Supporting Information

Table S1. Optimized structure for the complex $[UO_2(R_{hydO})_2(R_{hydOH})]$

Atom Type	Cartesian coordinates (Å)
U	-0.36671 -0.42006 -0.27795
C	-7.17809 -0.20729 0.64477
O	-5.85289 0.15446 0.34767
C	-4.93705 -0.86355 0.6436
C	-3.54309 -0.43877 0.28212
N	-3.36104 0.74108 -0.25582
O	-2.12894 1.14247 -0.58125
O	-2.57029 -1.20741 0.49223
O	0.29215 -2.55012 0.57621
N	1.57595 -2.84632 0.67918
C	2.50074 -2.05551 0.1909
O	2.1629 -0.9704 -0.35966
C	3.9322 -2.50365 0.26453
O	4.67118 -1.53668 0.95353
C	6.05381 -1.781 0.89855
O	-0.00127 0.3136 1.28952
O	-0.64883 -1.12128 -1.86983
O	3.57664 1.14463 -1.08436
N	2.87484 2.15838 -0.51777
C	1.56772 2.2807 -0.62844
O	0.85142 1.45994 -1.22997
C	0.94641 3.47113 0.05033
O	1.93176 4.30375 0.59539
C	1.38959 5.37978 1.32317
H	-5.16508 -1.78498 0.08581
H	-4.94684 -1.1172 1.71488
H	4.30359 -2.61541 -0.76751
H	4.00591 -3.48761 0.75595
H	6.31185 -2.74403 1.36334
H	6.4182 -1.77886 -0.13873

H	6.54346 -0.97762 1.45046
H	-7.49118 -1.08533 0.06266
H	-7.30011 -0.42896 1.71433
H	-7.8124 0.64031 0.38141
H	1.80845 -3.71733 1.13811
H	-4.13379 1.36735 -0.4356
H	0.77929 5.02155 2.16302
H	0.77091 6.02089 0.68047
H	2.22665 5.9626 1.70966
H	0.26777 3.07506 0.82083
H	0.33317 3.9936 -0.69825
H	3.41557 2.8429 -0.01037
H	3.12427 0.30451 -0.80132

Table S2. Optimized structure for the complex $[UO_2(R_{hydN})_2(R_{hydNH})]$

Atom Type	Cartesian coordinates (Å)
U	0.5725 -0.68232 -0.08389
C	-5.56163 -1.5626 -0.37355
O	-4.25254 -1.13801 -0.09633
C	-3.38289 -2.20906 0.08066
C	-2.01097 -1.69477 0.42605
O	-1.73544 -0.44911 0.42453
N	-1.00195 -2.49806 0.68105
O	-1.29563 -3.84024 0.42805
O	0.14355 -1.0894 -1.74098
O	1.01273 -0.27449 1.57733
N	-0.54654 2.47066 0.97427
C	-1.90625 2.77687 0.97832
C	-2.57779 2.78771 -0.37498
O	-3.8286 3.38252 -0.26084
C	-4.56687 3.28184 -1.44923
O	-0.06717 1.82891 -0.17544
O	-2.43814 3.03944 2.0257
H	-3.30374 -2.82978 -0.82715
H	-3.7126 -2.88104 0.8895
H	-2.65041 1.73759 -0.70378
H	-1.93904 3.31324 -1.103
H	-4.06318 3.79097 -2.28509
H	-4.73481 2.2313 -1.72897
H	-5.52973 3.76347 -1.27041
H	-5.6069 -2.15031 -1.30247
H	-5.96969 -2.1704 0.44736
H	-6.17252 -0.66578 -0.48746
H	-0.2458 1.97984 1.81128
H	5.6581 3.75438 -0.04837
C	5.75541 2.68437 0.14112
O	4.55508 2.08053 -0.26773
H	5.94071 2.52493 1.21353
H	6.61465 2.29656 -0.42556

