

Absorption Spectra of Benzoic Acid in Water at Different pH and in the Presence of Salts: Insights from the Integration of Experimental Data and Theoretical Cluster Models

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Simulation pH = 2.5

PhCOOH			
C	0.5008167286	-1.2184481684	0.0015685468
H	-0.0315152550	-2.1645435929	0.0030493814
C	1.8940193317	-1.1768767554	0.0016549940
H	2.4631554180	-2.1027694748	0.0033188169
C	2.5574435184	0.0551432175	-0.0003942490
H	3.6442265406	0.0866725574	-0.0003395998
C	1.8246944002	1.2463037687	-0.0025172562
H	2.3398656678	2.2033112241	-0.0041613470
C	0.4297550929	1.2102572479	-0.0025489954
H	-0.1431334014	2.1314305794	-0.0041997460
C	-0.2371980580	-0.0248701059	-0.0005699326
C	-1.7205587719	-0.1198075165	-0.0008557405
O	-2.3554918150	-1.1579183129	0.0012489724
O	-2.3360080818	1.0932657449	0.0004611239
H	-3.2951221653	0.9176638271	0.0014389430
PhCOOH_(H2O)			
C	3.2252481194	-0.0294890982	-0.0123923464

C	2.5478805118	1.1960714777	-0.0073224083
C	1.1533025816	1.2217531161	0.0014478486
C	0.4282133908	0.0196408323	0.0050862222
C	1.1090144832	-1.2086790117	0.0004770543
C	2.5050081157	-1.2296417790	-0.0083980872
C	-1.0577041406	0.0907069445	0.0157987465
O	-1.6586751840	-1.1081133982	0.0120856489
O	-1.6805924763	1.1512678460	0.0254319420
O	-4.1626069806	-0.0466676711	0.0630382889
H	3.1068443958	2.1281814174	-0.0097425662
H	0.6094537388	2.1612125775	0.0067068124
H	0.5436242205	-2.1344450271	0.0048714449
H	3.0307741266	-2.1808748354	-0.0114889422
H	4.3123327594	-0.0490006615	-0.0188222558
H	-2.6435839288	-0.9703108681	0.0179084352
H	-4.7389932793	-0.0042760203	-0.7143742069
H	-3.5906726989	0.7517980602	0.0388399173

PhCOOH_(H2O)₂

C	3.7622151910	0.0943426133	0.0002726034
C	3.0205023227	1.2815613840	0.0312732010
C	1.6263122270	1.2331586935	0.0310483974
C	0.9653269587	-0.0049813134	-0.0000642097
C	1.7113652418	-1.1943778320	-0.0311522220
C	3.1063919353	-1.1417359956	-0.0310436351
C	-0.5246473949	-0.0191652951	0.0012482107
O	-1.0511369248	-1.2384689822	-0.0124724046
O	-1.1907266478	1.0184338667	0.0134521785
O	-3.7144639990	-1.3084497655	-0.0560477421
O	-3.9103550070	1.3637508809	0.0478495030
H	3.5290099966	2.2418619599	0.0560091822
H	1.0338931666	2.1424610456	0.0559609002
H	1.1952545560	-2.1479899833	-0.0562126715
H	3.6817205066	-2.0635770620	-0.0557635930
H	4.8488429243	0.1326336272	0.0004133508
H	-2.0595806436	-1.2233119818	-0.0200217389
H	-4.0005297502	-0.3570521237	-0.0332648853
H	-4.1037557351	-1.7350993244	0.7214537757
H	-2.9223412733	1.3782777021	0.0397989982
H	-4.1997935261	1.8628424132	-0.7297153574

PhCOOH_(H2O)₃

C	4.2884578746	0.2094832339	-0.0542239994
C	3.4824216699	1.3532312636	-0.0023072721
C	2.0933403422	1.2265629990	0.0291270182
C	1.5017736273	-0.0460241907	0.0085502807
C	2.3121355948	-1.1916072008	-0.0443712537
C	3.7018067720	-1.0610946444	-0.0752853419
C	0.0136698523	-0.1445194528	0.0395680878
O	-0.4422431273	-1.3884761064	0.0012941290
O	-0.7083076010	0.8518395305	0.0956420021

