832	-1.2010206696470589	O	2.5153204732352941	0.6067089294117633	1.2262148710235294
H	0.9284148070588239	-1.6627975485294115	-1.915335696470588	O	0.35991137323529387	2.6904186329411764	2.2906674410235297
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H	-1.141325187058824	-3.3956246485294117	-0.35232676964705886	C	0.44647037323529393	-1.2328020370588238	-0.31368276897647057
H	1.226007792941177	-1.7478150485294117	0.283965385250615	C	-0.33716382676470613	-1.9519356370588239	-1.4141478589764707
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H	2.3511308792941175	1.0228387614705883	2.2908725303529409	O	-0.31063422676470620	-1.522186330588236	0.829853701202352940
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C	1.075728970588233	0.94570873611764705	0.85076888941176465	H	-1.397394417647062	-1.6248365370588236	-1.4606852589764707
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H	-1.1173100929411766	-1.666072538823531	-1.401146850882352	O	0.33426773647058816	2.5859976870588236	2.3511818948352943
H	0.43174239705882345	-1.8062935538823530	-2.153775050882354	O	-1.8130812835294117	2.5921427870588234	0.29157589483529417
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H				H	-0.38125166352941164	2.5232494670588235	3.0188413948352943
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C	0.3353764894117645	1.7632730053529411	1.3207159329411764	H	0.32852703647058834	-1.8590539129411767	-2.1963186051647057
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H	1.3729074894117646	-1.7666284946470587	-0.27559724705882360	C	-0.27289293235294121	-1.998593418823528	-1.42278344823526
H	8.936899411764632E-002	-1.8352244946470586	1.5556178329411765	O	-0.28671953235294123	-3.3915601418823527	-1.0554674344823529
H	2.7628359894117649	1.1973755653529412	2.0778597329411763	O	-0.38983633235294124	-1.4169824818823527	0.84610508551764707
H				H	0.23606806764705879	2.6845717581176469	2.975523865176472
C	0.60644742764705861	0.25178325941176471	-0.53286010823529417	H	1.3457400676470588	0.49462174811764709	-1.4026232344823530
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C	-0.828632528235294124	1.766323194117646	0.53371912176470593	H	-1.0406472023529412	-3.5366702418823528	-0.43596164448235292
O	-0.70768046235294124	0.93596512941176468	-0.57131409823529411	H	1.43272916764705870	-1.6022913418823528	0.22419534448235295
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O	-1.8596789223529413	2.4203898494117646	0.79252844176470583				
C	0.34049382764705860	-1.2455803505882352	-0.30806775823529409	C	0.68548337794117598	0.27954365758823518	-0.53634001647058827
C	-0.32375660235294135	-1.8597191505882353	-1.5224363982352942	C	1.0973545779411762	1.0596217735882352	0.64821218352941168
O	-0.42526596235294134	-3.2595545505882355	-1.168944982352941	C	0.14941137794117609	1.975832675882351	0.99237067352941177
O</td							

O	-0.52189850205882393	0.99194627258823520	-0.99259871647058828	H	1.5884562664705881	-1.5542253069411767	0.27443729705882358
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O	-0.22154342205882394	-1.4495523324117650	0.94790109352941165	C	-1.0914313941176472	1.6246860376470589	4.0701958823529671E-003
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H	-1.4104551170588240	-1.4745199324117650	-1.0411120164705883	O	-0.55408721411764728	2.7321389376470591	2.096843658823529
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H	2.6256330779411758	1.4200339075882351	1.6797622835294117	O	0.38333256411764727	1.3265257623529412	1.0617640558823529
				H	-0.45321227411764731	3.6533163376470590	1.7479515658823530
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O	-0.9406605941176473	1.7772028449241177	4.4627221764705904E-002	H	-0.9710927111764730	3.6626512623529406	-0.459751953411764707
O	-0.65364418941176472	0.75265715429411773	-0.77651904823529416	H	1.6207174358823526	-1.55862602623529411	0.4682373368235297
O	2.0777823005882352	0.66806106429411771	1.4578806517647058	H	0.19841003588235262	-1.1670752623529410	1.8803864658823530
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O	-2.0205128894117648	2.3118351542941178	-8.5082838232594056E-002				
C	0.47709600058823520	-1.3716414857058825	-6.4523382352940639E-003	C	0.69211851352941145	0.19525195095882341	-0.34398641941176461
C	-0.18884979941176483	-2.1325395857058824	-1.1918128482352941	C	0.913175912411764732	0.9989940005882344	0.93255876094058823541
O	-0.25502289941176470	-3.5484195857058825	-0.832255454823529418	C	-8.0069586470588261E-002	0.9132893905882353	0.97759754058823534
O	-0.38641456941176477	-1.4477483857058826	1.0906314917647060	C	-1.0304060264705883	1.7129071190588234	-0.11912263941176465
H	0.23836650058823516	3.8391596142941178	1.5817503517647058	O	-0.52185701647058835	0.775562277905882347	-0.94106114941176466
H	1.3544854005882354	0.27522710429411767	-1.1765594482352941	O	0.20022261235294113	0.84548336405882341	1.7127485505882354
H	-1.0954109794117648	-1.6510925857058822	-1.3914838482352940	O	-0.31499728647058833	2.8291161390588235	2.0264505505882355
H	0.51128490058823517	-2.0074198857058825	-2.04180120428352940	O	-2.1435445064705885	2.2296427390588232	-0.31621535941176465
H	-0.78061671941176480	-3.6812414857058822	-2.4571568235294106E-002	C	0.48910321352941155	-1.2969416609411764	2.5599210588235333E-002
H	1.5149290005882352	-1.8499259857058825	0.22420429176470591	C	0.11713221352941172	-2.0802032609411767	-1.1748448494117647
H	0.18117300058823527	-1.4872323857058825	1.8624622517647058	O	8.0790213529411625E-002	-3.4349667649411765	-0.702472941176470
H	2.2478632005882351	1.2009321742941177	2.2351950157647059	O	-0.66789943647058836	-1.4006800609411765	0.88612192058823536
C	0.63629340411764712	0.1694414988235309	-0.33156292470588233	H	1.52757851352941148	0.20786654905882340	-0.97988464941176479
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C	-3.3914595882352527E-002	1.9504687598823529	1.0517414952941175	H	0.84552791352941159	-1.9238747649411765	-1.9259525494117649
C	-1.0218045258823527	1.7219653398823529	-1.6546404705882367E-002	H	-0.7012400047058837	-3.4977371609411763	-0.15217597941176469
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O	2.1797301041176476	0.90412497188235308	1.4084457152941177	H	-0.43520848647058830	-1.4988549690411765	1.8442074505882353
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O	-2.07438674588235258	2.3365650598823531	-0.18615135470588234				
C	0.49611930411764726	-1.3463067401176469	5.574203529417642E-002	C	0.75771953176470586	0.3080784047647053	-0.31749798999999995
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O	-6.6697495882352720E-002	-3.4597198401176468	-1.071568647058823	C	-0.13861836823529416	1.8461225901764706	1.18620503000000000
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H	-0.70800586588235270	3.6429257598823530	1.792901152941177	O	-0.45142656823529426	0.91078311017647051	-0.9168261799999999
H	1.4147475041176474	0.21986784988235305	-1.0781934847058823	O	2.012745317317647060	0.77882209717647055	1.6945691199999999
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H	0.15338130411764728	-1.8136543041176470	1.9156812152941176	O	4.0629568235294178E-002	-3.342115808235293	-0.9987362799999992
H	2.4835513041176474	1.6271992098823529	1.9943924152941177	H	-0.5018826123529412	1.430578298235293	0.88221151000000009
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C	0.85447216647058832	1.0691689030588234	0.88642429705882364	H	-0.7065220982352942	-1.7236476098235296	-1.9038428800000002
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H	1.3580527664705881	0.50056135305882354	-1.1772750729411765	O	1.9811712370588230	0.61214725529411762	1.6882459394117646
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H	1.9832730764705884	1.5648926504529412	2.3118716235294117	H	-0.87164411823529442	-1.2178432358823530	0.73633615411764697
C	0.755						

H	-0.51021416823529442	-1.6518286358823531	-1.7331991658823531	O	-0.84257012941176512	2.5203743682352941	2.1556227570588233
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H	-0.23313572764705892	-1.6520633199999997	-1.9660851449999999	O	-7.4579617647062596E-002	2.794088339764705	1.9990417761764707
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H	-0.8050897746705881	-3.4576367319999997	-0.4745477449999999	C	0.22178123823529387	-1.2617914660235294	2.7529046176470590E-002
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C	0.65700115294117656	0.1111799299999993	-0.16983955717647059	H	1.6078135382352938	0.16986800397647067	-0.95009538382352932
C	0.81162565294117672	1.0101239199999998	1.0022392048235294	H	-1.0263781417647062	-1.9496715660235295	-1.6015041238235295
C	-0.15828754705882342	1.9508363499999999	0.97212130482352932	H	0.69052603823529402	-2.0627729660235294	-2.0407103238235296
C	-0.8806557705882330	1.8575681500000001	-0.30825989017647060	H	-0.49215982176470618	-3.7008825660235294	-8.5107382352941907E-004
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O	1.8531477529411766	0.8014171799999995	1.8066340048235294	H	-0.83342898176470614	-1.2546634660235294	1.66908847761764706
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C	0.28532665294117665	-1.3360772500000002	0.1965636448235293	C	0.6821131294117666	0.20745193176470589	-0.27285967352941187
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H	-0.62860320705882344	3.6163360317647060	2.0665661264705881	O	1.7252281535294118	0.672681149470588245	1.8584257054117646
H	1.494777129411765	0.40465308176470582	-0.98381696352941184	O	-0.32476314647058824	2.8051162547058826	2.048312054117646
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H	1.0446903129411764	1.9013016682352941	-1.924224735294119	O	0.21352105352941186	-1.28083614547058823	0.11804148341176469
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H	1.6660701129411766	0.76826594176470586	2.7737560264705881	H	-0.120872474647058810	3.7893759547058825	1.904844054117646
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C	0.74777676117647029	0.97733549652941176	1.0665426651764705	H	-0.73184259647058814	-1.7077818452941176	-1.6840710945882353
C	-0.22399723882352940	1.9259041565294117	1.1456402651764706	H	1.0535496465294119	-2.00938964652941173	-1.7309172945882353
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H	1.8932998936842105	-1.3819143810526318	1.5266104662631579	H	-0.15610569E+01	0.2209768E+01	-0.10466074E+01
H	1.6617555936842106	-2.5669805810526314	0.21684693626315793	H	-0.40614156E+00	-0.12936317E+01	-0.10033456E+01
H	3.4594793936842105	-0.33702811105263164	-0.10712672073684210	H	-0.11138054E+01	-0.25409428E+00	0.15649613E+01

H	4.012427699999999	-3.230566099999999	-0.875347639999999	H	-0.2022912100000001	-2.604508099999999	1.285147500000001
O	4.652482499999996	-3.712945899999998	2.712397400000000	O	4.013479399999996	-7.122546400000001	1.274909700000000
H	4.857309100000002	-4.61520199999997	2.757091800000000	H	3.714217699999998	-7.760301900000000	0.573051819999999
H	3.663546800000002	-3.749994000000001	2.681765000000002	H	3.138929699999998	-6.932865000000004	1.659828000000001
O	-1.440264100000000	-5.062708100000000	2.780371599999999E-002	O	5.119426500000003	-2.207315100000002	0.609519730000000
H	-0.6565861200000005	-4.516888599999997	0.1468473800000000	H	4.958923500000000	-2.835993999999999	1.294401900000000
H	-1.317792600000000	-5.731148100000004	0.7269698300000004	H	5.483353700000003	-1.430111900000000	1.069684099999999
O	3.950133199999998	-6.855448799999996	1.059905200000000				
H	3.616636999999999	-7.547132600000003	1.632546600000000	C	0.16882591E+01	-0.26991295E+01	0.22277372E+01
H	3.239650100000000	-6.291001099999999	1.249671100000000	C	0.17701170E+01	-0.13913474E+01	0.27153125E+01
O	2.903038200000001	-5.821033800000004	4.890371799999996	O	0.14083354E+01	-0.43179217E+00	0.17094152E+01
H	2.650640699999998	-5.149340099999999	4.270273699999997	C	0.11074573E+01	-0.11623065E+01	0.56177524E+00
H	2.218488900000001	-6.446715000000000	4.705411200000003	C	0.11001470E+01	-0.26412412E+01	0.97196453E+00
O	1.604416800000001	-3.514790699999998	5.798611000000002	O	0.19406862E+01	-0.10103694E+01	0.38898242E+01
H	2.215605699999998	-4.349009999999998	5.780015299999996	C	-0.18405623E+00	-0.66314047E+00	-0.41269318E-01
H	1.545161100000001	-3.324852700000001	4.859470599999999	O	-0.12331474E+01	-0.79080591E+00	0.89798956E+00
O	0.828649239999995	-7.316649000000000	3.717752700000001	O	0.853182879999998	-3.522797600000001	7.795389899999993E-002
H	0.613473990000002	-6.669767200000001	2.999610399999999	O	1.882844000000000	-3.825603999999998	2.935169600000000
H	1.588853400000001	-7.748885600000004	3.305823199999999	C	-0.10611843E+00	0.77580357E+00	-0.55961400E+00
O	-0.214372590000000	-3.470436600000002	-2.672412200000001	O	-0.14108678E+01	0.11479511E+01	-0.11091600E+01
H	3.595579000000001E-002	-4.358684199999999	-2.926068100000002	H	0.20123035E+01	-0.91491920E+00	-0.44517324E-01
H	3.790936100000003E-002	-3.589167300000002	-1.743355800000000	H	0.32987976E+00	0.14231814E+01	0.22643891E+00
O	-2.822797500000001	-3.107876899999999	1.021655699999999	H	0.64603599E+00	0.78296868E+00	-0.13656862E+01
H	-2.339212700000000	-3.880560300000000	0.623138480000005	H	-0.15308759E+01	0.21023075E+01	-0.10295375E+01
H	-2.302687500000002	-2.355242399999998	0.740250900000004	H	-0.44802145E+00	-0.13964769E+01	-0.86897069E+00
O	1.851460399999999	-1.830938699999999	-2.673470899999999	H	-0.98895706E+00	-0.37588637E+00	0.17195824E+01
H	2.376172700000001	-2.237604699999999	-2.021339900000001	O	1.517737700000001	-6.175871000000004	1.334123699999999
H	0.9778415700000005	-2.297584800000001	-2.492110400000001	H	1.717687000000000	-5.357998199999999	1.870618600000000
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C	0.15122821E+01	-0.28871651E+01	0.22007604E+01	O	-0.786615440000005	-4.126117800000003	3.886032699999999
C	0.14858721E+01	-0.15901309E+01	0.28065364E+01	H	1.438311999999999E-002	-0.429911400000001	3.468878900000000
O	0.10694795E+01	-0.59081960E+00	0.18820499E+01	H	-1.096055000000000	-4.832152899999996	3.282629399999998
C	0.88337540E+00	-0.13034403E+01	0.61075350E+00	O	3.210722899999999	-3.274818799999998	-1.318791300000000
C	0.97296960E+00	-0.27891703E+01	0.94192287E+00	H	2.514153600000002	-3.696162600000001	-0.7639252100000002
O	0.18069858E+01	-0.11977420E+01	0.39639582E+01	H	3.931944500000002	-3.049621300000001	-0.637291979999998
C	-0.30006780E+00	-0.71421104E+00	-0.84760462E-01	O	-1.513676999999999	-5.166480199999996	0.211269099999999
O	-0.14446668E+01	-0.785822269E+00	0.81349452E+00	H	-0.631722330000000	-4.817141999999996	0.362407910000000
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O	1.925693200000000	-3.918746300000000	2.878654500000001	O	4.590206900000001	-3.950800000000001	2.912682700000000
C	-0.95559121E-002	0.73752013E+00	-0.49092499E+00	H	4.909768200000002	-4.846350300000001	2.875244040000001
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H	0.17676420E+01	-0.98947378E+00	-0.10036895E-01	O	3.023026000000002	-5.969404239999999	4.398828000000000
H	0.22386065E+00	0.13518824E+01	0.34931102E+00	H	2.891228700000001	-5.291780000000002	3.670450500000002
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H	-0.11611478E+01	-0.55674763E+00	0.17313358E+01	H	1.6790487200000001	-3.377281200000001	4.810895000000004
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H	3.879378099999998	-2.975433999999999	-0.6723081699999998	H	5.152754500000003E-002	-3.706723900000001	-1.846309999999999
O	-0.868857320000004	-4.041207700000002	3.779136700000000	O	-2.805780800000000	-3.048593299999998	1.421464899999999
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H	-0.710195490000004	-4.690710700000003	2.743866550000000	H	3.909012699999999	-8.041642700000006	1.514293399999999
H	-1.514202799999999	-5.700806100000003	0.9693096399999997	H	3.254606900000002	-6.817569299999997	0.8352765500000001
O	4.645165699999997	-3.832937199999999	2.968627500000002	O	-1.144472800000000	-1.349633800000001	4.341379200000004
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H	3.611971399999998	-3.868364699999999	2.894628800000000	H	-0.2248554000000001	-1.198051000000000	4.592090200000003
O	3.099399399999998	-5.882707000000000	4.443267500000001				
H	2.754464800000000	-5.220301799999997	3.822225599999999	C	0.14317077E+01	-0.29184453E+01	0.22998025E+01
H	2.321279800000000	-6.522201200000002	4.360184999999996	C	0.15998344E+01	-0.16250058E+01	0.28623697E+01
O	1.517468300000000	-3.857137100000001	5.786136499999996	O	0.14019539E+01	-0.61137177E+00	0.19207035E+01
H	2.114250600000001	-4.568228000000004	5.940620300000000	C	0.10096264E+01	-0.12936437E+01	0.65063658E+00
H	1.690404599999999	-3.708750100000000	4.802896399999998	C	0.10353921E+01	-0.28013863E+01	0.96598155E+00
O	-3.167491100000000E-002	-3.531882299999999	-2.695391400000001	O	0.18386699E+01	-0.13565399E+01	0.40586199E+00
H	0.10737131400000000	-4.353307359999999	-3.257062700000001	C	-0.27334441E+00	-0.57009758E+00	0.66715958E-01
H	-3.476685100000001E-002	-3.820797499999998	-1.718230600000001	O	-0.12180299E+01	-0.37481197E+00	0.11272767E+01
O	1.023207999999999	-7.502110199999997	3.591982199999999	O	0.7661786400000002	-3.701141400000000	8.193756200000005E-002
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O	-2.809811900000001	-3.080177200000001	1.344663600000001	O	-0.11860391E+01	0.13521054E+01	-0.94281975E+00
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H	-0.88615373E+00	0.16864600E+00	0.18521782E+01	H	3.099695699999998	-6.624625499999996	1.097873000000001
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H	4.891564999999999	-5.085034000000003	2.549023099999999	H	1.379241299999999	-7.299291000000002	2.858243799999999
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O	4.162748599999996	-6.739089899999996	1.377292200000001	O	0.16846679E+01	-0.69724226E+00	0.1794133E+00
H	3.981490599999999	-7.498712000000003	0.839312460000004	C	0.12334282E+01	-0.14137964E+01	0.62495238E+00
H	3.249604199999998	-6.322089899999999	1.386357500000000	C	0.11439735E+01	-0.28645140E+01	0.11082466E+01
O	-9.34295910000000E-002	-3.422027100000002	-2.519785800000002	O	0.21742097E+01	-0.10106698E+01	0.39671633E+01
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H	0.1520826700000000	-3.472008999999998	-1.564530999999999	O	-0.10968870E+01	-0.59582691E+00	0.10826778E+01
O	1.664624799999999	-3.817016900000000	5.933564699999998	O	0.8269685599999996	-3.786254500000001	0.2520540499999997
H	1.931254000000000	-4.709217999999999	5.748465200000001	O	1.3427998000000001	-3.957917900000002	3.288057199999999
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O	-2.740915100000000	-2.607489300000001	1.539605600000000	O	-0.10042176E+01	0.11082730E+01	-0.10733564E+01
H	2.271162059999999	-3.363133899999998	1.167784800000000	H	0.201272172E+01	-0.13008736E+01	-0.9909361E-01
H	-2.029821699999998	-1.923926800000000	1.510670200000001	H	0.56317579E+00	0.12705724E+01	0.32216166E+00
O	4.681516900000001	-2.392923199999998	0.515074860000002	H	0.91506138E+00	0.62305157E+00	-0.13090517E+01
H	4.714076000000004	-3.128740800000001	1.121280600000000	H	-0.11512773E+01	0.2079846E+01	-0.94107853E+00
H	5.197803399999997	-1.666135100000000	0.988627600000002	H	-0.38963965E+00	-0.14846258E+01	-0.76047897E+00
O	1.255827100000001	-7.928443599999996	3.851003899999998	H	-0.70259042E+00	-0.74807667E+00	0.19547292E+01
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C	0.16885062E+01	-0.28885581E+01	0.24046318E+01	H	1.339522600000000	-5.606982500000000	0.6391306799999995
C	0.19585698E+01	-0.15592714E+01	0.28893593E+01	O	-1.511049200000000	-5.146537300000003	0.6122118899999998
O	0.16377522E+01	-0.53169847E+00	0.19186227E+01	H	-0.566720200000001	-5.024376400000004	0.5965372399999997
C	0.12204372E+01	-0.12173119E+01	0.69344733E+00	O	-1.734935700000001	-5.608991800000001	1.4419736000000001
C	0.11747421E+01	-0.27053657E+01	0.11085448E+01	H	-0.392231129999998	-3.934541499999996	4.384299999999996
O	0.23242773E+01	-0.11673562E+01	0.40015140E+01	H	-1.893851400000000	-4.304843499999996	3.8106575000000000
C	-0.15646207E+00	-0.63213244E+00	0.11128775E+00	O	3.452047600000002	-3.801185199999999	-1.122046700000001
O	-0.12021475E+01	-0.46882204E+00	0.11578417E+01	H	2.715341899999999	-4.139357600000003	-0.5560717499999998
O	0.712547959999998	-3.603760600000002	0.242913359999999	H	4.245159799999997	-3.788217500000000	-0.5277455500000001
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C	0.10881777E+00	0.75790567E+00	-0.48306258E+00	H	2.629904199999999	-4.740089399999996	4.199802199999997
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H	-0.67685824E+00	-0.24058622E+00	0.19494109E+01	H	-2.016192300000002	-2.000308299999999	1.145728499999999
O	1.441646400000001	-6.094556800000003	1.591852000000000	O	1.534843000000000	-3.586446899999999	6.007429100000004
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O	-1.740191199999999	-4.822112500000002	0.338912539999998	O	4.354565799999996	-6.348706499999996	0.5412790200000006
H	-0.8308125899999996	-4.509260000000003	0.556381209999996	H	4.476226999999997	-7.326326700000001	0.3636213799999999
H	-1.887740000000000	-5.339369099999999	1.188477599999999	H	3.347291499999999	-6.270872999999999	0.5595467899999996
O	-0.928951450000001	-3.764674600000002	4.172791400000004	O	1.625170999999999	-7.745131999999999	3.572972200000002
H	-6.275159900000005E-002	-4.136710100000002	3.979692500000001	H	1.520200400000000	-7.215741999999997	2.7785619000000001
H	-1.414565200000000	-4.238808999999998	3.478943900000000	H	2.266037700000000	-8.411762299999995	3.250631799999998
O	3.192521800000002	-3.412820700000002	-1.378763900000000	O	-0.6116098899999999	-1.325056599999999	4.827730700000000
H	3.021403600000002	-4.057289100000002	-0.6835517100000003	H	-0.8435800000000000	-2.2953453000000001	4.591984700000003
H	3.905927600000001	-2.865484200000000	-0.906973389999999	H	0.3526498800000003	-1.394048299999999	4.843726999999996
O	4.991653399999997	-4.327866300000002	2.315322399999999	O	4.727913199999997	-2.211757200000001	0.7838363600000001
H	4.705143200000002	-5.167545200000002	1.825995000000000	H	4.740632500000002	-2.782767600000001	1.566811800000000
H	4.098182800000000	-3.980669100000001	2.586758000000001	H	5.178131800000001	-1.393186100000001	1.102430000000000
O	3.194240999999999	-5.777398400000000	4.635641500000002				

C	0.14028332E+01	-0.30092635E+01	0.24581465E+01	O	-1.5483575000000001	-5.1830610999999998	0.6299714300000000
C	0.18723855E+01	-0.17268199E+01	0.28360600E+01	H	-0.7915974000000001	-4.5087278000000000	0.7442031200000000
O	0.17617132E+01	-0.84125694E+00	0.18166192E+01	H	-1.5955109000000001	-5.5451975999999998	1.5377075000000000
C	0.12249301E+01	-0.16007592E+01	0.62181759E+00	O	-0.7765393000000004	-4.4541902000000002	4.3143813000000000
C	0.10106946E+01	-0.29791535E+01	0.11136972E+01	H	0.10504980000000000	-4.486881999999999	3.8707957999999998
O	0.23446408E+01	-0.12563426E+01	0.38904146E+01	H	-1.3638583000000000	-4.8591781999999997	3.6571305999999999
C	-0.11768025E+00	-0.94994282E+00	0.19535063E+00	O	3.0651218999999998	-3.6753396999999999	-1.1879560000000000
O	-0.10278465E+01	-0.96025043E+00	0.12818282E+01	H	2.3148599000000001	-4.2143487000000004	-0.9079249000000003
O	0.60871209000000004	-3.9239369000000002	0.31109645000000002	H	3.4535714999999998	-3.4230977999999999	-0.3410220700000001
O	1.327603899999999	-4.0270685000000004	3.323197000000000	O	3.356614299999999	-5.6740832000000001	4.7465149999999996
C	0.10559049E+00	0.57250503E+00	-0.21641651E+00	H	2.833907599999999	-4.981581999999996	4.1817298999999997
O	-0.10221341E+01	0.10963007E+01	-0.87965156E+00	H	2.8511091999999998	-6.400520999999996	4.4418838999999997
H	0.20356575E+01	-0.15166379E+01	-0.14994861E+00	O	0.2981056799999998	-3.6880765000000002	-2.3389859000000000
H	0.25511847E+00	0.11194532E+01	0.70883299E+00	H	0.6566680999999998	-4.5595977000000003	-2.3977759000000000
H	0.10003751E+01	0.63854013E+00	-0.83542015E+00	H	0.12581279000000001	-3.7193901000000000	-1.3552119000000000
H	-0.85477051E+00	0.20575853E+01	-0.94723619E+00	O	1.7553893000000000	-3.7898309000000001	5.8775085000000002
H	-0.63879343E+00	-0.16030491E+01	-0.51213780E+00	H	2.3335670999999998	-4.5652920000000003	5.9094122999999996
H	-0.70783127E+00	-0.37056034E+00	-0.20099119E+01	H	1.4785360999999999	-3.8665848000000000	4.9605338999999997
O	1.7364733000000001	-6.079655999999999	1.609981799999999	O	-0.6205473900000003	-1.5042473999999999	4.7403430000000002
H	1.633240599999999	-5.469244299999997	2.378857800000000	H	-0.4849780200000001	-2.4967103000000002	4.5371755000000000
H	1.1632754000000001	-5.6121233000000004	0.898017799999999	H	0.30565205000000001	-1.1894608000000000	4.7369605999999997
O	-1.1349178000000000	-4.0373381000000004	4.265076299999996	O	-2.978456599999999	-2.7113931999999998	0.87923951000000000
H	-0.29965195000000000	-4.0639830000000003	3.7995461000000001	H	-2.4128234000000002	-3.4812671000000002	0.7737498299999997
H	-1.5072684000000001	-4.8829266000000002	3.9179963999999998	H	-2.2939136000000002	-2.0520149999999999	0.82236047000000001
O	-1.786561899999999	-5.2183628000000004	0.5493728799999995	O	4.6244709000000004	-6.7578379999999996	1.0162475000000000
H	-0.8673004600000005	-4.8768921000000001	0.5550819900000003	H	4.576235299999996	-7.656472199999996	0.64722214000000000
H	-1.9389525000000001	-5.567890399999996	1.4912635000000001	H	3.644509999999998	-6.656920099999998	1.30878860000000000
O	3.3875247000000002	-3.681884499999998	-1.042767599999999	O	4.7820647000000003	-2.1669020000000002	0.4845880100000001
H	2.6716880000000001	-3.8805345000000000	-0.3762685399999998	H	4.6684511000000004	-2.763425799999998	1.2719201000000000
H	3.952337999999999	-3.0576496000000000	-0.6172808100000001	H	5.623959499999998	-1.7734999000000000	0.83471132000000003
O	3.0770951000000002	-5.5511778200000002	4.720481099999998	O	1.6123710000000000	-7.956254099999998	3.8242055000000001
H	2.878266899999999	-4.7599073000000001	4.097285399999996	H	1.4873599000000000	-7.5256233000000003	2.950366799999998
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O	3.508964199999999	-4.036917299999998	-2.238839899999999				
H	1.0605902000000000	-4.676510699999997	-2.2918658999999999	C	0.14857108E+01	-0.28576461E+01	0.23987529E+01
H	0.3157626000000000	-3.9234011000000000	-1.3114277000000001	C	0.17869774E+01	-0.15663546E+01	0.28639913E+01
O	1.5109699000000001	-3.6907404000000001	6.041432699999997	O	0.16022816E+01	-0.64305760E+00	0.18402110E+01
H	1.9741413000000001	-4.5838326000000000	5.9510265000000002	C	0.12463888E+01	-0.13094361E+01	0.60965441E+00
H	1.361982999999999	-3.5405407000000002	5.059914799999996	C	0.11747409E+01	-0.27691922E+01	0.10114829E+01
O	-0.6958276900000000	-1.4430609000000001	4.8128612000000004	O	0.20822816E+01	-0.11484053E+01	0.40142144E+01
H	-0.7981729400000005	-2.3248761000000000	4.397873599999996	C	-0.16222850E-01	-0.69175585E+00	0.79583253E-01
H	0.2498153700000001	-1.4952953000000000	4.936634699999999	O	-0.11373806E+01	-0.80436948E+00	0.10225075E+01
O	-2.8724270000000001	-2.8974825000000002	0.8114723099999997	O	0.91823957000000000	-3.6974032999999999	0.21031510000000000
H	-2.402377299999999	-3.797598999999999	0.6423494300000000	O	1.4114176000000000	-3.9069348000000002	3.2281976999999999
H	-2.1308881000000000	-2.3083505999999998	1.0985328999999998	C	0.20677906E+00	-0.72688462E+00	-0.37996697E+00
O	4.455717599999999	-6.720678999999996	1.0567572000000001	O	-0.83346517E+00	0.10935782E+01	-0.11778605E+01
H	4.194863999999999	-7.354454699999999	0.3897251099999999	H	0.20489704E+01	-0.11178274E+01	-0.11028847E+00
H	3.5658994000000002	-6.579278099999998	1.3758893999999999	H	0.25096591E+00	0.13443938E+01	0.5402001E+00
O	1.8064293000000000	-7.983661999999998	6.3539142000000000	H	0.11381025E+01	-0.73580222E+00	-0.92087575E+00
H	1.7398905000000000	-7.6054268000000002	2.7587464000000002	H	-0.11259002E+01	0.20059114E+01	-0.95092875E+00
H	2.5936870000000001	-8.4912509000000007	3.4421574000000001	H	-0.33546142E+00	-0.11930733E+01	-0.79563826E+00
O	4.756308699999999	-2.217946899999998	0.8309933000000004	H	-0.82299424E+00	-0.44586506E+00	0.18905115E+01
H	4.844802399999998	-3.0530636000000002	1.3747761000000001	O	1.7648776000000001	-6.1400613999999996	1.4372175000000000
H	5.2184680000000001	-1.6071924000000000	1.4578070000000001	H	1.4461980000000001	-5.5642479999999999	2.1602665000000001
C	0.15686407E+01	-0.30190364E+01	0.23820805E+01	O	-1.3515995999999999	-5.0775059999999996	0.8033145999999999
C	0.19021299E+01	-0.16693253E+01	0.28110732E+01	H	-0.5093356100000005	-4.6631039000000003	0.8535892400000003
O	0.16956507E+01	-0.75938340E+00	0.18205836E+01	H	-1.3346138000000001	-5.7106224000000001	1.5949925000000000
C	0.12183966E+01	-0.14227525E+01	0.65775658E+00	O	-1.0153090000000000	-4.2648048000000003	4.3990530000000003
C	0.10432511E+01	-0.28396683E+01	0.11140431E+01	H	-0.1824481299999999	-4.2218787000000004	3.8865818999999999
O	-0.75677386E-01	-0.77798649E+00	0.20415454E+00	O	3.3555907000000000	-5.2009397999999996	4.4707781999999998
O	-0.11107471E+01	-0.80519276E+00	0.12076072E+01	H	2.6181854000000002	-4.8237832000000003	3.9636828000000000
O	0.5587142899999995	-3.7078338000000001	0.3295025799999999	H	2.9032159000000002	-6.037639299999996	4.590870999999998
O	1.6117500000000000	-4.1509312999999999	3.1250667999999999	O	3.2345579999999998	-3.2971455999999999	-1.6694376000000000
C	0.25712398E+00	-0.61923769E+00	-0.31564204E+00	H	2.5088265999999999	-3.5632104999999998	-1.0654881000000000
O	-0.84540418E+00	0.92375786E+00	-0.11958927E+01	H	3.7332291999999998	-2.6065114999999999	-1.2130280000000000
H	0.19929017E+01	-0.14376617E+01	-0.11293606E+00	O	-0.1449998000000001	-3.7637738000000001	-2.3371157999999999
H	0.17307470E+00	0.13124297E+01	0.51232962E+00	H	6.803631599999999E-002	-4.7161765999999998	-2.2135117000000002
H	0.11207653E+01	0.66984742E+00	-0.94244026E+00	H	0.15387543000000001	-3.5232770000000002	-1.4367635999999999
H	-0.94441311E+00	0.19280768E+01	-0.12037783E+01	O	-2.7813390000000000	-2.8978307999999999	1.0048477000000000
H	-0.42918678E+00	-0.13920353E+01	-0.63725819E+00	H	-2.2022962000000001	-3.7544453000000000	0.9991907399999997
H	-0.65763113E+00	-0.73962653E+00	0.20418368E+01	H	-2.0883459000000002	-2.2220282000000000	0.8839540700000004
O	2.0246374000000000	-6.4254832000000004	1.4233431999999999	O	1.9710318000000000	-3.4122232000000001	6.0337933000000001
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H	1.6118812000000000	-6.123826499999998	0.5978822000000003	H	1.7782688000000000	-3.0937445000000001	5.1162764999999997

O	4.672188399999996	-2.109883599999999	0.7972446500000000	O	1.2227980000000001	-3.847998899999999	0.3684799000000003
H	4.726914800000003	-2.928051299999999	1.2947715000000000	O	1.4219560000000000	-4.1464816000000004	3.3287105000000001
H	5.132331999999999	-1.4560556000000000	1.375428099999999	C	0.45690546E+00	0.55472457E+00	-0.45537762E+00
O	1.276769499999999	-7.865913899999999	3.7202576000000001	O	-0.69530555E+00	0.10744513E+01	-0.1144371E+01
H	1.4151088000000001	-7.291634799999997	2.977467600000002	H	0.23657517E+01	-0.11466632E+01	0.20532494E+00
H	2.045489599999998	-8.481026200000005	3.492109600000000	H	0.84812385E+00	0.12439635E+01	0.33838266E+00
O	4.541822899999997	-6.954208800000000	1.166730300000000	H	0.12441129E+01	0.51626608E+00	-0.12022512E+01
H	4.565363999999998	-7.718750700000002	0.6171911500000002	H	-0.87999560E+00	0.19093949E+01	-0.67134494E+00
H	3.595887499999999	-6.720355699999998	1.312971399999999	H	-0.12647592E+00	-0.15374702E+01	-0.78725821E+00
O	-0.1015894499999999	-1.546770100000000	4.481251699999996	H	-0.75774840E+00	-0.45356032E+00	0.18029163E+01
H	-1.1223356000000000	-2.581302200000001	4.646831899999996	O	2.1187697000000001	-6.214632499999996	1.5010128000000000
H	-0.10668606000000000	-1.390884100000001	4.631562599999996	H	1.916993600000001	-5.428833499999996	2.079800399999999
C	0.15031963E+01	-0.29591761E+01	0.25488906E+01	H	1.635448100000001	-5.797080499999999	0.7875691900000003
C	0.182375702E+01	-0.15893718E+01	0.30498554E+01	O	-1.1501423000000000	-5.276383100000003	0.4035255899999999
O	0.17986238E+01	-0.67182866E+00	0.20145519E+01	H	-0.2161524800000001	-4.913196000000000	0.4578070400000000
C	0.14925750E+01	-0.14194327E+01	0.78837526E+00	H	-1.3841654000000001	-3.385721000000004	1.339467000000000
C	0.13409976E+01	-0.28341760E+01	0.11856383E+01	O	-1.1653099000000000	-4.045135799999997	4.261265299999998
O	0.20964601E+01	-0.113139128E+01	0.41539814E+01	H	-0.2644452600000002	-4.198648000000004	3.945559499999999
C	0.25237767E+00	-0.83555382E+00	0.51544332E-01	O	3.788070799999998	-4.454037999999997	3.531345299999999
O	-0.95191510E+00	-0.86323664E+00	0.86578519E+00	H	2.986674499999999	-4.722463200000000	4.192306600000002
O	1.131355399999999	-3.763032200000000	0.322984669999997	H	3.4604471000000001	-6.128455299999997	4.549049600000000
O	1.385158099999999	-4.068083500000002	3.228661400000000	O	3.704587800000001	-3.323234900000001	-0.9876437200000000
C	0.55059806E+00	-0.56298491E+00	0.39075381E+00	H	2.970759339999999	-3.585934400000002	-0.4663175600000002
O	-0.62022504E+00	-0.11218903E+01	-0.10826748E+01	H	4.249655599999996	-2.801093199999999	-0.3947882200000002
H	0.23872600E+01	-0.12192338E+01	0.83967331E-01	O	0.1597563499999999	-3.836433899999998	-2.285503799999999
H	0.65228804E+00	-0.11634454E+01	0.55144524E+00	H	0.1916696099999999	-4.765714400000000	-2.347031200000000
H	0.13697366E+01	-0.49428946E+00	-0.106447450E+01	H	0.3989045399999999	-3.704370200000001	-1.339298600000000
H	-0.31402900E+00	-0.20233467E+01	-0.11364950E+01	O	1.696661100000000	-4.209310600000002	6.107826199999999
H	0.35065319E-01	-0.14373946E+01	-0.85830300E+00	H	2.486811900000002	-4.743951899999999	5.986353000000003
H	-0.81177332E+00	-0.21011633E+00	-0.15878995E+01	H	1.496133399999999	-3.977111490000001	5.207273299999998
O	1.843766999999999	-6.190844600000001	1.556693600000000	O	1.419162199999999	-7.934992699999996	3.706515399999998
H	1.691868800000000	-5.506304300000000	2.249172000000002	H	1.425217299999999	-7.209764899999997	3.026045200000000
H	1.459005700000000	-5.622607699999997	0.818264039999997	H	2.0869010000000001	-8.504060000000008	3.386313299999999
O	-1.233917399999999	-5.166190200000000	0.503020360000006	O	4.705899999999996	-6.919281500000003	1.338098599999999
H	-0.3823235000000001	-4.766048299999996	0.7090505900000004	H	4.498532300000001	-7.643523300000000	0.691808199999998
H	-1.4281117000000001	-5.604513899999997	1.332466600000001	H	3.784407200000000	-6.608595600000001	1.526203500000000
O	3.457839700000001	-5.107867999999999	4.113491400000000	O	-2.784262099999999	-3.109287100000000	0.3687167599999998
H	2.770025599999999	-4.701574400000002	3.626251100000002	H	-2.248063800000002	-3.943933500000000	0.3397846199999998
H	3.214752900000001	-6.038484699999997	4.052214000000002	H	-2.083045700000000	-2.465329000000001	0.4549113100000001
O	-0.9754947200000004	-4.149153600000000	4.434101300000000	O	-0.7152037399999998	-1.349845100000000	4.703900799999997
H	-0.1640177900000000	-4.134027100000000	3.856859300000000	H	-0.8617532399999998	-2.318894199999999	4.737317300000000
H	-1.462338100000000	-4.863182799999997	4.011348100000002	H	0.2270930499999999	-1.390697000000001	4.608689400000003
O	3.533781100000001	-3.303029000000000	-1.187702599999999	O	5.600437999999996	-4.607870300000001	2.401161600000000
H	2.650966600000000	-3.504774200000000	-0.8633767100000005	H	5.595817799999998	-5.399110799999999	1.732827399999999
H	3.909046200000001	-3.097584400000001	-0.290688720000001	H	4.993219299999998	-4.980806200000000	3.053893200000001
O	-2.811692700000000E-002	-3.990533699999999	-2.143643400000002				
H	8.197450100000005E-002	-4.943855100000004	-2.241203300000000	C	0.16019092E+01	-0.27646708E+01	0.24436244E+01
H	6.091359899999999E-002	-3.929456399999998	-1.208493700000000	C	0.18309432E+01	-0.15257748E+01	0.30079831E+01
O	1.890332399999999	-3.911834700000000	6.023831500000000	O	0.16922494E+01	-0.52897412E+00	0.19884341E+01
H	2.540313900000001	-4.688947599999997	5.887254399999998	C	0.16073505E+01	-0.12038975E+01	0.72114931E+00
H	1.602328400000000	-3.814985600000000	5.088579300000001	C	0.16098950E+01	-0.26112330E+01	0.10426953E+01
O	1.706255200000000	-7.709158900000001	3.715797900000001	O	0.20738336E+01	-0.11558369E+01	0.41814799E+01
H	1.718371799999999	-7.379341900000000	2.796601700000001	C	0.40817646E+00	-0.71794903E+00	-0.95040229E-01
H	2.304621700000002	-8.459136000000009	3.707093400000002	O	-0.77981619E+00	-0.83518769E+00	0.75549616E+00
O	-2.794284999999999	-3.074311799999998	0.785840899999995	O	1.412743300000000	-3.566517499999998	0.22444715000000001
H	-2.266593100000001	-3.884617700000002	0.569212619999995	H	1.534874400000001	-3.896070899999998	3.1819329000000001
H	-2.113893899999999	-2.380202100000000	1.037095300000001	C	0.44551483E+00	0.76101485E+00	-0.46719246E+00
O	4.424934200000000	-7.133303699999999	1.496788400000000	O	-0.61540995E+00	0.96263101E+00	-0.15074602E+01
H	4.216863300000000	-7.564912500000002	0.597960539999998	H	0.25500623E+01	-0.96751538E+00	0.21051363E+00
H	3.509631699999999	-6.888392800000001	1.794933200000000	H	0.13884079E+00	0.13634368E+01	0.44706535E+00
O	-0.8255928999999995	-1.371100599999999	4.939893299999996	H	0.14523772E+01	0.10474265E+01	-0.82976941E+00
H	-0.994524450000000	-2.286434100000001	4.691648299999998	H	-0.97087209E+00	0.18399246E+01	-0.14714635E+01
H	0.1503756300000001	-1.442754200000000	5.140850699999997	H	0.24400563E+00	-0.13600473E+01	-0.94278434E+00
O	5.629689700000001	-4.496088099999997	2.476987400000001	H	-0.53578229E+00	-0.43599749E+00	0.15969685E+01
H	5.502161300000000	-4.932284499999997	1.613709200000000	O	1.852857400000000	-6.061412200000004	1.563957100000001
H	4.968230700000003	-5.008988000000001	3.053643199999998	H	1.629181500000001	-5.382003400000003	2.273896000000000
H	-0.93221521E+00	-0.91293754E+00	0.93839320E+00	H	1.697020299999999	-5.519098200000002	0.7809073199999996
C	0.15339471E+01	-0.30045858E+01	0.26130672E+01	O	-0.8347352300000005	-5.266326600000002	0.5446290600000000
C	0.17059147E+01	-0.17148470E+01	0.31114058E+01	H	5.677981919999997E-002	-4.865661199999999	0.6813893500000000
O	0.16245936E+01	-0.78442501E+00	0.20237794E+01	H	-0.9676075800000002	-5.602600400000000	1.4003274000000001
C	0.14382958E+01	-0.14063494E+01	0.79388657E+00	O	3.6156366000000002	-5.631629099999996	4.2177695000000002
C	0.14230631E+01	-0.29120177E+01	0.11797100E+01	H	2.971784000000000	-5.152724000000001	3.613472400000000
O	0.19493885E+01	-0.11923206E+01	0.42239974E+01	H	2.988310199999999	-6.249820299999997	4.610348100000004
C	0.22358298E+00	-0.89321787E+00	0.47378581E-01	O	-1.064077500000000	-4.184491900000003	4.353143499999998
O	-0.93221521E+00	-0.91293754E+00	0.93839320E+00	H	-0.1851336999999997	-3.980376800000002	

