# Supplementary Information (SI)

# A Theoretical Study of the Oxidation of Benzene by Manganese Oxide Clusters: Formation of Quinone Intermediates

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**Content**

**Table S1.** Calculated equilibrium geometry, vibrational frequencies (cm$^{-1}$) and adiabatic electron affinity (EA, eV) of the ground state ($^4B_1$) of $MnO_2$

| Level of theory | Equilibrium geometry | | Vibrational frequencies (cm$^{-1}$) | | | EA (eV) |
|---|---|---|---|---|---|---|
| | rMn-O (Å) | <OMnO (°) | v1 (A1) | v2 (A1) | v3 (B2) | |
| **Expt.**[1] | 1.597 | 128.8 | 261.0 | 918.0 | 1012.0 | 2.060 |
| **PBE** | 1.598 | 127.8 | 270.0 | 904.0 | 1008.0 | 2.008 |
| **BP86** | 1.598 | 127.8 | 271.0 | 910.0 | 1013.0 | 2.113 |

[1] G.L. Gutsev, B.K. Rao, P. Jena, L. Xi, L.S. Wang, Experimental and theoretical study of the photoelectron spectra of MnOx- (x = 1 - 3) clusters, J. Chem. Phys. 113 (2000) 1473–1483.

| | | | | | | |
|---|---|---|---|---|---|---|
| **B3LYP** | 1.600 | 130 | 250.0 | 855.0 | 959.0 | 2.545 |
| **M06-2X** | 1.643 | 134.4 | 191.0 | 636.0 | 846.0 | 3.058 |

**Table S2.** Calculated the first vertical ionization energy (IE, eV), electron affinity (EA, eV) and proton affinity (PA, eV) of $C_6H_6$

| Level of theory | IE (eV) | EA (eV) | PA (eV) |
|---|---|---|---|
| **Expt.** | 9.244[2] | -1.150[3] | 7.780[4] |
| **PBE** | 9.254 | -0.594 | 7.875 |
| **BP86** | 9.344 | -0.508 | 7.857 |
| **B3LYP** | 9.262 | -0.528 | 8.164 |
| **M06-2X** | 9.415 | -0.883 | 7.634 |

**Table S3.** Comparison of calculated heats of reaction (kcal $mol^{-1}$) of some products of the $C_6H_6 + O_2$ reaction, in this work with available data at 298.15 K.

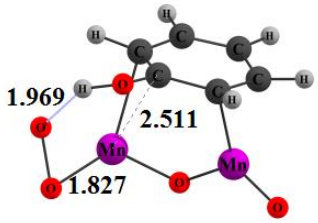
| Reaction paths | PBE/6-311++g(d,p) | NIST[5] |
|---|---|---|
| $C_6H_6 + O_2 \rightarrow$ catechol | -44.82 | -44.30 |
| $C_6H_6 + O_2 \rightarrow$ resorcinol | -44.58 | -43.80 |
| $C_6H_6 + O_2 \rightarrow$ hydroquinone | -42.56 | -44.20 |
| $C_6H_6 + O_2 \rightarrow$ benzoquinone + $H_2$ | -41.80 | -40.67 |

**Table S4.** Comparison of calculated heats of reaction (kcal $mol^{-1}$) of some products of the $C_6H_6 + Mn_2O_3 + O_2$ reaction in this work with available data at 298.15 K

| Reaction | PBE | M06-2X | B3LYP | BP86 | NIST |
|---|---|---|---|---|---|
| $C_6H_6 + Mn_2O_3 + O_2 \rightarrow$ hydroquinone | -76.42 | -84.13 | -74.24 | -75.14 | -76.77 |
| $C_6H_6 + Mn_2O_3 + O_2 \rightarrow$ *p*-benzoquinone + $H_2$ | -41.80 | -44.46 | -42.11 | -42.71 | -41.03 |
| $C_6H_6 + Mn_2O_3 + O_2 \rightarrow$ catechol | -78.69 | -86.78 | -76.39 | -77.34 | -77.44 |
| $C_6H_6 + Mn_2O_3 + O_2 \rightarrow$ *o*-benzoquinone + $H_2$ | -34.79 | -37.34 | -34.58 | -35.67 | -34.84 |

[2] webbook.nist.gov.
[3] N. Driver, P. Jena, Electron affinity of modified benzene, Int. J. Quantum Chem. 118 (2018) 1–10.
[4] E.P.L. Hunter, S.G. Lias, Evaluate Gas Phase Basicities and Proton Affinity of Molecules.Pdf, J. Phys. Chem. Ref. Data. 27 (1998) 413–656.
[5] Afeefy, H. Y; Liebman, J. F.; Stein, S. E. Neutral Thermochemical Data. In NIST Chemistry WebBook; Linstrom, P. J., Mallard, W. G., Eds; NIST Standard Reference Database Number 69; National Institute of Standards and Technology: Gaithersburg, MD, http://webbook.nist.gov, (retrieved September 13, 2011).

**Table S5.** Job cpu time to optimize the intermediate IM1 at PBE level with basis set 6-311++g(d,p) for C, H, O and different basis sets for Mn atom




**IM1**

| Basis set for Mn | CPU time | Single point energy (a.u) |
|---|---|---|
| **LanL2DZ** | 18 hours 51 minutes | -815.59763 |
| **LanL2TZ** | 1 days 1 hours 50 minutes | -815.612294 |
| **cc-pvTZ** | 2 days 22 hours 48 minutes | -2909.394603 |
| **cc-pvDZ** | 2 days 27 hours 56 minutes | -2909.366325 |
| **Aug-cc-pvDZ** | 3 days 24 hours 41 minutes | -2909.375627 |

**Table S6.** Theoretical predication of detailed energies for intermediates, transition states, and products of the $C_6H_6$ + $O_2$ gas phase reaction calculated at PBE/6-311++g(d,p) level. ZPE energies are reported unscaled

| Species | Single point energy (a.u) | ZPE (a.u) | Etotal (au) | Erelative (kcal.mol$^{-1}$) |
|---|---|---|---|---|
| $C_6H_6$ | -231.9948881 | 0.0975380 | -231.897350 | |
| $O_2$ | -150.2295138 | 0.0035290 | -150.225985 | |
| $CO_2$ | -188.4572427 | 0.0113260 | -188.445917 | |
| cyclopentadiene | -193.8893934 | 0.0896370 | -193.799756 | |
| $C_6H_6$+$O_2$ | -382.22440187 | 0.10106700 | -382.123335 | 0.00 |
| I1g | -382.52606469 | 0.104712 | -382.421353 | 28.09 |
| I2g | -382.20349795 | 0.103128 | -382.100370 | 14.41 |
| I3g | -382.20695210 | 0.103313 | -382.103639 | 12.36 |
| I4 | -382.26264918 | 0.101553 | -382.161096 | -23.70 |
| I5g | -382.18266272 | 0.104590 | -382.078073 | 28.40 |
| I6g | -382.24658535 | 0.105174 | -382.141411 | -11.34 |
| I7g | -382.14406796 | 0.10292900 | -382.041139 | 51.58 |
| I8g | -382.28193614 | 0.104843 | -382.177093 | -33.73 |
| I9g | -382.42966548 | 0.104911 | -382.324754 | 35.01 |
| I10g | -382.28280002 | 0.104858 | -382.177942 | -34.27 |
| I11g | -382.18281852 | 0.104179 | -382.078640 | 28.05 |
| I12g | -382.15915665 | 0.098295 | -382.060862 | 39.20 |
| I13g | -382.21804957 | 0.10049200 | -382.117558 | 3.63 |
| PR1g ($CO_2$+$C_5H_6$) | -382.22309722 | 0.09548300 | -382.127614 | -2.69 |

| | | | | |
|---|---|---|---|---|
| PR2g-resorcinol | -382.35260703 | 0.105101 | -382.247506 | -77.92 |
| PR3g-p-benzoquinone+$H_2$ | -382.28370235 | 0.09177900 | -382.191923 | -43.04 |
| PR4g-hydroquinone | -382.34927909 | 0.104839 | -382.244440 | -75.99 |
| T0g/1g | -382.50121451 | 0.104094 | -382.397121 | 42.07 |
| T1g/2g | -382.13558374 | 0.099085 | -382.036499 | 54.49 |
| T2g/3g | -382.60973829 | 0.104454 | -382.505284 | 47.60 |
| T3/4 | -382.20007338 | 0.100077 | -382.099996 | 14.65 |
| T4P1 | -382.24310236 | 0.100318 | -382.142784 | -12.20 |
| T0g/5g | -382.14063067 | 0.101774 | -382.038857 | 53.01 |
| T5g/6g | -382.14982272 | 0.101709 | -382.048114 | 47.20 |
| T6g/7g | -382.13881289 | 0.099721 | -382.039092 | 52.86 |
| T7g/8g | -382.13479915 | 0.101536 | -382.033263 | 56.52 |
| T8gP2g | -382.18661440 | 0.099253 | -382.087361 | 22.57 |
| T6g/9g | -382.14457545 | 0.099449 | -382.045126 | 49.08 |
| T9g/10g | -382.13274812 | 0.101580 | -382.031168 | 57.84 |
| T10gP2g | -382.17906631 | 0.098488 | -382.080578 | 26.83 |
| T0g/11g | -382.16851621 | 0.102331 | -382.066185 | 35.86 |
| T12g/13g | -382.13643209 | 0.095312 | -382.041120 | 51.59 |
| T12gP3g | -382.13595206 | 0.091602 | -382.044350 | 49.56 |
| T13gP4g | -382.17619556 | 0.096116 | -382.080080 | 27.14 |
| I11g+$O_2$ | -532.41233230 | 0.10770800 | -532.304624 | 0.00 |
| COM | -532.40046991 | 0.106056 | -532.294414 | 6.41 |
| T11g/COM | -532.37549400 | 0.105793 | -532.269701 | 21.91 |

**Table S7.** Cartesian coordinates (Å) for the reactants, intermediates, transition states, and products in the interaction of the $C_6H_6$ with $O_2$ by the method PBE/6-311++g(d,p)

| 12 | | | | 14 | | | |
|---|---|---|---|---|---|---|---|
| **$C_6H_6$** | | | | **T0-16g** | | | |
| C | 0.000000 | 1.401025 | 0.000000 | C | -0.513601 | 1.336561 | -0.691157 |
| C | 1.213323 | 0.700512 | 0.000000 | C | -1.384102 | 0.288177 | -0.653269 |
| C | 1.213323 | -0.700512 | 0.000000 | C | -0.829207 | -1.015344 | -0.271636 |
| C | 0.000000 | -1.401025 | 0.000000 | C | 0.509895 | -1.337828 | -0.691321 |
| C | -1.213323 | -0.700512 | 0.000000 | C | 1.380504 | -0.289358 | -0.658820 |
| C | -1.213323 | 0.700512 | 0.000000 | C | 0.827351 | 1.014677 | -0.277185 |
| H | 0.000000 | 2.493924 | 0.000000 | H | -0.838365 | 2.372309 | -0.796995 |
| H | 2.159801 | 1.246962 | 0.000000 | H | -2.463602 | 0.409090 | -0.755352 |
| H | 2.159801 | -1.246962 | 0.000000 | H | 0.834119 | -2.373702 | -0.797595 |
| H | 0.000000 | -2.493924 | 0.000000 | H | 2.459524 | -0.410347 | -0.765766 |
| H | -2.159801 | -1.246962 | 0.000000 | O | -0.551255 | -0.368597 | 1.424805 |

| | | | |
|---|---|---|---|
| H | -2.159801 | 1.246962 | 0.000000 |
| **$C_5H_6$** | | | |
| C | 0.995806 | -0.732765 | 0.000001 |
| C | 0.995013 | 0.733950 | 0.000001 |
| C | -0.287105 | 1.182050 | -0.000002 |
| C | -1.215324 | -0.000772 | 0.000002 |
| C | -0.285671 | -1.182380 | -0.000002 |
| H | 1.892837 | 1.353710 | 0.000001 |
| H | -0.618142 | 2.220156 | -0.000002 |
| H | -1.885063 | -0.001034 | 0.881350 |
| H | -0.615304 | -2.220949 | -0.000003 |
| H | 1.894430 | -1.351350 | 0.000000 |
| H | -1.885072 | -0.001034 | -0.881340 |
| 3 | | | |
| **$CO_2$** | | | |
| C | 0.000000 | 0.000000 | 0.000000 |
| O | 0.000000 | 0.000000 | 1.172289 |
| O | 0.000000 | 0.000000 | -1.172289 |
| 16 | | | |
| **COM** | | | |
| C | -0.516441 | -0.000275 | -1.104341 |
| C | 0.170139 | 1.261743 | -0.641596 |
| C | 1.391819 | 1.267109 | -0.087482 |
| C | 2.192020 | 0.000042 | 0.127119 |
| C | 1.391848 | -1.267141 | -0.086895 |
| C | 0.170171 | -1.262065 | -0.641019 |
| H | -0.398844 | 2.187382 | -0.768886 |
| H | 1.867222 | 2.190818 | 0.252918 |
| H | 2.952740 | -0.000149 | -0.726981 |
| H | 1.867274 | -2.190683 | 0.253927 |
| O | -1.908765 | -0.000236 | -0.863728 |
| O | 3.043198 | 0.000293 | 1.179872 |
| H | -0.398790 | -2.187774 | -0.767893 |
| H | -0.522109 | -0.000526 | -2.223419 |
| O | -2.110007 | 0.000221 | 0.853453 |
| O | -3.295030 | 0.000279 | 1.153606 |
| 14 | | | |
| **Resorcinol** | | | |
| O | 0.559294 | 0.371359 | 1.421006 |
| H | -1.534151 | -1.829967 | -0.090805 |
| H | 1.533128 | 1.829209 | -0.099641 |
| 14 | | | |
| **T0-1g** | | | |
| C | -1.655147 | -1.106404 | -0.113652 |
| C | -2.156760 | 0.197988 | -0.340623 |
| C | -1.348687 | 1.323052 | -0.060658 |
| C | -0.068791 | 1.168958 | 0.410994 |
| C | 0.530596 | -0.165434 | 0.569159 |
| C | -0.381132 | -1.300278 | 0.354652 |
| H | -3.166710 | 0.333235 | -0.715194 |
| H | -1.752596 | 2.320944 | -0.210324 |
| H | 0.559258 | 2.028371 | 0.625957 |
| H | 1.195793 | -0.266277 | 1.429180 |
| O | 1.673562 | -0.276728 | -0.601112 |
| O | 2.819334 | 0.169150 | -0.185510 |
| H | -0.000203 | -2.300138 | 0.540341 |
| H | -2.299193 | -1.962797 | -0.296211 |
| 14 | | | |
| **T0-5g** | | | |
| C | 0.192404 | -1.068703 | -0.693735 |
| C | 0.728410 | 0.353923 | -0.804366 |
| C | -1.090019 | -1.301552 | -0.232952 |
| C | -0.203983 | 1.426748 | -0.349915 |
| H | 1.206995 | 0.576004 | -1.773880 |
| C | -1.816070 | -0.246012 | 0.344088 |
| H | -1.493517 | -2.315657 | -0.215666 |
| C | -1.359315 | 1.103563 | 0.311085 |
| H | 0.138365 | 2.458999 | -0.444718 |
| H | -2.778169 | -0.460049 | 0.817510 |
| H | -1.972792 | 1.882220 | 0.770408 |
| H | 0.782297 | -1.861149 | -1.158661 |
| O | 1.800630 | 0.362996 | 0.207252 |
| O | 1.375403 | -0.599017 | 1.112719 |
| 14 | | | |
| **T10P3g** | | | |
| C | -0.292170 | -1.124487 | -0.384408 |

| | | | |
|---|---|---|---|
| C | -1.208098 | 1.121336 | 0.000197 |
| C | -1.219466 | -0.282678 | -0.000086 |
| C | -0.021980 | -1.008565 | -0.000192 |
| C | 1.199821 | -0.322154 | -0.000031 |
| C | 1.229892 | 1.079821 | -0.000077 |
| C | 0.019557 | 1.784856 | -0.000073 |
| H | -2.154088 | 1.664054 | 0.000657 |
| H | 2.185284 | 1.612293 | -0.000250 |
| H | 0.038199 | 2.877171 | -0.000021 |
| O | 2.339594 | -1.089934 | 0.000062 |
| H | 3.110226 | -0.497883 | 0.000593 |
| O | -2.445796 | -0.900799 | -0.000124 |
| H | -2.311144 | -1.863334 | 0.000817 |
| H | -0.017218 | -2.102125 | 0.000274 |

