

## Supporting Information

### **Biological Noncovalent N/O...V Interactions: Insights from Theory and Protein Data Bank Analyses.**

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## Cartesian coordinates of complexes 1 to 16

### 1

V	0.0002272	-0.0010834	0.7721433
O	0.0013417	-0.0014449	2.3286390
O	-1.4470166	-0.8353472	0.1986679
O	0.0002761	1.6702845	0.2014215
O	1.4465068	-0.8363775	0.1975512
H	2.0827821	-1.1967984	0.8208102
H	-2.0836690	-1.1968597	0.8208695
H	-0.0000357	2.4010832	0.8252204
O	-0.0004339	0.0011114	-2.5213587
C	0.0000214	-0.0045680	-3.6439642

### 2

V	0.0000594	-0.0005542	0.7571683
O	0.0003715	0.0003039	2.3136122
O	-1.4558324	-0.8418059	0.2089414
O	0.0000612	1.6809616	0.2096274
O	1.4554504	-0.8423332	0.2081692
H	2.0727742	-1.1954858	0.8545432
H	-2.0729062	-1.1949334	0.8555779
H	0.0003290	2.3934983	0.8545941
C	-0.0005412	0.0002974	-2.5693976
O	0.0002342	0.0000511	-3.6928362

### 3

V	-0.6095276	-0.0378574	-0.0692478
O	-2.1570113	0.0530416	0.0941354
O	-0.0844371	-0.9693165	1.3701924
O	-0.0827055	1.6757595	-0.0731757
O	-0.3773476	-0.8777032	-1.6105105
H	-1.1677900	-1.1428416	-2.0898305
H	-0.7763120	-1.2657942	1.9674767
H	-0.7750748	2.3389866	-0.0084195
O	1.8844528	-0.1008919	-0.1787729
H	2.0749484	0.8367833	-0.0741497
H	2.0708049	-0.5101661	0.6723022

### 4

V	0.0261656	1.5463605	0.4469121
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O	-0.0394437	3.0992257	0.5798606
O	-0.4419523	1.2527784	-1.2526139
O	1.7260774	1.1594572	0.8143544
O	-1.1590245	0.9667935	1.6448632
H	-1.6215330	1.6405650	2.1507542
H	-0.6407864	2.0344894	-1.7754049
H	2.3024547	1.9022706	1.0140173
O	0.1233189	-0.9475022	0.1929794
C	1.1065605	-1.4062444	-0.7077649
H	0.8248262	-1.1717999	-1.7412462
H	2.0336711	-0.8944902	-0.4586208
H	1.2418853	-2.4897321	-0.6055400
C	-1.1264648	-1.5586493	-0.0371322
H	-1.8165232	-1.1675986	0.7074644
H	-1.4949991	-1.3189716	-1.0419284
H	-1.0442328	-2.6469518	0.0690458

## 5

V	1.1943468	-0.0809612	0.0035149
O	2.6646806	0.4349669	-0.0105805
O	1.0437208	-1.0416829	1.4876590
O	0.1829699	1.3891009	0.0088494
O	1.0156421	-1.0472337	-1.4739389
H	1.7817066	-1.1352312	-2.0486145
H	1.8191843	-1.1221873	2.0508316
H	0.6428877	2.2332878	0.0028754
C	-2.6517862	0.1890739	-0.0074785
H	-3.7412411	0.1730100	-0.0212275
H	-2.1645963	1.1635316	-0.0174327
S	-1.7875153	-1.1556746	0.0255423

## 6

V	0.0497247	1.7575516	0.0431191
O	-0.0072373	3.2439747	-0.4318938
O	-0.3670167	0.8252208	-1.4259524
O	1.7373991	1.5428377	0.5776255
O	-1.1846787	1.6618160	1.3247439
H	-1.6656209	2.4718546	1.5190906
H	-0.5464253	1.3415402	-2.2169611
H	2.3086610	2.3129743	0.5026955
C	1.3042372	-1.6925854	-0.2857785
H	1.0002079	-1.3348362	-1.2707123
H	2.2964113	-1.3047741	-0.0551917
H	1.3250941	-2.7831235	-0.2623688

C	-1.3690806	-1.6669461	0.3391958
H	-2.1493808	-1.2709383	0.9891819
H	-1.5308811	-1.3036436	-0.6765485
H	-1.3940042	-2.7574680	0.3668315
S	0.1925903	-1.0434548	0.9629232