O	-3.0273678387	-1.9005963152	0.0932409152
O	-4.8797209088	0.0351574691	-0.1542347578
O	-3.1573414326	2.0933026975	-0.0262986372
H	3.9364885263	2.3406626783	0.0126311443
H	1.4516271434	2.1013365418	0.0674946969
H	1.8490550088	-2.1722388999	-0.0626697851
H	4.3267958724	-1.9494449006	-0.1169464573
H	5.3709717367	0.3082006164	-0.0794939144
H	-1.4495533228	-1.4418412274	0.0317619202
H	-3.7322445705	-1.2051819409	-0.0210313672
H	-3.2593722451	-2.3930796162	0.8939112497
H	-2.2878807534	1.6302437954	-0.0008950777
H	-3.1851262604	2.6504225216	0.7650180832
H	-5.3240326770	0.0569596454	-1.0144037694
H	-4.3291355916	0.8623942338	-0.1030837269

PhCOOH_(H2O)₄

C	4.6207911102	0.1619260700	-0.0005460578
C	3.8407537422	1.3247497400	-0.0001921328
C	2.4486821353	1.2306623383	0.0002740521
C	1.8279321864	-0.0282688310	0.0004439795
C	2.6125929167	-1.1928884366	0.0000362009
C	4.0052069013	-1.0950586218	-0.0004235582
C	0.3375814099	-0.1003198603	0.0011072290
O	-0.1449906129	-1.3235209656	0.0004505574
O	-0.3565943245	0.9265605229	0.0008173995
O	-2.6892680422	-1.6641117521	-0.0004565921
O	-2.9135405136	1.6956372052	0.0004433260
O	-3.8540635351	-0.0553032583	-1.9280000166
O	-3.8554540503	-0.0564522320	1.9272256806
H	4.3176529920	2.3014951330	-0.0002792446
H	1.8278246840	2.1211089870	0.0005792358
H	2.1263249462	-2.1623820644	0.0001578229
H	4.6099654552	-1.9981917999	-0.0006864803
H	5.7055811872	0.2354499703	-0.0009140428
H	-1.1766413961	-1.3738096611	0.0001263207
H	-3.1383397450	-1.2652832269	-0.7825636125
H	-3.1388921916	-1.2657571939	0.7815776882
H	-1.9693802126	1.3749111450	0.0007520899
H	-2.8779203662	2.6634106355	0.0006038595
H	-3.4292886235	0.0512606207	-2.7913074518
H	-3.6110139139	0.7337561328	-1.3937619453
H	-3.4312117778	0.0497148664	2.7908444635
H	-3.6122018327	0.7329323988	1.3935672296

PhCOOH_(H2O)₅

C	4.5663567448	-0.8415294209	0.0734684729
C	4.3579304835	0.5431020101	0.0706247479
C	3.0607500668	1.0533496515	0.0258144204
C	1.9625803354	0.1796681683	-0.0163503097
C	2.1746876152	-1.2087014382	-0.0128371849

C	3.4742456556	-1.7158051136	0.0318197405
C	0.5946760097	0.7632718799	-0.0627018305
O	-0.3850072359	-0.1420907288	-0.1039090940
O	0.3896321306	1.9762701369	-0.0689522209
O	-2.8525773081	0.7599510644	-0.2063961177
O	-3.5836972144	-0.7929366066	1.8552645789
O	-2.0404708729	3.3086757802	0.0129476507
O	-2.0562921531	-2.5079663273	0.3927603619
O	-3.3785188144	-1.4197798081	-1.7841105126
H	5.2058586056	1.2221516683	0.1039040551
H	2.8790307547	2.1234782807	0.0246622359
H	1.3259045176	-1.8832300113	-0.0458436154
H	3.6343750642	-2.7906622621	0.0353079481
H	5.5780005680	-1.2381713651	0.1086693471
H	-1.3039358353	0.2918923609	-0.1399821173
H	-3.2533824112	0.3789896859	0.6215992743
H	-2.8089014690	1.7471246852	-0.1290265379
H	-2.4848974397	-2.3044395086	-0.4718571102
H	-1.2192416926	-2.0137933737	0.3674526792
H	-4.4954583620	-1.1060336604	1.9442361551
H	-3.0644393486	-1.5451398272	1.4627401988
H	-2.1053087731	3.9751382909	-0.6858622818
H	-1.1172053855	2.9639499484	-0.0078935737
H	-3.2976236045	-0.5059954688	-1.4265639045
H	-3.0427976712	-1.3973144035	-2.6914219550