H	-1.4681929000000000	-4.845778199999998	3.731105200000000	H	-8.949881799999994E-002	-1.2381206000000000	4.168709999999999
O	4.0943186000000003	-3.1311043000000001	-1.1696196000000001	O	5.014831599999999	-2.400222799999999	1.2704389000000000
H	3.2219006000000001	-3.2405648000000000	-0.7995444000000004	H	5.3758504000000000	-3.0993490000000001	1.8418424000000000
H	4.553491099999996	-2.7633372000000000	-0.3870700000000003	H	5.4899960000000000	-1.6167654000000000	1.6211921000000000
O	-0.1480531700000001	-3.9450870000000000	-2.1989356000000000				
H	0.1505886400000000	-4.8556653000000001	-1.9863948000000000	C	0.15012376E+01	-0.26923015E+01	0.24924109E+01
H	1.425786800000000E-004	-3.622334999999999	-1.2686814000000000	C	0.17660620E+01	-0.13515910E+01	0.29226302E+01
O	4.4814122000000003	-6.8029567000000002	1.0416314000000000	O	0.19225876E+01	-0.45613624E+00	0.18865074E+01
H	4.261931699999999	-7.707462399999998	1.1109062000000001	C	0.14463008E+01	-0.10982164E+01	0.64473711E+00
H	3.583122599999998	-6.318308000000000	0.9797256800000004	C	0.13562997E+01	-0.25738431E+01	0.11077410E+01
O	1.9182386000000000	-3.8041426000000000	6.0783250000000004	O	0.18447682E+01	-0.91183169E+00	0.41370984E+01
H	2.5599580000000001	-4.459739999999999	6.353818699999997	C	0.14716005E+00	-0.37602346E+00	0.67879738E-01
H	1.862907899999999	-3.714635799999999	5.123896099999996	O	-0.91527385E+00	-0.50110869E+00	0.10473032E+01
O	-2.5893630000000000	-2.7997250000000000	1.2242618000000001	O	1.388659899999999	-3.541319699999998	0.2123860499999999
H	-1.942074499999999	-3.500977669999999	1.2608396000000000	O	1.560363699999999	-3.728548800000000	3.3006837999999998
H	-1.944654799999999	-2.101413099999998	0.9521209600000002	C	0.32035501E+00	0.10997451E+01	-0.22811500E+00
O	1.231392199999999	-7.767717199999999	3.4636518000000001	O	-0.73905918E+00	0.14165581E+01	-0.12021281E+01
H	1.412076399999999	-7.2923160220000001	2.7132122000000001	H	0.22418194E+01	-0.84462053E+00	-0.92515317E-01
H	2.051009699999999	-8.391478400000004	3.4047239000000000	H	0.18086343E+00	0.17428738E+01	0.65586028E+00
O	-0.952419319999996	-1.2280989000000000	4.3555786000000003	H	0.12927268E+01	0.12395447E+01	-0.61444950E+00
H	-1.110546599999999	-2.1744854000000000	4.336986999999997	H	-0.10447705E+01	0.23512287E+01	-0.11313958E+01
H	5.2626903000000003E-002	-1.3142081000000001	4.240563399999998	H	-0.15025539E+00	-0.90367486E+00	-0.89626612E+00
O	5.2608074000000000	-2.262849699999999	1.123337899999999	H	-0.59628161E+00	-0.44717058E+00	0.18921863E+01
H	5.3394066000000002	-3.126066999999999	1.5740765000000001	O	1.910689499999999	-5.8712717100000004	1.7029840000000001
H	5.8231313000000000	-1.6279416000000000	1.6324988000000000	H	1.678020999999999	-5.2083795000000004	2.403075499999999
C	0.15436674E+01	-0.26734821E+01	0.25162954E+01	O	-1.0206816000000001	-5.070401999999996	0.2684386999999999
C	0.1872557E+01	-0.14143625E+01	0.30001479E+01	H	-0.1386950999999999	-4.7186262000000001	0.4648361600000000
O	0.17986056E+01	-0.40560699E+00	0.19372802E+01	H	-1.2434390000000000	-5.511824299999998	1.124778899999999
C	0.14997864E+01	-0.11137019E+01	0.67678568E+00	O	-1.0927975000000001	-4.239181399999997	4.221876899999998
C	0.14699127E+01	-0.25518971E+01	0.11417748E+01	H	-0.15709616000000001	-4.329948000000004	3.783123799999998
O	0.22018243E+01	-0.10127382E+01	0.41692889E+01	H	-1.6117192000000000	-4.887299099999999	3.6628639000000001
C	0.27092757E+00	-0.56289340E+00	-0.30280634E-01	O	3.6059823000000000	-5.2097188000000001	4.2729654000000004
O	-0.82453183E+00	-0.61899759E+00	0.83874674E+00	H	2.9527749000000001	-4.624284000000003	3.8478159000000001
O	1.3580186000000001	-3.451042199999998	0.2134675299999999	H	3.188822699999998	-6.094096699999997	4.134077699999997
O	1.4707340700000000	-3.8286034000000000	3.2225838000000000	O	3.7527538000000000	-3.302138999999999	-1.134496699999999
C	0.42314417E+00	0.86283363E+00	-0.54391832E+00	H	3.1121286000000001	-3.393560299999999	-0.4728556099999998
O	-0.77265433E+00	0.12933927E+01	-0.12090822E+01	H	4.438762099999999	-2.7329780000000001	-0.6339156599999999
H	0.24111545E+01	-0.10419076E+01	0.51040874E-01	O	0.22858426000000001	-4.017798199999997	-2.214378299999999
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H	0.12883616E+01	0.88688501E+00	-0.11546211E+01	H	0.2979497400000002	-3.7230900000000000	-1.2808677000000000
H	-0.72551390E+00	0.22942453E+01	-0.10078922E+01	O	1.6631073000000001	-4.049849100000003	5.957845700000000
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O	2.0730984000000001	-5.9823082000000003	1.7590005000000000	O	4.3626389000000003	-6.812576599999999	0.9445494599999995
H	1.9122110000000001	-5.204761699999997	2.343049199999998	H	4.090415499999999	-7.7141491000000002	0.7414034400000002
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O	-0.9748036500000002	-5.0684649000000004	0.4345163699999999	O	1.5197601000000001	-7.694797200000000	3.669404600000000
H	-0.1767484300000001	-4.5371414000000003	0.6038148999999999	H	1.5946590000000000	-7.096716599999997	2.857690499999999
H	-1.1357221000000000	-5.4131988000000000	1.3181045000000000	H	2.0148693000000000	-8.408407300000004	3.281838599999999
O	-1.049440399999999	-4.079143799999998	4.276884299999999	O	5.037180099999996	-2.2125669000000001	0.9290526200000000
H	-9.718142800000000E-002	-3.849269099999999	3.9785742000000002	H	5.1167495000000001	-3.077264700000002	1.3954061000000000
H	-1.2284383000000001	-4.8093810000000001	3.6980697000000000	H	5.511475299999999	-1.641205999999999	1.5098114000000000
O	3.6671648000000001	-5.2134740400000003	4.1956585000000004	O	-2.6463054000000001	-2.7474012000000000	0.9266505000000004
H	2.887742799999999	-4.713983599999999	3.9293809000000000	H	-2.158114499999999	-3.5071229000000002	0.5997711599999997
H	3.499587599999999	-6.0516693000000004	3.7589459999999998	H	-1.8950240000000000	-2.0883354000000001	1.0924630000000000
O	4.000957099999999	-3.111967599999999	-1.083485199999999	O	-0.8620100400000003	-1.498827799999999	4.634618699999999
H	3.196173899999999	-3.161700499999999	-0.5863616800000000	H	-0.9738836899999999	-2.522575999999999	4.6547113000000000
H	4.598279899999999	-3.136273399999999	-0.3221900400000001	H	7.203854599999995E-002	-1.4758148000000000	4.8973008000000000
O	0.11882463000000000	-3.824542399999999	-2.3261280000000002				
H	0.3664734499999998	-4.761171999999997	-2.4302134000000000	C	0.15272479E+01	-0.26111224E+01	0.24286940E+01
H	9.6162355000000005E-002	-3.711192699999998	-1.3063895000000001	C	0.19321046E+01	-0.13241917E+01	0.29272073E+01
O	1.4866640000000000	-3.9605570000000001	5.980372199999997	O	0.18297018E+01	-0.34475325E+00	0.19797035E+01
H	1.7753254000000001	-4.876261099999998	5.701621799999999	C	0.14775802E+01	-0.93031821E+00	0.71889995E+00
H	1.4951532000000001	-3.5661596000000002	5.100917899999998	C	0.13294007E+01	-0.24864976E+01	0.10825658E+01
O	4.508347399999999	-6.9435038000000002	1.4856760000000000	O	0.22889765E+01	-0.98201691E+00	0.40469109E+01
H	4.228084199999996	-7.4149867000000000	0.6884491000000004	C	0.17575745E+00	-0.39436555E+00	0.88096624E-01
H	3.694072199999999	-6.4298212000000001	1.6043137000000001	O	-0.94207874E+00	-0.78717982E+00	0.91461773E+00
O	-2.584390899999998	-2.589030699999999	1.3192697000000000	O	1.2254687000000000	-3.398054199999998	0.17298530000000001
H	-2.1511307000000000	-3.294789199999999	0.8640998899999998	O	1.5362382000000001	-3.7220463000000001	3.1831589999999998
H	-1.937828099999999	-1.8587753000000000	1.261779299999999	C	0.19890691E+00	0.11431093E+01	-0.1691237E+00
O	1.361386299999999	-7.7426640000000004	3.5442806000000000	O	-0.90756652E+00	0.17003394E+01	-0.9427660E+00
H	1.3765383000000000	-7.191518799999999	2.7944909000000000	H	0.23025272E+01	-0.73809589E+00	0.33563561E-01
H	1.8363985000000000	-8.540686499999996	3.2286320000000002	H	0.19696410E+00	0.16853146E+01	0.77647955E+00
O	-1.0495156000000001	-1.3739238000000000	4.139112199999996	H	0.10881939E+01	0.12261338E+01	-0.85390558E+00
H	-1.0290940000000000	-2.390634299999999	4.243428699999999	H	-0.10846680E+01	0.25194589E+01	-0.46921094E+00

H	0.14587750E-01	-0.90685295E+00	-0.86584702E+00	H	2.380463199999999	-4.8043325000000001	6.073054400000002
H	-0.53515648E+00	-0.87358406E+00	0.17945224E+01	H	1.479254300000000	-4.034638099999996	5.159063800000002
O	1.815739599999999	-5.907957399999999	1.769313200000000	O	4.321119699999997	-6.677961400000000	0.9385284600000001
H	1.732665700000001	-5.250349899999998	2.518634300000000	H	4.190769699999997	-7.949480750000003	0.4303767000000000
H	1.788090200000001	-5.235821200000002	1.094683099999999	H	3.394053000000000	-6.415360899999996	1.220407700000000
O	-0.968819309999999	-4.802905000000000	0.534559519999995	O	-0.8227983700000000	-1.511606100000001	4.621011700000004
H	-6.373330800000002E-002	-4.530314599999996	0.4235981100000003	H	-1.060436399999999	-2.407828100000001	4.281696700000004
H	-0.977669899999999	-5.364887099999998	1.343060399999999	H	7.403580399999997E-002	-1.633748900000001	4.908694900000004
O	-1.059057799999999	-4.275141800000001	4.251998500000000	O	1.330133800000000	-7.914773200000000	3.511087900000002
H	-0.1145117200000000	-4.104102600000000	4.131025300000001	H	1.362281099999999	-7.262898999999999	2.819794299999999
H	-1.139450800000001	-5.128694999999996	3.854909399999999	H	2.043872900000002	-8.593102599999999	3.197092600000000
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H	3.167670400000000	-3.439358299999999	-0.721483329999998	H	-0.697310400000000	-6.863825099999997	3.199578499999999
H	4.589586500000002	-3.006315700000000	-0.836021640000001	H	-2.187257199999999	-6.553989500000001	3.259784999999999
O	3.731904099999999	-5.205270000000000	4.154110700000004	O	5.828586399999998	-4.637827100000000	2.609365100000002
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O	8.270863900000000E-002	-3.835060200000000	-2.350375999999998				
H	0.437018479999999	-4.704413200000003	-2.650745399999999	C	0.15695037E+01	-0.26664354E+01	0.25835940E+01
H	0.249073660000000	-3.902130699999998	-1.355056000000000	C	0.17950055E+01	-0.13111260E+01	0.29763773E+01
O	1.611876700000001	-3.874089699999997	6.010587799999997	O	0.17420916E+01	-0.39912410E+00	0.19521569E+01
H	2.169144999999999	-4.613682599999997	6.016629899999999	C	0.15273337E+01	-0.11235507E+01	0.67660233E+00
H	1.613094100000001	-3.674043900000000	5.011024100000002	C	0.15130291E+01	-0.26209812E+01	0.11734537E+01
O	4.385663600000000	-6.830824100000001	1.304456099999999	O	0.183490964E+01	-0.79906026E+00	0.41519687E+01
H	4.244437600000004	-7.648242400000000	0.7695966100000001	C	0.21444302E+00	-0.63255061E+00	0.11112860E+00
H	3.534306800000000	-6.363486100000003	1.463767300000000	O	-0.94752756E+00	-0.10215052E+01	0.71661289E+00
O	-2.720686900000000	-2.756595700000001	0.9130367600000000	O	1.323503099999999	-3.627492000000002	0.34169643000000000
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H	-1.896982600000001	-2.175099400000001	0.815147109999995	C	0.35762666E+00	0.96420709E+00	-0.34121033E-01
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H	-0.914085429999998	-2.563493600000001	4.496079550000003	H	0.23667551E+01	-0.10374159E+01	0.10535516E-01
H	0.254066870000000	-1.671791000000000	4.846800100000003	H	0.26371447E+00	0.13397798E+01	0.10193263E+01
O	0.9379902500000003	-8.030189599999999	3.492157900000000	H	0.13347571E+01	0.12019791E+01	-0.46881904E+00
H	1.337083400000000	-7.397647600000000	2.829061100000001	H	-0.10316166E+01	0.23911225E+01	-0.55137438E+00
H	1.667910700000000	-8.748623900000001	3.541576399999998	H	0.84948358E-01	-0.11204087E+01	-0.10019725E+01
O	-1.540084000000000	-6.464188700000002	2.696870999999998	H	-0.10316185E+01	-0.52205130E+00	0.148645314E+01
H	-1.366278099999999	-7.375652100000001	3.006029200000000	O	1.873614099999999	-5.804826499999999	1.720269199999999
H	-2.520178800000001	-6.475963000000001	2.992615400000000	H	2.004788200000001	-5.114786099999999	2.381314199999998
C	0.15383664E+01	-0.26431354E+01	0.25435197E+01	H	1.540226300000000	-5.226703099999999	0.9829381000000004
C	0.18253982E+01	-0.13091504E+01	0.30155248E+01	O	-1.121009900000000	0.5239097700000003	0.353064400000000
O	0.15753079E+01	-0.29937709E+00	0.20052917E+01	H	-0.4504123600000001	-4.526564900000003	0.4097308399999999
C	0.13551075E+01	-0.10444363E+01	0.37732232E+01	O	-1.031762899999999	-5.615349300000001	1.277756799999999
C	0.14023812E+01	-0.25458709E+01	0.11366968E+01	H	-0.1643237900000000	-4.284911900000000	3.973944700000001
O	0.20890824E+01	-0.87572364E+00	0.41734165E+01	H	-0.141575739999999	-5.090329900000004	3.849679399999999
C	0.79910181E-01	-0.49338954E+00	0.63685521E-02	O	0.3652964000000001	-5.458614700000000	3.957897900000000
O	-0.10900298E+01	-0.69663298E+00	0.78363701E+00	H	3.1103906000000001	-4.663001399999997	3.898413900000000
O	1.263866399999999	-3.536986900000001	0.2847973200000002	H	3.376292990000002	-5.939798599999996	3.206606700000000
O	1.442159000000000	-3.765419699999998	3.338396700000001	O	0.3628569300000001	-4.071590399999998	-1.262388600000000
C	0.27146061E+00	-0.10070107E+01	-0.20204517E+00	H	2.878271700000000	-4.344653799999997	-0.7832624700000004
O	-0.85097717E+00	-0.15323037E+01	-0.95119444E+00	H	4.071823600000001	-3.426268799999999	-0.6638370900000002
H	0.22752098E+01	-0.91552083E+00	0.89002999E-01	O	-7.939536999999999E-002	-3.494887900000002	-0.204774400000000
H	0.43151950E+00	-0.13977922E+01	0.79483317E+00	H	2.871467300000000E-002	-4.294189000000001	-2.652012000000000
H	0.12098571E+01	-0.10947962E+01	-0.81717807E+00	H	0.3655481800000000	-3.765680999999998	-1.203570800000001
H	-0.10187253E+01	-0.24472457E+01	-0.67844671E+00	O	-0.909612769999996	-3.104473000000000	4.383573999999997
H	-0.44763091E-01	-0.10270971E+01	-0.94835357E+00	H	-0.9413182100000004	-2.235343700000000	4.088775499999997
H	-0.91541744E+00	-0.61502123E+00	0.17564737E+01	H	4.268046000000000E-002	-1.316696000000001	4.667240600000004
O	1.751009500000001	-5.933741000000000	1.709618300000000	O	4.213690399999999	-4.071590399999998	1.070689500000001
H	1.737622900000001	-5.192677700000000	2.405332000000000	H	4.152678700000001	-7.623591050000000	0.6130930500000003
H	1.568284300000000	-5.296577000000003	0.939829669999995	H	3.340880900000002	-6.489054099999997	0.935449580000000
O	-0.9504926200000001	-5.182991799999999	0.4005353500000001	O	1.760073900000001	-3.960358799999998	6.209450000000004
H	-8.981641099999998E-002	-4.714053400000001	0.5371522500000000	H	2.188779700000000	-4.802739700000001	6.047163900000001
H	-1.135542700000000	-5.435789800000002	1.341276200000000	H	1.179785400000000	-3.891948900000000	5.455483100000004
O	-0.929917970999999	-4.024542900000001	4.421425700000003	O	1.063669299999999	-8.083979799999998	3.045703600000000
H	-0.10005430000000000	-3.836772799999999	3.908668200000001	H	1.492476799999999	-7.388817500000000	2.516855899999999
H	-1.367535800000000	-4.599370900000003	3.788260900000000	H	1.707611299999999	-8.803468300000005	3.043807199999998
O	3.732925799999998	-5.112487299999997	4.039420599999997	O	-1.121967900000000	-6.523529899999998	2.668725600000001
H	3.022186899999999	-4.394813799999997	4.021669100000004	H	-0.325998399999999	-7.102215000000002	2.639680100000001
H	3.218421199999999	-5.914670199999998	3.806028099999998	H	-1.7870638000000001	-7.155934499999999	3.098656300000000
O	-6.226924799999998E-002	-3.786793100000001	-2.091033200000000	O	-2.946995999999999	-3.2594077000000001	0.8241402700000001
H	-2.9154333000000001E-002	-4.752073499999998	-2.277133600000000	H	-2.433461799999999	-3.916900600000000	0.3007319199999999
H	0.450070939999997	-3.685110100000002	-1.246771400000001	H	-2.2933549000000002	-2.529907399999999	0.6356326599999996
O	3.813302100000000	-3.737939200000000	-1.536363500000000				
H	3.006009999999998	-4.007869300000003	-1.025341400000001	C	0.16538927E+01	-0.26938123E+01	0.26080880E+01
H	4.378781799999996	-3.277136000000000	-0.826897400000000	C	0.18239274E+01	-0.13489238E+01	0.30164745E+01
O	1.693122900000001	-4.019661199999998	6.125064300000000	O	0.1709649E+01	-0.46157986E+01	0.19835723E+01

C	0.13338591E+01	-0.12397239E+01	0.76681073E+00	O	3.690833300000000	-5.5074905999999997	3.788109800000000
C	0.13301804E+01	-0.27130987E+01	0.12408658E+01	H	2.996926000000000	-4.908499299999999	3.589520100000001
O	0.19841294E+01	-0.93104698E+00	0.41739996E+01	H	3.155026500000000	-6.241944600000001	3.937045900000002
C	0.27245421E-01	-0.71772742E+00	0.15564851E+00	O	-0.740826309999999	4.121270100000003	4.263174700000004
O	-0.10654091E+01	-0.98319844E+00	0.91317449E+00	H	0.1995684500000001	-4.216876799999996	4.062514099999996
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O	1.6229582000000000	-3.728479800000001	3.518616699999999	O	3.905981500000002	-6.020223800000001	0.4347351600000001
C	0.31841511E+00	0.78730522E+00	-0.66135676E-02	H	3.347397599999999	-6.444893699999997	-0.199544799999999
O	-0.78889505E+00	0.14244591E+01	-0.61044060E+00	H	3.269871100000000	-5.760617899999997	1.090225000000001
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H	0.61420317E+00	0.12494916E+01	0.93822754E+00	H	2.524802000000002	-3.449451900000001	-0.927818079999999
H	0.12791222E+01	0.85512891E+00	-0.55711450E+00	H	3.927578800000000	-2.918274000000002	-0.82242423000000000
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H	-0.13028388E+00	-0.12465223E+01	-0.84785771E+00	H	2.406837200000000	-4.711420999999998	6.082873900000001
H	-0.10353888E+01	-0.57400269E+00	0.17792690E+01	H	1.713484100000001	-3.525822199999999	5.464400200000000
O	1.8995567000000000	-5.791956599999998	1.758909600000000	O	0.3715766600000000	-3.721379799999998	-2.217742299999998
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O	-1.0836763000000000	-4.279462800000001	4.258575399999998	O	4.806123000000003	-2.144565600000002	0.5534084900000003
H	-0.1486290800000000	-4.079815100000002	3.966038699999999	H	5.110912099999997	-2.946555599999999	0.9821653500000005
H	-1.2789898999999999	-5.051280099999996	3.679703500000000	H	5.344568999999999	-1.513539500000000	1.015775400000001
O	3.5851850999999999	-5.651417600000003	3.903261399999999	O	-1.108884699999999	-1.264425900000000	4.478714000000001
H	2.824368199999999	-5.138505399999997	3.622490400000002	H	-1.025545100000000	-2.190108099999998	4.367776199999998
H	3.2918987000000000	-6.499707400000001	3.604196299999999	H	-0.2308660300000000	-1.0261735000000001	4.725119900000002
O	-1.3424805000000000	-5.233678099999997	0.300615180999998	O	1.063525600000000	-8.370491200000000	2.769729900000002
H	-0.5220052800000002	-4.655692499999998	0.3482532600000001	H	1.257583700000001	-7.565619400000001	2.292804100000001
H	-1.2992718000000001	-5.627195600000003	1.208892600000000	H	1.794709099999999	-8.901214100000002	2.5388787800000002
O	3.5008918000000002	-3.828719500000001	-1.352474400000000	O	5.749701000000001	-4.620828000000004	1.978215499999999
H	2.890546899999999	-4.237371399999998	-0.7302097800000003	H	5.264651500000003	-5.137703900000000	1.272791700000000
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H	7.04771629999995E-002	-4.469346599999997	-2.052685799999999	C	0.14610383E+01	-0.26553712E+01	0.26244650E+01
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O	4.264898999999999	-6.579517100000003	0.8696901500000005	O	0.154865621E+01	-0.40122772E+00	0.20853242E+01
H	3.862344900000001	-7.116573500000003	9.959684999999996E-002	C	0.14374531E+01	-0.11019323E+01	0.84285034E+00
H	3.491164100000002	-6.024258299999996	1.026975299999999	C	0.14223195E+01	-0.25654978E+01	0.12507241E+01
O	0.8305597200000000	-7.971867399999998	2.909551599999999	O	0.17091365E+01	-0.83202728E+00	0.42404217E+01
H	1.1856633000000001	-7.208044600000000	2.404530299999998	C	0.21237646E+00	-0.49227309E+00	0.97787947E-01
H	1.5063157000000000	-8.641285099999993	2.604709400000000	O	-0.92626479E+00	-0.65189569E+00	0.10103601E+01
O	-0.9998270500000005	-1.279034000000000	4.043131200000004	O	1.494867200000001	-3.491959300000000	0.3460174500000000
H	-1.1332409000000001	-2.263235200000000	3.960145400000000	O	1.419907999999999	-3.721246600000002	3.4527656000000002
H	-0.1456422400000001	-1.244547600000000	4.412951299999996	C	0.50933823E+00	-0.96415845E+00	-0.26753499E+00
O	1.8482611000000000	-4.031747499999998	6.549675800000002	O	-0.63409340E+00	-0.17028875E+01	-0.61852238E+00
H	2.4244378000000002	-4.733559999999998	6.253176800000003	H	0.23402108E+01	-0.98361316E+00	0.29868787E+00
H	1.4340605000000000	-3.963821199999999	5.683622899999999	H	0.91330681E+00	-0.14373662E+01	0.64525212E+00
O	-1.4382438000000000	-6.367076199999996	2.749381300000000	H	0.13152890E+01	-0.10685968E+01	-0.97365742E+00
H	-0.6480215299999996	-6.892152799999999	2.870863099999998	H	-0.38757985E+00	-0.26451123E+01	-0.50896012E+00
H	-2.0576699000000001	-7.009826799999999	3.173806299999999	H	0.47485319E-01	-0.12112228E+01	-0.78767020E+00
O	4.9323287300000001	-2.608201100000001	0.4589837300000002	H	-0.57599570E+00	-0.30943253E+00	0.18532443E+01
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H	5.2241030000000004	-1.782051799999999	0.9913659099999999	H	1.3617732000000000	-5.333924200000002	2.5520187000000001
C	0.16740883E+01	-0.27412630E+01	0.27685966E+01	H	1.359427999999999	-5.403866299999998	1.0783107000000001
C	0.17498577E+01	-0.13782966E+01	0.31632061E+01	O	-0.9222769500000005	-4.869256599999999	0.2121894600000000
O	0.16081440E+01	-0.43889482E+00	0.21987974E+01	H	-0.1662889999999999	-4.304074199999996	0.3170275000000002
C	0.14516949E+01	-0.12058991E+01	0.92395379E+00	O	-1.1501304000000001	-3.993427300000000	4.0996686000000002
C	0.14694952E+01	-0.26463315E+01	0.13802597E+01	H	-0.2391261799999999	-3.835118700000002	3.768186099999999
O	0.18813220E+01	-0.88918413E+00	0.43330184E+01	H	-1.3359699000000000	-4.851157600000002	3.642307100000000
C	0.24368098E+00	-0.67794686E+00	0.18942350E+00	O	3.467417800000002	-5.591167099999998	3.549024499999999
O	-0.91336767E+00	-0.74036462E+00	0.10323557E+01	H	3.016490000000001	-4.709811199999999	3.569434100000001
O	1.3713291999999999	-3.561251200000001	0.4773242699999999	H	2.7556278000000001	-6.162164599999997	3.250861000000000
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C	0.59323465E+00	0.71243676E+00	-0.25424156E+00	H	3.602446699999998	-6.733967999999996	-0.4120394399999998
O	-0.59612531E+00	0.12504333E+01	-0.85853818E+00	H	3.337816900000000	-5.572633699999999	0.5924098000000003
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H	0.14487721E+01	0.73349956E+00	-0.91582569E+00	H	4.204358599999999	-3.587206000000001	-0.5980165200000005
H	-0.54439557E+00	0.22132774E+01	-0.76948857E+00	O	0.6249058100000001	-3.550632799999998	-2.1971432000000002
H	0.10559428E+00	-0.13001144E+01	-0.72914561E+00	H	0.6302466500000002	-4.517881899999999	-2.3410418000000002
H	-0.56268224E+00	-0.47630691E+00	0.19151931E+01	H	0.4684543099999998	-3.533931999999998	-1.140262000000001
O	1.5512927999999999	-5.861680999999999	1.831170699999999	O	1.8433714000000001	-3.844490099999998	6.230327199999996
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H	1.2365116000000000	-5.453534600000002	0.9711172300000005	H	1.6133071000000001	-3.701213000000001	5.269315699999999
O	-0.8803534800000002	-4.963855699999999	0.2593372800000000	O	4.818022899999999	-2.156836199999999	0.5578716999999997
H	-0.10911619000000000	-4.393374599999996	0.4993501499999999	H	4.9834268000000002	-2.9963685600000000	1.0606412000000001
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O	-1.608942499999999	-6.257958999999996	2.594209600000001	O	-0.77729902E+00	0.18045519E+01	-0.31852530E+00
H	-0.714378909999998	-6.525643299999996	2.478791800000002	H	0.21752954E+01	-0.91275822E+00	0.20688925E-01
H	-1.822652800000000	-7.126676200000003	3.066143200000000	H	0.73294932E+00	0.14310873E+01	0.10408199E+01
O	5.405898200000002	-4.618722700000002	2.003290600000001	H	0.10661365E+01	0.11245754E+01	-0.6435169E+00
H	5.057665499999997	-5.231852899999998	1.301059699999999	H	-0.13011541E+01	0.20565865E+01	0.44078917E+00
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O	-1.235804200000000	-1.107529000000000	4.323159200000001	H	-0.55522583E+00	-0.59525020E+00	0.22864534E+01
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H	-0.3705139900000002	-0.8852617400000002	4.684737100000004	H	1.380742100000000	-4.933502200000004	2.172753100000000
C	0.12613630E+01	-0.26039101E+01	0.26093650E+01	H	0.9850416400000005	-5.587366000000003	0.9805114700000005
C	0.17490404E+01	-0.13097458E+01	0.30673537E+01	O	-1.162609700000000	-4.240543800000002	4.436685500000003
O	0.17470223E+01	-0.42329695E+00	0.20149058E+01	H	-0.3305954800000000	-4.267761199999998	3.873151899999999
C	0.13487315E+01	-0.112511392E+01	0.79755902E+00	H	-1.709663399999999	4.830471300000001	3.898548900000002
C	0.11637263E+01	-0.25844286E+01	0.12248818E+01	O	0.1351682700000000	-4.946159200000003	-0.202551399999999
O	0.21031040E+01	-0.92990773E+00	0.42114791E+01	H	-0.6886748000000003	-4.342246099999997	0.168165360000001
C	0.46665523E-01	-0.47926017E+00	0.29716970E+00	H	-1.388821800000001	-5.495086299999996	0.599176849999998
O	-0.9813242E+00	-0.63709821E+00	0.12586721E+01	O	3.224714500000002	-5.663605300000004	3.974845600000001
O	1.058247100000000	-3.534819399999999	0.376588639999997	H	0.2547140900000000	-4.977035200000004	3.764090899999998
O	1.254333900000000	-3.721042600000001	3.369437800000000	H	3.211682100000000	-6.26450100000002	3.170005999999999
C	0.35227559E+00	0.10407467E+01	0.18311533E+00	O	0.754753129999999	-3.558043800000001	-2.216707000000001
O	-0.59175006E+00	0.16141324E+00	-0.77085616E+00	H	0.6211581800000003	-4.487304599999999	-2.170771799999998
H	0.21160111E+01	-0.97472541E+00	0.11871260E+00	H	0.6267049000000001	-3.330426099999999	-1.273244100000001
H	0.1483175E+00	0.14262739E+01	0.11993734E+01	O	1.348226399999999	-3.711001299999999	6.168148900000003
H	0.13743515E+01	0.13001879E+01	-0.19637937E+00	H	0.1323844800000000	-4.622365699999996	6.352732500000001
H	-0.50996814E+00	0.25350262E+01	-0.58467725E+00	H	0.1563201200000000	-3.644954599999998	5.235265499999997
H	-0.15659124E+00	-0.92118763E+00	-0.69154447E+00	O	-1.521781400000001	-6.285547700000004	2.469431600000001
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O	1.3420433000000001	-6.094542200000002	1.669941399999999	H	-0.1967053200000001	-7.065218899999996	2.884516600000000
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H	-1.5388035000000000	-4.855384599999998	3.407332799999998	H	-1.154119700000001	-2.328454199999999	4.492126599999997
O	-1.3988588000000000	-4.946361900000003	3.504682900000002E-002	H	-0.2748227300000002	-1.208329800000000	4.875480300000004
H	-0.6477151800000003	-4.403084800000002	0.3112967500000001	O	3.833752000000000	-6.578875199999997	0.6334546500000001
H	-1.5491518000000000	-5.575751000000003	0.7573274800000005	H	0.375725059999999	-7.303284500000002	1.806421200000000E-002
O	3.181017400000000	-5.567004599999997	3.901625199999998	O	2.913484800000000	-6.440103500000002	0.834127900000003
H	2.635768980000000	-4.809695699999998	3.786978500000000	H	0.3249046400000001	-2.523128300000002	0.545277319999995
H	2.7539136000000002	-6.196796100000003	3.336842499999999	H	-2.913034699999999	-3.460918200000001	0.6501482800000002
O	3.5936012000000002	-3.789930899999999	-1.264395800000000	H	-2.411571299999999	-2.059802099999999	0.6119931359999998
H	2.826785099999999	-4.022002600000004	-0.7131840499999996	O	1.177904400000001	-8.206649900000004	3.249981699999999
H	4.2401922000000001	-3.261961500000000	-0.6802802599999997	H	1.332195400000000	-7.482582599999998	2.650739900000000
O	0.384420519999999	-3.634082900000001	-2.212018500000001	H	1.966384500000000	-8.791114500000008	3.214305800000000
H	0.5930854800000005	-4.512471599999996	-2.411123100000002	C	0.13886724E+01	-0.27135741E+01	0.26316515E+01
H	0.677544339999997	-3.571926100000002	-1.289183399999999	C	0.17366044E+01	-0.13984657E+01	0.29761915E+01
O	1.797617400000000	-3.507997300000000	6.140126399999998	O	0.17301576E+01	-0.49041809E+00	0.18939003E+01
H	1.9861131000000001	-4.471993099999997	6.059574099999999	C	0.12189317E+01	-0.12202131E+01	0.74371255E+00
H	1.5418056000000000	-3.426012800000001	5.167614600000003	C	0.11765098E+01	-0.26777111E+01	0.12239673E+01
O	-1.4507848000000001	-6.523232399999996	2.397087099999998	O	0.19693629E+01	-0.903771187E+00	0.41154284E+01
H	-0.5080006599999999	-6.572762199999997	2.615439400000001	C	-0.80770601E-01	-0.50258982E+00	0.37566291E+00
H	-1.7939309000000001	-7.313531700000004	2.836198099999998	O	-0.11008893E+01	-0.83651480E+00	0.1374423E+01
O	4.0819013000000002	-6.486480600000002	8.516557099999995E-002	O	1.050407300000000	-3.672802999999999	0.3526719099999998
H	4.095690999999999	-7.417687100000002	-0.133468649999999	O	1.364556900000000	-3.746768400000001	3.494084299999999
H	3.141947000000000	-6.372424699999998	0.1604704100000001	C	0.70958078E-01	0.10175324E+01	0.26233139E+00
O	5.218026499999997	-4.920843600000004	2.152141700000000	O	-0.95126391E+00	0.17760302E+01	-0.35295327E+00
H	4.713023599999996	-5.479611600000001	1.534806799999999	H	0.19886651E+01	-0.96992358E+00	-0.17795624E-01
H	4.615767899999998	-4.981256499999998	2.977739999999998	H	0.27207656E+00	0.14477384E+01	0.12653637E+01
O	-1.2640255000000000	-1.2878485000000000	4.410213299999997	H	0.91452322E+00	0.10847529E+01	-0.53264256E+00
H	-1.545897999999999	-2.192665799999999	4.269459600000002	H	-0.14917814E+01	0.21263549E+01	0.38973022E+00
H	-0.7698504000000005	-1.504971600000000	5.212655700000000	H	-0.41637769E+00	-0.98327909E+00	-0.56882684E+00
O	0.9636124400000001	-8.218762099999993	3.273264000000002	H	-0.63824457E+00	-0.11660503E+01	0.2184328E+01
H	1.1165479000000000	-7.444044500000004	2.714967699999999	O	1.323597900000000	-5.976690900000004	2.033604800000000
H	1.7580754000000001	-8.753178800000006	3.060859100000001	H	1.270875699999999	-5.157936499999999	2.589166399999999
C	0.15197156E+01	-0.26590324E+01	0.25955082E+01	H	1.183350100000000	-5.506973799999999	1.219639700000001
C	0.18771681E+01	-0.13342367E+01	0.30128506E+01	O	1.503262600000000	-4.644146700000003	0.3764325800000002
O	0.18560128E+01	-0.38342602E+00	0.19252912E+01	H	-0.566428080000000	-4.351124500000001	0.2970972399999998
C	0.14268350E+01	-0.11370708E+01	0.78516222E+00	O	-1.565312599999999	-5.092532499999999	1.272954700000001
C	0.12504204E+01	-0.25663672E+01	0.11947485E+01	H	-0.159378900000001	-4.156044600000004	4.472110299999998
O	0.21015297E+01	-0.80087398E+00	0.41743350E+01	H	-1.513567700000001	-4.735803800000002	4.300726199999997
C	0.76780219E-01	-0.52427338E+00	0.33302543E+00	O	3.417269999999998	-5.534279699999999	3.823536400000001
O	-0.90943467E+00	-0.71644022E+00	0.13956525E+01	H	2.670589300000001	-4.877188999999996	4.015203999999998
O	0.713356809999995	-3.384397499999999	0.3686005200000000	H	3.0580318000000002	-6.089176600000001	3.420854299999998
C	1.407829100000001	-3.619279399999999	3.420604800000000	O	-1.587754500000000	-6.090533500000003	2.754746500000000
C	0.27988078E+00	0.10016313E+01	0.11024099E+00	H	-0.6976835399999999	-6.263167300000001	2.411454599999999

H	-1.9759407000000000	-6.9287368999999996	2.936738399999999	H	1.9569302000000000	-8.899431200000004	2.8627292999999998
O	0.6448295200000004	-3.5023721000000001	-2.313171899999999	C	0.16666564E+01	-0.26513497E+01	0.27121938E+01
H	0.3945896500000001	-4.4256456000000002	-2.3516571000000002	C	0.17749742E+01	-0.13376307E+01	0.31531883E+01
H	0.9258290700000003	-3.376372599999998	-1.3658600000000001	O	0.18762317E+01	-0.43988274E+00	0.20862885E+01
O	1.5330245000000000	-3.7409783000000001	6.195566999999996	C	0.16742683E+01	-0.11513200E+01	0.83581494E+00
H	1.1680904000000001	-4.650757399999998	6.214805900000000	C	0.15734573E+01	-0.26067304E+01	0.12813091E+01
H	1.3346979000000001	-3.509476700000000	5.252132800000000	O	0.17874210E+01	-0.92733780E+00	0.43401813E+01
O	3.925334299999998	-3.852320400000000	-1.560120900000000	C	0.32944260E+00	-0.61559478E+00	0.20575346E+00
H	3.190268999999998	-3.6736276000000001	-0.9983205600000002	O	-0.76903099E+00	-0.95713592E+00	0.11186037E+01
H	4.595509299999998	-3.2863367000000001	-1.132147199999999	O	1.3434044000000001	-3.6193548000000000	0.5072423400000001
O	-0.9660899280000002	-1.299973899999999	4.579449300000003	O	1.3918159000000001	-3.713972399999998	3.487856799999999
H	-1.0666043000000001	-2.286011700000000	4.616435499999998	C	0.40587155E+00	0.85844793E+00	0.29293021E-01
H	3.528154199999998-E02	-1.343526199999999	4.838154399999996	O	-0.94134679E+00	0.14191742E+01	-0.37750676E+00
O	4.2315166000000000	-6.281990699999997	0.1043289200000001	H	0.25408874E+01	-0.10722191E+01	0.21512708E+00
H	3.8746349000000002	-7.146893099999998	0.197218189999999	H	0.70831370E+00	0.14110067E+01	0.98776225E+00
H	3.608847299999998	-5.709537199999998	-0.309836850000000	H	0.10493699E+01	0.11034120E+01	-0.77464864E+00
O	4.941059499999999	-2.097184899999998	0.6076995100000000	H	-0.14278317E+01	0.15987537E+01	0.44783498E+00
H	4.9094065000000002	-2.844007899999998	1.234305999999999	H	0.22811986E+00	-0.11895843E+01	-0.75572555E+00
H	5.3954101000000003	-1.376550900000000	1.1755644000000001	H	-0.38111044E+00	-0.15697274E+01	0.17683542E+01
O	5.132471599999997	-4.465746300000002	1.944208699999999	O	1.554945999999999	-6.0222651000000003	1.8789496000000001
H	4.7723364000000004	-5.173246800000003	1.3765764000000000	H	1.101742599999999	-5.3587799000000000	2.4387967000000002
H	4.900936299999997	-4.796506499999998	2.806927099999998	H	1.866268599999999	-5.393584999999999	1.2737961000000000
C	0.12018723E+01	-0.27028172E+01	0.27700512E+01	O	-1.3294888000000000	-4.4545192000000000	0.6741169599999999
C	0.15340874E+01	-0.13229461E+01	0.31183645E+01	H	-0.3560375000000001	4.176152899999999	0.6472142499999999
O	0.16035483E+01	-0.45706122E+00	0.20256751E+01	H	-1.3049352000000001	-5.314453000000000	1.0730010000000001
C	0.13588269E+01	-0.12222267E+01	0.85286545E+00	O	-1.2514611600000000	-4.3265345000000002	4.4296167999999998
C	0.12637269E+01	-0.26861965E+01	0.13621016E+01	H	-0.3915526600000000	-3.9908937999999998	4.0798411000000003
O	0.17330945E+01	-0.86868883E+00	0.42531601E+01	H	-1.397561199999999	-5.075676999999998	3.790759399999998
C	0.30604097E-01	-0.67212110E+00	0.22188273E+00	O	3.473507399999999	-5.547748300000003	3.7475298000000001
O	-0.10689745E+01	-0.86824529E+00	0.11278151E+01	H	2.856695100000000	-4.863247600000002	4.029416099999999
O	1.2206527000000000	-3.624678400000001	0.528073279999998	H	2.973718299999998	-5.857842400000000	2.992008999999999
O	1.3763631000000001	-3.713390800000000	3.617106900000000	O	1.6810520000000000	-4.189932999999999	6.1755250000000004
C	0.21651305E+00	0.87080507E+00	0.15263591E-01	H	1.206206899999999	-4.980456600000001	6.279921800000003
O	-0.10352825E+01	0.15169299E+01	-0.15094866E+00	H	1.642914700000000	-4.004119099999996	5.184235400000004
H	0.22309361E+01	-0.10851866E+01	0.14627787E+00	O	3.7797485000000002	-3.4014353000000002	-1.0969807000000000
H	0.63876142E+00	0.12447986E+01	0.95968018E+00	H	2.916992599999999	-3.640529799999999	-0.859203199999999
H	0.88431849E+00	0.10755563E+01	-0.79388348E+00	H	4.224394300000002	-3.103827700000001	-0.264543499999999
H	-0.14642394E+01	0.14012463E+01	0.72563717E+00	O	0.2717809699999999	-3.4840216000000002	-2.3313942000000001
H	-0.12997316E+00	-0.11772881E+01	-0.79835813E+00	H	0.6997730500000001	-4.4038775000000001	-2.609439099999999
H	-0.68154855E+00	-0.12492987E+01	0.19221258E+01	H	0.7657085500000004	-3.4737930000000001	-1.3331987000000001
O	1.319825199999999	-6.036664799999998	2.104497299999998	O	1.2212193000000000	-1.594201699999999	4.2755247000000001
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H	1.4615578000000000	-5.472576799999997	1.2999118000000001	H	-0.2909723900000003	-1.6384946000000000	4.4127150999999998
O	-1.4987136000000001	-4.2780239000000000	0.5937297900000004	O	2.0714128000000001	-6.4814388000000003	-1.0115759000000000
H	-0.4978947000000000	-4.342605599999997	0.6452522099999999	H	1.8260400000000001	-7.453263699999999	-0.9324124499999995
H	-1.7742359000000001	-5.057398000000001	1.1044537999999999	H	1.2316494000000000	-6.121041899999999	-0.6807110200000006
O	-1.2387576000000000	-4.130944800000000	4.290252299999997	O	5.488867899999998	-4.529968600000001	2.444345499999998
H	-0.3666851800000000	-3.8192170000000001	3.9801375000000001	H	0.5751846000000002	-5.243542500000002	1.8233050000000000
H	-1.3072078000000000	-4.9004181000000004	3.704386299999999	H	4.810812799999999	-4.978743100000000	3.0182625000000001
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H	2.9262288999999999	-5.946943000000001	3.2680655999999999	H	1.9917507000000001	-8.7535878000000000	3.3907661000000000
O	3.718474699999998	-3.894355099999998	-1.0326118000000000	O	1.152071499999999	-6.6124415000000001	2.736727399999999
H	2.775547899999998	-3.883603200000000	-0.709094099999995	H	-0.3405470500000002	-7.1399569000000001	2.9201310000000000
H	4.090194799999999	-3.175063300000001	-0.5349104799999997	H	-1.8185121000000000	-7.174715599999999	3.2042242000000001
O	0.9939512000000003	-3.3407510000000000	-2.3260602000000001				
H	0.5948111999999998	-4.142425099999997	-2.7763575000000000	C	0.15110328E+01	-0.27867062E+01	0.24547457E+01
H	1.0063248000000000	-3.497389800000001	-1.3325231000000000	C	0.18417033E+01	-0.14646509E+01	0.29235541E+01
O	1.4141741000000001	-3.972378599999999	6.477623399999997	O	0.19512783E+01	-0.55279290E+00	0.19417986E+01
H	1.1163673000000001	-4.886268999999999	6.655741899999998	C	0.16548828E+01	-0.12277634E+01	0.69276432E+00
H	1.2834166000000000	-3.956694800000002	5.4982479000000000	C	0.16195127E+01	-0.26909196E+01	0.10488402E+01
O	-1.3589729000000001	-1.5185980000000001	4.1286582000000003	O	0.20638210E+01	-0.11283635E+01	0.41111476E+01
H	-1.4228626000000000	-4.2812090000000002	4.078105599999998	C	0.29298854E+00	-0.82817301E+00	0.12316357E+00
H	-0.5263689700000005	-1.4824406000000001	4.590928999999998	O	-0.80241325E+00	-0.96179254E+00	0.10157471E+01
O	4.192797599999996	-6.248364699999998	0.4417571499999999	O	1.4738083000000000	-3.6833179000000000	0.2335768000000001
H	3.553760309999998	-7.023589099999997	0.5344773000000001	O	1.3956195000000000	-3.8396756000000001	3.164975699999998
H	3.6218156000000001	-5.5652381000000002	2.539373099999999E-002	C	0.32179459E+00	-0.65112765E+00	-0.28589350E+00
O	-1.521356399999999	-6.467160599999997	2.5504768000000002	O	-0.10383282E+01	0.11472787E+01	-0.48367240E+00
H	-0.6350441519999997	-6.775249699999998	2.4210802000000000	H	0.24163794E+01	-0.94110463E+00	-0.11429844E+00
H	-1.8747562000000000	-7.163523299999996	3.1660634999999999	H	0.80176340E+00	-0.12252238E+01	0.50684327E+00
O	5.454270799999998	-4.394453999999996	2.3160687000000002	H	0.84197937E+00	-0.81105124E+00	-0.12098770E+01
H	5.4470251000000003	-5.014644699999998	1.5579608000000000	H	-0.13970939E+01	0.12314605E+01	0.37237569E+00
H	4.770201199999998	-4.846408499999999	2.8699981000000001	H	0.17329360E+00	-0.15031571E+01	-0.73126090E+00
O	1.0556057000000001	-8.514435999999999	3.060820099999999	H	-0.66701595E+00	-0.17285266E+01	0.15805069E+01
H	1.1550252000000001	-7.5570325000000000	2.896816299999998	O	1.4074534999999999	-6.1129270000000000	1.5838649000000000

