

Electronic Supplementary Information for

**Theoretical Study of the Coordination Behavior of Formate and Formamidoximate
with Dioxovanadium (V) Cation: Implications for Selectivity towards Uranyl**

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Electronic supplementary information (ESI) available: Figure S1 showing structures of $\text{VO}_2(\text{HCOO})(\text{H}_2\text{O})_3$ complexes and relative energies in the gas phase and in aqueous solution, Table S1 listing relative electronic energies of $\text{VO}_2(\text{HCOO})(\text{H}_2\text{O})_3$ complexes at several levels of theory, and Cartesian coordinates of metal-ligand complexes accompanied with electronic energies of all species obtained with the B3LYP/aug-cc-pVDZ method and the MP2/aug-cc-pVDZ method, when available.

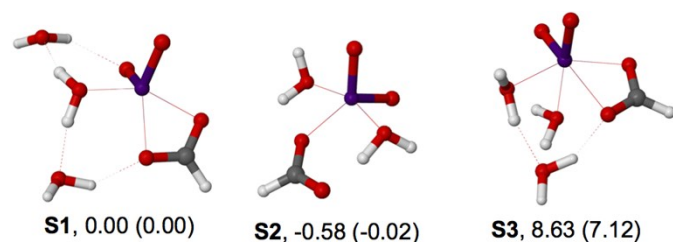


Figure S1. Structures of $\text{VO}_2(\text{HCOO})(\text{H}_2\text{O})_3$ complexes and relative energies in the gas phase and in aqueous solution (in parentheses) in units of kcal/mol.

Table S1. Relative gas phase electronic energies of five- and six-coordinate $\text{VO}_2(\text{HCOO})(\text{H}_2\text{O})_3$ in kcal/mol.^a All energies are given relative to complex **S1** in Figure S1.

Theory	S2 (c.n. = 5)	S3 (c.n. = 6)
MP2	-0.73	-1.53
MP2/aug- <i>qz</i> //MP2	-0.32	-1.46
CCSD(T)//MP2	-2.38	4.53
CCSD(T) + δ MP2	-1.97	4.60
B3LYP	-1.74	7.49
CCSD(T)//B3LYP	-2.52	2.75
M06		3.53
M06-L		2.03
ω B97XD		5.17
B97D3		5.98
PBE-D3		6.32
TPSS-D3		5.50
M06-L-D3		2.02
B3LYP-D3		5.15

^aThe aug-cc-pVDZ basis set was employed in all calculations unless otherwise specified. c.n. denotes coordination number.

Optimized Geometries and Absolute Energies Obtained at the MP2/aug-cc-pVDZ Level of Theory

VO₂⁺

Absolute Energy = -1093.236200 Hartrees

Cartesian Coordinates

V 0.0000 0.0000 0.4169
O 0.0000 1.2479 -0.5994
O 0.0000 -1.2479 -0.5994

VO₂(H₂O)₃⁺

Absolute Energy = -1322.251842 Hartrees

Cartesian Coordinates

V 0.9128 -0.2490 -2.6596
O 1.0976 1.1110 -1.6697
O 0.3804 -1.4041 -1.5435
O -1.0200 0.2633 -3.4321
H -1.7418 -0.3186 -3.1468
H -1.3199 1.1614 -3.2214
O 2.9741 -0.8371 -2.6660
H 3.1632 -1.6701 -2.2063
H 3.5853 -0.1901 -2.2802
O 1.2600 -0.4533 -4.7634
H 0.6120 -0.3039 -5.4668
H 2.0933 -0.7117 -5.1828

H₂VO₃(H₂O)₂⁺

Absolute Energy = -1322.218646 Hartrees

Cartesian Coordinates

V 2.0964 1.4268 0.8837
O 0.9126 2.2224 1.9232
O 1.4237 1.1868 -0.5742
O 3.5550 2.6244 0.2892
H 3.7139 2.9152 -0.6698
H 0.0277 2.5616 1.6993
O 3.7736 3.2285 -2.1682
H 4.4759 2.8811 -2.7372
H 3.5601 4.1060 -2.5176
O 2.6675 -0.1254 1.4998
H 4.2200 3.0163 0.8749
H 2.6848 -0.9931 1.0582

H₄VO₄(H₂O)⁺

Absolute Energy = -1322.166880 Hartrees

Cartesian Coordinates

V 0.2769 0.7656 -0.9472
O -0.9595 0.9964 -2.1769
O 0.0584 -0.6376 -0.1056
O 0.1799 -2.9404 0.6734
H 1.0681 -3.3237 0.5448
H -1.6165 0.3852 -2.5526
O 0.2475 2.1818 0.0973
H 0.2857 2.2621 1.0660
O 1.8848 0.5272 -1.6773
H -0.0845 -3.0626 1.6045
H 2.2328 1.2477 -2.2388
H 0.1327 -1.8927 0.3552

VO₂(AO)(H₂O)₃⁺

Absolute Energy = -1546.562308 Hartrees

Cartesian Coordinates

V 0.1324 1.0252 -0.4016

O -0.5392 1.0493 -1.9465
O -0.8109 -0.8847 2.7738
O -1.6651 0.3958 0.5191
N 2.2334 -0.7161 0.6384
C 2.8588 -0.0133 -0.3119
N 2.1653 0.8959 -0.9561
H 2.7120 1.4392 -1.6198
O 0.0763 2.6251 0.0840
H -0.6663 -0.2906 3.5218
H 0.0097 -0.8182 2.2286
H 3.9223 -0.2286 -0.4625
H 2.5784 -1.6144 0.9632
O 0.8746 -0.5209 0.7497
H -2.1129 -0.2092 -0.1126
H -1.5319 -0.0966 1.3639
O -2.5302 -0.9602 -1.7097
H -1.8887 -0.4097 -2.1954
H -3.3848 -0.7529 -2.1099

H₂VO₃(AO)(H₂O)₂⁺

Absolute Energy = -1546.539677 Hartrees

Cartesian Coordinates

V 1.4532 -1.8187 0.3581
O 1.9410 -0.1711 0.9352
O 1.4508 -1.4682 -1.2535
C -1.0003 -2.5549 1.6917
N -0.5267 -2.2037 0.4939
H -1.2482 -2.0833 -0.2133
N -0.1168 -2.7343 2.6557
O 1.1863 -2.5548 2.3650
O 1.8879 -2.2564 4.9041
H 1.9525 -0.4692 4.3057
H 1.8561 -2.4770 3.9407
O 2.8299 -3.0582 0.2319
H 2.9149 -3.4388 1.1250
H 2.6386 -2.7476 5.2606
O 1.8009 0.2749 3.6907
H 2.3699 0.9887 4.0037
H 1.9385 -0.1452 1.9264
H -2.0548 -2.7122 1.9336
H -0.3546 -2.9847 3.6138

Complex 1

Absolute Energy = -1398.545356 Hartrees

Cartesian Coordinates

O 0.3604 -2.6448 -0.7723
O -1.5204 -3.6351 0.7574
O -1.9947 -3.8756 -1.9453
O 0.8976 -4.9453 0.9184
O -1.1631 -6.3140 -0.6033
O 0.7302 -5.1609 -2.0823
V -0.4627 -4.1004 -0.4843
H 0.6016 -6.0947 -2.3027
H 1.4267 -4.8203 -2.6605
H 0.8333 -4.5267 1.7918
H 1.8381 -4.9171 0.6822
H -2.6714 -3.2356 -1.6721
H -1.0404 -6.8271 0.2097