PhCOOH_(H2O)₆

C	2.5218476502	-1.3351458173	-0.2203434672
C	2.4680799917	0.0564525846	-0.0380947313
C	3.6462441871	0.7730663276	0.2257667576
C	4.8672349937	0.1038859801	0.3075367938
C	4.9182194890	-1.2834679195	0.1245974926
C	3.7459510615	-2.0008656677	-0.1392564958
C	1.1858314859	0.8059343195	-0.1192973701
O	1.1194225572	2.0279938611	0.0054905371
O	0.1186050738	0.0361198324	-0.3433610015
O	-2.2260302882	1.1940101145	-0.3986595001
O	-1.1383661452	3.6322455576	-0.0881194126
O	-3.3702128440	-0.2138366657	1.6795794199
O	-5.3654239831	-1.0480688962	0.1261717892
O	-3.3397383251	-1.1332581229	-1.6248641133
O	-1.6738325970	-2.0876150054	0.3950854744
H	-0.7485083996	0.5695206464	-0.3824578853
H	-2.0638022460	2.1687939477	-0.3210154914
H	-2.6744630858	0.8883966495	0.4258206187
H	-3.5989850842	0.1070413100	2.5641301960
H	-4.2143817043	-0.5326225891	1.2453867924
H	-1.0866020332	4.2850072617	-0.8010877098
H	-0.2611804825	3.1836423545	-0.0492389971
H	-4.7409966897	-1.1307116842	-0.6520712105
H	-5.7736632310	-1.9178767875	0.2452924939

H	-2.6999434794	-1.6142480368	-1.0465981544
H	-3.0331172622	-0.2071501669	-1.5800425164
H	-2.1512401039	-1.5643412809	1.0713930119
H	-0.8433105406	-1.6026952924	0.2445704559
H	3.5845652363	1.8478922677	0.3643625470
H	5.7777182109	0.6610145317	0.5121084363
H	5.8703106150	-1.8046238275	0.1873532173
H	3.7852627610	-3.0773267389	-0.2826878488
H	1.6123823421	-1.8882453729	-0.4293127397