**7**

V	0.0025463	1.7819198	-0.0023683
O	0.4931230	3.2657337	0.0053244
O	-0.9372471	1.7222302	-1.5148934
O	1.6172296	0.9331368	-0.0127366
O	-0.9354705	1.7078451	1.5114552
H	-0.9578878	2.5288683	2.0114343
H	-0.9614440	2.5468516	-2.0086743
H	2.3649609	1.5358902	-0.0090941
C	-0.2565604	-1.5570514	-0.0059562
O	-0.7431269	-0.4297418	-0.0077645
N	-1.0580814	-2.6549752	-0.1475546
N	1.0687563	-1.7857589	0.1301937
H	-0.7494881	-3.5365662	0.2234862
H	1.6336376	-0.9434904	0.0741843
H	1.4600138	-2.6556731	-0.1822963
H	-2.0409613	-2.4592187	-0.0647397

**8**

V	-2.2532246	-0.0155435	-0.0000629
O	-3.8178963	-0.0716664	-0.0007472
O	-1.8374947	-0.9020338	1.4979258
O	-1.9473289	1.7532087	-0.0001277
O	-1.8365033	-0.9024468	-1.4975431
H	-2.5891588	-1.2368643	-1.9935950
H	-2.5904928	-1.2364822	1.9934538
H	-2.7368636	2.3008238	-0.0004550
C	0.8471289	-1.0869538	0.0002610
C	2.2283531	-1.1773071	-0.0000704
C	2.9691061	-0.0059307	-0.0001942
C	2.2983760	1.2054221	0.0000838
C	0.9124906	1.1978195	0.0004152
N	0.2013811	0.0754939	0.0004364
H	4.0527736	-0.0375108	-0.0005511
H	0.2226781	-1.9729796	0.0004327
H	2.7084956	-2.1479533	-0.0003419
H	2.8340639	2.1465458	-0.0000468
H	0.3341160	2.1143584	0.0007267

**9**

V	-0.0000111	-0.0001339	-0.6872906
O	-0.0007929	0.0002688	-2.3182548
O	1.3155034	1.1786091	-0.1518871
O	-1.1788165	1.3153203	-0.1528403
O	1.1793200	-1.3153860	-0.1535552
O	-1.3153192	-1.1792479	-0.1532566
H	-1.9104754	0.8928691	0.3053647
H	0.8926943	1.9109867	0.3048173
H	1.9104615	-0.8926380	0.3052007
H	-0.8929287	-1.9106963	0.3053121
Na	-0.0003604	0.0003651	-4.3474956
O	-0.0000699	-0.0011699	2.8107583
C	0.0007949	0.0008530	3.9331270

**10**

V	-0.0000101	-0.0000909	-0.7281926
O	0.0003498	0.0003381	-2.3591724
O	1.3214496	1.1735759	-0.1961974
O	-1.1736495	1.3213044	-0.1956326
O	1.1738060	-1.3215630	-0.1968123
O	-1.3215531	-1.1739636	-0.1967240
H	-1.9022907	0.9008523	0.2691910
H	0.9009060	1.9024347	0.2683397
H	1.9018862	-0.9011247	0.2689510
H	-0.9010123	-1.9020820	0.2688321
Na	-0.0004950	0.0004125	-4.3883207
C	-0.0001276	-0.0008233	3.0306865
O	0.0007406	0.0007294	4.1550515

**11**

V	0.0000000	0.0000000	-0.7957336
O	-0.0000000	-0.0000000	-2.4245256
O	-1.7566511	0.1161436	-0.1762087
O	-0.0745841	-1.7834398	-0.3937010
O	0.0745841	1.7834398	-0.3937010
O	1.7566511	-0.1161436	-0.1762087
H	0.2890026	-1.9173655	0.4877622
H	-2.0407426	-0.7848002	-0.0018727
H	-0.2890026	1.9173655	0.4877622
H	2.0407426	0.7848002	-0.0018727
Na	-0.0000000	-0.0000000	-4.4493829
O	-0.0000000	-0.0000000	2.2324632

