

Supplementary Information: Nanoconfinement Matters in Humidified CO₂ Interaction with Metal Silicates

S. Zare¹, K.M. Salah Uddin², A. Funk^{2,3}, Quin R.S. Miller⁴, M.Ja. Abdolhosseini Qomi^{1,*}

¹Department of Civil and Environmental Engineering, Henry Samueli School of Engineering, E4130 Engineering Gateway, University of California, Irvine, Irvine, CA, 92697-2175, USA.

²Construction Materials Chemistry Department, University of Kassel, Germany, Mönchebergstraße 19, 34125 Kassel, Germany.

³Chemistry Department, University of Siegen, Adolf-Reichwein-Straße 2, 57068 Siegen, Germany.

⁴Physical and Computational Sciences Directorate, Pacific Northwest National Laboratory, P. O. Box 999, MS K8-98, Richland, WA 99352, USA

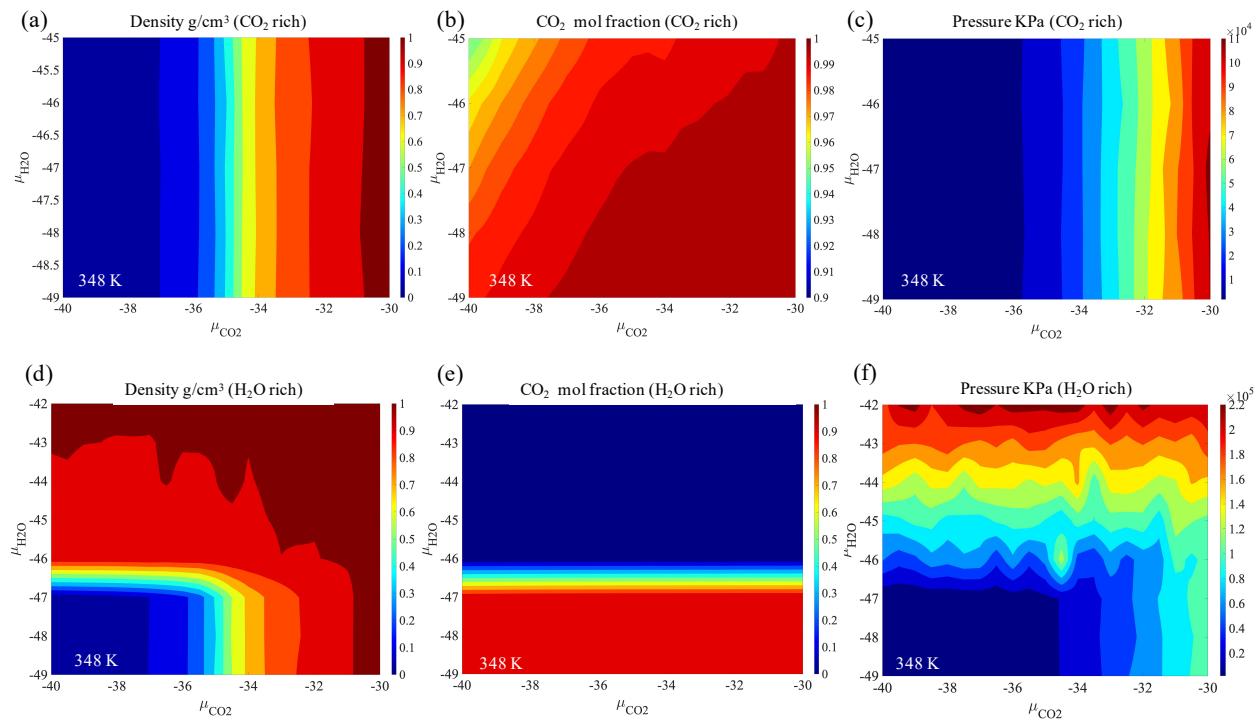
Supplementary Note 1: H₂O-CO₂ mixture adsorption in the macro-pore: Grand Canonical Monte Carlo (GCMC) simulations were used to determine the thermodynamic properties of the bulk H₂O-CO₂ mixture. We used the method of Configurational Biased Monte Carlo (CBMC)^{1,2} as implemented in Towhee³ to adsorb the mixture into a periodic box with dimensions (40 Å × 40 Å × 40 Å) in the grand canonical ensemble ($\mu_{H_2O}, \mu_{CO_2}, VT$). The cell dimensions are taken large enough to reduce the standard deviation of the solvent concentration as much as possible. The corresponding biased probabilities are given in the main text. We performed these GCMC simulations by considering 315 pairs of chemical potentials (μ_{H_2O}, μ_{CO_2}) in the ranges [-49,-42] kJ/mol and [-40, -30] kJ/mol for water and CO₂ respectively except for the simulations that were done at 348K with CO₂-rich condition where the chemical potential of water was in the range [-49,-45] kJ/mol. To examine whether phase coexistence exists, we assumed two different initial mixture compositions relevant to CO₂-rich and H₂O-rich conditions for all pairs of chemical potentials. Higher initial number of CO₂ molecules than water molecules were put on the lattice points for the CO₂-rich cases, and liquid water for the H₂O-rich cases were considered. We used rigid SPC⁴ model and EPM2 model⁵ for water and CO₂ respectively. All simulations are equilibrated for more than 25 million MC steps. The results are shown in **Fig. S1** and **Fig. S2** for temperatures of 348K and 300K respectively. The phase of the H₂O-CO₂ mixture is determined by μ_{H_2O} or μ_{CO_2} or both. At a specific range of chemical potentials, the mixture could be in coexisting CO₂-rich and H₂O-rich phases with two degrees of freedom (μ_{H_2O}, μ_{CO_2}) consistent with the Gibbs phase rule:

$$F = 2 + C - P$$

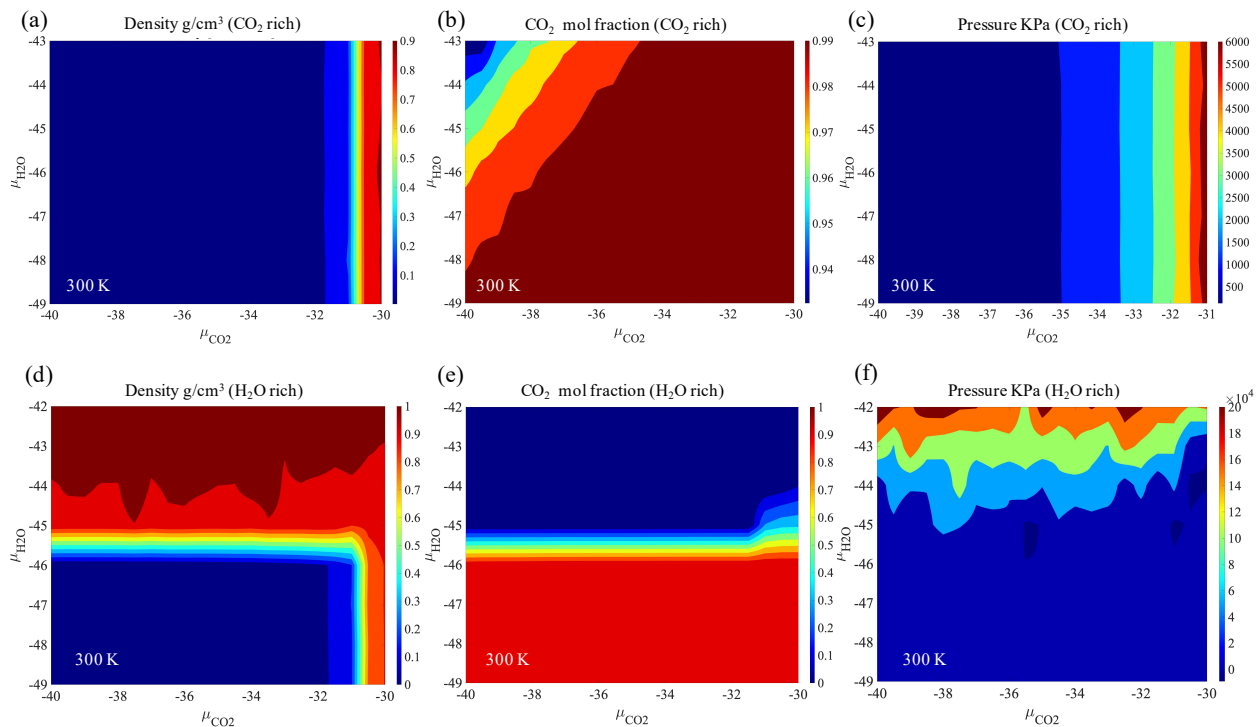
Where two degrees of freedom (F) is derived for a two-component immiscible mixture (C=2) with two phases (gas or liquid) (P=2). As expected for immiscible mixtures, CO₂ was calculated to be dominant when water is below saturation level ($\mu \leq 47 \frac{kJ}{mol}$ at 348K and $\mu \leq 46 \frac{kJ}{mol}$ at 300K) as

it could only be found in vapor form in that regime, see **Fig. S1.e** and **Fig. S2.e**. The density and pressure of CO₂-rich mixtures are merely controlled by the chemical potential of CO₂, see density and pressure colormaps in **Fig. S1** and **Fig. S2** for CO₂-rich phases. In the H₂O-rich phase, as water is found in liquid form the density is around 1 g/cm³ while the pressure is mostly controlled by the chemical potential of water. On the other hand, the molar fractions of components are sensitive to the chemical potential of both components, like in **Fig.S1.b** where the lowest CO₂ mole fraction is reached at the lowest μ_{CO_2} and highest μ_{H_2O} , and as we move from top left to bottom right of the diagram this molar fraction increases. To make the molar fractions clearer, H₂O molar fractions are depicted in **Fig. S3** for the regions of chemical potential space where CO₂ is dominant.

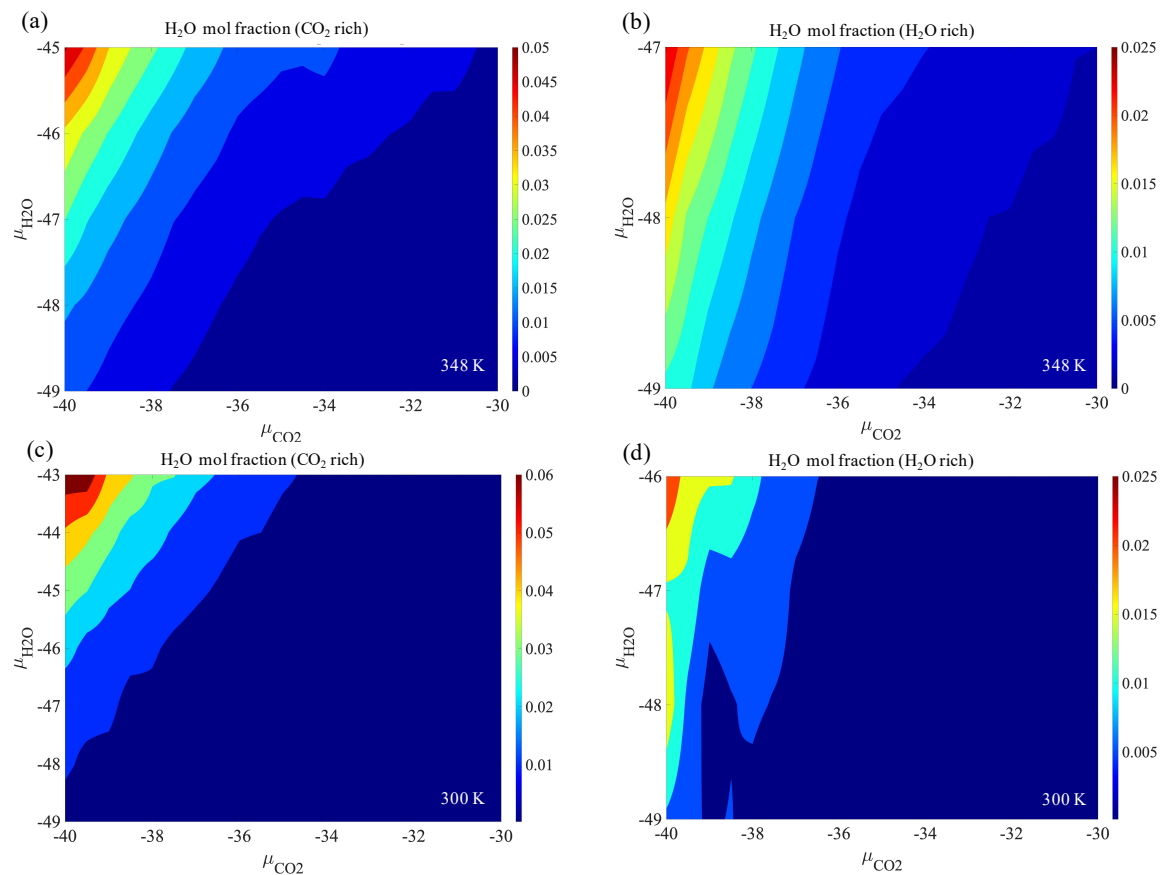
Supplementary Note 2: H₂O-CO₂ mixture adsorption in the slit nanopore: Upon GCMC calculations in the slit-pore of the mineral, CO₂ could only penetrate the slit pore when the interlayer distance is more than 30 Å, as could be seen in **Fig. S4.a**. At interlayer distances of less than 20 Å, the density of capillary water is found to be higher than its bulk value (1 g/cm³) consistent with the simulations on the ultra-confined nature of water in CSH^{6,7}, see **Fig S4-b**.



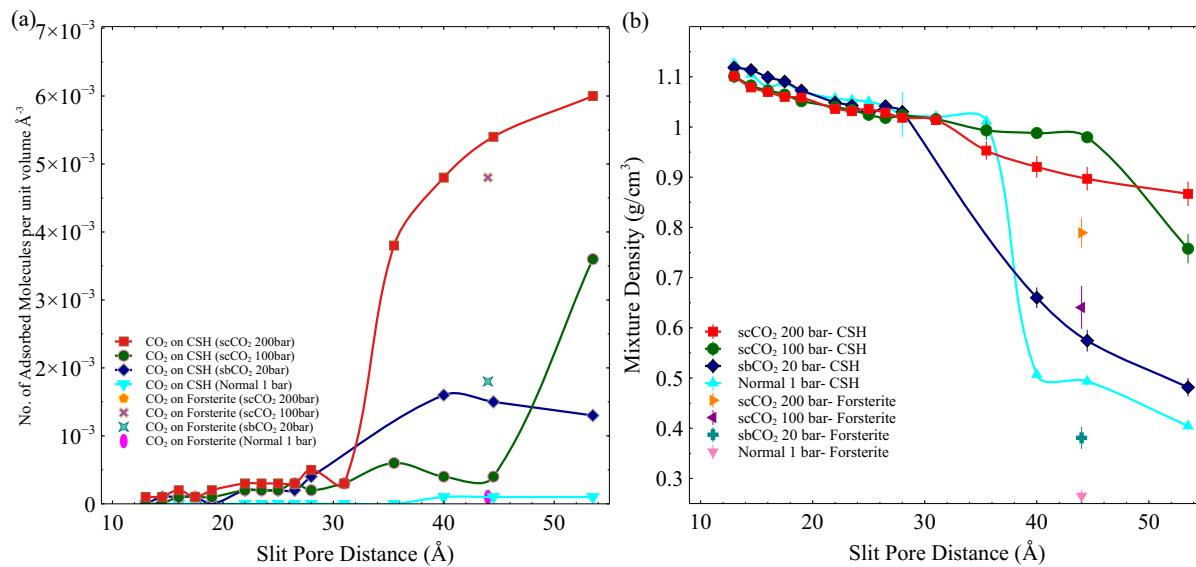
Supplementary Fig. S1. Adsorption of CO₂-H₂O mixture in the macro-pore at 348K. Colormaps of different thermodynamic properties are derived based on the independent variables (μ_{H_2O}, μ_{CO_2}). (a) density derived for a box initially at CO₂-rich condition. (b) CO₂ mole fraction derived for a box initially at CO₂-rich condition. (c) Pressure derived for a box initially at CO₂-rich condition. scCO₂ points at 100bar and 200bar were chosen for slit-pore adsorption. (d) Density for a box initially at H₂O-rich condition. (e) CO₂ mole fraction derived for a box initially at H₂O-rich condition. (f) Pressure derived for a box initially at H₂O-rich condition.



Supplementary Fig. S2. Adsorption of CO₂-H₂O mixture in the macro-pore at 300K. Colormaps of different thermodynamic properties are derived based on the independent variables ($\mu_{\text{H}_2\text{O}}, \mu_{\text{CO}_2}$). (a) density derived for a box initially at CO₂-rich condition. (b) CO₂ mole fraction derived for a box initially at CO₂-rich condition. (c) Pressure derived for a box initially at CO₂-rich condition. sbCO₂ at 20bar and normal condition at 1 bar were chosen for slit-pore adsorption (d) Density for a box initially at H₂O-rich condition. (e) CO₂ mole fraction derived for a box initially at H₂O-rich condition. (f) Pressure derived for a box initially at H₂O-rich condition.



Supplementary Fig. S3. H₂O mole fraction in the macropore dominated by CO₂. (a) Mole fraction of water at 348K in a cell initially rich with water. It was converged to the CO₂-rich phase for the below saturation conditions $\mu_{H_2O} \leq 47 \text{ kJ/mol}$. (b) Mole fraction of water at 348K in a cell initially rich with CO₂. (c) Mole fraction of water at 300K in a cell initially rich with CO₂. (d) Mole fraction of water at 300K in a cell initially rich with water. It was converged to the CO₂-rich phase for when $\mu_{H_2O} \leq 46 \text{ kJ/mol}$.



Supplementary Fig. S4. Adsorption of CO₂-H₂O mixture in the slit-pore of rock. (a) Number of adsorbed molecules per unit volume based on the slit-pore distance. 1/V dashed line shows that the number of water molecules is constant. It shows that after a certain distance only interfacial water exists. (b) The density of the mixture based on the slit-pore distance at various thermodynamic conditions.

Supplementary Table S1. Total energies of the structures in Density Functional Theory (DFT) calculations of the reactions between CO₂ and water/hydroxyl on the surface of C-S-H.

States	Total Energy (hartree)
2-ADS	-10151.30712
2-TS	-10151.30456
2-P	-10151.32684
1-ADS/3-ADS	-10151.30677
1-TS1/3-TS1	-10151.2408
1-INT/3-INT	-10151.28913
1-INT ^a	-10151.28611
3-TS2	-10151.28502
3-P	-10151.29313
3-INT ^b	-10151.28599
1-TS2	-10151.2798
1-P	-10151.31577

^a The geometry of this state is depicted in panel (d) of Fig. 8 in the main text. Compared to INT-1 in panel (c), the carbonic acid is rotated, and a weak hydrogen bond is formed between the hydroxyl group in carbonic acid and the surface hydroxide in C-S-H.

^b The geometry of this state is depicted in panel (e) of Fig. 8 in the main text. Compared to INT-3 in panel (c), the carbonic acid is rotated and two hydrogen bond are formed between carbonic acid and the silicate dimer on the surface of C-S-H.