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**hydroquinone**

| | | | |
|---|---|---|---|
| C | -0.680916 | 1.223647 | -0.000013 |
| C | 0.716558 | 1.196764 | 0.000015 |
| C | 1.404893 | -0.025229 | 0.000028 |
| C | 0.680916 | -1.223647 | 0.000013 |
| C | -0.716558 | -1.196764 | -0.000015 |
| C | -1.404893 | 0.025229 | -0.000028 |
| H | -1.220970 | 2.171983 | -0.000023 |
| H | 1.273104 | 2.139239 | 0.000027 |
| H | 1.220970 | -2.171983 | 0.000023 |
| H | -1.273104 | -2.139239 | -0.000027 |
| O | -2.780837 | 0.111632 | -0.000056 |
| H | -3.148047 | -0.787298 | -0.000063 |
| O | 2.780837 | -0.111632 | 0.000055 |
| H | 3.148047 | 0.787298 | 0.000065 |

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**I10g**

| | | | |
|---|---|---|---|
| C | -1.036730 | -1.031349 | -0.326212 |
| C | 0.421369 | -1.163518 | -0.286420 |
| C | 1.193526 | -0.075231 | 0.003520 |
| C | 0.637730 | 1.263174 | 0.043449 |
| C | -0.684278 | 1.483745 | -0.173336 |
| C | -1.631198 | 0.364364 | -0.266182 |
| C | 1.149103 | -0.821312 | -0.445839 |
| C | 1.583019 | 0.653163 | -0.420623 |
| C | 0.541110 | 1.601338 | -0.169455 |
| C | -0.750160 | 1.215314 | 0.113667 |
| C | -1.176676 | -0.154470 | -0.005162 |
| H | -0.658503 | -2.116161 | -0.658345 |
| H | 2.426667 | 0.125021 | 0.568093 |
| H | 0.802635 | 2.663726 | -0.167253 |
| H | -1.497032 | 1.967639 | 0.401031 |
| H | 1.719146 | -1.490485 | -1.104636 |
| O | 1.736978 | -0.734876 | 0.899547 |
| O | -2.500693 | -0.477733 | 0.163187 |
| H | -3.008543 | 0.333855 | 0.330156 |

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**T11-COMg**

| | | | |
|---|---|---|---|
| C | 1.714073 | 0.891441 | 0.178456 |
| C | 2.119660 | -0.485099 | 0.710452 |
| C | 1.231785 | -1.458053 | 0.488345 |
| C | -0.000637 | -1.042839 | -0.329072 |
| C | 0.401524 | -0.205599 | -1.539018 |
| C | 1.268753 | 0.778190 | -1.289024 |
| H | 3.033425 | -0.610729 | 1.294745 |
| H | 1.277066 | -2.462845 | 0.910754 |
| H | -0.601584 | -1.929233 | -0.601659 |
| H | -0.067918 | -0.381594 | -2.509076 |
| O | 0.639774 | 1.391125 | 0.922398 |
| O | -0.750229 | -0.253216 | 0.583626 |
| H | 1.592404 | 1.525736 | -2.015211 |
| H | 2.533538 | 1.632184 | 0.281928 |
| O | -3.323376 | 0.546218 | 0.343777 |
| O | -2.588404 | -0.264347 | -0.185092 |

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**T12-13g**

| | | | |
|---|---|---|---|
| C | -1.502584 | 0.000000 | 0.256230 |
| C | -0.692658 | -1.270180 | 0.106300 |
| C | 0.655169 | -1.252734 | 0.005342 |
| C | 1.415313 | 0.000000 | 0.065190 |
| C | 0.655170 | 1.252734 | 0.005342 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.602960 | -1.813528 | -0.844393 | C | -0.692658 | 1.270180 | 0.106300 |
| H | 1.343391 | 2.090214 | 0.150992 | H | -1.265128 | -2.199269 | 0.053353 |
| H | -1.060598 | 2.500950 | -0.307185 | H | 1.229225 | -2.172034 | -0.138191 |
| H | -2.602592 | 0.552421 | -0.737982 | H | 2.258889 | 0.000000 | 0.971254 |
| H | 0.871000 | -2.138695 | -0.495051 | H | 1.229225 | 2.172034 | -0.138191 |
| O | 2.556578 | -0.111413 | 0.161017 | O | -2.688155 | 0.000000 | -0.420507 |
| O | -1.707058 | -0.538966 | 0.860250 | O | 2.772709 | 0.000000 | -0.254630 |
| H | 2.853089 | -1.035439 | 0.094563 | H | -1.265128 | 2.199269 | 0.053353 |
| 14 | | | | H | -1.890027 | 0.000000 | 1.331299 |
| **I11g** | | | | 14 | | | |
| C | -1.233712 | 0.028334 | -0.072094 | **T1-2g** | | | |
| C | -0.641953 | 1.270204 | -0.697376 | C | -1.789651 | -1.007419 | -0.049277 |
| C | 0.699603 | 1.239467 | -0.697340 | C | -2.198533 | 0.366597 | -0.055207 |
| C | 1.233712 | -0.028334 | -0.072094 | C | -1.253263 | 1.378779 | -0.007199 |
| C | 0.641953 | -1.270204 | -0.697377 | C | 0.129851 | 1.089564 | 0.022078 |
| C | -0.699603 | -1.239466 | -0.697342 | C | 0.552438 | -0.320970 | 0.111642 |
| H | -1.258534 | 2.124370 | -0.980615 | C | -0.467832 | -1.361314 | 0.003442 |
| H | 1.354829 | 2.064370 | -0.980562 | H | -3.261183 | 0.610180 | -0.103189 |
| H | 2.322932 | -0.053464 | 0.057959 | H | -1.563648 | 2.425842 | -0.034820 |
| H | 1.258534 | -2.124369 | -0.980616 | H | 0.946863 | 1.811826 | 0.020940 |
| O | -0.738470 | 0.016873 | 1.338011 | H | 0.385111 | 0.165231 | 1.204454 |
| O | 0.738469 | -0.016874 | 1.338011 | O | 1.853663 | -0.665354 | -0.014240 |
| H | -1.354829 | -2.064370 | -0.980564 | O | 2.688963 | 0.453671 | -0.123327 |
| H | -2.322932 | 0.053464 | 0.057958 | H | -0.136921 | -2.401321 | -0.023118 |
| 14 | | | | H | -2.549291 | -1.789722 | -0.116601 |
| **I12g** | | | | 14 | | | |
| C | -1.249731 | -0.800796 | 0.210051 | **T12P3g** | | | |
| C | 0.119752 | -1.430633 | 0.056814 | C | 0.000176 | 1.305775 | 0.223867 |
| C | 1.249731 | -0.706576 | 0.056851 | C | -1.260598 | 0.663445 | -0.404774 |
| C | 1.249731 | 0.800796 | 0.210051 | C | -1.260598 | -0.663838 | -0.404624 |
| C | -0.119752 | 1.430633 | 0.056814 | C | -0.000176 | -1.305775 | 0.223867 |
| C | -1.249731 | 0.706576 | 0.056851 | C | 1.260598 | -0.663445 | -0.404774 |
| H | 0.127630 | -2.514826 | -0.084555 | C | 1.260598 | 0.663838 | -0.404624 |
| H | 2.231450 | -1.166760 | -0.084504 | H | -2.045770 | 1.335423 | -0.747824 |
| H | 1.521567 | 0.975040 | 1.306851 | H | -2.046495 | -1.335566 | -0.746570 |
| H | -0.127630 | 2.514826 | -0.084555 | H | 0.000239 | -0.600710 | 1.287395 |
| O | -2.273820 | -1.456985 | -0.385011 | H | 2.045770 | -1.335423 | -0.747824 |
| O | 2.273820 | 1.456985 | -0.385011 | O | -0.000565 | 2.571409 | 0.465024 |

| | | | |
|---|---|---|---|
| H | -2.231450 | 1.166760 | -0.084504 |
| H | -1.521567 | -0.975040 | 1.306851 |
| 14 | | | |
| **I13g** | | | |
| C | -0.700049 | -1.264954 | 0.252190 |
| C | 0.659048 | -1.219215 | 0.065312 |
| C | 1.346159 | 0.018232 | -0.026570 |
| C | 0.636150 | 1.245075 | 0.061190 |
| C | -0.720340 | 1.262533 | 0.244155 |
| C | -1.534095 | -0.008184 | 0.278093 |
| H | -1.232951 | -2.215781 | 0.307989 |
| H | 1.226016 | -2.154012 | -0.017286 |
| H | 1.201637 | 2.176357 | -0.025970 |
| H | -1.272529 | 2.202666 | 0.296309 |
| O | -2.570085 | -0.021558 | -0.639825 |
| H | -2.157119 | -0.007811 | 1.233646 |
| O | 2.701079 | 0.096697 | -0.207519 |
| H | 3.065752 | -0.803452 | -0.262149 |
| 14 | | | |
| **I1g** | | | |
| C | 0.018031 | 0.706670 | 0.910656 |
| C | -0.961883 | 1.406514 | 0.190858 |
| C | -1.926394 | 0.702926 | -0.531362 |
| C | -1.924975 | -0.705861 | -0.530210 |
| C | -0.959179 | -1.406337 | 0.193278 |
| C | 0.019339 | -0.703334 | 0.912025 |
| H | 0.771354 | -1.247334 | 1.487031 |
| H | -0.958040 | -2.498451 | 0.195910 |
| H | -2.685294 | -1.249262 | -1.096411 |
| H | -2.687808 | 1.243864 | -1.098446 |
| H | -0.962737 | 2.498634 | 0.191581 |
| H | 0.769466 | 1.253040 | 1.484205 |
| O | 1.932575 | -0.001278 | -0.729520 |
| O | 3.087854 | 0.000783 | -0.274898 |
| 14 | | | |
| **I2g** | | | |
| C | 1.759341 | -1.041634 | -0.000052 |
| C | 2.195766 | 0.333105 | -0.000048 |
| O | 0.000565 | -2.571409 | 0.465024 |
| H | 2.046495 | 1.335566 | -0.746570 |
| H | -0.000239 | 0.600710 | 1.287395 |
| 14 | | | |
| **T13P4g** | | | |
| C | -0.706431 | 1.260422 | -0.321814 |
| C | 0.643146 | 1.254012 | -0.098223 |
| C | 1.343637 | 0.017788 | 0.046091 |
| C | 0.665805 | -1.227458 | -0.099297 |
| C | -0.685331 | -1.261028 | -0.333022 |
| C | -1.470201 | -0.006167 | -0.244640 |
| H | -1.252774 | 2.195295 | -0.457176 |
| H | 1.218598 | 2.181889 | -0.050631 |
| H | 1.242861 | -2.158906 | -0.058201 |
| H | -1.212163 | -2.204532 | -0.483500 |
| O | -2.566101 | -0.022938 | 0.670955 |
| H | -2.766565 | -0.018234 | -0.513432 |
| O | 2.687624 | 0.095859 | 0.271542 |
| H | 3.054105 | -0.804286 | 0.328387 |
| 14 | | | |
| **T2-3g** | | | |
| C | 1.236126 | 1.350762 | -0.055555 |
| C | 2.155121 | 0.251562 | 0.134497 |
| C | 1.713519 | -1.020314 | 0.137233 |
| C | 0.262294 | -1.323993 | -0.017176 |
| C | -0.633100 | -0.151056 | -0.228792 |
| C | -0.108433 | 1.168900 | -0.208229 |
| H | 3.209595 | 0.470338 | 0.255658 |
| H | 2.396007 | -1.853190 | 0.263488 |
| H | 0.067715 | -2.063886 | -0.807778 |
| O | -2.389499 | 0.326584 | 0.669336 |
| O | -1.879157 | -0.419215 | -0.510108 |
| H | -0.796003 | 1.989858 | -0.353769 |
| H | 1.639952 | 2.356487 | -0.097293 |
| H | -0.121180 | -1.813723 | 0.893997 |
| 14 | | | |
| **T3-4g** | | | |
| C | -1.202436 | -1.131625 | -0.447315 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.296348 | 1.352602 | -0.000021 | C | -1.927752 | -0.013094 | -0.098662 |
| C | -0.171708 | 1.101290 | 0.000005 | C | -1.254355 | 1.185323 | 0.279835 |
| C | -0.536658 | -0.335196 | -0.000001 | C | 0.022072 | 1.473020 | -0.251986 |
| C | 0.422518 | -1.373581 | -0.000031 | C | 1.108169 | 0.015590 | -0.017238 |
| H | 3.267575 | 0.543939 | -0.000072 | C | 0.219157 | -1.264268 | -0.146057 |
| H | 1.632345 | 2.392358 | -0.000022 | H | -3.020750 | -0.052347 | -0.072252 |
| H | -0.698779 | 1.584715 | -0.853835 | H | -1.714367 | 1.843468 | 1.028172 |
| O | -1.806510 | -0.661345 | 0.000049 | H | 0.085427 | 1.356211 | -1.340617 |
| O | -2.679129 | 0.401404 | 0.000081 | O | 0.664005 | -0.654051 | 1.125134 |
| H | 0.079643 | -2.410003 | -0.000028 | O | 2.247289 | 0.291544 | -0.421413 |
| H | 2.509444 | -1.835698 | -0.000066 | H | 0.729232 | -2.203871 | -0.367722 |
| H | -0.698758 | 1.584696 | 0.853869 | H | -1.708428 | -1.990275 | -0.902517 |
| 14 | | | | H | 0.549415 | 2.357182 | 0.113709 |
| **I3g** | | | | 14 | | | |
| C | 1.342126 | 1.282146 | -0.034569 | **T4P1g** | | | |
| C | 2.112206 | 0.050165 | 0.089566 | C | 0.547404 | 1.372222 | 0.011196 |
| C | 1.504970 | -1.155968 | 0.050236 | C | 1.615604 | 0.824825 | -0.651759 |
| C | 0.025386 | -1.284888 | -0.153578 | C | 1.835170 | -0.560406 | -0.360512 |
| C | -0.760437 | 0.012350 | -0.041227 | C | 1.387680 | -1.029176 | 0.851482 |
| C | -0.010564 | 1.281124 | -0.116591 | C | -1.402549 | -0.298944 | -0.090892 |
| H | 3.195913 | 0.120646 | 0.207359 | C | -0.339265 | 0.473674 | 0.731865 |
| H | 2.085414 | -2.079303 | 0.124096 | H | 2.222518 | 1.390703 | -1.362279 |
| H | -0.162045 | -1.693339 | -1.166835 | H | 2.211297 | -1.242170 | -1.129425 |
| O | -1.864247 | 0.020417 | 0.859091 | H | 1.217506 | -2.092533 | 1.032614 |
| O | -2.043076 | -0.003789 | -0.638194 | O | -1.385154 | -1.383099 | -0.634105 |
| H | -0.603287 | 2.195275 | -0.182669 | O | -2.192936 | 0.696264 | 0.012760 |
| H | 1.882268 | 2.232735 | -0.050345 | H | -0.645993 | 0.693826 | 1.758387 |
| H | -0.421807 | -2.018609 | 0.538195 | H | 0.321968 | 2.442836 | -0.015826 |
| 14 | | | | H | 1.433163 | -0.391157 | 1.739011 |
| **I4g** | | | | 14 | | | |
| C | -0.298212 | -1.476456 | 0.100763 | **T5-6g** | | | |
| C | -1.495779 | -1.059334 | -0.370252 | C | 0.975290 | 0.433026 | 0.632829 |
| C | -2.035185 | 0.299943 | -0.385070 | C | 0.382322 | -0.972003 | 0.538307 |
| C | -1.855247 | 1.233748 | 0.565918 | C | -1.069477 | -1.161772 | 0.340599 |
| C | 1.397343 | 0.496980 | -0.052155 | C | -1.799150 | -0.072690 | -0.128191 |
| C | 0.774590 | -0.628420 | 0.653128 | C | -1.235780 | 1.232141 | -0.241983 |
| H | -2.146126 | -1.829893 | -0.801364 | C | 0.043703 | 1.510690 | 0.191100 |
| H | -2.677864 | 0.539526 | -1.240435 | H | 1.486510 | 0.664324 | 1.587777 |