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H	1.5196722000000000	-5.9741280999999997	0.6766103300000004	H	1.8081921000000001	-3.9280309999999998	5.3153252000000002
O	-1.3279491999999999	-4.636222499999997	0.5201207300000003	O	1.1674344999999999	-8.2263453999999996	3.2176265000000002
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H	-0.9916147899999997	-5.0465380000000000	1.3821243999999999	H	1.9794200000000000	-8.744196999999997	3.049934899999998
O	3.4435207000000001	-5.648201199999999	3.6427577000000002	O	-2.9453035999999999	-2.0276839999999998	0.3600449399999998
H	2.8665246000000000	-4.8227028000000001	3.6429643000000000	H	-2.3424372000000000	-2.8452500000000001	0.2685483200000001
H	2.9469348000000002	-6.117834799999998	2.9616022000000002	H	-2.258142299999998	-1.3257886000000001	0.6067612700000002
O	-1.3247201000000000	-4.173925699999998	3.937634899999999	O	4.214972999999996	-6.934897200000000	0.9572736400000004
H	-0.3727982799999998	-4.049604000000001	3.720531799999998	H	4.2039444000000001	-7.791975599999998	1.374924300000000
H	-1.604653799999999	-5.059633100000001	3.598029799999999	H	3.4965041000000001	-7.0763919000000000	0.1914643100000000
O	3.8950190000000000	-3.259782400000002	-1.234866199999999	O	5.8057964000000002	-4.764036199999996	2.427817999999998
H	2.9992835000000002	-3.416535399999999	-0.8594811000000000	H	5.579049600000003	-5.4480208000000001	1.7634344000000000
H	4.354797099999999	-2.867490999999998	-0.471886399999998	H	5.0760788000000003	-5.0756714000000001	3.0871368000000001
O	0.7906703899999995	-3.2981934000000002	-2.5357710000000000				
H	1.0567375000000001	-4.107789699999997	-3.0175079000000000	C	0.17806139E+01	-0.28677533E+01	0.24763352E+01
H	0.8658826299999999	-3.621708899999998	-1.6159185000000000	C	0.20075049E+01	-0.15147588E+01	0.28999208E+01
O	1.2347002000000000	-3.9949080800000001	6.2158796000000001	O	0.21319307E+01	-0.64986426E+00	0.18076622E+01
H	0.8460383999999997	-4.831220799999996	6.2704715000000002	C	0.16721675E+01	-0.13516335E+01	0.66914787E+00
H	1.3569624000000000	-3.8981636000000002	5.235205599999996	C	0.16779187E+01	-0.28118621E+01	0.10765811E+01
O	4.345475399999998	-6.4108377000000001	0.9459219700000000	O	0.21803123E+01	-0.974474249E+00	0.3938617E+01
H	4.200451199999998	-7.316212199999998	1.1444794000000000	C	0.34883733E+00	-0.71684165E+00	0.25343416E+00
H	3.6215155000000001	-6.2838015000000000	0.2609131599999998	O	-0.56965177E+00	-0.81947355E+00	0.13288251E+01
O	1.3035862000000000	-8.208832299999992	3.282264899999999	O	1.3913221000000000	-3.733794899999999	0.2350291000000001
H	1.3571504000000001	-7.299693399999998	2.8124055000000001	O	1.6131603000000001	-3.904844999999999	3.360209700000000
H	2.172387899999999	-8.6221285000000005	3.173976699999999	C	0.53198310E+00	0.73862440E+00	-0.11462869E+00
O	-0.9239463000000000	-1.5055649000000000	4.244019599999997	O	-0.70046386E+00	0.13355783E+01	-0.61631342E+00
H	-1.1484860000000000	-2.4497933000000001	4.138865599999999	H	0.23746991E+01	-0.12182113E+01	-0.14655920E+00
H	-1.121100000000000E-002	-1.5275557000000000	4.482240799999996	H	0.96229948E+00	0.13683868E+01	0.73472399E+00
O	5.8098856000000003	-4.509078500000002	2.5607979000000000	H	0.12154028E+01	0.73269045E+00	-0.9779081E+00
H	5.357491399999999	-5.032792599999996	1.8331229000000000	H	-0.95004375E+00	0.20503918E+01	-0.71943082E-01
H	5.4760162000000001	-4.960929300000001	3.377725799999999	H	-0.25877840E-01	-0.12343552E+01	-0.66588084E+00
O	3.4562206000000000	-2.3932992000000000	6.204177699999998	H	-0.43565089E+00	-0.16162233E+01	0.18684971E+01
H	2.832193499999999	-2.1687077000000001	5.5011013000000002	O	1.5583290000000001	-6.112690899999996	1.745619899999999
H	3.1169923000000002	-3.218638100000002	6.621979699999998	H	1.2457898999999999	-5.535569999999999	2.4413507000000001
C	0.14902415E+01	-0.28378975E+01	0.24159925E+01	O	1.6154520000000001	-5.538264599999999	0.944600789999999
C	0.19724024E+01	-0.15791860E+01	0.28144617E+01	H	-0.1677512999999999	-4.227280999999999	0.809477977999999
O	0.21284825E+01	-0.65897977E+00	0.17517874E+01	H	-0.3312855900000002	-4.232297000000004	0.361488499999999
C	0.16431497E+01	-0.13745512E+01	0.59427060E+00	O	-1.0966908000000000	-4.997409300000002	1.383262299999999
C	0.15278735E+01	-0.28219614E+01	0.99894820E+00	H	3.0033004000000001	-5.495034099999999	3.520642300000000
O	0.20922067E+01	-0.11768886E+01	0.39914516E+01	H	3.228292499999999	-6.196523599999999	2.996056700000000
C	0.29010940E+00	-0.84882254E+00	0.12633735E+00	O	-1.0328997000000000	-4.417420000000002	4.007434800000004
O	-0.71311275E+00	-0.95174405E+00	0.11234660E+01	H	-0.2220991400000000	-4.134728700000001	3.549330299999998
O	1.3499378000000000	-3.691583699999998	7.911526800000002E-002	H	-1.2150988000000000	-5.153310499999999	3.488460059999999
O	1.4018257999999999	-3.8932541000000001	3.217566999999998	O	3.9307030000000000	-3.426626199999999	-1.2358864000000001
C	0.48894645E+00	0.64257892E+00	-0.50107948E-01	H	3.187792299999999	-3.499025099999999	-0.5939097000000003
O	-0.71481535E+00	0.12048877E+01	-0.60175127E+00	H	4.5348344000000003	-2.858520200000001	-0.754181529999999
H	0.23592309E+01	-0.11765464E+01	-0.20339491E+00	O	-3.8839637500000005	-3.1574639000000002	-2.4745128000000002
H	0.78245644E+00	0.10390014E+01	0.92395794E+00	H	0.8907439999999998	-4.045973499999997	-2.8358945000000002
H	0.13663404E+01	0.8688583E+00	-0.69547553E+00	H	1.041314449999999	-3.3805380000000000	-1.5368037000000001
H	-0.94509103E+00	0.18945181E+01	0.35598234E-01	O	1.6253084000000000	-3.908136299999999	6.269550599999999
H	0.33180623E-01	-0.13590130E+01	-0.82281986E+00	H	1.2700157999999999	-4.7917075000000004	6.3929942000000004
H	-0.57225183E+00	-0.17870265E+01	0.16401117E+01	H	1.5073114000000001	-3.822488599999998	5.255917499999998
O	1.2910385000000000	-6.193271000000002	1.6537131500000001	O	4.454764649999999	-6.897303000000000	0.6109819300000001
H	1.2745329999999999	-5.206067400000002	1.865347099999999	H	4.364876699999999	-7.833727299999999	0.621764729999999
H	1.3508138000000001	-6.157465600000001	0.731545149999999	H	3.569039039999999	-6.658220000000000	0.304393729999999
O	-1.3615058000000001	-4.376584499999999	0.3802975900000002	O	5.7987140000000004	-6.494059900000001	2.1168493000000002
H	-0.3879989999999999	-4.278430400000004	0.2623568900000001	H	5.577288099999999	-5.354216100000004	1.3718773000000000
H	-1.5527016000000000	-5.0766719000000000	1.0566153000000000	H	5.018485999999998	-4.910868800000003	2.7354609000000001
O	-1.1200579999999999	-4.474369600000002	3.8605706000000000	O	1.250944499999999	-8.509893699999999	3.152469299999999
H	-0.16890383000000000	-4.487968399999997	3.5336560000000001	H	1.3537459000000001	-7.859372699999998	2.4396106000000000
H	-1.4617321000000001	-5.157644099999997	3.242230499999998	H	2.190920199999999	-8.792729999999995	3.2816041000000000
O	3.550826199999999	-5.5590586000000002	3.5460813000000000	O	-1.0141658000000000	-1.5141697000000001	4.7375737900000001
H	2.9996548000000001	-4.786391400000003	3.4239149000000002	H	-1.0892137000000000	-2.4577379000000001	4.670315399999998
H	3.324039299999999	-5.998011700000002	2.7212318000000000	H	-7.629757299999994E-002	-1.450424600000001	4.997159400000001
O	4.013113800000002	-3.425822800000002	-1.342186399999999	O	-1.435324899999999	-6.706883099999998	2.4130668000000002
H	3.1440378000000000	-3.604806099999998	-0.8189414299999997	H	-1.164615299999999	-7.264346899999996	1.7008198000000001
H	4.5195676000000002	-2.938880300000001	-0.6334649399999998	H	-1.761610799999999	-7.357833000000002	3.095548299999999
O	0.8930310500000005	-3.403940299999999	-2.577278000000002				
H	0.9174631699999999	-4.367953499999996	-2.7387489000000000	C	0.17499041E+01	-0.28835518E+01	0.25968427E+01
H	1.1288175000000000	-3.419405400000000	-1.6024548000000001	C	0.190269905E+01	-0.15157045E+01	0.31019972E+01
O	-1.1004973000000000	-1.657215099999999	4.3146806000000000	O	0.19587997E+01	-0.56899690E+00	0.20897162E+01
H	-1.3903269000000000	-2.6186596000000000	4.284957099999997	C	0.16807555E+01	-0.13615854E+01	0.78875384E+00
H	-0.11885724000000000	-1.8192058000000000	4.367815000000002	C	0.17613150E+01	-0.27843432E+01	0.11862112E+01
O	1.7162621000000000	-4.185622999999996	6.276415700000003	O	0.19369178E+01	-0.10901610E+01	0.42853442E+01

C	0.35256232E+00	-0.87414734E+00	0.21726297E+00	O	-0.9234858400000000	-4.4349059999999998	4.1861284999999997
O	-0.59840770E+00	-0.88481182E+00	0.12813742E+01	H	-2.376028499999999E-002	-4.3179430999999999	3.7678856999999999
O	1.5281545999999999	-3.6908960000000000	0.30773630000000002	H	-1.3074977999999999	-5.1660057999999998	3.6900667000000000
O	1.5979345000000000	-3.957892499999998	3.3127143000000001	O	3.7889438000000002	-3.9026000000000002	-1.3672461000000000
C	0.54682435E+00	0.55901242E+00	-0.29117606E+00	H	3.0156849999999999	0.4536707999999999	-0.8238284900000002
O	-0.79881918E+00	0.11404188E+01	-0.57202345E+00	H	4.1921732000000000	-3.1511868000000001	-0.8489325800000005
H	0.25102915E+01	-0.10507453E+01	0.12908948E+00	O	0.6252522299999996	-3.2291365000000001	-2.2000538000000001
H	0.94399168E+00	0.11687869E+01	0.47576759E+00	H	0.9819336800000003	-4.0669408999999996	-2.5587149000000000
H	0.12074402E+01	0.58878903E+00	-0.12286408E+01	H	0.7919554399999995	-3.2873720000000000	-1.2208741000000001
H	-0.10141069E+01	0.18231834E+01	0.82892096E-01	O	1.6227475000000000	-4.0886882000000000	6.3678704000000002
H	-0.77699708E-01	-0.15223936E+01	-0.55518721E+00	H	2.2133997000000001	4.8433124000000003	6.4506530000000000
H	-0.37620028E+00	-0.16554678E+01	0.18824124E+01	H	1.4763953999999999	-4.0034809999999998	5.3484540000000003
O	1.2928002999999999	-6.1214743000000000	1.6552572000000001	O	5.8147789000000003	-4.7489170999999999	2.1211232000000000
H	1.3496638000000001	-5.4125135999999996	2.3299775999999999	H	5.6368638000000004	-5.2903366800000001	1.3455804000000000
H	1.5414089000000000	-5.60008719010000003	0.8172790100000003	H	5.0561487999999999	-4.9507108000000004	2.6539804999999999
O	-1.1838256000000000	-4.1819965999999997	0.6883307400000005	O	-1.5514332000000000	-6.2957112999999998	2.1233765000000000
H	-0.2388758699999999	-4.0025798000000004	0.7375908599999996	H	-0.7385925899999999	-6.6889593999999999	1.8259269600000000
H	-1.2973110000000001	-4.8215189000000001	1.4195142999999999	H	-1.8334569000000001	-6.9807039999999999	2.7401477000000001
O	3.4189140999999998	-5.8754356000000003	3.5410355999999998	O	5.3286255999999996	-2.2912908000000001	0.5430884099999997
H	2.7241038999999998	-5.1826141000000003	3.5130669000000001	H	5.3839180999999998	-3.1207006000000002	1.0582026000000000
H	3.2349019000000001	-6.1649696000000000	2.6009050000000000	H	5.8045910999999997	-1.6183839000000000	1.1110454000000001
O	-0.8629450100000001	-4.5404021999999997	4.2204984999999997	O	4.3835968000000003	-6.8108097999999997	0.5511931300000003
H	9.706922699999994E-002	-4.5276114999999999	4.0783680000000002	H	4.4246240999999999	-7.7286112999999999	0.39301593000000001
H	-1.3428097000000001	-5.1294908000000001	3.5682309999999998	H	3.6341584999999998	-6.5523974000000003	-3.891987399999998E-002
O	3.9040431000000000	-3.6736650000000002	-1.2684816000000001	O	-0.9494514699999999	-1.5016791000000000	4.6750930999999998
H	3.0909018000000001	-3.6103740000000002	-0.7749687400000004	H	-1.1460106000000001	-2.4964944999999998	4.6811999000000002
H	4.5780731000000001	-3.3146958999999998	-0.6713795999999997	H	1.7782553000000000E-002	-1.6221563000000001	4.7706106999999998
O	0.7245764500000004	-3.2390574000000001	-2.3875378000000000				
H	0.8551838899999995	-4.1349267999999997	-2.6640682000000000	C	0.18737193E+01	-0.28953451E+01	0.26294164E+01
H	0.9260772499999996	-3.3503986000000001	-1.4323128000000001	C	0.18944772E+01	-0.15253158E+01	0.31014707E+01
O	-1.4364497000000001	-6.3962332999999996	2.3632314000000001	O	0.20758541E+01	-0.64521236E+00	0.20346482E+01
H	-0.5123823899999997	-6.5235820999999996	2.0642990000000001	C	0.18722828E+01	-0.13308195E+01	0.85063688E+00
H	-1.5702734000000000	-7.3164911000000004	2.6907827000000002	C	0.18165511E+01	-0.27767184E+01	0.12824290E+01
O	-1.0576421000000000	-1.5848154999999999	4.4382557000000000	O	0.17581777E+01	-0.10349883E+01	0.42360663E+01
H	-0.8152744699999997	-2.5192270000000000	4.1494074999999997	C	0.58842928E+00	-0.76288744E+00	0.13910617E+00
H	-0.3051368699999999	-1.4296039000000000	5.0030104000000000	O	-0.56464126E+00	-0.88651921E+00	0.10602894E+01
O	4.5368642000000001	-6.7191463999999996	0.7670234900000003	O	1.5676691000000000	-3.7629418000000001	0.3804626199999997
H	4.5403599999999997	-7.5546810999999998	0.2817493500000001	O	1.5839483000000001	-3.9289646999999999	3.4305303000000000
H	3.7785627000000002	-6.2751805000000003	0.2838454799999998	C	0.69037918E+00	0.72063714E+00	0.202304346E-01
O	1.7931250999999999	-4.1120380999999996	6.4513059000000004	O	-0.47234296E+00	0.14095365E+01	-0.40607288E+00
H	1.5597555999999999	-5.0354473999999998	6.4658293000000002	H	0.26969384E+01	-0.10161139E+01	0.13126222E+00
H	1.4761090000000000	-3.7935330999999999	5.5908085999999999	H	0.89280432E+00	0.10752304E+01	0.10457807E+01
O	1.2946000000000000	-8.5575462000000009	3.2993187000000002	H	0.14730470E+01	0.98745526E+00	-0.65360711E+00
H	1.6247638000000000	-7.7205775000000001	3.0780989999999999	H	-0.95922307E+00	0.14098743E+01	0.44311287E+00
H	2.1129999000000002	-9.0862216160000000	3.2364552000000000	H	0.43838215E+00	-0.12369623E+01	-0.82436661E+00
O	5.9292543000000002	-4.7418836000000004	2.1681572999999998	H	-0.45517005E+00	-0.15702556E+01	0.17513884E+01
H	5.3321731000000003	-5.4666123000000004	1.7782498000000000	O	1.1107402000000000	-6.1204919999999997	1.6577827000000001
H	5.5925946000000000	-4.6367544000000001	3.0765680999999998	H	1.2959390000000000	-5.2659564999999997	2.1438131000000000
C	0.17377136E+01	-0.27984279E+01	0.25997705E+01	O	-1.0674482999999999	-4.4603732000000003	0.15956276999999999
C	0.18527159E+01	-0.15209778E+01	0.31342084E+01	H	-0.15345878999999999	-4.1965339050000004	0.34880483000000000
O	0.21052264E+01	-0.56318635E+00	0.20841367E+01	H	-0.13068036000000001	-0.97801900000000003	1.0018894000000000
C	0.18006529E+01	-0.11783314E+01	0.82438271E+00	O	3.6964185999999999	-5.6564728999999998	3.5223176000000000
C	0.17323505E+01	-0.26638693E+01	0.12169668E+01	H	3.0144318999999999	-4.9137114000000004	0.35364822999999999
O	0.20264292E+01	-0.11588882E+01	0.43016431E+01	H	3.3065058000000001	-6.0743239999999999	2.7128106000000001
C	0.46098951E+00	-0.71922112E+00	0.34106958E+00	O	-1.0343058000000001	-4.2761193000000004	4.0015754000000001
O	-0.53949663E+00	-0.94651588E+00	0.13139809E+01	H	-7.2831477000000006E-002	-4.0540263000000003	3.8742679999999998
O	1.6570092000000001	-3.5684133999999998	0.3028039200000000	H	-1.2026211000000000	-5.1224572999999998	3.5379410000000000
H	1.5707078999999999	-3.9132939000000002	3.3615773999999998	O	3.6761626299999999	-3.6460655000000002	-1.4545078000000000
C	0.43560536E+00	-0.80762877E+00	-0.657657982E-01	H	2.8515628000000000	-3.6633439999999999	-0.9133640299999999
O	-0.86776904E+00	-0.12981598E+01	-0.589769781E+00	H	4.3817462000000003	-3.3514589000000001	-0.9113391699999999
H	0.26984085E+01	-0.94880666E+00	0.15512941E+00	O	0.9596241700000000	-2.9947789999999999	-2.3454820000000001
H	0.78517364E+00	-0.15304649E+01	0.70131395E+00	H	1.2512188000000000	-3.8862646999999999	-2.6047158000000001
H	0.11439748E+01	-0.80795461E+00	-0.89732797E+00	H	0.9003504599999997	-3.1016420999999998	-1.3718927000000001
H	-0.13585874E+01	-0.16660523E+01	0.21244548E+00	O	2.0620840000000000	-3.9340628000000000	6.3494975000000000
H	0.25061905E+00	-0.12739526E+01	-0.58976783E+00	H	2.2025336000000002	-4.9318350999999998	6.3231415999999996
H	-0.49117161E+00	-0.19148207E+01	0.16172013E+01	H	1.7451179000000001	-3.7857145999999999	5.4641706000000001
O	1.2502192000000001	-5.9416121000000004	1.6088967999999999	O	-1.5861628000000001	-6.3256462999999998	2.3826502999999999
H	1.3002602000000001	-5.2928892000000003	2.3623036000000002	H	-0.6960051000000000	-6.7032629999999997	2.1499044000000000
H	1.5302632000000000	-5.3364883000000001	0.9310873299999999	H	-1.9511537999999999	-7.0831895999999999	2.8043923999999998
O	-1.0266137000000000	-4.2487138000000000	0.3603861900000000	O	-1.1391433000000000	-1.5835695000000001	4.4086698000000002
H	-8.597522000000004E-002	-4.1299174000000001	0.3874563500000000	H	-1.1653989000000000	-2.5513439999999998	4.1497394999999999
H	-1.1936214999999999	-4.9368753999999999	1.0118670999999999	H	-0.26017258999999998	-1.5061382999999999	4.6982993999999998
O	3.6245640000000000	-5.7049225000000003	3.3768052000000002	O	4.3873711999999999	-6.6876432000000001	0.47792868999999999
H	2.9661141000000000	-4.9714102999999996	3.5152366000000002	H	4.3687982999999999	-7.6453784000000002	0.42679578000000001
H	3.3060279000000001	-6.0132433000000001	2.4793329000000002	H	3.6467532000000000	-6.4290468000000001	-0.10941948999999999

O	1.346216499999999	-8.775856400000003	2.500776699999999	H	0.13231791E+01	0.54651457E+00	-0.11825063E+01
H	1.376690800000000	-7.817022599999996	2.282886000000000	H	-0.78374151E+00	0.16902483E+01	0.36991125E+00
H	2.325859500000000	-8.953576599999999	2.643447300000001	H	0.19348718E+00	-0.12357055E+01	-0.60082951E+00
O	5.855416400000002	-4.745951999999999	2.109561000000001	H	-0.37741874E+00	-0.42829707E+00	0.20563993E+01
H	5.487129399999997	-5.296179399999998	1.391509399999999	O	1.114075900000000	-6.284846499999996	1.631789399999999
H	5.412149099999997	-5.117895599999998	2.911984900000002	H	1.124196100000000	-5.528892299999999	2.283217800000001
C	0.17873337E+01	-0.29106480E+01	0.26763491E+01	O	3.708426900000001	-5.622704200000003	3.794922199999998
C	0.18019193E+01	-0.16213183E+01	0.31911312E+01	H	2.953707899999999	-4.914739100000002	3.554352400000000
O	0.18661718E+01	-0.69427032E+00	0.21695984E+01	H	3.754717100000001	-6.122311800000003	2.910515000000002
C	0.18343621E+01	-0.13624619E+01	0.89942192E+00	O	-0.654543259999996	-4.573512400000003	-0.1150356600000000
C	0.17348356E+01	-0.28221016E+01	0.12375033E+01	H	0.3408163200000001	-4.671883999999999	-6.393845700000004-002
O	0.17527787E+01	-0.11483731E+01	0.43484023E+01	H	-1.054362399999999	-4.939205699999996	0.7853594800000000
C	0.57851439E+00	-0.81115349E+00	0.23288526E+00	O	-1.071634400000000	-4.305088300000004	3.991445699999999
O	-0.63803329E+00	-0.11182513E+01	0.96441699E+00	H	-0.1019539500000000	-4.319921999999997	4.037729100000000
O	1.793793400000000	-3.817739099999998	0.3968768899999998	H	-1.185513300000000	-4.670354999999998	3.096873500000001
O	1.549874100000000	-3.998558600000000	3.432705200000000	O	4.212996300000004	-3.468593499999999	-1.449381000000000
C	0.76368052E+00	0.67175118E+00	-0.12021165E+00	H	3.568403600000001	-3.635036800000000	-0.7266015599999998
O	-0.47489885E+00	0.12398720E+01	-0.53632229E+00	H	4.798439600000000	-2.791621100000000	-1.041924600000000
H	0.26381644E+01	-0.11233720E+01	0.16039748E+00	O	4.293757499999999	-6.395632100000003	0.5870057300000000
H	0.12584529E+01	0.13114210E+01	0.612331307E+00	H	4.235366000000000	-7.361673599999996	0.4850027900000002
H	0.14306366E+01	0.59478510E+00	0.98003669E+00	H	3.402660700000002	-6.179392199999997	0.2299849099999999
H	-0.88966809E+00	0.17374243E+01	0.19187282E+00	O	1.355415800000001	-3.173894499999998	-2.327515000000000
H	0.33882824E+00	-0.13207609E+01	-0.69585590E+00	H	1.351891600000001	-4.081788099999998	-2.741882800000000
H	-0.55794157E+00	-0.10906574E+01	0.19442811E+01	H	1.655107900000000	-3.279082400000001	-1.413372899999999
O	0.934089689999997	-6.289154800000004	1.686471800000001	O	-1.611568500000000	-6.186826100000002	1.764137600000000
H	1.097352600000000	-5.530025900000000	2.283071600000000	H	-0.6610764799999996	-6.289067499999998	1.809626999999999
H	1.442840100000000	-5.950622700000003	0.960239370000004	H	-2.000449199999998	-7.015498300000000	2.007668700000000
O	-0.937400380000003	-4.573149199999996	0.201165020000000	O	1.742432900000001	-4.094146000000003	6.412344499999997
H	-4.116147400000003-002	-4.182234399999996	0.383772199999999	H	1.641676300000001	-5.056161600000003	6.403601999999996
H	-0.109443800000000	-5.144598399999996	0.975825229999999	H	1.661172900000000	-3.869771500000001	5.472925599999999
O	3.641053499999999	-5.633351099999996	3.823490500000001	O	5.245528000000002	-1.812131699999999	0.2806973800000000
H	2.836248700000001	-5.028803000000003	3.769917000000000	H	4.973354399999998	-2.518918300000002	0.8465157700000000
H	3.458173400000002	-6.010186199999997	2.952353200000001	H	5.649305100000003	-1.255696799999999	0.9572135400000003
O	-1.104544800000000	-4.447091000000003	4.170576099999999	O	5.707031400000000	-4.547708600000000	2.172204000000001
H	-0.208311400000000	-4.392139499999999	3.780867000000002	H	5.453171399999998	-5.003562600000004	1.403251800000000
H	-1.455834699999999	-5.226725000000001	3.690589199999998	H	5.249091499999996	-5.127163399999997	2.796252200000001
O	3.910040700000001	-3.441461400000001	-1.551169599999999	O	2.195188400000002	-6.430448499999998	-1.076338700000000
H	3.174549100000001	-3.729835899999999	-0.9239390600000003	H	2.298296800000001	-7.368883200000000	-1.410935499999999
H	4.319085000000003	-2.686436699999998	-1.119840900000000	H	1.721552900000001	-6.042734399999996	-1.829394200000001
O	5.639425499999998	-4.449908999999999	2.366686699999998				
H	5.007689100000003	-4.758597100000002	1.653567800000000	C	0.15490616E+01	-0.28972425E+01	0.26405270E+01
H	4.995239400000000	-4.591794499999998	3.090084800000001	C	0.18438936E+01	-0.16032464E+01	0.32007920E+01
O	1.001279599999999	-3.174345699999999	-2.438758000000000	O	0.20586184E+01	-0.65137144E+00	0.22016011E+01
H	1.047309199999999	-4.124881600000001	-2.742497499999998	C	0.19190076E+01	-0.13162422E+01	0.90708303E+00
H	1.264989300000001	-3.226188099999999	-1.556827600000001	C	0.17404393E+01	-0.28461389E+01	0.12456455E+01
O	-1.866233199999999	-6.377092900000001	2.194730200000000	O	0.17616062E+01	-0.11131947E+01	0.43282001E+01
H	-0.895188920000005	-6.472093300000000	2.266566300000000	C	0.72646958E+00	-0.73312741E+00	0.18699444E+00
H	-2.276685800000001	-7.070830499999996	2.772336100000000	O	-0.49874385E+00	-0.10159703E+01	0.88631546E+00
O	1.513910700000001	-3.939006500000001	6.481750700000001	O	1.657383199999999	-3.701385699999999	0.3061212999999999
H	1.631633500000000	-4.914442300000002	6.512695800000004	O	1.260941899999999	-3.908798700000002	3.463441099999998
H	1.402910000000001	-3.786858099999999	5.563289000000002	C	0.92419432E+00	0.83674372E+00	-0.84421029E-01
O	4.341581500000002	-6.264765599999996	0.649792939999999	O	-0.32689977E+00	0.14350856E+01	-0.43351729E+00
H	4.566338799999996	-7.186779699999998	0.704597449999999	H	0.28152128E+01	-0.12774361E+01	0.35336388E+00
H	3.654204800000000	-6.333438000000001	-7.055613800000004-E02	H	0.14410165E+01	0.133222353E+01	0.77099978E+00
O	2.218966599999999	-6.583859900000002	-0.8956861600000001	H	0.15158464E+01	0.95188664E+00	-0.10210269E+01
H	2.012552100000002	-7.471653700000001	-1.252595500000000	H	-0.57608112E+00	0.20163594E+01	0.30422314E+00
H	1.724142000000001	-5.931699199999997	-1.332729899999999	H	0.58424108E+00	-0.13960856E+01	-0.72146339E+00
O	-1.155620099999999	-1.628886300000000	4.056267600000000	H	-0.53055120E+00	-0.60407864E+00	0.17623463E+01
H	-1.241646199999999	-2.618734299999998	4.250554400000004	O	1.597243500000000	-5.993682200000003	1.774948000000000
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C	0.16496266E+01	-0.29802481E+01	0.26626887E+01	H	1.602872700000000	-5.192348199999999	1.195063999999999
C	0.17281340E+01	-0.16318600E+01	0.32331404E+01	O	-0.751435349999999	-4.601286899999998	-0.3676188000000002
O	0.18467098E+01	-0.64658532E+00	0.22306798E+01	H	4.784963300000003-E02	-0.196431099999999	-5.064231200000002-E02
C	0.17544772E+01	-0.13833862E+01	0.87392140E+00	H	-1.013470499999999	-5.020540800000000	0.5037970800000001
C	0.18299046E+01	-0.28495823E+01	0.12340585E+01	H	0.354168519999999	-5.534565100000000	3.858274746000000
O	0.16441313E+01	-0.12182543E+01	0.43892110E+01	H	0.359906100000000	-5.794174299999999	2.920840200000002
C	0.48578705E+00	-0.69545276E+00	0.28270095E+00	O	-0.9643384000000004	-4.947082199999997	4.515402700000001
O	-0.63004126E+00	-0.72837699E+00	0.11508176E+01	H	-0.1154380800000000	-4.587354399999997	4.205833799999997
O	1.944649999999999	-3.753654300000000	0.3804674499999998	H	-1.385912899999999	-5.161334100000004	3.701388100000000
O	1.537147599999999	-4.111899999999998	3.329206399999999	O	3.972048000000000	-3.524628100000002	-1.536903799999999
C	0.78365362E+00	0.70772853E+00	-0.22513041E+00	H	3.344269100000000	-3.776112799999999	-0.8627122000000004
O	-0.39824780E+00	0.14652019E+01	-0.48168223E+00	H	4.522005400000003	-2.946718900000000	-0.9679033400000000
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H	1.7089383000000000	-4.244292999999999	5.261749300000000	C	0.19351772E+01	-0.16289609E+01	0.30364067E+01
O	1.1096854000000000	-3.063137400000000	-2.396835400000001	O	0.22601313E+01	-0.73041774E+00	0.20019683E+01
H	1.2535590000000001	-3.965395599999999	-2.679573400000002	C	0.19718931E+01	-0.14627304E+01	0.76458299E+00
H	1.468624699999999	-3.199053800000002	-1.486091300000000	C	0.16851431E+01	-0.28551446E+01	0.12004907E+01
O	-1.180490599999999	-2.154189300000001	4.2993279999999	O	0.19086730E+01	-0.12414771E+01	0.42425070E+01
H	-1.3657944000000000	-3.129831400000000	4.185532499999999	C	0.60582657E+00	-0.88481131E+00	0.20341876E+00
H	-0.2525986200000000	-2.100680699999998	4.416046500000002	O	-0.42384711E+00	-0.10782167E+01	0.11552740E+01
O	4.304081700000002	-6.306685299999998	1.107936300000000	O	1.604878100000001	-3.791668200000002	0.3194160999999998
H	4.112049200000004	-7.211652100000002	1.281116600000000	O	1.070792699999999	-3.832298999999999	3.359796499999999
H	3.743940199999999	-6.085694000000002	0.343432400000003	C	0.70612115E+00	0.63080173E+00	-0.68983321E-01
O	2.255258099999998	-6.475154899999997	-1.012773399999999	O	-0.49077256E+00	0.12101762E+01	-0.46926419E+00
H	2.269528600000001	-7.393613099999996	-1.263470400000001	H	0.27645271E+01	-0.14274527E+01	-0.38336303E-01
H	1.324908900000001	-6.482381799999997	-0.634850499999998	H	0.97583617E+00	0.10304143E+01	0.87961021E+00
O	-1.455198299999999	-6.261351000000003	1.925449400000000	H	0.14082250E+01	0.77680923B+00	-0.87989019E+00
H	-0.6679527400000004	-6.788392499999996	2.324818200000002	H	-0.96955449E+00	0.12203198E+01	0.32092251E+00
H	-2.1825065000000001	-6.911455100000004	2.038655799999999	H	0.32588386E+00	-0.13687865E+01	-0.77229000E+00
O	-2.739818699999998	-2.776819399999999	0.452505800000001	H	-0.12350424E+00	-0.17862302E+01	0.18427144E+01
H	-2.778659199999999	-2.905644999999998	-0.4919517299999998	O	1.335558900000001	-6.088892399999998	1.936613799999999
H	-1.835444000000001	-2.431375500000001	0.6213048599999996	H	0.158062999999998	2.419535000000002	1.1083177000000000
C	0.16462238E+01	-0.29146318E+01	0.25824248E+01	O	-0.865956450000004	-4.781761200000000	-0.2968534000000002
C	0.16997191E+01	-0.15202033E+01	0.31428029E+01	H	1.655699800000000E-002	-4.380461399999997	-2.493907700000000E-002
O	0.20460991E+01	-0.59704872E+00	0.21943690E+01	H	-1.223870500000001	-4.865541699999996	0.5711882999999998
C	0.20711727E+01	-0.12862379E+01	0.87071765E+00	O	3.589047700000001	-5.239972599999998	3.5575244000000001
C	0.19097183E+01	-0.28098841E+01	0.12055917E+01	H	3.304581100000000	-4.470203000000003	4.097508399999999
O	0.15727111E+01	-0.11558314E+01	0.43274870E+01	H	2.754522000000001	-5.568481000000002	3.199193000000002
C	0.77117866E+00	-0.75224621E+00	0.20534246E+00	O	-1.037434800000000	-2.480540300000002	4.685441700000002
O	-0.25651701E+00	-0.10122955E+01	0.11565734E+01	H	-0.4122993700000000	-3.137682400000001	4.272559600000001
O	2.002951599999998	-3.745060200000002	0.2940731100000003	H	-0.3942045499999999	-1.993129100000000	5.184488799999996
O	1.2991603000000000	-3.968849800000001	3.383936199999999	O	-0.9311834700000001	-5.443761600000002	4.606766099999998
C	0.89987630E+00	0.69033441E+00	-0.14471892E+00	H	-0.294133179999999	-4.878206200000002	4.214978600000002
O	-0.34076495E+00	0.12886711E+01	-0.52843236E+00	H	-1.452918500000000	-5.593293100000004	3.811987400000000
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H	-0.92262491E+00	0.14294354E+01	0.26825282E+00	O	1.080708999999999	-3.080885599999998	-2.353184499999998
H	0.60581647E+00	-0.13607162E+01	-0.63421165E+00	H	1.003327200000000	-4.002472700000002	-2.750349100000002
H	-0.14840628E+00	-0.42304869E+00	0.19244911E+01	H	1.096421499999999	-3.299638499999999	-1.399984300000001
O	0.125910269999999	-5.988166500000002	1.818637200000000	O	4.073562800000004	-3.749309900000001	-1.583265500000000
H	0.1569288000000000	-5.39234399999996	2.595434800000000	H	3.274345600000002	-3.899614800000002	-1.087299000000000
H	0.1760969599999999	-5.294506100000004	1.287377299999999	H	4.615953600000001	-3.240262800000000	-0.942770199999995
O	0.3558129699999998	-5.440173999999998	3.387457500000000	O	1.935860799999998	-4.347755799999998	6.181215500000004
H	0.2663136600000001	-5.017168800000003	3.280417200000000	H	1.336645099999999	-4.972234499999999	5.512651199999996
H	0.3596355899999998	-6.003514799999996	2.564791200000002	H	1.614925400000000	-4.267044600000002	5.321277300000002
O	-0.5667336400000004	-4.842649600000002	-0.256213709999998	O	-2.536439900000000	-2.704179100000002	0.4012806800000000
H	0.2268530000000000	-4.366293200000003	6.057744200000002E-002	H	-2.105876400000001	-3.217037299999999	-0.3044139100000001
H	-0.7617879499999999	-5.368558100000004	0.5343250699999996	H	-1.846152800000000	-2.086968600000001	0.7463099199999996
O	-0.1063987300000000	-5.068405900000001	4.363585399999998	O	2.452986500000002	6.419883099999998	-1.1254109000000001
H	-0.2023484999999999	-4.795543000000003	4.009274099999998	H	2.081131699999999	-7.275326300000001	-1.255176700000000
H	-0.1470605299999999	-5.567936300000004	3.615493900000001	H	1.740545599999999	-5.828192800000001	-1.438861200000001
O	0.4077698999999997	-3.800467199999999	-1.504272099999999	O	0.980357469999995	-8.646779600000003	2.579520999999999
H	0.3482445400000000	-3.926039900000001	-0.650166009999996	H	1.185449000000000	-7.722316300000001	2.265251699999999
H	0.4408233899999999	-2.969955300000001	-1.327156800000000	H	1.881293099999999	-8.973498499999998	2.5915501000000001
O	-0.141827600000001	-2.326095099999999	4.242618600000001				
H	-0.1254147500000000	-3.295808500000001	4.140336300000004	C	0.16188385E+01	-0.29120408E+01	0.26655029E+01
H	-0.1626862799999999	-2.250353300000000	4.159449099999998	C	0.18739273E+01	-0.15880918E+01	0.31370610E+01
O	0.1225881699999999	-3.145905800000000	-2.453280900000002	O	0.22748900E+01	-0.74278800E+00	0.20991965E+01
H	0.1309823400000000	-4.045595800000001	2.884694800000001	C	0.20739155E+01	-0.14566145E+01	0.86743005E+00
H	0.1532731700000000	-3.421734900000001	-1.509499700000001	C	0.18784657E+01	-0.29252301E+01	0.13022061E+01
O	0.1315805999999999	-4.398842600000000	6.220923000000000	O	0.18323970E+01	-0.11432443E+01	0.42926932E+01
H	0.1301710700000000	-5.032055600000004	6.436375199999996	C	0.79015318E+00	-0.87130398E+00	0.31188246E+00
H	0.1562481300000000	-4.348614000000004	5.260037200000002	O	-0.36556629E+00	-0.12066436E+01	0.11282198E+01
O	0.5822525999999997	-4.257807699999999	2.207369100000002	O	1.778654900000000	-3.824157099999999	0.3842373299999999
H	0.5579980700000001	-4.993609900000000	1.576420500000000	O	1.348508000000001	-3.909459500000002	3.532652999999998
H	0.4996532000000002	-4.276648700000000	2.829920800000000	C	0.82354063E+00	0.68131298E+00	0.15510016E+00
O	0.2763773700000002	-6.493416700000000	-1.149632999999999	O	-0.40510473E+00	0.12682098E+01	-0.30240674E+00
H	0.2264602700000002	-7.278633400000004	-1.003109000000000	H	0.29594468E+01	-0.12933140E+01	0.25596376E+00
H	0.2031179900000001	-5.889828299999996	-1.204068700000001	H	0.12112346E+01	0.13009487E+01	0.10277567E+01
O	0.4583390999999998	-6.708694099999998	1.036131799999999	H	0.15265371E+01	0.88233590E+00	-0.67831080E+00
H	0.4523820200000003	-7.590718899999997	0.677204200000003	H	-0.89632848E+00	0.16781598E+01	0.40770449E+00
H	0.4113835299999999	-6.274905900000003	0.2903259899999998	H	0.59438846E+00	-0.12277969E+01	-0.68399607E+00
O	-0.1435639300000001	-6.271981099999996	1.719382699999999	H	-0.25887987E+00	-0.19521748E+01	0.17362787E+01
H	-0.6888499799999997	-6.840520599999996	2.082832600000001	O	1.324557500000001	-6.102752599999996	1.8248598000000000
H	-2.181682800000002	-6.824322800000000	1.927625700000001	H	1.1109116000000001	-5.381562200000003	2.477055099999999
C	0.14376633E+01	-0.28429876E+01	0.25942007E+01	O	3.608059200000000	-5.288349000000002	3.8488554000000001