H	-0.7706165	0.0390136	2.8026097
H	0.7706165	-0.0390136	2.8026097

## 12

V	0.0012407	-0.0023236	-1.7900973
O	0.0018838	-0.0049766	-3.4177615
O	-1.7561343	-0.0897848	-1.1669859
O	0.1331115	-1.7834271	-1.3945636
O	-0.1306161	1.7810114	-1.4012761
O	1.7576928	0.0887960	-1.1657578
H	0.5122712	-1.8964057	-0.5170577
H	-1.9373688	-1.0195694	-1.0047650
H	-0.5132245	1.8978770	-0.5257961
H	1.9370303	1.0195202	-1.0068796
Na	-0.0056480	0.0090775	-5.4461833
O	0.0000125	-0.0000207	1.2817608
C	-1.1711629	0.0372567	2.0488876
H	-2.0030905	0.0855635	1.3463105
H	-1.2688969	-0.8596707	2.6778563
H	-1.1940264	0.9201798	2.7045584
C	1.1711402	-0.0374273	2.0489608
H	2.0030019	-0.0851450	1.3462679
H	1.2692050	0.8596828	2.6776336
H	1.1935784	-0.9202141	2.7048879

## 13

V	0.0001416	-0.0000925	-1.4511581
O	0.0003436	-0.0002657	-3.0821066
O	1.6775578	-0.0415933	-0.6657791
O	-0.0123930	1.8036949	-1.1247126
O	0.0125340	-1.8037443	-1.1243899
O	-1.6774522	0.0416463	-0.6660359
H	-0.3956720	2.0134342	-0.2669935
H	1.9329589	0.8687488	-0.4920316
H	0.3953031	-2.0136382	-0.2664990
H	-1.9327885	-0.8685839	-0.4916233
Na	-0.0009776	0.0005441	-5.1124360
C	0.0001294	-0.0000567	3.7944440
H	-0.0490084	-0.9208892	4.3771059
H	0.0492297	0.9208133	4.3770291
S	0.0000936	-0.0000176	2.1951864

## 14

V	0.0006030	-0.0011206	-2.1634290
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O	0.0017869	-0.0019942	-3.7928620
O	-1.7152211	-0.0597543	-1.4449863
O	0.1096399	-1.7916976	-1.8037253
O	-0.1097941	1.7900993	-1.8064086
O	1.7158077	0.0584680	-1.4439832
H	0.4541364	-1.9458146	-0.9172022
H	-1.9127918	-0.9866730	-1.2846325
H	-0.4542705	1.9446106	-0.9199225
H	1.9135403	0.9856726	-1.2855753
Na	-0.0029256	0.0051840	-5.8215075
C	-1.3769242	0.0036923	2.5034842
H	-2.2835356	0.0223104	1.8973399
H	-1.3813576	-0.8947096	3.1248181
H	-1.3608285	0.8901652	3.1414784
C	1.3768218	-0.0030513	2.5030210
H	2.2833280	-0.0215209	1.8966692
H	1.3813809	0.8953035	3.1243909
H	1.3608412	-0.8896584	3.1408106
S	-0.0002371	0.0004887	1.3522220

## 15

V	0.0020511	0.0000892	-2.1966825
O	0.0020807	-0.0000219	-3.8288391
O	1.7622673	0.0434631	-1.6117840
O	-0.0723482	1.7771003	-1.7369006
O	0.0749188	-1.7769113	-1.7391453
O	-1.7592330	-0.0395487	-1.6110459
H	-0.6772118	1.8641868	-0.9933906
H	1.9001032	0.9156062	-1.2334061
H	0.6692869	-1.8655669	-0.9874495
H	-1.9002865	-0.9128675	-1.2367094
Na	-0.0034119	-0.0008896	-5.8500741
O	-0.0001151	-0.0040097	1.1681625
C	0.0001214	-0.0018888	2.3790467
N	1.1497683	-0.1325565	3.1255688
H	1.9888778	-0.0380852	2.5777241
H	1.1795153	0.2985823	4.0339095
N	-1.1489444	0.1316317	3.1258353
H	-1.9888302	0.0373939	2.5791957
H	-1.1786097	-0.2957073	4.0359846

## 16

V	0.0023926	-0.0017553	-2.3159613
O	0.0031685	-0.0047220	-3.9425189

O	-0.0652018	1.7874831	-1.9339575
O	-1.7846967	-0.0277806	-1.7519115
O	1.7881077	0.0302457	-1.7518005
O	0.0673984	-1.7890375	-1.9298376
H	-2.0024319	-0.9524289	-1.6060559
H	-0.4459889	1.9235324	-1.0611396
H	2.0012752	0.9556633	-1.6040502
H	0.4321116	-1.9214876	-1.0495330
Na	-0.0029078	0.0068565	-5.9689981
C	1.1380781	-0.0983024	1.3620163
C	1.1897053	-0.1014917	2.7487334
C	0.0005634	0.0008418	3.4538521
C	-1.1885154	0.1016457	2.7483916
C	-1.1367631	0.0948335	1.3616977
N	0.0006691	-0.0028416	0.6831675
H	0.0005250	0.0019299	4.5382824
H	2.0327246	-0.1777482	0.7498711
H	2.1413622	-0.1827517	3.2604630
H	-2.1401962	0.1840794	3.2599078
H	-2.0313800	0.1732362	0.7493814



