

# Supplement Materials

## Structure and Vibrational Spectroscopy of Valent Isomers C<sub>82</sub> Fullerenols: an Experimental and Theoretical Joint Study

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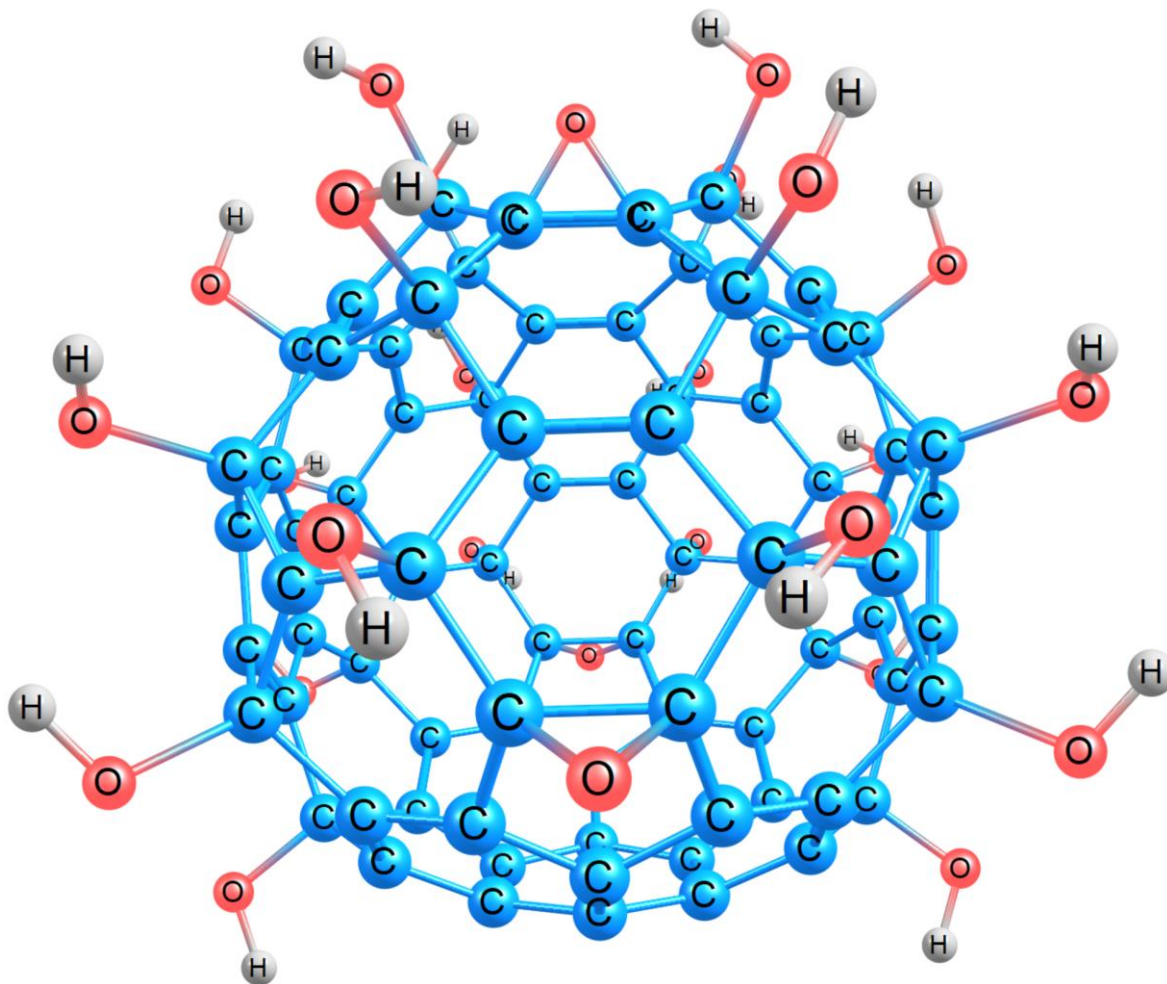
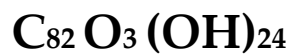
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**Abstract** Gd@C<sub>82</sub>O<sub>x</sub>H<sub>y</sub> endohedral complexes for advanced biomedical applications (computer tomography, cancer treatment, etc.) were synthesized using high-frequency arc plasma discharge through a mixture of graphite and Gd<sub>2</sub>O<sub>3</sub> oxide. The Gd@C<sub>82</sub> endohedral complex was isolated by high-efficiency liquid chromatography and consequently oxidized with formation of a family of Gd endohedral fullerenols with gross formula Gd@C<sub>82</sub>O<sub>8</sub>(OH)<sub>20</sub>. Fourier-transformed infra-red (FT-IR) spectroscopy was used to study structure and spectroscopic properties of the complexes in combination with DFTB3 electronic structure calculations and infra-red spectra simulations. It was shown that the main IR spectral features are formed by fullerene C<sub>82</sub> cage which allows one to consider the force constants at DFTB3 level of theory without consideration of gadolinium endohedral ions inside the carbon cage. Based on the comparison of experimental FT-IR and theoretical DFTB3 IR spectra it was found that oxidation of C<sub>82</sub> cage causes formation of Gd@C<sub>82</sub>O<sub>28</sub>H<sub>20</sub> with breakdown of the integrity of parent C<sub>82</sub> cage with formation of pores between neighboring carbonyl and carboxyl groups. The Gd@C<sub>82</sub>O<sub>6</sub>(OOH)<sub>2</sub>(OH)<sub>18</sub> endohedral complex with epoxy, carbonyl and carboxyl groups was considered as the most reliable fullerene structural model.