H	2.8927941000000001	-4.601168799999999	3.761901599999998	H	5.143015600000000	-4.908178000000003	1.7715263000000001
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H	0.33665663000000001	-4.711548600000004	-0.5943658699999996	H	1.154128300000000	-7.629546800000000	2.271662099999999
H	-0.892316239999998	-4.784196100000000	0.2828471699999998	H	2.108623000000001	-8.894395700000005	2.5949018000000001
O	-1.1370161000000001	-5.357685300000000	4.487983299999998	O	-1.048340400000001	-1.841157500000000	4.396027000000001
H	-0.4250001199999998	-4.981631000000001	3.945807299999998	H	-1.267824899999999	-2.796707000000001	4.426488199999997
H	-1.4965021000000001	-5.900512199999997	3.869836900000001	H	-8.32568110000000E-002	-1.706260900000000	4.761749199999997
O	1.112931200000000	-3.142085499999999	-2.232345800000000	O	4.444171800000003	-3.468257299999999	1.5840183000000001
H	0.9264500599999996	-4.001599200000002	-2.651764899999999	H	3.578744200000000	-3.593712500000001	1.2645728000000001
H	1.483409400000000	-3.361483400000000	-1.318536699999999	H	4.758589000000003	-2.759896200000000	-1.029743099999999
O	-1.024896700000000	-2.221121000000001	4.885980799999996				
H	-0.398420830000000	-2.874640299999998	4.503051999999997	C	0.15438651E+01	-0.28375602E+01	0.26628892E+01
H	-0.4794716700000002	-1.668569100000000	5.411731399999999	C	0.17679928E+01	-0.15829290E+01	0.32257970E+01
O	1.6196261000000001	-4.186396600000001	6.308266299999997	O	0.199826060E+01	-0.61385272E+00	0.22063739E+01
H	1.463280600000000	-5.047506300000002	5.673762999999996	C	0.17940289E+01	-0.12640603E+01	0.94607819E+00
H	1.428588400000000	-4.123394700000004	5.310576499999998	C	0.16087524E+01	-0.26931302E+01	0.12218910E+01
O	4.3827847000000002	-6.789653399999997	0.9403683299999997	O	0.20107500E+01	-0.12071864E+01	0.44290809E+01
H	3.683322000000001	-6.764634599999999	1.639749399999999	C	0.55102077E+00	-0.6085370E+00	0.25370766E+00
H	3.873794600000001	-6.475741600000001	0.1500032299999999	O	-0.67181312E+00	-0.10275979E+01	0.97845539E+00
O	4.374940099999999	-3.654785800000000	-1.628578899999999	O	1.602742099999999	-3.639483499999999	0.3800343000000003
H	3.664216600000000	-4.004057999999997	-1.117094700000000	O	1.247474299999999	-3.918932000000001	3.3677719000000002
H	4.702924999999996	-2.917855799999999	-1.086597599999999	C	0.7177988E+00	0.85508771E+00	0.27105992E+00
O	-1.923701099999999	-6.065560900000004	1.8591125300000001	O	-0.48880565E+00	0.15736672E+01	-0.15081445E+00
H	-1.185952799999999	-6.628526199999996	1.515570099999999	H	0.26191715E+01	-0.10135163E+01	0.27548856E+00
H	-2.232554800000000	-6.761312799999998	2.508759500000000	H	0.99644416E+00	0.11623222E+01	0.12718908E+01
O	5.252121299999998	-2.074977099999999	0.36334192900000001	H	0.15197337E+01	0.11752444E+01	-0.36266170E+00
H	5.272505800000002	-2.838816099999998	0.9726855500000001	H	-0.72277217E+00	0.23109200E+01	0.40962258E+00
H	5.761519700000000	-1.397068100000000	0.9798814300000005	H	0.42640393E+00	-0.99085473E+00	-0.75834606E+00
O	3.816622600000001	-2.583066500000002	5.738162299999999	H	-0.11602826E+01	0.19033388E+01	
H	0.3053448899999998	-2.238882300000002	5.277724199999998	O	1.023842100000000	-6.062133399999996	1.654105699999999
H	3.498259099999998	-3.420498400000000	6.104454600000004	H	0.8699686899999999	-5.420771300000002	2.366121900000000
C	0.15969875E+01	-0.29345006E+01	0.26342080E+01	O	-0.8274661599999995	-4.503284800000003	-0.4392355100000000
C	0.20306595E+01	-0.16541541E+01	0.31191330E+01	H	4.8432725000000003E-002	-4.211349700000004	-0.1257775499999999
O	0.21864192E+01	-0.74230658E+00	0.21185708E+01	H	-1.221507500000000	-4.828598000000001	0.3721474300000000
C	0.188221655E+01	-0.14599026E+01	0.86559388E+00	O	3.3554737000000001	-5.193266999999997	4.264774799999996
C	0.17126899E+01	-0.28943610E+01	0.12321599E+01	H	2.686302299999999	-4.516017400000000	3.991650700000001
O	0.20928552E+01	-0.12582341E+01	0.43230998E+01	H	2.887720799999999	-5.866600899999999	3.7644426000000002
C	0.69908643E+00	-0.74174493E+00	0.29711326E+00	O	-1.209834200000000	-4.560814800000002	4.4655680499999996
O	-0.52811789E+00	-0.99871819E+00	0.10690311E+01	H	-0.2977070399999998	-4.401098099999996	4.024969999999998
O	1.559272800000000	-3.831639500000001	0.3829348100000001	H	-1.813819000000001	-4.808923400000003	3.677709699999999
O	1.306691700000000	-3.980253899999999	3.480216599999999	O	1.5492763000000001	-2.878864999999998	-2.281120399999998
C	0.83391935E+00	0.78580771E+00	0.28409364E+00	H	1.514641700000001	-3.746299300000000	-2.695058599999999
O	-0.29685719E+00	0.13625938E+01	-0.33405593E+00	H	1.533227500000000	-3.056431100000002	-1.3198806000000001
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H	0.18310467E+01	0.11681937E+01	-0.10674961E+00	H	4.606429099999997	-4.360920000000001	2.886571599999999
H	-0.72931978E+00	0.17352827E+01	0.48809096E+00	O	-1.8625510000000001	-5.942646400000001	1.783943499999999
H	0.50319457E+00	-0.11281913E+01	-0.70907979E+00	H	-0.9691820500000002	-6.2243570000000004	1.8790878000000000
H	-0.35750692E+00	-0.74590196E+00	0.19606840E+01	H	-2.300000199999999	-6.488277499999997	2.4768164000000001
O	1.1820930000000001	-6.091339900000004	1.825371099999999	O	1.6782121000000001	-3.931046799999998	6.274181099999998
H	0.7998527399999995	-5.486376999999996	2.579671700000000	H	1.6772689000000001	-4.870503799999998	6.496500499999998
H	1.5205378000000001	-5.387842499999996	1.189434000000001	H	1.453415100000000	-3.928235200000000	5.309103999999996
O	-0.7512223000000001	-4.887084999999999	-0.5667902900000003	O	-1.042893099999999	-1.541273900000000	4.457429399999997
H	0.12903724000000000	-4.619407899999997	-0.2113416900000000	H	-0.9541704800000004	-2.4005512000000002	4.1122790000000000
H	-0.12745685000000000	-4.301997000000001	-6.914526100000003E-003	H	-0.2855489199999998	-1.508024999999999	4.9439054000000002
O	3.5997891000000002	-5.204264700000004	4.041127500000000	O	5.052662599999997	-1.926504000000000	0.518391289999995
H	2.908871899999998	-4.498272100000003	4.230916399999999	H	5.032764199999999	-2.607002899999999	1.2280838000000001
H	3.1322969000000001	-5.534510100000003	3.217801900000000	H	5.765682000000000	-1.407287000000001	0.833397379999999
O	-0.2217289000000000	-4.514862299999999	4.320285900000000	O	4.418403800000001	-6.367375100000003	0.6249024100000002
H	-0.3477947999999997	-4.381857000000001	3.881479399999999	H	4.071850399999998	-6.7366059000000001	1.4886801000000001
H	-0.17496171000000000	-4.951116599999998	3.602436260000000	H	3.615493700000000	-6.483909000000001	6.795278800000000-002
O	4.111031599999996	-6.299853100000000	0.8368652139999997	O	1.412870499999999	-8.683485299999999	2.2078788000000000
H	3.1653402000000002	-6.367476400000001	1.215445399999999	H	1.299240000000000	-7.750317400000001	1.9051572000000001
H	3.876509299999999	-6.174754199999997	-0.91412000000005E-002	H	2.284352399999999	-8.601576800000001	2.609658399999999
O	1.453138000000000	-3.015787800000000	-2.1250271000000001				
H	1.180162800000000	-3.920695300000002	-2.368687000000000	C	0.14862316E+01	-0.28878974E+01	0.24425595E+01
H	1.788073900000001	-3.130720900000000	-1.232076299999999	C	0.17117788E+01	-0.16050268E+01	0.30392992E+01
O	-1.689312900000000	-6.013363199999997	2.0292796000000002	O	0.19098927E+01	-0.59783660E+00	0.21384556E+01
H	-0.911492729999997	-6.239718299999998	1.5922506000000001	C	0.177653237E+01	-0.12105547E+01	0.83141495E+00
H	-2.115197700000000	-6.893314700000004	2.3623318000000002	C	0.16219440E+01	-0.27055284E+01	0.10652925E+01
O	1.250165000000000	-3.835457200000000	6.289664600000000	O	0.18836163E+01	-0.12481921E+01	0.42674631E+01
H	1.350673700000000	-4.789168400000003	6.386031899999999	C	0.59258260E+00	-0.55420382E+00	0.18562217E+00
H	1.169220799999999	-3.772293100000002	5.298910799999998	O	-0.64007836E+00	-0.83023880E+00	0.89228543E+00
O	5.492792299999996	-4.185676299999999	2.332845499999999	O	1.7939943000000000	-3.614806499999999	0.1344251999999999

O	1.373650700000000	-4.029518399999997	3.115676199999998	O	0.9872102000000004	-2.8744374000000001	-2.2085067000000000
C	0.73396789E+00	0.97107677E+00	0.29177275E+00	H	1.5283207000000001	-3.4616839000000001	-2.7004077000000000
O	-0.38715654E+00	0.17653048E+01	-0.38509460E+00	H	1.2264204999999999	-3.1753133999999998	-1.2906915000000001
H	0.26315151E+01	-0.98471767E+00	0.17098883E+00	O	3.995657099999999	-3.578361399999999	-1.5826811000000001
H	0.90834166E+00	0.13785377E+01	0.12605499E+01	H	3.4449103000000001	-4.1051659999999996	-0.9825993699999997
H	0.15913948E+01	0.13389897E+01	-0.27726936E+00	H	4.2391810000000003	-2.9049640999999999	-0.9212925800000003
H	-0.11357078E+01	0.19655120E+01	0.22532629E+00	O	1.7805591000000001	-3.661394899999999	6.1721028000000002
H	0.47047762E+00	-0.10332033E+01	-0.80620781E+00	H	1.5012489000000000	-4.5745405000000003	6.227546799999998
H	-0.39956848E+00	-0.85069377E+00	0.18223866E+01	H	1.6281671000000000	-3.4450064999999999	5.2235775999999996
O	1.1636416000000001	-6.171921199999999	1.3655940000000000	O	4.3976305000000000	-5.8938752000000001	0.6282615099999997
H	1.302412999999999	-5.561773299999996	2.1213201000000002	H	3.784171999999999	-6.2866514000000002	1.2053611000000000
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O	-0.8470602900000005	4.624517499999996	-0.302597899999998	O	5.147449499999996	-2.054107600000000	0.7331459500000005
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O	3.5528018000000001	-5.2299198000000002	4.020460199999996	O	-1.8668026000000000	-6.025197999999996	1.923919500000000
H	3.6264859000000000	-4.638097499999998	4.8078317000000004	H	-0.9733716100000005	-6.257659699999996	2.194804800000000
H	2.6746159999999999	-5.006000499999999	3.6264560000000001	H	-2.4314268000000001	-6.663099599999998	2.461062799999998
O	-0.9415839200000002	4.487931699999999	4.3654544000000001	O	-1.092201699999999	-1.585835099999999	4.2519429000000004
H	-0.1868284799999999	-4.232719399999997	3.8762059000000000	H	-1.159148499999999	-2.5512839000000000	4.200655399999996
H	-1.4573791000000000	-4.9985936000000004	3.763149499999999	H	-0.1183070000000000	-1.507727599999999	4.289842000000000
O	4.2369253000000002	-5.8252822000000002	0.785048639999996	O	5.7476475000000002	-4.179677899999997	2.703216700000000
H	3.951426099999999	-6.6170134000000003	1.2617818000000001	H	5.3646735000000003	-4.6631159000000002	1.9755341000000000
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O	0.9571318100000003	-3.038546999999999	-2.3458317000000002				
H	0.9701326399999999	-4.0320957000000002	-2.544764799999998	C	0.16251394E+01	-0.28581894E+01	0.26494446E+01
H	1.3826478000000000	-2.9681590000000000	-1.4371194000000000	C	0.18707965E+01	-0.15949903E+01	0.32925130E+01
O	4.274868699999999	-3.2286902000000000	-1.4766442000000000	O	0.19895217E+01	-0.59022187E+00	0.23498426E+01
H	3.5373803000000001	-3.7223752000000001	-0.9969643500000005	C	0.18805113E+01	-0.11537740E+01	0.10479014E+01
H	4.742674499999997	-2.769651999999998	-0.7259887200000003	C	0.17613333E+01	-0.26136454E+01	0.12673386E+01
O	5.567594399999999	-4.194816869999999	2.2024570000000000	O	0.18843738E+01	-0.12632368E+01	0.44882945E+01
H	5.233614499999998	-4.7551601000000003	1.487997199999999	C	0.75305492E+00	-0.55251195E+00	0.33361360E+00
H	4.7196524000000002	-4.145448199999997	2.7269258000000001	O	-0.48159576E+00	-0.99437900E+00	0.8867451671E+00
O	1.7304603000000001	-3.663877299999998	6.175437399999999	O	1.8741555000000001	-3.478678299999999	0.30743329000000003
H	1.3174515000000000	-4.551212099999999	6.320974099999999	O	1.4855155000000000	-3.931799499999999	3.417018399999999
H	1.4696170000000000	-3.488668099999999	5.243778800000003	C	0.70865857E+00	0.94830012E+00	0.44188360E+00
O	-1.815361599999999	-6.034820299999998	2.0189430000000002	O	-0.33494484E+00	0.16169523E+01	-0.20965112E+00
H	-0.9385410499999999	-6.495902600000000	1.9617312000000000	H	0.27883817E+01	-0.86776946E+00	0.48407088E+00
H	-2.2870979000000002	-6.6267123000000003	2.6531394000000001	H	0.75818217E+00	0.12184631E+01	0.14276187E+01
O	2.3680921000000001	-6.418171799999996	-1.2079362000000000	H	0.1569673972E+01	0.14181171E+01	-0.82408885E-02
H	2.266700699999999	-7.414512799999998	-1.2691732000000000	H	-0.1194276E+01	0.15733533E+01	0.40120881E+00
H	1.709114999999999	-6.099393199999997	-1.8745442000000001	H	0.73657635E+00	-0.87842511E+00	-0.69801409E-00
O	5.385146599999999	-1.7945473000000001	0.6696775000000004	H	-0.25268278E+00	-0.13800170E+01	0.17778187E+01
H	5.3449843000000001	-2.4284761000000001	1.3874025000000001	O	1.3315882999999999	-6.1705826000000004	1.574459099999999
H	6.2621770000000003	-1.3454140999999997	0.8575145899999997	H	1.2373320999999999	-5.486937799999998	2.2773250000000000
C	0.16102816E+01	-0.28314684E+01	0.25483858E+01	O	1.4855366000000001	-5.329947999999999	4.258327699999997
C	0.20131928E+01	-0.16259773E+01	0.30830961E+01	H	3.818673099999998	-4.4297601000000002	4.540922199999998
O	0.21751013E+01	-0.64135208E+00	0.21045203E+01	H	2.6254922000000001	-0.9468369000000001	3.9174601000000000
C	0.18630016E+01	-0.12027365E+01	0.86498375E+00	O	-0.8654614099999999	-4.922453499999996	-0.5501699199999998
C	0.17013273E+01	-0.27148838E+01	0.11530183E+01	H	-2.464183099999999	-4.641030899999996	-0.15707345000000000
O	0.21842724E+01	-0.12951637E+01	0.42997581E+01	H	-1.2448869000000000	-5.3298024000000002	0.2610034000000000
C	0.50629520E+00	-0.51793700E+00	0.31187706E+00	O	-0.1050753000000000	-4.258284899999996	4.0722883000000002
O	-0.65711381E+00	-0.10330262E+01	0.97034274E+00	H	-0.1274885299999999	-4.214703799999997	3.9498516000000001
O	1.6733070000000001	-3.6600728000000000	0.3252452599999997	H	-1.351213199999999	-3.9394420000000004	3.398044099999999
O	1.4245953000000000	-3.844339999999999	3.319323999999999	O	4.5609203000000003	-5.651500999999997	0.6817476399999999
C	0.57293364E+00	0.10054523E+01	0.31415873E+00	H	4.0996354000000004	-6.496203699999997	0.8333397200000001
O	-0.34896957E+00	0.17230739E+01	-0.47197717E+00	H	3.8974001000000000	-5.052481199999999	0.3290174499999999
H	0.26348684E+01	-0.92270023E+00	0.95937237E-01	O	0.9481635000000005	-2.949201299999999	-2.169581599999999
H	0.49916013E+00	0.13816797E+01	0.13450155E+01	H	0.9718672900000005	-3.8205133000000000	-2.570933999999998
H	0.15612553E+01	0.13973727E+01	0.47387684E-01	H	1.0215249000000000	-3.1313139000000002	-1.203967599999999
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H	0.44621577E+00	-0.70884857E+00	-0.75629941E+00	H	1.184041799999999	-4.6406887000000001	6.1610455000000002
H	-0.34912056E+00	-0.14234329E+01	0.18196474E+01	H	1.1274850000000001	-3.4771971000000002	5.313118199999999
O	0.9501502200000005	-6.105967599999996	1.637540199999999	O	5.075826099999996	-2.0816596000000001	0.6219324200000004
H	1.279351399999999	-5.3381039000000001	2.1473612000000002	H	5.0050659000000000	-2.4918965000000002	1.4583240000000000
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O	-0.9380375699999999	-4.530799199999997	-0.13539448000000001	O	-1.3935278000000000	-6.0947320000000003	1.9601360000000001
H	-1.889977400000001E-002	-4.3328128000000001	0.10318370000000000	H	-0.5205252299999995	-6.5705710000000002	1.9450780000000001
H	-1.1759636000000000	-5.0193477000000000	0.6948478099999995	H	-1.9915160000000001	-6.7533127000000004	2.2721030000000000
O	3.421075099999999	-5.480902999999996	4.020466899999997	O	4.1536087000000004	-2.685354999999999	5.4807043000000002
H	3.299103999999999	-4.9113613000000003	4.8431182000000002	H	3.619489699999999	-2.2857723000000001	4.7982911000000001
H	2.5447863000000002	-5.1176636000000002	3.622505299999998	H	3.488726499999998	-2.8938839000000001	6.1406235000000002
H	-1.0877827000000000	-4.3129533000000002	4.210375899999998	O	-1.0275831000000000	-1.571603099999999	4.1748830000000003
H	-0.1501604699999999	-4.2164428000000003	3.795277399999998	H	-1.108039999999999	-2.5555748000000000	4.2668273000000001
H	-1.4353031000000001	-5.044785799999997	3.6325606000000001	H	-0.1424208999999999	-1.3698577000000001	4.4638144000000004

O	5.809412700000002	-4.009374499999998	2.673083800000001	H	-0.28521497E+00	-0.14318513E+01	0.18861926E+01
H	5.496734700000002	-4.325876499999997	1.831756400000000	O	1.504052699999999	-6.234991400000002	1.508278199999999
H	5.808578500000003	-4.809073100000000	3.252270600000001	H	1.364404900000000	-5.557960399999998	2.210652600000000
C	0.18059173E+01	-0.29069395E+01	0.26111476E+01	H	1.830179800000000	-5.635357299999999	0.791613200000000
C	0.18229939E+01	-0.15746072E+01	0.30758342E+01	O	-0.8481457500000003	-4.585928799999996	4.079562900000000
O	0.20609104E+01	-0.67662942E+00	0.20771183E+01	H	0.1179108100000000	-4.604058400000004	3.890067100000000
C	0.18424985E+01	-0.13397820E+01	0.81837544E+00	O	-1.161308800000000	-4.967420200000003	3.249299699999999
C	0.18114103E+01	-0.282666402E+01	0.12266881E+01	H	9.330502699999999E-002	-4.232595599999998	-0.283319720000000
O	0.18212311E+01	-0.11478428E+01	0.42850916E+01	H	-0.888569999999997	-5.097576900000000	0.394439900000000
C	0.46902741E+00	-0.78707243E+00	0.19598354E+00	O	4.335609899999997	-5.556652699999999	1.026202700000000
O	-0.73288244E+00	-0.12569243E+01	0.77620056E+00	H	4.100356500000002	-6.380989800000000	1.515679400000000
O	1.840147200000001	-3.733548200000000	0.384598930000001	H	3.576421600000002	-5.601981900000002	0.375072450000000
O	1.773836400000000	-3.984788399999998	3.435537300000000	O	3.758978999999998	-3.531992000000001	4.728418500000001
C	0.61595570E+00	0.75478550E+00	0.26427926E+00	H	3.993029800000000	-4.421634000000002	4.700623700000004
O	-0.55172050E+00	0.13872865E+01	-0.15713632E+00	H	2.908946499999999	-5.337150699999996	4.312174500000002
H	0.26193066E+01	-0.12677206E+01	0.87452310E-01	O	-1.196946400000001	-6.299928000000004	1.798707499999999
H	0.77167608E+00	0.11204182E+01	0.12546579E+01	H	-0.2089789800000001	-6.414202099999998	1.610920399999999
H	0.13752534E+01	0.11652906E+01	-0.41148506E+00	H	-1.497597700000000	-6.911395200000003	2.495458900000000
H	-0.12599979E+01	0.12772251E+01	0.55422342E+00	O	1.891672400000000	-3.079872200000001	-2.194527599999998
H	0.57120909E+00	-0.12323297E+01	-0.83824202E+00	H	1.507181200000000	-3.917839299999998	-2.450275500000001
H	-0.50820191E+00	-0.19422923E+01	0.13934243E+01	H	1.754405000000000	-3.273646900000001	-1.194383200000001
O	1.435735400000000	-6.133732900000000	1.824676500000000	O	1.782432700000000	-3.941565199999999	6.459299800000001
H	1.481406500000001	-5.541518299999999	2.577488999999999	H	1.888960800000000	-4.939015699999997	6.645423199999998
H	1.840075100000000	-5.410435500000002	1.250505299999999	H	1.648371800000001	-3.914380500000000	5.494125099999998
O	-0.922849260000000	-4.201695700000001	3.812515799999999	O	6.048452600000001	-4.274764499999999	2.750265199999999
H	3.117232399999999E-002	-4.110237299999996	3.661016099999999	H	5.306051710000003	-4.715228599999997	2.269016999999999
H	-1.150084700000001	-4.856294400000003	3.117603599999998	H	5.879474100000004	-4.772041500000003	3.542134799999999
O	3.788129300000000	-5.214956500000004	4.649217900000000	O	-0.886611590000000	-1.729771699999999	4.153818499999999
H	4.038425100000004	-4.567647400000002	5.324374599999996	H	-0.933028900000005	-2.730415799999998	4.101076400000003
H	3.138438299999998	-4.739596099999999	4.050673200000003	H	-7.958228399999996E-004	-1.669267000000001	4.508520599999998
O	4.391776499999997	-5.445689500000003	0.936412470000005	O	1.158697899999999	-8.684889399999994	2.419675300000002
H	4.177240300000002	-6.350012999999997	1.264450000000001	H	1.190947100000000	-7.745911800000000	2.097197700000002
H	3.607948200000000	-5.151470599999997	0.3766388900000000	H	2.092960800000002	-8.735531599999998	2.667901899999999
O	-0.894874940000001	-4.591251200000002	-0.3903113999999998	O	5.119307199999997	-2.314761600000002	0.897418849999999
H	6.020731299999998E-002	-4.5770049375999999	-0.1087437599999998	H	5.562209400000004	-3.012606900000002	1.358938299999999
H	-1.215136700000000	-4.978559999999999	0.439732479999998	H	5.216953400000004	-1.579689200000000	1.475926800000001
O	1.502516200000001	-3.135386899999999	-0.207936910000001				
H	1.171522900000000	-4.031284299999997	-2.447677999999998	C	0.17798745E+01	-0.30190749E+01	0.2547503E+01
H	1.741487100000001	-3.393492999999999	-1.182138600000000	C	0.202099678E+01	-0.17552040E+01	0.30932571E+01
O	-1.399071000000000	-5.949391520000002	1.848893799999999	O	0.21746883E+01	-0.80904572E+00	0.21102091E+01
H	-0.458521330000000	-6.160879800000000	1.812322100000000	C	0.19335830E+01	-0.14866853E+01	0.84211068E+00
H	-1.806307799999999	-6.763737700000004	2.216441199999998	C	0.17979276E+01	-0.29544946E+01	0.11480922E+01
O	1.719844699999999	-4.000284999999999	6.307361000000002	O	0.20266871E+01	-0.13659203E+01	0.42972558E+01
H	1.596360900000001	-4.951598200000003	6.501389399999999	C	0.63508804E+00	-0.91561634E+00	0.27865067E+00
H	1.521150100000001	-3.894657099999999	5.379921999999996	O	-0.42603727E+00	-0.12400778E+01	0.11826841E+01
O	5.822159300000000	-3.987190300000000	2.713178800000001	O	1.714603499999999	-3.976967000000001	0.3715843600000000
H	5.263660500000003	-4.377956600000001	2.019801800000002	O	1.728007200000000	-4.089593500000003	3.327674000000000
H	5.626654000000003	-4.611660200000002	3.445167099999999	C	0.56422637E+00	-0.60806594E+00	0.18850991E+00
O	-0.988846479999997	-1.585610600000001	4.212105199999999	O	-0.66495894E+00	-0.10918429E+01	-0.24186241E+00
H	-0.922010799999995	-2.495225099999999	3.851303900000000	H	0.27861576E+01	-0.13081693E+01	0.14706568E+00
H	-4.44270030000000E-002	-1.316510200000000	4.297523899999998	H	0.83677155E+00	-0.94843702E+00	0.11489756E+01
O	4.067657099999998	-2.580214700000000	5.489943700000004	H	0.12816731E+01	-0.10401653E+01	-0.49141339E+00
H	3.396041900000002	-2.423965200000000	4.830561200000000	H	-0.13226610E+01	-0.95226778E+00	-0.44987442E+00
H	3.555837799999999	-2.544646800000002	6.346297200000004	H	0.36039137E+00	-0.13690026E+01	-0.72591108E+00
O	4.273976399999996	-3.430433400000001	-1.795514000000001	H	-0.19614395E+00	-0.79932995E+00	0.20281772E+01
H	3.479327099999999	-3.188635699999999	-1.338737300000001	O	1.507892500000001	-6.283080700000002	1.593124299999999
H	4.927056900000002	-3.063464980000000	-1.180004400000001	H	1.520581500000000	-5.621956599999999	2.344103800000001
C	0.19891018E+01	-0.30743361E+01	0.26178762E+01	H	1.468897899999999	-5.647153499999999	0.862843229999999
C	0.21068984E+01	-0.17649864E+01	0.31941614E+01	O	4.361180100000003	-5.772212500000002	1.105162000000000
O	0.20825925E+01	-0.81085916E+00	0.21758500E+01	H	3.877850399999999	-6.405974399999998	1.585636300000000
C	0.19357054E+01	-0.14375389E+01	0.90597785E+00	O	3.567590599999999	-5.406487699999996	0.697411099999995
C	0.18610834E+01	-0.29280509E+01	0.12449310E+01	H	4.030924500000002	-5.314199099999997	4.284787900000004
O	0.19898449E+01	-0.13626141E+01	0.43964929E+01	H	4.123281900000003	-4.543727399999999	4.905902700000004
C	0.63862999E+00	-0.91724563E+00	0.28846088E+00	H	3.313603600000000	-4.894184499999997	3.698615000000002
O	-0.51322062E+00	-0.14053607E+01	0.94281960E+00	O	-0.8434514100000001	-4.542236800000004	4.121670400000002
O	1.701213899999999	-3.854508000000000	0.401457239999999	H	0.1441480300000001	-4.513722300000004	3.936847000000002
O	1.748363099999999	-4.181157700000000	3.399773800000002	H	-1.142334299999999	-5.083886599999996	3.380280500000000
C	0.55174091E+00	0.59082891E+00	0.20468054E+00	O	-0.1086499000000000	-4.704101999999998	-0.592311649999999
O	-0.73533610E+00	0.10818731E+01	-0.24396167E+00	H	-0.1601804699999999	-4.550938000000004	-0.2443560200000001
H	0.27536554E+01	-0.11813502E+01	0.28222142E+00	O	-1.459253600000000	-4.935194899999999	0.277588699999999
H	0.86352549E+00	0.11166724E+01	0.11171023E+01	H	1.475527500000000	-4.183297500000001	-2.638901400000000
H	0.13056229E+01	0.92797063E+00	-0.58188451E+00	H	1.849535200000000	-3.490423799999999	-1.308367800000001
H	-0.13226078E+01	0.11622174E+01	0.52004679E+00	O	-1.301758400000000	-6.245445400000004	1.819065000000000
H	0.62374301E+00	-0.13844279E+01	-0.72365207E+00	H	-0.426772549999997	-6.546299499999999	1.787443500000000

H	-1.7104189000000001	-7.057183400000004	2.265016300000001	C	0.19413981E+01	-0.29579348E+01	0.12286550E+01
O	5.0086550000000001	-2.1726860000000001	0.7901748899999996	O	0.21197456E+01	-0.14492124E+01	0.42952678E+01
H	5.0858014000000002	-2.8657206000000002	1.435757299999999	C	0.69644683E+00	-0.99323129E+00	0.29084299E+00
H	5.0638679000000000	-1.4025760000000000	1.4011613000000001	O	-0.43380498E+00	-0.13782493E+01	0.10766495E+01
O	1.9016933000000000	-4.083882199999997	6.489716600000004	O	1.9206162000000000	-3.8433218000000000	0.3116314600000003
H	1.6165233000000001	-5.012892400000001	6.682049400000004	O	1.8143966000000000	-4.215015799999998	3.3053197000000001
H	1.8911270000000000	-4.061688799999998	5.510290500000000	C	0.64250825E+00	0.54772258E+00	0.35800261E-01
O	-0.9526890000000001	-1.8161540000000001	4.175746000000002	O	-0.62952699E+00	0.96511942E+00	-0.52454047E+00
H	-1.1131161999999999	-2.7700694000000001	3.9197660000000001	H	0.27922075E+01	-0.11633513E+01	0.24026814E+00
H	-2.538892400000002E-003	-1.8073413000000000	4.332312199999996	H	0.83010525E+00	0.10812296E+01	0.1015683E+01
O	1.3182343999999999	-8.712784799999997	2.4115058000000000	H	0.14773252E+01	0.78823043E+00	-0.65019383E+00
H	1.6375587000000000	-7.949382599999999	1.9553471000000000	H	-0.120757637E+01	0.12590655E+01	0.25470132E+00
H	2.1105255999999999	-9.227619799999994	2.558047199999999	H	0.46250176E+00	-0.14886926E+01	-0.66093572E+00
O	4.2581638000000002	-2.683260999999999	5.460049999999998	H	-0.24693170E+00	-0.11735759E+01	0.20567078E+01
H	3.4010395999999998	-2.340162299999998	5.0966956000000003	O	1.5965623000000000	-6.261157800000003	1.4710847000000000
H	4.0189959000000002	-2.861649400000001	6.384744699999997	H	1.376013699999999	-6.063569700000004	2.435871199999998
H				H	1.6178233000000000	-5.330847600000002	1.100924599999999
C	0.18376995E+01	-0.31244370E+01	0.24873294E+01	O	4.230466800000003	-5.644327200000000	1.017260199999999
C	0.19137574E+01	-0.18104579E+01	0.30616964E+01	H	3.504899200000001	-6.113737800000000	1.475099800000000
O	0.20461331E+01	-0.84161239E+00	0.2088809E+01	H	3.655450999999998	-4.858470900000004	0.771723089999994
C	0.18942010E+01	-0.14712227E+01	0.77298847E+00	O	-0.619592139999996	4.9316357720000002	-0.4415373400000000
C	0.18622574E+01	-0.294961945E+01	0.10970008E+01	H	0.2062746000000000	-0.4522198000000002	-0.1404080100000001
O	0.17709279E+01	-0.13937619E+01	0.42126700E+01	H	-0.8498504700000002	-5.385589000000004	0.3529161800000002
C	0.56081707E+00	-0.89530960E+00	0.21533416E+00	O	3.914464700000001	-5.46200299999997	4.393272900000004
O	-0.53893223E+00	-0.12679537E+01	0.10042009E+01	H	4.185908900000003	-4.577576900000004	4.746385700000003
O	1.7538975999999999	-3.8092766000000000	0.1079109699999999	H	3.024722699999999	-5.180022499999998	4.0524202000000002
O	1.6613789999999999	-4.237817899999996	3.2282060000000001	O	-0.8567532399999997	-4.787291899999996	4.0703101000000004
C	0.55231771E+00	0.58970849E+00	0.80295262E-01	H	0.1291865399999999	-4.787844899999996	3.915697699999999
O	-0.75211469E+00	0.10884975E+01	-0.31820307E+00	H	-1.169698799999999	-5.299985500000000	3.330428899999998
H	0.2680095E+01	-0.11526258E+01	-0.309592598E-02	O	1.7878543000000000	-3.48725709999999	-2.337441699999999
H	0.80569316E+00	0.10389390E+01	0.10515172E+01	H	1.542347399999999	-4.404396199999999	-2.468838200000000
H	0.13136422E+01	0.86770182E+00	-0.65825373E+00	H	1.876688300000001	-3.608479800000000	-1.343777800000000
H	-0.14142582E+01	0.91616375E+00	0.420023936E+00	O	1.718057299999999	-3.856640600000000	6.249927300000001
H	0.47358832E+00	-0.14112043E+01	-0.74277409E+00	H	1.814615499999999	-4.790814100000004	6.642972300000003
H	-0.45449835E+00	-0.11529329E+01	0.19758217E+01	H	1.782140099999999	-4.028758400000001	5.270046700000000
O	1.3039972000000000	-6.225977200000000	1.2149178000000000	O	5.911178999999998	-3.936921599999998	2.538164899999999
H	1.5163542999999999	-5.630737299999999	1.983136599999999	H	5.396071000000002	-4.564458700000003	1.986039900000000
H	1.3898862000000001	-5.531284600000002	0.559566699999997	H	6.202720000000002	-4.497432400000001	3.286109600000001
O	4.2737143000000000	-5.273451699999999	0.9942380499999998	O	2.358371599999999	-6.801516000000003	-1.6406406059999999
H	3.7718907000000002	-5.975423199999998	1.3209795000000000	H	2.226062000000002	-6.607668999999996	-0.707098079999996
H	3.6388770699999998	-4.690936899999996	0.591505309999995	H	1.4396773000000000	-6.715133400000000	-1.9931601000000001
O	-0.7907319400000002	-4.733264600000000	-0.550292409999995	O	-0.7849932200000005	-2.016405300000002	4.401684300000003
H	7.743069800000006E-002	-4.427415100000002	-0.272584769999998	H	-0.932253099999997	-2.949455099999999	4.063936599999999
H	-1.028183099999999	-5.230153800000001	0.263711509999998	H	-2.107569600000001E-002	-2.004686700000002	4.986100000000004
O	-0.994286399999998	-4.614851100000001	4.013169800000000	O	1.515835700000000	-8.654651299999994	2.837456406999999
H	-8.709729200000007E-002	-4.381839900000001	3.800891000000000	H	1.556425800000000	-7.892730499999999	2.206314900000002
H	-1.1814559000000000	-5.257318399999999	3.3175252000000000	H	2.472544300000000	-8.830832499999996	3.028312320000000
O	3.9564528999999999	-5.248721800000002	4.399738000000001	O	4.139127099999998	-7.805785799999998	3.342132200000000
H	4.2658044999999999	-4.377156300000002	4.706251100000002	H	3.9674589000000000	-6.8596573500000004	3.670787400000000
H	3.1137982000000002	-5.120590599999999	3.8955898000000002	H	5.104664699999998	-7.825008999999997	3.452428499999999
O	1.9266065999999999	-3.503793700000001	-2.401604799999999	O	3.8311066000000000	-0.2996006000000000	0.2996006000000000
H	1.4122155999999999	-4.344238100000001	-2.413746400000000	C	0.17778320E+01	-0.29799901E+01	0.25774516E+01
H	1.9968048000000000	-3.4259970000000002	-1.4041215000000000	C	0.19140873E+01	-0.16901018E+01	0.32218179E+01
O	2.5592226000000000	-6.559181800000002	-1.3809501000000000	O	0.21506295E+01	-0.69243550E+00	0.21750956E+01
H	2.1251978000000000	-6.331859399999999	-0.514768980000004	C	0.19593282E+01	-0.13509738E+01	0.81283132E+00
H	1.7297429000000000	-6.422980100000002	-1.981301200000001	C	0.19702065E+01	-0.28203902E+01	0.11878717E+01
O	-1.3855409999999999	-6.284958800000001	1.722150899999999	O	0.20955142E+01	-0.14020376E+01	0.43881743E+01
H	-0.5076913300000000	-6.685685999999996	1.560081499999999	C	0.60780192E+00	-0.95014263E+00	0.24618305E+00
H	-1.8422962000000001	-7.113572099999998	2.0176878000000000	O	-0.41475622E+00	-0.11029402E+01	0.11692500E+01
O	1.7371872000000001	-3.914761299999999	6.347293099999999	O	2.0500555999999999	-3.8311066000000000	0.2996006000000000
H	1.9867897999999999	-4.725190200000001	6.769103600000002	O	1.7877023000000001	-4.144859499999999	3.286682900000002
H	1.9158767999999999	-4.113887100000004	5.401571599999996	C	0.61718239E+00	-0.57782099E+00	-0.11874128E+00
O	6.1844561000000002	-4.012952399999996	2.559409200000002	O	-0.73192403E+00	0.90910528E+00	-0.59901979E+00
H	5.484074299999999	-4.546029599999998	2.063803000000001	H	0.27343401E+01	-0.10533610E+01	0.12370972E+00
H	6.1305636000000003	-4.403847800000003	3.443741000000002	H	0.97904707E+00	-0.12620795E+01	0.62250722E+00
O	1.4529231000000000	-8.693625199999996	2.6798947200000002	H	0.13344884E+01	0.68563130E+00	-0.9855732E+00
H	1.5317818000000001	-7.858785000000001	2.139578699999999	H	-0.12247871E+01	0.12874996E+01	0.16426232E+00
H	2.3459962999999999	-8.780828200000002	3.099029000000000	H	0.44706099E+00	-0.15688951E+01	-0.64117958E+00
O	4.255567499999997	-2.459387099999998	5.236828400000003	H	-0.22555599E+00	-0.18437782E+01	0.17369620E+01
H	3.3634848000000002	-2.367086599999999	4.887124400000003	O	1.4384950000000001	-6.289318299999997	1.2409363000000000
H	4.1550661000000000	-2.102823100000002	6.150736700000004	H	1.4325551000000001	-5.967685999999996	2.1254786000000001
C	0.18849973E+01	-0.31266583E+01	0.26027870E+01	O	4.333869899999998	-5.396023999999997	0.96992005000000003
C	0.21067717E+01	-0.17878803E+01	0.31381179E+01	H	3.8415105000000001	-6.002485899999999	1.536674099999999
O	0.22179083E+01	-0.76129564E+00	0.21326528E+01	H	3.6080518000000001	-4.929010100000002	0.5377267700000002
C	0.19927574E+01	-0.15007665E+01	0.84275431E+00	O	-0.4184520500000002	-4.8287882000000000	-0.33381094000000000

H	0.3945642400000001	-4.349541799999999	6.16129799999998E-002	H	2.334221799999999	-6.820450700000003	-0.6591764300000004
H	-0.7994014699999995	-5.366986400000000	0.4279739599999999	H	1.723223500000000	-7.076007899999996	-2.006851400000000
O	-0.6212018099999997	-5.112907899999997	3.950987300000000	O	-0.6569215999999999	-2.306906300000001	4.7010835000000002
H	0.2935020500000001	-4.870821099999997	3.663863900000000	H	-0.7379319600000005	3.166328599999999	4.263057599999998
H	-0.7642242799999998	-5.471845799999996	3.073215999999999	H	0.3107481300000001	-2.223800199999999	4.664079300000000
O	4.152996299999999	-5.307185099999999	4.561158800000003	O	4.123962999999998	-2.815218199999999	5.5931176000000002
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O	2.0821947000000001	-3.320883300000002	-2.278031700000001				
H	1.409236699999999	-3.961955999999998	-2.576243400000001	C	0.19524672E+01	-0.30067442E+01	0.26026166E+01
H	2.119438300000001	-3.544821999999999	-1.283915300000001	C	0.20091190E+01	-0.17152189E+01	0.31266408E+01
O	1.6357835000000001	-3.997486400000001	6.005527299999998	O	0.19467391E+01	-0.76563869E+00	0.21034360E+01
H	2.043138200000000	-4.804235099999996	6.362788700000003	C	0.16825424E+01	-0.14489877E+01	0.88018457E+00
H	1.680296400000000	-4.149079999999997	4.995976400000000	C	0.17597645E+01	-0.28830590E+01	0.12024833E+01
O	5.895906900000000	-3.691816499999998	2.408722200000001	O	0.20955333E+01	-0.12454968E+01	0.43206392E+01
H	5.448565000000002	-4.276951399999997	1.799607900000000	C	0.25306435E+00	-0.10812428E+01	0.32683048E+00
H	6.345194399999996	-4.293495799999996	2.990810499999998	O	-0.71517894E+00	-0.15092775E+01	0.13120642E+01
O	-0.79111686100000002	-2.287555300000002	4.733347000000002	O	1.704403099999999	-3.830326500000000	0.34344054000000002
H	-0.739009539999996	-3.138627899999997	4.347234900000001	O	1.915824999999996	-4.102794699999996	3.321463600000000
H	0.172769089999999	-2.182708200000000	4.832300100000003	C	0.26467064E+00	0.44547754E+00	0.15032379E+00
O	4.202873099999997	-7.708060200000003	3.134129300000001	O	-0.91570912E+00	0.98072123E+00	-0.52199885E+00
H	4.1598585000000003	-6.811939999999999	3.592544900000000	H	0.24023398E+01	-0.10796232E+01	0.12480821E+00
H	5.091144199999996	-7.992690500000001	3.399948600000001	H	0.34165597E+00	0.93243690E+00	0.11307589E+01
O	5.1518366000000002	-1.698123800000001	0.508348110000002	H	0.11489340E+01	0.68242727E+00	-0.45581294E+00
H	5.553612499999998	-2.389947900000001	1.023436999999999	H	-0.13679037E+01	0.16559314E+01	0.27935995E-01
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H	2.1062256000000001	-7.497312599999999	-0.160609059999999	H	-0.25713310E+00	-0.22117071E+01	0.17774756E+01
H	1.561965499999999	-7.115148500000001	-0.8776386009999999	O	1.6796234000000001	-6.247387999999999	1.5919964000000000
H	1.793907200000000	-6.907706100000004	-2.319211999999998	H	1.7492464000000001	-5.744150600000002	2.421473999999999
C	0.19784485E+01	-0.30599644E+01	0.25823416E+01	H	1.466546799999999	-5.403672900000001	1.122644800000000
C	0.19661840E+01	-0.17926298E+01	0.32260330E+01	O	-0.717584380000002	-4.426354899999998	3.493382299999999
O	0.18099115E+01	-0.81659943E+00	0.22375835E+01	H	0.2730585800000000	-4.379122500000003	3.384421100000000
C	0.18462337E+01	-0.13859394E+01	0.92748060E+00	O	-0.885339949999999	-5.097288599999999	2.8356229000000002
C	0.19792006E+01	-0.28933122E+01	0.12145260E+01	H	0.3154358400000002	-4.529640299999996	-0.3141794900000001
O	0.19884045E+01	-0.14239969E+01	0.44150748E+01	H	-0.7785045499999995	-5.323842400000002	0.3304499499999999
C	0.57163423E+00	-0.93430278E+00	0.13117802E+00	O	4.5551557000000003	-5.233006999999998	0.8831882300000002
O	-0.61866861E+00	-0.13082556E+01	0.89504733E+00	H	3.832566599999998	-5.711760100000002	1.276448800000001
O	2.080844799999999	-3.832892800000002	0.3105809700000001	H	4.076378400000003	-4.606886499999999	0.3596672400000000
O	1.996407199999999	-4.199094200000002	3.295024100000000	O	4.288774400000003	-5.232066500000000	4.232655200000000
C	0.46833873E+00	0.57336062E+00	0.87326659E-01	H	4.331708599999998	-4.453617800000000	4.7966432000000001
O	-0.73190660E+00	-0.10291057E+01	-0.57374634E+00	H	3.439335199999999	-5.065834599999996	3.761150999999999
H	0.27062826E+01	-0.10050495E+01	0.37241589E+00	O	2.112658199999998	-3.600723700000001	-2.282500400000000
H	0.51493645E+00	0.10908921E+01	0.10421975E+01	H	1.544401200000000	-4.351650099999996	-2.501708300000002
H	0.11513559E+01	0.10686357E+01	-0.55799499E+00	H	2.002319892000000	-3.587476199999999	-1.299575300000001
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H	-0.35771875E+00	-0.20133589E+01	0.15896013E+01	H	1.585246100000000	-4.134946300000002	5.071842799999998
O	1.414361100000000	-6.304605200000001	1.761103099999999	O	-0.866532399999999	-1.970825000000000	4.543887299999997
H	1.634497999999999	-5.820397500000003	2.604124199999998	H	-0.949132890000001	-2.870769999999998	4.223753499999999
H	1.545659100000000	-5.563198700000001	1.150968599999999	H	0.1027891500000000	-1.935820000000001	4.710526999999999
O	4.343518600000003	-5.368123899999996	0.924142040000000	O	0.1290683200000000	-8.606398699999997	2.800978900000000
H	3.867581400000002	-5.643385000000003	1.755372900000000	H	1.451963700000001	-7.741041300000000	2.352217099999998
H	3.651920200000002	-4.861760099999997	0.4826062600000001	H	2.182213400000002	-8.962960600000006	2.931622899999998
O	-0.6889535500000003	-5.009663539999997	3.747303699999998	O	3.647895699999996	-3.851538500000002	2.286016369999998
H	0.2703779399999998	-4.988387099999997	3.591678200000000	H	5.752691999999997	-4.554395200000001	1.932692899999999
H	-0.9291516400000002	-5.426622000000001	2.865889600000000	H	6.917125900000003	-4.384352100000001	2.908567000000001
O	-0.5905987799999999	-4.649626200000002	-0.4200369199999998	O	-1.503461800000000	-3.673519339999999	1.670573800000001
H	0.10843915000000000	-4.131880999999999	-8.774350799999998E-002	H	-1.213459899999999	-7.192517000000001	1.156696299999999
H	-0.9300124300000000	-5.055547599999997	0.4203738200000001	H	-2.297069599999999	-6.757099099999996	2.154131300000000
O	4.094471800000000	-5.399947000000001	4.569654599999998	O	5.580961799999999	-1.878198199999999	0.5345858000000000
H	4.438072400000003	-4.597162499999996	5.056680400000003	H	5.7105303000000003	-2.658621699999999	1.056895799999999
H	3.392875999999999	-4.867467999999997	3.992464800000000	H	5.767578999999996	-1.1762052000000001	1.1698705000000000
O	2.103779400000001	-3.782226399999999	-2.328369299999999	C	0.20488391E+01	-0.30105812E+01	0.25452406E+01
H	1.633397299999999	-4.611161899999999	-2.718946100000001	C	0.18711730E+01	-0.16873244E+01	0.31063182E+01
H	2.225313900000002	-4.034124699999996	-1.422214799999999	O	0.18689546E+01	-0.71646194E+00	0.21186544E+01
O	1.389523800000001	-4.093658300000004	6.043346500000002	O	0.17272650E+01	-0.13648316E+01	0.88115431E+00
H	1.612405899999999	-5.041620199999997	5.831885100000000	C	0.19257920E+01	-0.28449966E+01	0.11052007E+01
H	1.438078299999999	-3.784876999999998	5.086057399999996	O	0.17291290E+01	-0.13910113E+01	0.42865796E+01
O	5.072454800000000	-1.722248900000001	0.536493969999999	H	0.37936022E+00	-0.10758965E+01	0.29228315E+00
H	5.159178299999998	-2.517090200000002	1.038694300000000	O	-0.70322582E+00	-0.16007716E+01	0.10323570E+01
H	4.973749200000003	-1.081463899999999	1.235351800000001	O	0.1870595000000000	-3.681517800000000	0.16863288000000001
O	5.807857900000001	-3.631497299999999	2.458518000000002	O	1.922943499999999	-4.141302099999999	3.1942792000000000
H	5.620446699999996	-4.367528700000003	1.834609800000000	C	0.10815830E+00	-0.41203510E+00	-0.23802270E-01
H	6.360987000000001	-4.155221000000003	3.112749500000001	O	-0.12484575E+01	0.60208890E+00	-0.51510830E+00
O	2.5422853000000001	-7.177864099999999	-1.555033700000001				

