

Supporting Information

## **Formation of Environmentally-Persistent Free Radicals (EPFR) on $\alpha$ -Al<sub>2</sub>O<sub>3</sub>.**

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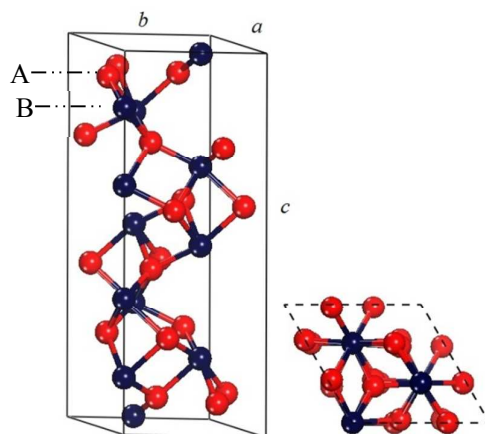


Figure S1. Side (left) and top (right) views of the hexagonal unit cell of bulk  $\alpha$ - $\text{Al}_2\text{O}_3$ . Blue spheres denote Al atoms and red spheres represent O atoms.

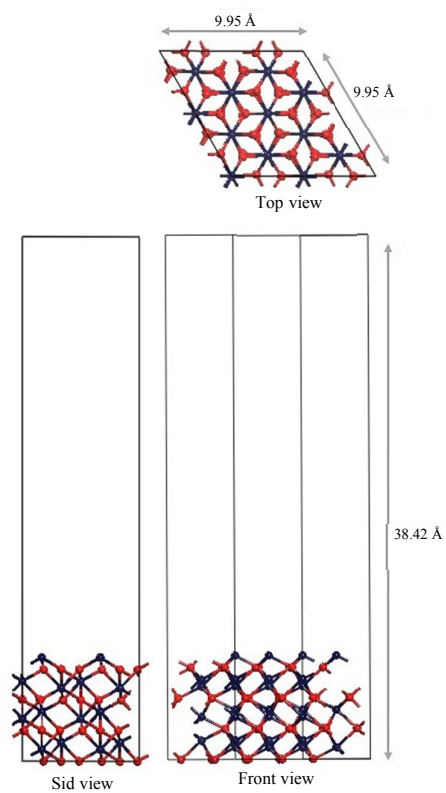


Figure S2. Unit cell (with slab and vacuum), employed the beginning of the coordinates in the periodic slab calculation for the  $\alpha$ - $\text{Al}_2\text{O}_3(0001)$  surface.

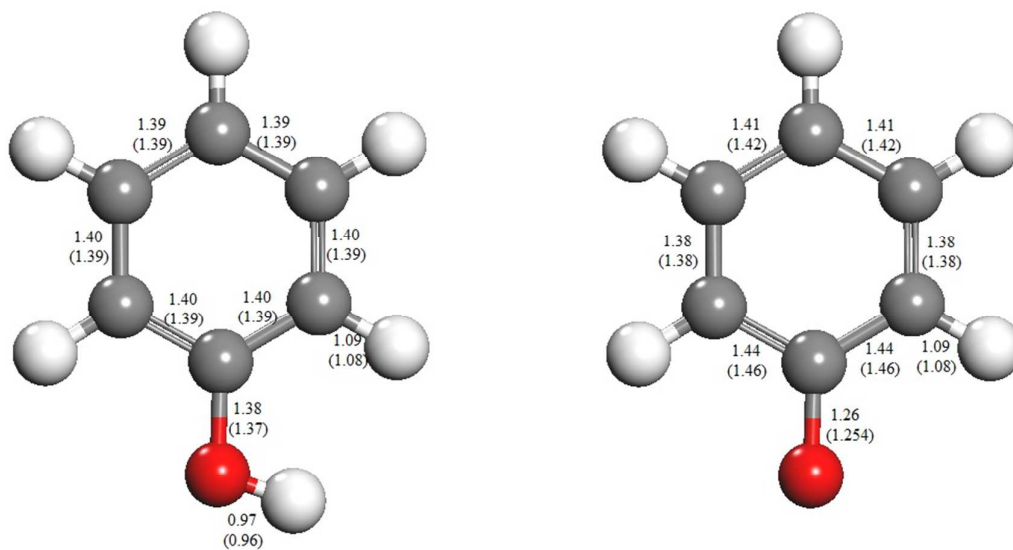


Figure S3: Coloured structure of a phenol molecule (left) and the phenoxy radical (right). Red, grey and white spheres represent O, C and H atoms, respectively. Bond lengths in parentheses signify the corresponding experimental or theoretical values from the previous studies.<sup>79,80</sup>



Scheme 1. Dissociation of phenol in gas phase.

### Cartesian coordinates for all structures involved in this study

\*Surface atoms are in red color and Al, O surface atoms which connected to H<sup>+</sup>, OH<sup>-</sup>, C<sub>6</sub>H<sub>5</sub>O<sup>-</sup> and C<sub>6</sub>H<sub>5</sub><sup>-</sup> groups are highlighted in yellow color.

#### Bulk Al<sub>2</sub>O<sub>3</sub>

| #  | Atom | X         | Y        | Z         |
|----|------|-----------|----------|-----------|
| 1  | O    | 1.468074  | 0.000000 | 3.251418  |
| 2  | O    | 3.867931  | 1.385558 | 7.586643  |
| 3  | O    | 1.468074  | 2.771116 | 11.921867 |
| 4  | O    | -0.734037 | 1.271389 | 3.251418  |
| 5  | O    | 1.665820  | 2.656947 | 7.586643  |
| 6  | O    | -0.734037 | 4.042506 | 11.921867 |
| 7  | O    | 1.665820  | 2.885285 | 3.251418  |
| 8  | O    | 1.665820  | 0.114169 | 7.586643  |
| 9  | O    | -0.734037 | 1.499727 | 11.921867 |
| 10 | O    | 3.331640  | 0.000000 | 9.754255  |
| 11 | O    | 0.931783  | 1.385558 | 1.083806  |
| 12 | O    | -1.468074 | 2.771116 | 5.419030  |
| 13 | O    | -1.665820 | 2.885285 | 9.754255  |
| 14 | O    | 3.133894  | 0.114169 | 1.083806  |
| 15 | O    | 0.734037  | 1.499727 | 5.419030  |
| 16 | O    | 0.734037  | 1.271389 | 9.754255  |
| 17 | O    | 3.133894  | 2.656947 | 1.083806  |
| 18 | O    | 0.734037  | 4.042506 | 5.419030  |
| 19 | Al   | 0.000000  | 0.000000 | 4.585018  |
| 20 | Al   | 2.399857  | 1.385558 | 8.920242  |
| 21 | Al   | 0.000000  | 2.771116 | 0.249793  |
| 22 | Al   | 0.000000  | 0.000000 | 1.917819  |
| 23 | Al   | 2.399857  | 1.385558 | 6.253043  |

|    |    |          |          |           |
|----|----|----------|----------|-----------|
| 24 | Al | 0.000000 | 2.771116 | 10.588267 |
| 25 | Al | 0.000000 | 0.000000 | 8.420655  |
| 26 | Al | 2.399857 | 1.385558 | 12.755880 |
| 27 | Al | 0.000000 | 2.771116 | 4.085431  |
| 28 | Al | 0.000000 | 0.000000 | 11.087854 |
| 29 | Al | 2.399857 | 1.385558 | 2.417406  |
| 30 | Al | 0.000000 | 2.771116 | 6.752630  |