H -2.0954 -6.4380 -0.8376
H -1.7129 -3.5977 -2.8310

Complex 2

Absolute Energy = -1398.541208 Hartrees

Cartesian Coordinates

O 0.2344 -4.0508 1.2520
O -1.9503 -3.4037 -0.0313
O 0.4409 -2.3565 -1.1153
O -1.1524 -6.1414 -0.1739
O 0.3930 -4.9437 -2.0790
V -0.4368 -4.1142 -0.2962
H 0.2818 -5.8616 -2.3607
H 1.0119 -4.4966 -2.6917
H -2.1205 -6.2032 -0.1656
H -0.8634 -6.6209 0.6178
H 0.6336 -1.6202 -0.5191
H 1.1733 -2.4132 -1.7597
O 2.0663 -3.1105 -3.2573
H 1.8573 -2.6801 -4.1008
H 3.0298 -3.2165 -3.2700

Complex 3

Absolute Energy = -1358.697173 Hartrees

Cartesian Coordinates

V 0.1482 -0.3605 0.2816
O 0.4640 0.7467 1.5104
O 1.0607 0.2100 -1.0092
O -1.7674 0.3620 -0.3385
C 0.0691 -2.7459 0.7624
O 1.1530 -2.0972 0.9161
O -1.0028 -2.1641 0.3548
H -2.2730 -0.4602 -0.4581
H -1.7442 0.7910 -1.2058
H 0.0457 -3.8266 0.9827

Complex 4

Absolute Energy = -1358.682407 sHartrees

Cartesian Coordinates

V -1.0412 0.6254 0.5267
O -1.6884 1.0175 2.0104
O -1.3013 -1.3900 0.2864
O -2.0086 1.4156 -0.5714
O 0.9345 0.6732 0.2769
O 1.1858 -1.5272 -0.2595
C 1.6246 -0.3651 -0.0807
H -0.3203 -1.6208 0.0540
H -1.5322 -1.8788 1.0894
H 2.7015 -0.1728 -0.2316

Complex 5

Absolute Energy = -1434.979157 Hartrees

Cartesian Coordinates

V 2.2016 9.6200 12.1816
O 0.4678 8.5264 12.6333
O 1.5059 9.7164 14.2020
O 3.7651 10.7849 12.9994
O 3.7483 12.6687 11.0781
O 1.7460 10.6456 10.9409
O 3.1425 8.4530 11.4161

C 0.5553 8.9355 13.8371
H -0.1966 8.6121 14.5770
H 2.9653 12.3242 10.6160
H 3.6364 13.6280 11.0927
H 3.8509 11.5959 12.4400
H 3.4340 11.0716 13.8652

Complex 6

Absolute Energy = -1434.981796 Hartrees

Cartesian Coordinates

V 2.2164 9.6024 12.2670
O 0.3634 8.6425 12.6844
O 1.3847 9.8438 14.2491
O 3.7834 10.8521 12.9654
O 1.8526 10.4634 10.8717
O 3.1369 8.3206 11.6976
C 0.3996 9.1079 13.8608
H -0.4175 8.8863 14.5682
H 3.6110 11.1868 13.8858
H 3.8877 11.6350 12.4086
H 2.2907 10.9979 15.3898
O 3.0493 11.6139 15.4242
H 3.5478 11.3691 16.2144

Complex 7

Absolute Energy = -1434.982087 Hartrees

Cartesian Coordinates

V -1.2912 0.5534 0.5708
O -1.1993 -1.5364 0.2383
O 0.7501 0.5665 0.1775
O 1.3540 -1.6036 -0.1432
C 1.6036 -0.3819 -0.0702
H -0.2161 -1.7266 0.0945
H -1.4671 -2.0428 1.0165
H 2.6437 -0.0377 -0.2274
O -0.6303 2.6056 0.8077
H 0.2840 2.4682 0.4936
H -1.0474 3.2018 0.1702
O -2.5339 0.8852 -0.5117
O -2.1046 0.4697 2.0459

Complex 8

Absolute Energy = -1434.978050 Hartrees

Cartesian Coordinates

V 2.6312 9.6650 12.0025
O 0.5409 9.6862 12.1563
O 1.6660 10.5968 13.8643
O 4.4977 10.4210 12.7276
O 2.5302 12.0248 11.6760
O 2.9527 9.5354 10.3426
O 2.8957 8.0757 12.5356
C 0.5798 10.2032 13.3287
H -0.3718 10.3051 13.8820
H 2.1980 12.1261 10.7719
H 1.8172 12.3133 12.2661
H 4.5076 10.2475 13.6823
H 4.3773 11.3823 12.6435

Complex 9

Absolute Energy = -1393.999430 Hartrees

Cartesian Coordinates

V 0.0922 1.0227 -0.4501
O -0.6263 1.0165 -1.9751
O -1.6361 0.2584 0.5978
N 2.0705 -0.8641 0.4704
C 2.7726 -0.0644 -0.3276
N 2.1349 0.9208 -0.9300
H 2.7301 1.4888 -1.5272
O -0.0549 2.6243 0.0567
H 3.8400 -0.2873 -0.4305
H 2.4624 -1.6265 1.0106
O 0.7396 -0.6035 0.6264
H -2.2598 -0.0708 -0.0658
H -1.2324 -0.5367 0.9929

Complex 10

Absolute Energy = -1393.984783 Hartrees

Cartesian Coordinates

V -2.1842 -1.1767 0.1110
O -3.1290 -2.2611 -0.7429
O -2.2679 -0.8376 1.9813
O -1.8981 0.1089 -0.9239
O 0.3097 -1.6836 1.4804
N -0.3317 -2.1122 0.2945
C 0.4157 -2.9114 -0.4007
N 1.6695 -3.2785 -0.0423
H 2.0133 -3.0013 0.8693
H 2.1466 -4.0049 -0.5544
H -2.8144 -1.3836 2.5642
H -0.4585 -1.3033 1.9776
H -0.0000 -3.2716 -1.3423

Complex 11

Absolute Energy = -1393.983631 Hartrees

Cartesian Coordinates

V 0.2862 -0.0973 -0.1309
O 0.9661 1.3911 -0.4753
O -0.0426 0.3226 1.9472
O -1.3259 0.0123 -0.5605
O 1.1909 -1.5301 -1.1350
N 1.3115 -1.8502 0.2160
C 1.9464 -2.9498 0.4807
N 2.5279 -3.7148 -0.5004
H 2.2145 -3.4932 -1.4426
H 2.6958 -4.6907 -0.2931
H 0.3302 1.2080 2.0795
H -1.0019 0.4454 2.0194
H 2.0646 -3.2322 1.5275

Complex 12

Absolute Energy = -1393.989084 Hartrees

Cartesian Coordinates

V -0.3341 0.3614 -0.9335
O -0.2779 0.5638 -2.6056
O -1.7827 1.0569 -0.4146
O 0.8691 -0.8493 0.1496
N -0.1855 -1.5742 -0.3988
C -0.2205 -2.8434 -0.1482
N 0.6914 -3.4528 0.6823