PhCOOH_(H2O)₇

C	2.8061019887	-0.7740215446	0.6871502178
C	2.2336329220	0.4308664563	0.2470072874
C	3.0504472224	1.4326427613	-0.3009862922
C	4.4263261366	1.2326202614	-0.4067231723
C	4.9941587486	0.0298226252	0.0309967482
C	4.1831931019	-0.9717643619	0.5762540240
C	0.7703610543	0.6787123204	0.3380743198
O	0.0851338225	-0.3125127689	0.9026744785
O	0.2483194363	1.7154930022	-0.0734714063
O	-2.5025870554	-0.2113174793	1.0018040400
O	-3.1237783108	0.0869622850	-1.5504272464
O	-2.1813614101	2.6600862149	-0.8131570543
O	-1.3191063846	-1.6275200773	-2.6493591483
O	-0.4354037669	-2.8414100873	-0.3897122432
O	-3.5055156866	2.2597746724	1.5762134829
O	-2.6226392190	-2.9345450782	1.2987306979
H	-0.9238910364	-0.1393817031	0.9414289517
H	-1.3003258305	2.3168690566	-0.5155806492
H	-2.0066181698	3.5014606142	-1.2599293196
H	-2.8033460464	-0.1681970724	0.0387697508
H	-2.8999781887	0.5952675222	1.4160966613
H	-4.4689527665	2.3212041865	1.4992604976
H	-3.1370319568	2.5915476679	0.7235639372
H	-2.5003876153	-0.4979714959	-2.0537064862
H	-2.8152644041	1.0074794976	-1.6582467024
H	-1.6437611817	-2.2773483986	-3.2890208528
H	-0.9920721852	-2.1461893408	-1.8641181521
H	-1.2097310035	-3.0387234087	0.1903812560
H	-0.0014586860	-2.0885869278	0.0506238189
H	2.5911464402	2.3566639053	-0.6373805972
H	5.0557346308	2.0104774065	-0.8308681316
H	6.0666520049	-0.1268089266	-0.0539052183
H	4.6224633937	-1.9066919063	0.9135910243
H	2.1766308697	-1.5488952972	1.1117648564
H	-2.7280551819	-1.9558771904	1.3641970819
H	-2.5179115689	-3.2651718445	2.2023485276

Simulation pH = 8.0

PhCOO⁻

C	0.42814171	-1.20551348	0.00213588
H	-0.14213234	-2.13076234	0.00377626
C	1.82787645	-1.20652485	0.00129756
H	2.37247133	-2.15091538	0.00250759
C	2.53258157	0.00491716	-0.00111171
H	3.62220407	0.00766598	-0.00185445
C	1.82176256	1.21278429	-0.00257570
H	2.36155820	2.15992689	-0.00450873
C	0.42203686	1.20470858	-0.00152782
H	-0.15290809	2.12707162	-0.00240393
C	-0.29404804	-0.00222653	0.00078053
C	-1.84777582	-0.00621430	0.00180962
O	-2.38627911	-1.14547896	0.00188811
O	-2.39226675	1.13012660	0.00245384

PhCOO⁻·(H₂O)₁

C	3.2124105685	-0.0158729675	0.0020922178
C	2.5140739655	1.1988053546	0.0009130267
C	1.1150161569	1.2044886907	0.0003203780
C	0.3915743966	0.0026007156	0.0007631280
C	1.0991371332	-1.2086310442	0.0018517466
C	2.4982341748	-1.2212428023	0.0025921227
C	-1.1480347723	0.0130328528	0.0001526280
O	-1.7110927768	-1.1181379453	-0.0011881970
O	-1.6958793579	1.1515819784	0.0010264549
O	-4.3109140350	0.0324675469	-0.0108884563
H	3.0622582662	2.1403994013	0.0004834215
H	0.5505543547	2.1327535785	-0.0003949765
H	0.5225941371	-2.1294629270	0.0020574475
H	3.0339440844	-2.1699878543	0.0035455591
H	4.3016208231	-0.0230207399	0.0026248611
H	-3.6629832040	-0.7047941263	-0.0083469242
H	-3.6545246944	0.7620626776	-0.0075478666

PhCOO⁻·(H₂O)₂

C	3.7383985151	0.1076317402	0.0095728540
C	3.0055643123	1.2968118547	0.1129213437
C	1.6070626333	1.2631672969	0.0967499444
C	0.9217320612	0.0455092529	-0.0246529544
C	1.6629085516	-1.1406526024	-0.1286497018
C	3.0612047708	-1.1127973952	-0.1109333091
C	-0.6122271742	0.0063362182	-0.0401990947
O	-1.1443445729	-1.1269325836	-0.1618254093
O	-1.1916409645	1.1289280899	0.0690181707
O	-3.9286484410	-1.4440979030	0.2567850371
O	-3.8667652809	1.4228935356	-0.1254370058