### Clean Surface

| #  | Atom | X         | Y        | Z        |
|----|------|-----------|----------|----------|
| 1  | O    | 3.874527  | 1.372226 | 2.203589 |
| 2  | O    | 1.511157  | 2.840949 | 6.558112 |
| 3  | O    | 1.674192  | 2.669961 | 2.205923 |
| 4  | O    | -0.814964 | 4.048217 | 6.557114 |
| 5  | O    | 1.649407  | 0.114787 | 2.203740 |
| 6  | O    | -0.696664 | 1.429442 | 6.557695 |
| 7  | O    | 3.306296  | 0.002033 | 4.387204 |
| 8  | O    | -1.468074 | 2.771116 | 0.000000 |
| 9  | O    | -1.654251 | 2.863480 | 4.388742 |
| 10 | O    | 0.734037  | 1.499727 | 0.000000 |
| 11 | O    | 0.746950  | 1.294179 | 4.388272 |
| 12 | O    | 0.734037  | 4.042506 | 0.000000 |
| 13 | Al   | 2.399043  | 1.386602 | 3.495858 |
| 14 | Al   | 2.399857  | 1.385558 | 0.834013 |
| 15 | Al   | -0.000027 | 2.772791 | 5.373806 |
| 16 | Al   | -0.000452 | 0.000392 | 3.039059 |
| 17 | Al   | 2.399946  | 1.387518 | 6.707380 |
| 18 | Al   | -0.000253 | 0.001569 | 5.665348 |
| 19 | Al   | 0.000000  | 2.771116 | 1.333600 |
| 20 | O    | 8.674000  | 1.372028 | 2.204353 |
| 21 | O    | 6.310753  | 2.841004 | 6.558026 |
| 22 | O    | 6.474163  | 2.670781 | 2.203679 |
| 23 | O    | 3.984854  | 4.048204 | 6.557041 |
| 24 | O    | 6.449497  | 0.115435 | 2.204171 |
| 25 | O    | 4.103051  | 1.429389 | 6.557436 |
| 26 | O    | 8.106240  | 0.001669 | 4.387845 |
| 27 | O    | 3.331626  | 2.771116 | 0.000000 |
| 28 | O    | 3.145833  | 2.863648 | 4.388771 |
| 29 | O    | 5.533737  | 1.499727 | 0.000000 |
| 30 | O    | 5.546732  | 1.294593 | 4.387816 |

|    |    |           |          |          |
|----|----|-----------|----------|----------|
| 31 | O  | 5.533737  | 4.042506 | 0.000000 |
| 32 | Al | 7.199264  | 1.385779 | 3.495555 |
| 33 | Al | 7.199557  | 1.385558 | 0.834013 |
| 34 | Al | 4.799773  | 2.772831 | 5.373677 |
| 35 | Al | 4.799721  | 0.000424 | 3.038808 |
| 36 | Al | 7.199597  | 1.387571 | 6.707196 |
| 37 | Al | 4.799444  | 0.001650 | 5.665004 |
| 38 | Al | 4.799700  | 2.771116 | 1.333600 |
| 39 | O  | 1.474625  | 5.529201 | 2.205245 |
| 40 | O  | -0.888755 | 6.997693 | 6.557656 |
| 41 | O  | -0.726151 | 6.827246 | 2.204376 |
| 42 | O  | -3.214687 | 8.204823 | 6.556957 |
| 43 | O  | -0.750634 | 4.271677 | 2.204457 |
| 44 | O  | -3.096571 | 5.586138 | 6.557537 |
| 45 | O  | 0.906537  | 4.158485 | 4.388101 |
| 46 | O  | -3.867924 | 6.927778 | 0.000000 |
| 47 | O  | -4.053826 | 7.020105 | 4.388403 |
| 48 | O  | -1.665813 | 5.656389 | 0.000000 |
| 49 | O  | -1.652966 | 5.451109 | 4.388079 |
| 50 | O  | -1.665813 | 8.199168 | 0.000000 |
| 51 | Al | -0.000694 | 5.542400 | 3.495605 |
| 52 | Al | 0.000007  | 5.542220 | 0.834013 |
| 53 | Al | -2.399887 | 6.929494 | 5.373544 |
| 54 | Al | -2.399923 | 4.157161 | 3.039176 |
| 55 | Al | 0.000053  | 5.544232 | 6.707059 |
| 56 | Al | -2.400124 | 4.158251 | 5.665346 |
| 57 | Al | -2.399850 | 6.927778 | 1.333600 |
| 58 | O  | 6.274299  | 5.528729 | 2.203514 |
| 59 | O  | 3.910994  | 6.997665 | 6.558068 |
| 60 | O  | 4.074064  | 6.826939 | 2.204810 |
| 61 | O  | 1.584911  | 8.204913 | 6.556801 |
| 62 | O  | 4.050035  | 4.271497 | 2.204256 |
| 63 | O  | 1.703206  | 5.586181 | 6.557659 |
| 64 | O  | 5.706533  | 4.158446 | 4.387443 |
| 65 | O  | 0.931776  | 6.927778 | 0.000000 |
| 66 | O  | 0.745581  | 7.020289 | 4.388480 |
| 67 | O  | 3.133887  | 5.656389 | 0.000000 |
| 68 | O  | 3.146916  | 5.451003 | 4.388274 |
| 69 | O  | 3.133887  | 8.199168 | 0.000000 |
| 70 | Al | 4.798876  | 5.542505 | 3.495706 |
| 71 | Al | 4.799707  | 5.542220 | 0.834013 |
| 72 | Al | 2.399823  | 6.929418 | 5.373679 |
| 73 | Al | 2.399721  | 4.157137 | 3.038720 |
| 74 | Al | 4.799735  | 5.544225 | 6.707517 |
| 75 | Al | 2.399575  | 4.158250 | 5.665303 |
| 76 | Al | 2.399850  | 6.927778 | 1.333600 |

## A1

| #  | Atom | X         | Y         | Z        |
|----|------|-----------|-----------|----------|
| 1  | O    | 3.866019  | 1.364978  | 2.198092 |
| 2  | O    | 1.501795  | 2.817356  | 6.577603 |
| 3  | O    | 1.671597  | 2.652033  | 2.206788 |
| 4  | O    | -0.772250 | 4.050979  | 6.427523 |
| 5  | O    | 1.635972  | 0.087600  | 2.233633 |
| 6  | O    | -0.723346 | 1.448891  | 6.532752 |
| 7  | O    | 3.299422  | 0.002437  | 4.400145 |
| 8  | O    | -1.468074 | 2.771116  | 0.000000 |
| 9  | O    | -1.653004 | 2.886762  | 4.321458 |
| 10 | O    | 0.734037  | 1.499727  | 0.000000 |
| 11 | O    | 0.747679  | 1.265015  | 4.394685 |
| 12 | O    | 0.734037  | 4.042506  | 0.000000 |
| 13 | Al   | 2.398830  | 1.368826  | 3.492724 |
| 14 | Al   | 2.399857  | 1.385558  | 0.834013 |
| 15 | Al   | 0.001325  | 2.766238  | 5.343810 |
| 16 | Al   | -0.029058 | 0.019430  | 3.047983 |
| 17 | Al   | 2.407539  | 1.368057  | 6.630346 |
| 18 | Al   | -0.031885 | 0.002765  | 5.706856 |
| 19 | Al   | 0.000000  | 2.771116  | 1.333600 |
| 20 | O    | 8.667036  | 1.378749  | 2.199006 |
| 21 | O    | 6.337604  | 2.803424  | 6.457606 |
| 22 | O    | 6.456409  | 2.687692  | 2.215640 |
| 23 | O    | 4.000126  | 4.051243  | 6.552786 |
| 24 | O    | 6.453107  | 0.122218  | 2.201122 |
| 25 | O    | 4.116345  | 1.413799  | 6.586869 |
| 26 | O    | 8.117465  | -0.005619 | 4.378806 |
| 27 | O    | 3.331626  | 2.771116  | 0.000000 |
| 28 | O    | 3.135632  | 2.836269  | 4.405233 |
| 29 | O    | 5.533737  | 1.499727  | 0.000000 |
| 30 | O    | 5.525051  | 1.291670  | 4.373876 |
| 31 | O    | 5.533737  | 4.042506  | 0.000000 |
| 32 | Al   | 7.185763  | 1.385255  | 3.522207 |
| 33 | Al   | 7.199557  | 1.385558  | 0.834013 |
| 34 | Al   | 4.783362  | 2.752312  | 5.394690 |
| 35 | Al   | 4.805730  | 0.004096  | 3.039121 |
| 36 | Al   | 7.207057  | 1.403529  | 6.975757 |
| 37 | Al   | 4.833528  | 0.001126  | 5.672391 |
| 38 | Al   | 4.799700  | 2.771116  | 1.333600 |
| 39 | O    | 1.499010  | 5.534609  | 2.228765 |
| 40 | O    | -0.867697 | 6.995091  | 6.525131 |