H 1.5261 -2.8969 0.8526
H 0.8355 -4.4462 0.5505
O 0.9861 1.8935 -0.2759
H -1.0434 -3.4219 -0.5688
H 0.4813 2.5334 0.2485
H 1.5311 1.4034 0.3635

Complex 13

Absolute Energy = -1393.988844 Hartrees

Cartesian Coordinates

V 0.0559 1.0320 -0.4447
O -0.6036 1.0557 -2.0034
O -1.6414 0.2373 0.5935
N 2.0612 -0.8921 0.5127
C 2.7652 -0.1273 -0.2621
O -0.0082 2.6337 0.0918
H 3.8332 -0.3292 -0.3633
O 0.7366 -0.5578 0.5675
H -2.2729 -0.1383 -0.0372
H -1.1761 -0.5268 0.9919
N 2.1443 0.9746 -0.9863
H 2.5985 1.8617 -0.7560
H 2.2436 0.8454 -1.9964

Complex 14

Absolute Energy = -1393.970530 Hartrees

Cartesian Coordinates

V -0.0489 0.9050 -0.1102
O -0.2718 1.3873 -1.7150
O -1.5886 -0.5829 -0.1615
N 0.9841 -0.8183 0.7460
C 2.0365 -0.3395 0.0524
N 2.0694 0.9901 0.0314
H 2.8261 1.3784 -0.5282
O -0.8177 2.0792 0.8041
H 2.7308 -1.0180 -0.4668
O 0.6823 -2.1905 0.3622
H -1.0956 -1.4024 0.0579
H -2.1899 -0.4293 0.5821
H 0.7131 -2.6565 1.2137

Complex 15

Absolute Energy = -1393.972482 Hartrees

Cartesian Coordinates

V -0.1737 0.8829 -0.1771
O -0.3814 1.5320 -1.7189
O -1.6384 -0.6264 -0.0436
N 0.8732 -0.8873 0.3365
C 2.1003 -0.4172 0.3810
N 2.0164 1.0022 0.0469
H 2.5230 1.2464 -0.8058
O -0.7026 2.0599 0.9095
H 3.0228 -0.9529 0.6254
O 0.4408 -2.0705 0.5690
H -1.0684 -1.4160 0.2485
H -2.3144 -0.4967 0.6354
H 2.3411 1.6114 0.7996

Complex 16

Absolute Energy = -1470.282922 Hartrees

Cartesian Coordinates

V 0.0385 0.9331 -0.3814
O -0.5396 1.3089 -1.9218
O -0.7049 -0.3735 2.7246
O -1.7939 0.0782 0.3027
N 2.0839 -0.9914 0.4157
C 2.7652 -0.0914 -0.3016
N 2.1116 0.9397 -0.7847
H 2.7038 1.6093 -1.2702
O -0.1307 2.3679 0.4781
H -0.4495 0.4620 3.1400
H 0.0368 -0.5807 2.1056
H 3.8410 -0.2689 -0.4102
H 2.4319 -1.9296 0.5863
O 0.7161 -0.8360 0.4811
H -1.8920 -0.8026 -0.0891
H -1.6210 -0.0919 1.2657

Complex 17

Absolute Energy = -1470.277878 Hartrees

Cartesian Coordinates

V -2.2756 -1.1028 0.0391
O -2.9869 -2.3132 -0.8846
O -2.1521 -0.8215 2.0474
O -1.7294 0.0169 -1.0848
O -4.0824 -0.0048 0.5571
O 0.2414 -1.6793 1.5457
N -0.4106 -2.0890 0.3716
C 0.3032 -2.9119 -0.3271
N 1.5237 -3.3849 0.0631
H 1.9736 -2.9077 0.8364
H 2.1159 -3.8125 -0.6345
H -2.5199 -1.5300 2.5977
H -0.5323 -1.2255 1.9977
H -0.1318 -3.2654 -1.2627
H -3.6838 0.1353 1.4462
H -4.0926 0.8590 0.1209

Complex 18

Absolute Energy = -1470.275822 Hartrees

Cartesian Coordinates

V -0.2477 0.3612 -0.8106
O -0.3348 0.5826 -2.4768
O 1.2178 0.8345 2.1906
O -1.6749 1.0006 -0.1892
O 0.9662 -0.9520 0.1865
N -0.1637 -1.6011 -0.3201
C -0.2269 -2.8796 -0.1294
N 0.7138 -3.5603 0.6061
H 1.5874 -3.0530 0.7281
H 0.7952 -4.5546 0.4341
O 1.1029 1.8789 -0.2614
H 0.4524 0.9336 2.7729
H 1.0547 -0.0095 1.7045
H -1.0949 -3.4096 -0.5230
H 0.7114 2.7586 -0.3548
H 1.2054 1.7190 0.7165

Complex 19

Absolute Energy = -1470.275291 Hartrees

Cartesian Coordinates

V 0.0922 1.0434 -0.4524
O -0.6022 0.7590 -1.9654
O -0.9112 -1.1538 2.4887
O -1.6669 0.6018 0.6571
N 2.2736 -0.4882 0.8450
C 2.8874 0.0772 -0.1458
O 0.0723 2.7176 -0.2862
H -0.8085 -0.8894 3.4119
H -0.0288 -0.9828 2.0639
H 3.9652 -0.0695 -0.2381
O 0.9221 -0.2477 0.8709
H -2.3268 0.1867 0.0856
H -1.5102 -0.0388 1.4083
N 2.1542 0.8734 -1.1143
H 2.5807 1.7957 -1.2256
H 2.1712 0.4270 -2.0351

Complex 20

Absolute Energy = -1470.262919 Hartrees

Cartesian Coordinates

V 0.4284 0.5952 -0.3818
O 0.9263 1.0703 -1.9171
O 0.2976 0.3788 1.9355
O 0.7845 2.5189 0.4548
O -1.2161 0.3618 -0.5399
O 1.5061 -1.0144 -0.2559
N 1.2648 -1.7769 0.9005
C 1.6689 -3.0055 0.7439
N 2.2871 -3.4702 -0.3900
H 2.1942 -2.8544 -1.1938
H 2.2561 -4.4658 -0.5653
H -0.6527 0.1922 1.9888
H 0.6997 -0.5459 1.8624
H 0.3686 3.2921 0.0510
H 0.4975 2.4683 1.3810
H 1.5530 -3.6799 1.5946

Complex 21

Absolute Energy = -1546.562308 Hartrees

Cartesian Coordinates

V 0.1324 1.0252 -0.4016
O -0.5392 1.0493 -1.9465
O -0.8109 -0.8847 2.7738
O -1.6651 0.3958 0.5191
N 2.2334 -0.7161 0.6384
C 2.8588 -0.0133 -0.3119
N 2.1653 0.8959 -0.9561
H 2.7120 1.4392 -1.6198
O 0.0763 2.6251 0.0840
H -0.6663 -0.2906 3.5218
H 0.0097 -0.8182 2.2286
H 3.9223 -0.2286 -0.4625
H 2.5784 -1.6144 0.9632
O 0.8746 -0.5209 0.7497
H -2.1129 -0.2092 -0.1126