**Keywords:** C<sub>82</sub>, Gd endohedral complexes, biomedical applications, fullerenols, DFTB3 electronic structure calculations, IR spectra

## CARTESIAN COORDINATES

Atomic Cartesian coordinates for equilibrium structures of studied complexes of  $C_{82}$  fullerenols (in Å: X, Y, Z) are presented below.



### DFTB3/3ob-3-1// Ground state

C	-2.633905408817	0.397581121835	3.485446169396
C	2.682739063779	0.283566937873	3.441110737430
C	-3.069223003628	1.505346063341	2.695103838800
C	3.103964922613	-0.970587089549	2.901719552697
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C	-3.115135761575	-0.837255108604	2.952054986657
C	-3.955905427232	0.975910383540	1.601788165265
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C	3.993662188175	0.804644688643	1.534591913286
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C	3.236088726545	2.761431789761	0.147777842919
C	-3.250914524502	-2.736017647769	0.822147546623
C	-2.315100314935	2.677981455769	2.617907541834
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C	-2.651765592782	-3.594673858356	-0.288437871890
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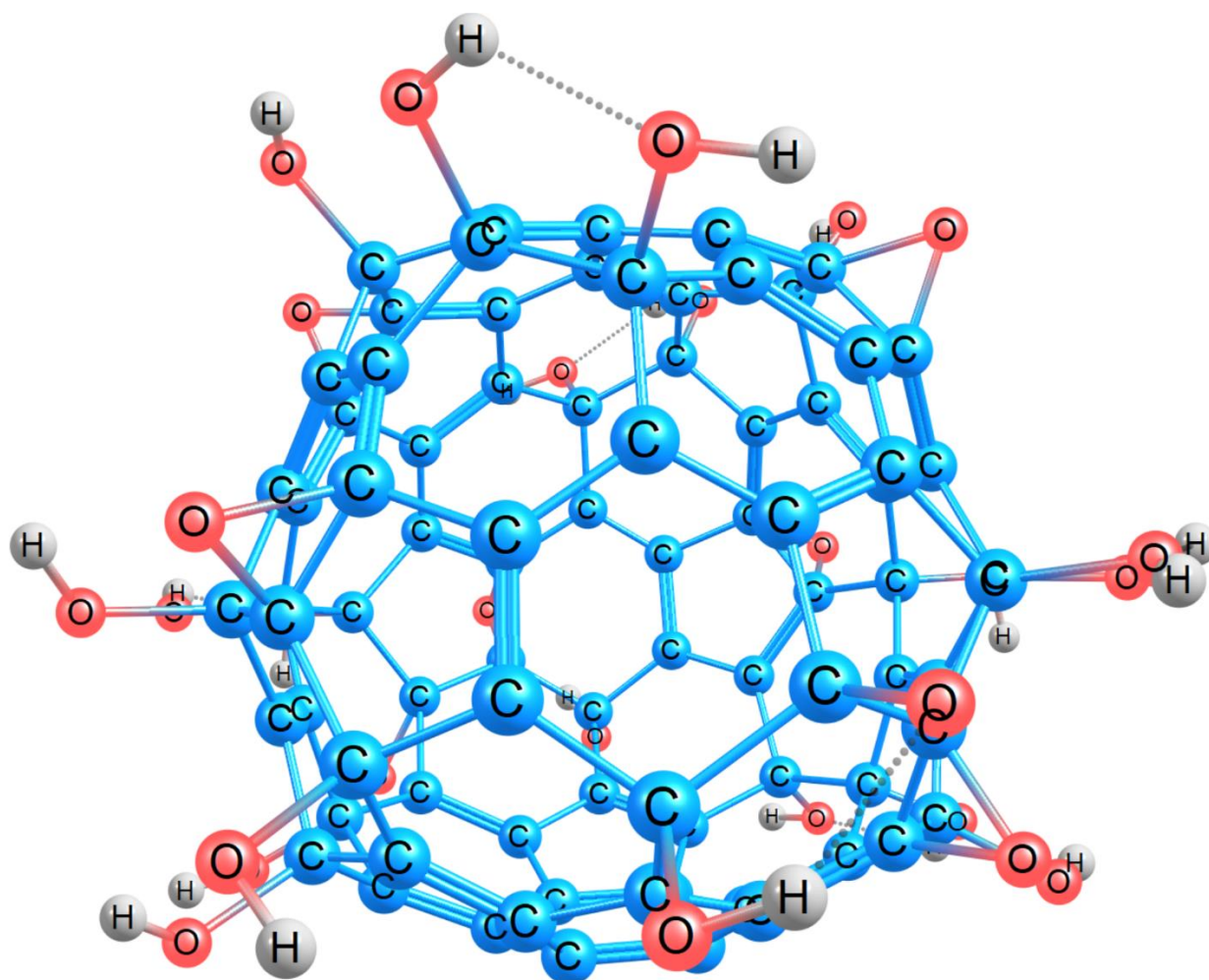
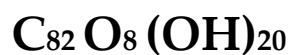
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C	-2.518842808835	-1.001892303563	-3.059105559609
C	-1.232397923443	2.308853057940	-2.904624047705
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C	1.249628982441	2.249495030968	-2.913901673671
C	-1.330512890385	-2.906675445698	-2.318820439939
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H	-3.605019316384	-4.910413564761	2.131308854057
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O	1.562593857282	-2.763325480763	-4.732418663843
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H    -2.647407990807    -3.091830970581    -4.562820263950

# First isomer



## DFTB3/3ob-3-1// Ground state

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C	-3.425757084427	-1.289839417424	2.486555171860
C	3.399060264462	-1.294617994400	2.431489772893
C	-3.743010316284	0.630278337705	1.076692924528
C	3.680921512346	0.644564036724	1.019519707536
C	-3.752357311301	-0.716332028655	1.071837746500
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C	2.614036759803	3.351843261500	1.190793347448