|    |    |           |          |          |
|----|----|-----------|----------|----------|
| 41 | O  | -0.720117 | 6.829583 | 2.209364 |
| 42 | O  | -3.218065 | 8.186795 | 6.567318 |
| 43 | O  | -0.727431 | 4.282512 | 2.190202 |
| 44 | O  | -3.048216 | 5.544779 | 6.616648 |
| 45 | O  | 0.946843  | 4.148093 | 4.371129 |
| 46 | O  | -3.867924 | 6.927778 | 0.000000 |
| 47 | O  | -4.067308 | 6.917714 | 4.498430 |
| 48 | O  | -1.665813 | 5.656389 | 0.000000 |
| 49 | O  | -1.669899 | 5.453847 | 4.351556 |
| 50 | O  | -1.665813 | 8.199168 | 0.000000 |
| 51 | Al | 0.020802  | 5.551775 | 3.530105 |
| 52 | Al | 0.000007  | 5.542220 | 0.834013 |
| 53 | Al | -2.356176 | 6.923317 | 5.386456 |
| 54 | Al | -2.366393 | 4.167006 | 3.004769 |
| 55 | Al | -0.061622 | 5.533539 | 6.978357 |
| 56 | Al | -2.366838 | 4.126812 | 5.611464 |
| 57 | Al | -2.399850 | 6.927778 | 1.333600 |
| 58 | O  | 6.267476  | 5.521357 | 2.202435 |
| 59 | O  | 3.910705  | 6.968487 | 6.563067 |
| 60 | O  | 4.080970  | 6.827629 | 2.217828 |
| 61 | O  | 1.602240  | 8.234373 | 6.593574 |
| 62 | O  | 4.039922  | 4.267196 | 2.223704 |
| 63 | O  | 1.632854  | 5.580888 | 6.610243 |
| 64 | O  | 5.649669  | 4.231763 | 4.471442 |
| 65 | O  | 0.931776  | 6.927778 | 0.000000 |
| 66 | O  | 0.766490  | 7.036306 | 4.395931 |
| 67 | O  | 3.133887  | 5.656389 | 0.000000 |
| 68 | O  | 3.196532  | 5.459568 | 4.471445 |
| 69 | O  | 3.133887  | 8.199168 | 0.000000 |
| 70 | Al | 4.787383  | 5.542646 | 3.439332 |
| 71 | Al | 4.799707  | 5.542220 | 0.834013 |
| 72 | Al | 2.385500  | 6.944023 | 5.437749 |
| 73 | Al | 2.386660  | 4.130092 | 3.061843 |
| 74 | Al | 4.830002  | 5.536770 | 6.175569 |
| 75 | Al | 2.375969  | 4.162979 | 5.730037 |
| 76 | Al | 2.399850  | 6.927778 | 1.333600 |
| 77 | C  | -2.830701 | 2.030279 | 9.313878 |
| 78 | C  | -1.666109 | 1.280710 | 9.559190 |
| 79 | C  | -0.423006 | 1.938571 | 9.591533 |
| 80 | C  | -0.342863 | 3.301509 | 9.331551 |
| 81 | C  | -1.502595 | 4.031319 | 9.029494 |
| 82 | C  | -2.753651 | 3.419620 | 9.075939 |
| 83 | O  | -1.369075 | 5.344603 | 8.583150 |
| 84 | H  | -3.813693 | 1.552920 | 9.321300 |
| 85 | H  | -1.727955 | 0.202202 | 9.703948 |
| 86 | H  | 0.486999  | 1.365210 | 9.758091 |



|    |   |           |          |          |
|----|---|-----------|----------|----------|
| 87 | H | 0.631628  | 3.787141 | 9.258797 |
| 88 | H | -3.651729 | 3.970094 | 8.800744 |
| 89 | H | -2.188353 | 5.551070 | 7.931780 |

## A2

| #  | Atom | X         | Y         | Z        |
|----|------|-----------|-----------|----------|
| 1  | O    | 3.883926  | 1.374719  | 2.211053 |
| 2  | O    | 1.528990  | 2.843512  | 6.544197 |
| 3  | O    | 1.669551  | 2.677439  | 2.207871 |
| 4  | O    | -0.822843 | 4.044576  | 6.558044 |
| 5  | O    | 1.658194  | 0.121354  | 2.198760 |
| 6  | O    | -0.684458 | 1.423814  | 6.561577 |
| 7  | O    | 3.319173  | -0.004755 | 4.373945 |
| 8  | O    | -1.468074 | 2.771116  | 0.000000 |
| 9  | O    | -1.672568 | 2.810265  | 4.433692 |
| 10 | O    | 0.734037  | 1.499727  | 0.000000 |
| 11 | O    | 0.744314  | 1.290674  | 4.379530 |
| 12 | O    | 0.734037  | 4.042506  | 0.000000 |
| 13 | Al   | 2.401704  | 1.391445  | 3.517762 |
| 14 | Al   | 2.399857  | 1.385558  | 0.834013 |
| 15 | Al   | 0.011839  | 2.754505  | 5.404876 |
| 16 | Al   | 0.020069  | 0.011404  | 3.049698 |
| 17 | Al   | 2.392195  | 1.408554  | 6.926541 |
| 18 | Al   | 0.025309  | -0.006415 | 5.694980 |
| 19 | Al   | 0.000000  | 2.771116  | 1.333600 |
| 20 | O    | 8.670628  | 1.364738  | 2.207238 |
| 21 | O    | 6.294933  | 2.824092  | 6.541065 |
| 22 | O    | 6.477439  | 2.663628  | 2.202604 |
| 23 | O    | 4.001096  | 4.067540  | 6.488962 |
| 24 | O    | 6.440634  | 0.102802  | 2.218342 |
| 25 | O    | 4.073527  | 1.443117  | 6.514503 |
| 26 | O    | 8.070344  | 0.033705  | 4.444666 |
| 27 | O    | 3.331626  | 2.771116  | 0.000000 |
| 28 | O    | 3.147419  | 2.885370  | 4.355103 |
| 29 | O    | 5.533737  | 1.499727  | 0.000000 |
| 30 | O    | 5.580725  | 1.290297  | 4.413502 |
| 31 | O    | 5.533737  | 4.042506  | 0.000000 |
| 32 | Al   | 7.198132  | 1.375866  | 3.453281 |
| 33 | Al   | 7.199557  | 1.385558  | 0.834013 |
| 34 | Al   | 4.787464  | 2.790446  | 5.363982 |
| 35 | Al   | 4.785043  | -0.010850 | 3.049042 |
| 36 | Al   | 7.211508  | 1.379308  | 6.304696 |
| 37 | Al   | 4.778687  | 0.007062  | 5.683557 |
| 38 | Al   | 4.799700  | 2.771116  | 1.333600 |

|    |    |           |          |          |
|----|----|-----------|----------|----------|
| 39 | O  | 1.466758  | 5.522222 | 2.200001 |
| 40 | O  | -0.900281 | 7.003026 | 6.575775 |
| 41 | O  | -0.726097 | 6.817187 | 2.205656 |
| 42 | O  | -3.198026 | 8.226413 | 6.589495 |
| 43 | O  | -0.764099 | 4.258858 | 2.224680 |
| 44 | O  | -3.129639 | 5.597275 | 6.563885 |
| 45 | O  | 0.876192  | 4.175010 | 4.419563 |
| 46 | O  | -3.867924 | 6.927778 | 0.000000 |
| 47 | O  | -4.052206 | 7.045066 | 4.390945 |
| 48 | O  | -1.665813 | 5.656389 | 0.000000 |
| 49 | O  | -1.625102 | 5.451694 | 4.435853 |
| 50 | O  | -1.665813 | 8.199168 | 0.000000 |
| 51 | Al | -0.005962 | 5.532568 | 3.468804 |
| 52 | Al | 0.000007  | 5.542220 | 0.834013 |
| 53 | Al | -2.414894 | 6.949248 | 5.404506 |
| 54 | Al | -2.419507 | 4.152638 | 3.052351 |
| 55 | Al | -0.005201 | 5.544416 | 6.389188 |
| 56 | Al | -2.428367 | 4.167031 | 5.699716 |
| 57 | Al | -2.399850 | 6.927778 | 1.333600 |
| 58 | O  | 6.281867  | 5.539676 | 2.215599 |
| 59 | O  | 3.928634  | 6.978559 | 6.556188 |
| 60 | O  | 4.071263  | 6.842934 | 2.220065 |
| 61 | O  | 1.578068  | 8.203671 | 6.552595 |
| 62 | O  | 4.059438  | 4.281912 | 2.193610 |
| 63 | O  | 1.707218  | 5.573342 | 6.553799 |
| 64 | O  | 5.728907  | 4.159445 | 4.362981 |
| 65 | O  | 0.931776  | 6.927778 | 0.000000 |
| 66 | O  | 0.725992  | 6.977223 | 4.424394 |
| 67 | O  | 3.133887  | 5.656389 | 0.000000 |
| 68 | O  | 3.130148  | 5.458100 | 4.361986 |
| 69 | O  | 3.133887  | 8.199168 | 0.000000 |
| 70 | Al | 4.799099  | 5.556377 | 3.522124 |
| 71 | Al | 4.799707  | 5.542220 | 0.834013 |
| 72 | Al | 2.409913  | 6.909314 | 5.405753 |
| 73 | Al | 2.414004  | 4.163049 | 3.027754 |
| 74 | Al | 4.785541  | 5.532386 | 6.947667 |
| 75 | Al | 2.412808  | 4.155245 | 5.647033 |
| 76 | Al | 2.399850  | 6.927778 | 1.333600 |
| 77 | C  | 5.414052  | 4.222692 | 9.305773 |
| 78 | C  | 4.600519  | 5.376448 | 9.297964 |
| 79 | C  | 3.194502  | 5.245463 | 9.246844 |
| 80 | C  | 2.609815  | 3.982683 | 9.167361 |
| 81 | C  | 3.444518  | 2.869827 | 9.144011 |
| 82 | C  | 4.831468  | 2.960189 | 9.211899 |
| 83 | O  | 2.827548  | 1.609494 | 8.924428 |
| 84 | H  | 6.498280  | 4.317669 | 9.284146 |