| | | | |
|---|---|---|---|
| H | -2.288537 | 2.230684 | 0.468447 |
| O | 1.453345 | 1.643680 | -0.393511 |
| O | 2.109290 | -0.624754 | -0.202533 |
| H | 1.039970 | -0.773366 | 1.707756 |
| H | -0.071512 | -2.548849 | 0.085855 |
| H | -1.282073 | 1.031726 | 1.474099 |
| 14 | | | |
| **I5g** | | | |
| C | -1.621388 | 0.892070 | -0.259356 |
| C | -0.464494 | 1.481904 | 0.110371 |
| C | 0.691009 | 0.672201 | 0.617364 |
| C | 0.528586 | -0.849246 | 0.506047 |
| C | -0.829821 | -1.394094 | 0.205584 |
| C | -1.820010 | -0.556997 | -0.172382 |
| H | -0.341218 | 2.567257 | 0.066336 |
| H | -2.455132 | 1.502123 | -0.617250 |
| H | -2.811561 | -0.952473 | -0.409048 |
| O | 1.800058 | 0.600740 | -0.344735 |
| O | 1.398522 | -0.823060 | -0.687131 |
| H | 1.071596 | 1.064506 | 1.576087 |
| H | 1.036026 | -1.406236 | 1.312407 |
| H | -0.991637 | -2.471655 | 0.280626 |
| 14 | | | |
| **I6g** | | | |
| C | 0.753261 | -0.982232 | 0.496577 |
| C | -0.753620 | -0.982112 | 0.496489 |
| C | -1.471629 | 0.298197 | 0.235150 |
| C | -0.675123 | 1.519264 | -0.004920 |
| C | 0.675894 | 1.518948 | -0.005242 |
| C | 1.471737 | 0.297659 | 0.235311 |
| H | 1.225257 | -1.722673 | 1.155182 |
| H | -2.474556 | 0.436848 | 0.655159 |
| H | -1.220414 | 2.455058 | -0.157312 |
| H | 1.221577 | 2.454444 | -0.158051 |
| H | 2.474948 | 0.435641 | 0.654847 |
| H | -1.226007 | -1.722362 | 1.155016 |
| O | -1.412887 | -0.771940 | -0.751553 |
| O | 1.412396 | -0.772472 | -0.751577 |
| H | -1.534185 | -2.136014 | 0.500557 |
| H | -2.856349 | -0.205397 | -0.376566 |
| H | -1.859965 | 2.033282 | -0.645945 |
| H | 0.445782 | 2.525085 | 0.129161 |
| H | 0.866793 | -1.683755 | 1.229384 |
| O | 0.593630 | -1.233012 | -0.831905 |
| O | 1.865116 | 0.356277 | -0.470637 |
| 14 | | | |
| **T6-7g** | | | |
| C | -0.746503 | -1.017174 | -0.537623 |
| C | 0.724460 | -0.943290 | -0.770817 |
| C | 1.382873 | 0.332242 | -0.342675 |
| C | 0.564514 | 1.514477 | 0.010958 |
| C | -0.785938 | 1.470437 | 0.039583 |
| C | -1.529899 | 0.214752 | -0.154506 |
| H | -1.257698 | -1.789080 | -1.127004 |
| H | 2.339857 | 0.589823 | -0.815960 |
| H | 1.084825 | 2.467198 | 0.139752 |
| H | -1.362993 | 2.384257 | 0.206403 |
| H | -2.579279 | 0.284284 | -0.463398 |
| H | 1.754763 | -1.492930 | 0.130509 |
| O | 1.575223 | -0.627607 | 0.773233 |
| O | -1.279787 | -0.856419 | 0.784289 |
| 14 | | | |
| **T6-9g** | | | |
| C | 0.285499 | -1.142553 | 0.484620 |
| C | -1.050087 | -0.438850 | 0.600710 |
| C | -1.137627 | 1.047893 | 0.350690 |
| C | 0.072978 | 1.692084 | -0.108833 |
| C | 1.312684 | 1.122604 | -0.021802 |
| C | 1.501519 | -0.316468 | 0.230335 |
| H | 0.410665 | -2.052390 | 1.086202 |
| H | -2.260081 | 0.530979 | -0.438176 |
| H | -0.003463 | 2.744366 | -0.401950 |
| H | 2.211220 | 1.728683 | -0.183851 |
| H | 2.474397 | -0.653822 | 0.601854 |
| H | -1.612879 | -0.812203 | 1.471670 |
| O | -1.813909 | -0.474989 | -0.631188 |

| | | | |
|---|---|---|---|
| 14 | | | |
| **I7g** | | | |
| C | -0.688073 | -1.040554 | -0.553100 |
| C | 0.772447 | -0.896766 | -0.837856 |
| C | 1.334276 | 0.402300 | -0.355568 |
| C | 0.485855 | 1.546037 | 0.032448 |
| C | -0.863874 | 1.436873 | 0.051349 |
| C | -1.538385 | 0.143344 | -0.137698 |
| H | -1.190059 | -1.826971 | -1.130825 |
| H | 2.305454 | 0.709522 | -0.766122 |
| H | 0.962199 | 2.523436 | 0.149820 |
| H | -1.487343 | 2.322079 | 0.206540 |
| H | -2.596589 | 0.155850 | -0.422959 |
| O | 1.533289 | -0.624755 | 0.748757 |
| O | -1.202305 | -0.914899 | 0.783768 |
| H | 2.345000 | -1.114079 | 0.505894 |
| 14 | | | |
| **I8g** | | | |
| C | -1.766291 | -0.531809 | 0.251103 |
| C | -1.261432 | 0.839168 | 0.363369 |
| C | 0.236048 | 1.050183 | 0.249787 |
| C | 1.070866 | -0.146969 | 0.036121 |
| C | 0.505412 | -1.362394 | -0.211846 |
| C | -0.920461 | -1.543337 | -0.095397 |
| H | -2.819187 | -0.721713 | 0.467910 |
| H | -1.837201 | 1.565294 | 0.948413 |
| H | 1.151221 | -2.220686 | -0.406094 |
| H | -1.314764 | -2.554396 | -0.227118 |
| O | 2.431185 | -0.025540 | 0.160369 |
| H | 2.672286 | 0.914678 | 0.105347 |
| H | 0.700447 | 1.894364 | 0.782465 |
| O | -0.648392 | 1.437217 | -0.814087 |
| 14 | | | |
| **I9g** | | | |
| C | -1.227093 | 1.117048 | -0.029375 |
| C | -1.169203 | -0.352432 | -0.190020 |
| C | 0.067237 | -1.121190 | 0.017128 |
| C | 1.230325 | -0.296381 | -0.013375 |
| O | 0.922703 | -1.184244 | -0.787571 |
| 14 | | | |
| **T7-8g** | | | |
| C | 0.714899 | -0.901058 | 0.653589 |
| C | -0.769852 | -0.891238 | 0.682222 |
| C | -1.408286 | 0.444831 | 0.439151 |
| C | -0.684510 | 1.532986 | -0.110738 |
| C | 0.700239 | 1.501410 | -0.177290 |
| C | 1.483399 | 0.318340 | 0.120701 |
| H | 1.232477 | -1.467235 | 1.439708 |
| H | -2.437575 | 0.624790 | 0.770760 |
| H | -1.208742 | 2.479073 | -0.273789 |
| H | 1.244626 | 2.432819 | -0.358148 |
| H | 2.521664 | 0.477351 | 0.432447 |
| H | -2.155015 | -1.356067 | -0.637976 |
| O | -1.267323 | -0.970288 | -0.757333 |
| O | 1.340727 | -0.932506 | -0.620017 |
| 14 | | | |
| **T8P2g** | | | |
| C | -1.635627 | 0.728385 | -0.250767 |
| C | -1.244821 | -0.687077 | -0.458452 |
| C | 0.236755 | -1.018673 | -0.471753 |
| C | 1.128113 | 0.037427 | -0.083119 |
| C | 0.690835 | 1.304604 | 0.233856 |
| C | -0.701383 | 1.646352 | 0.117049 |
| H | -2.672307 | 1.020871 | -0.431275 |
| H | -1.877741 | -1.232626 | -1.172514 |
| H | 1.410617 | 2.058135 | 0.565025 |
| H | -0.993590 | 2.683048 | 0.302132 |
| O | 2.468180 | -0.250684 | -0.053009 |
| H | 2.545089 | -1.200373 | -0.267098 |
| H | -0.190441 | -2.013414 | 0.387364 |
| O | -1.101288 | -1.422034 | 0.814944 |
| 14 | | | |
| **T9-10g** | | | |
| C | -0.549106 | -1.187695 | -0.408426 |
| C | 0.822793 | -0.668924 | -0.668314 |
| C | 1.193059 | 0.693857 | -0.462343 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 1.198760 | 1.088981 | 0.061704 | C | 0.211115 | 1.600107 | 0.077454 |
| C | -0.043500 | 1.797062 | 0.044078 | C | -1.119957 | 1.311018 | -0.064878 |
| H | -2.193545 | 1.606884 | -0.051321 | C | -1.559446 | -0.092954 | -0.181389 |
| H | -0.994064 | -0.448780 | -1.326170 | H | -0.832084 | -2.143754 | -0.873289 |
| H | 2.131331 | 1.638548 | 0.146489 | H | 0.532809 | 2.595955 | 0.398882 |
| H | -0.029553 | 2.879312 | 0.111751 | H | -1.893400 | 2.081579 | -0.008444 |
| O | 2.472861 | -0.916765 | 0.013545 | H | -2.589031 | -0.307237 | -0.485143 |
| H | 2.319733 | -1.885874 | 0.007813 | H | 1.447221 | -1.309170 | -1.309978 |
| H | -2.190666 | -1.936439 | 0.324430 | O | 1.903185 | -0.329249 | 0.635514 |
| O | -2.395661 | -0.989756 | 0.167226 | O | -1.086821 | -0.972261 | 0.893953 |
| | | | | H | 2.812836 | -0.437757 | 0.289613 |

**Table S8.** Theoretical predictions of detailed energies of reactants and intermediates in the interaction of the $C_6H_6$ with $MnO_x$ cluster by the method PBE-D3/6-311++g(d,p) (H, C, O)/LandL2DZ (Mn) with the BSSE correction. ZPE energies are reported unscaled.

| **Species** | **Single point energy (a.u)** | **ZPE (a.u)** | **BSSE energy (a.u)** |
|---|---|---|---|
| $C_6H_6$ | -231.9948881 | 0.097538 | |
| $MnO_2$ | -254.218000 | 0.005073 | |
| $Mn_2O_3$ | -433.349563 | 0.009255 | |
| A1 | -486.278115 | 0.104028 | 0.007956 |
| A2 | -486.243715 | 0.105238 | 0.009620 |
| A3 | -486.251774 | 0.104614 | 0.010966 |
| A4 | -486.237324 | 0.103756 | 0.008163 |
| A5 | -486.211873 | 0.102370 | 0.004337 |
| B1 | -665.42729533 | 0.107918 | 0.01254983 |
| B2 | -665.39773292 | 0.107916 | 0.00800227 |
| B3 | -665.37285880 | 0.107510 | 0.00951934 |

**Table S9.** Cartesian coordinates (Å) for the reactants, intermediates, transition states, and products in the interaction of the $C_6H_6$ with $MnO_x$ by the method PBE/6-311++g(d,p) (H, C, O)/ LandL2DZ (Mn).

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 5 | | | | 19 | | | |
| **$Mn_2O_3$** | | | | **I18** | | | |
| O | -2.166650 | 0.705772 | -0.615093 | C | 0.189229 | 1.636393 | 0.737236 |
| O | 2.204739 | 0.581863 | 0.688760 | C | -0.647944 | 2.206160 | -0.330447 |
| O | -0.001173 | -1.260102 | -0.091572 | C | -1.883454 | 1.725617 | -0.607350 |
| Mn | -1.172886 | -0.037950 | 0.393786 | C | -2.461686 | 0.528661 | 0.104722 |
| Mn | 1.161074 | 0.029140 | -0.388056 | C | -1.738892 | 0.235072 | 1.399365 |
| 3 | | | | C | -0.495868 | 0.731895 | 1.666443 |
| **$MnO_2$** | | | | O | -2.315682 | -0.669578 | -0.730899 |
| Mn | 0.000000 | 0.000000 | 0.274393 | O | 2.856907 | 1.093889 | -0.569424 |

| | | | |
|---|---|---|---|
| O | 0.000000 | 1.435438 | -0.428739 |
| O | 0.000000 | -1.435438 | -0.428739 |
| 15 | | | |
| **A1** | | | |
| C | 1.045649 | 2.149277 | 0.713161 |
| C | 1.045649 | 0.964953 | 1.415872 |
| C | 1.018955 | -0.294685 | 0.726653 |
| C | 1.018955 | -0.294685 | -0.726653 |
| C | 1.045649 | 0.964953 | -1.415872 |
| C | 1.045649 | 2.149277 | -0.713161 |
| H | 1.077095 | 3.100052 | 1.249623 |
| H | 1.100737 | 0.967426 | 2.506544 |
| H | 1.315744 | -1.198310 | 1.268389 |
| H | 1.100737 | 0.967426 | -2.506544 |
| H | 1.077095 | 3.100052 | -1.249623 |
| O | -0.938876 | -2.453924 | 0.000000 |
| O | -1.962607 | 0.240340 | 0.000000 |
| Mn | -0.843933 | -0.874568 | 0.000000 |
| H | 1.315744 | -1.198310 | -1.268389 |
| 15 | | | |
| **A2** | | | |
| C | 0.000000 | 1.462600 | -0.801232 |
| C | 1.253063 | 0.674121 | -1.138205 |
| C | 1.253063 | -0.674121 | -1.138205 |
| C | 0.000000 | -1.462600 | -0.801232 |
| C | -1.253063 | -0.674121 | -1.138205 |
| C | -1.253063 | 0.674121 | -1.138205 |
| H | 0.000000 | -2.439816 | -1.313435 |
| H | 2.181153 | -1.239954 | -1.262499 |
| H | 2.181153 | 1.239954 | -1.262499 |
| H | 0.000000 | 2.439816 | -1.313435 |
| H | -2.181153 | 1.239954 | -1.262499 |
| H | -2.181153 | -1.239954 | -1.262499 |
| Mn | 0.000000 | 0.000000 | 1.378018 |
| O | 0.000000 | -1.735551 | 0.634882 |
| O | 0.000000 | 1.735551 | 0.634882 |
| 15 | | | |
| **A3** | | | |
| O | 0.517389 | -0.366630 | -1.337228 |
| H | -2.478247 | 2.159491 | -1.414338 |
| H | 0.022650 | 0.440737 | 2.583408 |
| H | 0.918511 | 2.316729 | 1.200809 |
| H | -0.238272 | 3.036065 | -0.912016 |
| Mn | -0.650439 | -1.336381 | -0.405148 |
| Mn | 1.552879 | 0.334815 | -0.116876 |
| O | 1.646644 | -1.124484 | 0.942772 |
| O | 0.698520 | -2.123104 | 0.618423 |
| H | -3.547387 | 0.645820 | 0.266383 |
| H | -2.236777 | -0.423228 | 2.117381 |
| 19 | | | |
| **I19** | | | |
| C | 1.272001 | 1.342322 | 0.545331 |
| C | 0.840359 | 2.013608 | -0.685588 |
| C | -0.463107 | 2.292946 | -0.916105 |
| C | -1.538905 | 1.840639 | 0.024541 |
| C | -1.032248 | 1.497893 | 1.395506 |
| C | 0.275237 | 1.229457 | 1.617536 |
| O | -2.138981 | 0.632978 | -0.585317 |
| O | 2.693392 | -0.322090 | -1.205615 |
| O | 0.095526 | -1.193440 | -0.670418 |
| H | -0.776521 | 2.789932 | -1.837052 |
| H | 0.620323 | 0.911646 | 2.604248 |
| H | 2.296819 | 1.561877 | 0.873442 |
| H | 1.607664 | 2.284265 | -1.414826 |
| Mn | -1.589654 | -0.998947 | -0.335179 |
| Mn | 1.634743 | -0.595746 | -0.065393 |
| O | 2.094333 | -1.248838 | 1.295734 |
| O | -2.350949 | -1.987808 | 0.619808 |
| H | -2.373648 | 2.559833 | 0.069353 |
| H | -1.768448 | 1.412142 | 2.198293 |
| 19 | | | |
| **I20** | | | |
| C | 0.715900 | 1.168818 | 0.497758 |
| C | 0.352041 | 2.031752 | -0.598214 |
| C | -0.969263 | 2.284243 | -0.794480 |
| C | -1.991202 | 1.579022 | 0.055145 |