H -1.5319 -0.0966 1.3639
O -2.5302 -0.9602 -1.7097
H -1.8887 -0.4097 -2.1954
H -3.3848 -0.7529 -2.1099

Complex 22

Absolute Energy = -1546.563673 Hartrees

Cartesian Coordinates

V -2.0823 -0.5941 0.0231
O -2.7079 -0.6087 -1.5400
O -1.3896 1.4750 2.7171
O -2.2910 1.5321 0.2193
O -3.3635 -1.0535 0.9889
O -0.0793 -2.7566 0.6970
N -1.1547 -2.5170 -0.1693
C -1.4499 -3.5526 -0.8881
N -0.8222 -4.7616 -0.7765
H 0.0483 -4.7693 -0.2551
H -0.9138 -5.4153 -1.5416
H -1.9042 1.0126 3.3918
H -0.8603 0.7631 2.2679
H -3.1991 1.8143 0.0452
H -2.1202 1.6963 1.1864
H -2.2885 -3.4473 -1.5776
O -0.3087 -0.2239 0.9559
H 0.0917 -1.8073 0.9834
H 0.3243 0.3152 0.4585

Complex 23

Absolute Energy = -1546.556854 Hartrees

Cartesian Coordinates

V -0.1585 0.4500 -0.6771
O -0.2321 0.7318 -2.3303
O 1.4759 0.7222 2.3282
O -1.5644 1.1053 -0.0307
O 1.0152 -0.9461 0.2281
N -0.1343 -1.5333 -0.3019
C -0.2306 -2.8197 -0.1959
N 0.6993 -3.5705 0.4822
H 1.5877 -3.0960 0.6273
H 0.7506 -4.5542 0.2487
O 1.2092 1.9189 -0.1036
H 0.7629 0.8392 2.9701
H 1.2275 -0.0833 1.8213
H -1.1170 -3.2995 -0.6119
H 0.6948 2.7596 -0.0968
H 1.3981 1.7042 0.8438
O -0.7199 3.8634 -0.1361
H -1.3908 3.1644 -0.2345
H -0.8448 4.4334 -0.9066

Complex 24

Absolute Energy = -1546.554129 Hartrees

Cartesian Coordinates

V 0.1701 0.9200 -0.5032
O -0.4134 0.5316 -2.0368
O -0.8060 -1.2193 2.5221
O -1.5878 0.4063 0.5281
N 2.3963 -0.3600 0.9729

C	3.0149	0.1889	-0.0239
O	0.0587	2.5902	-0.4098
H	-0.7708	-0.8836	3.4268
H	0.0726	-0.9911	2.1258
H	4.1038	0.1233	-0.0611
O	1.0320	-0.2242	0.9186
H	-2.1880	-0.0604	-0.0954
H	-1.4422	-0.1926	1.3060
O	-2.9380	-0.6925	-1.5996
H	-2.2267	-0.4070	-2.1987
H	-3.7289	-0.2427	-1.9252
N	2.2663	0.8591	-1.0720
H	2.6328	1.7981	-1.2411
H	2.3444	0.3476	-1.9550

Complex 25

Absolute Energy = -1546.549250 Hartrees

Cartesian Coordinates

V	-0.3424	0.5467	-0.3443
O	-0.2937	0.5714	-2.0364
O	-0.2222	0.6725	2.0502
O	-1.9321	1.0415	-0.0244
O	1.3515	-0.7284	0.0978
N	0.1411	-1.3956	0.0314
C	0.1627	-2.6787	0.2070
N	1.3207	-3.3542	0.5354
H	2.1579	-2.8170	0.3163
H	1.3530	-4.3308	0.2668
O	0.8374	2.3109	-0.0988
H	-0.9685	1.2530	2.2553
H	0.5614	1.0513	2.4809
H	-0.7829	-3.2179	0.1460
H	1.2409	2.5135	-0.9549
H	1.5798	2.0221	0.4887
O	2.4336	1.0231	1.6800
H	3.3783	0.9009	1.8324
H	2.1021	0.1880	1.2380

Complex S1

Absolute Energy = -1511.261465 Hartrees

Cartesian Coordinates

V	2.1353	9.6790	12.2772
O	0.3723	8.5914	12.7249
O	1.4332	9.7085	14.3236
O	3.8002	10.7254	13.0077
O	3.9885	12.3891	10.8491
O	1.6300	10.7481	11.0997
O	2.9800	8.5112	11.4086
C	0.4584	8.9645	13.9337
H	-0.3067	8.6484	14.6630
H	3.1327	12.1160	10.4784
H	3.9716	13.3549	10.8315
H	3.5803	11.1827	13.8556
H	4.0038	11.4273	12.3477
H	2.2283	11.0522	15.3787
O	2.9070	11.7541	15.3651
H	3.4020	11.6476	16.1874

Complex S2

Absolute Energy = -1511.262636 Hartrees

Cartesian Coordinates

V -1.2331 0.4792 0.6384
O -1.1165 -1.6140 0.3712
O 0.7906 0.4839 0.2037
O 1.3943 -1.6806 -0.1608
C 1.6367 -0.4554 -0.0874
H -0.1406 -1.7997 0.1624
H -1.3257 -2.1055 1.1764
H 2.6673 -0.1039 -0.2852
O -0.6414 2.5245 0.8742
H 0.2639 2.4818 0.5210
H -1.1673 3.0553 0.2305
O -2.4434 0.7830 -0.4732
O -2.0742 0.3926 2.0956
O -2.2899 3.5771 -1.0253
H -2.7492 2.7412 -1.2121
H -2.9931 4.2138 -0.8416

Complex S3

Absolute Energy = -1511.263902 Hartrees

Cartesian Coordinates

V -0.4585 0.5784 -0.3167
O -0.3108 0.5745 -2.0087
O -0.2472 0.6006 1.9880
O -1.9906 1.2798 -0.1217
O 1.3500 -0.7847 0.1684
C 0.4676 -1.7112 0.1933
O 0.7869 2.3171 -0.0615
H -0.9215 1.2115 2.3166
H 0.6057 0.9089 2.3394
H 1.1399 2.5778 -0.9235
H 1.5638 2.0392 0.4780
O 2.4929 1.0540 1.6431
H 3.4136 1.0612 1.9309
H 2.3418 0.1957 1.1791
O -0.7589 -1.4868 -0.0554
H 0.7770 -2.7469 0.4215

Optimized Geometries and Absolute Energies Obtained at the B3LYP/aug-cc-pVDZ Level of Theory
VO₂⁺

Absolute Energy = -1094.198446 Hartrees

Cartesian Coordinates

V 0.010592 0.000000 0.008000
O 0.009996 0.000000 1.558220
O 1.501554 0.000000 -0.416515

Complex 1

Absolute Energy = -1400.211579 Hartrees

Cartesian Coordinates

O 0.379485 -2.745090 -0.830609
O -1.465735 -3.640096 0.701711
O -1.953706 -3.900414 -1.955501
O 0.901174 -4.956031 0.870030
O -1.191209 -6.278038 -0.561911
O 0.713230 -5.143943 -2.056998
V -0.461233 -4.039570 -0.463068