|    |   |          |          |          |
|----|---|----------|----------|----------|
| 85 | H | 5.051489 | 6.365773 | 9.419031 |
| 86 | H | 2.570168 | 6.134153 | 9.171442 |
| 87 | H | 1.538420 | 3.857950 | 9.024336 |
| 88 | H | 5.449016 | 2.072737 | 9.081988 |
| 89 | H | 3.518803 | 0.920263 | 9.025573 |

### A3

| #  | Atom | X         | Y         | Z        |
|----|------|-----------|-----------|----------|
| 1  | O    | 3.879256  | 1.366172  | 2.211910 |
| 2  | O    | 1.498528  | 2.818797  | 6.526677 |
| 3  | O    | 1.682370  | 2.665511  | 2.203734 |
| 4  | O    | -0.788887 | 4.078123  | 6.481684 |
| 5  | O    | 1.646362  | 0.111542  | 2.212851 |
| 6  | O    | -0.686354 | 1.440422  | 6.593851 |
| 7  | O    | 3.270305  | 0.039660  | 4.445606 |
| 8  | O    | -1.468074 | 2.771116  | 0.000000 |
| 9  | O    | -1.650120 | 2.856910  | 4.383879 |
| 10 | O    | 0.734037  | 1.499727  | 0.000000 |
| 11 | O    | 0.782067  | 1.297011  | 4.425473 |
| 12 | O    | 0.734037  | 4.042506  | 0.000000 |
| 13 | Al   | 2.401249  | 1.382023  | 3.446712 |
| 14 | Al   | 2.399857  | 1.385558  | 0.834013 |
| 15 | Al   | 0.001500  | 2.806451  | 5.347639 |
| 16 | Al   | -0.000881 | -0.018511 | 3.054776 |
| 17 | Al   | 2.422513  | 1.375785  | 6.261544 |
| 18 | Al   | -0.003333 | -0.013222 | 5.694672 |
| 19 | Al   | 0.000000  | 2.771116  | 1.333600 |
| 20 | O    | 8.689020  | 1.368502  | 2.221149 |
| 21 | O    | 6.327166  | 2.853967  | 6.565952 |
| 22 | O    | 6.477045  | 2.670855  | 2.202846 |
| 23 | O    | 3.972335  | 4.042825  | 6.562477 |
| 24 | O    | 6.461634  | 0.120360  | 2.203857 |
| 25 | O    | 4.121991  | 1.421859  | 6.555141 |
| 26 | O    | 8.115142  | 0.009883  | 4.415796 |
| 27 | O    | 3.331626  | 2.771116  | 0.000000 |
| 28 | O    | 3.131275  | 2.800190  | 4.447942 |
| 29 | O    | 5.533737  | 1.499727  | 0.000000 |
| 30 | O    | 5.562688  | 1.291688  | 4.392488 |
| 31 | O    | 5.533737  | 4.042506  | 0.000000 |
| 32 | Al   | 7.206736  | 1.385516  | 3.496762 |
| 33 | Al   | 7.199557  | 1.385558  | 0.834013 |
| 34 | Al   | 4.817686  | 2.761243  | 5.399142 |
| 35 | Al   | 4.821676  | 0.005949  | 3.050757 |

|    |    |           |           |          |
|----|----|-----------|-----------|----------|
| 36 | Al | 7.199739  | 1.394204  | 6.699471 |
| 37 | Al | 4.815373  | -0.022966 | 5.697058 |
| 38 | Al | 4.799700  | 2.771116  | 1.333600 |
| 39 | O  | 1.468978  | 5.541149  | 2.201401 |
| 40 | O  | -0.873250 | 6.960365  | 6.544400 |
| 41 | O  | -0.735014 | 6.842567  | 2.221162 |
| 42 | O  | -3.207860 | 8.200283  | 6.543595 |
| 43 | O  | -0.750662 | 4.275184  | 2.200666 |
| 44 | O  | -3.095206 | 5.571486  | 6.581132 |
| 45 | O  | 0.924007  | 4.150139  | 4.343934 |
| 46 | O  | -3.867924 | 6.927778  | 0.000000 |
| 47 | O  | -4.065926 | 7.005894  | 4.396823 |
| 48 | O  | -1.665813 | 5.656389  | 0.000000 |
| 49 | O  | -1.682393 | 5.452279  | 4.363867 |
| 50 | O  | -1.665813 | 8.199168  | 0.000000 |
| 51 | Al | -0.010400 | 5.553783  | 3.524452 |
| 52 | Al | 0.000007  | 5.542220  | 0.834013 |
| 53 | Al | -2.397167 | 6.906719  | 5.404891 |
| 54 | Al | -2.400523 | 4.162399  | 3.031495 |
| 55 | Al | 0.000495  | 5.535933  | 7.005189 |
| 56 | Al | -2.386611 | 4.166767  | 5.655323 |
| 57 | Al | -2.399850 | 6.927778  | 1.333600 |
| 58 | O  | 6.262429  | 5.525222  | 2.197638 |
| 59 | O  | 3.901703  | 6.986590  | 6.579369 |
| 60 | O  | 4.067934  | 6.820666  | 2.211876 |
| 61 | O  | 1.599209  | 8.201486  | 6.584022 |
| 62 | O  | 4.039758  | 4.255887  | 2.221457 |
| 63 | O  | 1.664451  | 5.588996  | 6.517165 |
| 64 | O  | 5.699316  | 4.151635  | 4.398177 |
| 65 | O  | 0.931776  | 6.927778  | 0.000000 |
| 66 | O  | 0.742754  | 7.047790  | 4.376057 |
| 67 | O  | 3.133887  | 5.656389  | 0.000000 |
| 68 | O  | 3.146325  | 5.437044  | 4.392821 |
| 69 | O  | 3.133887  | 8.199168  | 0.000000 |
| 70 | Al | 4.794459  | 5.530238  | 3.499218 |
| 71 | Al | 4.799707  | 5.542220  | 0.834013 |
| 72 | Al | 2.385059  | 6.917314  | 5.386197 |
| 73 | Al | 2.378849  | 4.169399  | 3.036019 |
| 74 | Al | 4.796628  | 5.532972  | 6.682209 |
| 75 | Al | 2.377274  | 4.168332  | 5.677608 |
| 76 | Al | 2.399850  | 6.927778  | 1.333600 |
| 77 | C  | 2.598609  | 5.037806  | 9.471749 |
| 78 | C  | 1.956354  | 6.278757  | 9.571465 |
| 79 | C  | 0.568158  | 6.338907  | 9.458521 |
| 80 | C  | -0.174345 | 5.153863  | 9.221945 |
| 81 | C  | 0.486643  | 3.894513  | 9.153041 |

|    |   |           |          |          |
|----|---|-----------|----------|----------|
| 82 | C | 1.886986  | 3.859458 | 9.253691 |
| 83 | O | -0.260663 | 2.778237 | 8.995675 |
| 84 | H | 3.685326  | 4.981383 | 9.556444 |
| 85 | H | 2.536438  | 7.190294 | 9.700846 |
| 86 | H | 0.044123  | 7.293749 | 9.496619 |
| 87 | H | -1.269103 | 5.163810 | 9.213628 |
| 88 | H | 2.404641  | 2.908551 | 9.150624 |
| 89 | H | -0.025715 | 2.317990 | 8.140591 |