| | | | |
|---|---|---|---|
| C | -0.921353 | 0.131386 | -1.409942 |
| C | -1.097241 | -1.155625 | -0.807533 |
| C | -1.112505 | -1.284797 | 0.585863 |
| C | -0.921000 | -0.131859 | 1.410004 |
| C | -1.097884 | 1.155023 | 0.807631 |
| C | -1.113407 | 1.284201 | -0.585729 |
| H | -0.852013 | 0.228743 | -2.492274 |
| H | -1.035057 | -2.049461 | -1.428707 |
| H | -1.053347 | -2.278024 | 1.031643 |
| H | -1.036120 | 2.048894 | 1.428795 |
| H | -1.054969 | 2.277486 | -1.031477 |
| O | 1.618346 | -1.332501 | -0.002183 |
| O | 1.617448 | 1.333469 | 0.002056 |
| Mn | 0.703078 | 0.000152 | -0.000042 |
| H | -0.851458 | -0.229151 | 2.492329 |
| 15 | | | |
| **A4** | | | |
| C | -0.566254 | 1.156081 | 0.551548 |
| C | -1.716953 | 1.186624 | -0.398505 |
| C | -2.402951 | 0.067163 | -0.732707 |
| C | -2.081795 | -1.231460 | -0.170600 |
| C | -1.059762 | -1.370016 | 0.719524 |
| C | -0.236363 | -0.234856 | 1.106679 |
| H | -0.663141 | 1.911390 | 1.351014 |
| H | -1.975882 | 2.159255 | -0.823723 |
| H | -0.828659 | -2.345347 | 1.154365 |
| H | 0.156323 | -0.250338 | 2.136092 |
| O | 1.891955 | -1.112076 | -1.044572 |
| O | 0.700930 | 1.556128 | -0.167631 |
| Mn | 1.474483 | -0.020228 | 0.053158 |
| H | -2.675442 | -2.099227 | -0.464721 |
| H | -3.233881 | 0.136338 | -1.439981 |
| 15 | | | |
| **A5** | | | |
| C | -0.666755 | -0.501334 | 0.823748 |
| C | -0.803022 | 0.981841 | 0.634043 |
| C | -1.869569 | 1.533239 | -0.029473 |
| C | -2.911532 | 0.719303 | -0.549910 |
| C | -1.482965 | 1.274826 | 1.442259 |
| C | -0.155223 | 1.060065 | 1.648771 |
| O | -2.270600 | 0.314354 | -0.640794 |
| O | 2.887586 | 0.454324 | -1.068158 |
| O | 0.473809 | -1.264018 | -0.706772 |
| H | -1.318610 | 2.849251 | -1.662393 |
| H | 0.238046 | 0.678283 | 2.593784 |
| H | 1.124550 | 2.349127 | -1.303323 |
| Mn | -1.266990 | -1.148753 | -0.405120 |
| Mn | 1.721027 | -0.263500 | 0.051867 |
| O | 2.277908 | -0.881963 | 1.389554 |
| O | -1.928521 | -2.368213 | 0.390129 |
| H | -2.950698 | 2.118441 | 0.085169 |
| H | -2.215585 | 1.091749 | 2.232495 |
| H | 3.434197 | -0.208760 | -1.533519 |
| 19 | | | |
| **I21** | | | |
| C | 2.051880 | 0.021185 | -0.031186 |
| C | 1.763483 | 1.015474 | -1.064034 |
| C | 0.904127 | 2.044666 | -0.843768 |
| C | 0.108563 | 2.148419 | 0.415907 |
| C | 0.662435 | 1.326070 | 1.528895 |
| C | 1.569879 | 0.318672 | 1.308491 |
| O | -1.271514 | 1.676299 | 0.075903 |
| O | -0.928463 | -0.830355 | -1.404423 |
| H | 0.685066 | 2.761385 | -1.638087 |
| H | 1.943443 | -0.297706 | 2.129061 |
| H | 2.259167 | 0.906435 | -2.034213 |
| Mn | -1.832272 | 0.052680 | -0.211052 |
| Mn | 0.297118 | -1.058805 | -0.124796 |
| O | 0.352467 | -2.400347 | 0.716197 |
| O | -2.933405 | -0.619378 | 0.682912 |
| H | -0.058832 | 3.193216 | 0.723168 |
| H | 0.262543 | 1.490068 | 2.531457 |
| O | 3.219175 | -0.728056 | -0.092866 |
| H | 3.419185 | -0.932496 | -1.022777 |
| 19 | | | |
| **I22** | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.861784 | -0.687716 | -0.385793 | C | 2.548923 | 0.303089 | -0.262986 |
| C | -1.817973 | -1.288772 | 0.274939 | C | 2.088008 | 1.657359 | -0.639557 |
| H | -0.551844 | -0.722243 | 1.908390 | C | 1.047241 | 2.259859 | -0.032075 |
| H | 0.004354 | 1.602012 | 1.034497 | C | 0.191201 | 1.618352 | 1.028848 |
| H | -1.921445 | 2.617396 | -0.161317 | C | 0.558261 | 0.176135 | 1.331674 |
| H | -3.670822 | -1.302067 | -0.790309 | C | 1.721816 | -0.425709 | 0.744412 |
| H | -1.767610 | -2.373769 | 0.389937 | O | -1.186854 | 1.743612 | 0.596209 |
| O | 2.744422 | 1.052878 | 0.295970 | O | 3.578944 | -0.190918 | -0.724233 |
| O | 0.543638 | -1.005652 | 0.198181 | O | -0.762063 | -0.469118 | -1.411868 |
| Mn | 2.037427 | -0.236663 | -0.394429 | H | 0.741994 | 3.271920 | -0.315762 |
| H | -3.748975 | 1.178077 | -1.079010 | H | 0.265547 | 2.213834 | 1.961062 |
| 17 | | | | H | 2.261097 | -1.223563 | 1.264309 |
| **B1** | | | | H | 2.671665 | 2.162645 | -1.413305 |
| C | 1.399288 | 0.280115 | 1.445816 | H | 0.201787 | -0.198374 | 2.299570 |
| C | 2.092640 | -0.748077 | 0.686465 | Mn | -1.855766 | 0.372879 | -0.317686 |
| C | 2.092640 | -0.748077 | -0.686465 | Mn | 0.036326 | -1.206207 | -0.051982 |
| C | 1.399288 | 0.280115 | -1.445816 | H | 1.149176 | -3.272300 | 0.795007 |
| C | 0.649578 | 1.291929 | -0.732762 | O | -3.301597 | -0.196003 | 0.001537 |
| C | 0.649578 | 1.291929 | 0.732762 | O | 0.329322 | -2.844506 | 0.491970 |
| O | -1.256880 | 0.322709 | -2.763531 | 19 | | | |
| O | -1.256880 | 0.322709 | 2.763531 | **I23** | | | |
| O | -1.333493 | -0.887395 | 0.000000 | C | -2.733927 | 0.223775 | 0.389189 |
| H | 1.691752 | 0.456414 | -2.484537 | C | -1.552467 | -0.309263 | 1.158486 |
| H | 2.645582 | -1.515882 | -1.231769 | C | -0.310550 | 0.384084 | 1.056928 |
| H | 2.645582 | -1.515882 | 1.231769 | C | -0.118560 | 1.647240 | 0.248068 |
| H | 1.691752 | 0.456414 | 2.484537 | C | -1.280627 | 1.962418 | -0.651735 |
| H | 0.380150 | 2.218606 | 1.244966 | C | -2.465698 | 1.326934 | -0.567886 |
| H | 0.380150 | 2.218606 | -1.244966 | O | 1.097595 | 1.542752 | -0.518973 |
| Mn | -0.567100 | -0.205401 | -1.434004 | O | 1.458181 | -1.463687 | -0.082845 |
| Mn | -0.567100 | -0.205401 | 1.434004 | H | 0.417869 | 0.237984 | 1.868644 |
| 17 | | | | H | -3.311775 | 1.613994 | -1.196889 |
| **B2** | | | | H | -1.814149 | -0.898579 | 2.039470 |
| C | -1.727487 | -1.645359 | 0.421579 | Mn | 2.181317 | 0.170880 | -0.111683 |
| C | -0.880098 | -1.026279 | -0.552413 | Mn | -0.280446 | -1.292277 | -0.140175 |
| C | -1.360975 | 0.152148 | -1.235824 | O | -0.931252 | -1.193056 | -1.547725 |
| C | -2.668249 | 0.656677 | -0.930018 | O | 3.492913 | 0.422470 | 0.762791 |
| C | -3.447556 | 0.035898 | 0.023522 | H | 0.011387 | 2.498456 | 0.951574 |
| C | -2.972520 | -1.121763 | 0.704380 | H | -1.120653 | 2.772883 | -1.368560 |

| | | | |
|---|---|---|---|
| H | -1.385638 | -2.559900 | 0.910671 |
| H | -3.045995 | 1.519755 | -1.482106 |
| H | -4.446046 | 0.418748 | 0.245111 |
| H | -3.614890 | -1.613161 | 1.438545 |
| H | -0.872817 | 0.478900 | -2.161901 |
| H | -0.031250 | -1.593419 | -0.945154 |
| Mn | 0.109514 | 0.751550 | 0.119521 |
| Mn | 2.362970 | -0.189913 | 0.219134 |
| O | 1.589883 | 1.182465 | -0.649638 |
| O | -0.429130 | 1.330731 | 1.469042 |
| O | 2.579977 | -1.638168 | -0.451764 |
| 17 | | | |
| **B3** | | | |
| C | -1.929328 | -1.118566 | 0.655258 |
| C | -1.220256 | 0.158791 | 1.111540 |
| C | -1.691553 | 1.440658 | 0.623589 |
| C | -2.787751 | 1.526879 | -0.195122 |
| C | -3.565304 | 0.350351 | -0.526977 |
| C | -3.208151 | -0.883153 | -0.092320 |
| O | 3.680612 | -0.771326 | -0.097025 |
| O | -0.951243 | -1.696638 | -0.299078 |
| O | 1.390103 | 0.969379 | -0.857444 |
| H | -3.807281 | -1.764238 | -0.334882 |
| H | -0.703308 | 0.131426 | 2.078666 |
| H | -4.470365 | 0.476726 | -1.126858 |
| H | -3.111844 | 2.500579 | -0.568903 |
| H | -1.156997 | 2.345323 | 0.924678 |
| Mn | 0.175021 | -0.279335 | -0.302461 |
| Mn | 2.575304 | 0.331225 | 0.227517 |
| H | -2.050046 | -1.848129 | 1.473454 |
| 17 | | | |
| **I1** | | | |
| C | 1.446100 | 1.399209 | 0.280124 |
| C | 0.686806 | 2.092662 | -0.748034 |
| C | -0.686124 | 2.092618 | -0.748121 |
| C | -1.445533 | 1.399368 | 0.280105 |
| C | -0.732541 | 0.649649 | 1.291953 |
| C | 0.732982 | 0.649508 | 1.291905 |
| O | -3.866041 | -0.200834 | 0.594206 |
| H | -0.944652 | -2.462085 | 0.544271 |
| 19 | | | |
| **I24** | | | |
| C | 2.421277 | -0.694824 | -0.446149 |
| C | 1.957221 | 0.222933 | 0.617840 |
| C | 0.764479 | -0.073521 | 1.389939 |
| C | 0.102657 | -1.421678 | 1.266414 |
| C | 0.511823 | -2.214334 | 0.058054 |
| C | 1.546828 | -1.867692 | -0.732325 |
| O | -1.373187 | -1.155456 | 1.204529 |
| O | -0.611825 | 0.960591 | -1.330101 |
| H | 0.666290 | 0.389454 | 2.377321 |
| H | 1.835333 | -2.477551 | -1.592150 |
| H | 2.718947 | 0.902352 | 1.012223 |
| Mn | -1.818940 | -0.014167 | -0.378240 |
| Mn | 0.400698 | 1.350077 | 0.006509 |
| O | 0.334386 | 2.765014 | 0.693630 |
| O | -3.314880 | -0.629135 | -0.605402 |
| H | 0.234756 | -2.016912 | 2.190081 |
| H | -0.058525 | -3.128765 | -0.144627 |
| O | 3.482833 | -0.540436 | -1.052519 |
| H | -1.905072 | -1.976250 | 1.246693 |
| 17 | | | |
| **I25** | | | |
| C | 2.115595 | -1.376973 | -0.270666 |
| C | 1.890559 | -0.131273 | 0.532668 |
| C | 0.666647 | 0.065637 | 1.260724 |
| C | -0.460274 | -0.850194 | 0.961355 |
| C | -0.177499 | -2.129105 | 0.315887 |
| C | 1.022165 | -2.369147 | -0.275844 |
| O | -1.651674 | -0.598457 | 1.536472 |
| O | -0.869666 | 1.327485 | -0.892139 |
| H | 0.618176 | 0.610812 | 2.209795 |
| H | 1.221719 | -3.302483 | -0.806502 |
| H | 2.812505 | 0.345280 | 0.880283 |
| Mn | -1.891625 | 0.093299 | -0.142360 |
| Mn | 0.761208 | 1.398049 | -0.241821 |