Optimized geometries of DFT calculations with revPBE

2-ADS

Si	3.54406144	12.17788652	13.35862272
Si	6.07550816	16.28779392	13.91083625
Si	6.63404103	12.59294670	18.27311905
Si	5.46256645	9.65651266	18.04776334
Si	7.28896976	19.03467240	14.57960618
Si	10.43002300	22.43139905	15.26500015
Si	5.98265228	6.50330447	13.41810595
Si	8.47015719	10.71912362	13.83081517
Si	9.20123247	7.20436737	18.18217090
Si	7.81529184	4.48380762	18.38155389
Si	10.03326257	13.42329348	13.98017214
Si	12.35989272	17.35305826	14.82031000
Si	13.14425113	13.41292619	18.97527327
Si	11.67779556	10.74493720	18.42085351
Si	9.04325012	0.72626843	14.91965528
Si	11.14574418	4.52389683	14.69772444
Si	12.93513768	1.14911147	18.84972967
Si	14.61199105	22.74514236	19.16923134
Si	12.71073186	7.45501323	14.63637780
Si	1.97974054	9.37534023	13.50012369
Si	3.10681350	5.80262574	17.83970865
Si	1.73516970	3.29769713	18.76268143
Si	14.46875519	19.67562972	14.50246197
Si	4.35496355	17.91023184	18.95144058
Si	2.45857805	16.11006230	17.53058345

Si	5.79869124	24.12238860	13.23014876
Si	4.31178742	3.64346921	13.69604122
Si	5.69338309	0.45950976	18.85675176
Si	7.66795597	21.71566448	18.61119994
Si	16.59055855	14.24046347	14.78185152
Si	19.20063568	17.37024133	15.03985230
Si	20.08715845	13.80702640	19.33845170
Si	18.69342844	11.25030326	18.29686311
Si	20.06976777	20.07329671	13.72168379
Si	22.61964634	23.43140355	13.32396740
Si	24.80675500	19.98346143	16.66519417
Si	22.61479303	19.04789529	18.35721878
Si	18.82956164	8.10253089	13.27891661
Si	20.95247580	12.38737247	13.82774393
Si	22.55261716	14.96197667	14.10049086
Si	26.28289838	15.32189229	16.89585195
Si	24.73954753	12.57412839	17.79788655
Si	21.39465252	1.65128966	13.06513066
Si	24.25026801	6.31029601	12.27984419
Si	25.76706635	3.34197460	16.84431572
Si	23.86968422	0.76615971	17.59149581
Si	25.41113556	9.04982702	12.89546411
Si	15.20533306	11.41100283	14.30720894
Si	16.65671185	7.51161890	18.41180939
Si	14.81393590	5.07298498	18.57032462
Si	29.96960083	23.74042486	12.73848106
Si	17.83065751	19.84281477	19.11512262

Si	15.86622292	17.31947174	19.32956779
Si	17.32864292	5.38247814	13.30454717
Si	18.39385707	2.30757449	17.76077073
Si	20.40785863	23.77165826	17.89495826
Ca	6.63247476	12.99316153	14.90445115
Ca	4.87033356	9.71296353	15.02213815
Ca	3.30471916	12.44802865	16.90947516
Ca	5.38363442	15.64101893	16.87447785
Ca	10.26003050	19.77181729	16.81229095
Ca	8.91669007	16.42430108	15.52179921
Ca	7.46346258	18.63379692	18.42602916
Ca	10.76901679	22.30055178	19.24812135
Ca	9.52038570	7.36907149	14.68399495
Ca	7.59085871	3.89009213	14.71815998
Ca	6.42892670	6.86387721	16.53340119
Ca	8.43922873	10.07234501	17.10454505
Ca	13.33434126	14.03326886	15.81671450
Ca	11.66412472	10.58984499	15.38514052
Ca	9.99401274	13.44121527	18.15042094
Ca	12.09114740	16.74592110	18.20279098
Ca	11.95613089	1.82472118	15.74953118
Ca	13.11681443	22.29941072	16.59657283
Ca	9.38773136	1.38964337	18.90795125
Ca	11.34178201	4.52420704	18.65698993
Ca	2.93927986	6.42968988	14.37168153
Ca	2.27991518	2.72416296	15.60755329
Ca	12.83814845	7.75989199	17.90262392

Ca	1.90910976	9.34243404	17.09558036
Ca	3.81973756	18.77512239	15.25832413
Ca	26.82026036	12.74787640	15.06300898
Ca	14.53192501	19.79123998	18.19402740
Ca	4.42437883	21.34110903	18.38296457
Ca	5.32172187	0.96162737	15.13819891
Ca	5.52305713	21.88488229	15.48894235
Ca	5.86228982	24.19903512	17.86237354
Ca	5.07089387	3.47281966	17.73207790
Ca	20.19937136	14.42571904	16.21181259
Ca	18.25732507	11.23462799	15.35979101
Ca	16.57684074	14.01295857	18.31094645
Ca	19.82972183	16.82856420	18.74024347
Ca	22.49567443	21.36696156	15.53748397
Ca	22.30249625	17.63220921	15.75420198
Ca	20.46080659	20.94637693	18.39521661
Ca	23.80468248	23.90847775	17.16829515
Ca	22.17065912	9.06327033	13.66368484
Ca	20.87533092	5.17106610	13.87038504
Ca	19.93003556	8.05673703	16.71342401
Ca	21.87002562	11.25115101	17.11562771
Ca	26.20005548	17.74937586	15.19373736
Ca	24.20379535	12.11635664	12.40933538
Ca	23.29235492	15.40721269	18.11798632
Ca	28.32933917	19.51165819	17.73430092
Ca	24.55037896	1.60205149	14.55006791
Ca	25.97562046	22.52074342	13.36044443

Ca	21.57959001	3.22652597	16.61433712
Ca	26.85955643	6.23851461	16.75155051
Ca	16.21270147	8.02599421	15.41711020
Ca	14.24745421	4.84846214	15.20896837
Ca	25.05112575	9.62847103	16.30965303
Ca	15.13863794	10.72137235	18.03309884
Ca	17.23938902	20.17790148	15.47126528
Ca	15.55683287	16.96805655	16.37713723
Ca	28.96749810	22.52734078	15.75874073
Ca	17.43730816	22.90632482	17.48228379
Ca	18.73063435	2.09351779	14.68129907
Ca	19.63639883	23.50321937	14.50104696
Ca	15.29144374	2.02052227	17.01034227
Ca	17.62472229	4.88992574	16.48263760
Ca	10.71507027	19.15357257	13.29339532
Ca	5.73688269	6.49801192	20.12994570
Ca	6.26589887	11.19820444	11.70845278
Ca	6.49119931	15.39349167	20.34059950
Ca	12.73597669	12.47838182	12.78882000
Ca	6.90644664	3.02794697	21.34259943
Ca	8.55539109	5.58756485	11.89749865
Ca	10.75388337	11.33219741	21.39362875
Ca	26.89133141	3.95787649	13.22165488
Ca	9.45140243	2.13061578	23.34722589
Ca	12.59334873	22.13564660	12.98190198
Ca	13.80436355	7.69543485	22.15198773
Ca	8.85716479	22.22610477	12.59293907

Ca	17.68972969	15.43969571	21.34974957
Ca	2.46994834	15.82010699	14.31727509
Ca	5.99960718	22.25531085	21.46712096
Ca	20.71950691	17.14241189	12.16870698
Ca	16.79323276	11.68577719	21.55103933
Ca	18.62271638	14.44056212	12.74250405
Ca	20.40940216	19.06929764	21.45624693
Ca	25.78237738	14.68259095	12.22938086
Ca	19.87712923	5.22173492	19.05584405
Ca	21.47593229	6.97167801	11.09934522
Ca	22.72445099	12.17223559	20.65793161
Ca	12.12273611	6.16421690	11.83244587
Ca	26.27319311	21.93079174	18.68613183
Ca	23.77918782	1.03131745	11.22992308
Ca	23.31578303	6.25910448	17.96104906
Ca	17.94216978	1.01058398	11.39898082
Ca	28.55130805	20.33257545	21.02534281
Ca	17.00735192	17.46804443	12.93502407
Ca	16.17976644	0.66785198	20.64554748
O	2.60363477	10.82561234	13.18275176
O	7.23252721	17.54252740	13.86614447
O	6.37141208	10.96543081	18.66401771
O	11.82770682	23.32640563	14.73811218
O	4.94347585	5.12286991	13.33462120
O	8.89853843	12.25331232	14.36450445
O	8.02828745	6.13116327	18.74708577
O	13.07807741	18.77726652	14.22448239

O	12.06939232	12.16278236	19.26318335
O	11.99404345	5.93137370	14.28128142
O	15.73757339	23.88656411	19.63295503
O	2.72590652	4.57115920	19.02845248
O	4.62217575	22.81531554	13.48192025
O	2.29019434	17.50460319	16.72970339
O	8.14129258	23.21830204	19.33140945
O	16.13231788	12.77295005	14.06994278
O	20.34747100	18.57922606	14.36530454
O	19.85384045	12.45682184	18.30947257
O	20.00062444	0.71840381	12.66809591
O	24.22857242	19.38176009	18.14620690
O	17.73478747	6.94499548	12.73551620
O	21.10316997	14.06185038	13.56006138
O	25.76311141	13.79303200	17.26479123
O	25.45668168	7.42475825	12.51943751
O	25.02273653	1.87887670	17.10824522
O	15.86199435	6.24283326	19.10734710
O	16.49686171	18.90605758	19.03529399
O	17.67615282	1.01000284	18.60083713
O	4.44161845	12.05242000	14.72268145
O	2.50093165	13.45987217	13.69707648
O	6.72428282	15.28751080	15.04635894
O	4.64411763	16.75771124	14.51695060
O	8.00965040	12.52662962	17.39206867
O	5.51455166	13.32035603	17.33269025
O	6.31467750	9.21428154	16.67715293

O	4.07486712	10.23166933	17.41100652
O	8.16950870	18.90938566	15.92594563
O	5.90349889	19.79802686	14.59345760
O	10.73371030	22.26943457	16.81624679
O	9.09191143	23.08078929	14.67178752
O	5.09762036	7.47412304	14.37348554
O	7.30637682	6.12649618	14.29708038
O	6.86139499	10.63478959	13.92043819
O	9.30424169	9.70230690	14.73361666
O	8.65267653	7.60535557	16.70865717
O	10.69584230	6.66644133	18.22904607
O	7.14087527	4.37876333	16.88598327
O	9.16602415	3.64240097	18.59110506
O	9.48056584	14.87310875	14.14914489
O	11.42837595	12.98672183	14.67460820
O	10.89757449	17.90595363	15.31762620
O	13.22592686	16.55870287	15.92613239
O	12.30217301	14.46758902	18.06138035
O	27.97045528	11.43859508	16.36909020
O	10.52921370	11.18356192	17.34563535
O	12.91029881	10.15716859	17.55743425
O	7.71397133	1.55111106	14.59084225
O	9.85799564	0.86830793	16.29307514
O	9.62442561	4.84937722	14.36845748
O	11.65720777	4.03504925	16.14363036
O	4.29118189	23.21200798	16.80329170
O	11.70844315	2.15713466	18.96125779

O	15.14895344	22.06863693	17.77992862
O	13.09370758	23.22036655	18.96416380
O	11.63729877	8.27550278	15.48226981
O	14.06660463	7.14309420	15.42095728
O	13.78697199	11.78494610	14.95893510
O	2.62162192	8.73885038	14.82216142
O	4.73295665	5.79730142	17.85838892
O	2.52684056	5.18511072	16.43092249
O	2.50045567	2.23119010	17.85244643
O	13.35790787	5.58838148	18.15443534
O	14.00772264	21.25797273	14.44032947
O	15.08197790	19.32394955	16.00418655
O	3.44161750	20.58351627	16.43615187
O	3.54634405	16.42166226	18.82009237
O	5.24392903	18.11735307	17.61716773
O	3.14403177	14.94441649	16.65106931
O	14.37863086	17.55278432	18.66444723
O	1.35776749	0.74057784	12.44627611
O	3.02870937	0.54649033	14.65732905
O	2.69809560	3.77040205	13.55927820
O	4.69619815	3.21881227	15.25362335
O	7.27777388	0.33629949	18.88954978
O	5.06653484	1.01061575	17.46529049
O	8.98709446	20.78926378	18.50876511
O	6.88896435	22.12824569	17.25490340
O	18.13827177	13.92994785	15.18139948
O	15.63740442	14.66863357	16.00859282

O	19.91636286	16.82336403	16.35659913
O	17.70977048	17.96686122	15.24485823
O	21.03421889	14.79486814	18.43214742
O	18.66477280	14.59854126	19.40222266
O	19.26345641	10.15636640	17.26741454
O	17.31653076	11.85424878	17.69137049
O	20.04796315	21.21560419	14.81327627
O	18.57762651	19.78183162	12.96400698
O	22.07432702	23.83026861	14.81837095
O	21.32440675	23.08546645	12.36234361
O	24.05684142	19.23697128	15.40702578
O	24.51478017	21.60867848	16.68393262
O	22.26866559	17.45946625	18.28778877
O	21.81387795	19.71325514	17.05340259
O	18.53156108	8.67761759	14.74757133
O	20.30530959	7.46925654	13.11034895
O	20.57148552	12.24039192	15.39884442
O	21.99671099	11.38605479	13.18243164
O	22.34395072	15.19960946	15.71059475
O	23.82177741	14.20520141	13.55600893
O	26.94115707	15.34444297	15.40774789
O	14.45496982	12.98874942	18.14789354
O	24.17729655	11.77800111	16.52089794
O	25.63071104	11.51189719	18.73833887
O	20.92550919	2.68777845	14.21137242
O	22.64691757	0.67294750	13.40406150
O	22.85282347	6.65754085	13.02437671

O	24.82380894	4.85559194	12.59493353
O	13.22222677	0.73747716	17.26865067
O	26.50649067	3.03079654	15.40707480
O	27.42487215	23.48764859	17.19473288
O	22.50100289	1.20201441	16.88423191
O	24.38185403	9.41386997	14.06220566
O	26.91009654	9.48572674	13.32891354
O	26.14982772	12.71950908	13.03660107
O	16.09595375	10.30163843	15.03839811
O	17.79437718	7.00496862	17.34299093
O	15.64095199	8.48660073	17.62529901
O	15.44208299	4.31193005	17.26073283
O	26.59922753	8.27102533	16.59219825
O	28.72451964	23.96293382	13.71732800
O	19.24173623	19.11994530	19.40874985
O	17.98083153	20.65922283	17.70230582
O	16.68506866	16.36200741	18.30458440
O	3.40595915	19.12404613	19.41562242
O	16.37130010	5.65331861	14.59346370
O	18.59410815	4.49494445	13.78098096
O	19.79104103	1.81146303	17.10390905
O	17.44054018	2.56020678	16.42982903
O	21.64949068	22.81397335	17.48113834
O	19.37761788	24.09344331	16.66161564
O	4.34875926	12.31538959	11.99190583
H	1.99565867	13.78843588	12.89717208
O	5.98445767	15.75159125	12.37953214

H	6.47552067	14.84974269	12.28969241
O	6.76608182	13.32366160	12.44518739
H	5.79052980	13.33019027	12.27861382
O	27.98117559	15.41486384	12.22038471
H	28.54628431	15.51471460	11.44100634
O	6.74696176	13.26477373	19.76965502
O	5.53202056	8.47638156	19.11643010
H	4.53722879	4.64857993	22.01254210
O	5.49681574	4.78531076	22.07919229
O	2.33286177	7.12640533	18.29171255
O	8.28257028	19.78871132	13.26675556
H	7.79319412	19.48640610	12.47850609
O	10.73188864	21.05490434	14.43169496
H	6.99503110	22.43777821	10.98048019
O	7.56660973	21.74441925	10.52040880
H	6.95750407	21.12661724	10.09190078
O	12.44463207	20.19007424	17.61663653
H	12.12243129	20.15461798	18.58123883
O	11.58107188	20.25786070	20.07497329
H	12.32342426	20.19294258	20.68893892
O	9.78583965	15.66591053	17.54588685
H	9.68520653	16.47027537	18.11696547
O	7.21368019	16.22018038	18.30110956
H	8.05231618	15.74847875	18.09046232
O	9.49043743	13.31602347	20.51949901
O	6.44065803	6.86537385	11.91871294
H	5.78138179	8.18097823	11.42486568

O	8.84443731	10.69464351	12.15684767
H	9.36464357	11.50582543	11.94926058
O	10.03181010	7.33688326	12.30268846
H	9.81639676	8.21397025	11.94942627
O	5.32561664	9.08329338	11.18376771
H	4.37831933	8.92789053	11.35999274
O	9.01387284	8.62023929	19.04838319
O	6.59160656	4.09961675	19.40111391
O	23.56165309	3.16795587	20.59589110
O	5.21948542	1.54611294	20.07336180
H	22.98878765	2.86611357	21.33366834
O	10.35735385	13.11901125	12.28895410
H	9.91936764	13.81832468	11.77566044
O	12.05823348	16.56171894	13.40342004
H	12.68731363	15.75046474	13.25131501
O	13.63208914	14.53374484	13.26688828
H	14.54951594	14.86738548	13.23293929
O	17.11500622	13.05778860	11.19540715
H	17.38599644	12.13748060	11.04432713
O	13.41446689	14.00106202	20.51476009
O	11.10948647	9.83709001	19.63761750
H	9.92454791	9.02311803	19.35449886
O	10.45135770	9.42958048	22.74213866
O	13.41490494	8.35079074	20.08122246
H	12.58463731	8.87181444	20.15563860
O	10.19856469	0.74430281	13.63763332
H	10.40934883	1.62371981	13.25921093

O	7.27187414	3.64328290	12.15395378
H	6.54637712	4.14506038	11.74015795
O	11.64416325	3.29700311	13.62895683
H	12.50525074	3.59313384	13.12323734
O	14.42010062	1.55531782	19.40361779
O	14.76139916	21.47209180	20.28666825
O	13.00590862	8.07057040	13.11003142
H	12.50858972	9.02556126	12.96575255
O	11.90606016	10.30426830	12.88916165
H	11.01513896	10.10193233	12.56227300
O	2.48775448	8.27076193	12.29311933
H	1.86704219	8.21914655	11.55034678
O	27.24375417	5.93236249	14.29213509
H	26.66664223	6.60451952	13.88707464
O	26.82770332	3.70414256	18.07389885
H	26.50867520	21.24663382	23.24281583
O	16.30912188	7.93660901	22.15240089
O	15.65391323	19.25424926	13.47120561
H	7.43965073	0.56332050	12.91575729
O	10.54699021	24.16210052	12.14668857
H	7.21597699	0.53449767	11.39624070
O	11.07518263	20.92094894	11.70121014
H	11.10519192	20.80291524	10.73990960
O	5.55522631	17.62931412	20.15050997
O	16.02819834	17.02896528	20.89311582
H	15.29339687	13.92150073	20.74967120
O	6.99288736	23.49038061	12.36962679