H	0.625811	-6.070566	-2.316494
H	1.398748	-4.731445	-2.599033
H	0.788398	-4.626840	1.775779
H	1.844072	-4.879571	0.660189
H	-2.694223	-3.344405	-1.665681
H	-1.060484	-6.798621	0.243289
H	-2.117570	-6.408802	-0.809267
H	-1.679856	-3.569867	-2.824237

Complex 2

Absolute Energy = -1400.217767 Hartrees

Cartesian Coordinates

O	0.615404	-4.247902	0.926937
O	-1.740188	-3.436919	0.245346
O	0.282589	-2.393399	-1.246156
O	-1.162574	-6.075436	-0.195001
O	0.209088	-4.884744	-2.172252
V	-0.396017	-4.093906	-0.280854
H	0.083957	-5.804695	-2.438585
H	0.917355	-4.473826	-2.711412
H	-2.115342	-6.092571	-0.010329
H	-0.742067	-6.605322	0.500826
H	0.157894	-1.541269	-0.805991
H	1.099231	-2.380284	-1.787937
O	2.158181	-3.150727	-3.094259
H	2.136388	-2.735788	-3.969347
H	3.095101	-3.316111	-2.911987

Complex 3

Absolute Energy = -1360.301270 Hartrees

Cartesian Coordinates

V	0.196334	-0.335346	0.298439
O	0.420268	0.676524	1.502307
O	0.962095	0.177703	-1.004582
O	-1.719799	0.302753	-0.347714
C	0.061038	-2.725671	0.765169
O	1.137612	-2.060532	0.857572
O	-0.998977	-2.122464	0.409197
H	-2.279184	-0.472171	-0.509582
H	-1.679474	0.818052	-1.165387
H	0.053387	-3.803647	0.991181

Complex 4

Absolute Energy = -1360.301193 Hartrees

Cartesian Coordinates

V	-1.101894	0.617275	0.529732
O	-1.550277	1.033081	1.996711
O	-1.246172	-1.365675	0.288622
O	-1.930489	1.435495	-0.548463
O	0.812308	0.635892	0.224801
O	1.193858	-1.549629	-0.188109
C	1.570016	-0.369834	-0.070025
H	-0.243434	-1.629352	0.075515
H	-1.582183	-1.909377	1.013373
H	2.632667	-0.120875	-0.221557

Complex 5

Absolute Energy = -1436.768243 Hartrees

Cartesian Coordinates

V	2.250554	9.574710	12.101873
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O	0.456199	8.720614	12.577831
O	1.622167	9.668291	14.158649
O	3.717094	10.778897	12.931635
O	3.687434	12.688349	11.137987
O	1.897841	10.605477	10.913050
O	3.110899	8.367745	11.543760
C	0.584088	9.031944	13.801891
H	-0.193059	8.751569	14.530519
H	2.968394	12.181882	10.707529
H	3.374029	13.597503	11.209815
H	3.813220	11.626252	12.407698
H	3.533441	10.989068	13.857262

Complex 6

Absolute Energy = -1436.766267 Hartrees

Cartesian Coordinates

V	2.241368	9.558049	12.212201
O	0.407852	8.716718	12.638706
O	1.382091	9.857572	14.220952
O	3.601423	10.939215	12.942459
O	1.958359	10.341864	10.851816
O	3.165701	8.297919	11.930235
C	0.398429	9.156028	13.822739
H	-0.447762	8.933291	14.492037
H	3.530405	11.236085	13.894177
H	3.699172	11.712395	12.373596
H	2.351715	10.952661	15.463990
O	3.123058	11.549714	15.459328
H	3.694189	11.270189	16.184864

Complex 7

Absolute Energy = -1436.767201 Hartrees

Cartesian Coordinates

V	-1.284791	0.532032	0.575229
O	-1.166014	-1.490446	0.226392
O	0.710811	0.524946	0.149055
O	1.337297	-1.632058	-0.066065
C	1.576923	-0.416797	-0.040482
H	-0.179355	-1.746373	0.122135
H	-1.566997	-2.021562	0.925450
H	2.614262	-0.066780	-0.191993
O	-0.626585	2.580570	0.775267
H	0.255596	2.601506	0.371471
H	-1.201568	3.167871	0.265553
O	-2.402671	0.955315	-0.483907
O	-1.921308	0.433376	2.034295

Four-Coordinate VO₂(HCOO)(H₂O)₂ Complex

Absolute Energy = -1436.766288 Hartrees

Cartesian Coordinates

V	1.751693	8.675161	12.238341
O	0.412477	8.831187	13.568829
O	1.266658	8.891759	15.661442
O	3.061388	10.132656	12.612263
O	1.182805	8.897184	10.768314
O	2.531447	7.291944	12.341841
C	0.373857	8.631217	14.859810
H	-0.585497	8.212191	15.211569
H	3.371509	10.202525	13.600002

H	2.966525	11.004509	12.210350
H	4.306469	9.659910	15.419131
O	3.546782	10.141523	15.069702
H	2.730187	9.663435	15.384207

Complex 9

Absolute Energy = -1395.740582 Hartrees

Cartesian Coordinates

V	0.115968	1.052107	-0.444132
O	-0.604067	0.964757	-1.880703
O	-1.608485	0.229875	0.560467
N	2.084562	-0.827141	0.499025
C	2.769797	-0.060840	-0.332825
N	2.104342	0.891860	-0.941320
H	2.631721	1.474661	-1.578549
O	0.045996	2.544863	0.126251
H	3.833844	-0.268446	-0.460632
H	2.465404	-1.582723	1.051419
O	0.758724	-0.553021	0.642584
H	-2.258111	0.026226	-0.126751
H	-1.306995	-0.614177	0.933566

Complex 10

Absolute Energy = -1395.741404 Hartrees

Cartesian Coordinates

V	-2.136784	-1.189736	0.070467
O	-3.099718	-2.264446	-0.627765
O	-2.349950	-0.831977	1.866563
O	-1.918682	0.104668	-0.845542
O	0.360890	-1.691129	1.527913
N	-0.302879	-2.103762	0.360249
C	0.406740	-2.911739	-0.361308
N	1.639981	-3.335341	-0.041753
H	2.078133	-3.012441	0.809317
H	2.135162	-3.972043	-0.643886
H	-2.939007	-1.379555	2.400433
H	-0.356936	-1.271306	2.045314
H	-0.046050	-3.258194	-1.288302

Complex 11

Absolute Energy = -1395.733252 Hartrees

Cartesian Coordinates

V	0.055457	1.049748	-0.432735
O	-0.538727	0.977084	-1.928280
O	-1.631024	0.218438	0.562479
N	2.064827	-0.842180	0.513937
C	2.768772	-0.111460	-0.261708
O	0.113181	2.549166	0.133138
H	3.834397	-0.303449	-0.371151
O	0.752346	-0.502250	0.555846
H	-2.307673	-0.068462	-0.066005
H	-1.260734	-0.578339	0.983246
N	2.130457	0.970729	-0.994829
H	2.554992	1.874111	-0.781496
H	2.199829	0.835863	-2.004539