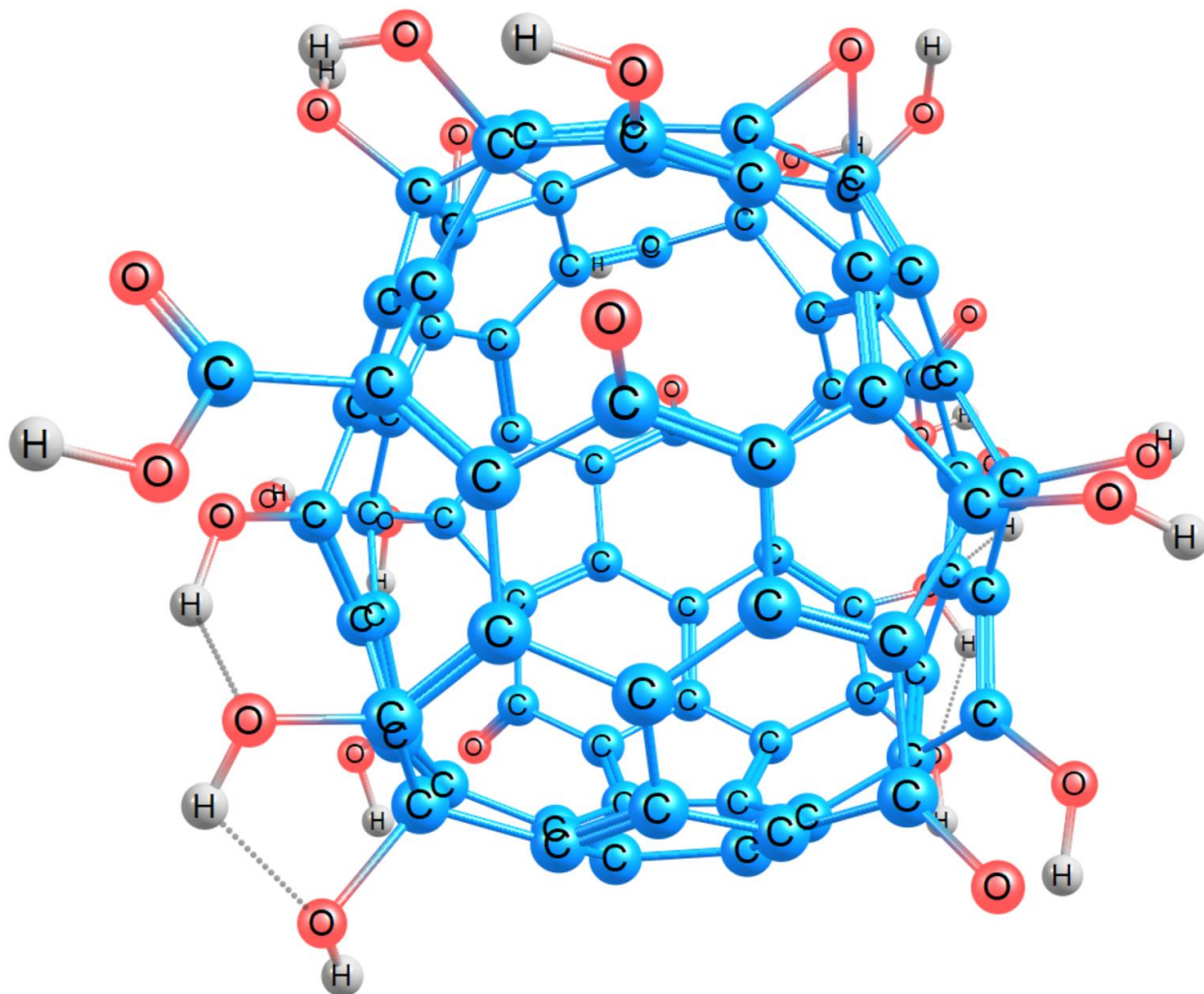
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C	4.004473681177	-1.527965935300	-0.234462225888
C	-4.123872027108	-1.545586647298	-0.169371561927
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C	-0.022017302006	4.272111075041	1.629324211239

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C	0.028146436003	3.113355899563	2.612356090796
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O	-5.455063287536	1.775070760191	-0.160195208951
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O	5.493677521526	1.643239689229	-0.128222422967
O	5.407606980568	-1.777623994168	-0.265310485875
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O	3.735990202320	1.442594771346	-4.052443095181
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O	-1.559571429303	-5.339298637570	-0.044089924996
O	0.149099091933	-5.552638559462	2.105022177047
O	-3.210430526524	-3.812402129273	2.356629768927
O	-4.628058466919	-1.650240780276	3.156349573562
O	-4.522812583970	1.676839813259	3.154985751550
O	-3.449532979436	4.448393140966	1.838299524161
O	-0.120076516951	5.504208243504	2.320569823934
O	1.840420209184	5.609157087463	0.767357490644
O	4.584990429917	1.528755903321	3.118063361573
O	3.241555313533	3.692587806313	2.355927411914
H	1.276370288432	-4.456531058999	-4.826447183837
H	-1.111175842472	-5.125277006686	-3.604896260342
H	-1.368067719354	4.481973615958	-4.648398208888