C	4.57069 0.70332 -0.06806
C	3.25917 0.11202 -0.51047
H	5.38179 0.21209 -0.62895
H	4.72444 0.4444 0.99269
N	3.02573 -1.18107 -0.48024
O	2.27269 0.8389 -0.86494
O	4.04427 -1.89797 0.15471
H	4.03705 -2.74844 -0.29138
H	-0.7687 -4.31616 1.07475
H	0.76227 2.27191 -0.40546

Table S3. Optimized structure for the complex $[UO_2(R_{carb})_2(R_{carbH})]$

Atom Type	Cartesian coordinates (Å)
U	0.29994 -0.36581 -0.16575
C	6.62826 -0.04455 0.51012
O	5.26264 0.18584 0.28477
C	4.48982 -0.93443 0.56695
C	3.02801 -0.68034 0.29953
O	2.61442 0.41124 -0.16311
O	2.22077 -1.62502 0.55802
O	0.47862 -0.96405 -1.80602
O	0.08575 0.29133 1.45632
O	-2.16773 -0.18746 -0.45776
C	-2.32541 -1.38693 -0.08279
O	-1.34757 -2.08683 0.27905
C	-3.72952 -1.93999 -0.10578
O	-3.77316 -3.24518 0.36724
C	-5.06799 -3.78329 0.31891
H	4.57913 -1.24477 1.62087
H	4.78312 -1.8035 -0.04502
H	-4.08634 -1.86644 -1.14675
H	-4.36065 -1.26291 0.49383
H	7.15574 0.87852 0.26457
H	6.82646 -0.30188 1.56148
H	7.01077 -0.85603 -0.12696
H	-5.00751 -4.80321 0.70155
H	-5.76836 -3.20763 0.94285
H	-5.45562 -3.80905 -0.71053
C	-3.40199 4.17367 1.5327
O	-2.42053 4.10649 0.52017
H	-3.82371 5.17849 1.50313
H	-4.1974 3.43922 1.35542
H	-2.95798 3.99496 2.5198
C	-1.78852 2.85771 0.43437
C	-0.81193 2.90446 -0.71114
H	-2.49254 2.03683 0.23773

H	-1.2299 2.60746 1.34754
O	-0.76178 4.02902 -1.38277
O	-0.10272 1.96469 -1.01533
H	-1.40375 4.63603 -0.97249

Table S4. Optimized structure for the complex $[UO_2(R_{HydO})_2(H_2O)]$

Atom Type	Cartesian coordinates (Å)
U	-0.08647 0.34153 0.03
C	4.98334 0.36855 4.35294
O	4.0216 0.06213 3.37673
C	3.95467 1.0363 2.37576
C	2.81431 0.70548 1.45002
O	1.61798 0.72422 1.82571
N	3.10862 0.41274 0.20038
O	2.14222 0.11817 -0.6645
O	0.00322 2.08734 -0.21529
O	-0.20155 -1.39041 0.31893
O	-1.16572 0.82839 2.31809
N	-3.13662 0.47525 -1.05654
C	-2.46042 0.2402 -2.15935
C	-3.22768 0.16032 -3.45143
O	-3.18213 -1.15624 -3.9218
C	-3.72848 -1.28043 -5.20972
O	-2.51053 0.56585 0.11495
O	-1.21198 0.10888 -2.11691
H	4.90321 1.0948 1.81647
H	3.75795 2.03054 2.80769
H	-2.74944 0.84996 -4.16421
H	-4.26931 0.4921 -3.30612
H	-4.78785 -0.98349 -5.22949
H	-3.17658 -0.6693 -5.93843
H	-3.64857 -2.33121 -5.49156
H	5.99299 0.43007 3.91991
H	4.75599 1.32102 4.8537
H	4.96084 -0.43621 5.08904
H	-2.03427 1.15587 2.05197
H	-0.70633 1.53278 2.78136
H	-4.14523 0.53837 -1.04606
H	4.05921 0.33332 -0.13304