H	0.24942751E+01	-0.89651411E+00	0.28314972E+00	O	1.301187499999999	-3.529534700000001	-2.596239300000001
H	0.25829266E+00	0.98315040E+00	0.90285515E+00	H	1.797548200000000	-4.229185900000001	-3.020585800000001
H	0.79238980E+00	0.71818822E+00	-0.83595961E+00	H	1.584441000000000	-3.701156900000000	-1.669406100000000
H	-0.17324011E+01	0.64671069E+00	0.33233247E+00	O	4.369110400000003	-2.893161300000000	-1.795901000000001
H	0.30376280E+00	-0.14609537E+01	-0.77034050E+00	H	3.484397500000000	-2.966396399999998	-1.379721699999999
H	-0.55652115E+00	-0.18359878E+01	0.19670847E+01	H	4.799647799999998	-2.308833700000001	-1.049247300000000
O	1.786942800000001	-6.117539299999998	1.420685800000000	O	1.576039900000000	-4.025423400000002	5.972835299999998
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H	1.712565200000000	-5.369654100000000	0.8055197100000000	H	1.701082500000001	-3.677932900000001	5.052814500000002
O	4.316021100000004	-5.282075599999998	0.7833895199999995	O	6.239209299999997	-3.941051299999998	1.506809400000001
H	3.799483599999999	-5.963014199999999	1.292144000000000	H	5.572065900000001	-4.644834200000000	1.246066700000001
H	3.692588900000001	-4.603847400000003	0.6365556700000002	H	7.049562400000001	-4.472993400000000	1.645419600000001
O	-0.774203360000001	-4.349862599999998	3.416169899999999	O	1.256287500000000	-8.594472500000002	2.613761600000001
H	0.212220419999999	-4.389343600000001	3.262676900000002	H	1.332170000000001	-7.647971000000002	2.307660799999998
H	-1.080916900000001	-4.996347600000000	2.691109700000002	H	2.209245999999998	-8.834798100000004	2.495625000000000
O	-0.6431519300000004	-4.883753500000001	0.6217475700000003	O	5.056869299999998	-1.724156000000000	0.531641049999995
H	0.1611003000000000	-4.349394300000002	-0.3428513899999998	H	5.547317999999997	-2.418334600000001	1.034459000000000
H	-0.824179169999996	-5.344528699999999	0.1675302499999999	H	5.175735300000004	-1.027463900000001	1.151219000000000
O	4.109319199999998	-5.315418700000004	4.449219499999999	O	4.346695200000001	-2.728673800000001	5.312408200000001
H	4.416884800000001	-4.521305700000001	4.972245100000003	H	3.522135899999999	-2.428133799999999	4.837718999999999
H	3.435761799999999	-4.954125099999997	3.833781300000001	H	4.226326199999999	-2.289463099999999	6.164363800000003
O	1.4816604000000000	-4.120185400000004	5.917345899999999				
H	1.908202000000000	-4.972643999999998	5.896607900000002	C	0.17716282E+01	-0.31085317E+01	0.25080918E+01
H	1.436025399999999	-4.018603899999996	5.016843400000001	C	0.19673800E+01	-0.17641130E+01	0.30062814E+01
O	1.656715699999999	-3.589549200000000	-2.634736100000000	O	0.18598245E+01	-0.78695702E+00	0.19076187E+01
H	1.971791499999999	-4.448375200000001	-2.840169299999999	C	0.16728326E+01	-0.15563914E+01	0.68430569E+00
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O	4.549010100000003	-2.750707499999999	-1.872802499999999	O	0.21217331E+01	-0.13374511E+01	0.41439634E+01
H	3.722303699999999	-3.147967899999998	-1.480581600000001	C	0.24588834E+00	-0.10676955E+01	0.21858956E-01
H	4.810034899999998	-2.050197400000001	-1.222227200000001	O	-0.86760964E+00	-0.14634482E+01	0.89666156E+00
O	6.413299499999999	-3.828897299999999	1.952986200000000	O	1.741034000000000	-3.969637399999999	0.25943089000000003
H	5.693254399999998	-4.331041100000002	1.501698699999999	O	1.910581400000001	-4.189164100000002	3.254942700000000
H	6.530683100000001	-4.376789699999998	2.764187800000002	C	0.14172970E+00	-0.44028593E+00	-0.97991209E-01
O	1.424316300000001	-8.772692400000004	2.381422900000000	O	-0.11403454E+01	-0.88788811E+00	-0.48458678E+00
H	1.607872500000000	-7.815365299999998	2.314056299999998	H	0.25144845E+01	-0.13886641E+01	-0.96164742E-01
H	2.362191199999998	-9.121930499999995	2.284328200000000	H	0.34693468E+00	-0.76525488E+00	0.96670554E+00
O	2.781384300000000	-7.163031700000003	-1.711105999999999	H	0.81978531E+00	-0.88179726E+00	-0.82613949E+00
H	2.765937399999999	-7.080916300000002	-0.7582658100000004	H	-0.17262210E+01	0.10669025E+01	0.27851241E+00
H	1.818978999999999	-7.214837099999996	-1.877187699999999	H	0.19596107E+00	-0.16306462E+01	-0.88384067E+00
O	-0.933564399999999	-1.892483500000000	4.841082700000003	H	-0.49810241E+00	-0.17530108E+01	0.17658723E+01
H	-0.951133659999999	-2.753972000000001	4.392166399999998	O	1.330900299999999	-6.379062399999996	1.712483100000000
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C	0.20479927E+01	-0.31355496E+01	0.23186531E+01	O	4.135002799999996	-5.312980399999998	0.5325255599999995
C	0.20488609E+01	-0.18195053E+01	0.29371629E+01	H	3.768912600000002	-5.421021500000002	1.406180200000001
O	0.19293460E+01	-0.79432846E+00	0.20156567E+01	H	3.405553700000000	-4.801832700000003	0.200478670000000
C	0.17300634E+01	-0.14374759E+01	0.65523858E+00	O	-0.7385633099999997	-4.576073199999997	3.775988299999999
C	0.19976889E+01	-0.28925511E+01	0.9679978E+00	H	0.2819509399999998	-4.577021000000002	3.779860400000000
O	0.21738854E+01	-0.14197811E+01	0.41235608E+01	H	-0.962983719999999	-5.229054699999998	3.063889699999998
C	0.34602389E+00	-0.10566862E+01	0.18779091E+00	O	-0.6972857900000002	-5.159964500000001	-0.3867150100000003
O	-0.66471531E+00	-0.15435868E+01	0.10908083E+01	H	-2.78396459999999E-002	-4.589663100000001	-4.30571759999999E-005
O	1.998404700000000	-3.821327199999998	1.705784700000000	H	-1.053467399999999	-5.522488600000000	0.4094369500000002
O	2.047729200000000	-4.285165799999997	3.055169300000002	O	3.946343300000001	-5.441974000000001	4.676875800000004
C	0.23607047E+00	-0.47668498E+00	-0.96036346E-01	H	4.418735299999998	-4.592872100000001	4.656656500000004
O	-0.11063319E+01	0.83150606E+00	-0.45390849E+00	H	3.116581899999999	-5.095832299999996	4.242878300000001
H	0.25573345E+01	-0.991156345E+00	0.80314533E-01	O	1.706235900000000	-3.765164599999999	5.864666599999996
H	0.62938362E+00	-0.10520768E+01	0.78536632E+00	H	2.154872999999998	-4.623627299999999	5.989813700000000
H	0.92067660E+00	-0.71923694E+00	-0.87336839E+00	H	1.903627600000001	-3.652838700000002	4.861081300000004
H	-0.15942524E+01	0.11794949E+01	0.32820257E+00	O	1.403073900000001	-3.417720900000000	-2.474021300000000
H	0.26657782E-01	-0.15937119E+01	-0.71840823E+00	H	1.621924200000000	-4.308229700000001	-2.808029799999999
H	-0.48868290E+00	-0.13859554E+01	0.20199805E+01	H	1.771890200000001	-3.540473200000001	-1.628849200000001
O	1.654938199999999	-6.233539000000004	1.051493100000001	O	4.484082199999996	-2.660735400000001	-1.510931999999999
H	1.645554400000000	-5.809110800000000	1.945638900000001	H	3.833756400000000	-3.195180100000000	-1.062839300000000
H	1.645122999999999	-5.395117100000002	0.5567995799999996	H	4.870959999999999	-2.198123400000001	-0.729225729999998
O	4.192419600000000	-5.430818200000000	0.3800873700000001	O	-1.278622500000000	-6.602941500000000	1.754284900000000
H	3.553737299999997	-5.978153799999997	0.8981261900000005	H	-0.3378157600000002	-6.945705099999996	1.793006900000000
H	3.528196200000000	-4.730732699999999	6.40360779999996-002	H	-1.834955399999999	-7.371738100000000	2.050687700000001
O	-0.9021456500000002	-4.912362800000004	-0.2981147200000000	O	-0.8152209500000006	-2.063359900000000	4.491519199999999
H	2.23385999999999E-002	-4.791245599999999	1.928015500000000	H	-1.218956500000000	-2.920747000000000	4.220977600000003
H	-1.130004700000000	-5.561763499999996	0.410372679999999	H	0.1060047900000000	-2.320771900000000	4.688360399999997
O	-0.692212049999997	-4.453194299999998	3.729696900000000	O	1.249994000000001	-8.830928699999994	2.681713999999999
H	0.284327319999999	-4.454179299999998	3.604108000000001	H	1.201334200000000	-7.870134900000000	2.523547699999999
H	-0.8515440500000000	-5.135459100000003	3.031473399999999	H	2.107207900000001	-9.079384700000003	2.214119199999998
O	4.027292100000004	-5.317019199999998	4.424563100000003	O	4.449454900000001	-2.799977300000001	5.310728600000000
H	4.390762999999997	-4.472250599999997	4.691981300000001	H	3.555162999999999	-2.546173200000001	5.063498600000000
H	3.272730199999998	-4.928011899999996	3.884671200000001	H	4.576085700000002	-2.316333300000002	6.126537299999999

C	0.19516266E+01	-0.30794290E+01	0.24351959E+01	H	1.756996300000000	-5.5089525999999998	1.0503226000000001
C	0.20563588E+01	-0.17367568E+01	0.29260739E+01	O	4.3557933000000002	-5.3586425000000002	0.7328910800000003
O	0.20509963E+01	-0.79597002E+00	0.18869772E+01	H	4.1043139999999996	-5.9328073000000003	1.4336894000000000
C	0.17344035E+01	-0.15318596E+01	0.64071733E+00	H	3.5016379999999998	-4.9495129999999996	0.6421259900000004
C	0.18767828E+01	-0.29886294E+01	0.10146918E+01	O	-0.3747801599999997	-5.193184189999999	-0.1260667000000000
O	0.20882927E+01	-0.13188189E+01	0.40806063E+01	H	0.30535109999999999	-4.5499276000000002	7.499552900000000E-002
C	0.27144694E+00	-0.12358737E+01	0.19267626E+00	H	-0.7300610499999999	-5.4697731000000003	0.7566329200000004
O	-0.70832582E+00	-0.13554264E+01	0.13061203E+01	O	-0.8553669099999998	-4.6655392000000004	3.472642000000000
O	1.891614399999999	-3.912899100000002	0.1320129499999999	H	0.10089115000000000	-4.4031399999999996	3.414095399999999
O	1.941802300000000	-4.196332700000001	3.1594299000000001	O	-0.9073537200000005	-5.408416599999998	2.9002669000000001
C	0.25240180E+00	0.26570556E+00	-0.22623572E+00	H	4.4350693999999997	-4.6318089000000002	4.2700357999999996
O	-0.10349340E+01	0.73601557E+00	-0.56937772E+00	H	3.1746694999999998	-5.191378199999999	3.630684599999999
H	0.23578728E+01	-0.11007184E+01	-0.97656675E-01	O	1.5693153000000000	-3.973274299999999	6.047275900000000
H	0.60836426E+00	0.79775386E+00	0.72139290E+00	H	2.2016452000000002	-4.6731809000000002	6.285807499999998
H	0.83443342E+00	0.39329693E+00	-0.11323751E+01	H	1.6112420000000001	-4.1008113000000002	5.073173999999999
H	-0.15233491E+01	0.10058546E+01	0.18209361E+00	O	3.9937892000000002	-2.807827399999999	-1.674871999999999
H	0.54475260E-02	-0.19703692E+01	-0.59391682E+00	H	3.4669105999999998	-3.2246967000000000	-0.9992216299999997
H	-0.19345351E+00	-0.17270159E+01	0.20519644E+01	H	4.6232666000000000	-2.3399526000000002	-1.074380399999999
O	1.794621599999999	-6.294125900000001	1.543209899999999	O	1.2055309999999999	-3.6783484000000000	-2.4661719999999998
H	1.969619999999999	-5.692875800000000	2.244223200000001	H	1.4446935999999999	-4.5797489999999997	-2.8190016999999998
H	1.758370500000001	-5.559316599999998	0.8752029000000004	H	1.4268054999999999	-3.6634487999999998	-1.5268459999999999
O	4.209443499999999	-5.453546799999998	0.6637355400000001	O	1.1375510000000000	-8.4536598000000005	2.847298799999999
H	3.592750699999999	-6.092486799999996	1.1212626000000001	H	1.4911158000000000	-7.630797499999999	2.4499187999999998
H	3.509663100000000	-4.846272729999997	0.3362583900000002	H	2.0043878999999998	-8.9461875000000006	2.726202199999999
O	-0.5612240200000005	-4.881939300000000	-0.2797620900000002	O	-0.6323367100000002	-2.0259510999999999	4.6473306000000001
H	0.3545731999999997	-4.609293199999998	-5.514735199999997E-002	H	-0.6364195099999997	-2.9991292000000001	4.7200129000000004
H	-0.9098211800000001	-5.335603299999998	0.516489789999996	H	0.3246354900000003	-1.8432126000000000	4.7035049999999998
O	-0.5713153699999999	-4.651114999999999	3.9412254000000000	O	4.292622299999997	-2.9269061000000001	5.585081599999996
H	0.4161266900000002	-4.5043914000000003	3.751620999999998	H	3.333632199999998	-2.826581599999999	5.2981670000000003
H	-0.9142126999999999	-4.994523499999997	3.0575993000000001	H	4.3580841000000001	-2.4225609000000001	6.384800199999999
O	4.2214555000000002	-5.387573899999996	4.270819099999998	O	6.490840099999998	-3.9061819000000000	1.762869199999999
H	4.666050799999998	-4.664050999999997	4.762237899999997	H	5.837915699999999	-4.4606937000000002	1.330051799999999
H	3.447877099999999	-4.846713900000001	3.990511999999998	H	7.1819490000000004	-4.549499199999996	1.7351182000000001
O	1.5443781000000001	-4.0785428000000001	6.0157359000000001				
H	1.878912600000000	-4.953683100000001	6.303585299999999	C	0.19481095E+01	-0.30234169E+01	0.27459011E+01
H	1.777469999999999	-4.070116600000004	5.035148699999999	C	0.19986026E+01	-0.16396065E+01	0.31943352E+01
O	1.069338200000000	-3.507407400000000	-2.601808900000000	O	0.20465640E+01	-0.72065369E+00	0.21639429E+01
H	1.528947600000000	-4.150414399999998	-3.151269800000001	C	0.18281005E+01	-0.15042912E+01	0.88855912B+00
H	1.479870700000000	-3.628936400000002	-1.694812000000000	C	0.18895180E+01	-0.29792890E+01	0.13460817E+01
O	4.426842299999997	-2.864789899999999	-1.806127500000001	O	0.19066616E+01	-0.12019640E+01	0.43454957E+01
H	3.742523199999999	-3.274959299999999	-1.271864799999999	C	0.49161933E+00	-0.11535762E+01	0.29615846E+00
H	4.866810000000001	-2.264511499999998	-1.085178699999999	O	-0.59031868E+00	-0.14370528E+01	0.12399795E+01
O	6.269805599999999	-3.941032299999998	1.750196099999999	O	1.9205260000000000	-3.9480748999999999	0.4642091000000002
H	5.529450999999999	-4.532877600000000	1.3732005000000000	O	1.8531563000000000	-4.0565629999999997	3.5185514000000002
H	6.956897399999999	-4.553294099999996	1.902859099999999	C	0.30836836E+00	0.32583559E+00	-0.11901900E+00
O	1.231972200000000	-8.560208199999999	3.073220500000001	O	-0.10293937E+01	0.59857449E+00	-0.70435568E+00
H	1.358315800000000	-7.773357999999999	2.467888299999998	H	0.26301072E+01	-0.12567892E+01	0.1977225E+00
H	2.171158100000000	-8.671893300000007	3.1963929000000002	H	0.48470605E+00	0.89643864E+00	0.76073632E+00
O	-1.152460599999999	-6.571466199999997	1.882287599999999	H	0.92992599E+00	0.66970849E+00	-0.91842563E+00
H	-0.6130084900000002	-7.052964799999998	1.218171399999999	H	-0.16657439E+01	0.33318375E+00	0.4655037E-01
H	-1.750424500000000	-7.270106499999998	2.1348139000000002	H	0.42862306E+00	-0.18144294E+01	-0.51006188E+00
O	-0.6649549099999995	-2.1330908000000002	4.7890230000000003	H	-0.12017326E+00	-0.21211234E+01	0.17712751E+01
H	-0.9234031200000002	-3.0506576000000001	4.5840727000000001	O	1.5904166000000000	-6.265993299999999	1.8979709999999999
H	0.2625324099999999	-2.222508899999998	4.9378479000000004	H	1.7068690000000000	-5.6314694000000003	2.6499451000000001
H				H	1.6798611999999999	-5.575026799999999	1.2330544999999999
C	0.20322237E+01	-0.30046114E+01	0.25833042E+01	O	4.213284200000004	-5.283533099999996	0.7104517900000003
C	0.20875884E+01	-0.17096825E+01	0.30580536E+01	H	3.838245500000002	-5.927296400000004	1.3441333000000000
O	0.19235738E+01	-0.71199813E+00	0.20453529E+01	H	3.426817199999999	-4.694716299999999	0.5996872300000002
C	0.17575753E+01	-0.14405476E+01	0.82618336E+00	O	-0.7750820100000005	-4.527143500000002	3.6196570000000001
C	0.19202197E+01	-0.29199039E+01	0.12139579E+01	H	0.1965751699999999	-4.576511499999999	3.7109570240000002
O	0.21518361E+01	-0.12666084E+01	0.42196149E+01	H	-0.9476907000000000	-5.0436730000000001	2.8806850000000002
C	0.47298234E+00	-0.11573362E+01	0.23408638E+00	O	4.378460399999999	-5.419960299999999	3.568630699999999
O	-0.69771849E+00	-0.14901265E+01	0.10304734E+01	H	5.1268034000000000	-4.858619599999999	3.366898599999999
O	1.9447703000000001	-3.7672891000000002	0.2401054999999999	H	3.6196202999999998	-4.8105168000000003	3.7055375000000002
O	1.8448277000000000	-4.096508799999996	3.3714430000000002	O	-0.3999755600000001	-5.2546111000000000	-0.3169404999999999
C	0.27167036E+00	0.32948719E+00	-0.2998558E+00	H	0.3754018399999999	-4.7690090000000004	1.9708967000000001E-002
O	-0.10553924E+01	0.46064781E+00	-0.70973213E+00	H	-0.7633931000000005	-5.598927599999999	0.4939983800000001
H	0.26180283E+01	-0.10865308E+01	0.23739624E+00	O	1.5333238000000000	-4.0211750000000004	6.2399696000000002
H	0.52114952E+00	0.10341117E+01	0.46868571E+00	H	1.8045838000000001	-4.9419535000000003	6.6048720000000003
H	0.98229376E+00	0.49620361E+00	-0.11827636E+01	H	1.5093306000000000	-4.084644899999999	5.227456799999997
H	-0.15634521E+01	0.69857932E+00	0.70092811E-01	O	0.9531475299999997	-3.776498699999999	-2.2092901000000000
H	0.43747551E+00	-0.18218374E+01	-0.56578688E+00	H	1.2604541000000000	-4.5853579000000000	-2.6236989999999998
H	-0.40986670E+00	-0.17123263E+01	0.19544338E+01	H	1.5558107000000001	-3.8249224000000002	-1.3691628000000000
O	1.9310008000000001	-6.231120899999996	1.7116141000000000	O	4.388210599999999	-3.042279699999999	-1.6261515000000000
H	1.6809605000000001	-5.784207699999998	2.5593693000000002	H	3.718927299999998	-3.4539453000000000	-1.0934834000000000

H	4.505623199999996	-2.254588399999998	-1.117606099999999	O	-0.68049538E+00	-0.18963480E+01	0.12217094E+01
O	-0.9384216699999999	-1.9509563000000001	4.6059256000000000	O	2.0722984000000002	-4.0119536000000000	0.37150201999999999
H	-0.8580323899999999	-2.746692799999999	4.163593099999999	O	1.8024860000000000	-4.0593940000000002	3.5212794000000001
H	-4.51253989999997E-002	-2.0355348000000002	5.0112598000000004	C	0.27929262E-01	-0.12120283E+00	-0.22773396E+00
O	1.0783094000000000	-8.732610499999998	2.728676099999999	O	-0.13167263E+01	-0.60067447E-01	-0.6982779E+00
H	1.3229795000000000	-7.834550199999998	2.480624699999999	H	0.24652460E+01	-0.12200810E+01	0.11420488E+00
H	1.950632799999999	-9.150361999999994	2.5436447000000002	H	0.22725046E+00	0.65839369E+00	0.54616329E+00
O	6.3059959000000001	-3.7784575000000000	1.9904077000000000	H	0.66536182E+00	-0.13308227E-01	-0.11346602E+01
H	5.8891888000000003	-4.3651846000000001	1.3495824000000001	H	-0.18321478E+01	-0.32026961E-01	0.12793200E+00
H	7.1592428000000004	-4.2244551000000001	2.1894524000000000	H	0.25062718E+00	-0.23088115E+01	-0.55623521E+00
O	4.3304925000000001	-3.0063102000000002	5.6951228000000000	H	-0.29386009E+00	-0.25631192E+01	0.18629597E+01
H	3.3721787000000001	-3.100413399999999	5.7155072000000002	O	1.8852622000000001	-6.3290620000000004	1.9445422000000001
H	4.342239499999998	-2.5196939000000000	6.513922199999997	H	2.0712581000000001	-5.8784060000000000	2.810869499999999
C	0.20068558E+01	-0.29384943E+01	0.26348319E+01	O	4.357369799999998	-5.5239247000000002	1.1899146000000000
C	0.19402167E+01	-0.15861835E+01	0.30835726E+01	H	3.6403428000000000	-6.193203299999997	1.3703555999999999
O	0.19717161E+01	-0.64307269E+00	0.20069292E+01	H	3.694699699999999	-4.9276140000000002	0.7527245599999999
C	0.17928251E+01	-0.14144289E+01	0.81264943E+00	O	-0.3515396499999998	-5.219523399999999	-0.1966881999999999
C	0.20147548E+01	-0.28545390E+01	0.12438491E+01	H	0.5523004799999998	-4.9020253000000000	6.937371599999997E-003
O	0.17536899E+01	-0.12001153E+01	0.42441335E+01	H	-0.5329457399999995	-5.705690899999996	0.6366318199999996
C	0.39455958E+00	-0.12113866E+01	0.24816252E+00	O	4.208117999999998	-5.544304699999996	3.893883699999999
O	-0.50284552E+00	-0.15225127E+01	0.13585564E+01	H	4.4402825000000004	-5.432297799999997	2.9529690000000000
O	2.0343513000000000	-3.851054899999998	0.4413051100000000	H	3.3510938000000001	-5.0856402000000003	3.9101778000000000
O	2.0447185999999999	-4.020279999999996	3.4029805000000000	O	-1.0496650999999999	-4.7622064000000002	3.6757493000000001
C	0.12036755E+00	0.24717369E+00	-0.83714470E-01	H	-7.303479799999998E-002	-4.6615628000000000	3.6779370000000000
O	-0.11465871E+01	0.48285072E+00	-0.67486926E+00	H	-1.1940640000000000	-5.5930431000000000	3.1790170000000000
H	0.25076035E+01	-0.10504213E+01	0.46901371E-01	O	4.4214368000000004	-3.330426699999999	-1.2298258000000000
H	0.13203711E+00	0.93260982E+00	0.83832098E+00	H	3.5946889000000000	-3.5643378000000001	-0.8139503399999999
H	0.82540947E+00	0.70141014E+00	-0.78783752E+00	H	4.488332999999999	-2.4572862000000000	-0.8510045299999998
H	-0.17992403E+01	0.64175298E+00	0.42232812E-01	O	1.5612393000000000	-4.3011080000000002	6.211846499999999
H	0.20188589E+00	-0.18737960E+01	-0.61425317E+00	H	2.410201999999999	-5.517622999999996	6.521745499999999
H	-0.13640104E+00	-0.22966940E+01	0.18318667E+01	H	1.693029399999999	-4.156271399999996	5.279616599999998
O	1.5393460000000001	-6.3702562600000000	2.0235316000000001	O	1.3688989000000000	-3.511854399999998	-2.4887850000000000
H	1.7602537000000000	-5.838296399999999	2.776043899999999	H	1.5976417000000001	-4.293084399999997	-3.0064388000000002
H	1.589789399999999	-5.677507099999997	1.3392067000000001	H	1.4218189000000001	-3.8329745000000002	-1.5721375000000000
O	4.228552099999999	-5.639484900000000	0.8131801199999995	O	-0.9521934199999996	-2.071428099999999	2.4057731000000002
H	4.252232399999999	-6.2053220000000004	1.6445554000000000	H	-1.0941816000000000	-3.0236201000000000	4.2153152000000000
H	3.5023355000000000	-4.9702723000000004	1.0710554999999999	H	4.119093100000000E-002	-1.9989218000000000	4.4249435999999998
O	4.298451599999999	-5.382929599999998	3.678782399999998	O	4.253918099999999	-2.8303137000000000	5.577426299999999
H	5.0162173000000001	-4.8330460000000004	3.4863411000000002	H	3.5630784000000002	-3.279636399999999	5.0698903000000000
H	3.5212838000000000	-4.784129199999997	3.421517399999999	H	4.3379946000000000	-2.1884785000000000	6.318087399999996
O	-0.7093892699999996	-4.403747700000003	3.2636528000000000	O	6.5403025000000001	-3.970396699999998	1.9652877000000000
H	0.2385306299999999	-4.338463700000001	3.3567562000000000	H	5.798261799999999	-4.5241210000000001	1.4675107000000001
H	-0.7863464000000000	-5.345211499999996	2.996605189999999	H	7.0915600000000003	-4.708501499999997	2.225516199999999
O	-0.5826408100000001	-5.101521599999999	-9.3329227000000001E-002	O	1.1933714000000000	-8.864208000000003	2.7013957000000000
H	0.3088162500000001	-4.738665499999998	0.1102383900000001	H	1.3730388000000000	-7.975827000000002	2.3179813000000000
H	-1.0303290000000001	-5.3120984000000000	0.7585039399999999	H	1.8624057000000001	-9.4078599999999994	2.2977194000000001
O	4.136166099999996	-3.183059600000000	-1.577098399999999	H	-	-	-
H	3.4378511000000000	-3.5760527000000000	-0.9634905060000000	C	0.18981901E+01	-0.32023805E+01	0.25020825E+01
H	4.5319520000000002	-2.5685270000000000	-1.0051782000000000	C	0.18898852E+01	-0.17921441E+01	0.28776919E+01
O	1.421201399999999	-4.0331307000000001	6.072812899999999	O	0.18613445E+01	-0.92805286E+00	0.17865132E+01
H	1.8595664000000001	-4.8899058000000002	6.3612950000000001	C	0.16197482E+01	-0.18053276E+01	0.64379884E+00
H	1.7819166000000000	-3.962820799999998	5.1499625000000000	C	0.20042861E+01	-0.31792893E+01	0.11270923E+01
O	0.959143749999996	-3.787455500000001	-2.3326680000000000	O	0.20229446E+01	-0.13322598E+01	0.40464877E+01
H	1.7146850000000000	-4.3094405000000000	-2.553310999999999	C	0.51084250E-01	-0.17532638E+01	0.24186598E+00
H	1.220719799999999	-3.766575899999999	-1.3441197000000000	O	-0.84368563E+00	-0.19554454E+01	0.13869113E+01
O	4.2924695000000002	-2.8312281000000001	5.445591399999999	O	2.097765299999998	-4.1465163000000000	0.22586355000000000
H	3.3671015000000000	-2.8927594000000001	5.0601145000000001	O	1.9711155000000000	-4.140513999999996	3.4276323000000000
H	4.1404920000000001	-2.3466705000000003	6.2656267000000003	C	-0.21333394E+00	-0.41999449E+00	-0.43857973E+00
O	6.365630999999996	-4.090293000000004	1.6814605000000000	O	-0.15477308E+01	-0.13876181E+00	-0.85103983E+00
H	5.769359999999999	-4.698834000000000	1.2736132000000000	H	0.22901275E+01	-0.15039771E+01	-0.21175789E+00
H	7.0445491000000002	-4.7161488000000000	1.759758999999999	H	0.24098945E+00	-0.36286323E+00	0.22616499E+00
O	-0.9752636300000005	-2.1253182000000002	4.4380549000000000	H	0.35853431E+00	-0.43143232E+00	-0.14401164E+01
H	-1.1138428000000000	-3.059815899999998	4.0287132000000003	H	-0.21162669E+01	0.36862469E-01	-0.91657848E-01
H	-4.202764500000000E-002	-2.1407001000000001	4.6433657000000004	H	-0.19590158E+00	-0.26027932E+01	-0.41803188E+00
O	1.2697274000000001	-8.954342300000004	2.7567986000000002	H	-0.44372274E+00	-0.27139446E+01	0.18501751E+01
H	1.3137938000000000	-8.096462799999994	2.3245350000000001	O	1.6316843999999999	-6.475434599999998	1.8436395000000001
H	2.1618471000000001	-9.3035463000000007	2.6070319000000000	H	1.6574918000000001	-5.792030399999998	-2.4959190000000002
C	0.19101670E+01	-0.30900019E+01	0.26550006E+01	O	4.313477899999996	-5.3301926000000002	0.9958399999999995
C	0.19230230E+01	-0.16645340E+01	0.30479069E+01	H	3.827782899999999	-5.8780456000000001	1.7108676000000000
O	0.18703492E+01	-0.81576953E+00	0.19753327E+01	H	3.6585384000000000	-4.7586461000000000	0.5033298499999997
C	0.17957817E+01	-0.16644273E+01	0.82127392E+00	O	4.189144599999997	-5.4912589000000001	4.037947599999999
C	0.19602084E+01	-0.31054988E+01	0.12646300E+01	H	4.6503214000000002	-4.7432568000000002	4.4276483000000004
O	0.18815966E+01	-0.11441197E+01	0.41757234E+01	H	3.3755930000000002	-5.0217026000000002	3.731703999999999
C	0.33309669E+00	-0.15353599E+01	0.23756847E+00	O	-0.8107597199999996	-5.1159207000000002	3.8403375999999998

H	-1.61884600000000E-002	-4.725068499999999	3.448136200000000	H	5.999425200000001	-4.179059299999996	1.294586000000000
H	-1.1194656000000001	-5.7512308000000001	3.162980100000000	H	7.199824800000000	-4.822165700000002	2.011775600000000
O	-0.8555259200000005	-5.2098443000000003	1.607795999999999E-002	O	4.580438700000002	-7.268277499999999	-1.165638500000000
H	5.8596263000000003E-002	-5.1628128000000002	0.2695908400000000	H	4.326625100000002	-6.690720000000003	-0.354518500000000
H	-1.221618099999999	-5.9691473000000004	0.583122899999995	H	5.413776300000003	-6.853871100000001	-1.402508500000001
O	4.400307699999999	-3.4580128000000001	-1.553541200000000	C	0.18922933E+01	-0.30255229E+01	0.24999430E+01
H	3.6339814000000001	-3.7629046000000002	-0.9833480100000005	C	0.19882449E+01	-0.16925406E+01	0.29506263E+01
H	4.735869799999999	-2.704955999999999	-1.018621500000001	O	0.18733102E+01	-0.74252108E+00	0.18815969E+01
O	1.618689899999999	-4.186407499999996	6.172250400000002	C	0.16070775E+01	-0.15210042E+01	0.73873866E+00
H	2.562911999999999	-4.060575600000000	6.218278800000002	C	0.17933349E+01	-0.29512582E+01	0.11526696E+01
H	1.482219100000000	-4.030112400000002	5.212225199999998	O	0.21588248E+01	-0.12337171E+01	0.41165701E+01
O	4.298646200000003	-2.969462699999998	5.361374399999999	C	0.1105657E+00	-0.14310670E+01	0.23357222E+00
H	3.526129899999999	-2.704684000000001	4.785032799999998	O	-0.80313855E+00	-0.15729981E+01	0.13592614E+01
H	4.369459999999999	-2.278572099999999	6.099439900000001	O	1.826566200000000	-3.886949200000001	0.2477312399999999
O	0.9239732499999997	-3.402445300000001	-2.541291199999999	O	1.946473500000000	-4.108412699999997	3.286520700000001
H	1.526121899999999	-3.682343400000002	-3.255910899999999	O	-0.18139433E-02	-0.33888842E-01	-0.42812851E+00
H	1.380127799999999	-3.719515100000002	-1.748535900000000	O	-0.13629840E+01	0.21951129E+00	-0.95066878E+00
O	6.556006000000000	-4.008947300000000	2.073096099999999	H	0.22439657E+01	-0.12368047E+01	-0.64470844E-01
H	5.774358999999998	-4.447814400000004	1.688082800000001	H	0.30043352E+00	0.78558974E+00	0.27359788E+00
H	7.098145599999996	-4.785700799999999	2.111519810000002	H	0.57047654E+00	0.48550602E+00	-0.13421583E+01
O	1.267374199999999	-8.893926699999997	2.812134799999999	H	-0.19817220E+01	0.30454842E+00	-0.20060008E+00
H	1.525070699999999	-8.024504399999996	2.485566200000001	H	-0.13954105E+00	-0.22326701E+01	-0.50576221E+00
H	2.041303600000000	-9.448547200000001	2.707920399999999	H	-0.46046902E+00	-0.23076602E+01	0.19021384E+01
O	-1.205750200000000	-2.305122999999998	4.671886899999996	O	1.587383599999999	-6.643779399999997	1.881284100000000
H	-1.192840700000001	-3.061963399999998	4.046202100000004	O	1.489538700000000	-5.719387799999998	2.261134499999998
H	-0.3019498600000001	-2.449443200000002	4.937542999999998	H	2.0369377000000002	-6.332835000000003	1.027589300000000
C	0.16933973E+01	-0.30444333E+01	0.25124590E+01	O	4.295136300000002	-5.075974699999997	0.846960669999999
C	0.18901861E+01	-0.16682460E+01	0.29435749E+01	H	4.296676599999996	-5.319217499999997	1.819691299999999
O	0.19082928E+01	-0.77491948E+00	0.18564988E+01	H	3.432488799999998	-4.631145600000000	0.7209375500000004
C	0.16273143E+01	-0.15552268E+01	0.69435848E+00	O	-0.548562279999996	-5.305925199999999	3.821770500000000
C	0.18768433E+01	-0.29910964E+01	0.11186895E+01	H	0.360721259999999	-4.936271299999996	3.586306099999998
O	0.21013355E+01	-0.12652279E+01	0.40780066E+01	H	-0.849916829999996	-5.678848799999999	2.913425900000000
C	0.23551949E+00	-0.14550257E+01	0.13792678E+00	O	-0.799166069999995	-5.119942000000002	-0.131559010000000
O	-0.82241893E+00	-0.17259095E+01	0.10914454E+01	H	8.418363099999995E-002	-5.004487600000000	0.245150819999999
O	2.174174100000001	-3.947105899999999	0.246947200000000	H	-1.277273600000000	-5.549460299999998	0.593802520000000
O	1.744216100000000	-4.107992399999997	3.399840100000000	O	4.220691399999999	-5.500689399999997	3.553316900000000
C	-0.11956429E+00	-0.37469583E-01	-0.38195887E+00	H	4.830084600000002	-4.716663200000002	3.708317399999999
O	-0.14416353E+01	0.10586765E+00	-0.80691799E+00	H	3.321124699999999	-5.128192900000002	3.605679499999999
H	0.23586096E+01	-0.12748490E+01	-0.13519623E+00	O	4.211027800000001	-3.347114700000001	-1.430830100000001
H	0.21808685E-01	0.70759649E+00	0.43475778E+00	H	3.482140300000002	-3.699669320000000	-0.925423129999998
H	0.47016665E+00	0.20409824E+00	-0.12904227E+01	H	4.433518600000002	-2.659596399999999	-0.806954400000005
H	-0.20392600E+01	0.24489657E+00	-0.68406087E-01	O	0.298684400000004	-3.579537000000001	-2.407386600000002
H	0.31700821E+00	-0.21611763E+01	-0.69473872E+00	H	1.447065800000001	-4.154149000000003	-2.904529399999999
H	-0.57900163E+00	-0.23095133E+01	0.18345244E+01	H	1.189686599999999	-3.779352499999999	-1.454401099999999
O	1.456727799999999	-6.356349800000003	1.703839099999999	O	1.731681500000001	-4.070094600000000	6.171452399999997
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H	1.828649299999999	-5.651537199999999	1.118560700000000	H	1.473424899999999	-4.198967200000002	5.192387600000000
O	4.131292900000000	-5.245722100000001	3.519875299999998	O	-1.004966000000000	-2.705725100000000	4.564862699999999
H	4.491554100000001	-4.419839299999996	3.808260000000002	H	-1.204847999999999	-3.617739100000001	4.398852699999999
H	3.190816299999998	-4.891997800000004	3.460310000000002	H	-5.566190900000002E-002	-2.808296200000000	4.813042699999996
O	4.476074099999999	-5.387796800000003	0.679484240000003	O	6.475516899999997	-3.791757399999998	2.177361000000000
H	4.477521900000002	-5.497878000000000	1.635795600000000	H	5.878750199999998	-4.119062600000004	1.459847400000001
H	3.511369999999999	-5.230071100000000	0.574826389999995	H	7.049572600000003	-4.570587299999997	2.151341400000002
O	-0.926402339999999	-4.829772700000004	0.356825750000000	O	4.639271100000002	-7.002162199999999	-1.092622500000001
H	6.5170000000000002E-003	-4.738893100000001	0.611134729999996	H	4.335297299999997	-6.502158599999996	-0.3079338500000001
H	-1.195698900000000	-5.654469260000003	0.6742632600000003	H	5.303864700000001	-6.334127099999999	-1.504411500000000
O	-0.7469076300000004	-5.218038400000002	3.687746600000001	O	4.164220799999998	-2.718867200000000	5.408763800000000
H	0.1853604700000000	-4.956398600000000	3.515720899999998	H	3.565692299999998	-2.022132800000001	5.061369899999999
H	-0.9899094400000003	-5.724028699999999	2.840497800000001	H	4.562764300000004	-2.260103700000002	6.232141099999998
O	4.053734999999997	-3.260729599999999	-1.541506199999999	C	0.18113028E+01	-0.31072160E+01	0.25672158E+01
H	3.379858000000000	-3.529097699999999	-0.836271479999996	C	0.18107691E+01	-0.17685011E+01	0.30638617E+01
H	4.457270200000000	-2.540378399999998	-1.039841400000000	C	0.18847921E+01	-0.79618945E+00	0.19922105E+01
O	1.573661200000001	-4.087906000000003	6.148412500000001	O	0.17754598E+01	-0.15975100E+01	0.77256737E+00
H	2.566117000000002	-4.037318000000000	6.208029100000001	C	0.19348717E+01	-0.29955239E+01	0.12056895E+01
H	1.492637800000000	-4.048434699999996	5.159190299999997	O	0.17343829E+01	-0.13816937E+01	0.42808088E+01
O	1.167299499999999	-3.616529599999998	-2.598033399999998	H	0.38517779E+00	-0.13613287E+01	0.15801885E+00
H	1.705567400000000	-4.277736499999996	-3.004109199999998	O	0.65076895E+00	-0.15991815E+01	0.12078435E+01
H	1.567263200000000	-3.570110300000001	-1.705934300000000	O	2.042293299999999	-3.928059300000001	0.2769688599999998
O	-1.215476300000000	-2.460228400000001	4.389065099999998	H	1.731640700000000	-4.117546400000002	3.397642199999999
H	-1.743024399999999	-3.262132999999999	4.101823999999997	O	0.14118259E+00	0.31124827E-01	-0.43729752E+00
H	-0.3440847200000001	-2.815513000000002	4.584888000000003	C	-0.11961687E+01	0.61412535E-01	-0.93231168E+00
O	4.202720199999999	-2.663804499999999	5.512440999999999	H	0.24166804E+01	-0.11550242E+01	-0.46564710E-01
H	3.273852999999999	-2.435597800000000	5.227815099999999	H	0.29348039E+00	0.78845448E+00	0.27352785E+00
H	4.455273000000000	-2.143317199999998	6.367108799999996	H	0.87788156E+00	0.19258027E+00	-0.12406377E+01