H	24.76822390	3.24398231	12.26386259
O	4.97841960	2.43615263	12.75547244
H	5.90929206	2.71373446	12.46426989
O	25.15711841	2.34477198	12.43316711
H	23.88502775	4.28372973	13.91328440
O	6.58205247	20.92931534	19.56443520
H	19.95532768	15.91456919	24.09996550
O	3.94924184	21.05296386	22.21929927
H	4.38451538	20.17698348	22.30846498
O	16.53020804	15.32740839	13.54749618
H	16.41281238	12.95024334	11.87183337
O	19.19695585	16.43183710	13.71855247
H	23.90266758	16.93179693	13.12441867
O	20.69236542	13.27137322	20.73033395
H	24.03510611	13.85183571	22.74754246
O	18.43741876	10.64027836	19.85252300
H	17.97562945	9.73629810	19.74545620
O	20.92964485	7.26545700	18.81677971
H	20.65754293	7.99733888	19.39321977
O	15.33240251	10.63503736	20.29091410
H	14.71576269	9.88770880	20.43463394
O	17.45509967	8.21312699	19.70751659
H	16.95516974	8.10387090	20.56557244
O	21.18101282	20.33162848	12.51534673
H	21.31181981	21.33267432	12.36064110
O	23.71595399	22.27297972	13.47368929
H	29.07186033	24.27352565	9.76910390

O	17.78028936	2.89148135	10.36886127
H	17.88268396	3.34838394	9.52639822
O	26.39341959	19.65636184	16.59153470
H	5.44180737	10.78232222	22.28572372
O	22.05821037	19.78313659	19.71291856
O	19.69846663	16.88387844	21.10899419
H	20.28924582	16.25840649	21.57151863
O	23.46553490	14.11979199	22.00258891
O	18.63990379	9.42514858	12.21525721
H	18.70647667	9.14675819	11.28729954
O	19.42583266	12.11721466	13.03775889
H	19.38332613	11.27133038	12.54208773
O	22.34884604	9.08225363	11.17813788
H	21.94712961	9.92976369	10.93672476
O	21.78856151	9.27394507	15.92835331
H	22.45057251	8.79332716	16.50407673
O	22.12795964	6.25542709	15.91813236
H	22.69022689	6.55489193	15.18167145
O	19.96463197	5.03806113	16.44962199
H	20.76145030	5.60989400	16.29264755
O	23.50884603	3.83752031	14.73489861
H	24.00397875	4.31726993	15.49892786
O	21.95770950	4.37349527	18.58522826
O	18.39172971	3.62416517	18.65881121
H	22.44718356	3.95868018	19.32464614
O	22.38748791	16.50154737	13.46916907
H	22.03111955	19.36063016	11.02554671

O	24.89283411	17.16297207	12.96663212
H	24.88170491	18.00407526	12.48613614
O	22.03402218	18.51083273	10.52800262
H	22.93888417	18.36513794	10.21432560
O	28.26042698	18.09697543	14.07517836
H	28.19246012	18.39039701	13.15407764
O	25.10425908	16.41675557	16.96781153
O	23.56923858	13.19443889	18.73384174
H	23.27088817	9.07937675	18.44019350
O	22.23944050	10.43981760	19.25996409
H	21.60922116	9.82277103	19.65838279
O	23.67344911	8.47993149	17.77090371
O	21.83862472	2.36930550	11.62401038
H	21.48035499	3.39024954	11.49278534
O	20.90101844	4.70265830	11.48083545
H	19.98723197	4.45588548	11.25376563
O	23.85229294	6.45352118	10.59840706
H	24.36571684	7.16226998	10.17958776
O	24.79671087	4.63495743	16.80560883
H	26.10240482	0.78192516	24.52592907
O	23.78626424	0.88585188	19.26648984
O	24.52619103	23.35111533	19.26477850
O	4.88315898	23.28925658	19.78602224
H	4.03197210	23.65645725	20.06883462
O	24.95262657	9.82517886	11.48047245
H	24.02619237	9.50464024	11.22721148
O	24.42645682	13.66666858	10.66377759

H	24.65542280	13.41366865	9.76054780
O	14.87231696	11.04296018	12.66158840
H	14.58054431	10.12265231	12.53729087
O	10.52259963	4.91333387	10.80625195
H	10.61580805	3.95865718	10.68012826
O	14.69735429	4.10362765	19.92862378
H	14.50954415	3.12971511	19.76554968
O	0.26368138	0.33844310	25.03732670
O	26.69019038	22.95216963	11.18217311
H	26.49902069	22.43266277	10.38958715
O	27.42627178	21.33444005	14.44451981
H	27.11815125	20.63412098	15.04989725
O	29.43820978	23.16046032	11.26275643
H	28.49270625	22.83379635	11.30689675
O	25.31056650	0.67453168	9.26625498
H	25.91606412	1.36024366	8.94374300
O	17.40147814	22.48181081	15.03423962
H	16.55733374	22.78432955	14.66293854
O	17.55212690	20.86177860	20.43727371
H	16.58597936	20.95420918	20.59212264
O	26.79088982	19.85420084	19.62857773
H	26.09297835	19.19075871	19.51482224
O	11.30239798	14.20137448	24.66185564
O	16.25859119	13.78633447	20.65765719
H	13.15758852	13.34791433	21.28015419
O	14.18397576	2.42117488	15.03369267
H	14.19400249	2.39153940	14.06620848

O	16.77944361	1.34608940	13.32896845
H	16.17480505	2.09895143	13.43008732
O	16.54184374	4.70870346	12.00308079
H	17.05506148	4.05373418	11.43761839
O	13.64892974	4.51322367	12.66597412
H	14.49896591	4.32256344	12.23185838
O	19.48616242	23.03524874	19.03561829
O	21.37729836	21.26653715	22.22935845
H	22.19042404	21.36817006	21.67007231
O	16.01361589	2.35428126	22.22227614
H	15.19198181	2.81133416	21.97937314
O	1.31135174	2.70017723	20.29267185
H	0.59864818	3.30898432	20.66481082
H	29.01287083	19.45830475	25.22387988
O	25.23284603	8.55121531	21.41542707
H	26.15892473	8.50290693	21.76419889
H	24.64791384	8.48182370	22.20387517
O	28.69317120	18.58349388	25.55065663
H	2.64033103	17.92901313	25.01552483
H	4.05294933	24.18203850	24.36721736
O	9.63475869	19.51479151	21.62681209
H	10.38549321	19.83301906	21.00225210
H	10.12193049	19.10568939	22.36100852
O	7.86820988	21.20085426	22.66320623
H	8.54956546	20.62612361	22.18255238
H	7.60394834	20.62414396	23.41914917
O	28.66137035	21.66908686	18.96627415

H	27.47758969	16.21511362	21.07053345
H	28.76755459	22.58301208	18.64649254
O	5.24994708	18.57599034	22.59889564
H	5.99418713	18.77724838	23.21520164
H	4.69376567	17.89814476	23.06565906
O	19.49011769	11.44754453	24.22917991
H	18.81595023	10.80612926	23.87190888
H	20.35385070	11.16276995	23.87806222
O	23.61944810	12.58355615	24.58818115
H	23.34978097	13.34522663	25.14931564
H	24.45660239	12.21917174	24.95809144
O	25.93551138	4.37916541	21.11116419
H	25.88215261	4.75399462	22.01691322
H	25.04680725	3.95360068	20.94128115
O	2.61458095	12.58871822	19.40999838
H	1.96414456	13.28070068	19.61540218
H	5.61667242	14.65888801	22.96948388
O	4.95378359	14.75050351	22.21979049
H	10.40374992	13.28220077	23.82729249
H	4.68495933	13.81483794	21.98282160
O	3.26670061	0.73609928	21.70534285
H	2.49483356	1.18599044	21.31444211
H	3.49212858	1.26197950	22.52240867
O	14.35948886	17.21826665	24.44994446
H	13.54836939	17.59744050	24.02424676
H	14.07578324	16.34424911	24.82833916
O	8.71496138	4.10527806	22.43135214

H	9.38262794	4.48965463	21.82637611
H	23.63528801	2.35585857	20.02118620
O	2.57636743	9.49058459	25.55027171
H	3.51043818	9.17449137	25.47468260
H	2.48904896	10.12912375	24.80960327
O	9.19739217	3.23485488	25.55387271
H	10.04043374	3.38272623	26.02018878
H	8.88767403	4.15337653	25.32031250
O	8.07788750	10.43533028	20.95374708
H	7.48795594	10.74049700	20.21832372
H	8.28748850	9.52087324	20.65310156
O	9.97938120	18.09855580	18.50117136
H	18.47873825	15.94527861	24.59842250
H	10.16812837	18.53608908	19.35179756
O	15.85505459	2.22551889	24.74886575
H	15.91993541	2.26923031	23.68583921
H	16.72977322	2.54932098	25.04382546
O	1.35476786	8.61577910	22.29321818
H	1.68800622	9.52310816	22.54956924
H	27.81156341	8.13345799	23.14859679
O	8.87663756	1.42521123	21.25113720
H	8.53805573	0.50987895	21.29820939
H	4.48040141	1.20953539	20.64901987
O	11.27177873	4.97351917	21.10579400
H	11.65791947	4.31069297	21.70555389
H	11.37517269	5.87370342	21.61440610
O	14.57974576	5.37526460	22.28874634

H	15.56235911	5.28433865	22.37103722
H	14.41952722	4.89061339	21.42574420
O	9.77788431	12.65867760	23.26046967
H	10.31617720	9.49038021	23.71051170
H	9.50831011	13.19520333	22.48128648
O	12.40978011	16.49290927	20.66503289
H	12.73068855	15.55115522	20.74621164
H	8.54977555	13.05171258	20.36992322
O	19.32991877	16.41944184	24.66861045
H	5.41992122	18.08390137	21.02936654
H	13.21305830	17.00538453	20.86175293
O	10.97697411	22.94292277	21.63720268
H	11.66893029	22.35566610	22.00154727
H	10.38165358	23.14498684	22.40599855
O	6.78597749	1.67447520	23.48462673
H	6.54453167	0.68511037	23.58543586
H	6.04224985	2.10928362	23.94787553
O	18.52655601	3.48981007	24.81920149
H	19.00204274	2.72260528	24.40871600
H	19.07027770	3.77409009	25.56793141
O	13.75933199	9.89600560	23.11390542
H	16.77312267	10.11698631	24.00963981
H	16.81969262	7.18054772	22.48802565
O	11.62845198	7.12605109	22.52180644
H	10.87888661	8.50082603	22.58237816
H	11.32599168	6.82751101	23.39747043
O	22.71678977	5.12081866	23.10613397

H	22.01580977	5.71908279	23.44261813
H	22.82298008	5.46786475	22.18135224
O	25.14899997	22.54730051	22.82190779
H	24.60126876	23.22305931	23.25458975
H	24.55190960	22.09669080	22.16122837
O	15.30162567	12.71675994	23.40191450
H	14.35367592	12.57674124	22.99237900
H	15.31736844	12.14452271	24.18825027
O	16.69308511	15.40440417	23.63715506
H	16.30254112	14.50459149	23.66289588
H	15.93245976	16.01030598	23.75257898
O	10.12522764	0.07008908	24.37478484
H	14.12115330	21.43587290	21.03340034
H	11.02111825	-0.11845600	24.69543617
O	20.82223536	23.90126359	22.30463473
H	21.03366018	22.93357589	22.17323820
H	20.33751055	23.87699343	23.19137713
O	24.94085930	1.81716911	23.33544538
H	23.95235065	1.87567606	23.31943035
H	25.22667666	2.73500189	23.47755292
O	17.37929632	9.96959645	23.25989918
H	14.22212900	10.03603652	23.96104394
H	16.73544427	8.78355431	22.61418362
O	25.68813987	15.41166826	24.44631710
H	19.53680890	13.26104982	21.74841016
H	24.77711898	15.29646029	24.82220049
O	18.70804614	13.32236473	22.37087144

H	19.01238053	12.84633255	23.18783245
H	25.99344777	14.54401346	24.13057669
O	27.37192366	22.61543960	21.25239700
H	26.65407748	22.91168300	21.85467002
H	28.00089993	23.35050224	21.14513387
O	7.29565477	23.49093359	25.56286356
H	8.19308678	23.50443634	25.05450018
H	7.20922007	24.35335709	26.00081317
O	20.38324380	9.22236028	21.40940566
H	20.81963966	9.95485786	21.88371301
H	19.63468616	9.66665434	20.94820953
O	19.69320484	5.11820700	21.41427654
H	20.03100043	5.77192697	22.06301239
H	18.78062101	4.88572259	21.75146176
O	9.18808673	18.29970864	25.77234144
H	9.52968560	17.59491128	25.17071355
H	9.97356516	18.83815321	26.00493838
O	15.39404312	10.03173405	25.55519483
H	15.00422700	10.68960465	26.16676763
H	14.92821352	9.18117046	25.69401819
O	1.49363901	4.64496505	24.81844259
H	0.52718312	4.56910326	24.70858136
H	1.83304716	4.65631709	23.88687233
O	2.33888470	2.08680753	25.92586565
H	2.00620425	3.00336241	25.81749171
H	1.55824960	1.51798316	25.71541600
O	23.75115742	21.40591556	20.81154930

H	23.91794026	22.20368569	20.19068908
H	23.16585110	20.74535059	20.28761443
O	22.17655841	11.03045897	22.89583030
H	22.59593743	11.63698820	23.57201760
H	22.62933526	10.16679498	23.08910857
O	22.21754041	18.16876227	22.82084066
H	22.08832895	18.54162546	23.74975846
H	23.12466744	18.41120234	22.50245861
O	27.16843416	20.52675535	23.18613477
H	26.74272363	19.76370098	23.61452562
H	24.65493798	0.75802204	19.72383796
O	13.77026163	14.54148201	25.18543169
H	14.22348363	14.13526625	24.42328450
H	12.72956567	14.41249464	24.95414728
O	18.44216585	7.87370896	24.66271797
H	18.49232193	8.18314665	25.57948209
H	18.11664328	8.67848357	24.14805690
O	11.56067132	22.34530688	24.88886041
H	11.90328202	21.88184548	24.10066738
H	12.69286964	23.58090389	24.71927426
O	25.01607376	11.43520405	21.26976516
H	25.12188873	10.46294774	21.38055974
H	25.38140973	11.55564977	19.71200808
O	13.08301594	21.06651786	22.59461610
H	11.00547668	13.89525373	25.53566691
H	13.92443216	21.20206873	23.11280412
O	27.02347170	15.41181130	20.73351923

H	12.78447960	20.14796322	22.79396207
H	25.42554347	15.81404432	20.48042384
O	6.15769336	10.36578978	22.81484539
H	6.92942405	10.37334041	22.16606664
H	24.82256675	24.10097013	19.80344929
O	8.50717841	15.41673304	21.64220120
H	9.02344530	14.60996584	21.20306856
H	8.19515368	15.12199676	22.52503705
O	9.41178739	23.35920015	23.99234855
H	8.89659219	22.67978786	23.51032847
H	10.62008155	22.73672764	24.57462243
O	23.32013369	8.55546337	23.48453278
H	23.87611566	8.62553892	24.32122411
H	22.54203422	7.99399817	23.66804693
O	3.74027935	16.68665817	23.85224287
H	4.42380250	16.64969117	24.58664553
H	3.91931279	15.87923249	23.30934840
O	27.49741463	15.61267163	18.07676094
H	27.24319832	15.42933771	19.76114612
H	2.10496863	11.72557698	19.46088429
O	14.38542119	12.45522476	26.81535697
H	14.18116118	13.28464249	26.27581154
H	14.86985819	12.77441639	27.59190647
O	11.51141580	11.90693415	26.96625554
H	12.48310739	12.03189836	27.02582823
H	11.20101804	11.93108099	27.88386397
O	2.26665330	11.09232219	23.04038961

H	3.04052249	11.43472822	22.56461763
H	28.03183399	11.75071835	22.86112176
O	7.52889504	10.15074921	26.44937938
H	7.42329417	10.95813861	25.89901521
H	6.81457364	9.55223737	26.15055959
O	13.35440774	0.66402277	24.06884153
H	16.98697017	24.42021865	23.33857092
H	14.08059937	0.98782237	24.63146838
O	13.19341869	6.18756103	9.48730060
H	13.99928787	5.64467899	9.49916219
H	12.49950829	5.60846979	9.11934874
O	27.82582648	10.29114415	19.33763660
H	27.64025304	9.76235715	20.12870675
H	26.95939473	10.71802700	19.03930259
O	26.72088532	12.58585856	22.74049767
H	26.95651429	13.43267028	22.32846781
H	25.74521947	11.92201896	21.88551519
O	8.47794713	5.65838577	24.38587621
H	8.56189670	5.06964060	23.51265446
H	7.50912558	5.79425060	24.52656908
O	3.38426083	21.19047163	24.73325178
H	30.06589071	21.14406591	23.68114966
H	29.31405151	21.92586377	24.89014728
O	15.48358719	21.25358238	23.78195941
H	16.09330387	21.99691956	23.64445808
H	15.88756794	20.46909779	23.32581403
O	7.03719553	7.53572213	21.99141664

H	6.74932382	8.37511237	22.38899342
H	7.63583421	7.11558118	22.63347710
O	22.58093287	21.46437191	24.51790630
H	23.52123630	21.30797489	24.34423773
H	21.80360319	21.32719834	23.17829966
O	28.23217817	17.83808214	21.85782302
H	27.62235764	17.80035095	22.64506381
H	29.06009976	17.45987335	22.20023562
O	24.44391501	16.01488742	20.36921530
H	24.37199814	16.95966492	20.61955557
H	23.91821565	14.85186589	21.49793765
O	25.97196864	0.74095003	20.89843898
H	26.66574652	1.35531920	20.55308961
H	25.64972010	1.16963204	21.72795540
O	14.61785641	4.71316816	25.03551977
H	14.43697905	4.79965620	24.07055720
H	15.06948511	3.83346256	25.09518540
O	25.05448979	8.88655892	25.48137445
H	25.83880094	8.29789504	25.42556058
H	25.42678110	9.78568299	25.32654036
O	11.67382961	19.84282629	25.93658623
H	11.55910860	20.81151550	25.74559503
H	12.59613269	19.74975645	26.27493471
O	17.27423444	4.64456846	22.51920502
H	16.88377598	3.72077676	22.29267032
H	17.59924207	4.51996892	23.43464323
O	13.96931066	7.53161671	24.96574926

H	13.01137301	7.44466673	25.12918123
H	14.34172003	6.66317357	25.22911378
O	5.26124081	8.61836975	25.03773197
H	5.37577901	7.66761174	24.77738843
H	5.50292582	9.13079083	24.23991799
O	12.84118111	12.37458283	22.44561688
H	12.38495015	12.84985902	23.16590767
H	13.37616317	10.78262923	22.85694774
O	22.27595281	23.62846610	25.70580954
H	22.45277043	22.66674940	25.25548592
H	22.58302322	23.57896806	26.62212307
O	16.25248204	18.77755421	22.81695086
H	16.15437818	18.19104118	21.97394532
H	15.73101694	18.27885558	23.47671212
O	17.53462798	23.42970593	21.63749868
H	17.79889556	22.51588043	21.38644839
H	16.79060011	23.61302288	21.00649365
O	23.07930043	15.14178165	25.33682748
H	22.63826940	15.72888445	26.01316004
H	22.48844971	15.25260558	24.55554678
O	22.97420532	6.53520584	20.66135506
H	23.60252655	7.27030178	20.79621600
H	22.17568979	6.93504450	20.22630828
O	22.20970617	2.35463450	22.96667161
H	22.11749170	3.31754462	23.15058020
H	21.34066735	1.93335206	23.16443554
O	5.69469270	20.92908110	26.37166288