Table S5. Optimized structure for the complex $[UO_2(R_{HydN})_2(H_2O)]$

Atom Type	Cartesian coordinates (Å)
U	0.03417 -0.18735 0.02356
C	-2.86123 -0.86938 -5.46468
O	-2.44644 -0.96878 -4.12733
C	-2.25578 0.28378 -3.54884
C	-1.824 0.12677 -2.1154
O	-1.57263 -1.01445 -1.60107
N	-1.61378 1.16173 -1.33635
O	-1.68315 2.37716 -2.01935
O	1.1938 0.05866 -1.28406
O	-1.13429 -0.48038 1.30637
O	0.28849 -2.69319 -0.69221
N	1.79759 -0.98643 1.64425
C	1.76964 0.19607 2.20983
C	2.16336 0.40381 3.6467
O	2.15167 1.76091 3.95295
C	2.48848 1.99799 5.29421
O	2.08171 -2.01374 2.54089
O	1.31663 1.14561 1.48009
H	-1.8976 3.01275 -1.33249
H	-3.17409 0.89221 -3.56963
H	-1.48485 0.86651 -4.07965
H	2.21799 -2.77734 1.97627
H	3.15622 -0.04731 3.80441
H	1.4595 -0.16532 4.27777
H	1.77665 1.51381 5.97933
H	3.50086 1.63522 5.52703
H	2.45344 3.07756 5.44897
H	-3.81802 -0.33355 -5.55108
H	-2.11236 -0.35084 -6.08158
H	-2.98875 -1.88632 -5.83929
H	-0.48383 -2.67803 -1.27841
H	1.0447 -2.7439 -1.28312

Table S6. Optimized structure for the complex $[UO_2(R_{Carb})_2(H_2O)]$

Atom Type	Cartesian coordinates (Å)
U	0.02158 -0.00318 0.02398
C	5.70381 2.61464 -1.07476
O	4.34826 2.29846 -0.89241
C	4.16153 0.96209 -0.56385
C	2.70165 0.64227 -0.36545
O	1.80975 1.52382 -0.48621
O	2.39971 -0.55079 -0.068
O	0.22981 -2.5001 0.57265
O	-0.10037 -0.43465 -1.67623
O	0.13424 0.41118 1.7265
O	-2.18898 0.96848 -0.06965
C	-2.77658 -0.11949 0.20555
O	-2.1204 -1.17253 0.40917
C	-4.28148 -0.09272 0.28252
O	-4.79835 -1.35614 0.5463
C	-6.19992 -1.34445 0.63472
H	4.6823 0.68754 0.3685
H	4.5385 0.28551 -1.34869
H	-4.64999 0.31487 -0.67286
H	-4.55228 0.63621 1.0641
H	5.7558 3.67512 -1.32543
H	6.28643 2.43331 -0.15931
H	6.14735 2.03014 -1.89462
H	-6.5184 -2.36723 0.84164
H	-6.54631 -0.68966 1.4479
H	-6.66019 -1.00884 -0.30634
H	-0.66466 -2.85062 0.4911
H	0.80644 -3.03217 0.01985

Table S7. Optimized structure for the complex $[UO_2(R_{HydO})_2(R_{HydOH})(H_2O)]$