H	1.015583234553	5.159390650669	-3.420076285430
H	-3.411023235462	2.109868667043	-5.072679550705
H	3.395871618470	-2.099140253071	-5.163701011668
H	-2.905339050678	5.065294246706	2.356668119937
H	-4.880740857798	2.454227821880	2.690822227790
H	4.652446279903	-2.364756249905	3.510575809400
H	2.796024005720	-4.420439137995	3.354308488484
H	-5.213099695638	-0.874641943588	3.197860213556
H	5.171189602652	0.750794949678	3.116770415604
H	5.746451318408	2.535741703856	-0.430062609824
H	4.157289241128	4.834190797826	-0.053870312000
H	-4.646801186877	-4.332002253012	0.794543182649
H	-5.724440326417	-2.650440855802	-0.423336672795
H	5.701971800421	-2.091722501034	0.605208824725
H	-5.614987267429	2.501170866870	-0.788482636639
H	-0.258910439903	-6.175787850214	1.475925596333
H	0.599570082725	6.080078922257	1.957854670127

## Second isomer



### DFTB3/3ob-3-1// Ground state

C	-2.815265689710	-0.004010644001	3.169549066584
C	2.842191235693	-0.032626075988	3.147448682585
C	-3.142173369572	1.146448036484	2.346297920914
C	3.523276714423	1.092677568483	2.476644576878
C	-3.537556951380	-1.111056647519	2.498733696863
C	3.164417208548	-1.168577408495	2.306297255973
C	-3.554642873410	0.644053804708	1.072738636528
C	3.639858459359	0.798993114624	1.117756752495
C	-3.671564438354	-0.793670358647	1.142213250463
C	3.552168942413	-0.646577850696	1.033423248557
C	2.161086188041	3.363489201458	1.306551419424

C	-2.723566331789	3.597832593345	1.749566194190
C	2.744949734750	-3.616755855350	1.678335749240
C	-2.138882508008	-3.322112884483	1.278923634435
C	3.818704707251	1.668764689251	-0.127950298965
C	-3.890423402246	1.243517234457	-0.175527807896
C	3.869962669244	-1.230636983433	-0.222678376888
C	-3.855794256277	-1.648083295262	-0.114467438934
C	3.095875475576	3.140755361555	0.019454645976
C	-3.952953388188	4.348447608047	-1.566378074276
C	3.944752805197	-4.325995081037	-1.647863879272
C	-3.078691709625	-3.110300377580	0.041525218986
C	-2.677512495769	2.526615261872	2.828095650692
C	2.211134601976	3.354410329493	2.823919504707
C	-2.200732027995	-3.322767165478	2.780900015749
C	2.707532844774	-2.556864822838	2.773494589732
C	-3.476449365413	0.597562138704	-1.401543698349
C	3.340184722467	0.860620440598	-1.395893211366
C	-3.365022184450	-0.829527410627	-1.373653725402
C	3.455871464419	-0.569167946729	-1.438956228329
C	-2.627434636825	3.704050835309	-1.438955835362
C	2.073464049064	3.455706039430	-1.118625723505
C	-2.096572694055	-3.426553803427	-1.133927650490
C	2.611653833798	-3.688922330344	-1.520683567336
C	2.115419993036	2.817082604713	-2.413440517919
C	-2.321549503957	2.670274977800	-2.484951925878
C	2.301674185934	-2.639528619782	-2.547122204855
C	-2.146002141003	-2.771773639753	-2.420229057885
C	-2.897393776712	1.410075973345	-2.502796059844
C	2.855744455712	1.581836883266	-2.511861460862
C	-2.889050902668	-1.539422412287	-2.503294071887
C	2.868556618717	-1.374321666367	-2.547309130844
C	-2.595415580800	0.707094421665	-3.835173818269
C	2.391077812926	0.840746495631	-3.706144575313
C	-2.433686036915	-0.785811710626	-3.694487188299