H	4.85666967	21.13347703	25.89061683
H	6.19541008	21.76731659	26.41557412
O	4.63748210	12.25465679	21.25518386
H	5.45621424	12.46466512	20.70447783
H	3.90695181	12.31168497	20.58363718
O	11.93192370	4.36901603	25.77713038
H	11.55330188	5.28311530	25.76374087
H	12.90883897	4.48954929	25.73077305
O	18.99549481	7.06783422	10.22066708
H	18.40685363	6.84530965	10.99158047
H	18.53760962	6.72747508	9.43862430
O	10.28341969	16.49249672	23.85476965
H	9.85382587	16.28381677	23.00236639
H	10.67096336	15.60401084	24.20398542
O	24.63665895	18.64101002	21.63582217
H	25.37192556	18.56678446	22.27003340
H	24.71805100	19.52682982	21.22507778
O	21.43371386	15.55811707	23.05080228
H	21.86954434	16.43777425	22.91650131
H	21.97761511	14.90428488	22.54637549
O	25.38445374	5.24944381	23.84553617
H	25.66412432	6.16523732	24.01926406
H	24.39813618	5.29113308	23.74112882
O	2.52946999	4.65435541	22.22289468
H	2.68791480	5.49208294	21.69544093
H	2.27394557	3.99838984	21.54719918
O	19.63961793	23.75556048	24.73784827

H	16.22141898	0.47552043	24.88851200
H	20.45405219	23.63056639	25.27827824
O	10.09989994	9.49700802	25.70310637
H	9.16254059	9.67114161	25.99520914
H	10.62552338	10.22497597	26.09087582
O	6.87952819	14.74988177	24.01465404
H	6.68664499	15.29348990	24.80340446
H	7.04486428	13.80552941	24.33063264
O	25.62365883	6.45394684	19.03520738
H	25.87659954	5.87591416	19.78630121
H	25.75585316	7.37606477	19.31653283
O	3.26116790	6.93233105	20.81726845
H	2.83943322	7.08233421	19.89494809
H	2.89020835	7.65999647	21.35782499
O	12.03422347	18.56995750	23.55529662
H	11.84269294	19.00334702	24.43433798
H	11.44930211	17.75952351	23.53983752
O	19.69784169	1.14574976	23.70779614
H	19.58153325	0.55960054	24.51129821
H	19.07215015	0.74827293	23.05602005
O	3.99626638	2.35267112	23.78368801
H	3.82217908	3.24956927	23.44491132
H	3.38840372	2.23343832	24.56989674
O	5.45945750	23.08258256	23.71579849
H	4.93825749	22.35501310	24.10882217
H	6.17275507	23.29511763	24.39888753
O	14.49533654	19.45324632	26.29973322

H	14.55978429	18.62557749	25.77536685
H	14.93844806	20.12524790	25.75314275
O	7.03856404	19.31430931	24.60241443
H	6.59124851	19.88883660	25.28172550
H	7.90470698	19.00589957	25.02645177
O	27.45648299	7.47435926	24.88704882
H	1.55455160	8.16810575	25.23458080
H	1.31123822	6.59777719	25.07607918
O	4.33142719	18.37139536	27.63109252
H	4.77514371	19.23811742	27.58843133
H	3.48045953	18.50599011	27.16670754
O	5.68574270	16.89099813	25.70327931
H	5.26603598	17.27105162	26.52067735
H	6.22948584	17.63633076	25.36755907
O	11.79888694	2.89455988	23.40881753
H	12.44163291	2.16092266	23.56778483
H	11.86965013	3.48412418	24.20876439
O	21.54966771	19.24059037	25.18838251
H	21.99586807	20.17129191	25.04737374
H	20.59891681	19.41081068	25.06566793
O	18.94233192	18.97246016	23.47814830
H	19.06861353	18.07981883	23.88923895
H	17.97201585	18.97525533	23.26257748
O	7.42818146	12.23737428	24.51826933
H	6.90985317	11.64698172	23.91487681
H	8.34104366	12.27842565	24.10900021
O	20.69096784	7.13975348	23.26147500

H	20.56536759	7.82191950	22.55322510
H	19.94202242	7.34962261	23.88833016
O	5.71157849	5.91780788	24.36456739
H	5.60318080	5.45580567	23.39921859
H	5.28913704	5.31291601	24.99220157
O	21.52379255	16.83243467	26.74812922
H	20.65653558	16.58100746	26.37711536
H	21.66180505	17.73515810	26.38287929
O	26.46767945	17.89367004	23.93594194
H	26.13334267	16.95959645	24.09757482
H	27.08166234	18.07520557	24.68940364
O	10.70266437	6.79915571	25.40856011
H	10.53004838	7.73011490	25.68668478
H	9.83079774	6.47547237	25.04695783
O	18.67692938	16.41754324	11.19080310
H	18.15699403	20.53207429	12.51537260
H	18.46792280	16.31757982	10.25005659
O	26.13439753	11.51230347	25.04281491
H	26.80389936	11.70377811	25.71661954
H	26.42627680	12.00645934	24.20020824
C	13.85571743	14.84299070	10.60354561
O	13.11848962	13.93426976	10.43477737
O	14.59911821	15.75027054	10.66084878

2-TS

Si	3.54407854	12.17786390	13.35841998
Si	6.07506351	16.28777416	13.91048375
Si	6.63303150	12.59261682	18.27318144

Si	5.46233404	9.65632095	18.04766580
Si	7.28913053	19.03482374	14.57908378
Si	10.43026190	22.43170938	15.26401041
Si	5.98267909	6.50329570	13.41792922
Si	8.47092723	10.71988731	13.83013142
Si	9.20096007	7.20405424	18.18113383
Si	7.81516546	4.48372067	18.38138009
Si	10.03531578	13.42465185	13.97795256
Si	12.36315219	17.35179633	14.80929777
Si	13.14331444	13.41079430	18.98112299
Si	11.67748212	10.74400294	18.41947456
Si	9.04328793	0.72667192	14.91957290
Si	11.14569337	4.52383953	14.69765691
Si	12.93522304	1.14908322	18.84963564
Si	14.61190097	22.74534748	19.16923408
Si	12.71032144	7.45476835	14.63646587
Si	1.97965530	9.37535961	13.50000774
Si	3.10671701	5.80264628	17.83964682
Si	1.73512443	3.29772012	18.76262937
Si	14.47070058	19.67630904	14.50163441
Si	4.35471247	17.91023038	18.95139374
Si	2.45851763	16.11004522	17.53047112
Si	5.79849989	24.12249607	13.23019909
Si	4.31175017	3.64353037	13.69605273
Si	5.69336860	0.45954113	18.85667859
Si	7.66815447	21.71549188	18.61089945
Si	16.59409730	14.23917417	14.78448132

Si	19.19848404	17.36870650	15.03698615
Si	20.08738243	13.80710657	19.33811238
Si	18.69351969	11.25029982	18.29637034
Si	20.06934312	20.07246111	13.72084063
Si	22.61968059	23.43151339	13.32385557
Si	24.80666094	19.98337929	16.66509229
Si	22.61486230	19.04782008	18.35689700
Si	18.82943214	8.10266308	13.27842189
Si	20.95266534	12.38792502	13.82761417
Si	22.55284771	14.96220927	14.09998100
Si	26.28311575	15.32190097	16.89577976
Si	24.73964040	12.57414149	17.79786410
Si	21.39466929	1.65131719	13.06501543
Si	24.25014091	6.31033298	12.27970278
Si	25.76701075	3.34194242	16.84424504
Si	23.86965260	0.76617056	17.59145824
Si	25.41107496	9.04981033	12.89533421
Si	15.20510731	11.42313557	14.30612700
Si	16.65703481	7.51108962	18.41153288
Si	14.81399880	5.07278808	18.57015955
Si	29.96947920	23.74042035	12.73837767
Si	17.83065610	19.84286311	19.11468737
Si	15.86564365	17.31961155	19.32909819
Si	17.32866976	5.38249425	13.30435321
Si	18.39389874	2.30757567	17.76067580
Si	20.40780978	23.77162981	17.89486291
Ca	6.63293011	12.99335091	14.90141499

Ca	4.87048666	9.71318963	15.02133952
Ca	3.30442454	12.44803408	16.90878014
Ca	5.38304591	15.64094667	16.87360933
Ca	10.25888122	19.77318307	16.80339702
Ca	8.91514743	16.42511502	15.51680344
Ca	7.46175038	18.63476465	18.42385691
Ca	10.76865136	22.30042791	19.24761883
Ca	9.52001248	7.36883926	14.68240705
Ca	7.59086642	3.89027577	14.71745833
Ca	6.42844583	6.86349011	16.53255976
Ca	8.43890752	10.07116415	17.10231336
Ca	13.33430889	14.01924175	15.86479209
Ca	11.66453785	10.59492399	15.37818266
Ca	9.98777118	13.44073160	18.15105889
Ca	12.09155285	16.74859546	18.20982721
Ca	11.95644375	1.82480919	15.74922280
Ca	13.11689596	22.30050012	16.59590466
Ca	9.38772030	1.38972421	18.90792741
Ca	11.34173243	4.52380985	18.65642500
Ca	2.93907333	6.42987181	14.37114727
Ca	2.27963557	2.72428146	15.60738394
Ca	12.83775748	7.75903729	17.90181763
Ca	1.90900486	9.34245783	17.09529844
Ca	3.81890988	18.77546818	15.25719786
Ca	26.81986578	12.74786202	15.06256687
Ca	14.53210502	19.79218446	18.19280239
Ca	4.42394107	21.34154173	18.38263720

Ca	5.32144239	0.96178537	15.13785948
Ca	5.52292818	21.88496771	15.48863462
Ca	5.86224145	24.19912073	17.86205097
Ca	5.07068207	3.47283243	17.73162049
Ca	20.20069612	14.42678420	16.20964350
Ca	18.25681491	11.23427673	15.35710060
Ca	16.58091599	14.01331830	18.31325484
Ca	19.83326276	16.83001675	18.73864201
Ca	22.49571011	21.36637557	15.53647510
Ca	22.30015080	17.63272176	15.75188817
Ca	20.46078867	20.94645012	18.39457966
Ca	23.80446789	23.90829042	17.16791477
Ca	22.17066625	9.06383029	13.66286961
Ca	20.87554078	5.17107477	13.86951173
Ca	19.93071659	8.05643212	16.71297550
Ca	21.87041770	11.25145275	17.11490390
Ca	26.19886978	17.74926165	15.19290672
Ca	24.20355830	12.11659251	12.40842532
Ca	23.29271174	15.40722432	18.11623377
Ca	28.32914414	19.51157444	17.73405933
Ca	24.55012935	1.60202740	14.54970230
Ca	25.97559503	22.52063969	13.35992629
Ca	21.57957107	3.22643456	16.61392446
Ca	26.85940306	6.23842710	16.75110639
Ca	16.21219592	8.02729591	15.41554984
Ca	14.24803478	4.84811307	15.20763362
Ca	25.05110503	9.62839201	16.30923674

Ca	15.14145939	10.71854872	18.03383804
Ca	17.24209566	20.17711041	15.46623786
Ca	15.56480887	16.97165883	16.37268033
Ca	28.96730845	22.52746109	15.75844192
Ca	17.43727055	22.90575221	17.48081980
Ca	18.73052884	2.09338093	14.68077146
Ca	19.63699110	23.50254771	14.50051430
Ca	15.29170287	2.02028829	17.01016221
Ca	17.62508332	4.88981044	16.48190690
Ca	10.71285503	19.15881768	13.27812058
Ca	5.73638021	6.49775348	20.12956382
Ca	6.26659179	11.19910474	11.70624666
Ca	6.48951902	15.39358841	20.34026828
Ca	12.73141309	12.48248744	12.75037849
Ca	6.90629819	3.02793855	21.34253643
Ca	8.55504867	5.58781964	11.89526709
Ca	10.75055521	11.33026643	21.39374043
Ca	26.89114202	3.95787425	13.22118783
Ca	9.45130817	2.13059374	23.34725037
Ca	12.59479477	22.13749310	12.98069141
Ca	13.80448636	7.69465974	22.15177521
Ca	8.85659578	22.22832628	12.59147775
Ca	17.69148037	15.44091607	21.35029032
Ca	2.46949485	15.82010926	14.31665029
Ca	5.99928119	22.25529357	21.46710586
Ca	20.71780402	17.13808991	12.16535377
Ca	16.79508225	11.68517061	21.55137530

Ca	18.61691175	14.43717535	12.73522530
Ca	20.40971940	19.06975805	21.45599514
Ca	25.78224996	14.68253492	12.22853206
Ca	19.87742102	5.22142263	19.05552078
Ca	21.47564581	6.97199350	11.09835369
Ca	22.72468272	12.17235175	20.65768004
Ca	12.12313386	6.16353193	11.83048246
Ca	26.27282372	21.93057722	18.68550110
Ca	23.77906578	1.03152804	11.22912302
Ca	23.31595981	6.25902182	17.96082114
Ca	17.94187226	1.01012376	11.39806097
Ca	28.55105262	20.33282806	21.02519905
Ca	16.99868486	17.46250214	12.91879120
Ca	16.17997909	0.66776817	20.64524790
O	2.60364283	10.82559648	13.18279736
O	7.23221317	17.54249060	13.86635571
O	6.37124314	10.96530811	18.66415710
O	11.82790667	23.32681980	14.73795069
O	4.94349463	5.12287599	13.33463354
O	8.90128099	12.25344937	14.36512103
O	8.02832000	6.13117380	18.74682190
O	13.08089457	18.77644875	14.22304782
O	12.06910368	12.16153893	19.26380966
O	11.99395771	5.93151769	14.28131511
O	15.73746043	23.88659399	19.63298246
O	2.72592013	4.57116404	19.02843210
O	4.62214184	22.81534261	13.48193207

O	2.29039974	17.50464786	16.72979905
O	8.14148240	23.21808913	19.33131847
O	16.13806780	12.77657963	14.07065600
O	20.34656250	18.57871243	14.36490749
O	19.85361729	12.45679603	18.30948526
O	20.00059324	0.71853165	12.66809191
O	24.22857679	19.38172611	18.14621997
O	17.73456535	6.94505809	12.73567108
O	21.10356750	14.06195377	13.56020941
O	25.76311136	13.79308332	17.26480703
O	25.45667082	7.42467758	12.51948202
O	25.02273674	1.87886347	17.10825593
O	15.86193641	6.24284301	19.10733056
O	16.49653737	18.90579590	19.03509745
O	17.67610509	1.01001222	18.60079299
O	4.44168829	12.05245995	14.72258845
O	2.50095087	13.45983984	13.69704091
O	6.72425531	15.28766461	15.04620071
O	4.64392413	16.75769375	14.51704625
O	8.00884652	12.52622783	17.39225222
O	5.51429580	13.32050881	17.33285197
O	6.31461965	9.21420295	16.67710264
O	4.07484506	10.23168064	17.41098916
O	8.16936540	18.90938847	15.92601429
O	5.90362192	19.79803724	14.59355193
O	10.73361377	22.26921399	16.81564631
O	9.09183098	23.08098644	14.67158167

O	5.09769841	7.47409585	14.37348579
O	7.30632257	6.12656736	14.29711606
O	6.86210842	10.63528716	13.92041793
O	9.30462920	9.70269262	14.73341301
O	8.65279913	7.60518241	16.70734245
O	10.69575333	6.66653062	18.22886621
O	7.14085878	4.37873929	16.88585594
O	9.16598026	3.64243263	18.59109960
O	9.48074267	14.87333847	14.14907032
O	11.43444112	12.99224446	14.67060873
O	10.89062989	17.90477668	15.26593072
O	13.22222437	16.55690673	15.92187855
O	12.30288102	14.46659339	18.06348994
O	27.97037929	11.43859591	16.36907079
O	10.53006255	11.18465585	17.34404072
O	12.91114432	10.15830421	17.55618069
O	7.71394541	1.55125363	14.59083965
O	9.85807118	0.86826411	16.29305398
O	9.62443472	4.84940998	14.36854577
O	11.65720057	4.03506878	16.14363453
O	4.29116455	23.21194198	16.80328088
O	11.70845529	2.15710711	18.96125735
O	15.14857766	22.06872012	17.77988126
O	13.09347316	23.22025095	18.96413075
O	11.63764678	8.27679639	15.48203672
O	14.06644858	7.14324138	15.42098495
O	13.79515822	11.83756449	14.95671902

O	2.62164947	8.73888160	14.82209294
O	4.73293828	5.79731857	17.85838619
O	2.52686099	5.18513760	16.43087119
O	2.50048000	2.23121860	17.85242296
O	13.35789602	5.58842540	18.15457526
O	14.00749466	21.25790928	14.44038758
O	15.08224700	19.32402023	16.00407378
O	3.44162946	20.58347306	16.43605341
O	3.54645641	16.42158873	18.82009620
O	5.24401634	18.11729057	17.61726429
O	3.14403265	14.94438237	16.65106869
O	14.37729532	17.55259928	18.66447371
O	1.35770299	0.74061233	12.44631983
O	3.02863107	0.54650793	14.65744478
O	2.69809819	3.77040914	13.55927515
O	4.69618358	3.21888458	15.25367213
O	7.27778183	0.33626284	18.88952966
O	5.06653610	1.01059170	17.46524816
O	8.98726450	20.78857315	18.50763156
O	6.88900055	22.12812337	17.25477276
O	18.14039735	13.93064456	15.18413727
O	15.63424348	14.66836909	16.00742487
O	19.91565594	16.82338704	16.35473039
O	17.70812938	17.96578202	15.24410399
O	21.03423626	14.79490930	18.43197208
O	18.66466559	14.59848221	19.40234060
O	19.26280531	10.15633399	17.26690436

O	17.31583112	11.85432683	17.69193492
O	20.04759361	21.21462190	14.81313057
O	18.57673318	19.78203256	12.96402750
O	22.07437025	23.83024621	14.81838602
O	21.32435818	23.08558628	12.36248264
O	24.05672721	19.23694793	15.40701391
O	24.51473348	21.60861613	16.68392340
O	22.26849316	17.45929917	18.28776678
O	21.81384060	19.71318504	17.05329647
O	18.53080707	8.67805128	14.74730089
O	20.30518486	7.46933009	13.11051565
O	20.57132955	12.24024935	15.39874035
O	21.99674986	11.38623900	13.18251744
O	22.34439988	15.19998605	15.71041897
O	23.82217130	14.20523633	13.55607164
O	26.94124512	15.34442603	15.40772251
O	14.45212023	12.98987420	18.14666172
O	24.17734192	11.77799146	16.52091904
O	25.63074511	11.51190639	18.73835743
O	20.92551736	2.68778045	14.21136562
O	22.64690042	0.67293975	13.40402757
O	22.85270828	6.65753587	13.02428927
O	24.82375739	4.85561468	12.59497668
O	13.22219927	0.73742055	17.26862263
O	26.50648457	3.03081847	15.40705527
O	27.42491174	23.48763420	17.19478500
O	22.50098267	1.20198642	16.88422294