H	-0.17127251E+01	-0.28301349E+00	-0.13676599E+00	O	1.6641248000000000	-3.8918457000000002	6.1642957000000003
H	0.25431518E+00	-0.21358409E+01	-0.63406915E+00	H	2.6456477999999999	-3.8732129000000000	6.2324846999999997
H	-0.57020364E+00	-0.95850406E+00	0.19033839E+01	H	1.6516717999999999	-3.7989437000000001	5.2002157000000002
O	1.6826242000000000	-6.3875798000000001	1.9180151999999999	O	-0.8683509700000006	-3.2816869000000000	4.5947554000000004
H	1.6207209000000000	-5.5574140999999999	2.5237854999999998	H	-1.2151921999999999	-4.1715451999999997	4.4883017000000001
H	1.8205392000000000	-6.0450096000000002	1.0443958000000000	H	8.9292544000000001E-002	-3.3765375000000000	4.6363674000000001
O	4.3979816999999999	-5.2851375000000003	0.9605638600000005	O	1.0990600000000001	-3.2850760999999999	2.3129482000000001
H	4.2563715999999996	-5.5393309000000004	1.9187988000000000	H	1.3935295000000001	-3.8153340999999998	3.0518730000000001
H	3.5155577999999998	-4.9707688000000001	0.7153265199999997	H	1.3487199999999999	-3.8590743999999999	-1.5589693000000000
O	-0.6650804799999997	-5.0497658999999997	-5.5640615999999997E-002	O	1.3342598999999999	-8.8865204000000002	3.0731071000000001
H	0.1888112899999999	-4.6133759000000003	0.1890873399999999	H	1.3546385999999999	-7.980370999999999	2.7441342999999998
H	-0.8641606899999995	-5.6292691000000001	0.6647280700000000	H	2.0162874999999998	-9.2450296999999999	2.5101996000000000
O	4.1964788000000004	-5.5540823000000001	3.6053779999999999	O	6.4423858999999997	-3.6612760999999998	2.3757720999999998
H	4.9153254000000004	-4.8778930999999996	3.7431619999999999	H	5.8200270999999999	-3.7090505999999999	1.6549714000000000
H	3.3872339999999999	-5.1179123000000004	3.6084711999999999	H	6.7164256000000000	-4.5821487999999999	2.3337995999999999
O	-0.4113342099999998	-5.8462708000000001	4.0028769999999998	O	-2.8813287000000001	-2.9625971000000000	0.6805034199999997
H	0.47659709000000000	-5.5504540999999996	3.8336858999999999	H	-2.7356064999999998	-3.5365117000000001	-7.714992399999995E-002
H	-0.5525294699999995	-6.3014260000000002	3.1685807000000001	H	-1.9839443999999999	-2.6574946000000002	0.86848093999999998
O	4.4704484000000004	-3.2160356000000001	-1.2206158000000000				
H	3.6538636000000002	-3.5431580999999999	-0.7702568600000004	C	0.18258432E+01	-0.31705324E+01	0.26749657E+01
H	4.5186647999999999	-2.3058209999999999	-0.8885455500000002	C	0.18928697E+01	-0.18269430E+01	0.30896851E+01
O	1.0083578000000000	-3.6049454999999999	-2.3479090000000000	O	0.16918416E+01	-0.94377040E+00	0.20458958E+01
H	1.3836583000000000	-4.3650041999999996	-2.8514278999999999	C	0.16433004E+01	-0.16596498E+01	0.79482389E+00
H	1.2739016000000001	-3.6239753000000001	-1.3754089000000000	C	0.18003935E+01	-0.31051389E+01	0.12544148E+01
O	-1.1698763000000001	-3.0887516000000002	4.4932037999999999	O	0.20468237E+01	-0.13993756E+01	0.42425001E+01
H	-1.3453271000000000	-4.0368282000000004	4.3578662000000001	C	0.20984536E+00	-0.14336864E+01	0.26735053E+00
H	-0.1808185000000001	-3.1716451000000001	4.5197313000000001	O	-0.735591115E+00	-0.17146490E+01	0.13105167E+01
O	1.8116560000000001	-4.1147194000000002	6.3078446000000001	O	1.8653865000000001	-4.0255630000000000	0.33389762000000001
H	2.7043020000000002	-3.8074276999999999	6.4159617999999998	O	1.8837212999999999	-4.3001429000000000	3.4119370999999998
H	1.7313778000000000	-3.9520461999999998	5.3441751000000002	C	0.947407057E-01	-0.26085237E-01	-0.34311985E+00
O	6.5333882000000001	-3.6097668000000001	2.5446802000000002	O	-0.11093101E+01	0.16189354E+00	-0.10943509E+01
H	5.7096628999999997	-3.6599753000000002	1.9158717000000001	H	0.24990702E+01	-0.12808714E+01	0.26665869E+00
H	6.9315154000000003	-4.5235158000000002	2.4769184000000002	H	0.31788031E+00	0.75519483E+00	0.34226504E+00
O	4.1943409999999997	-2.6136857000000000	5.5128598000000002	H	0.85617334E+00	-0.18906124E-01	-0.11256795E+01
H	3.4722371000000001	-2.2334501000000002	4.9967120999999999	H	-0.18561522E+01	0.12044007E+00	-0.51405030E+00
H	4.4083465999999998	-1.9668420400000000	6.2424004999999996	H	-0.47295036E-01	-0.20818253E+01	-0.58740993E+00
O	1.2784245999999999	-8.9573497999999994	2.9542690999999999	H	-0.57695170E+00	-0.12991802E+01	0.21470055E+01
H	1.3425586000000000	-8.1306805999999998	2.3939948000000002	O	1.9099760000000001	-6.4285188000000000	1.7146538000000000
H	2.0480181000000002	-9.4264077000000004	2.6171937999999999	H	2.0833366000000000	-5.6648712999999997	2.3249233999999999
C	0.19334847E+01	-0.31360828E+01	0.26076749E+01	H	1.7392718000000000	-5.8325883999999997	0.93643354000000001
C	0.19906093E+01	-0.17921053E+01	0.31577420E+01	O	4.6346993999999997	-5.2052364000000004	1.0612303999999999
O	0.19837126E+01	-0.83758552E+00	0.21157270E+01	H	4.2960513000000002	-5.7546992000000001	1.7652276000000000
C	0.18059672E+01	-0.15591466E+01	0.87644865E+00	O	3.7970608000000001	-4.7589673000000001	0.7616923300000003
C	0.19338736E+01	-0.30561720E+01	0.12162461E+01	H	4.1077992999999999	-5.8206471999999998	3.6737883000000000
O	0.19392664E+01	-0.13928422E+01	0.43373454E+01	H	4.6031972000000003	-4.9953424000000002	3.6426656999999998
C	0.40624877E+00	-0.13799329E+01	0.24905893E+00	O	-0.8074963600000002	-5.0153907999999996	-0.25485562000000000
O	-0.64470116E+00	-0.15410853E+01	0.12452134E+01	H	6.8180081000000003E-002	-4.8238731000000001	5.123411399999997E-002
O	1.8132302000000000	-4.0213074999999998	0.3748747399999998	H	-1.1776614999999999	-5.5969167999999998	0.46318028999999999
O	1.8590130000000000	-4.1681448000000003	3.4393961000000002	O	-0.5096144000000002	-5.7197177999999997	4.1892040000000001
C	0.19396673E+00	-0.21261845E-01	-0.43222618E+00	H	0.3827679600000002	-5.4291277999999998	3.9041949999999998
O	-0.10799695E+01	-0.17075111E+00	-0.95464911E+00	H	-0.7996684100000000	-6.1710172000000002	3.3547908000000000
H	0.25631695E+01	-0.12343668E+01	0.14213268E+00	O	1.7629992999999999	-3.8547668000000002	6.0787174000000004
H	0.38177857E+00	-0.82376275E+00	0.31246541E+00	H	2.4651375999999998	-4.5367449999999998	6.2448522999999998
H	0.91574074E+00	-0.24245254E+00	-0.12637151E+01	H	1.7346490000000001	-3.8316240000000001	5.0941650999999997
H	-0.17137286E+01	-0.65284579E-01	-0.28886510E+00	O	4.4095366000000000	-3.2211639999999999	-1.4371035000000001
H	0.18211176E+00	-0.21827423E+01	-0.48404550E+00	H	3.6075707000000001	-3.3014343999999998	-0.9464685900000005
H	-0.34611763E+00	-0.21837780E+01	0.19307316E+01	H	4.6744270999999999	-2.4087977000000000	-1.0110645000000000
O	1.8798288999999999	-6.4830439000000002	1.8541417000000000	O	1.2260187000000000	-3.2395491999999999	-2.4055209000000000
H	2.0542194999999999	-6.0443204000000001	2.6506064000000000	H	1.2332277000000000	-3.9852690000000002	-0.3053802800000002
H	1.6276527999999999	-5.7404792999999996	1.2025260000000000	H	1.4688028000000000	-3.6003398000000000	-1.4904288000000001
O	4.4232706000000004	-5.1782087000000002	0.9245457500000006	O	1.3788347000000001	-8.7427767999999997	2.8279814000000001
H	4.2332026999999997	-5.6539421000000001	1.8129137000000000	H	1.5302832000000000	-7.8270721999999999	2.5535301000000001
H	3.5412716999999998	-4.9175844000000000	0.7456003799999995	H	2.1557217999999998	-9.2242876000000003	2.5132017000000002
O	4.0362891999999997	-5.7136623999999996	3.6727794999999999	O	6.5383310999999997	-3.5001750000000000	2.0213454000000000
H	4.7817151999999998	-5.1446449999999997	3.5568168000000000	H	5.7832116999999998	-3.9385043999999998	1.5968747000000001
H	3.2664314999999999	-5.1014632999999998	3.5886947999999999	H	7.1878428999999997	-4.1364998999999996	2.0388736999999999
O	-0.6345466300000000	-4.8909244000000003	-0.1679791599999999	O	-0.9233847100000000	-2.9715349000000000	5.3640777000000002
H	0.2241396500000000	-4.5580489000000002	0.1451742100000000	H	-1.0250729000000001	-3.7473812000000000	4.7605046000000000
H	-0.7623453500000003	-5.6496583999999999	0.3950076000000002	H	1.6044249999999998	-2.9248083000000000	5.5709518999999998
H	-0.3216190299999997	-5.8638437999999997	4.0732751000000000	O	4.7785517000000004	-7.0933286999999998	-0.8405776400000001
H	0.5159194499999995	-5.3548315000000004	3.8095287000000000	H	4.6811053999999999	-6.6050088000000002	7.2472528999999998-003
H	-0.7249487700000002	-6.1044156999999997	3.1926931999999999	H	5.5265459000000003	-6.6956265999999998	-1.3101432000000000
O	3.9686875000000001	-3.0968618999999999	-1.3995015000000000	C	0.16735306E+01	-0.32075689E+01	0.27114432E+01
H	3.1420530000000002	-3.2805998000000001	-0.9229028400000000	C	0.15298403E+01	-0.18758704E+01	0.32132172E+01
H	4.4481275000000000	-2.5243837999999998	-0.8403605800000002				

O	0.14410989E+01	-0.90990138E+00	0.22360893E+01	H	3.146722599999999	-5.390212199999997	3.405552999999998
C	0.14107876E+01	-0.16238831E+01	0.99624583E+00	O	4.527096199999999	-4.936408900000000	1.056056600000000
C	0.16619734E+01	-0.31102646E+01	0.13397816E+01	H	4.3641829900000003	-5.2046982000000002	2.007704800000000
O	0.16184525E+01	-0.14957336E+01	0.44156570E+01	H	3.680691899999998	-4.724535300000003	0.6580402100000001
C	0.12971253E+00	-0.13300960E+01	0.10310809E+00	O	-0.923864099999997	-5.361300700000001	-0.4222858700000001
O	-0.10828104E+01	-0.15292072E+01	0.86745308E+00	H	-0.1234528700000001	-4.905818400000002	-0.1531746200000001
O	1.794939200000000	-3.990213100000001	0.4302968400000001	H	-1.284908800000000	-5.74883199999998	0.3901559000000000
O	1.707098800000000	-4.318538799999998	3.47013399999999	O	-0.993438489999995	-5.032283699999998	4.206097899999996
C	0.19261013E+00	-0.20859435E+01	-0.61256372E+00	H	-8.035020299999995E-002	-4.7086756000000003	4.0147066000000002
O	-0.97358251E+00	0.28472571E+00	-0.13526568E+01	H	-1.164778600000000	-5.683192700000002	3.546494399999998
H	0.22571881E+01	-0.11384578E+01	0.47207413E+00	O	1.860673100000001	-4.228324800000002	6.100488300000003
H	0.30163250E+00	0.76535531E+00	0.12912799E+00	H	2.766236999999998	-4.399067900000004	6.232173999999997
H	0.10496488E+01	-0.71342266E-01	-0.13041944E+01	H	1.771066199999999	-4.397883000000002	5.117180399999996
H	-0.18089191E+01	0.17219835E+00	-0.84641615E+00	O	0.810474629999999	-3.243842900000002	-2.186754300000000
H	0.16717133E+00	-0.21054895E+01	-0.64685816E+00	H	1.058930399999999	-3.994981999999999	-2.714059400000000
H	-0.98087045E+00	-0.10923069E+01	0.17373297E+01	H	1.055840300000001	-3.539922999999999	-1.283790100000000
O	1.631765600000000	-6.484349800000004	1.810352699999999	O	3.926758099999998	-3.240942399999998	-1.664123400000000
H	1.552038800000001	-5.777549900000003	2.497548699999998	H	3.015260800000001	-3.443643599999998	-1.3063990000000001
H	1.757011900000000	-0.938699100000000	0.9705967500000001	H	4.226263600000002	-2.572785699999998	-0.9849045100000001
O	3.914145500000001	-5.664802299999998	3.452836500000001	O	-0.8983679900000001	-2.304370300000000	4.876721899999997
H	4.062917399999999	-4.822785180000000	4.0044335700000004	H	-1.112522199999999	-3.214645500000000	4.777145599999999
H	2.950510299999999	-5.487373010000003	3.320040099999999	H	5.8007660000000003E-002	-2.411624700000000	4.805650899999998
O	4.544410199999997	-4.966789900000002	0.8649976299999996	O	-1.525228999999999	-6.974357399999997	2.051908999999998
H	4.304571199999998	-5.343424100000000	1.775720900000000	H	-1.014278800000000	-7.715829799999998	1.1631246000000000
H	3.701644299999999	-4.582403000000002	0.552227799999995	H	-2.012465100000000	-7.467659699999996	2.730323100000001
O	-0.68479456000000005	-5.362867899999997	4.109808400000004	O	1.214108699999999	-9.016807300000000	3.144244599999999
H	0.14279797600000000	-4.948675899999996	3.722626200000001	H	1.164227600000000	-8.310858400000008	2.456805100000000
H	-1.057707299999999	-5.855802020000003	3.351032000000000	H	2.002722500000000	-9.599685799999996	2.733636900000000
O	-0.84768701000000002	-5.440665000000001	-0.2853791000000000	O	-3.083115600000002	-3.023903700000000	0.3392341899999999
H	-2.852941499999998E-002	-5.117480800000002	-2.415259399999999E-002	H	-3.316985499999999	-2.568616599999999	-0.4410439800000000
H	-1.258977700000000	-5.837012800000001	0.5569320199999997	H	-2.167616100000000	-2.749570700000000	0.5560280399999995
O	1.823898100000001	-4.068101399999998	6.205076400000003				
H	2.435227199999999	-4.721859600000002	6.423554600000001	C	0.16579399E+01	-0.32868547E+01	0.24750892E+01
H	1.830717900000000	-4.042256499999997	5.218507800000003	C	0.18167588E+01	-0.19163540E+01	0.29766156E+01
O	4.033002100000000	-3.287534899999998	-1.443715300000000	O	0.17568874E+01	-0.10458593E+01	0.19000986E+01
H	3.198404899999999	-3.331408900000000	-0.970194859999999	C	0.15236215E+01	-0.17460771E+01	0.67536595E+00
H	4.634268699999999	-2.623708900000000	-0.993615429999999	C	0.16416707E+01	-0.31676548E+01	0.10542024E+01
O	1.324913599999999	-3.310335600000002	-2.350632399999998	O	0.18502000E+01	-0.14534965E+01	0.4119836E+01
H	1.172817100000001	-4.150802399999997	-2.795843699999996	C	0.12578802E+00	-0.14461836E+01	0.92452470E-01
H	1.386597700000000	-3.638977900000000	-1.429688999999999	O	-0.96557278E+00	-0.14975987E+01	0.10620773E+01
O	-1.027865400000000	-2.821213699999999	5.081340299999999	O	1.659749700000001	-4.069527400000001	7.878174999999998E-002
H	-1.081198700000001	-3.745808999999999	4.678755000000003	O	1.546868300000001	-4.333811899999997	3.303320700000000
H	-0.11120756000000000	-2.758575099999998	5.469002200000003	C	0.18782788E+00	-0.49041454E-02	-0.50609505E+00
O	-1.195757299999999	-7.029107999999999	2.031255799999998	O	-0.10326978E+01	0.31033650E+00	-0.10322346E+01
H	-0.39796943000000001	-7.499350899999996	1.775039199999999	H	0.22925681E+01	-0.14362316E+01	0.29579084E-01
H	-1.669646900000000	-7.740110900000003	2.479121999999998	H	0.37537503E+00	0.65789552E+00	0.30993545E+00
O	4.483203900000004	-2.901327499999998	5.601670200000000	H	0.96544118E+00	0.24597934E-01	-0.12911228E+01
H	3.538517300000001	-2.911584889999998	5.365033500000000	H	-0.17583072E+01	0.20259650E+00	-0.36646624E+00
H	4.561532300000004	-2.290786700000000	6.350451699999998	H	-0.15377072E+00	-0.21026551E+01	-0.65904997E+00
O	1.134482800000000	-8.999056100000007	2.811889299999998	H	-0.51578517E+00	-0.14518932E+01	0.19148752E+01
H	1.379816180000000	-8.165020500000007	2.410750600000001	O	1.208701400000000	-6.531840799999999	1.6420461000000000
H	2.004275300000002	-9.473209400000000	2.734291900000001	H	1.227646700000000	-5.999685799999998	2.454151000000000
C	0.15025866E+01	-0.33091353E+01	0.25947376E+01	O	1.527808199999999	-5.817730199999997	1.0465675000000000
C	0.17603171E+01	-0.19997639E+01	0.31498269E+01	H	4.292325199999996	-4.620669099999998	0.7108433600000004
O	0.17475398E+01	-0.10210112E+01	0.21408051E+01	H	4.162747000000004	-4.900605599999996	1.604185000000000
C	0.14467639E+01	-0.17522008E+01	0.86504618E+00	H	3.405640200000001	-4.261447099999998	0.4536342800000000
C	0.15438909E+01	-0.32205881E+01	0.12293311E+01	H	3.918047699999998	-5.487394199999998	3.292586000000000
O	0.20439516E+01	-0.15653943E+01	0.43245616E+01	H	-5.124592700000000	4.057177099999996	3.151828700000000
C	0.10338522E+00	-0.13085786E+01	0.23816946E+00	O	-5.285604799999998	-0.2572844100000002	
O	-0.10001162E+01	-0.14237939E+01	0.12036258E+01	H	-1.868567800000001	-5.195103000000000	2.083347700000000-002
O	1.533701999999999	-4.127887999999996	0.3828844499999998	H	-1.143841700000001	-6.028680500000001	0.3826249299999997
O	1.466273399999999	-4.406136799999996	3.375106800000002	O	-1.088405300000000	-4.9409368050000002	3.8566636300000001
C	0.45020629E-01	0.95797117E-01	-0.48004312E+00	H	-0.1126012900000001	4.813549300000001	3.5884922000000001
O	-0.12033257E+01	0.41185885E+00	-0.11356969E+01	H	-1.258919200000000	-5.584095099999999	3.098791700000000
H	0.22713222E+01	-0.15332997E+01	0.21368265E+00	O	0.5194104000000002	-3.545663700000000	-2.533677200000001
H	0.25513760E+00	0.88286235E+00	0.24384723E+00	H	0.940775079999999	-4.315610500000000	-2.950103700000001
H	0.79612175E+00	0.14287979E+00	-0.12773040E+01	H	0.7530884500000002	-3.724518999999999	-1.616189499999999
H	-0.19314043E+01	0.27549939E+00	-0.50909259E+00	O	4.109958299999997	-3.429898699999999	-1.719536100000000
H	-0.52626112E-01	-0.19969149E+01	-0.57431010E+00	H	3.239303000000000	-3.666359100000002	-1.387281299999999
H	-0.64546465E+00	-0.21698619E+01	0.18691612E+01	H	4.506281699999997	-3.010392200000001	-0.9281840999999996
O	1.341761699999999	-6.789070100000000	1.495269299999999	O	1.327643900000000	-4.449547400000002	6.158700500000001
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H	1.414943200000000	-6.251386600000000	0.721538679999999	H	1.304262700000000	-4.282647200000004	5.209326199999996
O	4.082038700000000	-5.653903599999996	3.611080900000001	O	4.496299900000003	-7.160270399999999	-0.59780672000000001
H	4.374497200000004	-4.974266300000000	4.249907000000003	H	4.179303400000002	-6.487522399999996	8.197113799999999-002

H	5.2627506000000004	-6.690762499999999	-0.9981362700000005	C	0.34053405E+00	0.20428599E+00	-0.10130456E+00
O	6.2364075000000003	-3.6797764000000002	2.4057556999999998	O	-0.90222195E+00	0.54414672E+00	-0.79080484E+00
H	5.6078951000000004	-3.8521314000000002	1.6939347000000000	H	0.24394351E+01	-0.13713686E+01	0.25788775E+00
H	6.3686322000000004	-4.5676335000000003	2.8105375000000001	H	0.27463775E+00	0.74427732E+00	0.90473652E+00
O	-1.5237141000000001	-7.1238529000000002	1.6505627000000000	H	0.11764860E+01	0.54724426E+00	-0.70361034E+00
H	-0.6755177599999997	-7.5168600000000003	1.8490977000000000	H	-0.16058572E+01	0.61069964E+01	-0.34176223E+00
H	-2.192921999999998	-7.608842799999997	2.1917216000000002	H	0.29350359E+00	-0.17103166E+01	-0.91068062E+00
O	1.3858330000000001	-8.871158499999999	3.2738440000000000	H	-0.79774878E+00	-0.19127352E+01	0.17715092E+01
H	1.3996820000000001	-8.1317339000000004	2.6058490999999999	O	1.8770781000000001	-6.524484199999998	1.7320907999999999
H	2.2115881000000002	-9.3193640000000002	2.9686281999999999	H	1.7960035000000001	-5.9554482000000002	2.5087000000000002
				H	1.8992015000000000	-5.8239616999999999	1.0518797000000000
C	0.15105499E+01	-0.32443828E+01	0.26064736E+01	O	4.3784460000000003	-4.7440163999999996	1.2392192000000000
C	0.16990512E+01	-0.19408369E+01	0.31782256E+01	H	3.955847299999998	-5.4926936000000000	1.7615784000000001
O	0.15975459E+01	-0.94476619E+00	0.21922342E+01	H	3.5812392000000002	-0.4951730000000003	0.7658586200000005
C	0.15739139E+01	-0.15728235E+01	0.88730602E+00	O	3.8923958600000001	-5.5248495999999996	4.0003612999999998
C	0.15940519E+01	-0.30795837E+01	0.11929434E+01	H	4.4269249000000004	-4.7555006999999998	4.4000135000000000
O	0.18171574E+01	-0.15051904E+01	0.43496643E+01	H	3.0810431000000000	-4.9965191000000004	3.7220787000000000
C	0.21905475E+00	-0.12639742E+01	0.20532846E+00	O	-1.0804043000000001	-5.4597302000000001	3.8287148000000002
O	-0.86227089E+00	-0.15183285E+01	0.10612328E+01	H	-9.871253900000002E-002	-0.3765700000000001	3.6778510999999998
O	1.6891331300000001	-3.9328723000000001	0.24200289000000000	H	-1.3562528000000000	-5.9497416999999997	3.0598887000000001
O	1.4091681000000000	-4.3097782999999996	3.3632536000000002	O	-0.9794412900000002	-5.2300373000000002	-0.4138128200000003
C	0.15825870E+00	0.25394053E+00	-0.25821701E+00	H	-0.10324375000000000	-0.5031948999999998	-3.1565432999999997E-002
O	-0.93420843E+00	0.40723078E+00	-0.11890956E+01	H	-1.2836350000000001	-5.9347035000000004	0.2165175199999999
H	0.24434733E+01	-0.13542067E+01	0.26781727E+00	O	3.5849443999999999	-3.1123406000000000	-1.3651708000000000
H	0.20336763E+00	0.10453018E+01	0.48704482E+00	H	2.9296467000000002	-3.2786878000000002	-0.6806104200000005
H	0.10927540E+01	0.42552240E+00	-0.81324728E+00	H	4.0267410000000003	-2.4059773999999998	-0.8857899299999995
H	-0.17548588E+01	0.12222943E+00	-0.68030928E+00	O	-0.9670830999999997	-2.6858930000000001	4.8396338999999999
H	0.99693525E+00	-0.17452473E+01	-0.73699193E+00	H	-0.8071654999999998	-3.5126496999999999	4.3298800000000000
H	-0.61003493E+00	-0.15269716E+01	0.20340987E+01	H	-6.9845163000000002E-002	-2.4703051000000000	4.9915867000000000
O	1.3126600000000000	-6.3837751000000003	1.8687206000000001	O	1.5798529999999999	-4.4039529000000002	6.3017909999999999
H	1.3014036000000000	-5.6244475799999999	2.5124564999999999	H	2.1280655900000002	-5.1885299999999999	6.1128704000000003
H	1.5734562000000001	-5.8407963000000001	1.1725660000000000	H	1.3149493000000001	-4.2685143999999999	5.3590470999999997
O	4.1916595000000001	-4.9420295000000003	0.8778517500000004	O	0.8646825500000005	-3.4521742100000002	-2.5568276000000001
H	3.8874930999999999	-5.0910679999999997	1.7626596000000001	H	1.5998899000000000	-3.9406539999999999	-2.9062139000000000
H	3.2576724000000001	-4.6114268999999997	0.6279150199999999	H	0.9096921300000004	-3.7681651999999999	-1.6265889000000000
O	3.8285070999999999	-5.2660803999999999	3.6293785999999999	O	3.9144304000000001	-7.0756553999999996	-0.5843796700000002
H	4.1432976000000004	-4.5198461999999999	4.2320829999999998	H	3.3464467000000000	-6.9267159999999999	0.21176033999999999
H	2.8456758000000000	-5.0834333000000003	3.4866780999999998	H	4.7677671999999998	-7.2600218999999999	-0.2368342900000000
O	-0.12358579999999999	-5.2460839000000004	3.6611348000000001	O	1.4328959999999999	-8.6290558999999991	3.4264716000000002
H	-0.33990988000000000	-4.9260126000000000	3.3882191000000002	H	1.7541635000000000	-7.8399360000000003	2.9768189999999999
H	-1.42335468000000000	-5.9068157000000001	2.9898028999999999	H	1.9128706000000000	-9.2655869000000006	2.8968340000000001
O	-0.96260520999999999	-5.3607703999999998	-0.4314765500000001	O	4.2687033000000003	-3.2257603000000001	5.5030231000000001
H	-0.10177946000000000	-5.1363940000000001	-2.7034656000000001E-002	H	3.3208628999999998	-3.2210497999999999	5.4481431999999999
H	-1.2463120000000001	-6.0790744999999999	0.21765298000000000	H	4.4126475999999997	-2.4960410000000000	6.1744326999999997
O	1.3427040000000000	-4.0825506000000003	5.9578844999999999				
H	2.1733248999999999	-4.5192418999999999	6.1388951000000000	C	0.16888298E+01	-0.32565825E+01	0.25625045E+01
H	1.3475193999999999	-4.1278094499999999	4.9868446999999999	C	0.16794285E+01	-0.19219012E+01	0.32017489E+01
O	3.7752555999999999	-3.2626267000000002	-1.7325771000000001	O	0.16061273E+01	-0.93546956E+00	0.22784840E+01
H	3.0042496000000001	-3.5444273000000002	-1.2013408999999999	C	0.14525264E+01	-0.15346256E+01	0.91779838E+00
H	4.3086045000000004	-2.7782461999999999	-1.1255160000000000	C	0.14854087E+01	-0.30791256E+01	0.11783066E+01
O	0.4511670800000000	-3.4341238000000001	-2.6355197000000001	O	0.17168852E+01	-0.16657862E+01	0.44187640E+01
H	1.1142010000000000	-3.8706502999999999	-3.2249154000000000	C	0.14193906E+00	-0.11477384E+01	0.29960819E+00
H	0.6905312300000005	-3.8595036000000000	-1.7626567000000000	O	-0.98865256E+00	-0.16805685E+01	0.10025597E+01
O	3.9868549999999999	-3.4761926999999999	5.5225302000000003	O	1.4760275000000000	-3.9637916000000000	0.23359288000000000
H	3.0852726299999999	-3.3237686000000002	5.1600390999999999	O	1.6440405000000000	-4.3346584999999997	3.3601752000000000
H	4.2679577999999996	-2.5522783000000002	5.6116653999999997	C	0.21140425E-01	0.38622703E+00	0.16941869E+00
O	-1.1349020999999999	-2.2749335999999999	4.8268483000000000	O	-0.97467650E+00	0.87298278E+00	-0.7078204E+00
H	-1.1478347000000000	-3.2218949000000001	4.6577469999999996	H	0.23090388E+01	-0.12209476E+01	0.37734982E+00
H	-0.20048326000000000	-2.0774468000000001	4.6731047999999999	H	-0.94858064E-01	0.81113715E+00	0.11523804E+01
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H	1.3364119999999999	-7.9780404000000003	2.8749937000000001	H	-0.17554050E+01	0.78808920E+00	-0.24121295E+00
H	2.0180949999999999	-9.2440668000000006	2.6740629999999999	H	0.26374438E+00	-0.15422003E+01	-0.73509788E+00
O	0.436165529800000004	-7.2556938000000004	-0.5304038199999997	H	-0.69798635E+00	-0.23654992E+01	0.16195664E+01
H	4.1864204999999997	-6.2667954000000003	-0.35676898000000001	O	1.8367434000000000	-6.3992623000000002	1.6984222000000000
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				H	1.7630988999999999	-5.8366055000000001	0.9260041500000003
C	0.15157770E+01	-0.33074633E+01	0.26855336E+01	O	4.0054689000000003	-5.6971752000000002	3.4195538000000001
C	0.17023073E+01	-0.18763114E+01	0.31529444E+01	H	4.3583385999999997	-4.8513653999999997	3.8632659000000000
O	0.16319375E+01	-0.10254394E+01	0.20958922E+01	H	3.0075265000000000	-5.4557317000000003	3.4437062000000001
C	0.15684757E+01	-0.17337873E+01	0.82420036E+00	O	-0.9928342000000000	-5.1035953000000003	-0.4057734800000002
C	0.15512647E+01	-0.31830480E+01	0.12596751E+01	H	-0.17381693000000001	-4.8187981000000004	1.5378085000000000E-002
O	0.18313202E+01	-0.14021944E+01	0.43082776E+01	H	-1.3153923000000001	-5.7700304999999998	0.1659280400000000
C	0.30377997E+00	-0.12578918E+01	0.96087325E-01	O	-1.0533553000000000	-5.2406338000000003	3.7525921000000002
O	-0.91391346E+00	-0.17156838E+01	0.76957509E+00	H	-0.13704864000000000	-4.8671077000000000	3.7108638399999998
O	1.5217159000000000	-4.1387887000000001	0.29285106000000000	H	-1.0820372000000000	-5.8726513000000002	2.9709649999999998
O	1.5018138000000001	-4.3695959999999999	3.5306955000000002	O	4.7807382000000000	-4.7272501000000000	0.9076281000000000

H	4.335198400000003	-5.113238100000002	1.729952600000001	H	3.504027199999999	-7.423326999999996	0.3364312099999998
H	4.028447800000004	-4.536744099999999	0.3575806300000001	H	4.952736800000003	-7.439397600000004	0.39196646000000002
O	3.594987499999998	-3.083117800000001	-1.455999499999999				
H	2.826719300000002	-3.339213899999998	-0.954437219999998	C	0.15483187E+01	-0.33747145E+01	0.27016728E+01
H	4.076822100000002	-2.568301200000001	-0.773934670000005	C	0.17090685E+01	-0.20596923E+01	0.34041706E+01
O	1.336004000000000	-4.616469200000001	6.126262299999996	O	0.16359573E+01	-0.10979792E+01	0.24359403E+01
H	2.128838700000002	-5.027491200000000	6.474622300000001	C	0.14752693E+01	-0.16427269E+01	0.11213146E+01
H	1.518973399999999	-4.614176299999996	5.177028000000000	C	0.15544418E+01	-0.30904688E+01	0.13049437E+01
O	0.8611617579999999	-3.202943700000001	-2.494726300000000	O	0.17821660E+01	-0.17745815E+01	0.46335505E+01
H	1.316254300000000	-3.923496399999999	-3.008412400000001	C	0.11440298E+00	-0.10508081E+01	0.54188130E+00
H	0.959571610000002	-3.554955800000001	-1.599186599999999	O	-0.91629883E+00	-0.14247355E+01	0.14775118E+01
O	1.230566700000000	-8.645671900000000	3.306824000000001	O	1.652919000000000	-3.945319800000000	0.32888895000000001
H	1.349786900000000	-7.762404799999997	2.879512300000000	O	1.579680400000000	-4.583147399999996	3.206836899999999
H	1.918081999999999	-9.102037199999998	2.889609999999998	C	0.18544692E-01	0.37890887E+00	0.19080207E+00
O	-0.971582940000001	-2.560150999999998	4.605917100000001	O	-0.11241884E+01	0.65162413E+00	-0.56048495E+00
H	-1.161424199999999	-3.494756100000000	4.402796200000000	H	0.22653015E+01	-0.11546879E+01	0.45292733E+00
H	-4.607431699999997E-002	-2.533692299999998	4.947113400000001	H	0.17393530E-01	0.90500852E+00	0.11241747E+01
O	4.137156499999997	-3.351205400000000	5.315574700000000	H	0.81375588E+00	0.72879998E+00	-0.45238415E+00
H	3.312295499999998	-2.900783900000000	5.018405300000004	H	-0.18906237E+01	0.29434530E+00	-0.20127393E-01
H	4.317902100000004	-2.719070200000000	6.018812299999996	H	-0.33611490E-01	-0.16906582E+01	-0.35037096E+00
O	-1.308331399999999	-6.969602139999997	1.604813700000000	H	-0.51591539E+00	-0.20047498E+01	0.21041059E+01
H	-0.585729899999999	-7.626811000000000	1.437684800000000	O	2.080385600000001	-6.558966400000001	1.37888280000000000
H	-2.097114299999999	-7.468020600000000	1.871262900000001	H	2.062609199999998	-6.276456500000001	2.356082100000001
C	0.17519745E+01	-0.32884620E+01	0.25457687E+01	O	-0.896036689999999	1.866321500000000	1.00072750000000000
C	0.17583701E+01	-0.20097804E+01	0.313121916E+01	H	7.92006710000000E-002	-5.159889500000002	0.1479270199999999
O	0.16125219E+01	-0.96718985E+00	0.22098383E+01	H	-1.150094699999999	5.701868000000002	0.6786645999999997
C	0.15571217E+01	-0.15414050E+01	0.88700918E+00	O	4.021562399999996	-5.354438899999999	3.8251998000000000
C	0.17891280E+01	-0.30150497E+01	0.11293366E+01	H	4.315129599999997	-4.665561099999997	4.488831099999996
O	0.18203013E+01	-0.17603879E+01	0.43489228E+01	H	3.095140300000002	-5.058358499999998	3.7001023000000002
C	0.27696503E+00	-0.11308656E+01	0.31000532E+00	O	4.684618200000001	-4.179718799999998	1.1847369000000001
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O	1.758172899999999	-3.965574199999998	0.2324125300000001	H	3.979700900000001	-4.435389899999997	0.5464959999999997
O	1.660229500000000	-4.431805500000003	3.179631800000001	O	-1.081838099999999	-5.429869899999999	3.638680100000002
C	0.16904468E+00	0.32583372E+00	0.11239126E+00	H	-8.31334720000000E-002	-5.428745100000004	3.473767099999999
O	-0.10357582E+01	0.65646108E+00	-0.62994065E+00	H	-1.370062100000000	-6.012188300000000	2.8978025000000001
H	0.24061856E+01	-0.10949815E+01	0.35297667E+00	O	3.571940800000001	-3.587799700000001	-1.5384918000000001
H	0.33013261E-01	0.86330857E+00	0.10688593E+01	H	2.892538500000001	-3.661842699999998	-0.8864571000000000
H	0.11100243E+01	0.64950591E+00	-0.44647480E+00	H	4.094002100000000	-2.950275800000002	-0.9738444499999997
H	-0.17415417E+01	0.100008816E+01	-0.56124070E-01	O	0.773354349999999	-3.549283099999998	-2.182995200000001
H	0.16397197E+00	-0.16551054E+01	-0.58269832E+00	H	1.338348300000000	-4.052731900000004	-2.774035599999999
H	-0.55441797E+00	-0.18326531E+01	0.19975519E+01	H	1.258774000000000	-3.582042400000002	-1.376372300000001
O	1.952568000000001	-6.530115900000002	1.384739000000001	O	1.522743400000000	-4.267047999999997	6.138129400000004
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O	4.665794599999999	-4.488614400000003	1.168546009999999	O	-1.054551300000000	2.786734899999999	4.822618900000002
H	3.951426500000002	-4.870223000000002	1.778446699999999	H	-1.036360699999999	-3.575972600000001	4.221590000000000
H	4.172157799999999	-4.443338999999998	0.308651960000000	H	-8.923156000000001E-002	-2.672619000000002	4.932454999999999
O	4.108704989999997	-5.497972700000000	3.694284000000001	O	4.474464199999999	-7.077744899999999	-0.4399081200000001
H	4.551456299999999	-4.896918799999999	4.279586999999998	H	3.714953099999998	-6.921808000000004	0.14012622000000000
H	3.272336999999998	-5.021501200000000	3.459408600000002	H	4.903091899999997	-7.745840399999996	0.10611286000000000
O	-0.869115949999999	-5.353091400000003	-0.2587242320000001	O	1.472397000000000	-6.871581790000004	2.976275100000001
H	2.899041700000001E-002	-4.973008700000003	-0.1081932800000000	H	1.916674500000001	-7.981450200000003	2.4303417000000000
H	-1.050518300000000	-5.757972399999999	0.609835829999999	H	2.138030000000001	-9.357500999999992	2.999794999999998
O	-0.987405160000000	-5.291339700000000	3.531267999999999	O	4.383450700000000	-3.088011299999998	5.5177768000000000
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H	-1.251615200000000	-5.845621500000000	2.821973299999998	H	4.463379299999997	-2.418454300000001	6.288601400000001
O	3.910721000000001	-3.448753000000000	-1.519379300000000				
H	3.013929899999999	-3.473904000000002	-1.112682200000001	C	0.15506501E+01	-0.35051760E+01	0.26782111E+01
H	4.288852000000003	-2.825607600000001	-0.884686210000003	C	0.15213863E+01	-0.22124750E+01	0.33464953E+01
O	0.700732040000000	-3.461651400000000	-2.428618600000001	O	0.16148934E+01	-0.11208366E+01	0.24333501E+01
H	1.329480800000000	-3.999782199999998	-2.981991400000001	C	0.15113740E+01	-0.17192408E+01	0.11371520E+01
H	1.022133000000000	-3.690287500000002	-1.509919999999999	C	0.16044554E+01	-0.32000468E+01	0.13022617E+01
O	1.370067200000000	-4.604637600000002	6.083829399999999	O	0.14953266E+01	-0.19623184E+01	0.45946547E+01
H	2.046281700000002	-5.249561800000004	6.351014900000000	C	0.15344018E+00	-0.13163197E+01	0.51515910E+00
H	1.651548000000000	-4.485360599999999	5.164968899999999	O	0.99788032E+00	-0.16570645E+01	0.13603380E+01
O	1.317868899999999	-8.391770400000004	3.241756200000002	O	1.765133200000000	-3.991540300000000	0.30470638000000000
H	1.397797500000000	-7.809213699999999	2.488017199999998	O	1.673414200000000	-4.698528099999999	3.222792699999998
H	1.903754299999999	-9.108255500000003	3.077331399999998	C	0.12932069E+00	0.18405185E+00	0.36461593E+00
O	-1.140725500000001	-2.860231900000000	4.665575600000004	O	-0.92650081E+00	0.81438884E+00	-0.42593312E+00
H	-1.200310400000000	-3.754542810000002	4.205286000000001	H	0.22486046E+01	-0.13488583E+01	0.39033941E+00
H	-0.200467360000001	-2.807519000000001	4.953280000000003	H	0.72524018E-01	0.61732641E+00	0.13724034E+01
O	4.168581299999996	-3.253692700000002	5.490127900000001	H	0.10452457E+01	0.40559829E+00	-0.23092940E+00
H	3.505974199999998	-2.863800599999998	4.925313700000002	H	-0.16963994E+01	0.15081617E+00	-0.27571068E+00
H	4.103421499999996	-2.690771900000001	6.296190499999998	H	0.96523946E-01	-0.19893633E+01	-0.35361004E+00
O	4.267323199999999	-7.218239900000004	-0.217976160000000	H	-0.85208973E+00	-0.25353273E+01	0.17930459E+01

O	1.8681633000000000	-6.459626199999998	1.126246099999999	O	1.2051371000000000	-4.648639400000004	6.067496900000001
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O	-1.068114999999999	-5.116887400000004	0.2896523200000002	O	1.422007199999999	-8.496914999999996	2.846682100000002
H	-0.1447448600000000	-5.211598099999998	0.5851011400000002	H	1.796539200000000	-7.72641039999998	2.390856499999999
H	-1.474684799999999	-5.706389899999996	0.9315093700000000	H	2.120354299999998	-9.136542099999998	2.810836900000000
O	4.838495899999998	-4.368301500000003	1.354886000000000	O	4.124002299999999	-7.201607199999998	-0.3089203400000002
H	4.525600299999998	-4.986335200000001	2.049512399999998	H	3.425726000000000	-7.071711399999999	0.404277649999999
H	4.031345800000004	-3.835009599999998	1.187585200000000	H	4.903017499999998	-7.101405200000003	0.2330550000000000
O	4.118172600000003	-5.221041699999998	3.966704899999999	O	-1.176061400000000	-2.785902600000000	4.797307100000003
H	4.230265700000004	-4.307875900000000	4.228090500000004	H	-1.315381600000000	-3.729214100000001	4.436506299999996
H	3.167325200000001	-5.125548000000003	3.579429199999999	H	-0.2753629100000002	-2.845947799999998	5.039869300000003
O	-1.047160099999999	-5.215620699999997	3.499064900000000	O	-2.153738100000000	-3.709813300000000	-1.614747900000000
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H	-1.459662500000001	-5.975095200000002	3.085074999999998	H	-1.802286300000000	-4.269562500000001	-0.8470201200000004
O	3.608731999999998	-3.226989900000000	-1.661827800000000				
H	3.007548599999998	-3.694192900000000	-1.108711500000001	C	0.15158330E+01	-0.34589808E+01	0.26396849E+01
H	4.118937299999998	-2.689787299999998	-1.029831200000001	C	0.16863780E+01	-0.22461615E+01	0.33413523E+01
O	1.397672900000001	-4.625974700000004	6.051599099999998	O	0.18002204E+01	-0.11067104E+01	0.25120758E+01
H	2.086684599999999	-5.262272000000003	6.182436100000003	C	0.17007551E+01	-0.16099246E+01	0.11398238E+01
H	1.503030499999999	-4.613260099999998	5.065138000000001	C	0.16567470E+01	-0.30997499E+01	0.12513009E+01
O	0.7531574800000005	-3.420217000000001	-2.322130399999998	O	0.17008524E+01	-0.19972147E+01	0.45494520E+01
H	1.266441900000000	-3.866794500000001	-3.030813600000001	C	0.30419570E+00	-0.11117393E+01	0.54076210E+00
H	1.156448300000001	-3.835585500000001	-1.526715700000000	O	-0.76758367E+00	-0.14542247E+01	0.13870272E+01
O	1.482105000000000	-8.513685600000005	2.869614099999998	O	1.603859000000000	-3.945360000000000	0.2338873499999999
H	1.382897199999999	-7.872944200000001	2.153333400000002	O	1.353834999999999	-4.699255000000000	3.170306000000000
H	2.432218799999998	-8.828260300000002	2.900283700000001	C	0.28828249E+00	0.34146934E+00	0.24283456E+00
O	4.207218300000001	-7.234069599999998	-0.534837149999998	O	-0.92372000E+00	0.74121302E+00	-0.48791258E+00
H	3.549507900000000	-6.934873999999998	7.44997699999995E-002	H	0.24595902E+01	-0.12385365E+01	0.49534725E+00
H	5.007133399999998	-7.163203600000001	-9.697017199999997E-003	H	0.31259439E+00	0.92032315E+00	0.11799387E+01
O	-1.269056400000000	-2.789081599999998	4.729564299999998	H	0.11062474E+01	0.50780827E+00	-0.44627086E+00
H	-1.076189600000000	-3.446409000000000	4.057183900000001	H	-0.16422394E+01	0.34565694E+00	0.37200514E-01
H	-0.432010349999999	-2.303592300000000	4.815228099999999	H	0.18039835E+00	-0.15854332E+01	-0.42486555E+00
O	5.352390400000000	-7.330028699999997	2.778845599999999	H	-0.42245860E+00	-0.19027129E+01	0.22105956E+01
H	4.977201799999996	-6.488588599999999	3.178950200000001	O	2.187102900000002	-6.464735499999997	1.366714299999999
H	6.314651300000004	-7.107313000000004	2.849232499999998	H	1.887800200000000	-5.949380699999999	2.127191000000000
C	0.14503695E+01	-0.33998685E+01	0.26051323E+01	H	1.860334800000000	-5.839685799999998	0.6469412399999997
C	0.16150657E+01	-0.21456922E+01	0.33859209E+01	O	-1.174725800000000	-5.054657599999996	0.1355068800000000
O	0.17327150E+01	-0.11081148E+01	0.24997411E+01	H	-0.339107949999999	-4.598174700000004	0.3575699000000000
C	0.15350808E+01	-0.15912319E+01	0.10993454E+01	H	-1.133340000000001	-5.757483239999996	0.874231400000000
C	0.16315317E+01	-0.30865102E+01	0.125154258E+01	O	-1.249860000000000	-4.853657300000001	3.798269100000002
O	0.17796143E+01	-0.19106153E+01	0.45596217E+01	H	-0.2741066500000001	-4.671272900000000	3.558176599999999
C	0.27507257E+00	-0.11351878E+01	0.45014312E+00	O	-1.317809800000000	-5.619177500000002	3.186220200000002
O	-0.82199073E+00	-0.15606417E+01	0.13066348E+01	H	4.604041399999998	-4.427729600000002	1.086710899999999
O	1.689482800000000	-3.891545600000002	0.2288940600000001	H	0.477429399999999	-5.223396799999997	1.299817000000000
O	1.368219000000001	-4.586029100000002	3.225007699999999	O	3.934554900000002	-3.797308800000002	0.765077699999998
C	0.23775259E+00	-0.46285814E+00	0.37156087E+00	H	3.852223899999999	-5.328568200000003	4.099291199999997
O	-0.94359845E+00	-0.85846393E+00	-0.26188922E+00	H	4.033516900000004	-4.420686899999998	4.361651499999998
H	0.23016497E+01	-0.11704121E+01	0.50977090E+00	H	2.983894799999999	-5.344032999999996	3.749031000000001
H	0.33255195E+00	-0.99709323E+00	0.13381281E+01	O	0.4986176700000001	-3.577720600000001	-2.161905500000000
H	0.11306565E+01	-0.73251766E+00	-0.25755740E+00	H	1.276861999999999	-3.806953599999999	-2.678347899999999
H	-0.16942285E+01	-0.284343462E+00	-0.30060106E-01	O	0.896387469999999	-3.596373679999999	-1.220073900000000
H	0.22015150E+00	-0.15413295E+01	-0.54943516E+00	O	3.438595000000000	-3.202609199999999	-1.626560500000001
H	-0.59856934E+00	-0.12824561E+01	0.22063523E+01	H	2.851459999999999	-3.490652799999999	-0.917320339999999
O	2.156719499999999	-6.414159999999999	1.288839300000000	H	4.009304000000002	-2.669669700000000	-1.049124000000000
H	1.867318100000001	-5.891035300000004	2.030031999999998	O	1.140075900000000	-4.424792400000003	6.122884100000003
H	1.969574900000000	-5.784673699999999	0.641444829999997	H	1.829706300000000	-4.879787099999997	6.456502800000000
O	-0.935541729999996	-5.255677699999997	0.1254681199999999	O	1.067335200000000	-4.664919900000001	5.188394200000003
H	1.653680800000000E-002	-4.945635799999998	0.3499076999999999	H	4.224055500000004	-7.422823199999998	-0.2880022999999999
H	-1.104233000000000	-5.856363600000004	0.861195929999997	H	3.383910499999998	-7.272998300000002	8.005760000000003E-002
O	4.718079300000003	-4.466688999999997	1.300963300000000	H	4.751452900000003	-7.258951399999999	0.4969875300000001
H	4.240238100000000	-4.899491300000002	0.5722590800000003	O	1.240131200000000	-8.682579699999998	3.112813500000001
H	3.984243799999998	-3.886948400000002	1.656772200000000	H	1.498992999999999	-8.150908799999998	2.281248199999998
O	-1.190327000000001	-5.293530299999996	3.580573999999999	H	2.111901099999999	-8.852525000000000	3.426983000000000
H	-0.2309244300000001	-5.103581400000004	3.527482099999998	O	-1.177155800000000	-2.231309500000001	4.548957399999999
H	-1.313875500000000	-5.986548799999996	2.915842899999999	H	-1.352200899999999	-3.112742999999998	4.301395600000002
O	3.768736500000002	-5.145456099999996	4.390027199999996	H	-0.279221139999998	-2.417141400000002	4.718799000000001
H	3.987610900000000	-4.215405699999998	4.521468500000001	O	-3.070420200000000	-2.497445400000001	0.532508309999998
H	2.932393799999998	-5.102599800000001	3.913383800000001	H	-2.765978399999998	-2.568192799999998	-0.4042042900000002
O	0.6683087199999997	-3.802833600000000	-2.245061499999998	H	-2.231535800000001	-2.488497999999999	0.9515174300000000
H	1.423610400000001	-4.284514599999996	-2.703923600000000	C	0.16167241E+01	-0.32651595E+01	0.25896290E+01
H	0.949116779999999	-3.866049400000001	-1.275788600000001	C	0.18584688E+01	-0.20122833E+01	0.32135015E+01
O	3.625361700000000	-3.245251199999998	-1.612152100000001	O	0.18603033E+01	-0.95091262E+00	0.2252657E+01
H	2.858862499999999	-3.467591399999999	-0.966955820000002	C	0.15567084E+01	-0.15331939E+01	0.97245961E+00
H	4.081356000000004	-2.589803400000001	-1.104247999999999	C	0.14562771E+01	-0.30507545E+01	0.12407698E+01