| | | | |
|---|---|---|---|
| O | -2.763938 | -1.256358 | 0.322632 |
| O | 2.763124 | -1.257402 | 0.322787 |
| O | -0.000164 | -1.333493 | -0.887395 |
| H | -2.484232 | 1.691949 | 0.456340 |
| H | -1.231398 | 2.645483 | -1.516002 |
| H | 1.232141 | 2.645680 | -1.515763 |
| H | 2.484842 | 1.691555 | 0.456487 |
| H | 1.245199 | 0.379926 | 2.218519 |
| H | -1.244733 | 0.380374 | 2.218693 |
| Mn | -1.434087 | -0.567040 | -0.205323 |
| Mn | 1.433922 | -0.567161 | -0.205479 |
| 17 | | | |
| **I2** | | | |
| C | 0.727483 | 1.723583 | 0.019021 |
| C | -0.366528 | 2.018863 | -0.914506 |
| C | -1.648031 | 1.630168 | -0.701185 |
| C | -2.067058 | 0.737546 | 0.436790 |
| C | -0.877285 | 0.274702 | 1.275137 |
| C | 0.434903 | 0.912490 | 1.173691 |
| O | -2.572066 | -0.539581 | -0.103306 |
| O | 3.078926 | -0.139137 | 0.329398 |
| O | 0.707256 | -1.382756 | -0.916744 |
| H | -2.435716 | 1.913138 | -1.404092 |
| H | -2.874775 | 1.191273 | 1.041935 |
| H | 1.049758 | 0.979724 | 2.076204 |
| H | 1.558755 | 2.433274 | 0.062965 |
| H | -0.126989 | 2.617770 | -1.797688 |
| H | -1.147273 | -0.153378 | 2.249386 |
| Mn | -0.902534 | -1.323526 | -0.026802 |
| Mn | 1.584230 | -0.127438 | -0.150685 |
| 17 | | | |
| **I3** | | | |
| C | -0.466071 | 0.953851 | 0.568767 |
| C | 0.702697 | 0.312376 | 1.159642 |
| C | 1.985482 | 0.733509 | 0.627395 |
| C | 2.081168 | 1.920793 | -0.171838 |
| C | 0.950625 | 2.626633 | -0.525048 |
| C | -0.337384 | 2.086177 | -0.213612 |
| O | 1.367049 | 2.747252 | 0.308884 |
| O | -2.748267 | -0.812495 | -1.118748 |
| H | -1.001939 | -2.845820 | 0.268882 |
| O | 3.185909 | -1.581930 | -0.846053 |
| 19 | | | |
| **T18-19** | | | |
| C | 0.255610 | 1.692784 | 0.548071 |
| C | -0.823249 | 2.114693 | -0.363606 |
| C | -2.044971 | 1.530732 | -0.349441 |
| C | -2.371242 | 0.360320 | 0.546236 |
| C | -1.388659 | 0.231314 | 1.685016 |
| C | -0.160334 | 0.815463 | 1.652886 |
| O | -2.280171 | -0.893764 | -0.218481 |
| O | 2.617042 | 1.411048 | -1.241374 |
| O | 0.425929 | -0.396725 | -1.504674 |
| H | -2.821845 | 1.858920 | -1.043971 |
| H | 0.558689 | 0.620066 | 2.452093 |
| H | 0.982810 | 2.470302 | 0.823521 |
| H | -0.608019 | 2.920747 | -1.069921 |
| Mn | -0.524786 | -1.340463 | -0.362263 |
| Mn | 1.556798 | 0.495492 | -0.522920 |
| O | 1.984023 | -0.803748 | 0.494064 |
| O | 0.883708 | -2.067859 | 0.398871 |
| H | -3.411467 | 0.411900 | 0.909979 |
| H | -1.672380 | -0.413824 | 2.521060 |
| 19 | | | |
| **T19-20** | | | |
| C | 0.857727 | 1.307781 | 0.373856 |
| C | 0.295820 | 2.018150 | -0.753600 |
| C | -1.044178 | 2.250692 | -0.800099 |
| C | -1.951790 | 1.590946 | 0.196633 |
| C | -1.281792 | 1.315059 | 1.514945 |
| C | 0.069914 | 1.137161 | 1.570159 |
| O | -2.336280 | 0.309643 | -0.435350 |
| O | 2.884783 | 0.635987 | -0.728786 |
| O | 0.393390 | -1.166064 | -0.969225 |
| H | -1.499802 | 2.751526 | -1.657672 |
| H | 0.559188 | 0.773570 | 2.477978 |

| | | | |
|---|---|---|---|
| O | 2.048170 | -2.182696 | 0.318370 |
| O | -3.531859 | 0.088765 | 0.285411 |
| O | -0.423084 | -1.195813 | -0.948603 |
| H | 3.070773 | 2.270366 | -0.475456 |
| H | 2.899144 | 0.341886 | 1.084507 |
| H | 0.615684 | -0.226986 | 2.109087 |
| H | -1.223595 | 2.543560 | -0.665594 |
| H | 1.025214 | 3.546866 | -1.108558 |
| Mn | -1.815796 | -0.350253 | -0.049873 |
| Mn | 1.149094 | -1.033046 | -0.263001 |
| H | -3.964600 | 0.624723 | 0.964598 |
| 17 | | | |
| **I4** | | | |
| C | -0.383183 | 2.138743 | -0.753320 |
| C | -1.600699 | 1.556035 | -0.975427 |
| C | -2.079725 | 0.420130 | -0.190514 |
| C | -1.282655 | 0.012142 | 0.947422 |
| C | 0.031618 | 0.605306 | 1.181298 |
| C | 0.503500 | 1.672141 | 0.305333 |
| O | -1.821448 | -0.685840 | 2.024700 |
| O | 2.867696 | -0.155055 | 0.839385 |
| O | 0.953281 | -1.059432 | -1.270824 |
| H | -3.155833 | 0.212915 | -0.185274 |
| H | -2.250892 | 1.939551 | -1.765291 |
| H | -0.068171 | 2.990375 | -1.359307 |
| H | 1.242807 | 2.377650 | 0.697867 |
| H | 0.415055 | 0.519247 | 2.202174 |
| Mn | -0.785516 | -1.180127 | -0.655711 |
| Mn | 1.564301 | -0.039840 | -0.036918 |
| H | -2.781975 | -0.764923 | 1.890724 |
| 17 | | | |
| **I5** | | | |
| C | 1.699795 | 1.277722 | 0.281319 |
| C | 0.981425 | 2.173224 | -0.606369 |
| C | -0.395297 | 2.189747 | -0.660233 |
| C | -1.102893 | 1.303040 | 0.207720 |
| C | -0.489461 | 0.619526 | 1.322040 |
| C | 0.973450 | 0.516428 | 1.288168 |
| H | 2.214766 | 1.380489 | 0.081595 |
| H | 0.954546 | 2.312093 | -1.573942 |
| Mn | -1.284373 | -1.124111 | -0.369273 |
| Mn | 1.720284 | -0.417656 | -0.097169 |
| O | 2.103711 | -1.108137 | 1.281656 |
| O | -1.793973 | -2.379383 | 0.477186 |
| H | -2.901783 | 2.132357 | 0.327924 |
| H | -1.911958 | 1.139068 | 2.389962 |
| 19 | | | |
| **T20-21** | | | |
| C | 0.810750 | 1.113584 | 0.177421 |
| C | 0.321183 | 1.836930 | -0.983126 |
| C | -0.986600 | 2.179622 | -0.973952 |
| C | -1.842555 | 1.694775 | 0.164688 |
| C | -1.082694 | 1.672536 | 1.471034 |
| C | 0.246161 | 1.397784 | 1.481243 |
| O | -2.254098 | 0.345489 | -0.207504 |
| O | 2.708191 | 1.020456 | -0.412718 |
| O | 0.334942 | -1.371111 | -1.126319 |
| H | -1.468504 | 2.626500 | -1.846218 |
| H | 0.804476 | 1.176818 | 2.392365 |
| H | 0.978294 | 1.975808 | -1.842186 |
| Mn | -1.232883 | -1.138093 | -0.305087 |
| Mn | 1.529501 | -0.543419 | -0.143979 |
| O | 1.920062 | -1.201142 | 1.228410 |
| O | -1.641281 | -2.303038 | 0.708103 |
| H | -2.774835 | 2.273459 | 0.259888 |
| H | -1.652152 | 1.707082 | 2.403055 |
| H | 3.357267 | 0.981527 | 0.316135 |
| 19 | | | |
| **T21-22** | | | |
| C | 1.726939 | 0.408660 | 0.131130 |
| C | 1.655876 | 1.318468 | -1.006785 |
| C | 0.720924 | 2.298754 | -0.991016 |
| C | -0.274344 | 2.348795 | 0.135040 |
| C | 0.292366 | 1.856858 | 1.435371 |
| C | 1.213372 | 0.864463 | 1.422064 |
| O | -1.394723 | 1.482147 | -0.277046 |

| | | | |
|---|---|---|---|
| O | -3.280067 | -0.831411 | 0.164486 |
| O | 2.585499 | -1.665260 | 0.244656 |
| O | -0.144578 | -1.055169 | -0.949925 |
| H | -0.920247 | 2.797611 | -1.400458 |
| H | 1.559610 | 2.819575 | -1.271652 |
| H | 2.772499 | 1.440739 | 0.421753 |
| H | 1.498048 | 0.185245 | 2.188671 |
| H | -0.993030 | 0.515141 | 2.289891 |
| Mn | -1.565135 | -0.415792 | -0.082279 |
| Mn | 1.438432 | -0.686757 | -0.272414 |
| H | -4.038245 | -0.258009 | -0.030480 |
| 17 | | | |
| **I6** | | | |
| C | 0.513233 | 1.717815 | 0.336934 |
| C | -0.432271 | 2.029795 | -0.700938 |
| C | -1.629895 | 1.342106 | -0.801412 |
| C | -1.992144 | 0.333819 | 0.140808 |
| C | -1.136114 | -0.013234 | 1.239160 |
| C | 0.195831 | 0.642436 | 1.261911 |
| O | -3.281959 | -0.172305 | 0.185524 |
| O | 3.031387 | 0.009735 | 0.486737 |
| O | 0.807633 | -0.905384 | -1.328229 |
| H | -2.325726 | 1.573789 | -1.614583 |
| H | 0.726147 | 0.603143 | 2.217128 |
| H | -0.200041 | 2.819754 | -1.417275 |
| H | -1.585825 | -0.367561 | 2.172321 |
| Mn | -0.457758 | -1.447900 | -0.051509 |
| Mn | 1.591754 | 0.043730 | -0.150109 |
| H | 1.264373 | 2.467440 | 0.603871 |
| H | -3.797179 | 0.234882 | -0.532028 |
| 17 | | | |
| **I7** | | | |
| C | 2.327790 | -0.237445 | 0.503870 |
| C | 2.389970 | 0.823439 | -0.502104 |
| C | 1.441017 | 1.789418 | -0.626441 |
| C | 0.202370 | 1.833997 | 0.221941 |
| C | 0.063737 | 0.645294 | 1.170324 |
| C | 1.202916 | -0.259191 | 1.396302 |
| O | -0.922120 | -1.304471 | -1.224133 |
| H | 0.593285 | 2.980314 | -1.833960 |
| H | 1.555787 | 0.359539 | 2.327605 |
| H | 2.337589 | 1.153028 | -1.844338 |
| Mn | -1.749316 | -0.222372 | -0.160480 |
| Mn | 0.641405 | -1.218763 | -0.357349 |
| O | 1.053670 | -2.142861 | 0.993009 |
| O | -2.623166 | -0.780623 | 1.013371 |
| H | -0.723819 | 3.348338 | 0.238207 |
| H | -0.141013 | 2.219025 | 2.369038 |
| O | 2.613628 | -0.651588 | 0.015881 |
| H | 2.246824 | -1.428685 | 0.765683 |
| 19 | | | |
| **T22-23** | | | |
| C | 2.387057 | -0.971091 | -0.349129 |
| C | 1.861279 | -0.330791 | 0.908171 |
| C | 0.665657 | -0.741398 | 1.462372 |
| C | -0.220970 | -1.760563 | 0.795375 |
| C | 0.224022 | -2.140399 | -0.591333 |
| C | 1.416219 | -1.782462 | -1.113056 |
| O | -1.594589 | -1.358541 | 0.817252 |
| O | -1.073687 | 1.326353 | 0.219630 |
| H | 0.356133 | -0.401913 | 2.455771 |
| H | 1.733429 | -2.108153 | -2.106724 |
| H | 2.589751 | 0.246763 | 1.490897 |
| Mn | -2.186091 | 0.075393 | -0.046093 |
| Mn | 0.714471 | 1.404736 | 0.145245 |
| O | 1.485624 | 2.644591 | -0.619608 |
| O | -3.196199 | 0.018213 | -1.246379 |
| H | -0.175394 | -2.676814 | 1.428258 |
| H | -0.480417 | -2.759824 | -1.154628 |
| O | 3.560361 | -0.835883 | -0.683438 |
| H | 1.315328 | 2.699062 | 0.833563 |
| 19 | | | |
| **T23-24** | | | |
| C | 2.171743 | -0.951372 | -0.558875 |
| C | 2.026975 | 0.196593 | 0.377929 |
| C | 1.066195 | 0.150283 | 1.446053 |

| | | | |
|---|---|---|---|
| O | -0.972397 | 1.660220 | -0.636704 |
| O | -0.827692 | -1.214296 | -1.138648 |
| H | 1.537908 | 2.567449 | -1.387394 |
| H | 0.092796 | 2.807408 | 0.737658 |
| H | 1.251833 | -0.809575 | 2.341544 |
| H | 3.250626 | -0.749633 | 0.785603 |
| H | 3.252248 | 0.833026 | -1.175600 |
| H | -0.563884 | 0.830176 | 2.048132 |
| Mn | -1.479101 | 0.025554 | -0.144022 |
| Mn | 0.737900 | -1.423607 | -0.203139 |
| O | -2.707200 | -0.208500 | 0.818566 |
| 17 | | | |
| **T1-2** | | | |
| C | 0.813295 | 1.717534 | 0.030456 |
| C | -0.253813 | 2.090156 | -0.874847 |
| C | -1.564720 | 1.732964 | -0.674571 |
| C | -1.963294 | 0.924916 | 0.457548 |
| C | -0.917273 | 0.437161 | 1.343703 |
| C | 0.475872 | 0.873575 | 1.161461 |
| O | -2.593383 | -0.823693 | -0.250962 |
| O | 3.023353 | -0.363238 | 0.370785 |
| O | 0.589052 | -1.302733 | -1.003689 |
| H | -2.340092 | 2.083502 | -1.356981 |
| H | 1.109897 | 0.878373 | 2.052759 |
| H | 1.697477 | 2.360742 | 0.070779 |
| H | -0.004880 | 2.733107 | -1.723473 |
| H | -1.222515 | 0.092821 | 2.337784 |
| Mn | -0.939156 | -1.192030 | 0.042920 |
| Mn | 1.570799 | -0.175628 | -0.203643 |
| H | -2.975071 | 1.024682 | 0.847337 |
| 17 | | | |
| **T1-3** | | | |
| C | -0.576450 | 1.152906 | 0.685418 |
| C | 0.533180 | 0.375136 | 1.234554 |
| C | 1.847272 | 0.611758 | 0.675506 |
| C | 2.050784 | 1.728949 | -0.200913 |
| C | 1.000959 | 2.540842 | -0.588801 |
| C | -0.325868 | 2.174507 | -0.227709 |
| C | 0.123995 | -1.031085 | 1.628363 |
| C | 0.268309 | -2.098727 | 0.578108 |
| C | 1.173900 | -2.046069 | -0.421829 |
| O | -1.241975 | -0.462285 | 1.566963 |
| O | -0.631025 | 0.705836 | -1.340325 |
| H | 1.236958 | 0.756924 | 2.341659 |
| H | 1.238992 | -2.839402 | -1.170890 |
| H | 2.899438 | 0.854117 | 0.442621 |
| Mn | -1.811136 | -0.098857 | -0.266916 |
| Mn | 0.408899 | 1.308781 | -0.097791 |
| O | 0.525548 | 2.837833 | 0.205000 |
| O | -3.025912 | -0.888898 | -0.955123 |
| H | 0.194800 | -1.464006 | 2.640437 |
| H | -0.426752 | -2.941404 | 0.657884 |
| O | 3.083360 | -1.017341 | -1.382205 |
| H | -0.754192 | 0.666772 | 1.152963 |
| 19 | | | |
| **T24-25** | | | |
| C | 2.684257 | -0.370613 | -0.285068 |
| C | 1.946333 | 0.403389 | 0.745696 |
| C | 0.762579 | -0.128771 | 1.375444 |
| C | 0.209999 | -1.397113 | 0.900244 |
| C | 0.848304 | -2.048729 | -0.236102 |
| C | 2.009916 | -1.587373 | -0.779963 |
| O | -1.240808 | -1.502596 | 0.960059 |
| O | -0.760897 | 0.713572 | -1.345619 |
| H | 0.423346 | 0.232551 | 2.351635 |
| H | 2.494296 | -2.109307 | -1.608701 |
| H | 2.521743 | 1.193265 | 1.236091 |
| Mn | -1.867199 | -0.275188 | -0.356514 |
| Mn | 0.236421 | 1.236051 | -0.020956 |
| O | -0.010932 | 2.650093 | 0.598158 |
| O | -3.463056 | -0.174109 | -0.298474 |
| H | 0.244985 | -2.375488 | 1.971054 |
| H | 0.355560 | -2.944225 | -0.625477 |
| O | 3.796250 | -0.028327 | -0.699357 |
| H | -0.754964 | -2.361156 | 1.905628 |
| 19 | | | |