#### A4

| #  | Atom | X         | Y        | Z        |
|----|------|-----------|----------|----------|
| 1  | O    | 3.876405  | 1.369965 | 2.204139 |
| 2  | O    | 1.511715  | 2.846361 | 6.567093 |
| 3  | O    | 1.675721  | 2.662329 | 2.200297 |
| 4  | O    | -0.804870 | 4.062539 | 6.564401 |
| 5  | O    | 1.646808  | 0.109452 | 2.211949 |
| 6  | O    | -0.701950 | 1.432989 | 6.565173 |
| 7  | O    | 3.304038  | 0.000914 | 4.388863 |
| 8  | O    | -1.468074 | 2.771116 | 0.000000 |
| 9  | O    | -1.654875 | 2.864852 | 4.398936 |
| 10 | O    | 0.734037  | 1.499727 | 0.000000 |
| 11 | O    | 0.748077  | 1.290949 | 4.397479 |
| 12 | O    | 0.734037  | 4.042506 | 0.000000 |
| 13 | Al   | 2.398134  | 1.380756 | 3.496752 |
| 14 | Al   | 2.399857  | 1.385558 | 0.834013 |
| 15 | Al   | 0.001009  | 2.785369 | 5.384079 |
| 16 | Al   | -0.003494 | 0.004455 | 3.044579 |
| 17 | Al   | 2.400158  | 1.387122 | 6.689929 |
| 18 | Al   | -0.004220 | 0.003358 | 5.679727 |
| 19 | Al   | 0.000000  | 2.771116 | 1.333600 |
| 20 | O    | 8.674093  | 1.375588 | 2.208603 |
| 21 | O    | 6.309226  | 2.847423 | 6.561155 |
| 22 | O    | 6.472132  | 2.678445 | 2.212186 |
| 23 | O    | 3.965643  | 4.047907 | 6.553410 |
| 24 | O    | 6.452026  | 0.122560 | 2.199804 |
| 25 | O    | 4.105298  | 1.419850 | 6.558995 |
| 26 | O    | 8.104404  | 0.008481 | 4.391348 |
| 27 | O    | 3.331626  | 2.771116 | 0.000000 |
| 28 | O    | 3.144873  | 2.856196 | 4.387492 |
| 29 | O    | 5.533737  | 1.499727 | 0.000000 |
| 30 | O    | 5.554011  | 1.297026 | 4.398120 |
| 31 | O    | 5.533737  | 4.042506 | 0.000000 |
| 32 | Al   | 7.197477  | 1.393651 | 3.494005 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 33 | Al | 7.199557  | 1.385558  | 0.834013  |
| 34 | Al | 4.796040  | 2.766379  | 5.381263  |
| 35 | Al | 4.802819  | -0.002939 | 3.035636  |
| 36 | Al | 7.189836  | 1.386823  | 6.671762  |
| 37 | Al | 4.798335  | -0.017184 | 5.666764  |
| 38 | Al | 4.799700  | 2.771116  | 1.333600  |
| 39 | O  | 1.476912  | 5.530427  | 2.205875  |
| 40 | O  | -0.886436 | 6.977101  | 6.535851  |
| 41 | O  | -0.727781 | 6.825460  | 2.202484  |
| 42 | O  | -3.215907 | 8.202873  | 6.564191  |
| 43 | O  | -0.748206 | 4.269927  | 2.203335  |
| 44 | O  | -3.084078 | 5.586434  | 6.564967  |
| 45 | O  | 0.916877  | 4.145301  | 4.371299  |
| 46 | O  | -3.867924 | 6.927778  | 0.000000  |
| 47 | O  | -4.063343 | 7.004118  | 4.412740  |
| 48 | O  | -1.665813 | 5.656389  | 0.000000  |
| 49 | O  | -1.664412 | 5.443291  | 4.372001  |
| 50 | O  | -1.665813 | 8.199168  | 0.000000  |
| 51 | Al | -0.000440 | 5.541405  | 3.517956  |
| 52 | Al | 0.000007  | 5.542220  | 0.834013  |
| 53 | Al | -2.385803 | 6.921685  | 5.377461  |
| 54 | Al | -2.394136 | 4.165575  | 3.040461  |
| 55 | Al | -0.030745 | 5.545725  | 6.970982  |
| 56 | Al | -2.383774 | 4.163528  | 5.671663  |
| 57 | Al | -2.399850 | 6.927778  | 1.333600  |
| 58 | O  | 6.269764  | 5.528353  | 2.203041  |
| 59 | O  | 3.893517  | 6.989123  | 6.563326  |
| 60 | O  | 4.074581  | 6.830591  | 2.207880  |
| 61 | O  | 1.583940  | 8.192042  | 6.566176  |
| 62 | O  | 4.048170  | 4.270290  | 2.202283  |
| 63 | O  | 1.674225  | 5.594602  | 6.490470  |
| 64 | O  | 5.691431  | 4.171063  | 4.409632  |
| 65 | O  | 0.931776  | 6.927778  | 0.000000  |
| 66 | O  | 0.749474  | 7.037703  | 4.364113  |
| 67 | O  | 3.133887  | 5.656389  | 0.000000  |
| 68 | O  | 3.158327  | 5.452992  | 4.386280  |
| 69 | O  | 3.133887  | 8.199168  | 0.000000  |
| 70 | Al | 4.799589  | 5.540753  | 3.481774  |
| 71 | Al | 4.799707  | 5.542220  | 0.834013  |
| 72 | Al | 2.388004  | 6.932818  | 5.343028  |
| 73 | Al | 2.395023  | 4.150574  | 3.027545  |
| 74 | Al | 4.807027  | 5.537972  | 6.551586  |
| 75 | Al | 2.387156  | 4.152192  | 5.643741  |
| 76 | Al | 2.399850  | 6.927778  | 1.333600  |
| 77 | C  | 2.651918  | 6.054550  | 11.878266 |
| 78 | C  | 1.648361  | 5.660466  | 12.771426 |

|    |   |           |          |           |
|----|---|-----------|----------|-----------|
| 79 | C | 0.374890  | 5.337425 | 12.286436 |
| 80 | C | 0.095576  | 5.394287 | 10.917868 |
| 81 | C | 1.111940  | 5.787071 | 10.046943 |
| 82 | C | 2.387466  | 6.123836 | 10.509766 |
| 83 | O | 0.864549  | 5.860049 | 8.692368  |
| 84 | H | 3.645593  | 6.316357 | 12.243046 |
| 85 | H | 1.856223  | 5.607702 | 13.840308 |
| 86 | H | -0.408170 | 5.028842 | 12.979430 |
| 87 | H | -0.887314 | 5.135937 | 10.523650 |
| 88 | H | 3.148521  | 6.443666 | 9.796239  |
| 89 | H | 1.695739  | 5.917172 | 8.084009  |

### D<sub>H1</sub>

| #  | Atom | X         | Y         | Z         |
|----|------|-----------|-----------|-----------|
| 1  | O    | 3.874441  | 1.363928  | 2.202397  |
| 2  | O    | 1.507302  | 2.823786  | 6.501813  |
| 3  | O    | 1.665433  | 2.646776  | 2.193460  |
| 4  | O    | -0.781228 | 4.026574  | 6.298791  |
| 5  | O    | 1.641348  | 0.088730  | 2.225123  |
| 6  | O    | -0.701013 | 1.429093  | 6.539443  |
| 7  | O    | 3.309060  | -0.009845 | 4.395735  |
| 8  | O    | -1.468074 | 2.771116  | 0.000000  |
| 9  | O    | -1.698397 | 2.850623  | 4.330544  |
| 10 | O    | 0.734037  | 1.499727  | 0.000000  |
| 11 | O    | 0.745891  | 1.258770  | 4.369099  |
| 12 | O    | 0.734037  | 4.042506  | 0.000000  |
| 13 | Al   | 2.407146  | 1.351429  | 3.476300  |
| 14 | Al   | 2.399857  | 1.385558  | 0.834013  |
| 15 | Al   | -0.002312 | 2.745530  | 5.279448  |
| 16 | Al   | -0.016252 | 0.005409  | 3.019568  |
| 17 | Al   | 2.396722  | 1.380699  | 6.717836  |
| 18 | Al   | -0.008319 | -0.006611 | 5.693989  |
| 19 | Al   | 0.000000  | 2.771116  | 1.333600  |
| 20 | C    | 1.310732  | 5.571990  | 11.549620 |
| 21 | C    | 0.102716  | 5.682253  | 12.259352 |
| 22 | C    | -1.096423 | 5.714613  | 11.533952 |
| 23 | C    | -1.101289 | 5.559049  | 10.173411 |
| 24 | C    | 0.129416  | 5.313526  | 9.551278  |
| 25 | C    | 1.365090  | 5.479561  | 10.179782 |
| 26 | O    | 0.136647  | 4.728470  | 8.407707  |
| 27 | H    | 2.226241  | 5.378288  | 12.031206 |

