**Table S1**

Coordinates of the optimized structure, Mulliken charges and spin densities for the model shown in Figure 7A

| Atom Number | Element | Coordinates, Å x | y | z | Mulliken charges | Spin densities |
|---|---|---|---|---|---|---|
| 1 | Al | 3.828655 | -0.000008 | 0 | 0.209384 | 0.012665 |
| 2 | O | 4.591375 | 0.000967 | 1.527606 | -0.435184 | -0.00181 |
| 3 | H | 5.532936 | -0.000206 | 1.710864 | 0.356951 | 0.000817 |
| 4 | O | 4.591379 | -0.000942 | -1.527605 | -0.435183 | -0.00181 |
| 5 | H | 5.532942 | -0.000139 | -1.710853 | 0.356951 | 0.000817 |
| 6 | C | 0.136676 | -0.000004 | 0 | -0.010263 | -0.18939 |
| 7 | C | -0.54969 | 1.228672 | -0.000062 | 0.083639 | 0.239159 |
| 8 | C | -0.54971 | -1.228671 | 0.000064 | 0.083611 | 0.239161 |
| 9 | C | -1.93634 | 1.18853 | -0.000062 | 0.081871 | -0.15352 |
| 10 | H | -0.016 | 2.169722 | -0.000108 | 0.209695 | -0.00857 |
| 11 | C | -1.93636 | -1.188514 | 0.000065 | 0.081891 | -0.15352 |
| 12 | H | -0.01603 | -2.169727 | 0.000109 | 0.209694 | -0.00857 |
| 13 | C | -2.66597 | 0.000014 | 0.000002 | -0.057372 | 0.251893 |
| 14 | H | -3.7474 | 0.000024 | 0.000003 | 0.214004 | -0.00901 |
| 15 | N | 1.516727 | -0.000013 | -0.000002 | -0.813274 | 0.439192 |
| 16 | O | 2.251912 | 1.097606 | -0.000008 | 0.264329 | 0.172295 |
| 17 | O | 2.2519 | -1.097636 | 0.000006 | 0.264323 | 0.172305 |
| 18 | N | -2.67719 | 2.473121 | -0.000137 | -0.367579 | 0.012237 |
| 19 | O | -3.90405 | 2.414514 | -0.000125 | 0.019168 | -0.00683 |
| 20 | O | -2.01335 | 3.506919 | -0.000203 | 0.015882 | -0.00646 |
| 21 | N | -2.67723 | -2.473098 | 0.000141 | -0.367592 | 0.012237 |
| 22 | O | -3.90409 | -2.414488 | 0.000122 | 0.019171 | -0.00683 |
| 23 | O | -2.01342 | -3.506914 | 0.000197 | 0.015884 | -0.00646 |

**Table S2**

Coordinates of the optimized structure, Mulliken charges and spin densities for the model shown in Figure 7B

| Atom Number | Element | Coordinates, Å x | y | z | Mulliken charges | Spin densities |
|---|---|---|---|---|---|---|
| 1 | Al | -0.00612 | -0.03484 | -0.02236 | -0.07097 | 0.004268 |
| 2 | O | -0.0344 | -0.05411 | 1.735699 | -0.46824 | 0.001464 |
| 3 | H | 0.742409 | 0.332521 | 2.151685 | 0.326375 | 0.000038 |
| 4 | O | -0.48964 | -1.48422 | -0.88693 | -0.52159 | 0.003925 |
| 5 | H | -1.41895 | -1.71352 | -0.77585 | 0.338269 | -0.0007 |
| 6 | C | -3.34259 | 2.251265 | -0.73906 | 0.208784 | -0.11069 |
| 7 | C | -2.76251 | 3.481965 | -1.12155 | 0.23027 | 0.201131 |
| 8 | C | -4.74722 | 2.117746 | -0.66333 | -0.43705 | 0.196464 |
| 9 | C | -3.6085 | 4.541691 | -1.41556 | 0.051171 | -0.15313 |
| 10 | H | -1.68808 | 3.583233 | -1.17808 | 0.206707 | -0.00718 |
| 11 | C | -5.53086 | 3.219226 | -0.97197 | 0.345746 | -0.15214 |
| 12 | H | -5.18615 | 1.174885 | -0.36925 | 0.199594 | -0.00786 |
| 13 | C | -5.00464 | 4.458363 | -1.3548 | -0.09554 | 0.364334 |
| 14 | H | -5.63769 | 5.299992 | -1.58925 | 0.189392 | -0.01334 |
| 15 | N | -2.54341 | 1.156993 | -0.43553 | -0.97176 | 0.27002 |
| 16 | O | -1.23706 | 1.33662 | -0.53365 | 0.455354 | 0.108504 |
| 17 | O | -3.04651 | 0.04861 | -0.0965 | 0.025154 | 0.286253 |
| 18 | N | -3.00758 | 5.828052 | -1.81569 | -0.41385 | 0.015407 |
| 19 | O | -3.77381 | 6.762466 | -2.06962 | -0.01061 | -0.01427 |
| 20 | O | -1.77985 | 5.905089 | -1.87672 | 0.003998 | 0.004196 |
| 21 | N | -6.99689 | 3.079602 | -0.89386 | -0.41433 | 0.015325 |
| 22 | O | -7.68171 | 4.069167 | -1.1683 | -0.01052 | -0.01376 |
| 23 | O | -7.4627 | 1.988063 | -0.56118 | -0.00095 | 0.002634 |
| 24 | O | 1.526135 | 0.608189 | -0.60443 | -0.4939 | -0.00092 |
| 25 | H | 1.784377 | 0.3479 | -1.4936 | 0.328491 | 0.000032 |