O	24.38184823	9.41376223	14.06219973
O	26.91005488	9.48571159	13.32895264
O	26.14977301	12.71948807	13.03650700
O	16.08830555	10.30567982	15.03876509
O	17.79451363	7.00491780	17.34279194
O	15.64109233	8.48640416	17.62517244
O	15.44205400	4.31192015	17.26061901
O	26.59920665	8.27098843	16.59223321
O	28.72456121	23.96292303	13.71744236
O	19.24161798	19.11988305	19.40870693
O	17.98066060	20.65905638	17.70199595
O	16.68381639	16.36166745	18.30371985
O	3.40591285	19.12406722	19.41559974
O	16.37128160	5.65345814	14.59341574
O	18.59406038	4.49505724	13.78112992
O	19.79107747	1.81145109	17.10393313
O	17.44058479	2.56022479	16.42972925
O	21.64946177	22.81396363	17.48113494
O	19.37762235	24.09338364	16.66147905
O	4.34883036	12.31528654	11.99185012
H	1.99567416	13.78837386	12.89709182
O	5.98424200	15.75156341	12.37944494
H	6.47591905	14.85011750	12.28892912
O	6.76573670	13.32364340	12.44551526
H	5.79013458	13.33024390	12.27925000
O	27.98117998	15.41487084	12.22040118
H	28.54586716	15.51492229	11.44072400

O	6.74722603	13.26479836	19.76965286
O	5.53204863	8.47637828	19.11648221
H	4.53720772	4.64858481	22.01265872
O	5.49680786	4.78533567	22.07921476
O	2.33291035	7.12644363	18.29178032
O	8.28208356	19.78892945	13.26618398
H	7.79178166	19.48736439	12.47816549
O	10.73188277	21.05484745	14.43135403
H	6.99312970	22.43643329	10.97869875
O	7.56674170	21.74415108	10.52037061
H	6.96042223	21.12678002	10.08732105
O	12.44321949	20.18862254	17.61472637
H	12.12105602	20.15377263	18.57928251
O	11.58112706	20.25762703	20.07465976
H	12.32355795	20.19406493	20.68870095
O	9.78837017	15.66720555	17.54468084
H	9.68441042	16.47094650	18.11570656
O	7.21380153	16.22024800	18.30122471
H	8.05179368	15.74835387	18.08972817
O	9.49024005	13.31566391	20.51933169
O	6.44070748	6.86532234	11.91865164
H	5.78125445	8.18127728	11.42460794
O	8.84475446	10.69512585	12.15661312
H	9.36132327	11.50835424	11.94718657
O	10.03188037	7.33682093	12.30260918
H	9.81689223	8.21349788	11.94801207
O	5.32562983	9.08350881	11.18383354

H	4.37828796	8.92820060	11.35979454
O	9.01351356	8.62000248	19.04770324
O	6.59158872	4.09963780	19.40107625
O	23.56167188	3.16794709	20.59588057
O	5.21948913	1.54605234	20.07336413
H	22.98878130	2.86612845	21.33363961
O	10.35634637	13.11763723	12.28944078
H	9.94256037	13.82620853	11.76904502
O	12.06298901	16.55366235	13.39586600
H	12.71145110	15.79189534	13.18385726
O	13.70854307	14.54237246	13.04779807
H	14.62689589	14.85893551	13.17176382
O	17.11989000	13.05761978	11.19025416
H	17.36078782	12.11985724	11.11106231
O	13.41419653	14.00039547	20.51709607
O	11.10946661	9.83691154	19.63665135
H	9.92386369	9.02210351	19.35382843
O	10.45140406	9.42921891	22.74231917
O	13.41497949	8.35098141	20.08102023
H	12.58448586	8.87150096	20.15558142
O	10.19861067	0.74435911	13.63758583
H	10.40959015	1.62361575	13.25885913
O	7.27192054	3.64340826	12.15399794
H	6.54627230	4.14488250	11.74009504
O	11.64420714	3.29700920	13.62899959
H	12.50526623	3.59321551	13.12309467
O	14.42006947	1.55540278	19.40365495

O	14.76136075	21.47208489	20.28654049
O	13.00614600	8.07023816	13.11000420
H	12.51010423	9.02389798	12.96487049
O	11.90730606	10.30588163	12.88950540
H	11.01717629	10.10350142	12.56005725
O	2.48775801	8.27072594	12.29315327
H	1.86758361	8.21953512	11.54988830
O	27.24371646	5.93233269	14.29210006
H	26.66654340	6.60434828	13.88683396
O	26.82768595	3.70412699	18.07388222
H	26.50869997	21.24667146	23.24288719
O	16.30910284	7.93654241	22.15240646
O	15.65501600	19.25474005	13.47100074
H	7.43941707	0.56401450	12.91529447
O	10.54704811	24.16222981	12.14668569
H	7.21766996	0.53400387	11.39539748
O	11.07582037	20.92336371	11.69953763
H	11.10834186	20.80453871	10.73832479
O	5.55518683	17.62933889	20.15048156
O	16.02792579	17.02865378	20.89263365
H	15.29434075	13.92273277	20.75196645
O	6.99271348	23.49059817	12.36971234
H	24.76808286	3.24389908	12.26374998
O	4.97851333	2.43611433	12.75569028
H	5.90928402	2.71369670	12.46424135
O	25.15706301	2.34473285	12.43310822
H	23.88506469	4.28376537	13.91319277

O	6.58226458	20.92920774	19.56428107
H	19.95564293	15.91451443	24.10026134
O	3.94922683	21.05300488	22.21928584
H	4.38436523	20.17697704	22.30846391
O	16.52915421	15.32737728	13.55185578
H	16.36082079	13.01681705	11.80689688
O	19.19573118	16.42985385	13.71660590
H	23.90238138	16.93164151	13.12409369
O	20.69217989	13.27151029	20.73026291
H	24.03533670	13.85220944	22.74736574
O	18.43736185	10.64026135	19.85234742
H	17.97627944	9.73589088	19.74527561
O	20.92959356	7.26548404	18.81677476
H	20.65739201	7.99719633	19.39337087
O	15.33233721	10.63554512	20.29099877
H	14.71541255	9.88851901	20.43535421
O	17.45500811	8.21315531	19.70736274
H	16.95524055	8.10354862	20.56542453
O	21.18102720	20.33167863	12.51529377
H	21.31154417	21.33258773	12.36051745
O	23.71597380	22.27305692	13.47372751
H	29.07236063	24.27371030	9.76852334
O	17.78027668	2.89155056	10.36904530
H	17.88259648	3.34863581	9.52665357
O	26.39335063	19.65633437	16.59149048
H	5.44161863	10.78231203	22.28584520
O	22.05817030	19.78301348	19.71275897

O	19.69856876	16.88389998	21.10883200
H	20.29002985	16.25885481	21.57110639
O	23.46549477	14.11996769	22.00255467
O	18.63973792	9.42527643	12.21532789
H	18.70437100	9.14795693	11.28687561
O	19.42594973	12.11697636	13.03787195
H	19.38637723	11.27243995	12.53980330
O	22.34893237	9.08222397	11.17824300
H	21.94712392	9.92898035	10.93428037
O	21.78855360	9.27400166	15.92828985
H	22.45068376	8.79341775	16.50389467
O	22.12792935	6.25549547	15.91817727
H	22.68973795	6.55519545	15.18144041
O	19.96468978	5.03817401	16.44971074
H	20.76165390	5.60973624	16.29218682
O	23.50884634	3.83754911	14.73484852
H	24.00393461	4.31733362	15.49880526
O	21.95777366	4.37346340	18.58514345
O	18.39169428	3.62414860	18.65879345
H	22.44730212	3.95858713	19.32448465
O	22.38747124	16.50167843	13.46892868
H	22.03089043	19.36024973	11.02615050
O	24.89275370	17.16293389	12.96665931
H	24.88151373	18.00288551	12.48414397
O	22.03372442	18.51068191	10.52832122
H	22.93760155	18.36663181	10.21118163
O	28.26034185	18.09702256	14.07516852

H	28.19203916	18.39047407	13.15408763
O	25.10467162	16.41683618	16.96787779
O	23.56926262	13.19449386	18.73377540
H	23.27103882	9.07949675	18.44009466
O	22.23941690	10.43998300	19.25987980
H	21.60947034	9.82242796	19.65789921
O	23.67346763	8.47992719	17.77086524
O	21.83864864	2.36942753	11.62401452
H	21.48025772	3.39041698	11.49269403
O	20.90103462	4.70268419	11.48081734
H	19.98745399	4.45611913	11.25265432
O	23.85224842	6.45347705	10.59840865
H	24.36582685	7.16184868	10.17913534
O	24.79672625	4.63497337	16.80563115
H	26.10232286	0.78195888	24.52604182
O	23.78624864	0.88587073	19.26648247
O	24.52616369	23.35105353	19.26471730
O	4.88332240	23.28929388	19.78595743
H	4.03218171	23.65665911	20.06872176
O	24.95262173	9.82516474	11.48047502
H	24.02622151	9.50462819	11.22700868
O	24.42652416	13.66667211	10.66379803
H	24.65276519	13.41512107	9.75949152
O	14.87046983	11.04308734	12.66414986
H	14.58571232	10.12043713	12.54200399
O	10.52239495	4.91316379	10.80637262
H	10.61580925	3.95879820	10.67814708

O	14.69733939	4.10362287	19.92860280
H	14.50964231	3.12961935	19.76557391
O	0.26367189	0.33844973	25.03732374
O	26.69026812	22.95224723	11.18212303
H	26.49923415	22.43285350	10.38941019
O	27.42626034	21.33445647	14.44453845
H	27.11786895	20.63421385	15.04987270
O	29.43821089	23.16044189	11.26278548
H	28.49260920	22.83395204	11.30668649
O	25.31052271	0.67455925	9.26622947
H	25.91564525	1.35968591	8.94178828
O	17.40145117	22.48201346	15.03420139
H	16.55767559	22.78477014	14.66229139
O	17.55199919	20.86158797	20.43710990
H	16.58586919	20.95451165	20.59170339
O	26.79086218	19.85418800	19.62856259
H	26.09292690	19.19075554	19.51488481
O	11.30236651	14.20126279	24.66174081
O	16.25893570	13.78640905	20.65763873
H	13.15699127	13.34675837	21.28484446
O	14.18395747	2.42119681	15.03371474
H	14.19485821	2.39017040	14.06628890
O	16.77955011	1.34602845	13.32888010
H	16.17519705	2.09921490	13.42914485
O	16.54184824	4.70862048	12.00310791
H	17.05505720	4.05369645	11.43738659
O	13.64889790	4.51324698	12.66612600

H	14.49844186	4.32230088	12.23115563
O	19.48608278	23.03524309	19.03556937
O	21.37734972	21.26655012	22.22936803
H	22.19046364	21.36829195	21.67003689
O	16.01363642	2.35427646	22.22226673
H	15.19185872	2.81106122	21.97937063
O	1.31136610	2.70019659	20.29266646
H	0.59862751	3.30898532	20.66478482
H	29.01290626	19.45834265	25.22394580
O	25.23283611	8.55122817	21.41543094
H	26.15891530	8.50286883	21.76416767
H	24.64792695	8.48177413	22.20388546
O	28.69315628	18.58353551	25.55067532
H	2.64035439	17.92904732	25.01561495
H	4.05287839	24.18217220	24.36710464
O	9.63478869	19.51470191	21.62673964
H	10.38558890	19.83291434	21.00233306
H	10.12186104	19.10618196	22.36131946
O	7.86816238	21.20089209	22.66321807
H	8.54936590	20.62622782	22.18245945
H	7.60390005	20.62417909	23.41915677
O	28.66133357	21.66909252	18.96625960
H	27.47755107	16.21511933	21.07058788
H	28.76693981	22.58310275	18.64651131
O	5.24996868	18.57596869	22.59889232
H	5.99408179	18.77736008	23.21530089
H	4.69372008	17.89818311	23.06565090

O	19.49020529	11.44760976	24.22916526
H	18.81630548	10.80593308	23.87204302
H	20.35411584	11.16282165	23.87842678
O	23.61943443	12.58353590	24.58817097
H	23.34981389	13.34517319	25.14936437
H	24.45657914	12.21907135	24.95803991
O	25.93551751	4.37915759	21.11116680
H	25.88213889	4.75398256	22.01691262
H	25.04680614	3.95360564	20.94125074
O	2.61463587	12.58869625	19.41001507
H	1.96407280	13.28064045	19.61516439
H	5.61652002	14.65881405	22.96957673
O	4.95376147	14.75032692	22.21979652
H	10.40395274	13.28205937	23.82777074
H	4.68486374	13.81462438	21.98295662
O	3.26669928	0.73610948	21.70533415
H	2.49486936	1.18605924	21.31440672
H	3.49211445	1.26196798	22.52241930
O	14.35946494	17.21827115	24.44986629
H	13.54820143	17.59782190	24.02472159
H	14.07566059	16.34444722	24.82854990
O	8.71493627	4.10528618	22.43140195
H	9.38250372	4.48962764	21.82631930
H	23.63529125	2.35583405	20.02117122
O	2.57634197	9.49060221	25.55028956
H	3.51039188	9.17450402	25.47480910
H	2.48905334	10.12914017	24.80962316

O	9.19738498	3.23482752	25.55387235
H	10.04023956	3.38256095	26.02055576
H	8.88771732	4.15337828	25.32044455
O	8.07798229	10.43523995	20.95348752
H	7.48804919	10.74065078	20.21805862
H	8.28638310	9.52039803	20.65307035
O	9.98215897	18.09917989	18.49407589
H	18.47903934	15.94488665	24.59889630
H	10.16851118	18.54016874	19.34380077
O	15.85504298	2.22554932	24.74886433
H	15.91995792	2.26920678	23.68582879
H	16.72981736	2.54922018	25.04381788
O	1.35477841	8.61576443	22.29322653
H	1.68794466	9.52310615	22.54958408
H	27.81152956	8.13345190	23.14861033
O	8.87663621	1.42523323	21.25112943
H	8.53796133	0.50993369	21.29813536
H	4.48035160	1.20951295	20.64899966
O	11.27177247	4.97340930	21.10569577
H	11.65792210	4.31064068	21.70552373
H	11.37498111	5.87344381	21.61406855
O	14.57987558	5.37513996	22.28860816
H	15.56247162	5.28398776	22.37133703
H	14.41996622	4.89036621	21.42553633
O	9.77802459	12.65870116	23.26050986
H	10.31592133	9.48994090	23.71070434
H	9.50838488	13.19591249	22.48192726

O	12.41011495	16.49283277	20.66538362
H	12.73019015	15.55111841	20.74871351
H	8.54905995	13.05216954	20.37073907
O	19.32999439	16.41944983	24.66861226
H	5.41993349	18.08406465	21.02928085
H	13.21381449	17.00506085	20.86160150
O	10.97694352	22.94290497	21.63716894
H	11.66911680	22.35605958	22.00171875
H	10.38160560	23.14503359	22.40596533
O	6.78597372	1.67450581	23.48462545
H	6.54450136	0.68515539	23.58544715
H	6.04224735	2.10934249	23.94786476
O	18.52655290	3.48981320	24.81919550
H	19.00204906	2.72258008	24.40875591
H	19.06993104	3.77369445	25.56833062
O	13.75937167	9.89588503	23.11384825
H	16.77324425	10.11686274	24.00982057
H	16.81961966	7.18035186	22.48786472
O	11.62842001	7.12634479	22.52185712
H	10.87914786	8.50017281	22.58262885
H	11.32616541	6.82752860	23.39751948
O	22.71680779	5.12081017	23.10613122
H	22.01586930	5.71903137	23.44273337
H	22.82294850	5.46792799	22.18136338
O	25.14899862	22.54729275	22.82192586
H	24.60133754	23.22307936	23.25464872
H	24.55187973	22.09674511	22.16123757

O	15.30206319	12.71670313	23.40211520
H	14.35456957	12.57648909	22.99297531
H	15.31823637	12.14437704	24.18840771
O	16.69315153	15.40450515	23.63710610
H	16.30288887	14.50463944	23.66324781
H	15.93258772	16.01034027	23.75323836
O	10.12526020	0.07008510	24.37479782
H	14.12140759	21.43601112	21.03350152
H	11.02099180	-0.11788987	24.69623603
O	20.82222838	23.90128233	22.30462831
H	21.03367392	22.93360346	22.17325843
H	20.33749353	23.87704301	23.19135353
O	24.94086153	1.81716641	23.33545311
H	23.95235274	1.87568010	23.31943912
H	25.22668434	2.73498527	23.47763633
O	17.37921065	9.96973978	23.25985856
H	14.22170104	10.03598967	23.96126455
H	16.73544956	8.78329547	22.61424935
O	25.68813532	15.41165488	24.44631869
H	19.53703112	13.26119811	21.74804244
H	24.77718412	15.29644491	24.82235217
O	18.70812496	13.32233145	22.37077121
H	19.01281552	12.84646945	23.18773410
H	25.99361147	14.54389700	24.13103738
O	27.37194198	22.61544348	21.25243643
H	26.65401525	22.91164334	21.85462835
H	28.00081300	23.35058719	21.14515407

O	7.29563740	23.49095545	25.56290502
H	8.19306145	23.50455362	25.05467858
H	7.20922746	24.35321008	26.00119925
O	20.38325159	9.22236995	21.40943929
H	20.82018251	9.95475239	21.88344138
H	19.63512148	9.66698343	20.94793528
O	19.69322406	5.11819896	21.41419589
H	20.03111151	5.77178691	22.06299455
H	18.78068363	4.88568909	21.75136486
O	9.18808877	18.29977544	25.77241331
H	9.52986509	17.59496012	25.17099653
H	9.97347259	18.83821533	26.00533563
O	15.39399606	10.03175192	25.55512076
H	15.00452107	10.68932501	26.16721703
H	14.92865238	9.18095753	25.69421951
O	1.49363608	4.64497259	24.81844691
H	0.52717230	4.56910148	24.70865032
H	1.83297743	4.65632582	23.88686082
O	2.33889983	2.08679291	25.92585715
H	2.00621914	3.00336388	25.81766983
H	1.55822038	1.51800331	25.71548355
O	23.75112786	21.40592719	20.81152997
H	23.91802556	22.20373174	20.19065673
H	23.16590120	20.74539036	20.28750514
O	22.17654273	11.03047360	22.89584072
H	22.59607249	11.63706702	23.57190331
H	22.62936793	10.16682396	23.08912714