O	0.20696705E+01	-0.17356032E+01	0.43811755E+01	H	-1.4786824999999999	-6.0057396000000001	0.9484533000000002
C	0.26457452E+00	-0.99713742E+00	0.37141566E+00	O	4.6370243000000002	-4.3059821999999999	1.1932474000000000
O	-0.83363645E+00	-0.12507020E+01	0.13230876E+01	H	3.7982659000000001	-3.8740676999999999	0.9469282999999995
O	1.3575699999999999	-3.8818345999999999	0.2115361199999999	H	4.3457071999999997	-4.8054429000000001	1.9314378000000001
O	1.5354614000000000	-4.3818913000000004	3.3622461000000001	O	4.0308999999999999	-5.2369449000000001	3.7026292000000001
C	0.25954511E+00	0.52851996E+00	0.10753386E+00	H	4.3816531999999997	-4.4003034999999997	4.0813060999999999
O	-0.10399651E+01	0.89386345E+00	-0.28724430E+00	H	3.0768325000000001	-4.9525281999999997	3.7649313000000002
H	0.23890528E+01	-0.12665674E+01	0.30249773E+00	O	3.2143259999999998	-3.2078327000000000	-1.5869396000000000
H	0.65365948E+00	0.11252097E+01	0.10428614E+01	H	2.5154003000000000	-3.4452791999999999	-0.9660210400000000
H	0.10461547E+01	0.80818720E+00	-0.68984413E+00	H	3.7209685000000001	-2.5385515000000001	-1.0683199999999999
H	-0.16891750E+01	0.26824216E+00	-0.11420388E-01	O	0.8360156300000001	-4.6643207999999996	5.9211030999999998
H	-0.35567478E-01	-0.13416916E+01	-0.60092070E+00	H	1.5512077000000000	-5.2858720999999997	6.1394346000000004
H	-0.62999771E+00	-0.19523653E+01	0.19544041E+01	H	1.0526895000000001	-4.4757321000000001	5.0171554000000000
O	1.8066295999999999	-6.2736027999999999	1.3444217000000001	O	0.2434063700000001	-3.5281650999999998	-2.3910233999999999
H	1.8981090000000000	-5.5813638000000001	2.0464839000000001	H	1.0437643999999999	-3.5895373139999998	-3.0072464999999999
H	1.5500809000000000	-5.7117975999999997	0.6130115900000005	H	0.6157907099999996	-3.6784924999999999	-1.4770231000000000
O	4.3423448000000002	-4.3073782999999999	1.0950238000000001	O	1.2613645000000000	-2.3452323000000002	4.5006561999999999
H	3.4882594000000000	-4.2410728999999998	0.9595117160000003	H	-1.3399580000000001	-3.2828721000000001	4.1523360000000000
H	4.0367711999999996	-4.4115520000000004	2.0019049000000000	H	-0.3421895500000001	-2.4681943999999998	4.8059710999999998
O	-0.2513112000000000	-4.7024027000000004	3.5149173999999999	O	4.0106283999999999	-7.1528450000000001	-0.1434934400000000
H	-0.2712332000000001	-4.5725254000000000	3.4149596000000000	H	3.1895819999999998	-7.1388018999999997	0.4040385599999999
H	-1.5177080000000001	-5.4138780999999998	2.8613259999999998	H	4.6854326000000004	-7.1901840000000002	0.5285518900000002
O	3.9491567000000001	-5.2734538000000004	3.6990329000000002	O	1.1294831000000001	-8.8675873000000003	2.6232020999999999
H	4.2353862000000004	-4.4107184000000004	4.0591737999999999	H	1.2163663000000000	-8.0456705999999993	2.1006019000000000
H	2.9510141000000001	-5.0935376000000003	3.6284535999999998	H	2.0599178000000000	-9.082627999999997	2.9015624999999998
O	-1.1155082000000001	-5.3221993000000003	-0.2201251700000001	O	4.4978892000000004	-2.9617192000000001	5.1520143999999997
H	-0.4657294799999999	-4.7072735999999997	1.9077255000000001E-002	H	3.5304278999999998	-2.6898875000000002	4.9679975000000001
H	-0.98877086000000003	-5.9606029999999999	0.4314527599999999	H	4.6091534999999997	-2.3930072000000000	5.9340865000000003
O	3.3204658999999999	-3.1067161699999998	-1.6666673999999999				
H	2.6196692999999999	-3.3268377000000000	-1.1168380000000000	C	0.16237398E+01	-0.33006049E+01	0.26766736E+01
H	3.8645122000000001	-2.5618162000000000	-1.0247440000000001	C	0.16454705E+01	-0.20419993E+01	0.33947132E+01
O	0.6104531600000005	-3.3948121000000002	-2.3203792999999999	O	0.14830272E+01	-0.10293796E+01	0.24609800E+01
H	1.1953503000000001	-4.0303089999999998	-2.6937671000000001	C	0.14433203E+01	-0.15438866E+01	0.11219185E+01
H	8.8116468300000004	-3.3781287000000000	-1.3895950000000001	C	0.14291739E+01	-0.30199922E+01	0.13180370E+01
O	1.0160536000000000	-4.5915134000000002	6.1407286000000001	O	0.17359514E+01	-0.17550762E+01	0.45999325E+01
H	1.7199629999999999	-5.0369549999999998	6.5606115999999997	C	0.13929682E+00	-0.10221689E+01	0.38845020E+00
H	1.3994065000000000	-4.3369906000000000	5.2833107999999998	O	-0.130030576E+01	-0.16661406E+01	0.82691377E+00
O	3.9712790999999998	-7.4590091999999997	-6.349214899999998E-002	O	1.4616564999999999	-3.9414278999999999	0.36291373999999998
H	3.3131816000000001	-6.7457308999999999	0.16221416999999999	O	1.6108350000000000	-4.5492977999999997	3.2227079000000001
H	4.6782918000000002	-7.3278886699999999	0.5382284999999996	C	0.60902709E-01	0.53090265E+00	0.455045446E+00
O	1.1835975000000001	-8.4955665000000007	2.8152970000000002	O	-0.10665979E+01	0.99827212E+00	-0.28443739E+00
H	1.5189847000000001	-7.8477931999999999	2.2694879999999999	H	0.23830740E+01	-0.11538286E+01	0.6162760E+00
H	1.6234313000000000	-9.2987862999999997	2.5732189000000001	H	0.41458392E-01	0.97307754E+00	0.14970999E+01
O	-1.2868539999999999	-2.1746089000000000	4.7313359000000004	H	0.93910025E+00	0.89510992E+00	0.14495994E-01
H	-1.5379668000000000	-3.0344057000000002	4.2092698999999998	H	-0.17422873E+01	0.31251792E+00	-0.10653465E+00
H	-1.1506787999999999	-2.5935600000000001	5.6057736000000000	H	0.26770419E+00	-0.12606874E+01	-0.66428330E+00
O	4.7275860999999999	-2.9570061000000001	5.3214967000000000	H	-0.9807005E+00	-0.16209336E+01	0.18447515E+01
H	3.8283393999999999	-2.7221069999999998	5.0247985000000002	O	1.8410010999999999	-6.8027417999999997	1.6187465000000001
H	4.6981466999999997	-2.4868138000000002	6.1469579000000002	H	1.7714204000000000	-6.0034023000000003	2.2056936000000000
C	0.16308611E+01	-0.32315515E+01	0.26305411E+01	H	1.7122801999999999	-6.2792039999999997	0.8081744800000003
C	0.17960257E+01	-0.20255364E+01	0.33343628E+01	H	1.7122801999999999	-6.2792039999999997	0.8081744800000003
O	0.16670772E+01	-0.92998803E+00	0.24725737E+01	C	-1.1025509230000001	-4.8199757999999999	3.3566380000000000
C	0.15676646E+01	-0.14282576E+01	0.10525418E+01	H	-1.1025509230000001	-4.8199757999999999	3.3566380000000000
C	0.14534264E+01	-0.29619065E+01	0.12435767E+01	O	4.0542845999999999	-5.0795868999999998	3.9333545999999999
O	0.20742300E+01	-0.17955948E+01	0.44851933E+01	H	4.1957284000000001	-4.0887320999999996	4.1547067000000002
C	0.32801033E+00	-0.91096675E+00	0.35485824E+00	O	3.0675881000000000	-4.9795606000000001	3.6193667999999999
O	-0.93488414E+00	-0.13651481E+01	0.94876758E+00	H	4.6633509000000002	-4.3087567000000000	1.2252955000000001
O	1.1335694000000001	-3.7083922000000000	0.22306296000000000	H	4.0351138999999999	-4.7479838000000001	1.8391204000000001
O	1.5742560999999999	-4.3947960999999998	3.3250552000000000	O	-1.0510971000000000	5.4017043999999999	1.2520028000000001E-002
C	0.22408536E+00	0.58831630E+00	0.27834744E+00	H	-0.4306954399999999	-4.6879626999999999	0.1212416900000000
O	-0.90520973E+00	0.90833659E+00	-0.54271857E+00	H	-0.9804316600000000	-5.9517572000000003	0.82684250999999998
H	0.24462389E+01	-0.11065438E+01	0.52540850E+00	O	0.8741541640000001	-4.6250210100000004	5.7232832000000000
H	0.84940414E+01	0.95605193E+00	0.13476738E+01	H	1.5875117999999999	-5.2741483999999996	5.8664717100000000
H	0.11063059E+01	-0.10292185E+01	-0.14864557E+00	H	1.1056097000000000	-4.2543473000000001	4.8280802999999999
H	-0.17108122E+01	0.36742120E+00	-0.50041943E+00	O	3.1442792000000002	-3.2081262000000001	1.6907279000000000
H	0.41628471E+00	-0.13397429E+01	-0.62366326E+00	H	2.5884553000000001	-3.6217090000000001	-1.0240149999999999
H	-0.68794503E+00	-0.22740473E+01	0.11767050E+01	H	3.7716224000000000	-2.7924834000000001	-1.1056185999999999
O	1.7886711000000000	-6.3413582000000002	1.3790243000000000	O	0.1683524100000001	-3.6678970999999998	2.2685564999999999
H	1.6726060000000000	-5.6199203000000004	2.0276926000000000	H	0.7983443799999996	-3.4859844999999998	-2.9782454000000000
H	1.5732375999999999	-5.7514099999999999	0.6734703600000005	H	0.5992914099999997	-3.6132970000000002	-1.4296835999999999
O	-1.1693469000000001	-4.8980101999999999	3.3491181000000001	O	-1.2813775000000001	-2.2942743000000001	4.2727127999999999
H	-0.1957591700000001	-4.9492598000000001	3.3506738999999999	H	-1.4671010000000000	-3.2116400000000001	3.9400053000000002
H	-1.3575262000000000	-5.6818989000000002	2.8120539000000000	H	-0.5561740499999998	-2.5114269000000000	4.8833647999999998
O	-1.4098404000000000	-5.2972479300000003	0.21445987000000000	O	5.1523800000000003	-6.9791730000000003	2.1680044000000001
H	-0.5130882100000004	-4.9379052999999997	0.4956945300000002	H	4.7441114000000004	-6.2575476999999999	2.7015047999999999

H	6.078326399999999	-6.810176799999998	2.343926699999999	H	-0.40917389E-01	0.88878004E+00	0.12013910E+01
O	3.958156799999998	-7.652628199999997	-0.1186327200000000	H	0.97685740E+00	0.79921219E+00	-0.26404858E+00
H	3.194382399999998	-7.647410100000001	0.4969781700000000	H	-0.18166025E+01	0.51431229E+00	-0.26500110E+00
H	4.555143099999996	-7.136658999999997	0.4760044800000001	H	0.39060881E-01	-0.15801285E+01	-0.62570212E+00
O	1.018588000000001	-9.308042300000003	2.392886600000002	H	-0.80004832E+00	-0.16108281E+01	0.20252826E+01
H	0.9894587200000001	-8.407707500000008	2.097735600000000	O	1.423550900000000	-6.468693499999997	1.439740300000000
H	1.940012400000001	-9.232800400000004	2.699987199999998	H	1.418759200000000	-5.662024599999996	2.041066900000001
C	0.15346113E+01	-0.32792958E+01	0.26500966E+01	O	1.339246100000000	-5.969032500000000	0.5793711099999997
C	0.17250216E+01	-0.1996666E+01	0.32565327E+01	H	-1.359062000000000	-4.312908700000004	3.412158900000001
O	0.17405960E+01	-0.94065595E+00	0.23437680E+01	H	-0.3850056600000003	-4.436252200000002	3.171976700000001
C	0.14988705E+01	-0.15010803E+01	0.10335426E+01	O	-1.261766800000000	-5.545473000000002	-7.723359000000003
C	0.14855237E+01	-0.30690815E+01	0.12659661E+01	H	-0.4980172500000002	-5.068024300000003	0.3027857500000002
O	0.18762447E+01	-0.18029806E+01	0.45283915E+01	H	-1.509269000000001	-6.070532000000000	0.7631934000000002
C	0.24425862E+00	-0.93037853E+00	0.40774948E+00	O	4.369244799999997	-3.814946099999998	1.580622999999999
O	-0.95493177E+00	-0.13842759E+01	0.99844098E+00	H	3.587401299999998	-3.256136800000002	1.717325800000000
O	1.392062600000000	-3.917875700000002	0.336663949999999	H	4.466101499999997	-4.067445000000002	2.448977800000002
O	1.555755999999999	-4.435056799999999	3.3293913600000001	O	3.838913600000001	-5.531533900000001	3.934863999999998
C	0.16458325E+00	0.58063612E+00	0.27044432E+00	H	3.945632199999997	-4.625555300000003	4.334451999999997
O	-0.84139220E+00	0.92561648E+00	-0.67574801E+00	H	2.875262100000000	-5.460882700000000	3.743774900000000
H	0.24225536E+01	-0.11875622E+01	0.48996413E+00	O	0.3345765800000001	-3.763363300000000	-2.323628700000000
H	-0.92759949E-01	0.10190393E+01	0.12751949E+01	H	0.107599299999999	-4.293169599999997	-2.635319400000002
H	0.10870328E+01	0.94335933E+00	-0.17137510E+00	H	0.6167990800000006	-3.661392900000001	-1.337232200000001
H	-0.16088078E+01	0.43061928E+00	-0.42050082E+00	O	3.147577099999999	-3.235028400000000	-1.786953999999999
H	0.25610823E+00	-0.12391349E+01	-0.6639276E+00	H	2.558677700000001	-3.544043700000000	-1.087152600000000
H	-0.10904077E+01	-0.14412189E+01	0.19723499E+01	H	3.664083499999998	-2.543284900000002	-1.221993300000001
O	2.018420900000002	-6.485953900000002	1.464835300000000	O	1.006493200000000	-4.579850500000000	5.923441500000000
H	1.940718200000001	-6.045538000000004	2.383301700000001	H	1.583335500000000	-5.295146400000001	6.125081800000002
H	1.668604000000000	-5.645442899999999	1.016074600000000	H	1.067257200000000	-4.441307100000004	4.923834699999996
O	4.404661800000004	-4.265524199999998	1.340091100000000	O	3.514542099999999	-7.428778999999996	-0.258613900000000
H	3.575813600000000	-3.721738700000000	1.350268300000000	H	2.766097199999999	-7.044536500000004	0.2924968199999999
H	4.208725600000002	-4.901767900000003	2.112748700000000	H	4.189572400000003	-7.408423100000003	0.485585949999999
O	-1.258748100000000	-4.630256100000004	3.469744100000000	O	-1.173194600000000	-1.878303400000001	4.602255600000003
H	-0.294697409999999	-4.497660899999996	3.354972200000002	H	-1.345268700000001	-2.799642599999999	4.242749400000001
H	-1.402485000000000	-5.420497799999997	2.916821399999999	H	-0.2334293500000001	-1.965730900000001	4.977547999999996
O	-1.204463700000000	-5.389607299999998	-3.175528200000003E-002	O	1.038839700000000	-9.034062499999992	2.704966900000001
H	-0.445623029999999	-4.799773100000003	0.221303260000000	H	1.101599599999999	-8.171149210000000	2.263878099999999
H	-1.295707400000000	-5.942619500000002	0.754084520000004	H	1.966427100000000	-9.257822799999996	2.784844500000002
O	4.027056499999996	-5.127148100000003	3.914438699999998	O	0.135935680000000	-7.115929999999996	-1.922378600000000
H	4.386406700000002	-4.405154999999997	4.488012499999999	H	-0.300786119999999	-6.662185899999999	-1.146787000000000
H	3.058199000000000	-4.851151400000000	3.850944600000001	H	0.6230314500000004	-6.367712499999997	-2.341713299999999
O	0.370805039999999	-3.578276100000001	-2.075694299999999	H	1.209915400000001	-2.548228599999998	0.25827372E+01
H	-3.405962100000000	-3.749946219999999	-2.548228599999998	C	0.14448477E+01	-0.31846865E+01	0.33100503E+01
H	0.8166255500000003	-3.799466999999999	-1.214788299999999	C	0.16651311E+01	-0.19634750E+01	0.24169297E+01
O	3.265586400000001	-3.375807700000002	-1.758459100000000	O	0.16611525E+01	-0.86245173E+00	0.10924548E+01
H	2.702430699999999	-3.834841299999999	-1.112057700000000	C	0.15192537E+01	-0.14490427E+01	0.12205404E+01
H	3.881959900000000	-2.815263499999999	-1.208909100000001	C	0.14304997E+01	-0.28920115E+01	0.45313310E+01
O	0.934001599999999	-4.622787500000003	5.993815299999996	O	0.17180648E+01	-0.17235498E+01	0.41938445E+00
H	1.887157299999999	-4.733861900000000	6.254314599999998	C	0.14550683E+00	-0.93183107E+00	0.12313531E+01
H	0.9788111699999995	-4.746894400000004	5.021721900000002	O	-0.99133041E+00	-0.12384489E+01	0.71951228E-01
O	3.960068600000000	-7.404748599999996	-0.464401369999998	O	1.3007223000000001	-3.7682093000000001	0.2402913999999999
H	3.439441899999999	-7.263177899999996	0.375584809999999	O	1.268915000000000	-4.409948499999996	3.120834999999999
H	4.837522200000004	-7.148271900000000	-0.1029386100000000	C	0.28795704E+00	-0.53802970E+00	0.71951228E-01
O	4.365413099999996	-2.894186200000000	5.155971400000003	O	-0.70881029E+00	-0.91321674E+00	-0.81896113E+00
H	3.489365499999999	-2.567627500000000	4.856705700000000	H	0.23192582E+01	-0.10232943E+01	0.44353092E+00
H	4.419774000000003	-2.459608999999999	6.048045799999997	H	0.28164846E+00	-0.12009453E+01	0.10127394E+01
O	-0.945246999999995	-2.116848600000000	4.821300599999998	H	0.12171940E+01	-0.73965970E+00	-0.49384006E+00
H	-1.175065999999999	-3.033770200000002	4.593525900000004	H	-0.15619787E+01	-0.51370725E+00	-0.56611933E+00
H	-2.0785943000000001E-002	-2.257257300000000	5.048638999999997	H	0.10033066E+00	-0.15070215E+01	-0.51993537E+00
O	1.147625399999999	-9.060218900000006	2.711613400000001	H	-0.65439398E+00	-0.15212027E+01	0.21343826E+01
H	1.100936999999999	-8.296078400000007	2.143381999999999	O	1.660745600000000	-6.297545000000004	0.9543941900000003
H	2.0879362000000001	-9.330790999999996	2.571538799999999	H	1.488413000000000	-5.890905999999996	1.860408499999999
C	0.15242178E+01	-0.33482575E+01	0.24865492E+01	H	1.815631400000000	-5.378076300000000	0.5720491800000005
C	0.17700501E+01	-0.2118997E+01	0.31169397E+01	O	4.319298100000001	-3.664972000000001	1.513029699999999
O	0.16495601E+01	-0.10005662E+01	0.22895477E+01	H	3.348738000000000	-3.640141700000000	1.176067699999999
C	0.14457841E+01	-0.15099791E+01	0.93358124E+00	O	4.207188000000001	-5.428171899999997	-1.105410800000000E-002
C	0.12783631E+01	-0.30391604E+01	0.11431537E+01	H	-0.5472415200000004	-4.809194999999997	0.2754742399999998
O	0.18734163E+01	-0.17962243E+01	0.43216516E+01	H	-1.063349799999999	-6.111701600000000	0.6636996400000004
C	0.13026822E+00	-0.10989120E+01	0.37170658E+00	O	-1.759025099999999	-4.454759600000000	3.285593599999999
O	-0.99425687E+00	-0.16209825E+01	0.11180891E+01	H	-0.7525496699999995	-4.609698599999998	3.4056413000000001
O	0.9947579600000005	-3.857479060000002	0.246172079999999	H	-2.031315699999999	-5.192922000000003	2.6503665000000001
O	1.357365699999999	-4.501757500000001	3.121204200000002	O	3.761321999999998	-5.130355700000000	4.166357399999999
C	0.76386873E-01	0.43824180E+00	0.17872733E+00	H	3.910804900000000	-4.344687300000004	4.691606900000000
O	-0.10033300E+01	0.85757242E+00	-0.70940715E+00	H	2.795265800000001	-5.105167400000000	3.956739400000000
H	0.23519088E+01	-0.12181577E+01	0.30380799E+00	O	3.205492300000000	-3.345965699999998	-1.8162313000000001

H	2.5488268999999999	-3.4334783000000000	-1.0828481000000001	C	0.14146099E+01	-0.34071596E+01	0.26390927E+01
H	3.7575126999999999	-2.6559930000000000	-1.3614236000000000	C	0.16790736E+01	-0.21903960E+01	0.32973441E+01
O	-0.12270389000000000	-3.8107147000000001	-2.2449360000000000	O	0.18591705E+01	-0.11484028E+01	0.23712010E+01
H	0.6737450000000004	-4.1104361999999997	-2.6122163999999999	C	0.15451510E+01	-0.16576957E+01	0.10304130E+01
H	0.1451828199999999	-3.6501598999999998	-1.3060006000000000	C	0.14325951E+01	-0.32010648E+01	0.12297545E+01
O	1.0660470000000000	-4.6314750000000000	5.9584118000000004	O	0.19647488E+01	-0.19754924E+01	0.45062777E+01
H	1.6149610000000001	-5.4192822999999999	6.1535076000000002	C	0.35773707E+00	-0.94869610E+00	0.40705125E+00
H	1.2489459999999999	-4.4256469999999997	5.0010881999999999	O	-0.85231984E+00	-0.11974701E+01	0.12210833E+01
O	3.5015196000000000	-7.6380609000000002	-0.2846770399999999	O	1.2887092000000000	-4.0941669000000003	0.3068214100000002
H	2.6918749000000002	-7.1327106999999997	3.7080180999999997E-002	O	1.3276876000000000	-4.5937036000000004	3.239098300000002
H	4.0339184000000001	-7.4117753000000004	0.4557381400000001	C	0.49429049E+00	0.59237660E+00	0.21948239E+00
O	-3.3034309999999999	-2.9804971999999998	0.8033625500000001	O	-0.59273321E+00	0.10771503E+01	-0.61125943E+00
H	-3.3082460999999999	-2.9393394000000002	0.1844356299999999	H	0.24279097E+01	-0.14305856E+01	0.37228102E+00
H	-2.3968756999999999	-2.6440970000000000	1.0405009000000001	H	0.41429002E+00	0.11190985E+01	0.11224470E+01
O	1.0822887999999999	-8.7159355000000005	3.1855232000000000	H	0.14400254E+01	0.89094313E+00	-0.22647495E+00
H	0.9463846799999998	-8.0973641999999995	2.4596507999999999	H	-0.13938184E+01	0.10135844E+01	-0.10203007E+00
H	2.0125611999999999	-8.8314872999999992	3.2876596000000000	H	0.21191596E+00	-0.13559838E+01	-0.60055048E+00
O	-1.3052589000000001	-2.0940249999999998	4.5192794000000003	H	-0.61357923E+00	-0.17720527E+01	0.19216781E+01
H	-1.8513991000000001	-2.8012288000000001	4.1004752000000000	O	1.2307378500000000	-6.5800240000000001	1.2915934000000000
H	-0.9837495000000005	-2.5486130000000000	5.3103677999999999	H	1.1137123000000000	-6.1025288000000000	2.1419074000000000
H				H	1.4309426000000001	-5.7061818999999998	0.9094789399999996
C	0.13260192E+01	-0.34153959E+01	0.26991770E+01	O	-1.4458225000000000	4.8156768000000003	3.5184513000000002
C	0.17466525E+01	-0.21514813E+01	0.33473631E+01	H	-0.5100079800000003	-4.7738725000000004	3.2516213000000000
O	0.16821593E+01	-0.11319245E+01	0.24064307E+01	H	-1.8454904999999999	-5.4583354000000002	2.8204889000000000
C	0.15193873E+01	-0.16389557E+01	0.11144455E+01	O	-1.2070916000000000	-5.5237625000000001	-0.1869202200000000
C	0.13550417E+01	-0.31364821E+01	0.13314529E+01	H	-0.4247040799999998	-5.0227976999999999	0.1145309999999999
O	0.21042992E+01	-0.18761121E+01	0.44877674E+01	H	-1.5703527000000001	-6.0844136999999998	0.5791220299999997
C	0.259117748E+00	-0.10144338E+01	0.45449235E+00	O	3.8848052000000002	-5.2166952000000002	3.7112017000000002
O	-0.90175594E+00	-0.11729058E+01	0.12907069E+01	H	4.0829908000000001	-4.3581070999999998	4.1895699999999998
O	1.2237644999999999	-3.9191698000000001	0.3104691800000001	H	2.8888321000000001	-5.1293803999999996	3.6958457000000000
O	1.2873915000000000	-4.6265761999999997	3.2614212999999997	O	4.6701762000000002	-3.9792293000000001	1.2944363999999999
C	0.39587173E+00	0.46327217E+00	0.16694140E+00	H	4.1741406999999997	-4.2514963000000003	2.0876209000000001
O	-0.63591422E+00	0.10416628E+01	-0.61901060E+00	H	4.1249804000000001	-3.2033239999999999	1.1009028000000001
H	0.24643563E+01	-0.14542219E+01	0.56619322E+00	O	2.9297342999999998	-2.8707365999999999	-1.7237107000000000
H	0.45478040E+00	0.10033288E+01	0.11104543E+01	H	2.4651188999999998	-3.4910814999999999	-1.1139827000000000
H	0.13320397E+01	0.64533090E+00	-0.43229467E+00	H	3.6879637399999999	-2.6273898000000000	-1.1287020000000001
H	-0.14857636E+01	0.63762804E+00	-0.40172708E+00	O	1.0228105000000001	-4.7214393000000001	5.9264608000000001
H	0.11491458E+00	-0.16481136E+01	-0.41536013E+00	H	1.7076990000000001	-5.3588221000000003	6.0804425999999996
H	-0.57202164E+00	-0.90453149E+00	0.21453185E+01	H	1.0520389999999999	-4.5751822000000004	4.9887287000000002
O	1.5362213000000000	-6.4153342999999996	1.1607422000000001	O	0.20100978000000000	-3.6430418000000002	-2.1787635000000001
H	1.3511229000000000	-5.9821477999999999	2.0402211000000001	H	0.8146382199999997	-4.2987526999999996	-2.4707219000000000
H	1.7778702000000000	-5.5917092000000004	0.6777583600000000	H	0.39107121000000000	-3.6371812000000001	-1.2562472000000000
O	-1.2471018000000000	-5.2730091999999997	9.2183888000000005-002	O	3.2612165000000002	-7.435980299999998	-0.3561555000000000
H	-0.3882329199999999	-4.9197218999999999	0.4252156300000001	H	2.3414126999999998	-7.4492858000000002	-1.2477401000000001E-002
H	-1.5080507000000001	-5.8152473000000002	0.8725755499999999	H	3.7730448999999999	-7.1199165000000004	0.3619514500000002
O	4.5686568000000003	-3.8717304000000001	1.3746271000000001	O	1.1576417000000001	-8.8601030999999999	3.2281487000000002
H	4.6272824999999997	-3.1183971000000001	2.0077056999999998	H	1.1609721000000000	-8.0132282999999997	2.6837023000000002
H	3.7466140999999999	-4.1634509000000000	1.7554828000000000	H	1.9410741000000000	-9.3148458999999999	2.8525684000000000
O	3.7758194999999999	-5.0239744000000002	3.9032822000000000	O	4.6019268000000002	-7.1781400000000001	2.0620235000000000
H	3.8646368999999998	-4.1422891000000002	4.3608468000000000	H	4.4906796000000000	-6.2843619999999998	2.4316518999999999
H	2.7983254999999998	-4.9637840000000004	3.6299739999999998	H	5.5884480999999997	-7.1366759000000002	1.8405130000000001
O	-1.6804338999999999	-4.5973750999999998	3.5678484000000000	O	1.3023845000000001	-2.1964901000000001	4.5282830000000003
H	-0.7306439500000004	-4.6657057959999996	3.4472599000000002	H	-1.8256186000000001	-2.9872429999999999	4.2339054000000003
H	-1.8947927000000000	-5.3299269999999999	2.9089285999999999	H	-0.7156027999999998	-2.6203379000000000	5.2310127000000000
O	2.9598599999999999	-3.0706381999999999	-1.6764996000000001	H			
H	2.3902166999999999	-3.2826914999999999	-0.9000760700000001	C	0.15107713E+01	-0.33491638E+01	0.27139394E+01
H	3.7851431999999998	-2.9092489999999998	-1.1724926000000000	C	0.17610736E+01	-0.20531694E+01	0.32342887E+01
O	0.8162511799999997	-4.5601437000000002	5.8006732000000003	O	0.18689340E+01	-0.10618562E+01	0.23372738E+01
H	1.4062593999999999	-5.2608109000000001	6.0842492000000004	C	0.15613790E+01	-0.16884598E+01	0.10047942E+01
H	1.1824625000000000	-4.4511096999999999	4.8869674999999999	C	0.15165973E+01	-0.32000799E+01	0.13376109E+01
O	4.7992545999999997-002	-3.9334223000000001	-2.3305946000000000	O	0.19183672E+01	-0.17117382E+01	0.44686841E+01
H	0.9226458500000003	-4.0298527000000002	-2.7847251000000002	C	0.26814784E+00	-0.10242815E+01	0.42183047E+00
H	0.4016130000000000	-3.9243082000000000	-1.3950427999999999	O	-0.92986213E+00	-0.12255276E+01	0.12823213E+01
O	4.5579986000000003	-7.0971415000000002	1.9415929999999999	O	1.5552931000000001	-4.1002691999999996	0.407581050000000000
H	4.1486501000000002	-6.3104449999999996	2.3812628999999998	O	1.3287051000000001	-4.5314629000000002	3.38708540000000001
H	5.5058465999999999	-6.8461828999999996	1.8622889000000000	C	0.49399444E+00	-0.45470527E+00	0.31865045E+00
O	1.3202479000000000	-8.3489336000000005	3.3100377000000001	O	-0.35813549E+00	0.11729370E+01	-0.52935337E+00
H	1.5139841999999999	-7.7767605000000000	2.5645308000000000	H	0.23623535E+01	-0.13913683E+01	0.26873045E+00
H	2.1885351000000002	-8.7660850999999997	3.4883346999999998	H	0.46447220E+00	0.88186440E+00	0.13302932E+01
O	3.5067233999999998	-7.7329309999999998	-0.3859715200000001	H	0.14894145E+01	0.54607779E+00	-0.13787054E+00
H	2.6518994000000000	-7.3577624000000004	-1.9577424000000000-002	H	-0.12179654E+01	0.75326254E+00	-0.37386812E+00
H	4.0795705999999996	-7.4692765999999997	0.3576112400000000	H	0.17987829E+00	-0.14898691E+01	-0.53126090E+00
O	-1.1455914000000000	-1.8945495000000001	4.8101279000000003	H	-0.73577737E+00	-0.14633063E+01	0.22036432E+01
H	-1.2763723000000001	-2.8282289000000000	4.5941796999999998	O	1.3197357000000001	-6.5794772999999998	1.8202691000000000
H	-0.9326424899999999	-1.9235903999999999	5.7471524000000000	H	1.2316638000000000	-5.7787082999999999	2.4146789000000002
H				H	1.0948891999999999	-6.0947658999999996	1.0028459000000000

O	4.6578669000000001	-4.3729880999999997	1.396013699999999	O	-1.6014725000000001	-1.9898705000000001	4.5347299999999997
H	4.6627080999999997	-4.7253515000000004	2.3032430000000002	H	-1.1600189000000001	-2.892148199999998	4.3688986999999999
H	3.7212524000000000	-4.3886573999999996	1.183167099999999	H	-1.4530478000000000	-1.9780924000000000	5.4793816000000000
O	3.7165564999999998	-5.357312699999996	4.079957200000000	O	3.453018399999999	-7.735472299999996	0.14981201000000000
H	3.7743916000000000	-4.465239999999997	4.3856214000000001	H	2.5958689000000001	-7.5189269000000003	0.62149639000000001
H	2.8001296999999998	-5.238764100000000	3.8333267000000002	H	4.128013799999997	-7.317509399999996	0.77725367000000001
O	-1.4086183000000001	-5.495194399999999	0.414786319999999	O	1.1839386000000001	-8.741006900000004	3.424781799999999
H	-0.8053706299999998	-4.894002099999998	0.8345906800000003	H	1.2674547000000000	-8.142654600000002	2.7119260000000001
H	-1.6554721999999999	-6.2000804000000000	1.119625499999999	H	2.0542329000000001	-9.1068633000000005	3.3475465000000000
O	-1.4761207999999999	-4.676186999999996	3.760304900000000	O	5.060361200000000	-7.177503899999996	2.172639400000000
H	-0.4899016800000001	-4.772291899999999	3.6966733000000001	H	4.8505558000000004	-6.5350057000000001	2.8751655999999999
H	-1.7878076000000001	-5.3973861000000001	3.2508181000000000	H	6.0205817000000001	-6.939637499999999	2.1071925999999999
O	3.175887500000000	-2.951633999999999	-1.6079583000000000				
H	2.6824102000000001	-3.352579500000000	-0.8600016400000001	C	0.14637178E+01	-0.33108193E+01	0.27032038E+01
H	3.911471900000000	-2.4631093000000002	-1.1815245000000001	C	0.16130472E+01	-0.20641054E+01	0.34687659E+01
O	1.5858863000000001	-4.464889399999997	6.1039608000000003	O	0.16355267E+01	-0.99049409E+00	0.26250927E+01
H	1.994474899999999	-5.322562099999999	6.187281800000001	C	0.15931201E+01	-0.14291550E+01	0.12074299E+01
H	1.5083261999999999	-4.347156000000000	5.125082199999996	C	0.15480209E+01	-0.30005933E+01	0.13641240E+01
O	0.2502167000000001	-3.736992400000001	-2.064125999999999	O	0.18318554E+01	-0.18080914E+01	0.46674736E+01
H	0.9008847800000005	-4.296497399999998	-2.590841999999999	C	0.24502519E+00	-0.84922783E+00	0.69905130E+00
H	0.7008815000000005	-3.826998699999999	-1.2159424000000001	O	-0.86455697E+00	-0.12325903E+01	0.14833096E+01
O	3.4110543000000000	-7.597347499999997	-0.13991523000000000	O	1.3195276000000000	-3.738371299999998	0.29578868000000003
H	2.7277650000000002	-7.0728748000000001	0.2540335899999998	O	1.2994068000000001	-4.4375602000000001	3.402990299999999
H	4.1659253999999999	-7.574695199999999	0.4470508000000003	C	0.28795044E+00	0.70847587E+00	0.61990620E+00
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H	1.0815904999999999	-8.055556999999993	2.752146999999999	H	0.24576940E+01	-0.95133889E+00	0.67554159E+00
H	2.0583895999999999	-8.780761099999994	3.6266421000000002	H	-0.19422889E+00	0.11023646E+01	0.15584121E+01
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H	4.6199056000000001	-6.5449713000000003	2.964686599999998	H	-0.12622495E+01	0.13522239E+01	-0.34278050E+00
H	6.0241576999999999	-6.9530088000000001	2.379118699999998	H	0.13415224E+00	-0.11488256E+01	-0.33602452E+00
O	-1.5355530000000000	-1.916480699999999	4.353928899999999	H	-0.57013576E+00	-0.14921455E+01	0.23671399E+01
H	-1.7591308000000001	-2.798637499999999	4.0579023000000003	O	1.6065507000000001	-6.337931700000004	1.6295766000000000
H	-0.8887487400000004	-2.1593881000000001	5.0036493000000002	H	1.521834600000000	-5.817011800000004	2.5161821999999998
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C	0.15420413E+01	-0.32992388E+01	0.28628421E+01	O	-1.1131557000000001	-5.3500882000000001	0.1858917200000001
C	0.18455660E+01	-0.19385852E+01	0.337655991E+01	H	-0.3893817800000001	-4.730037799999998	0.4525282700000001
O	0.16512537E+01	-0.98413994E+00	0.24009563E+01	H	-1.5896125000000001	-0.4569572500000003	1.0544123000000001
C	0.14834779E+01	-0.16652073E+01	0.11223807E+01	O	4.5204516000000003	-4.870071199999999	1.0676555999999999
C	0.14588676E+01	-0.31520533E+01	0.143425959E+01	H	4.6683981000000001	-5.776947599999999	1.4136854999999999
O	0.20158193E+01	-0.15200422E+01	0.45441532E+01	H	3.5855130000000001	-0.6743808500000001	1.1891198000000001
C	0.23279254E+00	-0.10368133E+01	0.48720270E+00	O	-1.4441583000000000	-4.8504896000000004	4.0392180000000004
O	-0.10567438E+01	-0.12919636E+01	0.12489658E+01	H	-0.4633529599999998	-4.713785900000004	3.874846499999999
O	1.3689783000000000	-4.103109999999997	0.5516138400000002	H	-1.6633492100000000	-5.594411899999999	3.454286499999999
O	1.5204340999999999	-4.3909311000000004	3.5915070000000000	O	3.7726264000000000	-5.5787778000000001	4.3328436000000004
C	0.37736027E+00	-0.57736991E+00	0.50549342E+00	H	3.8305107000000000	-4.814119400000000	4.8057670000000003
O	-0.66524883E+00	-0.12516520E+01	-0.13774253E+00	H	2.8363209000000000	-5.488016599999999	4.0706762000000003
H	0.23993964E+01	-0.13601423E+01	0.54732017E+00	O	3.0064570000000002	-2.819286599999999	-1.6930334000000000
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H	0.12517535E+01	-0.72904281E+00	-0.87992303E+00	H	3.472860799999999	-3.280274399999999	-0.940238369999999
H	-0.15219849E+01	-0.78870459E+00	-0.65126087E-01	O	0.788369769999999	-4.167429399999996	6.222299099999999
H	0.50057647E-01	-0.13610230E+01	-0.55653975E+00	H	1.106437399999999	-5.0749338000000002	6.4155578000000002
H	-0.71701072E+00	-0.15137139E+01	0.21583624E+01	H	0.9973049000000003	-4.026306199999996	5.273583499999999
O	1.7911096000000000	-6.391227599999997	1.771495199999999	O	3.327010999999999E-03	-3.5638431000000002	-2.330982199999998
H	1.7946228000000000	-5.8749703000000002	2.6361530000000002	H	0.6156464699999995	-3.946135999999999	-2.9625430000000001
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O	4.4923222999999997	-4.3995927000000004	1.2700864000000001	O	3.3938969000000001	-7.552428299999999	0.15131642000000001
H	4.1240442000000002	-5.2355304000000000	1.5991166999999999	H	2.6324773000000001	-6.979128499999998	0.45633040000000002
H	3.6497077999999998	-3.886554799999999	1.2085352010000000	H	3.8552301000000000	-7.5355146000000000	0.9945287699999995
O	3.9488772999999999	-5.3910888000000003	4.2015997000000000	O	0.8745300499999995	-8.552013499999993	3.3032645000000000
H	4.1445857999999998	-4.6514042000000000	4.7983924000000000	H	1.1249974000000000	-7.841387400000003	2.627552999999998
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O	-1.3333573000000001	-4.9949734000000001	3.981696299999999	O	-0.3232511749999999	-6.7479078000000001	-2.1006046000000000
H	-0.4122299200000003	-4.7707546000000001	3.7070853000000001	H	-0.3257465470000000	-6.259826799999999	-1.2608024000000000
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O	-1.0595958000000001	-5.7658132000000002	0.13627425000000001	O	-1.572965299999999	-2.0334143000000000	4.5586279000000003
H	-0.3596851200000002	-4.9896243000000000	0.12835715000000000	H	1.7270823000000000	-2.9679617000000000	4.4221763000000003
H	-1.1826026999999999	-5.942780999999996	1.1149973000000000	H	-1.4875631000000000	-1.954943799999999	5.5029474000000000
O	1.1750449000000001	-4.267413099999997	6.214775399999997				
H	1.6087648999999999	-5.0459261000000000	6.453318699999996	C	0.12544972E+01	-0.33575950E+01	0.27369362E+01
H	1.4258036000000001	-4.1335670000000002	5.281693899999996	C	0.15682297E+01	-0.21173269E+01	0.34348418E+01
O	2.9603310000000000	-3.0928338000000002	-1.626557199999999	O	0.17257318E+01	-0.11154225E+01	0.25181044E+01
H	2.5715070999999998	-3.7027554000000000	-1.0365160000000000	C	0.15793398E+01	-0.16544654E+01	0.11949770E+01
H	3.6236446000000000	-2.6513194000000002	-1.0429169000000000	C	0.13822307E+01	-0.31332158E+01	0.13884221E+01
O	5.7944606000000003E-002	-3.9045928000000001	-2.3138431000000002	O	0.17918861E+01	-0.17156856E+01	0.45802312E+01
H	0.7789386000000004	-4.171963899999997	-2.924836099999998	C	0.38190971E+00	-0.82449629E+00	0.57265537E+00
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C	0.69618811E+00	0.62101239E+00	0.55144131E+00	H	3.619835900000000	-4.602468100000003	4.948803599999997
O	-0.31076938E+00	0.12811291E+01	-0.35084934E+00	H	2.409354599999999	-5.216261000000004	4.195312600000003
H	0.24791468E+01	-0.14104013E+01	0.67463645E+00	O	0.5236263599999996	-4.543896300000001	5.955347300000003
H	0.55441355E+00	0.92585104E+00	0.16169187E+01	H	1.011456399999999	-5.309035500000002	6.250752499999999
H	0.16827721E+01	0.87949752E+00	-0.19287036E-01	H	0.6471888599999998	-4.556450400000001	4.955128700000004
H	-0.12611245E+01	0.12094771E+01	-0.63847202E-01	O	3.115150200000000	-3.088810300000000	-1.490496800000001
H	0.70814938E-01	-0.12021285E+01	-0.42185959E+00	H	2.538186300000000	-3.649000899999999	-0.821336399999997
H	-0.65050162E+00	-0.12499952E+01	0.22144423E+01	H	3.590321400000001	-2.470130399999999	0.947271839999998
O	1.6412458000000001	-6.412188300000004	1.458954499999999	O	0.156499699999999	-3.570603000000002	-2.188979700000000
H	1.473402399999999	-5.958997000000001	2.370760100000000	H	0.798032900000005	-3.940949600000002	-2.900079900000002
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O	-1.088472799999999	-5.948387099999997	0.423329989999999	O	0.806163269999999	-8.703949599999996	2.651927800000002
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H	-1.289512000000000	-6.357377999999998	1.304364800000001	H	1.617603700000001	-9.197027999999995	2.627072899999999
O	4.202178400000002	-5.027054599999996	0.9939889400000004	O	3.673000000000000	-7.630474099999998	-0.232727490000001
H	3.703344899999998	-5.439312699999998	1.670762870000000	H	3.120432600000000	-7.051774000000000	0.3032992900000000
H	3.635209999999998	-4.364477400000002	0.6503438000000003	H	4.511091200000001	-7.656889000000002	0.2839368800000000
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H	3.702106800000001	-4.649899399999998	4.940940399999997	H	-2.988106300000001	-3.269214499999999	-0.30701811000000001
H	2.585741899999999	-5.163755600000000	4.102955200000002	H	-2.253256200000000	-2.557675999999998	0.7547759200000004
O	-1.774046700000000	-4.721162200000002	3.903245699999998	O	4.435363899999996	-7.559406700000003	2.950185900000001
H	-0.829584600000003	-4.794712699999998	3.656038800000001	H	3.860413499999999	-6.977808699999998	3.498069399999999
H	-2.104202599999998	-5.529344400000003	3.506813699999999	H	5.327486399999997	-7.093052000000001	3.007680100000000
O	0.2807308399999998	-3.513863900000000	-1.973452000000000				
H	0.884695299999996	-4.057515900000003	-2.545534599999999	C	0.14526639E+01	-0.34432261E+01	0.28498919E+01
H	0.7802852000000001	-3.517667700000001	-1.123661400000000	C	0.17211146E+01	-0.21369190E+01	0.34723102E+01
O	3.116570700000000	-3.066455100000002	-1.584149100000001	O	0.18459034E+01	-0.11814004E+01	0.25814670E+01
H	2.523715300000001	-3.569153200000001	-0.934332150000003	C	0.16472122E+01	-0.16731060E+01	0.12462494E+01
H	3.840273100000001	-2.782737300000000	-1.041809000000001	C	0.14966897E+01	-0.32071166E+01	0.14770255E+01
O	0.744844920000002	-4.338768899999998	6.127637899999999	O	0.18001810E+01	-0.18499307E+01	0.47397130E+01
H	1.415603200000001	-4.897731499999999	6.414883599999996	C	0.27853206E+00	-0.10446790E+01	0.68626494E+00
H	0.746421400000001	-4.246908600000003	5.189775400000003	O	-0.92974993E+00	-0.13178084E+01	0.14068543E+01
O	3.637170100000001	-7.521588699999997	-6.263721099999998E-002	O	1.352343499999999	-4.042574900000000	0.4622986399999998
H	2.983593500000000	-7.153473800000004	0.6181423200000002	O	0.9870536000000005	-4.526328699999996	3.523841899999999
H	4.417653999999997	-7.199001599999999	0.3391064300000001	C	0.42150581E+00	-0.45950515E+00	0.69145854E+00
O	0.810436530000004	-8.653293200000002	2.818583900000001	O	-0.58265792E+00	-0.11594656E+01	0.39458126E-02
H	0.815568929999997	-7.925433400000002	2.231069699999999	H	0.24798222E+01	-0.14950800E+01	0.61990512E+00
H	1.758564599999999	-8.889926000000009	2.710624000000001	H	0.39529729E+00	-0.78413607E+00	0.17970620E+01
O	-1.871865799999999	-1.867526400000000	4.211576499999996	H	0.13885539E+01	-0.81391078E+00	0.25223600E+00
H	-1.771611300000000	-2.784857000000001	3.882719139999999	H	-0.15150324E+01	-0.10942630E+01	0.34122269E+00
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O	4.007067700000003	-3.031517500000001	5.555589500000000	H	-0.72887957E+00	-0.18280084E+01	0.2239945E+01
H	3.204571000000002	-2.790973000000001	5.052275500000004	O	1.843389800000000	-6.429546600000001	1.795461300000000
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C	0.13434138E+01	-0.33335752E+01	0.27672288E+01	O	1.682868999999999	-5.622737500000004	1.242084800000000
C	0.15982676E+01	-0.20466316E+01	0.33740080E+01	H	-0.5338930600000005	-6.231100000000002	0.5918755000000000
O	0.16813559E+01	-0.10859654E+01	0.23792148E+01	H	-2.852472700000000	-5.441300000000000	0.623179200000004
C	0.14998226E+01	-0.16348386E+01	0.11353840E+01	O	-0.2163553100000000	-6.766316700000000	1.291818300000001
C	0.13243565E+01	-0.31287635E+01	0.13871206E+01	H	-0.1579229200000000	-5.017409999999999	3.915829399999998
O	0.18287509E+01	-0.16877204E+01	0.45354827E+01	H	-0.6360957200000003	-4.843066000000000	3.757928600000001
C	0.26668634E+00	-0.94350167E+00	0.54819227E+00	H	-0.1711771000000000	-5.913979000000003	3.416265800000001
O	-0.89258277E+00	-0.12521199E+01	0.13883142E+01	O	3.486895200000002	-5.204513200000001	4.494722900000002
O	1.234008000000000	-4.041423499999996	0.4447781599999998	H	2.596905000000000	-5.107447699999998	4.156279699999998
O	1.102680000000000	-4.502375800000003	3.400980300000002	O	4.392577099999996	-4.888201200000000	1.254431099999999
C	0.57554932E+00	0.52698811E+00	0.36630426E+00	H	4.060536299999999	-4.043128900000001	1.525616899999999
O	-0.54711010E+00	0.12453417E+01	-0.22655484E+00	H	3.666528800000000	-5.415284400000000	1.518127100000001
H	0.23344254E+01	-0.14326358E+01	0.45394825E+00	O	3.241503300000002	-3.553260499999999	-1.457855000000000
H	0.91687123E+00	0.10204660E+01	0.12152744E+01	H	2.537172599999999	-3.867616800000000	-0.7990940600000005
H	0.13828500E+01	0.80470922E+00	-0.29766564E+00	H	3.777109600000002	-3.082315400000001	-0.8704666100000003
H	-0.13828052E+01	0.92501141E+00	0.17907624E+00	O	0.1206253500000000	-3.577755100000001	-1.978669000000000
H	0.18978207E-01	-0.13640371E+01	-0.44030696E+00	H	0.738031149999999	-4.147883300000002	-2.576294499999999
H	-0.15543967E+00	-0.15542456E+01	0.22333736E+01	H	0.5264081699999995	-3.735622100000001	-1.127872500000001
O	0.1978426400000000	-6.436947800000004	1.799205299999999	O	0.3928822200000000	-4.458286000000002	6.133709099999999
H	1.634689099999999	-5.981197800000003	2.660673300000000	H	0.816789129999997	-5.393979200000004	6.029226900000003
H	1.638122899999999	-5.761908000000000	1.197125700000000	H	0.568330769999999	-4.185494300000002	5.182086400000002
O	-0.8194026800000005	-6.062379100000002	0.5346898500000002	O	0.5404084500000004	-8.551894999999993	2.703317900000001
H	-0.2408610200000001	-5.272454899999996	0.531447169999997	H	1.130692000000000	-7.785181299999996	2.485452899999999
H	-1.0548706000000001	-6.210978100000002	1.449582200000000	H	1.116439800000000	-9.029304000000002	3.294121699999998
O	4.285387000000004	-4.952034999999998	1.132291000000000	O	3.529062699999999	-7.701502299999996	0.1736290600000000
H	4.193578999999997	-5.300221200000002	2.039547600000001	H	2.819832200000000	-7.129380600000002	0.5295742799999995
H	3.344409100000000	-4.739205600000000	1.017678800000001	H	4.274968999999997	-7.708047999999998	0.7873406000000001
O	-1.756399899999999	-4.777590400000002	3.571969000000002	O	-1.799974500000000	-2.369004799999999	4.665802700000004
H	-0.7689062800000005	-4.771740399999997	3.465318299999999	H	-1.913438699999999	-3.243965799999998	4.144411400000001