Complex 12

Absolute Energy = -1395.733252 Hartrees

Cartesian Coordinates

V	-0.345890	0.339344	-0.939562
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O	-0.254246	0.474853	-2.532130
O	-1.687847	0.995296	-0.339476
O	0.895931	-0.803697	0.121334
N	-0.150061	-1.543359	-0.378786
C	-0.206557	-2.808961	-0.160990
N	0.705473	-3.473266	0.597104
H	1.547222	-2.975039	0.854562
H	0.737507	-4.479479	0.565392
O	0.958156	1.870147	-0.267264
H	-1.047849	-3.356534	-0.579984
H	0.428287	2.585964	0.112129
H	1.496375	1.502332	0.449371

Complex 13

Absolute Energy = -1395.727057 Hartrees

Cartesian Coordinates

V	0.2935	0.3275	-0.4283
O	0.7283	1.5664	-1.3326
O	0.3787	0.5041	1.6239
O	-1.2027	-0.1438	-0.7583
O	1.5853	-1.0163	-0.3021
N	1.2904	-1.7748	0.8525
C	1.6182	-3.0193	0.7155
N	2.1500	-3.5681	-0.3972
H	2.2783	-2.9850	-1.2123
H	2.3497	-4.5526	-0.4475
H	-0.4673	0.5985	2.0819
H	0.7023	-0.4515	1.7578
H	1.4589	-3.6640	1.5793

Complex 14

Absolute Energy = -1395.704388 Hartrees

Cartesian Coordinates

V	-0.045643	0.921272	-0.161637
O	-0.240843	1.305859	-1.701388
O	-1.603684	-0.538405	-0.098822
N	0.977463	-0.845730	0.638759
C	2.070065	-0.348136	0.055864
N	2.014160	0.971374	0.007096
H	2.751012	1.448346	-0.497514
O	-0.741728	1.997616	0.796100
H	2.855528	-0.984886	-0.371947
O	0.733100	-2.221873	0.322890
H	-1.217371	-1.411945	0.093754
H	-2.240763	-0.331542	0.598204
H	0.718402	-2.659451	1.186741

Complex 15

Absolute Energy = -1395.709269 Hartrees

Cartesian Coordinates

V	-0.201170	0.892330	-0.182218
O	-0.283156	1.447956	-1.680005
O	-1.597082	-0.609665	-0.011577
N	0.868110	-0.854346	0.327095
C	2.075221	-0.405679	0.369564
N	1.997688	1.008913	0.048898
H	2.477705	1.272706	-0.810719
O	-0.629114	1.980211	0.914740
H	2.992428	-0.948223	0.602973

O	0.400665	-2.030654	0.547495
H	-1.039012	-1.431961	0.272390
H	-2.326282	-0.479071	0.606857
H	2.302700	1.625384	0.801007

Complex 16

Absolute Energy = -1472.203027 Hartrees

Cartesian Coordinates

V	0.135064	1.052678	-0.483787
O	-0.567201	0.890058	-1.920452
O	-0.931333	-1.020202	2.639665
O	-1.613907	0.440393	0.527825
N	2.232691	-0.642426	0.638105
C	2.827309	-0.028604	-0.377913
N	2.102027	0.806058	-1.071821
H	2.571650	1.301543	-1.818989
O	0.171630	2.592703	-0.056295
H	-0.872415	-0.544514	3.476956
H	-0.059614	-0.908452	2.194177
H	3.881345	-0.250775	-0.556550
H	2.608832	-1.456587	1.105570
O	0.891227	-0.409674	0.786096
H	-2.236049	0.032811	-0.086110
H	-1.544157	-0.121709	1.344423

Complex 17

Absolute Energy = -1472.200707 Hartrees

Cartesian Coordinates

V	-2.193113	-1.079742	0.130545
O	-2.843768	-2.263261	-0.740663
O	-2.127662	-0.879946	2.048333
O	-1.705161	0.147091	-0.788935
O	-4.121065	-0.068127	0.513196
O	0.351736	-1.694721	1.591301
N	-0.350066	-2.046706	0.435400
C	0.300466	-2.853799	-0.334610
N	1.534142	-3.331070	-0.071770
H	2.009526	-3.047392	0.772459
H	1.985080	-3.966516	-0.707776
H	-2.562341	-1.551350	2.588912
H	-0.369113	-1.256389	2.108027
H	-0.200750	-3.154746	-1.252024
H	-3.904996	0.419708	1.323057
H	-4.242514	0.589767	-0.186152

Complex 18

Absolute Energy = -1472.198576 Hartrees

Cartesian Coordinates

V	-0.316064	0.326026	-0.845738
O	-0.268944	0.471304	-2.440152
O	1.319439	0.935225	2.239345
O	-1.682751	0.905429	-0.231917
O	0.892301	-0.888282	0.234737
N	-0.163792	-1.581454	-0.316474
C	-0.214022	-2.860892	-0.202027
N	0.692942	-3.580704	0.510840
H	1.548130	-3.109569	0.777271
H	0.724406	-4.581073	0.393799
O	1.007275	1.812775	-0.238948

H 0.622214 1.097528 2.886866
H 1.110632 0.064817 1.837694
H -1.049794 -3.376237 -0.670438
H 0.678270 2.705850 -0.402236
H 1.164160 1.708557 0.741378

Complex 19

Absolute Energy = -1472.197307 Hartrees

Cartesian Coordinates

V 0.4809 0.5694 -0.9697
O 0.8750 1.1169 -2.4192
O 0.3655 0.4828 2.4567
O 0.7875 1.9983 0.4450
O -1.0746 0.1877 -0.8894
O 1.6167 -0.7619 -0.3761
N 1.2496 -1.4625 0.7867
C 1.5433 -2.7200 0.6881
N 2.0921 -3.3201 -0.3906
H 2.2935 -2.7632 -1.2090
H 2.2868 -4.3067 -0.3946
H -0.5619 0.3253 2.6744
H 0.6742 -0.3511 1.9890
H 0.3381 2.8492 0.3750
H 0.5705 1.5580 1.3432
H 1.3268 -3.3378 1.5592

Complex 20

Absolute Energy = -1472.192635 Hartrees

Cartesian Coordinates

V 0.0751 1.0538 -0.4499
O -0.5058 0.6976 -1.9085
O -0.9234 -1.0980 2.5194
O -1.6393 0.5360 0.6170
N 2.2535 -0.5000 0.7872
C 2.8725 0.0603 -0.1783
O 0.1821 2.6361 -0.2210
H -0.8438 -0.8132 3.4374
H -0.0355 -0.9667 2.1055
H 3.9430 -0.0995 -0.2945
O 0.9182 -0.2294 0.8224
H -2.3153 0.1601 0.0398
H -1.5240 -0.0702 1.4095
N 2.1382 0.8946 -1.1069
H 2.5218 1.8386 -1.1573
H 2.1471 0.5117 -2.0531

Complex 21

Absolute Energy = -1548.668264 Hartrees

Cartesian Coordinates

V 0.163038 0.937158 -0.486461
O -0.483931 0.722657 -1.962446
O -0.839831 -1.058608 2.730425
O -1.534546 0.216641 0.451738
N 2.355881 -0.518503 0.769037
C 2.921675 0.053410 -0.284738
N 2.142814 0.770604 -1.050483
H 2.580414 1.236547 -1.835079
O 0.124044 2.481547 -0.094747
H -0.864432 -0.504997 3.520098