## Cartesian coordinates of the H-optimized PDB models

### 2JJ9@SER236

O	3.20859480	2.40747300	-2.66605450
C	-3.81742340	-0.25033730	-5.86304000
O	-2.88376900	-0.82756590	-6.76580410
C	1.25240670	2.36456350	-6.29213060
O	1.48717560	2.76295750	-4.95645410
V	0.34362410	-1.81329760	-4.83765800
O	1.34204210	-2.82514810	-5.57722520
O	0.55080250	-0.27242090	-5.45486180
O	-1.35596780	-2.35469600	-4.78788700
P	1.86951830	-1.72576640	-1.95469430
O	2.85271800	-2.95563340	-1.83142950
O	2.65424440	-0.24173090	-1.99965600
O	1.05325270	-1.58246180	-3.22995420
P	0.87974870	-0.35004830	0.48469540
O	-0.11493970	0.77959730	-0.32107240
O	2.22106180	0.18773280	1.00742320
O	0.97018490	-1.57437290	-0.59921850
O	-0.13773630	-1.01799510	1.54169790
C	-1.59727980	-1.10992960	1.45009280
C	-2.19474410	-0.82278960	2.79809210
O	-1.56476190	-1.72667230	3.76554220
C	-1.83468670	0.55373930	3.38273110
O	-2.65408280	1.60643600	2.79892330
C	-2.10676810	0.32798620	4.88735790
O	-3.52797500	0.17199450	5.16742640
C	-1.45300220	-1.07758800	5.07782900
N	-0.04713170	-1.04940880	5.49948310
C	1.09486440	-1.51531330	4.80757380
N	2.21339680	-1.34787070	5.48239230
C	1.82198030	-0.74889810	6.68022010
C	2.54077960	-0.31871110	7.83798990
N	3.88883110	-0.45079630	7.96302510
N	1.83855080	0.25119370	8.87925430
C	0.48079210	0.39228480	8.78362530
C	0.42024720	-0.54952850	6.70702690
N	-0.29509780	0.01443110	7.73353910
Mg	1.84872610	0.95423900	-3.71458030
O	3.52353450	0.52177410	-4.75784340
O	0.05243820	2.25254840	-2.27963950
H	-4.29681220	-1.08901840	-5.33617660

H	-2.44741590	-0.11361730	-7.24375800
H	2.00337500	1.65443570	-6.71839280
H	1.20200350	3.21899960	-6.99867250
H	-2.02489104	-1.62062939	-4.72441949
H	-1.84151310	-2.13096090	1.12110300
H	-1.94859000	-0.36852910	0.71492420
H	-3.28897920	-0.96374310	2.77964340
H	-0.77658230	0.78694780	3.20636020
H	-3.50458610	1.52190780	3.25179510
H	-1.65251100	1.09107580	5.53604370
H	-3.63727570	0.37056640	6.10313080
H	-2.02503950	-1.65638220	5.81904910
H	0.98856380	-1.91503270	3.79908460
H	4.33884660	-0.04837320	8.77183450
H	-0.02332420	0.85365980	9.63802120
H	2.67518360	3.21147710	-2.63147890
H	3.19016320	2.02336220	-1.77179070
H	4.09809690	0.17456080	-4.05301740
H	3.86848210	1.40707570	-4.95708710
H	0.18454710	3.17768950	-2.06335360
H	0.01621090	1.70922730	-1.40537390
H	0.22135950	1.89065430	-6.45495450
H	-4.60886720	0.28715640	-6.41484170
H	4.42808550	-0.78093350	7.17645140
H	-3.30720380	0.39814168	-5.18182713
H	2.43285072	2.81018276	-4.79812424
H	-0.01983973	0.33997340	-4.98481854