H	3.5255372778	2.2492152095	0.2078190318
H	1.0172361088	2.1714631695	0.1795898764
H	1.1147044534	-2.0738006683	-0.2216343752
H	3.6248778461	-2.0413674261	-0.1908278587
H	4.8270949147	0.1316398818	0.0235416559
H	-2.9538516352	-1.4299472696	0.1066729930
H	-4.1336610539	-0.4895928246	0.3132556412
H	-2.8782935253	1.3154882354	0.0063206426
H	-3.9855304970	1.2612483260	-1.0728342914

PhCOO \cdot ·(H₂O)₃

C	4.0135479300	0.0572823158	-0.3515878104
C	3.4176877848	1.2959455216	-0.0817971371
C	2.0305052519	1.3887171565	0.0680684890
C	1.2219916398	0.2489435693	-0.0498092711
C	1.8252597799	-0.9880640807	-0.3182036211
C	3.2122920266	-1.0852583724	-0.4693512619
C	-0.2943282787	0.3558069748	0.1096025306
O	-0.9494580180	-0.7289918975	0.0041085988
O	-0.7634090088	1.5022415001	0.3297707302
O	-3.3363763749	-1.2098639114	1.3791722188
O	-3.4208019580	-0.4636229810	-1.4257453095
O	-3.5278745286	1.5643821274	0.5672112218
H	4.0354359613	2.1878054164	0.0116494238
H	1.5448168536	2.3376798491	0.2758550328
H	1.1828730370	-1.8593813222	-0.4052627511
H	3.6697929546	-2.0508722732	-0.6791193938
H	5.0934629879	-0.0170329571	-0.4695458368
H	-2.3996444581	-1.0694389072	1.0995449965
H	-3.7643310813	-1.3119453167	0.5072213766
H	-2.5441212890	1.6524197186	0.4804198748
H	-3.6188919459	0.7659213469	1.1269547526
H	-2.4927366326	-0.6217246505	-1.1445228639
H	-3.6192356167	0.3827814979	-0.9659000179

PhCOO \cdot ·(H₂O)₄

C	4.4690847155	0.0199861822	-0.0097958059
C	3.8136774735	1.2138619684	-0.3364859225
C	2.4226440598	1.3024051732	-0.2263421848
C	1.6702579939	0.2012355970	0.2072236720
C	2.3325522372	-0.9911353220	0.5322707695
C	3.7237858292	-1.0827523169	0.4257936868
C	0.1521872589	0.2949595505	0.3243095365
O	-0.4588365284	-0.7497905440	0.6917523712
O	-0.3663947380	1.4154111526	0.0485040490
O	-2.7621130328	-1.9743291542	-0.5257532468
O	-3.0011103581	1.7228791392	0.1232762301
O	-3.9736247529	0.1007120887	-2.0820231246
O	-3.0104917457	-0.4881928921	1.8907180674

H	4.3875654238	2.0740707184	-0.6771371963
H	1.8928138627	2.2172852414	-0.4740590048
H	1.7330592976	-1.8335078125	0.8643701827
H	4.2278963394	-2.0134227720	0.6806672488
H	5.5521171035	-0.0508791660	-0.0953651679
H	-1.8510895564	-1.6425262909	-0.3848380381
H	-3.5809753137	-0.7127086739	-1.6952332642
H	-3.1893031538	-1.6769716156	0.3053938407
H	-2.0033281170	1.5726629819	0.0689723066
H	-3.1086840615	2.6659446598	0.3090051351
H	-3.7178041387	0.7859376739	-1.4340105386
H	-2.0535964522	-0.5743998921	1.6736553527
H	-3.2488938882	0.3353016159	1.4165311662