|    |    |           |          |           |
|----|----|-----------|----------|-----------|
| 28 | H  | 0.105453  | 5.707008 | 13.348715 |
| 29 | H  | -2.071928 | 5.723892 | 11.956340 |
| 30 | H  | -2.013201 | 5.458793 | 9.584486  |
| 31 | H  | 2.266467  | 5.358909 | 9.545533  |
| 32 | H  | 2.265820  | 5.827395 | 7.320893  |
| 33 | O  | 8.674000  | 1.372028 | 2.204353  |
| 34 | O  | 6.313093  | 2.833137 | 6.545593  |
| 35 | O  | 6.449198  | 2.687516 | 2.205817  |
| 36 | O  | 3.962389  | 4.070600 | 6.500910  |
| 37 | O  | 6.445904  | 0.115586 | 2.209074  |
| 38 | O  | 4.103051  | 1.429389 | 6.557436  |
| 39 | O  | 8.113095  | 0.025173 | 4.355207  |
| 40 | O  | 3.343090  | 2.736086 | 0.036288  |
| 41 | O  | 3.155666  | 2.841677 | 4.345639  |
| 42 | O  | 5.540733  | 1.493083 | 0.061782  |
| 43 | O  | 5.543379  | 1.289143 | 4.397860  |
| 44 | O  | 5.532567  | 4.028682 | 0.033947  |
| 45 | Al | 7.171341  | 1.392668 | 3.459049  |
| 46 | Al | 7.199557  | 1.385558 | 0.834013  |
| 47 | Al | 4.783632  | 2.754197 | 5.387453  |
| 48 | Al | 4.799721  | 0.000424 | 3.038808  |
| 49 | Al | 7.197613  | 1.380646 | 6.689311  |
| 50 | Al | 4.799444  | 0.001650 | 5.665004  |
| 51 | Al | 4.800437  | 2.767119 | 1.241071  |
| 52 | O  | 1.474625  | 5.529201 | 2.205245  |
| 53 | O  | -0.861868 | 6.976939 | 6.528694  |
| 54 | O  | -0.726510 | 6.828848 | 2.210244  |
| 55 | O  | -3.210864 | 8.198091 | 6.560097  |
| 56 | O  | -0.744703 | 4.261856 | 2.204432  |
| 57 | O  | -3.096571 | 5.586138 | 6.557537  |
| 58 | O  | 0.955699  | 4.164151 | 4.352643  |
| 59 | O  | -3.841653 | 6.932105 | 0.044926  |
| 60 | O  | -4.086810 | 6.933462 | 4.458506  |
| 61 | O  | -1.665410 | 5.656432 | 0.072834  |
| 62 | O  | -1.673316 | 5.454055 | 4.338874  |
| 63 | O  | -1.686811 | 8.200544 | 0.064110  |
| 64 | Al | -0.000414 | 5.546509 | 3.486003  |
| 65 | Al | 0.000007  | 5.542220 | 0.834013  |
| 66 | Al | -2.377000 | 6.909576 | 5.385008  |
| 67 | Al | -2.399923 | 4.157161 | 3.039176  |
| 68 | Al | -0.099735 | 5.481094 | 6.876254  |
| 69 | Al | -2.400124 | 4.158251 | 5.665346  |
| 70 | Al | -2.401536 | 6.922127 | 1.269687  |
| 71 | O  | 6.274299  | 5.528729 | 2.203514  |
| 72 | O  | 3.868090  | 6.944166 | 6.492986  |
| 73 | O  | 4.069406  | 6.840565 | 2.191763  |



|    |    |          |          |          |
|----|----|----------|----------|----------|
| 74 | O  | 1.596470 | 8.182529 | 6.545592 |
| 75 | O  | 4.039652 | 4.262586 | 2.171046 |
| 76 | O  | 1.703206 | 5.586181 | 6.557659 |
| 77 | O  | 5.633498 | 4.226785 | 4.456685 |
| 78 | O  | 0.926216 | 6.917785 | 0.059249 |
| 79 | O  | 0.761638 | 7.013792 | 4.381595 |
| 80 | O  | 3.108450 | 5.659085 | 0.054981 |
| 81 | O  | 3.190302 | 5.459870 | 4.395866 |
| 82 | O  | 3.127032 | 8.212905 | 0.062468 |
| 83 | Al | 4.783999 | 5.538474 | 3.352977 |
| 84 | Al | 4.794034 | 5.544916 | 0.708964 |
| 85 | Al | 2.414714 | 6.986817 | 5.253736 |
| 86 | Al | 2.394182 | 4.137185 | 2.975310 |
| 87 | Al | 4.827866 | 5.531807 | 6.082886 |
| 88 | Al | 2.411639 | 4.087466 | 5.585028 |
| 89 | Al | 2.394892 | 6.930201 | 1.244205 |

## D<sub>H2</sub>

| #  | Atom | X         | Y         | Z         |
|----|------|-----------|-----------|-----------|
| 1  | O    | 3.875456  | 1.366990  | 2.215028  |
| 2  | O    | 1.498184  | 2.811413  | 6.515972  |
| 3  | O    | 1.662956  | 2.635385  | 2.191830  |
| 4  | O    | -0.771134 | 4.057754  | 6.284496  |
| 5  | O    | 1.639323  | 0.076925  | 2.242142  |
| 6  | O    | -0.696274 | 1.421067  | 6.552094  |
| 7  | O    | 3.295582  | -0.010042 | 4.408855  |
| 8  | O    | -1.468074 | 2.771116  | 0.000000  |
| 9  | O    | -1.702693 | 2.834039  | 4.348402  |
| 10 | O    | 0.734037  | 1.499727  | 0.000000  |
| 11 | O    | 0.735019  | 1.262622  | 4.359048  |
| 12 | O    | 0.734037  | 4.042506  | 0.000000  |
| 13 | Al   | 2.411691  | 1.354967  | 3.484180  |
| 14 | Al   | 2.399857  | 1.385558  | 0.834013  |
| 15 | Al   | 0.010184  | 2.774621  | 5.286735  |
| 16 | Al   | -0.025833 | 0.004556  | 2.998201  |
| 17 | Al   | 2.404422  | 1.384089  | 6.738670  |
| 18 | Al   | 0.035161  | 0.053994  | 5.642757  |
| 19 | Al   | 0.000000  | 2.771116  | 1.333600  |
| 20 | C    | 1.232755  | 5.539936  | 11.609727 |
| 21 | C    | 0.027407  | 5.656872  | 12.324146 |
| 22 | C    | -1.174516 | 5.683417  | 11.602721 |

|    |    |           |           |           |
|----|----|-----------|-----------|-----------|
| 23 | C  | -1.186214 | 5.509124  | 10.246661 |
| 24 | C  | 0.039955  | 5.265223  | 9.605307  |
| 25 | C  | 1.281649  | 5.439621  | 10.238512 |
| 26 | O  | 0.004386  | 4.704569  | 8.454869  |
| 27 | H  | 2.152257  | 5.378288  | 12.105191 |
| 28 | H  | 0.035270  | 5.701898  | 13.412908 |
| 29 | H  | -2.145912 | 5.723892  | 12.030325 |
| 30 | H  | -2.099308 | 5.411751  | 9.659470  |
| 31 | H  | 2.192482  | 5.358909  | 9.619518  |
| 32 | H  | 3.581069  | 6.969058  | 7.474650  |
| 33 | O  | 8.674000  | 1.372028  | 2.204353  |
| 34 | O  | 6.301897  | 2.847420  | 6.531618  |
| 35 | O  | 6.446850  | 2.684369  | 2.224058  |
| 36 | O  | 3.991558  | 4.072685  | 6.504028  |
| 37 | O  | 6.450114  | 0.116754  | 2.219127  |
| 38 | O  | 4.103051  | 1.429389  | 6.557436  |
| 39 | O  | 8.102854  | -0.007247 | 4.414034  |
| 40 | O  | 3.345765  | 2.735538  | 0.041986  |
| 41 | O  | 3.138974  | 2.852949  | 4.361198  |
| 42 | O  | 5.537386  | 1.492793  | 0.073353  |
| 43 | O  | 5.550052  | 1.292101  | 4.415556  |
| 44 | O  | 5.533561  | 4.023743  | 0.045251  |
| 45 | Al | 7.174788  | 1.376606  | 3.464155  |
| 46 | Al | 7.199557  | 1.385558  | 0.834013  |
| 47 | Al | 4.756551  | 2.754349  | 5.391117  |
| 48 | Al | 4.799721  | 0.000424  | 3.038808  |
| 49 | Al | 7.195591  | 1.403293  | 6.564287  |
| 50 | Al | 4.799444  | 0.001650  | 5.665004  |
| 51 | Al | 4.799374  | 2.769054  | 1.248883  |
| 52 | O  | 1.474625  | 5.529201  | 2.205245  |
| 53 | O  | -0.839133 | 6.965750  | 6.538066  |
| 54 | O  | -0.731035 | 6.828840  | 2.208303  |
| 55 | O  | -3.214251 | 8.206321  | 6.572096  |
| 56 | O  | -0.748185 | 4.255600  | 2.205368  |
| 57 | O  | -3.096571 | 5.586138  | 6.557537  |
| 58 | O  | 0.963549  | 4.157061  | 4.327297  |
| 59 | O  | -3.843566 | 6.940678  | 0.050306  |
| 60 | O  | -4.120412 | 6.906048  | 4.531631  |
| 61 | O  | -1.668086 | 5.646810  | 0.077263  |
| 62 | O  | -1.687917 | 5.447806  | 4.329275  |
| 63 | O  | -1.688604 | 8.200946  | 0.070080  |
| 64 | Al | -0.009566 | 5.542557  | 3.486486  |
| 65 | Al | 0.000007  | 5.542220  | 0.834013  |
| 66 | Al | -2.343777 | 6.895575  | 5.433969  |
| 67 | Al | -2.399923 | 4.157161  | 3.039176  |
| 68 | Al | 0.005605  | 5.483191  | 6.897404  |