Atom Type	Cartesian coordinates (Å)
U	-0.2047 -0.74981 -0.32422
C	-7.01409 0.40782 0.85556
O	-5.67391 0.53787 0.45273
C	-4.8833 -0.54805 0.85093
C	-3.47122 -0.37989 0.36578
O	-2.59575 -1.24002 0.62628
O	0.68355 1.33164 -1.24252
C	1.04318 2.38664 -0.69671
C	0.03375 3.3585 -0.14721
O	0.67444 4.49547 0.3663
C	-0.22494 5.40437 0.9512
N	-3.16967 0.67861 -0.34198
O	-1.93693 0.8413 -0.82242
O	1.1975 -2.619 0.52564
N	2.49918 -2.45811 0.70686
C	3.11193 -1.3892 0.2581
C	4.60314 -1.30599 0.42996
O	4.90214 -0.19385 1.22413
C	6.27706 0.09351 1.24718
O	2.44939 -0.49169 -0.32363
O	-0.04872 -0.08107 1.30018
O	-0.25359 -1.3545 -1.9718
N	2.31306 2.71089 -0.5496
O	3.32347 1.9169 -0.98802
H	-5.27018 -1.49548 0.44397
H	-4.85912 -0.64622 1.94737
H	5.0516 -1.20262 -0.5715
H	4.99606 -2.23297 0.87939
H	6.85694 -0.74074 1.66929
H	6.65481 0.31398 0.23857
H	6.41005 0.9734 1.87806
H	-7.47652 -0.48766 0.41716
H	-7.09747 0.35026 1.95002
H	-7.54614 1.29268 0.50332
H	2.99502 -3.19522 1.18911

H	-3.87044 1.36603 -0.58318
H	-0.76856 4.94227 1.78658
H	-0.95193 5.7735 0.21453
H	0.36094 6.2449 1.32601
H	-0.54243 2.82375 0.62175
H	-0.66112 3.60847 -0.96123
H	2.5891 3.5658 -0.09186
H	3.05394 0.98798 -0.74387
O	-1.15333 -3.24717 -0.00705
H	-0.40084 -3.61651 0.47244
H	-1.86736 -3.0821 0.61722

Table S8. Optimized structure for the complex $[UO_2(R_{HydN})_2(R_{HydNH})(H_2O)]$

Atom Type	Cartesian coordinates (Å)
U	0.56096 -0.63815 -0.12415
C	-5.47176 -1.70659 -0.79377
O	-4.23949 -1.17088 -0.38809
C	-3.37344 -2.15154 0.08181
C	-2.07416 -1.5207 0.50919
N	-1.07968 -2.20432 1.04288
O	2.12061 1.02925 -1.00475
C	3.15576 0.38793 -0.62972
N	3.0209 -0.91744 -0.65631
O	4.05187 -1.60059 0.00655
O	-1.8185 -0.29464 0.3284
O	-1.23414 -3.61636 0.97785
O	0.02986 -1.16971 -1.7167
O	1.09434 -0.12883 1.48442
O	-0.15995 1.88363 -0.20704
N	-0.57994 2.49807 0.97887
C	-1.93512 2.80609 1.05178
O	-2.42774 3.02659 2.12921
C	-2.65918 2.86509 -0.27268
O	-3.90882 3.44886 -0.08917
C	-4.69803 3.36564 -1.24432
C	4.38718 1.07367 -0.10432
O	4.26065 2.45121 -0.25833
C	5.3802 3.14059 0.23384
H	-3.15058 -2.90835 -0.68811
H	-3.79962 -2.69508 0.94123
H	-2.73825 1.827 -0.63524
H	-2.0514 3.42114 -1.00398
H	-4.23854 3.89809 -2.0914
H	-4.86787 2.31966 -1.54012
H	-5.65706 3.83252 -1.01248
H	-5.34724 -2.42766 -1.61524
H	-5.98774 -2.20719 0.039
H	-6.0855 -0.87385 -1.14055
H	-0.24472 1.98246 1.78758

H	5.19681 4.20477 0.07834
H	5.52684 2.95493 1.30815
H	6.2977 2.85316 -0.30074
H	5.26508 0.67615 -0.63831
H	4.51068 0.79009 0.95416
H	4.1774 -2.38397 -0.53643
H	-1.28388 -3.88568 1.9011
H	0.68217 2.30139 -0.44516
O	1.42639 -3.04182 0.25734
H	2.07391 -3.01855 0.96749
H	0.65308 -3.53683 0.57892