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|---|---|---|---|
| O | 1.525078 | -2.347542 | 0.467918 |
| O | -2.942026 | 0.293624 | 0.683449 |
| O | -0.252099 | -0.964630 | -1.414526 |
| H | 3.064659 | 1.943007 | -0.548875 |
| H | 2.723938 | 0.154613 | 1.143765 |
| H | 0.400808 | -0.128747 | 2.197205 |
| H | -1.910862 | 0.989312 | 1.050844 |
| H | -1.172176 | 2.689699 | -0.693173 |
| H | 1.174912 | 3.405098 | -1.232511 |
| Mn | -1.617631 | -0.391477 | -0.201376 |
| Mn | 0.893304 | -1.064891 | -0.169837 |
| 17 | | | |
| **T1-5** | | | |
| C | -1.704410 | 1.397357 | -0.101330 |
| C | -1.272172 | 0.917779 | 1.187030 |
| C | 0.131912 | 0.710526 | 1.380084 |
| C | 1.085696 | 1.206645 | 0.452565 |
| C | 0.607165 | 1.960980 | -0.682119 |
| C | -0.736551 | 2.053336 | -0.958122 |
| O | 3.136448 | -0.207906 | 0.486847 |
| O | -2.550944 | -1.489073 | 0.283421 |
| O | 0.009231 | -1.226576 | -1.062931 |
| H | 0.466761 | 0.202252 | 2.290119 |
| H | 2.453577 | 0.810869 | 0.667802 |
| H | -1.095044 | 2.608368 | -1.828446 |
| H | -2.765702 | 1.586062 | -0.274105 |
| H | -1.984617 | 0.728936 | 1.993989 |
| H | 1.337432 | 2.445398 | -1.335870 |
| Mn | 1.601103 | -0.707780 | -0.174733 |
| Mn | -1.274708 | -0.671148 | -0.098900 |
| 17 | | | |
| **T2-7** | | | |
| C | -1.152839 | 1.952183 | 0.273834 |
| C | -2.063727 | 1.229029 | -0.584849 |
| C | -2.340568 | -0.098491 | -0.433196 |
| C | -1.652899 | -0.968388 | 0.582846 |
| C | -0.514334 | -0.218255 | 1.253478 |
| C | -0.438694 | 1.235303 | 1.250005 |

| | | | |
|---|---|---|---|
| **I26** | | | |
| C | 1.670650 | 1.832594 | -1.009892 |
| C | 0.349496 | 2.162410 | -1.175980 |
| C | -0.644409 | 1.778990 | -0.206333 |
| C | -0.242844 | 1.165455 | 1.003074 |
| C | 1.130758 | 0.756160 | 1.187403 |
| C | 2.096714 | 1.068639 | 0.139017 |
| O | -1.080737 | 0.934267 | 2.033828 |
| O | 2.474538 | -1.937149 | 0.638896 |
| O | 0.225759 | -1.240146 | -1.135201 |
| H | -1.655258 | 2.192228 | -0.271060 |
| H | 0.026696 | 2.733340 | -2.048398 |
| H | 2.418341 | 2.152417 | -1.737268 |
| H | 3.162159 | 1.037630 | 0.384293 |
| H | 1.444159 | 0.513336 | 2.206404 |
| Mn | -1.330845 | -0.458566 | -0.572726 |
| Mn | 1.475688 | -0.884780 | 0.004857 |
| H | -2.008784 | 0.858943 | 1.681000 |
| O | -2.776853 | -1.366138 | 0.078733 |
| O | -2.989029 | 0.047949 | 0.178495 |
| 19 | | | |
| **I27** | | | |
| C | 1.866861 | 1.765316 | -0.830950 |
| C | 0.571244 | 2.127322 | -1.113182 |
| C | -0.528782 | 1.716366 | -0.280134 |
| C | -0.269541 | 1.153390 | 1.057485 |
| C | 1.105284 | 0.667241 | 1.285619 |
| C | 2.158419 | 0.977439 | 0.341016 |
| O | -1.178711 | 1.003231 | 1.923169 |
| O | 2.150989 | -2.107410 | 0.680402 |
| O | 0.234013 | -1.113069 | -1.296678 |
| H | -1.485786 | 2.243399 | -0.386241 |
| H | 0.354530 | 2.727367 | -2.000352 |
| H | 2.686471 | 2.068667 | -1.483738 |
| H | 3.199533 | 0.859839 | 0.655685 |
| H | 1.341734 | 0.354312 | 2.306498 |
| Mn | -1.273648 | -0.322143 | -0.709932 |
| Mn | 1.360862 | -0.916379 | 0.013184 |

| | | | |
|---|---|---|---|
| O | -0.908544 | -2.078915 | -0.068022 |
| O | 2.092513 | -0.753201 | 0.475464 |
| O | 0.732066 | -0.037612 | -1.560719 |
| H | -3.093177 | -0.576748 | -1.064613 |
| H | -2.358929 | -1.448190 | 1.288432 |
| H | 0.029855 | 1.742638 | 2.103580 |
| H | -1.157667 | 3.043640 | 0.275421 |
| H | -2.592621 | 1.791344 | -1.359142 |
| H | -0.065146 | -0.729154 | 2.110325 |
| Mn | 0.622198 | -1.203592 | -0.324394 |
| Mn | 1.293417 | 1.073013 | -0.051538 |
| 17 | | | |
| **T3-4** | | | |
| C | -2.137269 | 1.689956 | -0.211826 |
| C | -2.705091 | 0.525836 | -0.701012 |
| C | -2.107034 | -0.745511 | -0.453644 |
| C | -0.963991 | -0.787243 | 0.331490 |
| C | -0.452953 | 0.358702 | 1.068981 |
| C | -0.991682 | 1.636424 | 0.646265 |
| O | -0.437306 | -2.354235 | 1.188758 |
| O | 1.967013 | 2.082864 | 0.550867 |
| O | 1.488138 | -0.241421 | -1.180654 |
| H | -2.456267 | -1.627655 | -0.996818 |
| H | -3.580088 | 0.572706 | -1.353945 |
| H | -2.577108 | 2.660220 | -0.448744 |
| H | -0.731227 | 2.519907 | 1.235383 |
| H | -0.009297 | 0.198086 | 2.055853 |
| Mn | 0.691024 | -1.606200 | -0.283828 |
| Mn | 0.948631 | 1.136377 | -0.222483 |
| H | -1.184976 | -2.943370 | 0.985471 |
| 17 | | | |
| **T5-6** | | | |
| C | 1.229059 | 1.599299 | 0.175017 |
| C | 0.307214 | 2.230098 | -0.753197 |
| C | -1.025914 | 1.876809 | -0.793903 |
| C | -1.437175 | 0.891006 | 0.146741 |
| C | -0.699642 | 0.465480 | 1.279453 |
| C | 0.715997 | 0.799215 | 1.283304 |
| H | -2.591468 | 0.392576 | 1.160935 |
| O | -2.567099 | -1.346309 | 0.191003 |
| O | -3.027475 | 0.047863 | 0.302952 |
| 19 | | | |
| **I28** | | | |
| C | -0.978878 | 0.628373 | 1.976396 |
| C | 0.352252 | 0.909750 | 1.725536 |
| C | 0.829358 | 1.373631 | 0.429151 |
| C | -0.216995 | 1.781339 | -0.570974 |
| C | -1.563076 | 1.159105 | -0.370916 |
| C | -1.981365 | 0.777691 | 0.951989 |
| O | -0.005582 | 2.583363 | -1.472278 |
| O | -2.648301 | -1.466006 | -0.870133 |
| O | 0.213379 | -1.544487 | -0.461989 |
| H | 1.736117 | 1.989981 | 0.414980 |
| H | 1.091958 | 0.761877 | 2.514693 |
| H | -1.281291 | 0.284060 | 2.967722 |
| H | -3.042224 | 0.740349 | 1.212565 |
| H | -2.312645 | 1.435768 | -1.115983 |
| Mn | 1.508267 | -0.444830 | -0.194713 |
| Mn | -1.395313 | -0.869152 | -0.101707 |
| H | 3.198460 | -1.502487 | 1.038628 |
| O | 2.321962 | -0.068814 | -1.477519 |
| O | 2.510792 | -0.833974 | 1.223269 |
| 19 | | | |
| **I29** | | | |
| C | -1.543957 | 1.779310 | -0.784923 |
| C | -0.246564 | 1.416796 | -1.165520 |
| C | 0.172274 | 0.051680 | -1.105343 |
| C | -0.826267 | -0.981722 | -1.034876 |
| C | -2.183940 | -0.605655 | -0.800274 |
| C | -2.507990 | 0.748075 | -0.534602 |
| O | -1.635360 | -0.620979 | 1.933783 |
| O | 0.704777 | 0.758522 | 1.319790 |
| H | 0.530609 | 2.183598 | -1.215950 |
| H | -1.814021 | 2.825121 | -0.635585 |
| H | -3.512643 | 1.007427 | -0.200760 |
| H | -2.927485 | -1.384751 | -0.604734 |

| | | | |
|---|---|---|---|
| O | -3.067074 | -0.247884 | 0.399406 |
| O | 3.004389 | -0.884692 | 0.234207 |
| O | 0.297133 | -1.281174 | -0.980670 |
| H | -1.707755 | 2.302209 | -1.532720 |
| H | 0.687940 | 2.983356 | -1.447166 |
| H | 2.219973 | 2.045802 | 0.291415 |
| H | 1.271772 | 0.713130 | 2.220651 |
| H | -1.200214 | 0.113628 | 2.186087 |
| Mn | -1.302905 | -1.015447 | -0.126251 |
| Mn | 1.536614 | -0.426051 | -0.135742 |
| H | -3.527263 | 0.017866 | -0.416489 |
| 19 | | | |
| **I10** | | | |
| C | 0.517575 | 0.950247 | 0.659748 |
| C | 0.080901 | 2.225929 | 0.160290 |
| C | -1.250113 | 2.438165 | -0.051654 |
| C | -2.193492 | 1.282410 | 0.095718 |
| C | -1.790145 | 0.301890 | 1.185777 |
| C | -0.407495 | 0.098888 | 1.394173 |
| O | -2.009805 | 0.381943 | -1.057831 |
| O | 2.550508 | 0.860248 | -1.159448 |
| O | 0.599529 | -1.196847 | -0.837825 |
| H | -1.611205 | 3.370285 | -0.492268 |
| H | -0.026874 | -0.594165 | 2.150361 |
| H | 3.189917 | -0.212594 | 1.741882 |
| H | 0.831174 | 2.959569 | -0.142327 |
| Mn | -1.088086 | -0.955323 | -0.290989 |
| Mn | 1.792716 | -0.098416 | -0.156634 |
| O | 2.756277 | -0.835348 | 1.130117 |
| O | -1.889542 | -2.254642 | 0.089811 |
| H | -3.250499 | 1.580855 | 0.149410 |
| H | -2.547389 | -0.188477 | 1.800607 |
| 19 | | | |
| **I11** | | | |
| C | 1.051856 | 1.551725 | 0.461968 |
| C | 0.416566 | 2.512525 | -0.439191 |
| C | -0.920878 | 2.497870 | -0.629739 |
| C | -1.818909 | 1.460476 | -0.011791 |
| Mn | 1.687634 | -0.042633 | 0.114129 |
| Mn | -0.922484 | 0.174603 | 0.770372 |
| H | 3.614483 | 1.288988 | -0.091134 |
| O | 2.134138 | -1.535635 | 0.371645 |
| O | 2.852942 | 1.059990 | -0.656652 |
| O | -0.437720 | -2.262601 | -1.204228 |
| H | -1.151246 | -2.864911 | -0.925838 |
| 19 | | | |
| **I30** | | | |
| C | 0.257949 | -1.051426 | 1.972839 |
| C | -1.042420 | -0.731046 | 1.665136 |
| C | -1.519361 | -0.745325 | 0.284404 |
| C | -0.620818 | -1.230293 | -0.722044 |
| C | 0.767056 | -1.469655 | -0.442071 |
| C | 1.228134 | -1.382987 | 0.948541 |
| O | -1.121165 | -1.560939 | -1.915078 |
| O | 3.241223 | 0.202265 | -0.802872 |
| O | 0.982002 | 1.675726 | 0.318355 |
| H | -1.772330 | -0.489773 | 2.439830 |
| H | 0.576571 | -1.067488 | 3.016838 |
| H | 2.122362 | -1.940013 | 1.242015 |
| H | 1.323037 | -2.056148 | -1.179273 |
| Mn | -0.783884 | 1.240589 | -0.048235 |
| Mn | 1.812620 | 0.249940 | -0.125966 |
| H | -2.098856 | -1.425528 | -1.830502 |
| O | -2.382568 | 1.673907 | -0.250041 |
| O | -2.862896 | -0.835116 | -0.032718 |
| H | -3.145208 | 0.133360 | -0.115851 |
| 19 | | | |
| **I31** | | | |
| C | 0.884266 | 1.684635 | -1.573036 |
| C | -0.424583 | 1.829165 | -1.232552 |
| C | -0.917244 | 1.416164 | 0.088259 |
| C | 0.084427 | 1.168178 | 1.115728 |
| C | 1.464553 | 1.061259 | 0.782295 |
| C | 1.840485 | 1.149395 | -0.617937 |
| O | -0.245633 | 1.083233 | 2.409425 |
| O | 2.754359 | -1.508066 | 0.139325 |