O	22.21750846	18.16876769	22.82084552
H	22.08821297	18.54172334	23.74972440
H	23.12468480	18.41114717	22.50249497
O	27.16844153	20.52677830	23.18614444
H	26.74282571	19.76378432	23.61472308
H	24.65491769	0.75796843	19.72377939
O	13.77035014	14.54153307	25.18543778
H	14.22380870	14.13514280	24.42356578
H	12.72987340	14.41248109	24.95413031
O	18.44214165	7.87365748	24.66279341
H	18.49232031	8.18283895	25.57964568
H	18.11687816	8.67847903	24.14828020
O	11.56064547	22.34530524	24.88888238
H	11.90335226	21.88201088	24.10065077
H	12.69289450	23.58103283	24.71951942
O	25.01604494	11.43518387	21.26981432
H	25.12187019	10.46291692	21.38056121
H	25.38147577	11.55568691	19.71199622
O	13.08305145	21.06654024	22.59459948
H	11.00577353	13.89510701	25.53566989
H	13.92445003	21.20220704	23.11282103
O	27.02349370	15.41180529	20.73353479
H	12.78451289	20.14805294	22.79409563
H	25.42547051	15.81406533	20.48033304
O	6.15759541	10.36580918	22.81488316
H	6.92912155	10.37312895	22.16606098
H	24.82267322	24.10094668	19.80325593

O	8.50685687	15.41697397	21.64246394
H	9.02288771	14.61061993	21.20383414
H	8.19417621	15.12228188	22.52514975
O	9.41185830	23.35920478	23.99231756
H	8.89651597	22.67984438	23.51039535
H	10.62000781	22.73676138	24.57458697
O	23.32015181	8.55550458	23.48455114
H	23.87621989	8.62559519	24.32120225
H	22.54216850	7.99391664	23.66812916
O	3.74027153	16.68669409	23.85227189
H	4.42378099	16.64970109	24.58668660
H	3.91899757	15.87916021	23.30952824
O	27.49752693	15.61263529	18.07681675
H	27.24320153	15.42940327	19.76115436
H	2.10502401	11.72551904	19.46069909
O	14.38546844	12.45515553	26.81545767
H	14.18125032	13.28474344	26.27635439
H	14.86927507	12.77399645	27.59255970
O	11.51140184	11.90694347	26.96623216
H	12.48309859	12.03163251	27.02619067
H	11.20064360	11.93102130	27.88373335
O	2.26662956	11.09237030	23.04039639
H	3.04036799	11.43474371	22.56441905
H	28.03172691	11.75074924	22.86113631
O	7.52890626	10.15062045	26.44939070
H	7.42297252	10.95815214	25.89936436
H	6.81445672	9.55214185	26.15078877

O	13.35442103	0.66405564	24.06885784
H	16.98708111	24.42030039	23.33861365
H	14.08055419	0.98793181	24.63152572
O	13.19359394	6.18772055	9.48735612
H	14.00123044	5.64746711	9.49442446
H	12.50174431	5.61026213	9.11333212
O	27.82584564	10.29116217	19.33761188
H	27.64022602	9.76237866	20.12866913
H	26.95940994	10.71800899	19.03920465
O	26.72090965	12.58585272	22.74051961
H	26.95642948	13.43271120	22.32852003
H	25.74517541	11.92196934	21.88553592
O	8.47794192	5.65841775	24.38587477
H	8.56189272	5.06957819	23.51267801
H	7.50910962	5.79411025	24.52672357
O	3.38425060	21.19050960	24.73328559
H	30.06579995	21.14416094	23.68120694
H	29.31401808	21.92586212	24.89029543
O	15.48357035	21.25371263	23.78197103
H	16.09323868	21.99715222	23.64475614
H	15.88775868	20.46940455	23.32582371
O	7.03724034	7.53575149	21.99132292
H	6.74817736	8.37425365	22.38988037
H	7.63490364	7.11481429	22.63378461
O	22.58093393	21.46434630	24.51789785
H	23.52126406	21.30800759	24.34430993
H	21.80370952	21.32720262	23.17832297

O	28.23216627	17.83810550	21.85783226
H	27.62223226	17.80045993	22.64499348
H	29.06006722	17.46009175	22.20048495
O	24.44385583	16.01483052	20.36916604
H	24.37188920	16.95962754	20.61935739
H	23.91801325	14.85200343	21.49757770
O	25.97199768	0.74094865	20.89845257
H	26.66567142	1.35541285	20.55307021
H	25.64969890	1.16963196	21.72794843
O	14.61788030	4.71317686	25.03553220
H	14.43686274	4.79939123	24.07059457
H	15.06961839	3.83351106	25.09531567
O	25.05448252	8.88655965	25.48137089
H	25.83877678	8.29786600	25.42568636
H	25.42682788	9.78567456	25.32664184
O	11.67384553	19.84283000	25.93646768
H	11.55905518	20.81155345	25.74554112
H	12.59605529	19.74985063	26.27508147
O	17.27418421	4.64455461	22.51922686
H	16.88372040	3.72071864	22.29265868
H	17.59930877	4.51987927	23.43462217
O	13.96933415	7.53159447	24.96572690
H	13.01147118	7.44461359	25.12958990
H	14.34186743	6.66316503	25.22904910
O	5.26125277	8.61833870	25.03776337
H	5.37570867	7.66754866	24.77746332
H	5.50270284	9.13073593	24.23989434

O	12.84092406	12.37555358	22.44488868
H	12.38444076	12.85093687	23.16499063
H	13.37630487	10.78211037	22.85654461
O	22.27593921	23.62848082	25.70582454
H	22.45274857	22.66679514	25.25558999
H	22.58288608	23.57903172	26.62218682
O	16.25243546	18.77753213	22.81693984
H	16.15444549	18.19152457	21.97388020
H	15.73067145	18.27876047	23.47640177
O	17.53463476	23.42969413	21.63750130
H	17.79904673	22.51595680	21.38632421
H	16.79069668	23.61304856	21.00641939
O	23.07930808	15.14177691	25.33687825
H	22.63832232	15.72883184	26.01327946
H	22.48844170	15.25267540	24.55564877
O	22.97420300	6.53519809	20.66137017
H	23.60266215	7.27021176	20.79603451
H	22.17578884	6.93503316	20.22613784
O	22.20971066	2.35463018	22.96667693
H	22.11752196	3.31753215	23.15061676
H	21.34068067	1.93335340	23.16446743
O	5.69470639	20.92905748	26.37165226
H	4.85661854	21.13349960	25.89074108
H	6.19530547	21.76734291	26.41584993
O	4.63735918	12.25462818	21.25520550
H	5.45606183	12.46437651	20.70454461
H	3.90674502	12.31171032	20.58365284

O	11.93192744	4.36898515	25.77712899
H	11.55329104	5.28306125	25.76392465
H	12.90884408	4.48951267	25.73101673
O	18.99562510	7.06781096	10.22060749
H	18.40566396	6.84486315	10.99013875
H	18.53600319	6.73484531	9.43639681
O	10.28344756	16.49248165	23.85476540
H	9.85285683	16.28383310	23.00288686
H	10.67076187	15.60395607	24.20401093
O	24.63662575	18.64102911	21.63585685
H	25.37184571	18.56687856	22.27012903
H	24.71787937	19.52691758	21.22522138
O	21.43372870	15.55817044	23.05076018
H	21.86949885	16.43793572	22.91680603
H	21.97820313	14.90448752	22.54666676
O	25.38446267	5.24944051	23.84554497
H	25.66408456	6.16521887	24.01942133
H	24.39814577	5.29109142	23.74113855
O	2.52948565	4.65434171	22.22288031
H	2.68786568	5.49208538	21.69543821
H	2.27387218	3.99841495	21.54716929
O	19.63960842	23.75554919	24.73785472
H	16.22136582	0.47547719	24.88858035
H	20.45404674	23.63056061	25.27828956
O	10.09985866	9.49704270	25.70306249
H	9.16246772	9.67107343	25.99521725
H	10.62546699	10.22483076	26.09119231

O	6.87959725	14.74998554	24.01463983
H	6.68660876	15.29378456	24.80326977
H	7.04479462	13.80567724	24.33078826
O	25.62366417	6.45394726	19.03517650
H	25.87670773	5.87601435	19.78629844
H	25.75611717	7.37611202	19.31621100
O	3.26113962	6.93234246	20.81723098
H	2.83935470	7.08229777	19.89485393
H	2.89008923	7.65997507	21.35777583
O	12.03425229	18.56993724	23.55537972
H	11.84280946	19.00359326	24.43440129
H	11.44908761	17.75971217	23.54010199
O	19.69783557	1.14575923	23.70780884
H	19.58154536	0.55960388	24.51130628
H	19.07217398	0.74826370	23.05601852
O	3.99625841	2.35267085	23.78370469
H	3.82195531	3.24952036	23.44491104
H	3.38840226	2.23336679	24.56993340
O	5.45946660	23.08257295	23.71580750
H	4.93819573	22.35513697	24.10899432
H	6.17271677	23.29522668	24.39888999
O	14.49534517	19.45329630	26.29976379
H	14.56026944	18.62567354	25.77546677
H	14.93883779	20.12537970	25.75358972
O	7.03852001	19.31434451	24.60243382
H	6.59116161	19.88895317	25.28170058
H	7.90460486	19.00599046	25.02653055

O	27.45647721	7.47434791	24.88704493
H	1.55449163	8.16808507	25.23464789
H	1.31120149	6.59776507	25.07614735
O	4.33144216	18.37135039	27.63108628
H	4.77504030	19.23815063	27.58893647
H	3.48031410	18.50613580	27.16706855
O	5.68574624	16.89100363	25.70327935
H	5.26592486	17.27095786	26.52070259
H	6.22931983	17.63650509	25.36765423
O	11.79888082	2.89457235	23.40881347
H	12.44162702	2.16090924	23.56771112
H	11.86963645	3.48404782	24.20882870
O	21.54970156	19.24062250	25.18839035
H	21.99600194	20.17132299	25.04737088
H	20.59893792	19.41108311	25.06619736
O	18.94240651	18.97248526	23.47814152
H	19.06880555	18.07992694	23.88933010
H	17.97213056	18.97529540	23.26273041
O	7.42807367	12.23740250	24.51829101
H	6.90972673	11.64691376	23.91499633
H	8.34092614	12.27823775	24.10922878
O	20.69100069	7.13972161	23.26147330
H	20.56539325	7.82185654	22.55322551
H	19.94211834	7.34951214	23.88835046
O	5.71159883	5.91781693	24.36454178
H	5.60314884	5.45571769	23.39917726
H	5.28908141	5.31304507	24.99224637

O	21.52383100	16.83245958	26.74815368
H	20.65645257	16.58119394	26.37736574
H	21.66190857	17.73520244	26.38298136
O	26.46768492	17.89367088	23.93595825
H	26.13338494	16.95960061	24.09761045
H	27.08164733	18.07523467	24.68942925
O	10.70266307	6.79914232	25.40852710
H	10.52990818	7.72996254	25.68696079
H	9.83076083	6.47535001	25.04704976
O	18.67652584	16.41712674	11.19060992
H	18.15921962	20.53100538	12.51041189
H	18.45744578	16.31260537	10.25247121
O	26.13438446	11.51230789	25.04283255
H	26.80361283	11.70402347	25.71684118
H	26.42631692	12.00649176	24.20026618
C	13.84926411	14.82937295	10.80454511
O	13.04967585	13.99350835	10.50826925
O	14.66316511	15.68569888	10.73759538

2-P

Si	3.54178817	12.17735981	13.35662620
Si	6.07398444	16.28813882	13.90761980
Si	6.62824402	12.59221847	18.27408352
Si	5.46275944	9.65533632	18.04709331
Si	7.28675883	19.03711747	14.57888159
Si	10.43206527	22.42685221	15.26283882
Si	5.98260056	6.50278184	13.41710599
Si	8.47927531	10.76422606	13.83083313

Si	9.20000422	7.20495955	18.17029764
Si	7.81500339	4.48425476	18.38054472
Si	10.05433717	13.46215678	13.95072012
Si	12.35031010	17.37231098	14.81222792
Si	13.12282583	13.40832449	19.00694604
Si	11.67514368	10.75156894	18.41734169
Si	9.04351774	0.72122412	14.91809586
Si	11.14437562	4.52548421	14.69797241
Si	12.93505346	1.14882741	18.84924392
Si	14.61293608	22.74329547	19.16982467
Si	12.70893569	7.45343237	14.63763177
Si	1.97877143	9.37481918	13.49970755
Si	3.10646925	5.80281015	17.83936038
Si	1.73493438	3.29793262	18.76242298
Si	14.48750284	19.67274846	14.50374889
Si	4.35402967	17.91035621	18.95130899
Si	2.45805329	16.11002445	17.53022567
Si	5.79799940	24.12257642	13.23010672
Si	4.31164712	3.64331811	13.69616540
Si	5.69313264	0.46004436	18.85647772
Si	7.66708968	21.71585235	18.61144997
Si	16.59878889	14.21728883	14.84250509
Si	19.18388750	17.36057343	15.02778560
Si	20.08873185	13.80613135	19.33866469
Si	18.69372257	11.25154938	18.29450135
Si	20.04229704	20.07463824	13.71027518
Si	22.61937297	23.43148701	13.32351071

Si	24.80533800	19.98292704	16.66465265
Si	22.61362173	19.04632739	18.35545709
Si	18.82862393	8.10450507	13.27310230
Si	20.94751360	12.38713596	13.82525839
Si	22.55271705	14.96114827	14.09937553
Si	26.28344124	15.32174746	16.89563827
Si	24.73950255	12.57445031	17.79785486
Si	21.39464102	1.65189090	13.06426627
Si	24.24887425	6.31055133	12.27895020
Si	25.76674973	3.34181564	16.84398730
Si	23.86937460	0.76623496	17.59130463
Si	25.41014922	9.04961639	12.89469253
Si	15.21444565	11.41317430	14.31357190
Si	16.65758319	7.50852204	18.41321602
Si	14.81344833	5.07181181	18.56980212
Si	29.96893469	23.74050655	12.73806688
Si	17.82959997	19.84278873	19.11433211
Si	15.88480311	17.30723189	19.32123018
Si	17.32901382	5.38237412	13.30369921
Si	18.39416128	2.30719937	17.76044598
Si	20.40754139	23.77143544	17.89455152
Ca	6.61606760	12.99268761	14.89961786
Ca	4.87195789	9.71353528	15.02043476
Ca	3.30034292	12.44829196	16.90837907
Ca	5.38022799	15.64452679	16.87104185
Ca	10.25521715	19.77897896	16.80986258
Ca	8.90736129	16.42175400	15.48155282

Ca	7.45911270	18.63410952	18.41852294
Ca	10.76640339	22.30247823	19.24909028
Ca	9.51624440	7.39337191	14.66668818
Ca	7.59307186	3.88993022	14.71719562
Ca	6.42880609	6.86127425	16.52908772
Ca	8.44075685	10.08159106	17.10057215
Ca	13.33248977	13.95001955	15.99296462
Ca	11.65442106	10.60550342	15.36092087
Ca	9.96799646	13.44918895	18.14923667
Ca	12.07633633	16.75232950	18.20589615
Ca	11.95687643	1.82464585	15.74599024
Ca	13.12090231	22.30522511	16.60182477
Ca	9.38856742	1.39038751	18.90821245
Ca	11.34136034	4.52385776	18.65400486
Ca	2.93822791	6.43011074	14.36964848
Ca	2.27867962	2.72404415	15.60663970
Ca	12.83677353	7.75863040	17.90084631
Ca	1.90832657	9.34207208	17.09448263
Ca	3.81376900	18.77724218	15.25329487
Ca	26.81518756	12.74663400	15.06172404
Ca	14.53215544	19.77642672	18.19250567
Ca	4.42187737	21.34241114	18.38216551
Ca	5.32149762	0.96067734	15.13729389
Ca	5.52218175	21.88683112	15.48830707
Ca	5.86091080	24.19964293	17.86273713
Ca	5.06987059	3.47308535	17.73031072
Ca	20.21400199	14.42715759	16.21018232

Ca	18.25210668	11.19822201	15.34735931
Ca	16.58120904	14.00609375	18.33264020
Ca	19.81321299	16.82629426	18.72878313
Ca	22.49295858	21.36162914	15.53089205
Ca	22.28524489	17.63338316	15.74679553
Ca	20.46141782	20.94696676	18.39541235
Ca	23.80306235	23.90663541	17.16542588
Ca	22.16822117	9.06801776	13.65799432
Ca	20.87580286	5.17274645	13.86593103
Ca	19.93418255	8.05231802	16.71173275
Ca	21.87074496	11.25176486	17.11130685
Ca	26.19258880	17.74878074	15.19097365
Ca	24.20067979	12.11742567	12.40508756
Ca	23.29245548	15.40987589	18.11473013
Ca	28.32750037	19.51112071	17.73381219
Ca	24.54882731	1.60220933	14.54839766
Ca	25.97523265	22.52083811	13.35853259
Ca	21.57927724	3.22607992	16.61204713
Ca	26.85855716	6.23799997	16.74932594
Ca	16.20992044	8.01484657	15.42123325
Ca	14.24840336	4.84538310	15.20265083
Ca	25.04995431	9.62746101	16.30742905
Ca	15.14606934	10.70813778	18.02747123
Ca	17.25269429	20.17429315	15.46503722
Ca	15.59408582	16.94901726	16.35598577
Ca	28.96619743	22.52791117	15.75766152
Ca	17.43689160	22.90543784	17.47673530

Ca	18.73025797	2.09335583	14.67890759
Ca	19.63673165	23.50204122	14.49895553
Ca	15.29223959	2.01980246	17.01000884
Ca	17.62623773	4.88797890	16.48079060
Ca	10.69405364	19.15265796	13.26980489
Ca	5.73487980	6.49705674	20.12835442
Ca	6.27063110	11.20164752	11.70145085
Ca	6.48620820	15.39438362	20.34108688
Ca	12.72598770	12.44084397	12.67485108
Ca	6.90616800	3.02838294	21.34236565
Ca	8.55637237	5.58405891	11.89516506
Ca	10.74240441	11.32633602	21.39214341
Ca	26.88996464	3.95821724	13.21976706
Ca	9.45141695	2.13082285	23.34735188
Ca	12.61023294	22.11473730	12.99109360
Ca	13.80474301	7.69309051	22.15106722
Ca	8.86058159	22.23860607	12.58406028
Ca	17.69880703	15.44183640	21.35520623
Ca	2.46612022	15.82027376	14.31517093
Ca	5.99725617	22.25479781	21.46760323
Ca	20.71346115	17.10941891	12.15193632
Ca	16.79853211	11.68087775	21.55268948
Ca	18.58687733	14.41419682	12.74063604
Ca	20.41278050	19.06753626	21.45235795
Ca	25.78149756	14.68140293	12.22531304
Ca	19.87837128	5.22019187	19.05479845
Ca	21.47107193	6.97610161	11.09511420