Table S9. Optimized structure for the complex $[UO_2(R_{Carb})_2(R_{CarbH})(H_2O)]$

Atom Type	Cartesian coordinates (Å)
U	0.16054 -0.67417 0.04525
C	6.48467 0.19765 -0.10693
O	5.08605 0.29574 -0.07602
C	4.47265 -0.94993 -0.06953
C	2.96968 -0.82759 -0.03014
O	2.29874 -1.90351 -0.02258
O	-2.08754 -1.76122 -0.00508
C	-2.71311 -0.67712 -0.02401
C	-4.22056 -0.6287 -0.07078
O	-4.77076 -1.90517 -0.11071
C	-6.17352 -1.87504 -0.14217
O	2.39262 0.28439 -0.00321
O	0.05586 -3.22924 0.20049
O	0.13828 -0.73481 -1.71091
O	0.15193 -0.58836 1.79851
O	-2.09664 0.42654 -0.00345
O	-0.10591 2.05394 -0.0314
C	0.46582 3.27403 -0.04484
O	1.64551 3.44163 -0.0822
C	-0.52116 4.42366 -0.00937
O	-1.82954 3.92963 0.01028
C	-2.81254 4.935 0.06792
H	4.77163 -1.5537 0.80362
H	4.72718 -1.54092 -0.96535
H	-4.50164 -0.03157 -0.95388
H	-4.55579 -0.06423 0.8151
H	6.87853 1.21515 -0.10842
H	6.87186 -0.33544 0.77464
H	6.83349 -0.323 -1.01171
H	-6.51834 -2.90985 -0.16927
H	-6.58605 -1.38346 0.75158
H	-6.54597 -1.34981 -1.03444
H	-0.75098 -3.56549 -0.19976
H	0.81804 -3.6267 -0.22879
H	-3.78196 4.43589 0.07977

H	-2.70574 5.53986 0.97835
H	-2.75548 5.59402 -0.80877
H	-0.29704 5.02449 0.88383
H	-0.3325 5.05053 -0.89249
H	-1.07927 2.13965 -0.00776

Table S10. Optimized structures in gas phase and solvent for the complex $[UO_2(R_{HydO})_2(H_2O)_2]$

Atom Type	Cartesian coordinates (Å)	
	Gas Phase	*Solvent (ethanol)*
U	0.00245 0.05585 -0.01272	-0.00408 0.01244 0.11807
C	4.43542 0.89506 4.96114	-6.58417 -0.80663 0.2315
O	3.65555 0.42613 3.89214	-5.2553 -0.3908 0.38485
C	3.70282 1.28145 2.78708	-4.7554 0.3449 -0.6935
C	2.74101 0.78473 1.7414	-3.28818 0.54725 -0.37111
N	3.22996 0.45813 0.5658	-2.82144 1.76825 -0.25893
O	2.42381 0.03048 -0.39993	-1.50909 1.94715 0.02024
O	-1.49301 0.02829 -2.08327	2.50829 0.45556 -0.25441
C	-2.72196 0.21301 -1.92677	3.28312 -0.53288 -0.39067
C	-3.67376 0.33728 -3.086	4.75725 -0.36153 -0.70462
O	-3.65963 -0.85481 -3.81652	5.29326 0.31412 0.39733
C	-4.43054 -0.77041 -4.98675	6.6442 0.65853 0.25649
O	1.50788 0.70556 1.9462	-2.51139 -0.43699 -0.23164
O	0.03548 1.79094 -0.32733	-0.00816 0.01498 -1.61126
O	-0.03012 -1.67195 0.29939	-0.00063 0.00662 1.83311
O	-0.97896 0.3083 2.3756	-0.94562 -2.40367 0.25289
O	-2.41562 0.25709 0.34442	1.49382 -1.91906 -0.00065
N	-3.214 0.33888 -0.71443	2.80399 -1.74936 -0.28648
H	4.72429 1.34079 2.37572	-5.27602 1.30558 -0.82565
H	3.39599 2.30179 3.06929	-4.83815 -0.22037 -1.63411
H	-3.33682 1.18157 -3.7093	4.85924 0.22121 -1.63299
H	-4.69049 0.5703 -2.72806	5.24188 -1.33769 -0.85992
H	-5.4882 -0.56783 -4.76061	7.2793 -0.23019 0.13435
H	-4.05682 0.01799 -5.65665	6.80109 1.32047 -0.60713
H	-4.35399 -1.73422 -5.49204	6.93877 1.18418 1.16607
H	5.4976 0.97121 4.68402	-7.26832 0.04808 0.13352
H	4.09045 1.88084 5.30646	-6.70415 -1.45282 -0.64949
H	4.33158 0.17541 5.77442	-6.84807 -1.37218 1.1266
H	-1.8309 0.73118 2.21914	-0.26342 -2.93915 -0.18171
H	-0.39459 0.90582 2.85129	-1.76432 -2.43658 -0.26108
H	-4.20543 0.42322 -0.53856	3.37789 -2.59521 -0.32768
H	4.2226 0.44334 0.37753	-3.4017 2.60953 -0.3015
O	0.97716 -0.57431 -2.33238	0.93683 2.42401 0.23154