| | | | |
|---|---|---|---|
| C | -1.185307 | 0.628144 | 1.103374 |
| C | 0.256581 | 0.721555 | 1.284024 |
| O | -2.099278 | 0.428632 | -1.030873 |
| O | 2.341875 | 1.267651 | 0.385291 |
| O | 0.158822 | -1.560815 | -0.439652 |
| H | -1.391221 | 3.211608 | -1.311877 |
| H | 0.729611 | 0.242797 | 2.151012 |
| H | 3.938598 | -1.080333 | -0.477899 |
| H | 1.072012 | 3.214004 | -0.960824 |
| Mn | -1.428081 | -0.958712 | -0.134273 |
| Mn | 1.637791 | -0.533527 | -0.020241 |
| O | 3.071370 | -1.520828 | -0.520339 |
| O | -2.448983 | -1.969830 | 0.551564 |
| H | -2.787826 | 1.890364 | 0.291183 |
| H | -1.793839 | 0.435286 | 1.991464 |
| 19 | | | |
| **I12** | | | |
| C | 2.015574 | 1.071355 | 0.258624 |
| C | 1.523248 | 2.200439 | -0.558681 |
| C | 0.231566 | 2.587613 | -0.568995 |
| C | -0.839650 | 1.947577 | 0.259809 |
| C | -0.400636 | 0.732926 | 1.072399 |
| C | 0.984493 | 0.254603 | 0.982545 |
| O | -1.863311 | 1.401604 | -0.629885 |
| O | 2.377201 | -2.109624 | -0.097529 |
| O | -0.891909 | -1.440185 | -1.038875 |
| H | -0.099733 | 3.406282 | -1.216081 |
| H | 1.394809 | -0.228295 | 1.881762 |
| H | 2.278947 | 2.708238 | -1.163578 |
| Mn | -1.759085 | -0.294352 | -0.099750 |
| Mn | 0.730792 | -1.411742 | -0.185003 |
| O | -2.827158 | -0.876690 | 0.924785 |
| H | -1.323287 | 2.702736 | 0.908368 |
| H | -0.880157 | 0.629755 | 2.052142 |
| O | 3.218683 | 0.799937 | 0.326903 |
| H | 3.141140 | -1.533778 | 0.098803 |
| 19 | | | |
| **I13** | | | |
| O | -0.118710 | -1.649976 | -0.466607 |
| H | -1.853992 | 1.866288 | 0.437895 |
| H | -1.159574 | 2.206611 | -1.944206 |
| H | 1.234640 | 1.960951 | -2.568775 |
| H | 2.904114 | 1.206818 | -0.855989 |
| H | 2.196764 | 1.044810 | 1.593194 |
| Mn | -1.466726 | -0.553484 | -0.170704 |
| Mn | 1.355039 | -0.783366 | -0.067631 |
| H | -1.179293 | 0.774722 | 2.469854 |
| O | -2.105452 | -0.721569 | 1.287080 |
| O | -2.402302 | -0.390090 | -1.437992 |
| 19 | | | |
| **I32** | | | |
| C | 1.109977 | 1.281883 | -1.773303 |
| C | -0.235776 | 1.425599 | -1.607720 |
| C | -0.875761 | 1.340091 | -0.288078 |
| C | 0.013728 | 1.444938 | 0.922624 |
| C | 1.438287 | 1.114903 | 0.707687 |
| C | 1.985214 | 1.061589 | -0.628512 |
| O | -0.438707 | 1.730869 | 2.039415 |
| O | 2.688771 | -1.528816 | 0.705785 |
| O | -0.108406 | -1.575388 | -0.161209 |
| H | -1.814214 | 1.896539 | -0.168150 |
| H | -0.885922 | 1.578318 | -2.472391 |
| H | 1.553943 | 1.322930 | -2.769442 |
| H | 3.066174 | 1.151993 | -0.766044 |
| H | 2.092679 | 1.252485 | 1.572262 |
| Mn | -1.539014 | -0.581911 | -0.118144 |
| Mn | 1.478275 | -0.793571 | 0.010781 |
| O | -2.280574 | -0.334606 | 1.435604 |
| O | -2.505318 | -0.702824 | -1.349997 |
| H | -1.954324 | 0.456901 | 1.934855 |
| 17 | | | |
| **I33** | | | |
| C | -1.873795 | -0.075890 | 1.549845 |
| C | -0.450758 | -0.165198 | 1.644036 |
| C | 0.353338 | 0.644495 | 0.820898 |
| C | -0.210139 | 1.784583 | 0.032008 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 2.163751 | 0.900675 | 0.334215 | C | -1.585637 | 1.427510 | -0.390678 |
| C | 1.792302 | 2.012030 | -0.571068 | C | -2.430018 | 0.734258 | 0.523460 |
| C | 0.542606 | 2.512079 | -0.632858 | O | 0.399453 | 2.772905 | -0.342378 |
| C | -0.584094 | 2.015534 | 0.216743 | O | -2.317391 | -1.464325 | -1.087284 |
| C | -0.298308 | 0.766457 | 1.044942 | O | 0.507161 | -1.049457 | -1.035079 |
| C | 1.023247 | 0.103338 | 0.931260 | H | 0.005546 | -0.940890 | 2.264635 |
| O | -1.681117 | 1.555420 | -0.643972 | H | -2.514707 | -0.681339 | 2.192096 |
| O | 1.339829 | -2.774594 | 0.220170 | H | -3.499862 | 0.665843 | 0.316672 |
| O | -0.897770 | -1.318037 | -0.924094 | H | -2.019097 | 1.970329 | -1.233433 |
| H | 0.297766 | 3.330769 | -1.317048 | Mn | 1.771716 | -0.322419 | -0.043574 |
| H | 1.347709 | -0.449776 | 1.823832 | Mn | -1.132422 | -0.682869 | -0.401676 |
| H | 2.608632 | 2.433066 | -1.163629 | O | 2.651812 | 0.755683 | -0.775605 |
| Mn | -1.784179 | -0.104360 | -0.057373 | O | 2.412443 | -1.262342 | 1.054577 |
| Mn | 0.759622 | -1.432801 | -0.358382 | 17 | | | |
| O | -2.892424 | -0.499687 | 0.977596 | **I34** | | | |
| H | -0.979725 | 2.834652 | 0.845687 | C | 2.462227 | 1.712974 | -0.419997 |
| H | -0.733220 | 0.763787 | 2.050568 | C | 1.164476 | 2.119233 | -0.783500 |
| O | 3.333099 | 0.633652 | 0.594226 | C | 0.053823 | 1.538444 | -0.151548 |
| H | 1.622816 | -1.118161 | -1.576342 | C | 0.252005 | 0.653373 | 0.982203 |
| 19 | | | | C | 1.566922 | 0.179252 | 1.273626 |
| **I14** | | | | C | 2.669813 | 0.735749 | 0.561601 |
| C | 2.407072 | -0.067032 | -0.115871 | O | -0.847354 | 0.166181 | 1.547525 |
| C | 2.318781 | -1.388791 | 0.555637 | O | 1.887863 | -2.466872 | -0.102912 |
| C | 1.332587 | -2.273235 | 0.308695 | O | -0.833565 | -1.135381 | -0.788556 |
| C | 0.180342 | -1.999998 | -0.612166 | H | 0.997486 | 2.821238 | -1.603037 |
| C | 0.102882 | -0.568168 | -1.143047 | H | 3.320078 | 2.139115 | -0.943629 |
| C | 1.230507 | 0.358064 | -0.930045 | H | 3.677790 | 0.393539 | 0.799026 |
| O | -1.058031 | -2.118526 | 0.137765 | H | 1.718239 | -0.492236 | 2.122743 |
| O | -0.079821 | 2.910464 | -0.437831 | Mn | -1.900101 | -0.016921 | -0.020464 |
| O | -0.846476 | 0.522308 | 1.555698 | Mn | 0.967555 | -1.170196 | -0.402321 |
| H | 1.319342 | -3.250935 | 0.801699 | O | -3.427116 | -0.315513 | 0.093207 |
| H | 1.491864 | 1.034503 | -1.752982 | O | -1.206770 | 1.649349 | -0.571737 |
| H | 3.145857 | -1.629523 | 1.229295 | 19 | | | |
| Mn | -1.574820 | -0.417908 | 0.124577 | **T26-27** | | | |
| Mn | 0.023531 | 1.478551 | 0.191052 | C | 1.803285 | 1.822946 | -0.809381 |
| O | -2.847822 | 0.007580 | -0.689846 | C | 0.503322 | 2.169311 | -1.082372 |
| H | 0.161247 | -2.743016 | -1.434200 | C | -0.585659 | 1.735067 | -0.244791 |
| H | -0.401644 | -0.480802 | -2.112491 | C | -0.311027 | 1.122767 | 1.041664 |

| | | | |
|---|---|---|---|
| O | 3.416281 | 0.634226 | -0.004141 |
| H | -1.040513 | 0.540239 | 2.505579 |
| 19 | | | |
| **I15** | | | |
| C | -2.583806 | -0.674320 | -0.353072 |
| C | -1.764188 | -1.877338 | -0.621112 |
| C | -0.647445 | -2.159764 | 0.077713 |
| C | -0.108844 | -1.302151 | 1.192011 |
| C | -0.808255 | 0.045473 | 1.342989 |
| C | -2.032581 | 0.303356 | 0.631309 |
| O | 1.319125 | -1.146529 | 1.079084 |
| O | -0.544910 | 2.801184 | 0.494536 |
| O | 0.883063 | 0.678188 | -1.050247 |
| H | -0.068327 | -3.065683 | -0.127782 |
| H | -2.760294 | 1.025827 | 1.014072 |
| H | -2.132863 | -2.543212 | -1.405402 |
| Mn | 2.059261 | -0.330271 | -0.299412 |
| Mn | -0.493715 | 1.357223 | -0.150077 |
| O | 3.552714 | 0.112086 | -0.243712 |
| H | -0.238890 | -1.859254 | 2.143718 |
| H | -0.630838 | 0.551924 | 2.297244 |
| O | -3.672326 | -0.492321 | -0.899974 |
| H | 2.061931 | -1.415811 | -1.341174 |
| 19 | | | |
| **I16** | | | |
| C | -2.421172 | -0.695032 | -0.446012 |
| C | -1.546431 | -1.867640 | -0.732429 |
| C | -0.511298 | -2.214144 | 0.057842 |
| C | -0.102388 | -1.421624 | 1.266378 |
| C | -0.764326 | -0.073531 | 1.389957 |
| C | -1.957187 | 0.222764 | 0.617983 |
| O | 1.373396 | -1.155175 | 1.204895 |
| O | -0.334547 | 2.765011 | 0.693488 |
| O | 0.611612 | 0.960503 | -1.330227 |
| H | 0.059293 | -3.128389 | -0.144996 |
| H | -2.718981 | 0.902068 | 1.012433 |
| H | -1.834809 | -2.477423 | -1.592351 |
| Mn | 1.818719 | -0.014143 | -0.378290 |
| C | 1.057953 | 0.684113 | 1.292261 |
| C | 2.108571 | 1.015528 | 0.347481 |
| O | -1.242991 | 0.884237 | 1.910065 |
| O | 2.236088 | -2.048487 | 0.660632 |
| O | 0.250886 | -1.121736 | -1.295879 |
| H | -1.560126 | 2.225708 | -0.350241 |
| H | 0.271129 | 2.780451 | -1.957414 |
| H | 2.617661 | 2.154313 | -1.454973 |
| H | 3.150302 | 0.920550 | 0.666887 |
| H | 1.289779 | 0.360240 | 2.310527 |
| Mn | -1.292481 | -0.354763 | -0.758085 |
| Mn | 1.378137 | -0.894184 | 0.010130 |
| H | -2.246073 | 0.485773 | 1.263870 |
| O | -2.487232 | -1.364158 | 0.232459 |
| O | -2.897095 | 0.024924 | 0.361605 |
| 19 | | | |
| **T26-31** | | | |
| C | -0.997802 | 0.453621 | 1.843481 |
| C | 0.408632 | 0.545782 | 1.781276 |
| C | 1.054348 | 1.252076 | 0.702627 |
| C | 0.233945 | 1.670221 | -0.401023 |
| C | -1.185373 | 1.551206 | -0.344159 |
| C | -1.821722 | 1.067567 | 0.850808 |
| O | 0.756175 | 2.284881 | -1.487838 |
| O | -3.045780 | -1.085334 | -0.621988 |
| O | -0.097829 | -1.601306 | -0.615258 |
| H | 2.071111 | 1.633869 | 0.823520 |
| H | 1.021691 | 0.176653 | 2.605684 |
| H | -1.467841 | -0.032537 | 2.701209 |
| H | -2.888900 | 1.217866 | 1.013329 |
| H | -1.770014 | 2.021724 | -1.137684 |
| Mn | 1.183937 | -0.602571 | -0.065151 |
| Mn | -1.542620 | -0.624278 | -0.261462 |
| H | 1.717378 | 2.115932 | -1.522425 |
| O | 2.776917 | -1.069712 | 0.753421 |
| O | 2.626952 | -0.491669 | -0.892883 |
| 19 | | | |
| **T27-28** | | | |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Mn | -0.400822 | 1.350036 | 0.006451 | C | 1.799296 | 1.712617 | -1.012492 |
| O | 3.314774 | -0.628837 | -0.605407 | C | 0.476388 | 2.054562 | -1.222404 |
| H | -0.234654 | -2.017013 | 2.189926 | C | -0.548370 | 1.717599 | -0.284924 |
| H | -0.666099 | 0.389455 | 2.377332 | C | -0.193886 | 1.224025 | 1.062829 |
| O | -3.482839 | -0.540870 | -1.052222 | C | 1.203088 | 0.742647 | 1.209515 |
| H | 1.905476 | -1.975841 | 1.247105 | C | 2.185158 | 1.023488 | 0.185271 |
| 17 | | | | O | -1.025984 | 1.148891 | 1.994653 |
| **I17** | | | | O | 2.165736 | -2.077786 | 0.720215 |
| C | 2.499920 | -0.053831 | -0.202885 | O | 0.192165 | -1.157144 | -1.228498 |
| C | 2.431747 | -1.361940 | 0.496279 | H | -1.517330 | 2.222549 | -0.359344 |
| C | 1.331923 | -2.160250 | 0.452478 | H | 0.196416 | 2.594379 | -2.130527 |
| C | 0.167906 | -1.752789 | -0.302026 | H | 2.563574 | 1.973454 | -1.745962 |
| C | 0.187766 | -0.578275 | -1.144855 | H | 3.248058 | 0.927016 | 0.426209 |
| C | 1.279771 | 0.377319 | -0.952642 | H | 1.519063 | 0.488111 | 2.225357 |
| O | -1.027595 | -2.228625 | -0.030964 | Mn | -1.310389 | -0.410180 | -0.558044 |
| O | -0.316892 | 2.837239 | -0.243398 | Mn | 1.368666 | -0.909551 | 0.019297 |
| O | -1.007379 | 0.411180 | 1.413186 | H | -2.807790 | 0.451516 | 1.113443 |
| H | 1.265638 | -3.097189 | 1.011743 | O | -2.553724 | -1.465287 | 0.126852 |
| H | 1.487815 | 1.101171 | -1.748904 | O | -3.051814 | 0.237152 | 0.175870 |
| H | 3.324900 | -1.646452 | 1.058166 | 19 | | | |
| Mn | -1.593123 | -0.415157 | 0.015409 | **T28-29** | | | |
| Mn | 0.049061 | 1.402810 | 0.328104 | C | -1.221304 | 1.434891 | 1.564426 |
| O | -2.989418 | -0.052404 | -0.576451 | C | 0.151302 | 1.487145 | 1.255787 |
| H | -0.379981 | -0.612998 | -2.083434 | C | 0.548830 | 1.231688 | -0.093084 |
| O | 3.529908 | 0.625451 | -0.175308 | C | -0.449777 | 1.365498 | -1.149748 |
| 19 | | | | C | -1.831320 | 1.193940 | -0.844869 |
| **I8** | | | | C | -2.205245 | 1.249176 | 0.531219 |
| C | 0.922373 | 1.734920 | 0.605272 | O | 0.174134 | 1.604765 | -2.248038 |
| C | 0.257135 | 2.440623 | -0.486998 | O | -2.098281 | -1.524094 | -0.145022 |
| C | -1.073691 | 2.323635 | -0.705111 | O | 0.386370 | -1.284717 | 1.017732 |
| C | -1.948874 | 1.392621 | 0.082203 | H | 1.201486 | 1.531767 | -1.326167 |
| C | -1.202339 | 0.565337 | 1.133901 | H | 0.894309 | 1.485337 | 2.055600 |
| C | 0.209660 | 0.845512 | 1.396663 | H | -1.550735 | 1.487905 | 2.602804 |
| O | -2.460800 | 0.347375 | -0.833333 | H | -3.257915 | 1.181401 | 0.806694 |
| O | 0.099358 | -1.206510 | -0.660360 | H | -2.577980 | 1.077309 | -1.631581 |
| H | -1.561819 | 2.899178 | -1.495614 | Mn | 1.595054 | -0.554097 | 0.013684 |
| H | -2.837355 | 1.905190 | 0.492247 | Mn | -1.046367 | -0.464741 | 0.327469 |
| H | 0.658846 | 0.438142 | 2.308897 | H | 3.335861 | -0.696927 | 1.589957 |