Ca	22.72569928	12.17221889	20.65678317
Ca	12.12672056	6.15825755	11.82506450
Ca	26.27070641	21.92968183	18.68305814
Ca	23.77745818	1.03351510	11.22657571
Ca	23.31657438	6.25852036	17.95982994
Ca	17.94209513	1.00918394	11.39540139
Ca	28.54969035	20.33415292	21.02497088
Ca	16.98990624	17.44806786	12.88530237
Ca	16.18061064	0.66776416	20.64436292
O	2.60317350	10.82485197	13.18245195
O	7.23062410	17.54445246	13.86566005
O	6.37053018	10.96525067	18.66485990
O	11.83154140	23.31679178	14.73660503
O	4.94339960	5.12282275	13.33473088
O	8.90559659	12.30907094	14.36263286
O	8.02869409	6.13294934	18.74295822
O	13.08574755	18.78023391	14.22738701
O	12.06442202	12.15456881	19.28610031
O	11.99379586	5.93202333	14.28063558
O	15.73712200	23.88601768	19.63283076
O	2.72607144	4.57122409	19.02830414
O	4.62204796	22.81540373	13.48185665
O	2.29117482	17.50477253	16.73003815
O	8.14178406	23.21805897	19.33134711
O	16.20551072	12.73126931	14.14680675
O	20.29747882	18.58247992	14.35958098
O	19.85407080	12.45632318	18.30958933

O	20.00051730	0.71854544	12.66802322
O	24.22772282	19.38181900	18.14610311
O	17.73332250	6.94426308	12.73639065
O	21.10530288	14.06180209	13.56144216
O	25.76339336	13.79301138	17.26481828
O	25.45648696	7.42419907	12.51967885
O	25.02274124	1.87877942	17.10830145
O	15.86225007	6.24056782	19.10806824
O	16.49383418	18.90440849	19.03544407
O	17.67592917	1.00991250	18.60072045
O	4.43775051	12.05185367	14.72257976
O	2.50055095	13.46001337	13.69636759
O	6.72821061	15.28729843	15.04331493
O	4.64466590	16.75697795	14.51806142
O	8.00322250	12.52529945	17.39216913
O	5.51257433	13.32156137	17.33267137
O	6.31857314	9.21480408	16.67775182
O	4.07565083	10.23135980	17.41038163
O	8.16941777	18.90970482	15.92406649
O	5.90150535	19.79908953	14.59340608
O	10.73416814	22.26808255	16.81561385
O	9.09527339	23.07931813	14.67084148
O	5.09838451	7.47439304	14.37340499
O	7.30624768	6.12694021	14.29678798
O	6.87189250	10.64980476	13.92395412
O	9.31868615	9.75733914	14.74142864
O	8.65680187	7.60578522	16.69136155

O	10.69466884	6.66729882	18.22691308
O	7.14057328	4.37851194	16.88539845
O	9.16562222	3.64274442	18.59106135
O	9.55302439	14.93663307	14.07280918
O	11.45400409	13.05416795	14.66278164
O	10.89930321	17.90706890	15.32588265
O	13.22206800	16.49191321	15.84127192
O	12.29311985	14.46787020	18.07796037
O	27.96986333	11.43850959	16.36897283
O	10.54135749	11.23376383	17.34166033
O	12.90845432	10.16216004	17.55426831
O	7.71499460	1.54845244	14.59105088
O	9.85779069	0.86498842	16.29229524
O	9.62375863	4.85124992	14.36792167
O	11.65674393	4.03505344	16.14345088
O	4.29100986	23.21192717	16.80342932
O	11.70828313	2.15701950	18.96139649
O	15.14850822	22.06483126	17.78107004
O	13.09442386	23.21958099	18.96394576
O	11.63649155	8.28007588	15.48040552
O	14.06436302	7.14152105	15.42262580
O	13.78471623	11.85807308	14.88954764
O	2.62201751	8.73915199	14.82196137
O	4.73298715	5.79750088	17.85818749
O	2.52694203	5.18525731	16.43065794
O	2.50056695	2.23135927	17.85237624
O	13.35745312	5.58890535	18.15532832

O	14.06195548	21.26179412	14.44033477
O	15.08543083	19.31396155	16.00721959
O	3.44148258	20.58331839	16.43588035
O	3.54693958	16.42136224	18.81995845
O	5.24448898	18.11650862	17.61750069
O	3.14429963	14.94457619	16.65085694
O	14.38836733	17.50208392	18.65316893
O	1.35762187	0.74066008	12.44642015
O	3.02866125	0.54615098	14.65762798
O	2.69812765	3.77041046	13.55933925
O	4.69624225	3.21845900	15.25377929
O	7.27771214	0.33639307	18.88954431
O	5.06650432	1.01054591	17.46506266
O	8.98646594	20.78847601	18.50875527
O	6.88920318	22.12810683	17.25471932
O	18.16341587	13.99266957	15.19046588
O	15.62914107	14.60708562	16.07344767
O	19.91878038	16.82199751	16.33893904
O	17.69677174	17.95829586	15.24628617
O	21.03371565	14.79593567	18.43370920
O	18.66463071	14.59477837	19.40484135
O	19.26071899	10.15529429	17.26599565
O	17.31392601	11.85577385	17.69313523
O	20.04257344	21.21281249	14.80953519
O	18.53383638	19.79133242	12.96679668
O	22.07430839	23.82998713	14.81839156
O	21.32389092	23.08550839	12.36274415

O	24.05550979	19.23605335	15.40694334
O	24.51404124	21.60827518	16.68265116
O	22.26700567	17.45844473	18.28655787
O	21.81098223	19.71280536	17.05275248
O	18.52728669	8.67991644	14.74569914
O	20.30458900	7.46874511	13.11233014
O	20.56717847	12.23866087	15.39786565
O	21.99577475	11.38785252	13.18271992
O	22.34717875	15.20091393	15.71068787
O	23.82371048	14.20618422	13.55609281
O	26.94147841	15.34429157	15.40772255
O	14.40710468	12.98416235	18.13987378
O	24.17762176	11.77795167	16.52089963
O	25.63083913	11.51206297	18.73833700
O	20.92549557	2.68774059	14.21145191
O	22.64675232	0.67307621	13.40380120
O	22.85200270	6.65759256	13.02430893
O	24.82342926	4.85579256	12.59500735
O	13.22168325	0.73735829	17.26837058
O	26.50650556	3.03088404	15.40701003
O	27.42502207	23.48755553	17.19505562
O	22.50086751	1.20183938	16.88407783
O	24.38130299	9.41343348	14.06204884
O	26.90960109	9.48545931	13.32910671
O	26.14922446	12.71923112	13.03608425
O	16.02908707	10.29293391	15.11042542
O	17.79420176	7.00434962	17.34281856

O	15.64033452	8.48295786	17.62786627
O	15.44097399	4.31178473	17.26003854
O	26.59908689	8.27090970	16.59238302
O	28.72472722	23.96288774	13.71800404
O	19.24019866	19.11942345	19.40845787
O	17.98015736	20.65863861	17.70195721
O	16.74211153	16.36924562	18.30355069
O	3.40585057	19.12417107	19.41546210
O	16.37107430	5.65272317	14.59346650
O	18.59383068	4.49476361	13.78169024
O	19.79126954	1.81124282	17.10399564
O	17.44068544	2.56003785	16.42959274
O	21.64913214	22.81376822	17.48113416
O	19.37746385	24.09326421	16.66115316
O	4.34909116	12.31458598	11.99189327
H	1.99525723	13.78943608	12.89655388
O	5.98385613	15.75094185	12.37853252
H	6.47690303	14.84891508	12.28708565
O	6.76335461	13.32458013	12.44611588
H	5.78784816	13.33009887	12.27902387
O	27.98111487	15.41492531	12.22046966
H	28.54346495	15.51802639	11.43947369
O	6.74718031	13.26544542	19.76956446
O	5.53211940	8.47635735	19.11655170
H	4.53716663	4.64833066	22.01324248
O	5.49678490	4.78540955	22.07927193
O	2.33310334	7.12663141	18.29196078

O	8.28093330	19.78972545	13.26577202
H	7.78458929	19.49883182	12.47733277
O	10.73414743	21.04767516	14.43235309
H	6.98863561	22.43296714	10.97589512
O	7.56700348	21.74366122	10.52056682
H	6.96773336	21.13151927	10.07068978
O	12.44614542	20.18626835	17.61668322
H	12.12302338	20.15601886	18.58157595
O	11.58160213	20.25768347	20.07437857
H	12.32241710	20.21052714	20.69199027
O	9.79005559	15.66723110	17.48524212
H	9.67498034	16.46502725	18.06140457
O	7.21383422	16.21947255	18.30173689
H	8.04341527	15.74402202	18.07322294
O	9.48919017	13.31683607	20.51887017
O	6.44105375	6.86525548	11.91842136
H	5.78088769	8.18171856	11.42388584
O	8.84572856	10.70304501	12.15947250
H	9.36552665	11.51292749	11.93591011
O	10.03190546	7.33834530	12.30166594
H	9.81504124	8.20652823	11.92740007
O	5.32602338	9.08428253	11.18433494
H	4.37834721	8.92972072	11.35898300
O	9.01194605	8.61928882	19.04170695
O	6.59187970	4.10046307	19.40097822
O	23.56171852	3.16792037	20.59581807
O	5.21950196	1.54608188	20.07341764

H	22.98855592	2.86610091	21.33334285
O	10.35439397	13.06245031	12.28004750
H	10.04696352	13.78985034	11.71389884
O	11.93338799	16.68918017	13.33224381
H	12.60030625	16.09054072	12.94100095
O	14.02397682	14.67666400	12.73582819
H	14.94397794	14.98349646	13.05511687
O	17.17070383	13.16890031	11.15978199
H	16.70773423	12.42088435	11.58244147
O	13.41298126	14.00072357	20.52833126
O	11.10519980	9.83659696	19.62890329
H	9.92265855	9.01960336	19.34809792
O	10.45156416	9.42856567	22.74237097
O	13.41454079	8.35195392	20.08068477
H	12.58401898	8.87207274	20.15435714
O	10.19872261	0.74318584	13.63763514
H	10.40613647	1.62267627	13.25768560
O	7.27174201	3.64286591	12.15434968
H	6.54606842	4.14419427	11.74028217
O	11.64364468	3.29746000	13.62957909
H	12.50427540	3.59251980	13.12348579
O	14.41959162	1.55537235	19.40372187
O	14.76143405	21.47096543	20.28745520
O	13.00779250	8.06614750	13.10997123
H	12.52098327	9.01391932	12.96272242
O	11.90297678	10.30417196	12.88885436
H	11.01868730	10.09667496	12.54661383

O	2.48769013	8.27037206	12.29325597
H	1.86770579	8.21860497	11.54981177
O	27.24359839	5.93246782	14.29192382
H	26.66596331	6.60360767	13.88553658
O	26.82764126	3.70407263	18.07380524
H	26.50905772	21.24718272	23.24280771
O	16.30903733	7.93625627	22.15249737
O	15.65644624	19.24473496	13.46474882
H	7.44125129	0.56371608	12.91512311
O	10.54685596	24.16290118	12.14607351
H	7.22263073	0.53609276	11.39486648
O	11.07615366	20.92187695	11.70242664
H	11.11436416	20.80115218	10.74147199
O	5.55528394	17.62933270	20.15028750
O	16.02987051	17.02595061	20.88928547
H	15.29479194	13.92575629	20.76415266
O	6.99255582	23.49092021	12.36990233
H	24.76778826	3.24389224	12.26341941
O	4.97843407	2.43572837	12.75607717
H	5.90911025	2.71296149	12.46429237
O	25.15686712	2.34466508	12.43284745
H	23.88463016	4.28410809	13.91265312
O	6.58184524	20.92911189	19.56443241
H	19.95638866	15.91464582	24.10052196
O	3.94910480	21.05292066	22.21925442
H	4.38355233	20.17660717	22.30853188
O	16.44761356	15.33511042	13.63170668

H	16.45222498	13.75919341	10.83974169
O	19.18470503	16.42313322	13.70757351
H	23.90195930	16.93100614	13.12438072
O	20.69221528	13.27017234	20.73126134
H	24.03576375	13.85344563	22.74707941
O	18.43737871	10.64064548	19.85144296
H	17.97757676	9.73579279	19.74397865
O	20.92945417	7.26544183	18.81676178
H	20.65734580	7.99725304	19.39324904
O	15.33276458	10.63706065	20.28955935
H	14.71390103	9.89167711	20.43428692
O	17.45526064	8.21291173	19.70774209
H	16.95590531	8.10347562	20.56594921
O	21.17211202	20.32816130	12.51666515
H	21.30408143	21.32862474	12.36162527
O	23.71580462	22.27293996	13.47356101
H	29.07475163	24.27594604	9.76750990
O	17.78015737	2.89159461	10.36948627
H	17.88253347	3.35206796	9.52890335
O	26.39258238	19.65631845	16.59129302
H	5.44109220	10.78216250	22.28616207
O	22.05824392	19.78286574	19.71207459
O	19.69803438	16.88313128	21.10760586
H	20.29372868	16.25839829	21.56475385
O	23.46540112	14.12037674	22.00241761
O	18.63840607	9.42543395	12.22068154
H	18.65183257	9.17193019	11.28406637

O	19.41810346	12.12145875	13.04418018
H	19.36883967	11.31132619	12.49419142
O	22.35021612	9.08238148	11.17864966
H	21.94126357	9.92296699	10.92467619
O	21.78811217	9.27355274	15.92790411
H	22.45086186	8.79302580	16.50264866
O	22.12768349	6.25576198	15.91856727
H	22.68596723	6.55843838	15.18023092
O	19.96469913	5.03884662	16.45020122
H	20.76261514	5.60884228	16.29026770
O	23.50886308	3.83762789	14.73462841
H	24.00365221	4.31784548	15.49806269
O	21.95796707	4.37334056	18.58474952
O	18.39159898	3.62390488	18.65864832
H	22.44776824	3.95830635	19.32378159
O	22.38469027	16.50226880	13.47068731
H	22.02255363	19.35807837	11.02989808
O	24.89221292	17.16270591	12.96670504
H	24.87935787	17.99894486	12.47778116
O	22.03072441	18.50977473	10.53026726
H	22.93165090	18.37837155	10.19995693
O	28.25990416	18.09714618	14.07522812
H	28.18905274	18.39272440	13.15498447
O	25.10626462	16.41713697	16.96843520
O	23.56920239	13.19493377	18.73361201
H	23.27091510	9.07981891	18.43957113
O	22.23935837	10.44034903	19.25931713

H	21.60917308	9.82230102	19.65606933
O	23.67350635	8.47978192	17.77087126
O	21.83846677	2.37095094	11.62414027
H	21.47838968	3.39398397	11.49274348
O	20.90131050	4.70232423	11.48060615
H	19.98832326	4.45809288	11.24742823
O	23.85186594	6.45348231	10.59825677
H	24.36222008	7.16453230	10.17950055
O	24.79685026	4.63506190	16.80574129
H	26.10265639	0.78255783	24.52597197
O	23.78621764	0.88599260	19.26644304
O	24.52592870	23.35083159	19.26424696
O	4.88211483	23.28935270	19.78638772
H	4.03118186	23.65650067	20.07027361
O	24.95229372	9.82511991	11.48041776
H	24.02497916	9.50598245	11.22664811
O	24.42660132	13.66706279	10.66375082
H	24.63563682	13.42306090	9.75338994
O	14.94587556	11.04187556	12.66236228
H	14.70199151	10.11206249	12.51344418
O	10.52172250	4.91265721	10.80667454
H	10.61514158	3.95972870	10.66838140
O	14.69706655	4.10316902	19.92865637
H	14.50893837	3.12910717	19.76588070
O	0.26365734	0.33852514	25.03732250
O	26.69055263	22.95277688	11.18195530
H	26.49793514	22.43534932	10.38829100

O	27.42608595	21.33437856	14.44463125
H	27.11557121	20.63542886	15.05049745
O	29.43817724	23.16046433	11.26283916
H	28.49186030	22.83535322	11.30539514
O	25.31023374	0.67468498	9.26607479
H	25.91286114	1.35819580	8.93377827
O	17.40129488	22.48187588	15.03466438
H	16.55363756	22.77229505	14.66147874
O	17.55092511	20.86108460	20.43668987
H	16.58484315	20.95587996	20.59058050
O	26.79069118	19.85411274	19.62848350
H	26.09175206	19.19158067	19.51549343
O	11.30228284	14.20095149	24.66154278
O	16.25760622	13.78636257	20.65978866
H	13.15509837	13.34570454	21.30304680
O	14.18382041	2.42106841	15.03382535
H	14.19980686	2.38276175	14.06677017
O	16.77987456	1.34609235	13.32835976
H	16.17776677	2.10165921	13.42365646
O	16.54162314	4.70803944	12.00335054
H	17.05493161	4.05333955	11.43698072
O	13.64942307	4.51328658	12.66634689
H	14.49808060	4.32257500	12.22937196
O	19.48544654	23.03546475	19.03546033
O	21.37726438	21.26646152	22.22912939
H	22.19050919	21.36857671	21.67001181
O	16.01369831	2.35427843	22.22224059

H	15.19193364	2.81083692	21.97893259
O	1.31140779	2.70033472	20.29262448
H	0.59855894	3.30908712	20.66468160
H	29.01313385	19.45807209	25.22372646
O	25.23277123	8.55128105	21.41545219
H	26.15874326	8.50274274	21.76428711
H	24.64768770	8.48193250	22.20378747
O	28.69307946	18.58352896	25.55078257
H	2.64026762	17.92860694	25.01632711
H	4.05291581	24.18242845	24.36711738
O	9.63500957	19.51435712	21.62637227
H	10.38582636	19.83218300	21.00196324
H	10.12205324	19.10729043	22.36179372
O	7.86800294	21.20099411	22.66323756
H	8.54859339	20.62648893	22.18203298
H	7.60382890	20.62424221	23.41918902
O	28.66100234	21.66900950	18.96615308
H	27.47739678	16.21534097	21.07038697
H	28.76402444	22.58324721	18.64612520
O	5.25005776	18.57585949	22.59880840
H	5.99367175	18.77767043	23.21568986
H	4.69357231	17.89816973	23.06541731
O	19.49048171	11.44774798	24.22911644
H	18.81732836	10.80546593	23.87222220
H	20.35472352	11.16361666	23.87841768
O	23.61940705	12.58354725	24.58815498
H	23.34986538	13.34530983	25.14921921

H	24.45654688	12.21908028	24.95803147
O	25.93553437	4.37916759	21.11121084
H	25.88166755	4.75394850	22.01694845
H	25.04673446	3.95401727	20.94066871
O	2.61466595	12.58853328	19.41025654
H	1.96462924	13.28042451	19.61740116
H	5.61595150	14.65860872	22.97029281
O	4.95384020	14.74981369	22.21994068
H	10.40449578	13.28144440	23.82907830
H	4.68463328	13.81405320	21.98355951
O	3.26669779	0.73612754	21.70530538
H	2.49464199	1.18608638	21.31476434
H	3.49219362	1.26180906	22.52250033
O	14.35946684	17.21833645	24.44969830
H	13.54784160	17.59834397	24.02556635
H	14.07563403	16.34492782	24.82913541
O	8.71493288	4.10535319	22.43145956
H	9.38261463	4.48960159	21.82644142
H	23.63513992	2.35589914	20.02087927
O	2.57627100	9.49064357	25.55036448
H	3.51028462	9.17463313	25.47513687
H	2.48891511	10.12917355	24.80971910
O	9.19741069	3.23474997	25.55387882
H	10.03996033	3.38203801	26.02124808
H	8.88795138	4.15341888	25.32085730
O	8.07819497	10.43490142	20.95279338
H	7.48759980	10.73937748	20.21729683