H	0.40878 -0.16281 -2.98996	1.75537 2.45772 -0.28265
H	1.84283 -0.15043 -2.32878	0.25087 2.96724 -0.18609

Table S11. Optimized structure in gas phase and solvent for the complex $[UO_2(R_{HydN})_2(H_2O)_2]$

Atom Type	Cartesian coordinates (Å)	
	Gas Phase	*Solvent (ethanol)*
U	0.00023 -0.00248 0.00904	-0.00061 -0.00321 0.00295
C	6.22063 0.80937 -0.413	6.20162 -0.87748 0.35063
O	4.87865 0.86169 -0.00695	4.85836 -0.83646 -0.03318
C	4.2755 -0.39325 -0.04055	4.30873 0.43582 0.06047
C	2.83833 -0.28548 0.39078	2.85449 0.33204 -0.34919
N	2.07764 -1.33353 0.57549	2.08241 1.36556 -0.54473
O	-2.24483 -0.83931 -0.52708	-2.25568 0.80799 0.48008
C	-2.83592 0.28473 -0.39266	-2.85065 -0.32385 0.35425
C	-4.28119 0.40117 0.00822	-4.30108 -0.43053 -0.0687
O	-4.88932 -0.85118 -0.03011	-4.86239 0.83732 0.03138
C	-6.23955 -0.79011 0.34614	-6.20655 0.87103 -0.35648
O	2.24517 0.83524 0.54154	2.2551 -0.79827 -0.46875
O	2.66825 -2.53919 0.19568	2.63379 2.61153 -0.24361
O	0.50422 -0.07231 -1.68097	0.46949 0.07667 1.67682
O	-0.50286 0.06913 1.6992	-0.4659 -0.06484 -1.6727
O	0.35154 2.60175 0.29914	0.35311 -2.64778 -0.33494
N	-2.06804 1.32891 -0.56729	-2.07662 -1.35918 0.55281
O	-2.65984 2.53955 -0.20901	-2.64061 -2.59391 0.22099
H	2.16522 -3.19012 0.69234	2.09438 3.2276 -0.76858
H	4.78398 -1.11329 0.62001	4.81786 1.17929 -0.57007
H	4.29851 -0.8293 -1.05377	4.3502 0.81987 1.09252
H	-2.12409 3.18603 -0.67646	-2.07776 -3.23084 0.69675
H	-4.7725 1.11925 -0.6674	-4.81013 -1.17931 0.55555
H	-4.32332 0.84401 1.01791	-4.33282 -0.80816 -1.10349
H	-6.35462 -0.41793 1.37513	-6.32988 0.57213 -1.40717
H	-6.81785 -0.14045 -0.32779	-6.82781 0.21492 0.26733
H	-6.63677 -1.80489 0.28897	-6.54921 1.90041 -0.24132
H	6.8165 0.15821 0.24395	6.8254 -0.23022 -0.27997
H	6.31479 0.44422 -1.44662	6.33043 -0.57177 1.39864
H	6.61437 1.82563 -0.358	6.53678 -1.91002 0.24186
H	1.30401 2.53744 0.4647	1.30971 -2.54547 -0.49296
H	-0.04749 2.83231 1.14243	-0.07133 -2.82865 -1.18493
O	-0.34633 -2.60119 -0.28291	-0.35514 2.63473 0.32601