|    |    |           |          |          |
|----|----|-----------|----------|----------|
| 69 | Al | -2.400124 | 4.158251 | 5.665346 |
| 70 | Al | -2.401440 | 6.921096 | 1.266880 |
| 71 | O  | 6.274299  | 5.528729 | 2.203514 |
| 72 | O  | 3.940838  | 6.944392 | 6.573017 |
| 73 | O  | 4.062987  | 6.840791 | 2.200356 |
| 74 | O  | 1.614516  | 8.187686 | 6.553567 |
| 75 | O  | 4.022178  | 4.268178 | 2.176010 |
| 76 | O  | 1.703206  | 5.586181 | 6.557659 |
| 77 | O  | 5.617843  | 4.236760 | 4.455977 |
| 78 | O  | 0.916382  | 6.925383 | 0.066009 |
| 79 | O  | 0.737047  | 7.029116 | 4.358713 |
| 80 | O  | 3.107522  | 5.666489 | 0.050461 |
| 81 | O  | 3.247016  | 5.499013 | 4.460816 |
| 82 | O  | 3.122568  | 8.209708 | 0.067127 |
| 83 | Al | 4.777688  | 5.530545 | 3.333582 |
| 84 | Al | 4.793449  | 5.545625 | 0.686060 |
| 85 | Al | 2.316579  | 6.915420 | 5.314648 |
| 86 | Al | 2.379397  | 4.116599 | 2.999791 |
| 87 | Al | 4.862698  | 5.479815 | 5.929662 |
| 88 | Al | 2.382437  | 4.150306 | 5.687528 |
| 89 | Al | 2.387835  | 6.925211 | 1.243306 |

D<sub>OHI</sub>

|    |    |           |          |           |
|----|----|-----------|----------|-----------|
| 1  | O  | 3.868218  | 1.376319 | 2.206529  |
| 2  | O  | 1.501471  | 2.814354 | 6.530174  |
| 3  | O  | 1.661412  | 2.663088 | 2.198346  |
| 4  | O  | -0.887264 | 4.157594 | 6.620270  |
| 5  | O  | 1.630871  | 0.102921 | 2.226156  |
| 6  | O  | -0.722129 | 1.474974 | 6.582787  |
| 7  | O  | 3.307359  | 0.025526 | 4.363888  |
| 8  | O  | -1.468074 | 2.771116 | 0.000000  |
| 9  | O  | -1.679563 | 2.887111 | 4.415065  |
| 10 | O  | 0.734037  | 1.499727 | 0.000000  |
| 11 | O  | 0.727769  | 1.296882 | 4.389403  |
| 12 | O  | 0.734037  | 4.042506 | 0.000000  |
| 13 | Al | 2.378364  | 1.388174 | 3.476504  |
| 14 | Al | 2.399857  | 1.385558 | 0.834013  |
| 15 | Al | -0.032874 | 2.865998 | 5.437223  |
| 16 | Al | -0.027058 | 0.012329 | 3.016488  |
| 17 | Al | 2.401043  | 1.364982 | 6.697563  |
| 18 | Al | -0.018110 | 0.066268 | 5.656603  |
| 19 | Al | 0.000000  | 2.771116 | 1.333600  |
| 20 | C  | 1.282974  | 4.488169 | 10.158436 |

|    |    |           |          |           |
|----|----|-----------|----------|-----------|
| 21 | C  | 2.012319  | 5.465312 | 10.845734 |
| 22 | C  | 2.656808  | 6.478546 | 10.122662 |
| 23 | C  | 2.524572  | 6.550163 | 8.725536  |
| 24 | C  | 1.811011  | 5.565763 | 7.969761  |
| 25 | C  | 1.216550  | 4.518185 | 8.749363  |
| 26 | O  | -1.616059 | 5.747788 | 9.205193  |
| 27 | H  | 0.767422  | 3.696737 | 10.750562 |
| 28 | H  | 2.098249  | 5.425403 | 11.932507 |
| 29 | H  | 3.293325  | 7.191820 | 10.691292 |
| 30 | H  | 3.050274  | 7.324153 | 8.185693  |
| 31 | H  | 0.720850  | 3.690102 | 8.264933  |
| 32 | H  | -0.840286 | 5.681609 | 9.782104  |
| 33 | O  | 8.674000  | 1.372028 | 2.204353  |
| 34 | O  | 6.278148  | 2.869506 | 6.561196  |
| 35 | O  | 6.459878  | 2.688351 | 2.242506  |
| 36 | O  | 3.953431  | 4.073947 | 6.505539  |
| 37 | O  | 6.444056  | 0.124830 | 2.209060  |
| 38 | O  | 4.103051  | 1.429389 | 6.557436  |
| 39 | O  | 8.104205  | 0.037472 | 4.361256  |
| 40 | O  | 3.343324  | 2.748614 | 0.047095  |
| 41 | O  | 3.124339  | 2.863865 | 4.365821  |
| 42 | O  | 5.538791  | 1.514523 | 0.077849  |
| 43 | O  | 5.540212  | 1.318116 | 4.403137  |
| 44 | O  | 5.535296  | 4.031327 | 0.062753  |
| 45 | Al | 7.182169  | 1.402584 | 3.484403  |
| 46 | Al | 7.199557  | 1.385558 | 0.834013  |
| 47 | Al | 4.759284  | 2.767028 | 5.394920  |
| 48 | Al | 4.799721  | 0.000424 | 3.038808  |
| 49 | Al | 7.168700  | 1.425709 | 6.703582  |
| 50 | Al | 4.799444  | 0.001650 | 5.665004  |
| 51 | Al | 4.798640  | 2.772258 | 1.268293  |
| 52 | O  | 1.474625  | 5.529201 | 2.205245  |
| 53 | O  | -0.940419 | 7.005579 | 6.493890  |
| 54 | O  | -0.733122 | 6.825071 | 2.224603  |
| 55 | O  | -3.232477 | 8.200719 | 6.523689  |
| 56 | O  | -0.744714 | 4.256197 | 2.216709  |
| 57 | O  | -3.096571 | 5.586138 | 6.557537  |
| 58 | O  | 0.910680  | 4.176285 | 4.403665  |
| 59 | O  | -3.843174 | 6.932469 | 0.051518  |
| 60 | O  | -4.072707 | 6.945126 | 4.425071  |
| 61 | O  | -1.668527 | 5.655560 | 0.080346  |
| 62 | O  | -1.692718 | 5.441641 | 4.353077  |
| 63 | O  | -1.682459 | 8.200307 | 0.074308  |
| 64 | Al | -0.005517 | 5.554064 | 3.533477  |
| 65 | Al | 0.000007  | 5.542220 | 0.834013  |
| 66 | Al | -2.374980 | 6.968341 | 5.265836  |