H	8.28366691	9.51858703	20.65501219
O	9.98358807	18.09516258	18.48897269
H	18.48001923	15.94359409	24.60074913
H	10.15987636	18.52932287	19.34441292
O	15.85496916	2.22563536	24.74879752
H	15.92004348	2.26929721	23.68568676
H	16.72983328	2.54879810	25.04401817
O	1.35482993	8.61567900	22.29327097
H	1.68787870	9.52303110	22.54955467
H	27.81138381	8.13349358	23.14872841
O	8.87664115	1.42530654	21.25110238
H	8.53738238	0.51027745	21.29813893
H	4.48014215	1.20972101	20.64898428
O	11.27168807	4.97315279	21.10536938
H	11.65870562	4.31061583	21.70488931
H	11.37451315	5.87280601	21.61319747
O	14.58015658	5.37487712	22.28821916
H	15.56271910	5.28327082	22.37188418
H	14.42095705	4.88980217	21.42496251
O	9.77835412	12.65869089	23.26061969
H	10.31560740	9.48960075	23.71075571
H	9.50823984	13.19824271	22.48416139
O	12.40926901	16.49498448	20.66434952
H	12.72917777	15.55423185	20.75140738
H	8.54734831	13.05383482	20.37254054
O	19.33026225	16.41944950	24.66859112
H	5.42049874	18.08466089	21.02892587

H	13.21494213	17.00649092	20.85501560
O	10.97676926	22.94297284	21.63757715
H	11.67003512	22.35855246	22.00377313
H	10.38083956	23.14553107	22.40605264
O	6.78596868	1.67467872	23.48459733
H	6.54439328	0.68545156	23.58544010
H	6.04221729	2.10962256	23.94774574
O	18.52656965	3.48989618	24.81906320
H	19.00212469	2.72276279	24.40845016
H	19.07122933	3.77523495	25.56671992
O	13.75949803	9.89558330	23.11372711
H	16.77374878	10.11637034	24.01065542
H	16.81955842	7.17961224	22.48703798
O	11.62837058	7.12702987	22.52198006
H	10.87975529	8.49878851	22.58321406
H	11.32663192	6.82761240	23.39765550
O	22.71685545	5.12084504	23.10602817
H	22.01597074	5.71904007	23.44271378
H	22.82305324	5.46813292	22.18129604
O	25.14897481	22.54729406	22.82189655
H	24.60197002	23.22356497	23.25469539
H	24.55141031	22.09711353	22.16135191
O	15.30313484	12.71651422	23.40277665
H	14.35648572	12.57559039	22.99510583
H	15.32048254	12.14465007	24.18945694
O	16.69306327	15.40449267	23.63734483
H	16.30280470	14.50476338	23.66447649

H	15.93291279	16.01070395	23.75419391
O	10.12532900	0.07005614	24.37474643
H	14.12378456	21.43684368	21.03628281
H	11.02087842	-0.11665552	24.69746260
O	20.82218273	23.90126784	22.30456197
H	21.03349083	22.93350854	22.17332947
H	20.33740335	23.87722138	23.19122261
O	24.94091567	1.81718609	23.33537412
H	23.95239538	1.87555868	23.31934769
H	25.22660211	2.73541160	23.47518415
O	17.37895786	9.96995219	23.25992115
H	14.22047392	10.03598012	23.96190993
H	16.73535577	8.78228424	22.61473560
O	25.68812451	15.41167041	24.44632128
H	19.53791279	13.26046658	21.74731774
H	24.77719123	15.29659842	24.82246711
O	18.70838292	13.32203566	22.37063241
H	19.01344698	12.84661644	23.18779544
H	25.99324649	14.54389920	24.13075612
O	27.37184204	22.61546438	21.25253222
H	26.65278804	22.91154018	21.85346937
H	27.99869995	23.35198709	21.14334570
O	7.29564074	23.49103862	25.56315347
H	8.19302883	23.50514942	25.05545102
H	7.20958520	24.35224057	26.00359906
O	20.38322723	9.22239537	21.40948112
H	20.82165809	9.95487530	21.88195961

H	19.63611039	9.66746166	20.94694847
O	19.69326848	5.11819681	21.41400724
H	20.03119914	5.77187183	22.06264374
H	18.78074425	4.88579099	21.75103236
O	9.18806215	18.29987974	25.77257512
H	9.53032840	17.59496175	25.17173102
H	9.97324117	18.83811710	26.00660972
O	15.39389297	10.03177110	25.55494081
H	15.00517128	10.68851762	26.16835572
H	14.92987703	9.18032678	25.69466036
O	1.49357385	4.64498347	24.81850450
H	0.52704638	4.56891526	24.70930645
H	1.83238734	4.65636065	23.88676257
O	2.33894845	2.08672668	25.92585033
H	2.00637545	3.00338704	25.81823510
H	1.55806926	1.51812468	25.71566816
O	23.75102422	21.40582049	20.81140462
H	23.91826464	22.20378195	20.19059067
H	23.16568312	20.74549967	20.28690432
O	22.17649019	11.03052767	22.89586531
H	22.59645517	11.63741856	23.57142945
H	22.62932786	10.16692830	23.08938508
O	22.21759468	18.16866603	22.82097107
H	22.08780213	18.54205431	23.74967837
H	23.12512258	18.41046865	22.50306584
O	27.16840752	20.52688753	23.18616942
H	26.74234947	19.76417056	23.61480860

H	24.65507443	0.75843318	19.72331926
O	13.77042546	14.54168652	25.18552259
H	14.22438108	14.13514199	24.42414589
H	12.73042856	14.41252743	24.95410195
O	18.44215501	7.87355122	24.66303109
H	18.49435494	8.18318076	25.57963723
H	18.11753357	8.67830687	24.14860651
O	11.56053713	22.34533441	24.88900093
H	11.90304236	21.88167872	24.10098909
H	12.69310083	23.58120474	24.72003144
O	25.01603111	11.43497963	21.26995589
H	25.12194589	10.46265637	21.38033662
H	25.38178655	11.55591794	19.71186904
O	13.08303680	21.06638692	22.59469511
H	11.00644776	13.89505612	25.53586356
H	13.92440505	21.20278060	23.11299676
O	27.02361166	15.41178550	20.73355377
H	12.78476694	20.14792970	22.79504185
H	25.42530162	15.81430367	20.48029797
O	6.15726924	10.36580847	22.81505301
H	6.92837691	10.37252139	22.16634041
H	24.82167866	24.10157624	19.80197280
O	8.50587818	15.41753188	21.64389724
H	9.02121410	14.61110690	21.20647889
H	8.19173128	15.12376265	22.52654990
O	9.41209582	23.35918144	23.99208870
H	8.89608338	22.67976086	23.51098917

H	10.61978602	22.73690050	24.57455943
O	23.32018091	8.55559906	23.48459636
H	23.87629688	8.62571098	24.32124201
H	22.54237703	7.99380191	23.66816718
O	3.74025361	16.68682817	23.85237868
H	4.42380477	16.64980914	24.58677362
H	3.91782358	15.87880771	23.31029314
O	27.49799357	15.61242004	18.07701470
H	27.24295259	15.42942093	19.76107693
H	2.10483825	11.72529518	19.46122680
O	14.38559905	12.45498368	26.81565378
H	14.18143550	13.28500763	26.27764608
H	14.86829658	12.77289177	27.59386357
O	11.51138628	11.90694230	26.96620160
H	12.48312839	12.03084557	27.02683241
H	11.20017665	11.93009593	27.88360627
O	2.26656109	11.09254713	23.04044816
H	3.04033854	11.43507330	22.56476168
H	28.03155648	11.75109784	22.86122917
O	7.52889480	10.15014597	26.44947225
H	7.42194958	10.95798545	25.90027917
H	6.81410185	9.55166173	26.15167494
O	13.35445428	0.66406762	24.06881151
H	16.98704291	24.42075097	23.33820431
H	14.08076531	0.98831260	24.63108910
O	13.19421067	6.18844610	9.48731940
H	14.00884098	5.65918570	9.47503284

H	12.50956767	5.61708070	9.09238106
O	27.82579650	10.29144332	19.33744480
H	27.63898872	9.76277818	20.12830165
H	26.95957846	10.71857380	19.03816357
O	26.72104044	12.58587759	22.74055638
H	26.95560190	13.43303166	22.32861682
H	25.74497806	11.92157043	21.88559595
O	8.47789046	5.65848429	24.38593522
H	8.56186788	5.06945808	23.51284955
H	7.50903728	5.79369652	24.52721049
O	3.38418402	21.19067122	24.73339574
H	30.06550123	21.14440507	23.68144052
H	29.31307257	21.92527100	24.89054216
O	15.48337626	21.25440736	23.78196341
H	16.09299653	21.99843530	23.64753733
H	15.88891916	20.47116601	23.32562742
O	7.03736517	7.53583694	21.99102682
H	6.74416359	8.37102848	22.39342454
H	7.63203785	7.11201795	22.63442421
O	22.58094155	21.46432441	24.51794737
H	23.52130719	21.30829839	24.34428562
H	21.80334331	21.32690465	23.17806234
O	28.23209141	17.83819184	21.85782231
H	27.62167254	17.80082350	22.64465961
H	29.05986495	17.46080011	22.20138258
O	24.44377299	16.01487632	20.36918664
H	24.37158620	16.95972189	20.61903640

H	23.91731372	14.85247759	21.49675258
O	25.97209736	0.74097543	20.89838388
H	26.66507118	1.35600679	20.55263552
H	25.64955602	1.16950696	21.72787748
O	14.61791739	4.71320653	25.03553298
H	14.43677502	4.79888515	24.07061620
H	15.07012866	3.83373751	25.09555023
O	25.05445339	8.88656477	25.48135170
H	25.83875410	8.29790925	25.42549371
H	25.42673975	9.78574988	25.32699214
O	11.67385804	19.84274712	25.93640067
H	11.55882699	20.81157828	25.74608302
H	12.59576525	19.74991482	26.27586082
O	17.27409921	4.64455048	22.51927676
H	16.88372364	3.72064025	22.29246460
H	17.59982942	4.51933737	23.43443131
O	13.96942791	7.53152751	24.96567083
H	13.01176867	7.44414025	25.13050017
H	14.34250805	6.66317497	25.22869380
O	5.26127605	8.61824226	25.03787889
H	5.37544883	7.66736534	24.77771211
H	5.50224155	9.13064498	24.23996049
O	12.84042712	12.37792789	22.44417551
H	12.38323164	12.85228734	23.16461890
H	13.37662683	10.78075790	22.85538601
O	22.27588037	23.62850248	25.70579157
H	22.45273875	22.66671604	25.25578178

H	22.58212330	23.57927438	26.62240648
O	16.25225226	18.77734733	22.81647406
H	16.15585323	18.19324547	21.97323883
H	15.72960524	18.27801226	23.47480300
O	17.53464972	23.42982221	21.63755302
H	17.79965574	22.51628557	21.38657572
H	16.79130183	23.61308552	21.00578464
O	23.07932153	15.14179452	25.33690746
H	22.63847193	15.72879379	26.01344937
H	22.48851563	15.25305769	24.55569802
O	22.97417245	6.53521413	20.66134580
H	23.60296250	7.27017238	20.79474702
H	22.17599471	6.93468700	20.22533048
O	22.20971401	2.35465597	22.96665572
H	22.11767679	3.31762973	23.15029153
H	21.34058065	1.93358299	23.16438310
O	5.69471192	20.92898241	26.37167712
H	4.85624757	21.13355244	25.89151041
H	6.19478381	21.76749475	26.41694112
O	4.63694992	12.25446828	21.25541485
H	5.45552637	12.46385285	20.70512940
H	3.90617912	12.31133741	20.58376475
O	11.93195622	4.36889858	25.77711018
H	11.55339997	5.28296367	25.76432701
H	12.90890476	4.48929724	25.73148617
O	18.99588771	7.06730989	10.21972093
H	18.40004917	6.84540153	10.98384830

H	18.52549967	6.77213248	9.42689598
O	10.28348276	16.49248498	23.85481492
H	9.85071007	16.28385513	23.00410642
H	10.67043738	15.60392847	24.20400148
O	24.63644969	18.64119598	21.63586510
H	25.37187653	18.56858051	22.27002050
H	24.71514026	19.52765680	21.22585506
O	21.43373005	15.55814066	23.05076201
H	21.86902564	16.43824430	22.91726996
H	21.97932893	14.90482124	22.54724254
O	25.38446490	5.24946663	23.84548310
H	25.66420640	6.16542280	24.01819109
H	24.39813845	5.29115018	23.74111364
O	2.52951283	4.65413385	22.22284064
H	2.68773137	5.49181607	21.69529024
H	2.27357913	3.99820248	21.54721209
O	19.63959007	23.75551972	24.73787728
H	16.22126560	0.47536304	24.88873745
H	20.45420881	23.63060128	25.27812064
O	10.09979676	9.49713046	25.70296285
H	9.16235425	9.67083922	25.99527956
H	10.62537267	10.22442141	26.09207345
O	6.87966371	14.75035865	24.01532289
H	6.68617298	15.29438843	24.80379272
H	7.04469065	13.80612102	24.33171909
O	25.62370061	6.45421380	19.03496824
H	25.87763917	5.87791851	19.78693718

H	25.75654501	7.37711963	19.31336659
O	3.26101792	6.93238619	20.81714596
H	2.83907413	7.08223629	19.89462946
H	2.88924364	7.65958086	21.35784079
O	12.03429687	18.57012225	23.55560846
H	11.84291103	19.00386874	24.43476199
H	11.44880608	17.76023076	23.54016446
O	19.69779984	1.14578907	23.70780278
H	19.58147991	0.55968432	24.51134850
H	19.07226757	0.74817228	23.05596297
O	3.99621232	2.35263374	23.78380054
H	3.82076100	3.24932269	23.44517590
H	3.38852574	2.23277110	24.57017018
O	5.45942454	23.08250466	23.71612125
H	4.93775738	22.35586720	24.11034646
H	6.17256150	23.29578430	24.39904359
O	14.49533441	19.45340783	26.29982833
H	14.56130566	18.62592910	25.77560043
H	14.93939655	20.12576377	25.75447914
O	7.03840551	19.31445404	24.60247716
H	6.59094185	19.88928022	25.28162046
H	7.90434765	19.00618948	25.02673537
O	27.45643970	7.47431983	24.88701778
H	1.55438710	8.16788224	25.23491665
H	1.31071613	6.59761252	25.07649883
O	4.33145523	18.37121890	27.63112128
H	4.77464054	19.23830228	27.59118574

H	3.47975696	18.50688785	27.16846396
O	5.68572427	16.89102568	25.70330936
H	5.26553782	17.27069107	26.52077383
H	6.22894231	17.63695646	25.36805800
O	11.79890981	2.89458313	23.40881993
H	12.44177126	2.16094863	23.56755365
H	11.86976465	3.48399848	24.20888347
O	21.54977700	19.24068441	25.18835394
H	21.99634490	20.17137460	25.04731086
H	20.59909330	19.41156110	25.06619683
O	18.94308727	18.97258747	23.47785185
H	19.06921485	18.08011723	23.88907784
H	17.97315839	18.97589591	23.26247877
O	7.42783066	12.23745569	24.51837711
H	6.90940830	11.64671791	23.91540750
H	8.34073191	12.27760588	24.10988450
O	20.69109215	7.13968517	23.26140230
H	20.56578799	7.82184301	22.55317147
H	19.94219134	7.34938267	23.88811807
O	5.71166530	5.91783392	24.36449635
H	5.60305840	5.45540864	23.39915354
H	5.28933272	5.31326698	24.99253909
O	21.52392398	16.83254016	26.74818783
H	20.65640836	16.58159918	26.37760410
H	21.66211279	17.73537793	26.38327321
O	26.46766375	17.89381480	23.93587285
H	26.13318017	16.95982432	24.09745358

H	27.08153943	18.07531683	24.68940486
O	10.70268448	6.79913040	25.40847373
H	10.52969692	7.72969996	25.68745701
H	9.83071805	6.47514572	25.04728156
O	18.67218427	16.41504411	11.19095555
H	18.12325123	20.53806501	12.50316995
H	18.43111305	16.30749002	10.25818375
O	26.13436451	11.51233370	25.04284679
H	26.80299870	11.70509747	25.71714468
H	26.42608841	12.00660318	24.20028511
C	14.10868738	14.59055195	11.28225053
O	13.18919032	13.86013205	10.81308209
O	15.05166263	15.20437449	10.74061708

Reference:

- (1) Martin, M. G.; Siepmann, J. I. Novel Configurational-Bias Monte Carlo Method for Branched Molecules. Transferable Potentials for Phase Equilibria. 2. United-Atom Description of Branched Alkanes. *J. Phys. Chem. B* **1999**, *103* (21), 4508–4517. <https://doi.org/10.1021/jp984742e>.
- (2) Martin, M. G.; Thompson, A. P. Industrial Property Prediction Using Towhee and LAMMPS. *Fluid Phase Equilibria* **2004**, *217* (1), 105–110. <https://doi.org/10.1016/j.fluid.2003.06.007>.
- (3) M. G. Martin; “MCCCS Towhee: a tool for Monte Carlo molecular simulation”, *Mol. Simulat.* **39** 1212-1222 (2013) (accessed 2018 -09 -29).
- (4) Berendsen, H. J. C.; Postma, J. P. M.; van Gunsteren, W. F.; Hermans, J. Interaction Models for Water in Relation to Protein Hydration. In *Intermolecular Forces: Proceedings of the Fourteenth Jerusalem Symposium on Quantum Chemistry and Biochemistry Held in Jerusalem, Israel, April 13–16, 1981*; Pullman, B., Ed.; The Jerusalem Symposia on Quantum Chemistry and Biochemistry; Springer Netherlands: Dordrecht, 1981; pp 331–342. https://doi.org/10.1007/978-94-015-7658-1_21.
- (5) Harris, J. G.; Yung, K. H. Carbon Dioxide’s Liquid-Vapor Coexistence Curve And Critical Properties as Predicted by a Simple Molecular Model. *J. Phys. Chem.* **1995**, *99* (31), 12021–12024. <https://doi.org/10.1021/j100031a034>.
- (6) Qomi, M. J. A.; Bauchy, M.; Ulm, F.-J.; Pellenq, R. J.-M. Anomalous Composition-Dependent Dynamics of Nanoconfined Water in the Interlayer of Disordered Calcium-Silicates. *The Journal of Chemical Physics* **2014**, *140* (5), 054515. <https://doi.org/10.1063/1.4864118>.
- (7) Youssef, M.; Pellenq, R. J.-M.; Yildiz, B. Glassy Nature of Water in an Ultraconfining Disordered Material: The Case of Calcium–Silicate–Hydrate. *J. Am. Chem. Soc.* **2011**, *133* (8), 2499–2510. <https://doi.org/10.1021/ja107003a>.