H	-1.29358 -2.54115 -0.47641	-1.30453 2.54466 0.50747
H	0.08002 -2.84179 -1.1098	0.09371 2.83767 1.15809

Table S13. Optimized structure in gas phase and solvent for the complex $[UO_2(R_{Carb})_2(H_2O)_2]$

Atom Type	Cartesian coordinates (Å)	
	Gas Phase	*Solvent (ethanol)*
U	0.00254 0.00971 0.04165	-0.00079 0.00153 0.09938
C	6.01525 1.90445 -1.1891	6.37907 0.2971 -0.25395
O	4.63246 1.76719 -0.99325	4.99057 0.45876 -0.18122
C	4.28284 0.47386 -0.61873	4.2971 -0.74207 -0.10976
C	2.79711 0.3479 -0.38657	2.80244 -0.44915 -0.04207
O	2.35015 -0.79239 -0.07584	2.01493 -1.43535 -0.01964
O	-2.03676 -1.35654 0.38258	-2.3618 -0.72765 -0.01028
C	-2.81285 -0.38855 0.18876	-2.80314 0.45134 -0.04659
C	-4.31194 -0.5531 0.24243	-4.30038 0.73794 -0.11656
O	-4.67158 -1.87697 0.4732	-4.97673 -0.47227 -0.20549
C	-6.06328 -2.04026 0.5494	-6.37194 -0.32977 -0.23547
O	2.02829 1.33535 -0.48965	2.36179 0.73089 -0.0108
O	0.34804 -2.48525 0.55256	-0.43975 -2.56 0.08134
O	-0.12573 -0.35213 -1.67659	0.00107 -0.00189 -1.63827
O	0.13052 0.3716 1.75522	-0.00237 0.01339 1.82491
O	-2.36132 0.76651 -0.05291	-2.01712 1.44083 -0.02913
H	4.78404 0.16633 0.31393	4.56516 -1.33788 0.7792
H	4.55984 -0.2662 -1.38723	4.47652 -1.39043 -0.98359
H	-4.71881 -0.17618 -0.71013	-4.48127 1.385 -0.99043
H	-4.68367 0.11783 1.03446	-4.57647 1.32278 0.77725
H	6.19962 2.94077 -1.47674	6.81545 1.29723 -0.30677
H	6.57657 1.68313 -0.26906	6.77604 -0.21843 0.633
H	6.37787 1.241 -1.98856	6.67717 -0.26857 -1.14913
H	-6.25497 -3.09887 0.73183	-6.79402 -1.3351 -0.30182
H	-6.49368 -1.45148 1.3732	-6.74759 0.15581 0.67699
H	-6.55683 -1.74337 -0.38818	-6.70243 0.2549 -1.10605
H	-0.44867 -2.97204 0.32049	-1.31046 -2.74499 -0.30092
H	1.09466 -2.86027 0.07909	0.23132 -3.0576 -0.40787
O	-0.34103 2.50931 -0.45017	0.43548 2.57583 0.0759
H	0.40158 2.83416 -0.96845	1.30721 2.75567 -0.30916
H	-1.1565 2.68174 -0.92716	-0.23149 3.06789 -0.4253