PhCOO⁻·(H₂O)₅

C	4.4411660495	-0.8832418912	0.0385789508
C	4.2391095034	0.4743276983	-0.2408918690
C	2.9425565228	0.9923799907	-0.2966209875
C	1.8339737988	0.1631065628	-0.0712968851
C	2.0425326836	-1.1951842010	0.2080212424
C	3.3389440325	-1.7164917588	0.2624535983
C	0.4302462462	0.7428420866	-0.1372974402
O	-0.5371086935	-0.0544460839	0.1377677788
O	0.3015037205	1.9466614092	-0.4505540995
O	-2.6584685664	1.0967794387	1.5718738953
O	-4.0584526241	-1.0746636323	0.5657345873
O	-2.4246205651	2.6692901915	-0.7402855215
O	-1.6414375135	-2.5321325264	-0.1194266642
O	-2.6906589142	-0.0535791781	-1.6815007996
H	5.0921870740	1.1267772889	-0.4177652905
H	2.7611147073	2.0405419963	-0.5152061683
H	1.1813470236	-1.8342085293	0.3755308786
H	3.4881511663	-2.7728391700	0.4769277825
H	5.4503943325	-1.2891387264	0.0801376187
H	-1.8223074373	0.6886066677	1.2525637665
H	-3.7012794445	-0.2936613689	1.0592875291
H	-2.7821546264	1.8063304145	0.8987111841
H	-1.9399714316	-2.3364221246	-1.0237474859
H	-1.0842368836	-1.7449654461	0.0906068473
H	-3.3304864740	-1.7300924219	0.5886218583
H	-2.7064681960	1.9024964534	-1.2816346688
H	-1.4498219352	2.5337984790	-0.6538260866
H	-3.3737433651	-0.3588627187	-1.0406868186
H	-1.8814050798	-0.0031853528	-1.1235125887

PhCOO⁻·(H₂O)₆

C	2.4000942114	-1.2926543499	0.1743838203
C	2.4179447031	0.1026923661	0.0333143143
C	3.6501596366	0.7603375493	-0.0918977966

C	4.8463039358	0.0371194934	-0.0768636117
C	4.8219844639	-1.3558121580	0.0665433449
C	3.5950316772	-2.0183812501	0.1919367298
C	1.1205412084	0.8982793571	0.0220783331
O	1.2094769216	2.1510935898	-0.0828596057
O	0.0446129600	0.2325554785	0.1215938880
O	-2.3883741388	1.3598152857	0.1429106106
O	-0.9890126839	3.7250916872	-0.2897671356
O	-3.4623610774	-0.6623238240	1.7636331887
O	-5.3755583709	-1.4804248462	-0.1951339960
O	-3.2466688972	-0.6134286332	-1.6231720037
O	-1.5862093621	-1.9976683771	0.1383081056
H	-1.4698451280	0.9661017838	0.1544380467
H	-2.1916823596	2.3193642080	0.0571976187
H	-3.1726565648	0.1933350437	1.3737744128
H	-4.2531036838	-0.9125192630	1.2383010765
H	-1.0165183556	3.8611976950	-1.2478618095
H	-0.1746998717	3.1587681611	-0.1493667309
H	-4.6799697267	-1.1383767121	-0.8276525598
H	-5.2717089447	-2.4429863929	-0.2183524675
H	-2.5948216285	-1.2188680229	-1.1892080741
H	-3.0475623365	0.2440938668	-1.1790373681
H	-2.1836007919	-1.6646528732	0.8508568278
H	-0.8468492233	-1.3500594434	0.1343446327
H	3.6446303805	1.8410209679	-0.1981142627
H	5.7971126593	0.5581828580	-0.1750074957
H	5.7523680530	-1.9207910946	0.0811510385
H	3.5683606929	-3.1005293291	0.3041924689
H	1.4430378678	-1.7959573688	0.2721734799

PhCOO⁻·(H₂O)₇

C	2.6885493175	-0.8442388045	0.4173550029
C	2.2611574972	0.4665515715	0.1591086658
C	3.2179385283	1.4520049203	-0.1264909656
C	4.5791573453	1.1364027565	-0.1481696088
C	4.9991952742	-0.1746749035	0.1089168602
C	4.0494565910	-1.1638522198	0.3890862561
C	0.7820458019	0.8232907887	0.1784042464
O	-0.0265112876	-0.0901302397	0.5334217619
O	0.4702976366	1.9969160446	-0.1563087866
O	-2.7084391413	-0.2921735467	1.0291595784
O	-3.2797267820	0.2121872845	-1.5955687349
O	-2.0178059333	2.5943784042	-0.8447018282
O	-1.7224618985	-1.8685087004	-2.6485415853
O	-0.3711248456	-2.6236590358	-0.4112927756
O	-3.4818250912	2.4137730630	1.6629689277
O	-2.5016134254	-2.9468190784	1.3821973947
H	-1.7455663646	-0.0852388778	0.9061881420
H	-1.0970608586	2.3361207398	-0.5233513186
H	-1.8822678356	3.3569682940	-1.4240459005