C	2.548240259860	-0.649548346701	-3.864061527243
C	-1.442160504365	2.872706414692	-3.842403255278
C	1.056171749535	2.822870221736	-3.381978669461
C	-1.084350116517	-2.768513630769	-3.398198234459
C	1.403130590374	-2.815363857699	-3.916588041246
C	-1.295657200408	1.401281380372	-4.254007880076
C	1.141788708490	1.540413611282	-4.166686452104
C	-1.188178025476	-1.478329087330	-4.171686351114
C	1.241637993434	-1.331841751403	-4.271856244074
C	-1.623411932281	4.085174052141	-0.499754056783
C	0.931835249577	3.994704958192	-0.569657256717
C	-0.933994351598	-3.951101998187	-0.604531771751
C	1.622536616277	-4.086251871155	-0.573304206720
C	-1.610101236258	3.944899458205	0.945420224571
C	0.928217844598	3.806930110280	0.860604501620
C	-0.902635887589	-3.761429067314	0.817503440624
C	1.629782532237	-3.951386731213	0.875859357602
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C	-1.288874405401	2.334260364921	3.361347138469
C	1.324627545384	-2.372300326923	3.328510577467
C	-0.986510412550	-2.582601562817	3.291646090488
C	-0.751467347638	1.138731408472	3.861341217246
C	0.731584313681	1.258144934435	3.818890984257
C	-0.694047026673	-1.299232110390	3.815983942266
C	0.789394189642	-1.182015032444	3.851226746251
C	1.541273943314	0.049652530984	3.793571477255
C	-1.506730077328	-0.094463376955	3.799111497270
C	-0.095929435958	0.775841542669	-4.441316223000
C	0.042815047996	-0.704628709690	-4.450729185994
C	-0.101654526932	3.585161747389	-3.675891868336
C	0.073551655976	-3.528393763381	-3.711238660306
C	-0.312779725882	4.586886147932	-1.083705703513
C	0.290717829844	-4.572526782943	-1.126178914489
C	-0.303905257837	3.803529666280	1.618776403240

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C	-0.224058253873	3.129387514561	2.861818549718
C	0.255726206879	-3.151401210595	2.818546995697
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O	-4.209147462105	5.360237231546	-0.689778195663
O	4.088263120152	4.135247253109	-0.014303483978
O	5.216521478658	1.965501771129	-0.352376352828
O	4.578518152945	-2.342803318924	-0.310036413872
O	4.171364383112	-5.373671957561	-0.805321111631
O	-5.233470362620	-1.924324507139	-0.361931343821
O	-4.093821390168	-4.123269909126	0.061138779960
O	-2.388644669905	-1.469161702321	-4.977638000721
O	-3.659313413317	1.000191439565	-4.763865048853
O	3.680735138342	-3.026146318652	3.786078860290
O	-2.221703475993	3.656795360367	-4.742063677834
O	-0.075944920940	4.856704703787	-3.951682643215
O	3.598139100375	-0.930294958595	-4.814628785807
O	2.334086519928	1.532364280325	-4.983488221741
O	0.085328969954	-4.812697139832	-3.949337047226
O	2.176340570038	-3.526277067402	-4.859478806822
O	-2.949290407649	-4.001687053204	3.474467317422
O	-4.287499246064	-2.028505825060	3.117681400588
O	4.211666117099	2.055111324061	3.096977703578
O	2.878753579714	4.088424890166	3.531846460406
H	3.049545295630	-3.097994723617	-4.935907754761
H	-3.118588198563	3.271169647536	-4.794668156844
H	5.698411328405	1.135923403485	-0.504178438757
H	4.897012673758	3.803051126266	0.411225344837
H	-4.273571811050	-4.379041940003	0.982293081547
H	-5.343488712559	-2.895453688667	-0.445724471797
O	4.758029316865	-4.074636446150	-2.542625044869
O	3.950580606194	-4.160236550121	1.518932960306
O	-4.732869414854	4.141906186138	-2.503636534870
O	-3.924670362224	4.141686800098	1.602346243265



H	-4.867720425815	2.680262031803	0.629817348702
H	4.815862629822	-2.709125635749	0.557970903757
H	-5.027024266700	5.805561412345	-0.966669595561
H	4.994039740755	-5.813382636369	-1.076613975516
H	-3.690626260342	0.276151542898	-5.415695940551
H	3.604114234372	-0.206756036886	-5.468317921516
H	4.019249315194	2.104444660038	4.045311088169
H	-4.059030317177	-2.135289299024	4.053713177147
O	-3.641567149360	2.984058054650	3.853387144226
H	-4.440942948989	3.935155040225	2.411993516916
H	-3.612908069351	2.359442398923	4.599688890894
H	4.462705265985	-3.976884550205	2.336345548923
H	3.627531843363	-2.434944160905	4.557655609942
O	0.297754584845	-5.631045318428	-1.746059830230
O	-0.376674590815	5.621635938440	-1.736844887215
H	-0.970886692562	5.162910590671	-4.196958448121
H	-0.758715535673	-5.247276914605	-3.748203558298