### 7B19@OH<sub>2</sub>

C	23.94800000	42.81100000	51.65600000
O	23.69800000	42.37300000	50.31600000
H	23.11400000	42.89400000	52.14300000
C	21.88400000	43.46500000	46.62100000
O	22.27800000	43.66500000	47.97300000
H	21.68600000	42.52400000	46.49400000
H	22.61700000	43.73100000	46.04400000
V	18.70600000	40.40100000	48.82900000
O	19.23300000	38.72300000	48.08600000
O	19.95900000	41.76000000	48.44800000
O	17.03000000	41.11200000	48.08400000
P	20.15900000	40.10900000	51.59500000
O	21.32600000	40.54700000	50.89200000
O	20.33200000	38.76100000	52.05300000

O	18.75500000	40.12000000	50.83000000
P	20.38000000	42.08600000	53.79800000
O	21.71700000	41.70000000	54.14700000
O	20.45500000	43.48100000	53.35800000
O	19.67900000	41.12000000	52.74100000
O	19.42200000	42.02700000	55.08300000
C	18.23800000	42.71600000	54.95300000
H	16.66900000	41.54700000	48.68900000
H	18.32000000	43.36300000	54.23400000
H	17.52100000	42.09400000	54.75500000
Mg	21.98300000	41.86500000	49.27100000
O	22.99200000	40.29300000	48.30400000
O	18.68200000	40.88000000	46.25000000
O	21.13400000	43.51500000	50.26800000
H	18.48671660	40.02842090	45.83871150
H	17.81360570	41.25619480	46.46719460
H	24.47990360	43.77704040	51.64921700
H	24.57469160	42.07163280	52.17586460
H	18.01652380	43.24572120	55.89244640
H	20.98997350	44.06705240	46.41322270
H	19.28795640	38.02419450	48.76326770
H	21.42124990	44.38419150	49.97348430
H	20.95339870	43.57264560	51.22882570
H	24.05228680	39.99840670	48.81831120
H	22.55750420	39.43646820	48.23467260
H	24.57453810	42.05012610	49.92236440
H	23.22372500	43.85577790	48.02097930

### 6MI8@SER139

C	2.79780540	3.54332960	3.65967760
C	3.04580540	2.20232960	2.98667760
O	3.31480540	1.18732960	3.62867760
N	2.94880540	2.20232960	1.67167760
C	3.35780540	1.02732960	0.92867760
C	4.81880540	1.15532960	0.53367760
O	5.44280540	2.20532960	0.70567760
C	2.48980540	0.83932960	-0.30132240
O	2.89680540	-0.29567040	-1.04432240
N	5.35680540	0.06432960	-0.01632240
C	6.78580540	-0.00367040	-0.27332240
P	0.87480540	-2.45867040	-2.51932240
O	1.07280540	-3.54967040	-3.53832240
O	1.42080540	-2.86567040	-1.17732240

O	1.57680540	-1.04267040	-2.99632240
P	-1.33019460	-1.57567040	-0.91932240
O	-2.77619460	-1.22167040	-1.07032240
O	-1.15719460	-2.57067040	0.19167760
O	-0.73719460	-2.19867040	-2.32232240
O	-0.56919460	-0.17467040	-0.51632240
C	-1.01719460	0.45032960	0.66567760
C	-1.88519460	1.62632960	0.30467760
O	-2.87319460	1.65532960	1.11467760
C	-1.03919460	3.05332960	0.47667760
O	-1.52819460	4.03032960	-0.48132240
C	-1.28019460	3.46032960	1.64667760
O	-1.30019460	4.95832960	1.64467760
C	-2.72319460	2.94432960	1.96567760
N	-2.89019460	2.75732960	3.26767760
C	-2.47919460	3.60232960	4.19767760
N	-2.80219460	3.16132960	5.40167760
C	-3.45019460	1.99932960	5.26367760
C	-4.03019460	1.07432960	6.14167760
N	-3.98319460	1.31532960	7.57867760
N	-4.61919460	-0.01467040	5.67567760
C	-4.66319460	-0.24067040	4.37167760
N	-4.12619460	0.61632960	3.52167760
C	-3.51019460	1.74332960	3.91267760
V	3.36580540	-1.30167040	-4.08032240
O	3.73480540	-2.92867040	-2.80432240
O	5.40980540	-0.99067040	-3.70032240
O	3.39180540	0.78532960	-3.84632240
O	3.02880540	-1.87767040	-6.06932240
H	2.05795550	4.14918820	3.11438490
H	1.44423340	0.73906250	0.02826760
H	2.54870630	1.75313300	-0.92843090
H	2.67347366	-1.08983224	-0.52561321
H	3.24807540	0.16436010	1.59991080
H	7.23138390	0.93932920	0.06424980
H	7.24149990	-0.84479190	0.27349060
H	-1.54832920	-0.25492430	1.32569000
H	-0.13734430	0.84006390	1.19797820
H	-1.49488690	4.85234990	0.04563080
H	-0.46931120	5.24521760	2.04793050
H	-1.96202930	4.52845730	3.96448930
H	-3.81974640	2.27884220	7.84147670
H	-5.14832450	-1.14481150	3.99259080
H	6.98136390	-0.13099320	-1.35046730