H	-3.0766750099	-0.1710732033	0.1137518178
H	-3.3169983329	1.4484807436	1.6643802940
H	-3.0412340120	2.6921634932	0.8367306714
H	-2.6552811911	-0.4167542244	-2.0263311737
H	-2.8158878719	1.0760907382	-1.5198756028
H	-2.4108627244	-2.5423312429	-2.7471018863
H	-1.1812018724	-2.1685167068	-1.8644512299
H	-1.0943705361	-2.8947544811	0.2001371143
H	-0.1198325034	-1.7253672868	-0.0808339299
H	2.8699213008	2.4602139543	-0.3296901204
H	5.3125442094	1.9101428683	-0.3681758274
H	6.0586878698	-0.4237693125	0.0885888024
H	4.3675979139	-2.1863527368	0.5827123103
H	1.9480973850	-1.6084479763	0.6296697551
H	-2.6811770165	-1.9646130668	1.2879129056
H	-2.1571125442	-3.0501101443	2.2809933730

PhCOO⁻·(H₂O)₈

C	-3.9680724949	1.1739174404	-0.2931586848
C	-2.8681865734	0.5625843526	-0.9011958132
C	-2.0966622582	-0.3751834142	-0.2004250515
C	-2.4471250152	-0.6993720653	1.1190822006
C	-3.5378762747	-0.0786986767	1.7346366258
C	-4.3016738852	0.8608231229	1.0296466057
C	-0.8497199704	-0.9743273548	-0.8304333779
O	-0.3053451018	-1.9402891749	-0.2184026434
O	-0.4218348285	-0.4401142974	-1.8941575415
O	2.2140374123	0.5549814082	-1.8334625569
O	3.9270207243	-1.3420221009	-0.8747070754
O	2.6165499823	2.1464021615	0.3886867826
O	1.9241850009	-3.3083467685	-0.9402254553
O	-0.1907520667	2.2543909124	-1.6148673611
O	-0.2459984019	1.9184032673	1.0947679910
O	0.8241159276	-0.5904671348	2.0019321200
O	3.5781601341	-0.1850242782	1.6353379254
H	2.4094872325	1.5929900733	-0.4077518603
H	1.7754287121	2.2283083233	0.8692195241
H	-0.3844839459	1.3119135072	-1.8535756546
H	1.3858455690	0.0288311553	-1.8849079691
H	2.9230892762	-0.1069385922	-1.6080098697
H	2.6543892752	-0.4474212805	1.8582580492
H	3.2970206481	-2.0977089593	-0.9133895968
H	3.8923977140	-1.0205977060	0.0611578912
H	-1.8355396437	-1.4142924254	1.6590818398
H	-3.7873337418	-0.3218781982	2.7653108359
H	-5.1478417469	1.3482171619	1.5098892092
H	-4.5540259159	1.9050759968	-0.8457231877
H	-2.5863338909	0.8181366425	-1.9173724096
H	1.9829003846	-3.8644809220	-0.1501089039
H	1.0995927033	-2.7677960963	-0.8008276527

H	0.5176955989	-1.1965645190	1.2946202196
H	3.4526785971	0.7265987875	1.2861051813
H	0.5219129791	0.2910423474	1.6929096632
H	-1.1561102696	1.7104755949	1.3591489683
H	-0.2882089806	2.0742529981	0.1114868380
H	0.7611981437	2.3345538559	-1.8005372791