|    |    |           |          |          |
|----|----|-----------|----------|----------|
| 67 | Al | -2.399923 | 4.157161 | 3.039176 |
| 68 | Al | -1.372116 | 5.643193 | 7.499119 |
| 69 | Al | -2.400124 | 4.158251 | 5.665346 |
| 70 | Al | -2.400877 | 6.927369 | 1.276756 |
| 71 | O  | 6.274299  | 5.528729 | 2.203514 |
| 72 | O  | 3.921125  | 6.996792 | 6.432368 |
| 73 | O  | 4.061804  | 6.835469 | 2.187899 |
| 74 | O  | 1.593364  | 8.223501 | 6.541927 |
| 75 | O  | 4.039897  | 4.267763 | 2.196926 |
| 76 | O  | 1.703206  | 5.586181 | 6.557659 |
| 77 | O  | 5.618406  | 4.246773 | 4.480192 |
| 78 | O  | 0.918207  | 6.922938 | 0.063422 |
| 79 | O  | 0.751982  | 7.046344 | 4.386424 |
| 80 | O  | 3.108218  | 5.662738 | 0.055186 |
| 81 | O  | 3.172975  | 5.480411 | 4.413710 |
| 82 | O  | 3.118221  | 8.211096 | 0.057022 |
| 83 | Al | 4.784458  | 5.556406 | 3.368595 |
| 84 | Al | 4.789878  | 5.549086 | 0.725793 |
| 85 | Al | 2.388962  | 6.987069 | 5.329299 |
| 86 | Al | 2.389480  | 4.146825 | 3.001129 |
| 87 | Al | 4.795067  | 5.536544 | 6.076368 |
| 88 | Al | 2.371457  | 4.125821 | 5.625679 |
| 89 | Al | 2.387630  | 6.933081 | 1.246601 |

## D<sub>OH2</sub>

| #  | Atom | X         | Y         | Z        |
|----|------|-----------|-----------|----------|
| 1  | O    | 3.870255  | 1.373907  | 2.198408 |
| 2  | O    | 1.531164  | 2.822060  | 6.502212 |
| 3  | O    | 1.656017  | 2.699926  | 2.229678 |
| 4  | O    | -0.797965 | 4.068805  | 6.505964 |
| 5  | O    | 1.649901  | 0.127641  | 2.190171 |
| 6  | O    | -0.758619 | 1.415187  | 6.493446 |
| 7  | O    | 3.312306  | 0.006952  | 4.377148 |
| 8  | O    | -1.468074 | 2.771116  | 0.000000 |
| 9  | O    | -1.651968 | 2.900100  | 4.332426 |
| 10 | O    | 0.734037  | 1.499727  | 0.000000 |
| 11 | O    | 0.757158  | 1.316948  | 4.377198 |
| 12 | O    | 0.734037  | 4.042506  | 0.000000 |
| 13 | Al   | 2.402775  | 1.386952  | 3.483415 |
| 14 | Al   | 2.399857  | 1.385558  | 0.834013 |
| 15 | Al   | -0.058149 | 2.742570  | 5.405225 |
| 16 | Al   | 0.004789  | -0.002485 | 3.002020 |
| 17 | Al   | 2.408153  | 1.374071  | 6.736479 |

|    |    |           |          |           |
|----|----|-----------|----------|-----------|
| 18 | Al | 0.004716  | 0.037262 | 5.627447  |
| 19 | Al | 0.000000  | 2.771116 | 1.333600  |
| 20 | C  | 1.288257  | 4.481271 | 10.175889 |
| 21 | C  | 2.037477  | 5.440432 | 10.864193 |
| 22 | C  | 2.677863  | 6.452746 | 10.149164 |
| 23 | C  | 2.530775  | 6.532853 | 8.750031  |
| 24 | C  | 1.815539  | 5.551991 | 8.045401  |
| 25 | C  | 1.209263  | 4.509670 | 8.771400  |
| 26 | O  | 7.220767  | 1.329138 | 8.930954  |
| 27 | H  | 0.767422  | 3.696737 | 10.750562 |
| 28 | H  | 2.125162  | 5.395160 | 11.950312 |
| 29 | H  | 3.293325  | 7.191820 | 10.691292 |
| 30 | H  | 2.990614  | 7.354953 | 8.231196  |
| 31 | H  | 0.720850  | 3.690102 | 8.264933  |
| 32 | H  | 7.135596  | 2.182393 | 9.382160  |
| 33 | O  | 8.674000  | 1.372028 | 2.204353  |
| 34 | O  | 6.335543  | 2.801322 | 6.482593  |
| 35 | O  | 6.475085  | 2.670253 | 2.196508  |
| 36 | O  | 3.982508  | 4.042036 | 6.550412  |
| 37 | O  | 6.449061  | 0.080685 | 2.231904  |
| 38 | O  | 4.103051  | 1.429389 | 6.557436  |
| 39 | O  | 8.145336  | 0.003944 | 4.312671  |
| 40 | O  | 3.337883  | 2.752952 | 0.056074  |
| 41 | O  | 3.159792  | 2.882500 | 4.351873  |
| 42 | O  | 5.536782  | 1.479351 | 0.072457  |
| 43 | O  | 5.525768  | 1.255738 | 4.348044  |
| 44 | O  | 5.536307  | 4.033416 | 0.038931  |
| 45 | Al | 7.198020  | 1.398885 | 3.504866  |
| 46 | Al | 7.199557  | 1.385558 | 0.834013  |
| 47 | Al | 4.847632  | 2.744622 | 5.368247  |
| 48 | Al | 4.799721  | 0.000424 | 3.038808  |
| 49 | Al | 7.184880  | 1.395424 | 7.164901  |
| 50 | Al | 4.799444  | 0.001650 | 5.665004  |
| 51 | Al | 4.811664  | 2.761835 | 1.247219  |
| 52 | O  | 1.474625  | 5.529201 | 2.205245  |
| 53 | O  | -0.867807 | 6.975889 | 6.502258  |
| 54 | O  | -0.720661 | 6.832145 | 2.215863  |
| 55 | O  | -3.234334 | 8.212775 | 6.572531  |
| 56 | O  | -0.748765 | 4.276552 | 2.203516  |
| 57 | O  | -3.096571 | 5.586138 | 6.557537  |
| 58 | O  | 0.843507  | 4.267861 | 4.511782  |
| 59 | O  | -3.865287 | 6.920463 | 0.053464  |
| 60 | O  | -4.021384 | 7.033966 | 4.367177  |
| 61 | O  | -1.657897 | 5.674277 | 0.074666  |
| 62 | O  | -1.553455 | 5.488869 | 4.448738  |
| 63 | O  | -1.681408 | 8.204656 | 0.051731  |

|    |    |           |          |          |
|----|----|-----------|----------|----------|
| 64 | Al | 0.013080  | 5.540108 | 3.366436 |
| 65 | Al | 0.000007  | 5.542220 | 0.834013 |
| 66 | Al | -2.408586 | 6.968465 | 5.406207 |
| 67 | Al | -2.399923 | 4.157161 | 3.039176 |
| 68 | Al | -0.058119 | 5.540195 | 5.923103 |
| 69 | Al | -2.400124 | 4.158251 | 5.665346 |
| 70 | Al | -2.409426 | 6.931596 | 1.253200 |
| 71 | O  | 6.274299  | 5.528729 | 2.203514 |
| 72 | O  | 3.941901  | 6.971678 | 6.444214 |
| 73 | O  | 4.078633  | 6.822478 | 2.190625 |
| 74 | O  | 1.643908  | 8.245753 | 6.442364 |
| 75 | O  | 4.079118  | 4.268861 | 2.183589 |
| 76 | O  | 1.703206  | 5.586181 | 6.557659 |
| 77 | O  | 5.725848  | 4.186925 | 4.380539 |
| 78 | O  | 0.947675  | 6.898915 | 0.054761 |
| 79 | O  | 0.744020  | 6.889250 | 4.475139 |
| 80 | O  | 3.122312  | 5.641800 | 0.069415 |
| 81 | O  | 3.136921  | 5.448427 | 4.372099 |
| 82 | O  | 3.133505  | 8.218397 | 0.065973 |
| 83 | Al | 4.820499  | 5.559239 | 3.467509 |
| 84 | Al | 4.798579  | 5.533493 | 0.784353 |
| 85 | Al | 2.471187  | 7.022320 | 5.290869 |
| 86 | Al | 2.456545  | 4.177146 | 2.972120 |
| 87 | Al | 4.816312  | 5.525830 | 6.709400 |
| 88 | Al | 2.453403  | 4.097559 | 5.592596 |
| 89 | Al | 2.411835  | 6.938734 | 1.240325 |