H	2.45611360	3.36448400	4.68616430
H	3.74444920	4.10457950	3.70010870
H	3.07562680	3.08302890	1.18561060
H	4.72726110	-0.65786560	-0.35198500
H	-4.67640420	0.80054040	8.10642220
H	5.57411280	-1.81058650	-3.20789110
H	4.27009810	0.83358630	-3.43032640
H	3.37759880	-2.71608550	-1.91846380
H	-3.27142100	-1.71033530	-0.39044940
H	2.05340800	-3.74631210	-3.48719320
N	-3.37419460	-1.64867040	-4.49232240
C	-4.23619460	-2.42567040	-3.63132240
C	-3.88419460	-3.89167040	-3.55232240
O	-4.68519460	-4.68767040	-3.05932240
N	-2.68619460	-4.24867040	-4.01732240
C	-2.31519460	-5.65367040	-4.13632240
H	-4.21307450	-1.97651590	-2.63105190
H	-5.26745630	-2.36994640	-4.00600000
H	-3.74324370	-0.70809900	-4.68291650
H	-2.44118070	-1.51060270	-4.06211200
H	-3.20973990	-2.11835830	-5.39460280
H	-3.19594590	-6.22584590	-4.45187820
H	-1.96391110	-6.05946040	-3.17506430
H	-1.51542580	-5.74668870	-4.88156180
H	-1.89588430	-3.61400130	-3.93260210
H	-2.23786204	1.52748274	-0.70068551
H	-3.43384246	3.66863880	1.62618414

## 2JJ9@OH<sub>2</sub>

C	68.62900000	42.32000000	-25.22900000
O	68.47400000	41.90500000	-26.60000000
C	66.65500000	42.71600000	-30.20700000
O	67.17900000	43.01600000	-28.92900000
V	63.47400000	40.17300000	-28.25500000
O	63.58300000	38.69200000	-28.85700000
O	64.54100000	41.18200000	-29.05600000
O	61.81000000	40.80900000	-28.15100000
P	64.93000000	39.58800000	-25.39400000
O	64.95400000	38.03400000	-25.11300000
O	66.45600000	40.25300000	-25.61600000
O	64.28700000	40.07600000	-26.68300000
P	65.17200000	41.51900000	-23.15000000
O	65.02900000	42.93300000	-24.09600000

O	66.59300000	41.16000000	-22.68800000
O	64.41300000	40.40000000	-24.07400000
O	64.03700000	41.73600000	-22.02600000
C	62.82800000	42.55900000	-22.11600000
Mg	66.43796880	41.50947920	-27.47102300
O	67.41300000	40.03000000	-28.44100000
O	65.92800000	43.77800000	-26.22000000
O	63.24000000	40.20100000	-30.74800000
H	67.69131700	42.13044020	-24.69317700
H	69.35915130	41.74304260	-27.01810970
H	66.78081860	41.63591450	-30.36160500
H	67.22580110	43.23527200	-30.99452250
H	66.94378690	43.90771250	-28.63768630
H	63.98552190	37.91515550	-28.41497950
H	65.32520742	40.73398290	-29.42730309
H	61.99227890	41.93518310	-22.46759800
H	63.01143840	43.39088170	-22.81047390
H	63.30004240	39.28006910	-31.03536100
H	62.47001940	40.57393810	-31.19855430
H	68.40352380	39.99876510	-28.24640360
H	67.16772480	39.24227980	-27.92600800
H	66.83143380	43.98931070	-25.95707670
H	65.53680210	43.39918160	-25.32359360
H	68.90889200	43.38816660	-25.17069370
H	69.41261850	41.72367010	-24.73906230
H	65.59475950	43.00132640	-30.30308670
H	62.62831780	42.92222310	-21.10029380