H	-1.1442230000000000	-2.7383586000000002	5.269436400000000	H	-0.75364012E-01	-0.12442200E+01	-0.36562322E+00
O	-3.082919899999998	-2.8171501000000001	0.4338024300000002	H	-0.56833391E+00	-0.16095103E+01	0.22889065E+01
H	-2.8089312000000000	-3.3349766000000001	-0.2708899000000000	O	2.1111304000000000	-6.466048299999997	1.963208099999999
H	-2.216823199999999	-2.475418799999999	0.7448715299999995	H	1.7933380000000001	-5.91205499999999	2.769441200000002
C	0.13501424E+01	-0.33051602E+01	0.28641344E+01	O	-0.4105638899999999	-6.250594000000004	0.3333267999999998
C	0.18344268E+01	-0.20889042E+01	0.34218565E+01	H	0.2488841000000000	-5.532153900000000	0.4416213099999999
O	0.19325007E+01	-0.10270280E+01	0.24891957E+01	H	-0.5711580499999997	-6.498749300000001	1.277504299999999
C	0.15994428E+01	-0.15789906E+01	0.11862378E+01	O	3.641866499999999	-4.929327800000003	4.145309400000004
C	0.13970174E+01	-0.31019271E+01	0.14849324E+01	H	3.7009059000000000	-4.541850499999998	5.000237600000002
O	0.19494882E+01	-0.16277995E+01	0.45753246E+01	H	2.647965999999998	-4.718106200000002	3.989958500000002
C	0.30060712E+00	-0.89327390E+00	0.66951033E+00	O	-1.796338000000000	-4.854238600000004	3.809759800000001
O	-0.94819974E+00	-0.11201129E+01	0.14262020E+01	H	-0.774248579999996	-4.793639699999999	3.743137299999999
O	1.174388999999999	-4.044290700000003	0.6053946300000004	H	-1.883976200000000	-5.612490000000002	3.200489000000001
O	1.114191900000000	-4.412269700000004	3.502658600000002	O	3.317428599999999	-3.301907899999998	-1.111940999999999
C	0.45849808E+00	0.62988194E+00	0.72255321E+00	H	2.566808000000000	-3.579574300000000	-0.552390499999997
O	-0.54178686E+00	0.12947794E+01	-0.23090229E-01	H	3.908860199999999	-2.989014899999999	-0.4060088000000000
H	0.24257259E+01	-0.12211661E+01	0.54254565E+00	O	0.3399932900000000	-3.376638700000000	-1.914009000000000
H	0.34576885E+00	0.92307393E+00	0.17352769E+01	H	1.174826699999999	-3.824372599999998	-2.215321299999998
H	0.14593573E+01	0.95927494E+00	0.43069254E+00	H	0.426208199999999	-3.510560200000000	-0.9837798700000000
H	-0.14382975E+01	0.91910409E+00	0.14084429E+00	O	4.681390999999998	-4.711257899999997	1.722838000000001
H	0.21283747E+00	-0.11615157E+01	-0.33557626E+00	H	5.047481599999997	-3.809261499999999	1.542832900000001
H	-0.63470042E+00	-0.15256817E+01	0.22594552E+01	H	4.262615799999998	-4.702530699999996	2.620794399999999
O	1.923677800000001	-6.519825899999998	1.796397100000001	O	0.6904110700000002	-4.542762899999996	6.386209000000004
H	1.700255000000001	-5.938101200000002	2.553109300000000	H	1.2032905000000000	-5.312987100000000	6.715347099999998
H	1.920888900000000	-5.776153599999998	1.154433700000000	H	0.8410550900000001	-4.601581799999999	5.403251799999996
O	-0.5993672400000003	-6.201462000000003	0.4692857200000003	O	0.9365577899999995	-8.648606199999997	3.100210000000001
H	-1.8599211100000001E-002	-5.450013700000004	0.5821718400000000	H	1.199384599999999	-7.786415200000004	2.612985300000000
H	-0.2156066000000001	-6.873288900000004	1.045934600000000	H	1.5113558000000000	-9.256754400000002	2.661620600000000
O	-1.646046799999999	-4.930254299999996	3.908119800000001	O	4.626823400000001	-7.349533600000000	2.623223700000000
H	-0.657181029999996	-4.699477400000001	3.757258300000002	H	3.712896900000001	-7.014877939999999	2.560296160000000
H	-1.7181010000000001	-5.590980700000002	3.182182300000000	H	5.098123900000000	-6.494310200000001	2.718717199999999
O	3.488047500000000	-5.395718200000001	4.559290200000004	O	3.675500000000000	-7.474289500000003	-8.947618699999999E-002
H	3.834295300000000	-4.513163500000001	4.904432100000002	H	2.891923600000001	-7.378117699999998	0.480839369999999
H	2.579414900000002	-5.130916799999996	4.208922600000002	H	4.333735100000002	-7.334003000000000	0.6699595000000001
O	4.495935399999996	-4.826339700000001	1.605446200000000	O	-1.127434199999999	-2.351137000000000	4.743701699999998
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H	4.074827700000002	-5.101224300000002	2.422047399999999	H	-0.3823410199999998	-2.728215000000001	5.193785799999997
O	0.5754125599999996	-4.512679600000002	6.132475900000000				
H	1.238504800000001	-5.203558400000004	6.376091299999997	C	0.12739277E+01	-0.32871721E+01	0.27407748E+01
H	0.7233166800000005	-4.513344499999996	5.156474099999996	C	0.16576097E+01	-0.20001430E+01	0.32748647E+01
O	0.1220226200000000	-3.494374600000000	-1.854713899999999	O	0.18733521E+01	-0.10940615E+01	0.22866174E+01
H	0.7280096000000003	-4.018130099999996	-2.398536599999999	C	0.15944258E+01	-0.17891065E+01	0.10297440E+01
H	0.4543610499999999	-3.535324300000001	-0.942725629999998	C	0.13261697E+01	-0.32548874E+01	0.13758415E+01
O	3.519637100000002	-3.694664299999999	-1.184457200000000	O	0.18791802E+01	-0.17292350E+01	0.44803904E+01
H	2.721462600000002	-3.925605399999998	-0.737500190000000	C	0.34377965E+00	-0.11029811E+01	0.43778160E+00
H	4.106372799999999	-3.279211099999999	-0.590011900000003	O	-0.85198274E+00	-0.13798078E+01	0.12815121E+01
O	3.685075400000001	-7.434756700000003	-0.1647475300000000	O	1.396587000000000	-4.199860799999997	0.5226824500000002
H	2.916293800000000	-6.868750300000003	0.2367088300000001	O	1.088931099999999	-4.439898000000003	3.502119800000000
H	4.346838599999999	-7.264286199999999	0.5175397699999995	C	0.57200965E+00	0.39076728E+00	0.31685233E+00
O	0.815209019999995	-8.745843799999994	3.1531964000000001	O	-0.39396676E+00	0.11263051E+01	-0.48175668E+00
H	0.936840079999996	-7.840289300000002	2.950431000000000	H	0.24548863E+01	-0.15137533E+01	0.38065964E+00
H	1.603543500000000	-9.173814399999995	2.812193999999999	H	0.52863346E+00	0.81522425E+00	0.13434511E+01
O	-1.464217700000001	-2.173707299999998	4.682461299999999	H	0.15371168E+01	0.63221574E+00	-0.44343745E-01
H	-2.056836999999999	-2.840886400000000	4.244163200000000	H	-0.13229631E+01	0.87040183E+00	-0.27738325E+00
H	-0.871432129999997	-2.802070699999998	5.041114200000000	H	0.13207563E+00	-0.14905979E+01	-0.57967461E+00
O	-3.081027999999999	-2.955430199999999	0.4570352100000003	H	-0.56266302E+00	-0.15647942E+01	0.22043193E+01
H	-2.551337000000002	-3.630043000000001	-5.829922099999998E-002	O	1.6137056000000001	-6.669124400000003	1.929401600000000
H	-2.257086399999999	-2.406894700000001	0.694455300000000	H	1.372328599999999	-6.042789800000004	2.620967300000002
C	0.12849221E+01	-0.34216006E+01	0.27696341E+01	O	-0.6611590760000006	-6.027909799999998	0.302491769999999
C	0.17614761E+01	-0.21672592E+01	0.33045682E+01	H	-6.4442868000000002	-5.243971499999998	0.446170889999999
O	0.19032614E+01	-0.11762066E+01	0.24167659E+01	H	-0.2598096100000002	-6.598457800000003	0.9802270400000005
C	0.14387332E+01	-0.16934910E+01	0.10807656E+01	O	3.596685799999999	-5.116672300000003	4.278147299999997
C	0.13227643E+01	-0.32312528E+01	0.14294698E+01	H	3.559412599999999	-4.346254899999999	4.9500621000000002
O	0.21368328E+01	-0.18866383E+01	0.44862559E+01	H	2.693154299999998	-5.058284699999997	3.886845000000001
C	0.23007241E+00	-0.86356571E+00	0.66782752E+00	O	-1.5824658000000000	-4.973987999999999	3.982618399999998
O	-0.89846412E+00	-0.10507897E+01	0.15540012E+01	H	-0.6061152199999995	-4.746228500000000	3.8685067000000002
O	1.1232517000000001	-4.086662399999998	0.4797904000000001	H	-1.6708407000000001	-5.614017600000004	3.267175899999998
O	1.107561199999999	-4.576819000000004	3.5010606000000002	O	4.599452200000000	-4.297978699999998	1.709716400000000
C	0.54130873E+00	0.64999714E+00	0.55338024E+00	H	4.812699200000000	-3.328046000000001	1.673417100000000
O	-0.35929943E+00	0.13796066E+01	-0.27447529E+00	H	4.1238625000000004	-4.298029200000002	2.5926919000000002
H	0.22807958E+01	-0.14998624E+01	0.42124551E+00	O	0.2671526599999999	-3.800399999999998	-1.987316700000000
H	0.61949592E+00	0.11357394E+01	0.15074007E+01	H	1.046890499999999	-4.212106300000003	-2.3955590000000000
H	0.15241922E+01	0.73437604E+00	0.10288120E+00	H	0.4134571400000000	-3.991719999999999	-1.0091755000000000
H	-0.12566712E+01	0.10883285E+01	0.25440453E-02	O	0.8045179399999999	-4.295823200000001	6.121390299999998

H	1.2870621000000000	-5.145534200000002	6.288084999999997	C	0.16461734E+01	-0.17688466E+01	0.10817010E+01
H	0.9704702200000005	-4.245247100000003	5.160279300000000	C	0.15022681E+01	-0.32447639E+01	0.13574831E+01
O	3.749969800000001	-3.582248200000000	-1.059052900000000	O	0.18446402E+01	-0.15978704E+01	0.44353691E+01
H	3.006970799999999	-3.963595100000000	-0.627838279999997	C	0.41312425E+00	-0.11038407E+01	0.48162084E+00
H	3.890639800000002	-2.878650599999998	-0.389365499999998	O	-0.7753366E+00	-0.13778761E+01	0.13571812E+01
O	-1.432678100000000	-2.187138399999998	4.944251399999997	O	1.488724200000001	-4.143115200000004	0.5108836100000004
H	-1.898279499999999	-3.021523000000001	4.894564800000004	O	1.281211600000000	-4.425654200000003	3.445767000000000
H	-0.563892360000004	-2.594301600000001	5.049482499999999	C	0.57687707E+00	0.32352497E+00	0.30731417E+00
O	4.614320900000001	-7.331847700000000	2.439629699999998	O	-0.44369623E+00	0.96244324E+00	-0.47356504E+00
H	4.100733100000002	-6.819253400000000	3.161160900000001	H	0.24408319E+01	-0.15449885E+01	0.32185093E+00
H	5.359289600000003	-6.786314000000000	2.227795500000000	H	0.55601626E+00	0.80587056E+00	0.12775492E+01
O	-2.892963500000000	-3.078795700000001	0.519614919999998	H	0.15507487E+01	0.49277117E+00	-0.24020995E+00
H	-2.795711100000001	-3.071114100000000	-0.428264340000002	H	-0.12682720E+01	0.52578320E+00	-0.40933270E+00
H	-2.087657900000000	-2.560029199999998	0.764407850000000	H	0.28677464E+00	-0.15748979E+01	-0.45637235E+00
O	0.857563060000004	-9.070298400000004	3.052216500000001	H	-0.53397976E+00	-0.20566903E+01	0.18823821E+01
H	1.305268499999999	-8.228284399999997	2.871275400000000	O	1.467733800000000	6.660948200000000	1.860832399999999
H	1.584148900000000	-9.757608499999999	2.989876499999998	H	1.465458100000000	-5.941138800000001	2.611763400000001
C	0.13992176E+01	-0.33646787E+01	0.27481709E+01	O	3.822341799999998	-5.179687000000004	4.077564200000003
C	0.18438073E+01	-0.21240672E+01	0.32393651E+01	H	3.759410299999999	-4.529440300000001	4.833204399999996
O	0.21068793E+01	-0.11985395E+01	0.22376798E+01	H	2.947375899999999	5.011888199999996	3.613586800000002
C	0.16620098E+01	-0.17512470E+01	0.10005456E+01	O	-0.828599179999999	-6.157952599999998	0.251345199999999
C	0.14225821E+01	-0.32621555E+01	0.13275015E+01	H	-4.132653700000003E-002	-5.721584199999997	0.6353108800000002
O	0.21330305E+01	-0.16063213E+01	0.43496219E+01	H	-1.250314600000001	-6.577590700000000	1.064421600000000
C	0.39108655E+00	-0.11110938E+01	0.43838629E+00	O	-1.600326100000000	-4.640988499999997	3.876728400000002
O	-0.70581355E+00	-0.13169897E+01	0.12808979E+01	H	-0.6682460000000001	-4.830232299999996	3.667888999999999
O	1.222013100000001	-4.171151600000000	0.444694089999999	H	-2.075043700000002	-5.321441100000004	3.3004424000000001
O	1.212401600000000	-4.422199400000002	3.523232339999999	O	0.364880089999999	-3.774206400000002	-1.986284100000000
C	0.52940465E+00	0.40958228E+00	0.33126890E+00	H	0.7630244800000000	-4.394339999999997	-2.597925000000000
O	-0.55931473E+00	0.10707587E+01	-0.41460362E+00	H	0.6904060300000000	-4.034110100000004	-1.111770000000000
H	0.25077744E+01	-0.16277313E+01	0.22234792E+00	O	4.516002600000002	-7.135293400000001	-4.331860199999998E-002
H	0.62450058E+00	0.84111081E+00	0.13187586E+01	H	4.837383000000000	-3.580714899999998	1.304977800000001
H	0.14997032E+01	0.63901978E+00	-0.22624059E+00	H	4.602563199999996	-6.439785200000004	2.439752000000001
H	-0.14217193E+01	0.69601678E+00	-0.87016147E-01	O	0.8841543100000000	-4.083512299999998	6.062545799999997
H	0.20609766E+00	-0.16219759E+01	-0.55527704E+00	H	1.346295599999999	-4.941656600000000	6.229424800000003
H	-0.41756231E+00	-0.18974458E+01	0.20506024E+01	H	1.152615699999999	-3.944870299999998	5.183061200000000
O	1.616905400000000	-6.651140299999998	1.779976599999999	O	3.462039299999998	-7.135293400000001	-4.331860199999999E-002
H	1.698471600000000	-5.946719599999998	2.401556499999999	H	2.611655299999998	-7.445824199999997	0.301413519999999
H	1.374514800000000	-6.070278400000003	1.009672200000000	H	3.510606699999999	-6.325242700000004	0.498846120000000
O	3.761652999999999	-5.027452499999999	4.174042400000003	O	3.9791338000000001	-3.829354400000002	-1.124009500000001
H	3.559267600000001	-4.558642299999998	4.994219000000002	H	3.116678299999998	-4.144026199999999	-0.872027199999996
H	2.867121700000002	-4.776967899999998	3.780142699999999	H	4.177088999999996	-3.257287400000001	-0.440106290000001
O	-0.821217100000005	-6.021690530000000	0.153853300000000	O	4.867345099999996	-7.243764000000002	2.626057600000002
H	-0.210501329999999	-5.239086999999996	0.178207239999999	H	4.182744300000004	-6.601918200000001	2.859821900000000
H	-0.572475839999996	-6.416558499999998	0.983353680000001	H	5.668630499999999	-6.730803999999997	2.457821500000001
O	-1.442439100000001	-4.826773700000004	4.024982399999998	O	1.0905609000000001	-9.055444200000002	3.180050800000001
H	-0.4534834370000000	-4.804267000000003	3.973577500000002	H	1.042011300000000	-8.174154599999996	2.735291600000000
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O	8.622590600000005E-002	-3.827506699999998	-1.921421119999999	O	-3.046669300000000	-3.102230899999999	0.3463131900000001
H	0.612175290000004	-4.408809599999997	-2.460041599999998	H	-2.833039400000001	-3.510375199999999	-0.490790249999999
H	0.473825950000000	-3.954054100000000	-1.090846200000001	H	-2.185143899999999	-2.679114480000000	0.697701789999999
O	0.605347230000001	-4.295282199999999	6.230688229999997	H	-	-	-
H	1.059928000000000	-5.114128400000002	6.476592400000004	C	0.15662633E+01	-0.32526762E+01	0.27469064E+01
H	0.930240740000001	-4.287263399999996	5.303991400000001	C	0.16159668E+01	-0.19490276E+01	0.32832259E+01
O	3.873968600000000	-3.546809800000001	-1.138725299999999	O	0.17948473E+01	-0.93776898E+00	0.23962709E+01
H	2.988610000000000	-3.827382699999998	-0.951837460000002	C	0.17071634E+01	-0.15821177E+01	0.11239615E+01
H	4.093849099999999	-2.955623999999998	-0.333355069999998	C	0.16313408E+01	-0.30935094E+01	0.13716045E+01
O	4.794432800000001	-4.614909100000002	1.599775500000000	O	0.16136369E+01	-0.16440159E+01	0.45215580E+01
H	5.097976199999997	-3.731237300000001	1.419170599999999	C	0.47080737E+00	-0.10413938E+01	0.38700870E+00
H	4.631049000000000	-4.522014699999997	2.542920300000000	O	-0.71237381E+00	-0.13642610E+01	0.10781492E+01
O	3.880748899999999	-7.165157599999997	-0.163187880000001	O	1.553337500000000	-4.028435000000000	0.5282825199999998
H	2.952699500000000	-7.140648500000002	0.140351079999999	O	1.455131800000000	-4.3944040040000003	3.353018099999999
H	4.300910499999996	-6.585443699999999	0.463172270000000	C	0.51593517E+00	0.50955071E+00	0.20355520E+00
O	-2.893561399999998	-2.990070100000001	0.742750050000005	O	-0.60506640E+00	0.11378480E+01	-0.47979540E+00
H	-2.859613899999998	-3.338471300000001	-0.1522548200000001	H	0.25819638E+01	-0.13990035E+01	0.49860205E+00
H	-1.986681300000001	-2.566905900000001	0.803970489999998	H	0.72302112E+00	0.98902322E+00	0.12072936E+01
O	0.858019369999995	-9.127351100000003	2.696869599999999	H	0.14766160E+01	0.66104160E+00	-0.41419090E+00
H	0.814490669999997	-8.229946299999999	2.359321200000001	H	-0.13460317E+01	0.72745749E+00	0.13111015E-01
H	1.849559299999999	-9.142414000000005	2.626510500000002	H	0.49808391E+00	-0.16331999E+01	-0.56809302E+00
O	-1.096097000000001	-2.235217599999999	5.436450500000003	H	-0.51863525E+00	-0.19346547E+01	0.17988567E+01
H	-1.422002700000000	-2.806935000000002	4.724646700000001	O	1.254419400000000	-6.644340999999998	1.785421900000000
H	-0.4865796000000000	-2.904471000000000	5.813820299999997	H	1.293827400000001	-6.408331399999998	2.741767799999999
C	0.14395272E+01	-0.32740384E+01	0.27426258E+01	O	3.730110400000000	-5.149190299999999	4.273598899999996
C	0.18035445E+01	-0.20213813E+01	0.32456897E+01	H	3.936528300000000	-4.528569600000000	4.998459999999997
O	0.20281644E+01	-0.10801368E+01	0.22599319E+01	H	2.849025000000001	-4.819432299999999	3.963496000000000

O	-1.4145194000000001	-4.952993499999998	4.038747200000004	O	-0.7506506899999995	-1.926555999999999	4.881881899999998
H	-0.5096561200000005	-4.926269099999998	3.605338699999999	H	-1.3973802000000000	-2.6642458000000002	4.901333000000001
H	-1.873789399999999	-5.699108700000000	3.671000900000001	H	5.396697200000002E-002	-2.3912007200000002	4.985751999999997
O	-0.8666925100000003	-6.433076899999997	3.13410000000003E-002	O	4.334890500000002	-7.623383500000001	2.875472199999999
H	-0.1071381300000000	-6.379724699999997	0.653368449999999	H	3.899167600000002	-6.869964800000000	3.323812699999999
H	-1.5404670000000000	-6.471517999999997	0.7578657399999995	H	5.141625999999996	-7.203595299999999	2.581882799999998
O	4.7658499000000001	-4.620975099999999	1.5973531000000001	O	0.7172280100000003	-9.084025000000005	2.880086799999999
H	4.7996306000000004	-3.664080400000000	1.7988966000000000	H	0.7816676400000000	-8.311664199999992	2.300925599999998
H	4.409947599999997	-4.961429400000001	2.3861786000000000	H	1.472325099999999	-9.581572899999994	2.563202400000002
O	3.5967180000000001	-7.120150200000003	0.1295905599999999				
H	2.787329499999998	-6.790837999999999	0.4600392600000002	C	0.15045093E+01	-0.32110083E+01	0.26680412E+01
H	4.090053199999998	-7.231270900000002	0.9853956000000004	C	0.19915883E+01	-0.19540609E+01	0.31279319E+01
O	0.1425835300000001	-4.161300599999997	-2.08260699999999	O	0.20754057E+01	-0.98571582E+00	0.20727055E+01
H	0.7473310500000000	-4.777329400000002	-2.576311399999998	C	0.18212021E+01	-0.17360099E+01	0.79264380E+00
H	0.5681228999999999	-4.022221700000002	-1.254965399999999	C	0.1546749484E+01	-0.32303695E+01	0.12351678E+01
O	0.7601270399999998	-4.049819000000003	6.150447700000000	O	0.22764863E+01	-0.16308411E+01	0.43078686E+01
H	1.2829782000000001	-4.905790599999998	6.321027800000004	C	0.61402758E+00	-0.11825241E+01	0.14585221E+00
H	1.0341416000000001	-3.921388100000002	5.230519799999997	O	-0.55018457E+00	-0.13784118E+01	0.99489632E+00
O	4.3195728000000004	-3.393626900000001	-1.089435600000001	O	1.2393445000000001	-4.1870488000000003	0.4179990100000000
H	3.629363699999999	-3.925826600000002	-0.647376619999996	O	1.3247897000000000	-4.185263599999999	3.5555226000000002
H	4.639942200000001	-2.808084300000000	-0.3125241400000001	C	0.71614697E+00	0.35320917E+00	-0.14300564E+00
O	4.432342600000001	-7.175747200000000	2.677151200000000	O	-0.46488432E+00	0.83417625E+00	-0.72616085E+00
H	3.831230399999999	-6.562898699999999	3.208314699999999	H	0.27048404E+01	-0.16598402E+01	0.23370974E+00
H	5.2500717000000003	-6.665117299999998	2.455182600000001	H	0.92545755E+00	0.92317455E+00	0.78399623E+00
O	3.7339473000000001	-2.892893200000001	5.995032000000004	H	0.15297809E+01	0.60621016E+00	-0.84280544E+00
H	2.9231368000000000	-2.775450000000002	5.507693599999996	H	-0.12335801E+01	0.63700557E+00	-0.17589174E+00
H	4.1434851000000004	-1.991894700000000	5.987127499999997	H	0.38124960E+00	-0.17216535E+01	0.79535805E+00
O	0.1025785000000000	-9.156748399999997	3.317482800000001	H	-0.31748074E+00	-0.18064722E+01	0.18453509E+01
H	0.9279784899999999	-8.475743899999994	2.593296699999998	O	1.364381899999999	-6.527383800000000	1.899266399999999
H	1.9242163000000001	-9.555820999999999	3.051346999999998	H	1.107248400000000	-5.856396400000000	2.582603300000002
C	0.15549846E+01	-0.33313730E+01	0.27446831E+01	H	1.6383483800000001	-5.783501700000004	1.2726401000000001
C	0.19700836E+01	-0.20443995E+01	0.31675962E+01	O	-1.358856300000000	-4.625233299999997	3.627362400000000
O	0.20983832E+01	-0.11084801E+01	0.21005525E+01	H	-0.373083310000000	-4.567777999999997	3.620742500000000
C	0.17080653E+01	-0.18829267E+01	0.93119380E+00	H	1.493279999999999	-5.371309799999997	3.044849100000000
C	0.15709492E+01	-0.33221313E+01	0.13365417E+01	O	3.741207999999999	-5.183677499999999	4.140157900000002
O	0.20779266E+01	-0.16194025E+01	0.43156635E+01	H	3.803357300000001	-4.470008100000003	4.750645300000004
C	0.38426206E+00	-0.12958987E+01	0.35811888E+00	O	2.780535200000001	-5.096353599999996	3.863221100000001
O	-0.82368898E+00	-0.16731345E+01	0.10666312E+01	H	4.605881199999998	-4.800350999999996	1.741836900000000
O	1.3725825000000000	-4.277532500000004	0.492798179999997	H	4.723601699999997	-3.880379399999998	1.493097600000000
O	1.3442118000000001	-4.301549299999996	3.605807899999998	H	4.303727600000002	-4.639059900000003	2.635065899999998
C	0.48865137E+00	-0.19250805E+00	0.19794568E+00	O	2.6135815000000003	-4.207983800000001	-1.953040099999999
O	-0.46118937E+00	-0.82541701E+00	-0.76954670E+00	H	0.477956139999997	-4.976042900000004	-2.309999000000002
H	0.25103469E+01	-0.16186008E+01	0.21708024E+00	H	0.5557336000000005	-4.153075600000002	-1.128000600000000
H	0.32824517E+00	-0.50609069E+00	0.12388261E+01	O	-0.798821239999999	-6.732572900000001	-0.1276474599999999
H	0.14609629E+01	-0.55961711E+00	-0.20805109E+00	H	-4.570419000000001E-002	-6.774774466999999	0.4574366599999999
H	-0.13241784E+01	-0.41063063E+00	-0.46851108E+00	H	-1.5254326000000000	-6.746948999999999	0.5447864300000004
H	0.33757168E+00	-0.17161265E+01	-0.68760754E+00	O	0.9211856899999995	-4.463057600000000	6.276444599999996
H	-0.52849048E+00	-0.21899701E+01	0.18331370E+01	H	1.478209399999999	-5.244013599999997	6.407910199999999
O	1.494005599999999	-6.550794299999997	2.071319900000002	H	1.220628899999999	-4.180446000000000	5.374255200000003
H	1.4732320000000001	-5.966946300000000	2.857595900000002	O	3.530743600000001	-6.703617699999997	-0.1450765300000001
H	1.3417173000000000	-5.936870700000001	1.414062300000001	H	2.873308000000002	-7.257744400000000	0.3326540499999998
O	3.8447653000000002	-5.219466800000002	4.315865299999996	H	3.871001100000000	-6.227782300000003	0.6053509200000001
H	3.8785123000000001	-4.415063700000001	4.854942900000002	O	4.215332199999998	-3.788615399999999	-1.260192500000000
H	2.9539846000000001	-5.024932699999999	3.912127799999999	H	3.343342400000000	-4.053902199999996	-0.973338429999998
O	-1.431548599999999	-4.548192499999999	4.048146300000000	O	4.577887679999998	-3.364884299999999	-0.4913982900000002
H	-0.4494796300000002	-4.540274799999997	4.077314900000002	H	-0.9900969699999998	-2.115749399999999	4.655109999999996
H	-1.5614389000000000	-5.256444600000000	3.366997200000001	H	-1.480734999999999	-2.823361300000000	4.133926400000000
O	-1.0050066999999999	-6.238881499999997	-9.548162600000000E-002	H	-0.2156664460000000	-4.943689000000000	-0.627782300000000
H	-0.4236711699999999	-5.575958000000000	0.2804776700000001	O	4.405285199999998	-7.433123600000001	2.743333799999998
H	-1.3749520000000000	-6.520792900000000	0.7656929300000005	H	3.884221199999998	-6.749078800000004	3.156063000000002
O	0.1970086000000000	-3.872485199999998	-1.863080700000000	O	5.200645100000000	-7.010697300000004	2.488788800000000
H	0.6139284600000001	-4.622535199999997	-2.377259300000000	H	0.9206259700000002	-8.865000999999996	3.022041100000000
H	0.6243874700000006	-4.015451399999999	-0.944201839999996	H	1.188472500000000	-7.983039000000001	2.641557100000000
O	4.469001099999998	-4.860440299999996	1.571216800000000	H	1.515983300000000	-9.402294999999997	2.510861499999999
H	4.590967899999999	-3.919976300000001	1.593102400000000	C	0.15228785E+01	-0.34224646E+01	0.26940265E+01
H	4.343226399999998	-5.105979800000001	2.547324699999999	C	0.18759526E+01	-0.20742920E+01	0.31207802E+01
O	4.084478700000000	-3.546555699999999	-1.023272000000000	O	0.19475394E+01	-0.12559390E+01	0.20255322E+01
H	3.144822399999998	-3.649194200000002	-0.6070526000000005	C	0.16632525E+01	-0.19911156E+01	0.87673486E+00
H	4.606179000000000	-3.050299299999998	-0.3558465599999998	C	0.13760896E+01	-0.33900021E+01	0.13319735E+01
O	3.307372099999998	-6.784955400000003	-0.1454836700000001	O	0.20338255E+01	-0.15416814E+01	0.42171007E+01
H	2.606186199999998	-6.982292300000001	0.4616006500000000	C	0.39199041E+00	-0.13181199E+01	0.10596946E+00
H	3.5827265000000001	-6.017610999999996	0.3222260900000002	O	-0.80515249E+00	-0.15650301E+01	0.91124416E+00
O	1.006392699999999	-4.319856699999999	6.305916500000004	O	1.152007000000000	-4.363893799999996	0.4942440799999997
H	1.5270353000000001	-5.106651199999999	6.642733400000000	O	1.378101400000000	-4.424441500000004	3.567778000000000
H	1.2592989000000004	-4.179389300000004	5.369381999999999	C	0.51784809E+00	0.11250931E+00	-0.444245030E-01

O	-0.59360697E+00	0.77599476E+00	-0.76639235E+00	H	-1.097598499999999	-6.960927299999998	0.5461694299999996
H	0.25484351E+01	-0.19308239E+01	0.22617045E+00	O	4.699373699999998	-5.005923900000000	1.644796100000000
H	0.69902658E+00	0.65952472E+00	0.92243190E+00	H	4.574547599999998	-4.026071400000002	1.495378000000001
H	0.15133610E+01	0.37565155E+00	-0.56918538E+00	H	4.944895800000003	-5.008823399999998	2.600763600000001
H	-0.13243149E+01	0.15872208E+00	-0.61764082E+00	O	3.321213600000001	-6.904538099999999	-0.127825040000000
H	0.19029769E+00	-0.19267650E+01	-0.79820279E+00	H	2.568970300000002	-7.302971600000002	0.337149880000001
H	-0.65572586E+00	-0.22598915E+01	0.15346451E+01	H	3.661890699999998	6.279395199999997	0.519162429999995
O	1.577530999999999	-6.543957299999998	2.042973599999998	O	0.8492951100000002	-4.546358800000001	6.188235200000003
H	1.437340400000001	-5.809238599999996	2.660580400000002	H	1.2977358000000001	-5.384695899999996	6.448524199999996
H	1.416089600000001	-5.950041399999999	1.245994100000001	H	1.184948300000001	-4.362839000000001	5.268946699999999
O	-1.197722400000000	-4.848878199999997	3.863263700000001	O	0.1562099300000000	-4.006797200000003	-2.071218099999998
H	-0.2578465799999999	-4.733800300000004	3.827265699999999	H	0.8541944899999996	-4.397928799999999	-2.600766800000002
H	-1.294807000000000	-5.440892599999997	3.151310500000001	H	0.6038732000000005	-4.037979400000002	-1.177007399999999
O	-0.7091832399999999	-6.458776399999996	-3.282831499999997E-02	O	0.6881629000000002	-8.718533700000001	3.485589899999999
H	-2.036841799999999E-002	-5.814552299999999	0.1983968000000000	H	1.0155391000000000	-7.974851600000000	2.999738499999999
H	-1.060075499999999	-6.694794700000001	0.8913132299999996	H	1.3347198000000000	-9.341564500000005	3.135574699999998
O	3.948335600000001	-5.149711700000001	4.288704000000001	O	4.577717599999997	-7.685169600000000	3.136993299999999
H	4.105301800000003	-4.413458399999997	4.997554899999999	H	4.202634899999996	-6.872886499999999	3.622505299999998
H	3.032590200000000	-4.839750900000003	4.119407899999997	H	5.488309499999997	-7.365710899999998	2.944776999999998
O	0.8269592900000001	-4.571848199999998	6.167322099999998	O	4.8218052000000000	-2.2604706000000001	0.9712917800000005
H	1.282228300000001	-5.477726099999999	6.154994999999997	H	4.6542164000000001	-1.532834999999999	1.5848156000000000
H	1.077335699999999	-4.393501399999999	5.239944800000000	H	5.756997100000004	-2.008508800000000	0.6149100600000004
O	3.428836800000000	-6.580496799999997	-8.370781600000004E-002				
H	2.711949000000002	-6.876321899999998	0.546348000000003	C	0.162255096E+01	-0.3431697E+01	0.26317527E+01
H	4.032527400000002	-6.185412900000002	0.578905160000003	C	0.19432184E+01	-0.207696633E+01	0.31141704E+01
O	-2.315961600000001E-002	-4.204331299999998	-2.062758500000002	O	0.18880464E+01	-0.10897577E+01	0.20677335E+01
H	0.426013640000003	-4.716067200000003	-2.735147099999998	C	0.161110429E+01	-0.18585577E+01	0.87826413E+00
H	0.533850649999999	-3.145221999999999	-1.259769300000001	C	0.14998020E+01	-0.33207002E+01	0.12291224E+01
O	4.920174399999996	-4.812440299999996	1.745515300000001	O	0.22786455E+01	-0.16849696E+01	0.42462837E+01
H	4.952554499999997	-3.818313900000001	1.623201300000001	C	0.33580513E+00	-0.13823395E+01	0.11245411E+00
H	4.562712200000000	-4.869172299999998	2.706122699999999	O	-0.90161077E+00	-0.17006226E+01	0.72716302E+00
O	4.292826100000001	-3.797684700000000	-1.041154200000000	O	1.230066000000001	-4.248798599999998	0.3432606000000003
H	3.565746299999998	-4.338958100000002	-1.236418000000000	O	1.457517299999999	-4.515841399999999	3.371197099999998
H	4.098301499999998	-3.554963799999999	-0.117999300000000	C	0.37353966E+00	0.99952620E-01	-0.10218593E+00
O	-0.8729858700000005	-2.239691399999999	4.766716500000002	O	-0.68198961E+00	0.70957797E+00	-0.88761873E+00
H	-1.096554900000001	-3.150819900000001	4.789815499999997	H	0.24013436E+01	-0.17690953E+01	0.17385482E+00
H	9.509587299999997E-002	-2.412687899999998	4.889765999999998	H	0.24679115E+00	0.54333840E+00	0.81694244E+00
O	0.805726759999999	-8.888070499999995	3.373488699999998	H	0.13389293E+01	0.40822345E+00	-0.64705085E+00
H	0.939328880000003	-8.046651999999999	2.869486100000000	H	-0.15450947E+01	0.67634522E+00	-0.31923849E+00
H	1.573652199999999	-9.352949600000005	2.929293299999999	H	0.25342077E+00	-0.18808489E+01	-0.86550518E+00
O	4.825095600000000	-2.288239400000001	1.192510500000000	H	-0.74177949E+00	-0.26046862E+01	0.10611269E+01
H	4.554759100000001	-1.483756200000000	1.747101000000000	O	1.119400100000000	-6.660540300000001	1.663269000000001
H	5.678521599999998	-1.929947200000000	0.8266854399999999	H	1.144325999999999	-6.206872599999996	2.559929000000001
C	0.17573252E+01	-0.34471008E+01	0.27094534E+01	O	1.323915000000000	5.915348599999997	1.0724879700000000
C	0.20337527E+01	-0.20850401E+01	0.32308399E+01	H	-1.267854899999999	-4.812867100000001	4.026912600000000
O	0.19686685E+01	-0.11505246E+01	0.22099043E+01	H	-0.366458230000000	4.739262000000001	3.686501100000001
C	0.17331119E+01	-0.19106598E+01	0.97764294E+00	H	-1.751442699999999	-5.499907000000004	3.489727400000000
C	0.15956051E+01	-0.33860256E+01	0.1331314313E+01	O	0.564416800000001	-4.826238700000002	1.504452500000000
O	0.22267031E+01	-0.16199571E+01	0.44109715E+01	H	4.704963199999999	-3.912484099999999	1.329651700000001
C	0.52782008E+00	-0.13863539E+01	0.22666593E+00	O	4.010093399999997	-4.616172299999997	2.240404600000002
O	-0.67628262E+00	-0.17303058E+01	0.95954814E+00	H	-0.4293049600000001	-6.338136900000003	-0.563279690000000
O	1.383367999999999	-4.325440399999997	0.4364372899999998	H	-0.288861729999999	-5.445945150000000	-0.213085650000001
O	1.763419099999999	-4.465193199999999	3.585860300000001	O	-0.145817179999999	-6.760602600000004	0.2312259300000000
C	0.44875389E+00	0.14615207E+00	0.21686090E-01	O	3.896718100000002	-5.301105400000000	4.381523399999998
O	-0.66654917E+00	0.69612625E+00	-0.70557988E+00	H	4.107273300000001	-4.460396900000001	4.864640900000004
H	0.26774671E+01	-0.17037300E+01	0.39445756E+00	H	2.986745400000002	-5.182682700000000	4.049298300000002
H	0.66685604E+00	0.63616163E+00	0.98997403E+00	O	3.682556100000002	-3.848667400000001	-1.248121400000000
H	0.13605108E+01	0.35401588E+00	-0.57149506E+00	H	4.080562000000003	-6.338136900000003	-0.895105489999995
H	-0.15728201E+01	0.59219987E+00	-0.38721144E+00	H	4.146373900000004	-3.601940599999998	-0.411105889999997
H	0.48977558E+00	-0.18289890E+01	-0.75566899E+00	H	0.196044904000000	-4.092458999999998	-2.231649399999998
H	-0.56732258E+00	-0.25326971E+01	0.15061248E+01	H	0.646809830000003	-4.117724499999996	-1.315555300000000
O	1.370087000000001	-6.593163200000002	1.789820200000001	O	0.804347530000003	-4.360591099999997	6.068252900000001
H	1.513402700000001	-5.962105600000001	2.473504699999999	H	1.378328599999999	-5.062307299999996	6.275251899999998
H	1.401447099999999	-5.965783799999996	1.026489100000000	H	0.9102205100000004	-4.397301200000002	5.108341399999996
O	-1.266490100000000	-4.763004600000004	3.765307999999999	O	3.554458500000000	-6.783087799999998	-9.176599700000002
H	-0.2957368000000002	-4.895558900000002	3.738528600000000	H	2.629064800000001	-6.878516200000000	0.112465109999999
H	-1.664466400000000	-5.331974200000003	3.058980300000000	H	3.927843000000002	-6.164396100000003	0.5863680100000005
O	4.215703999999997	-5.221323900000002	4.436802799999997	O	-0.9841436599999998	-2.498373299999999	5.341039900000002
H	4.357526100000003	-4.393075900000004	5.007234399999998	H	-1.151025400000000	-3.336959000000001	4.812634400000003
H	3.348762199999999	-5.043450299999999	4.024645200000001	H	-0.1835266399999999	-2.765933299999999	5.782902899999998
O	3.735756600000000	-3.986629999999999	-1.142600200000000	O	4.885464200000004	-2.279189500000002	0.887137819999997
H	2.882260099999999	-4.103812200000001	-0.630845050000002	H	4.853208399999998	-1.442409300000000	1.379938700000001
H	4.387626499999997	-3.738041899999998	-0.468851579999999	H	5.849480400000000	-2.121541100000000	0.6123680900000003
O	-0.7171281400000003	-6.665554799999998	-0.322154800000002	O	4.560916999999999	-7.673194500000001	2.9307118000000001
H	-0.1016901500000001	-5.942023200000004	1.880789600000001E-002	H	4.309279100000004	-6.955808600000000	3.4918589000000000

H 5.233793999999996 -7.202792699999998 2.4317049000000002