H 0.029177 -0.888886 2.305320
H 3.991320 -0.102463 -0.437300
H 2.783924 -1.251064 1.319383
O 1.000637 -0.372172 0.880139
H -2.140822 -0.228683 -0.192734
H -1.474892 -0.292505 1.294918
O -2.767109 -0.734031 -1.723045
H -2.003341 -0.277955 -2.141669
H -3.550717 -0.273495 -2.045955

Complex 22

Absolute Energy = -1548.666049 Hartrees

Cartesian Coordinates

V -2.0884 -0.6701 0.0672
O -2.6011 -0.6710 -1.4606
O -1.3719 1.6328 2.6976
O -2.3515 1.4460 0.2394
O -3.2575 -1.1018 1.0745
O -0.0798 -2.8274 0.7424
N -1.1095 -2.5288 -0.1525
C -1.3969 -3.5049 -0.9482
N -0.7768 -4.7025 -0.9411
H -0.0389 -4.8787 -0.2751
H -1.0393 -5.4203 -1.5950
H -1.8706 1.2526 3.4310
H -0.8609 0.8840 2.3077
H -3.2452 1.7148 -0.0068
H -2.1859 1.7076 1.1845
H -2.1970 -3.3232 -1.6625
O -0.3825 -0.2296 0.9531
H 0.1054 -1.9223 1.0985
H 0.2780 0.2443 0.4323

Complex 23

Absolute Energy = -1548.664163 Hartrees

Cartesian Coordinates

V -0.095822 0.436709 -0.902649
O 0.204145 0.515865 -2.467487
O 1.745260 0.813882 2.289002
O -1.528982 1.109467 -0.536229
O 0.919122 -0.844467 0.278812
N -0.127088 -1.468842 -0.359807
C -0.263814 -2.744156 -0.271577
N 0.537808 -3.526901 0.498559
H 1.399713 -3.115982 0.834085
H 0.513489 -4.526153 0.370550
O 1.087225 1.910587 -0.099852
H 1.218165 1.026015 3.068660
H 1.362857 -0.005390 1.917340
H -1.090217 -3.200816 -0.811844
H 0.529529 2.728281 -0.016314
H 1.405630 1.673493 0.807701
O -0.890307 3.711776 0.082912
H -1.446098 2.935476 -0.145745
H -1.051815 4.360955 -0.612118

Complex 24

Absolute Energy = -1548.656813 Hartrees

Cartesian Coordinates

V 0.1255 0.9275 -0.4831
O -0.3892 0.5091 -1.9690
O -0.8391 -1.1228 2.5871
O -1.5694 0.3341 0.4963
N 2.3644 -0.4027 0.8841
C 2.9762 0.1441 -0.0934
O 0.1623 2.5143 -0.2934
H -0.8098 -0.7569 3.4788
H 0.0487 -0.9628 2.1935
H 4.0590 0.0597 -0.1661
O 1.0129 -0.2352 0.8561
H -2.1977 -0.1105 -0.1290
H -1.4715 -0.2033 1.3286
O -2.8469 -0.7000 -1.6155
H -2.0563 -0.3711 -2.0914
H -3.5966 -0.2295 -1.9991
N 2.2131 0.8600 -1.0939
H 2.5320 1.8229 -1.2014
H 2.2725 0.4151 -2.0107

Figure 11, reactant

Absolute Energy = -454.595311445 Hartrees

Cartesian Coordinates

N -0.8180 -1.5483 0.0757
C -0.2680 -1.4795 -1.0963
H 0.2683 -2.3811 -1.3967
O -1.5130 -0.3258 0.3504
N -0.3102 -0.4497 -1.9733
H -0.5179 0.4986 -1.6431
H 0.2850 -0.5110 -2.7850
O -0.2304 2.3209 -1.0678
H 0.2968 2.1343 -0.2596
O 1.2991 1.7224 1.1980
H 2.2234 1.9945 1.1830
H 1.3084 0.7834 1.4855
H -1.0401 2.7295 -0.7413
H 0.6060 -1.3848 1.3434
O 1.3245 -0.9925 1.8880
H 1.1798 -1.3099 2.7863
H -1.9858 -0.5317 1.1651

Figure 11, transition state

Absolute Energy = -454.549629140 Hartrees

Cartesian Coordinates

N 2.2915 -0.5455 0.6658
C 2.8815 -0.4352 -0.5225
H 3.6606 -1.1846 -0.6829
O 1.3106 0.4317 0.9307
N 2.5875 0.4517 -1.4404
H 2.3530 1.4878 -1.0801
H 3.1431 0.3915 -2.2850
O 2.5970 2.7835 -0.4683
H 3.3523 2.4643 0.2897
O 4.2445 1.9274 1.1332
H 5.0667 2.4275 1.1452
H 4.2547 0.7599 1.9506
H 1.8441 3.1304 0.0238
H 2.9753 -0.6272 1.5035

O 4.1452 -0.1916 2.4288
H 3.9968 -0.0245 3.3657
H 0.5740 -0.0783 1.2966

Figure 11, product

Absolute Energy = -454.583306000 Hartrees

Cartesian Coordinates

N -0.7500 -1.3440 0.1420
C -0.1067 -1.2667 -1.0683
H 0.7131 -1.9988 -1.1097
O -1.6946 -0.3243 0.4017
N -0.4450 -0.4845 -2.0301
H -0.5205 1.2725 -1.3983
H 0.1372 -0.6604 -2.8478
O -0.3508 2.1366 -0.9504
H 0.8758 1.8152 0.2606
O 1.5461 1.5898 0.9529
H 2.3727 1.9837 0.6548
H 1.4802 -0.0053 1.7023
H -1.1701 2.3119 -0.4716
H -0.1208 -1.4225 0.9537
O 1.3519 -0.9252 2.0335
H 1.3425 -0.8568 2.9944
H -2.5498 -0.7508 0.2539

Figure 12, reactant

Absolute Energy = -1701.56628149 Hartrees

Cartesian Coordinates

V -1.3462 -0.3894 -0.6491
O -1.9510 -1.0907 -1.9582
N 0.9005 -1.7244 0.6227
C 1.4462 -1.2163 -0.4140
O -1.6296 1.2039 -0.6279
H 2.5040 -1.3919 -0.6035
O -0.4237 -1.4174 0.7536
N 0.6869 -0.3230 -1.2480
H 1.0798 0.6552 -1.0817
H 0.8034 -0.5375 -2.2384
O 1.8512 2.0389 -0.5964
H 2.3684 1.8632 0.2163
O 3.2916 1.2385 1.6720
H 4.2155 1.4347 1.8583
H 3.0869 0.4062 2.1511
H 1.1792 2.7160 -0.3647
H 1.9968 -1.5886 2.2088
O 2.6299 -1.2043 2.8515
H 2.1768 -1.2180 3.7024
O -0.3758 3.5933 -0.0354
H -0.9682 2.8307 -0.2093
H -0.6767 4.2933 -0.6256
O -2.8693 -1.0575 0.6943
H -3.5380 -1.5745 0.2244
H -2.3783 -1.6687 1.2724