### 3MNQ@OH<sub>2</sub>

C	2.33015750	1.18562880	1.63232590
O	2.10815750	0.80362880	0.26632590
C	0.27715750	1.71162880	-3.31367410
O	0.72515750	1.88262880	-1.98267410
V	-2.80384250	-1.02837120	-1.33967410
O	-2.68384250	-2.50037120	-1.91367410
O	-1.74784250	0.05362880	-2.11567410
O	-4.47584250	-0.46137120	-1.26467410
P	-1.37184250	-1.64037120	1.54532590
O	0.13015750	-0.88937120	1.40132590
O	-1.33084250	-3.18037120	1.74032590
O	-2.02084250	-1.11637120	0.24532590
P	-1.16684250	0.29762880	3.81832590
O	0.29315750	-0.01637120	4.19632590
O	-1.39884250	1.69762880	2.89132590

O	-1.92284250	-0.85637120	2.89232590
O	-2.22784250	0.52262880	5.03332590
C	-3.53484250	1.20062880	4.98132590
Mg	0.10615750	0.28662880	-0.52067410
O	1.07415750	-1.16137120	-1.55167410
O	-0.35984250	2.02662880	0.39732590
O	-3.15684250	-0.84337120	-3.68467410
H	1.43489550	0.95512140	2.22444940
H	2.97522700	0.48355590	-0.11761940
H	0.39023530	0.66687650	-3.65429680
H	0.82994530	2.36367910	-4.00887760
H	1.69158680	1.82320490	-1.93059240
H	-2.58061740	-3.32636760	-1.39938520
H	-0.90505448	-0.30500301	-2.43321541
H	-4.30809640	0.47915250	4.67782020
H	-3.47524960	2.03538480	4.26802940
H	0.70988790	-2.05429470	-1.58027080
H	-0.70944880	1.93090350	1.36007500
H	-3.97742140	-0.35848010	-3.86004220
H	-3.27890760	-1.71160550	-4.09446840
H	0.37035710	2.65168040	0.42803150
H	2.00968570	-1.35005560	-1.17507230
H	2.57804060	2.26002460	1.70009990
H	3.16352370	0.60269560	2.04883490
H	-0.77803410	2.01257230	-3.34248710
H	-3.72485500	1.55829720	6.00032890

### 3MJX@OH<sub>2</sub>

C	24.10800000	42.05900000	51.49500000
O	23.78900000	41.59700000	50.17300000
C	22.17100000	42.55900000	46.53000000
O	22.50500000	42.66600000	47.90600000
V	18.97900000	39.86700000	48.53600000
O	19.09900000	38.36500000	48.00400000
O	20.01600000	40.91800000	47.67500000
O	17.30400000	40.42700000	48.58000000
P	20.40600000	39.33200000	51.43300000
O	21.91400000	40.09100000	51.29300000
O	20.44900000	37.78300000	51.67800000
O	19.75900000	39.82900000	50.11400000
P	20.56100000	41.31900000	53.67000000
O	22.00700000	41.01300000	54.11300000
O	20.34800000	42.70200000	52.70100000
O	19.82600000	40.13800000	52.75200000

O	19.46300000	41.57200000	54.84400000
C	18.22900000	42.35700000	54.76000000
Mg	21.75100000	41.16500000	49.37800000
O	22.91900000	39.73900000	48.42500000
O	21.43400000	43.02600000	50.38600000
O	18.57800000	39.86700000	46.12300000
H	23.28870220	41.78884350	52.17585390
H	24.63379070	41.40376150	49.68668450
H	22.37580030	41.51878270	46.24136440
H	22.81095570	43.21303530	45.91606110
H	22.25767130	43.53126130	48.25780760
H	19.25203680	37.57481830	48.56260700
H	20.63608586	40.49564776	47.05714268
H	17.40142430	41.70268980	54.44629100
H	18.37220150	43.17625020	54.04123150
H	23.84289710	39.52763390	48.84435800
H	20.96382070	42.89729500	51.32941100
H	18.48127160	38.95567870	45.81508490
H	17.75024460	40.31084930	45.88956870
H	22.62224270	38.85467550	48.18655960
H	22.34003030	43.22134210	50.65829820
H	18.04543570	42.73983150	55.77146870
H	24.28449690	43.15281080	51.50529430
H	21.11440060	42.80968710	46.33310990
H	25.02188250	41.56580950	51.85779310