**Table S3**

Coordinates of the optimized structure, Mulliken charges and spin densities for the model shown in Figure 8

| Atom | | Coordinates, Å | | | Mulliken | Spin |
|---|---|---|---|---|---|---|
| Number | Element | x | y | z | charges | densities |
| 1 | Al | -3.25275 | -1.30146 | 0.338327 | -0.07557 | 0.008453 |
| 2 | O | -3.80246 | -2.74363 | -0.41958 | -0.37969 | -0.00051 |
| 3 | H | -4.4339 | -2.76582 | -1.14229 | 0.350313 | 0.000043 |
| 4 | O | -2.62163 | -1.39033 | 1.948675 | -0.46952 | 0.008274 |
| 5 | H | -2.57543 | -2.21607 | 2.437913 | 0.360729 | -0.00027 |
| 6 | C | 0.533245 | 0.107197 | -0.232 | -0.12434 | -0.18295 |
| 7 | C | 1.289036 | 1.279103 | -0.05972 | 0.420071 | 0.226629 |
| 8 | C | 1.143974 | -1.15863 | -0.27618 | 0.306652 | 0.207295 |
| 9 | C | 2.665312 | 1.146196 | 0.068654 | -0.30088 | -0.13477 |
| 10 | H | 0.822458 | 2.253568 | -0.02764 | 0.20951 | -0.00765 |
| 11 | C | 2.52398 | -1.21396 | -0.14297 | -0.28341 | -0.13293 |
| 12 | H | 0.558668 | -2.05866 | -0.40743 | 0.214814 | -0.00766 |
| 13 | C | 3.319617 | -0.08305 | 0.032312 | 0.286703 | 0.217965 |
| 14 | H | 4.393818 | -0.15674 | 0.134283 | 0.214853 | -0.00775 |
| 15 | N | -0.85486 | 0.183009 | -0.35472 | -0.98638 | 0.454043 |
| 16 | O | -1.40563 | 1.407281 | -0.33222 | 0.349405 | 0.107555 |
| 17 | O | -1.55597 | -0.86262 | -0.62681 | 0.323016 | 0.236604 |
| 18 | N | 3.475991 | 2.374248 | 0.250174 | -0.31492 | 0.010712 |
| 19 | O | 4.690972 | 2.234366 | 0.362556 | 0.011342 | -0.00548 |
| 20 | O | 2.877156 | 3.446933 | 0.275251 | -0.00258 | -0.00612 |
| 21 | N | 3.183841 | -2.54157 | -0.18917 | -0.32103 | 0.010609 |
| 22 | O | 4.40554 | -2.5655 | -0.06236 | 0.010064 | -0.00545 |
| 23 | O | 2.464462 | -3.52344 | -0.3518 | 0.005584 | -0.00597 |
| 24 | O | -4.05257 | 0.232574 | 0.024214 | -0.07451 | 0.002369 |
| 25 | Al | -3.1915 | 1.642135 | -0.21086 | 0.280964 | 0.006327 |
| 26 | O | -3.51301 | 3.292376 | -0.39392 | -0.38322 | 0.000765 |
| 27 | H | -4.37099 | 3.719922 | -0.3286 | 0.372012 | -0.00014 |