Figure 11, transition state 1

Absolute Energy = -1701.55792713 Hartrees

Cartesian Coordinates

V -1.2429 -0.3415 -0.6726
O -1.9605 -1.1591 -1.8504

N 1.0052 -1.7109 0.5571
C 1.4613 -1.2724 -0.5628
O -1.5684 1.2590 -0.7595
H 2.4657 -1.5744 -0.8657
O -0.2917 -1.2678 0.7732
N 0.7245 -0.3361 -1.2938
H 1.2465 0.9227 -0.8336
H 0.9123 -0.3801 -2.2934
O 1.7084 1.8642 -0.4406
H 2.2077 1.6745 0.4171
O 2.9935 1.3376 1.7644
H 3.9387 1.5165 1.8172
H 2.8520 0.4498 2.1884
H 0.9849 2.5600 -0.2749
H 2.0195 -1.5336 2.0454
O 2.5941 -1.1346 2.7480
H 2.1175 -1.2542 3.5774
O -0.2994 3.4310 -0.0411
H -0.9486 2.7093 -0.2731
H -0.4854 4.1656 -0.6371
O -2.7089 -0.8670 0.8241
H -3.3882 -1.4145 0.4070
H -2.1565 -1.4569 1.3710

Figure 11, intermediate

Absolute Energy = -1701.55812653 Hartrees

Cartesian Coordinates

V -1.2262 -0.3433 -0.6988
O -1.9891 -1.1878 -1.8282
N 1.0319 -1.6868 0.5495
C 1.4667 -1.2838 -0.5960
O -1.5470 1.2620 -0.8217
H 2.4650 -1.5990 -0.9070
O -0.2668 -1.2297 0.7610
N 0.7168 -0.3887 -1.3417
H 1.2897 1.0092 -0.7902
H 0.9287 -0.4112 -2.3360
O 1.7059 1.8836 -0.3881
H 2.2018 1.6679 0.4796
O 2.9568 1.3501 1.7873
H 3.9042 1.5224 1.8230
H 2.8162 0.4532 2.2034
H 0.9469 2.5688 -0.2239
H 2.0147 -1.5016 2.0101
O 2.5816 -1.1104 2.7300
H 2.1000 -1.2511 3.5531
O -0.3025 3.3733 -0.0136
H -0.9439 2.6484 -0.2898
H -0.4691 4.1253 -0.5938
O -2.6740 -0.8071 0.8421
H -3.3572 -1.3666 0.4478
H -2.1095 -1.3834 1.3917

Figure 11, transition state 2

Absolute Energy = -1701.55148707 Hartrees

Cartesian Coordinates

V 0.1654 0.5355 -0.9477
O -0.7239 -0.3468 -1.9529

N	2.5005	-0.6880	0.3052
C	2.8637	-0.3965	-0.9103
O	-0.1179	2.1347	-1.1491
H	3.8595	-0.7090	-1.2338
O	1.1972	-0.2445	0.5388
N	2.0360	0.3290	-1.6991
H	2.7714	2.0533	-0.9095
H	2.2821	0.3582	-2.6823
O	3.1593	2.8113	-0.4175
H	3.6910	2.4751	0.7332
O	4.1864	2.2173	1.7078
H	5.1242	2.4423	1.6656
H	4.0568	1.1532	2.0413
H	2.4200	3.4898	-0.3513
H	3.3327	-0.4987	1.5187
O	3.9061	-0.1167	2.3389
H	3.3989	-0.2666	3.1463
O	1.0344	4.3341	-0.2652
H	0.4561	3.5852	-0.5820
H	0.8767	5.0657	-0.8725
O	-1.2034	0.2047	0.7015
H	-1.8996	-0.3767	0.3656
H	-0.6172	-0.3393	1.2601

Figure 11, product

Absolute Energy = -1701.58206042 Hartrees

Cartesian Coordinates

V	-1.5381	-0.6618	-0.8354
O	-2.6368	-1.6383	-1.4788
N	0.9651	-1.4151	0.3392
C	1.1923	-1.4926	-0.9522
O	-1.7168	0.8539	-1.3899
H	2.1991	-1.7540	-1.2805
O	-0.3145	-1.0832	0.6876
N	0.1719	-1.2552	-1.7567
H	2.7870	2.9542	-0.3137
H	0.3430	-1.3509	-2.7491
O	2.1661	2.8944	0.4202
H	2.5892	1.9623	1.7996
O	2.8792	1.4451	2.5906
H	3.5159	2.0025	3.0497
H	2.9849	-0.2613	2.4490
H	1.2701	2.9327	0.0027
H	1.6729	-1.4394	1.0958
O	2.9425	-1.2352	2.2794
H	2.8544	-1.6495	3.1448
O	-0.1889	3.0468	-0.8859
H	-0.7455	2.2519	-1.0725
H	-0.8099	3.7644	-0.7218
O	-2.6860	-0.4784	0.9836
H	-3.4160	-1.1109	0.9330
H	-2.0769	-0.7892	1.6746

Complex S1

Absolute Energy = -1513.230730 Hartrees

Cartesian Coordinates

V	2.298649	9.569206	12.238981
O	0.404562	8.835654	12.575136

O	1.378086	9.880853	14.220310
O	3.620293	10.923347	12.964298
O	3.756400	12.553923	10.878925
O	2.113916	10.307843	10.819722
O	3.160702	8.253082	12.054246
C	0.375497	9.243589	13.771820
H	-0.504680	9.046356	14.404398
H	3.132474	11.922560	10.468670
H	3.346379	13.422887	10.795687
H	3.575196	11.216893	13.910383
H	3.768011	11.686184	12.345867
H	2.388369	10.931344	15.512651
O	3.168166	11.514745	15.530055
H	3.734982	11.191934	16.240749

Complex S2

Absolute Energy = -1513.233497 Hartrees

Cartesian Coordinates

V	-1.206642	0.513868	0.560514
O	-1.107426	-1.524236	0.252912
O	0.784945	0.439194	0.164409
O	1.396377	-1.731358	0.063294
C	1.645885	-0.517417	0.043888
H	-0.123170	-1.805565	0.198953
H	-1.549698	-2.028313	0.946997
H	2.690515	-0.182395	-0.090388
O	-0.590366	2.526283	0.666158
H	0.311452	2.585571	0.320249
H	-1.188371	3.098209	0.109724
O	-2.362890	0.866093	-0.507223
O	-1.829352	0.421887	2.021768
O	-2.410615	3.577487	-0.942397
H	-2.726038	2.654511	-1.030076
H	-3.155906	4.079381	-0.590682

Complex S3

Absolute Energy = -1513.218789 Hartrees

Cartesian Coordinates

V	-0.553966	0.596639	-0.376712
O	-0.321587	0.691419	-1.953707
O	-0.259843	0.651189	1.986457
O	-1.994439	1.203531	-0.064929
O	1.395137	-0.820188	0.192076
C	0.492631	-1.692706	0.164818
O	0.803267	2.197874	-0.077219
H	-0.992171	1.198187	2.298541
H	0.556572	0.981417	2.391405
H	1.150093	2.422447	-0.951305
H	1.568949	1.960131	0.500128
O	2.532610	1.069490	1.659882
H	3.458798	1.152339	1.911143
H	2.414773	0.196584	1.222867
O	-0.720118	-1.383034	-0.080785
H	0.721094	-2.756618	0.348339