| | | | |
|---|---|---|---|
| H | 1.932261 | 2.037166 | 0.895578 |
| H | 0.856046 | 3.117076 | -1.101596 |
| H | -1.791089 | 0.275457 | 2.010937 |
| Mn | -1.507856 | -0.977038 | -0.138728 |
| Mn | 1.633552 | -0.355111 | -0.135564 |
| O | -2.229403 | -2.177789 | 0.613970 |
| O | 3.254528 | -1.104910 | -0.514597 |
| O | 3.413206 | -0.006211 | 0.343231 |
| 19 | | | |
| **I9** | | | |
| C | 0.710146 | 1.126465 | 0.979983 |
| C | 0.305661 | 2.252682 | 0.126031 |
| C | -0.959991 | 2.416594 | -0.321568 |
| C | -2.022701 | 1.394678 | -0.050213 |
| C | -1.706265 | 0.482939 | 1.120442 |
| C | -0.364564 | 0.248238 | 1.483579 |
| O | -1.996728 | 0.377469 | -1.109948 |
| O | 2.632609 | 0.681153 | -1.049179 |
| O | 0.481206 | -1.115800 | -0.961419 |
| H | -1.217345 | 3.262461 | -0.962625 |
| H | -0.127892 | -0.420557 | 2.314649 |
| H | 1.498850 | 1.346876 | 1.710970 |
| H | 1.084082 | 2.970111 | -0.143937 |
| Mn | -1.130607 | -0.925964 | -0.225359 |
| Mn | 1.732540 | -0.244405 | -0.139824 |
| O | 2.428926 | -1.100804 | 0.995950 |
| O | -1.858369 | -2.254446 | 0.185709 |
| H | -3.034501 | 1.826618 | -0.000710 |
| H | -2.526364 | 0.043560 | 1.692810 |
| 19 | | | |
| **T10-11** | | | |
| C | 0.365832 | 1.232293 | 0.473655 |
| C | -0.439990 | 2.238392 | -0.157554 |
| C | -1.798991 | 2.127071 | -0.155741 |
| C | -2.412673 | 0.823375 | 0.250216 |
| C | -1.619666 | 0.073551 | 1.308902 |
| C | -0.223317 | 0.276708 | 1.385686 |
| O | -2.217985 | -0.131523 | -0.858768 |
| O | 1.918792 | -1.159256 | -1.403632 |
| O | 2.921574 | 0.010492 | 1.060211 |
| 19 | | | |
| **T29-30** | | | |
| C | -0.883757 | 1.404222 | 1.893935 |
| C | 0.452369 | 1.399411 | 1.602028 |
| C | 0.774111 | 0.949121 | 0.267621 |
| C | -0.118523 | 1.299134 | -0.832172 |
| C | -1.504741 | 1.303916 | -0.529410 |
| C | -1.855406 | 1.086590 | 0.863310 |
| O | 0.308138 | 1.475743 | -2.091404 |
| O | -2.859506 | -1.377455 | -0.103065 |
| O | 0.084790 | -1.753590 | -0.418914 |
| H | 1.229305 | 1.484500 | 2.362512 |
| H | -1.225537 | 1.569702 | 2.918419 |
| H | -2.913681 | 1.109408 | 1.123137 |
| H | -2.230889 | 1.605396 | -1.288038 |
| Mn | 1.434765 | -0.780238 | -0.000216 |
| Mn | -1.405167 | -0.724690 | -0.201187 |
| H | 1.297153 | 1.465461 | -2.043116 |
| O | 2.368712 | 0.908917 | -0.724564 |
| O | 2.450463 | -1.174727 | 1.147816 |
| H | 3.098603 | 1.103270 | -0.108673 |
| 19 | | | |
| **T31-32** | | | |
| C | 1.164093 | 1.849442 | -1.237265 |
| C | -0.175042 | 1.942747 | -1.010610 |
| C | -0.794260 | 1.375598 | 0.192286 |
| C | 0.099184 | 0.950908 | 1.286422 |
| C | 1.509068 | 0.837732 | 1.030097 |
| C | 2.036401 | 1.201660 | -0.266176 |
| O | -0.396468 | 0.571420 | 2.420905 |
| O | 2.597151 | -1.752137 | 0.120058 |
| O | -0.157911 | -1.385857 | -0.717859 |
| H | -1.718553 | 1.853068 | 0.540395 |
| H | -0.835316 | 2.418404 | -1.738017 |
| H | 1.605225 | 2.248227 | -2.152083 |
| H | 3.118591 | 1.292238 | -0.384248 |

| | | | |
|---|---|---|---|
| O | 2.042655 | 1.687127 | -0.143778 |
| O | 0.661547 | -0.762501 | -1.323568 |
| H | -2.430236 | 2.898893 | -0.600262 |
| H | -3.487114 | 0.887815 | 0.476565 |
| H | 0.384749 | -0.229726 | 2.140752 |
| H | 0.066969 | 3.074730 | -0.642342 |
| H | -2.141077 | -0.571477 | 2.020591 |
| Mn | -0.803187 | -1.045136 | -0.252546 |
| Mn | 1.761250 | 0.052399 | -0.278732 |
| O | -1.044982 | -2.519639 | 0.231505 |
| O | 2.658848 | -0.899845 | 0.903439 |
| H | 3.627307 | -0.859105 | 0.785030 |
| 19 | | | |
| **T11-12** | | | |
| C | 1.918742 | 0.881209 | 0.244090 |
| C | 1.597961 | 2.100936 | -0.477422 |
| C | 0.353423 | 2.631709 | -0.463977 |
| C | -0.795503 | 1.993335 | 0.251843 |
| C | -0.450474 | 0.780343 | 1.107402 |
| C | 0.914393 | 0.225857 | 1.063931 |
| O | -1.689590 | 1.390923 | -0.749043 |
| O | 3.128360 | 0.410135 | 0.144196 |
| O | -0.813608 | -1.491141 | -1.043469 |
| H | 0.128949 | 3.526313 | -1.051955 |
| H | -1.379210 | 2.744299 | 0.813545 |
| H | 1.295759 | -0.258199 | 1.976727 |
| H | 2.410024 | 2.548685 | -1.054793 |
| H | -0.947186 | 0.730845 | 2.081271 |
| Mn | -1.667351 | -0.274549 | -0.133995 |
| Mn | 0.629662 | -1.427388 | -0.079495 |
| H | 2.966973 | -0.712037 | 0.113999 |
| O | -2.838473 | -0.737578 | 0.805467 |
| O | 2.242769 | -1.786314 | -0.144243 |
| 19 | | | |
| **T12-13** | | | |
| C | 2.317056 | 0.702831 | 0.308829 |
| C | 1.993903 | 1.768527 | -0.670240 |
| C | 0.784374 | 2.357389 | -0.729074 |
| H | 2.162151 | 0.604190 | 1.874090 |
| Mn | -1.602119 | -0.466637 | -0.269159 |
| Mn | 1.430331 | -0.756923 | -0.275083 |
| H | -1.358952 | 0.041482 | 2.107267 |
| O | -2.145104 | -0.645842 | 1.287661 |
| O | -2.612055 | -0.139729 | -1.437003 |
| 19 | | | |
| **T31-33** | | | |
| C | -0.892784 | 1.082506 | 1.964161 |
| C | 0.428638 | 1.255628 | 1.656610 |
| C | 0.797538 | 1.131384 | 0.255881 |
| C | -0.204068 | 1.628635 | -0.761211 |
| C | -1.562024 | 1.193244 | -0.468228 |
| C | -1.866974 | 0.839482 | 0.914455 |
| O | 0.152197 | 2.340160 | -1.710941 |
| O | -2.727463 | -1.559666 | -0.496037 |
| O | 0.137205 | -1.673755 | 0.091451 |
| H | 1.875808 | 2.086236 | -0.214412 |
| H | 1.211354 | 1.275767 | 2.417192 |
| H | -1.211826 | 1.028167 | 3.006884 |
| H | -2.921280 | 0.777525 | 1.192044 |
| H | -2.349576 | 1.493986 | -1.162732 |
| Mn | 1.531854 | -0.579168 | -0.036585 |
| Mn | -1.360568 | -0.814376 | -0.208743 |
| O | 2.075112 | -0.496273 | -1.513779 |
| O | 2.522477 | -0.748042 | 1.186679 |
| H | 1.635213 | 2.492241 | -0.934784 |
| 19 | | | |
| **T32-33** | | | |
| C | -0.863503 | 1.251535 | 1.946612 |
| C | 0.461928 | 1.350862 | 1.636085 |
| C | 0.853842 | 1.097903 | 0.259087 |
| C | -0.115737 | 1.520013 | -0.859869 |
| C | -1.510646 | 1.201599 | -0.493492 |
| C | -1.837564 | 0.974065 | 0.901928 |
| O | 0.226468 | 2.011432 | -1.922555 |
| O | -2.850895 | -1.438825 | -0.475094 |
| O | 0.078699 | -1.640819 | -0.230342 |

| | | | |
|---|---|---|---|
| C | -0.346967 | 2.001668 | 0.183450 |
| C | -0.150312 | 0.733714 | 1.013223 |
| C | 1.151381 | 0.040200 | 0.993790 |
| O | -1.538936 | 1.688787 | -0.600092 |
| O | 1.416549 | -2.727502 | -0.274685 |
| O | -1.111298 | -1.218608 | -0.998746 |
| H | 0.577055 | 3.153821 | -1.450687 |
| H | 1.438384 | -0.483309 | 1.918027 |
| H | 2.818581 | 2.087187 | -1.312802 |
| Mn | -1.808034 | 0.027686 | -0.065607 |
| Mn | 0.432773 | -1.429647 | -0.136218 |
| O | -2.905259 | -0.302377 | 1.007938 |
| H | -0.594369 | 2.862119 | 0.835420 |
| H | -0.647148 | 0.747213 | 1.990398 |
| O | 3.474532 | 0.388199 | 0.567793 |
| H | 1.607694 | -1.571974 | -1.152267 |
| 19 | | | |
| **T13-14** | | | |
| C | 2.638790 | 0.064917 | 0.191520 |
| C | 2.402061 | -1.338163 | 0.601397 |
| C | 1.419881 | -2.089552 | 0.067252 |
| C | 0.431140 | -1.599633 | -0.958325 |
| C | 0.614367 | -0.140571 | -1.361165 |
| C | 1.665822 | 0.642251 | -0.781012 |
| O | -0.889036 | -1.851624 | -0.416242 |
| O | -0.530573 | 2.544292 | -0.627833 |
| O | -0.803862 | 0.527921 | 1.519972 |
| H | 1.271121 | -3.125628 | 0.387522 |
| H | 2.020600 | 1.551523 | -1.277273 |
| H | 3.090479 | -1.740513 | 1.349141 |
| Mn | -1.772790 | -0.517080 | 0.351143 |
| Mn | -0.136594 | 1.180064 | -0.019370 |
| O | -3.217646 | -0.115608 | -0.159601 |
| H | 0.510027 | -2.233134 | -1.864075 |
| H | 0.206448 | 0.128960 | -2.341184 |
| O | 3.602254 | 0.709433 | 0.605246 |
| H | 0.314468 | 1.093377 | 1.521194 |
| 19 | | | |
| H | 1.981016 | 1.859437 | -0.303339 |
| H | 1.237681 | 1.430437 | 2.401541 |
| H | -1.197535 | 1.315035 | 2.984173 |
| H | -2.895331 | 0.979715 | 1.176077 |
| H | -2.275919 | 1.504079 | -1.213507 |
| Mn | 1.517111 | -0.633584 | 0.005977 |
| Mn | -1.449580 | -0.781375 | -0.155824 |
| O | 2.382176 | -0.180747 | -1.268217 |
| O | 2.313817 | -0.964537 | 1.323099 |
| H | 2.329761 | 1.617379 | -1.055993 |
| 17 | | | |
| **T33-34** | | | |
| C | -1.924021 | 0.332250 | 1.447493 |
| C | -0.518077 | 0.353057 | 1.670696 |
| C | 0.323625 | 0.876504 | 0.676131 |
| C | -0.160684 | 1.803818 | -0.384962 |
| C | -1.493046 | 1.280438 | -0.788530 |
| C | -2.405239 | 0.803859 | 0.191488 |
| O | 0.443350 | 2.708139 | -0.930966 |
| O | -2.037940 | -1.604272 | -1.135188 |
| O | 0.522513 | -1.682712 | 0.068715 |
| H | -0.084545 | -0.234481 | 2.482494 |
| H | -2.602481 | -0.081471 | 2.194018 |
| H | -3.451292 | 0.646871 | -0.077191 |
| H | -1.847519 | 1.530387 | -1.791909 |
| Mn | 1.727014 | -0.441230 | 0.010894 |
| Mn | -1.059151 | -0.804761 | -0.195680 |
| O | 2.538274 | -0.176641 | -1.305062 |
| O | 2.078041 | 0.329100 | 1.419796 |

**T14-15**

| | | | |
|---|---|---|---|
| C | 2.423025 | 0.614368 | 0.199478 |
| C | 2.007183 | 1.651042 | -0.779066 |
| C | 0.811836 | 2.268731 | -0.708842 |
| C | -0.218201 | 1.945548 | 0.332067 |
| C | 0.027141 | 0.636137 | 1.072315 |
| C | 1.331144 | 0.000972 | 1.020041 |
| O | -1.524472 | 1.819406 | -0.295135 |
| O | 1.355961 | -2.713762 | -0.244421 |
| O | -1.049278 | -1.144831 | -1.139268 |
| H | 0.540064 | 3.064174 | -1.409510 |
| H | 1.685845 | -0.547351 | 1.902381 |
| H | 2.760140 | 1.939720 | -1.516711 |
| Mn | -1.824346 | 0.092637 | -0.063485 |
| Mn | 0.405816 | -1.425618 | -0.079893 |
| O | -3.003903 | -0.372311 | 0.859926 |
| H | -0.294614 | 2.778040 | 1.062125 |
| H | -0.520247 | 0.552036 | 2.019832 |
| O | 3.601061 | 0.303405 | 0.350147 |
| H | -2.035668 | -0.298126 | -1.539607 |

19

**T15-16**

| | | | |
|---|---|---|---|
| C | 2.622153 | 0.024857 | -0.270836 |
| C | 2.249787 | 1.401774 | -0.680817 |
| C | 1.261051 | 2.094512 | -0.082996 |
| C | 0.408319 | 1.552831 | 1.028195 |
| C | 0.658022 | 0.093221 | 1.363404 |
| C | 1.751649 | -0.617083 | 0.749603 |
| O | -1.013899 | 1.787514 | 0.700725 |
| O | -0.476297 | -2.571762 | 0.639277 |
| O | -0.721228 | -0.475257 | -1.418751 |
| H | 1.039056 | 3.124306 | -0.383206 |
| H | 2.187632 | -1.494842 | 1.237044 |
| H | 2.856557 | 1.843045 | -1.475530 |
| Mn | -1.754392 | 0.376264 | -0.293348 |
| Mn | -0.015437 | -1.226179 | -0.002204 |
| O | -3.299256 | 0.128602 | -0.223695 |
| H | 0.545381 | 2.180353 | 1.929371 |

| | | | |
|---|---|---|---|
| H | 0.310486 | -0.219338 | 2.353504 |
| O | 3.615621 | -0.536881 | -0.732762 |
| H | -1.238819 | 1.855948 | -0.630022 |
| 19 | | | |
| **T16-17** | | | |
| C | -2.667970 | -0.347830 | -0.306325 |
| C | -1.990461 | -1.557249 | -0.814738 |
| C | -0.833811 | -2.028315 | -0.268672 |
| C | -0.203190 | -1.394050 | 0.881908 |
| C | -0.758204 | -0.132182 | 1.371370 |
| C | -1.936794 | 0.410397 | 0.740810 |
| O | 1.246702 | -1.501935 | 0.950760 |
| O | 0.025337 | 2.655807 | 0.640207 |
| O | 0.783233 | 0.746529 | -1.327890 |
| H | -0.339077 | -2.918439 | -0.667701 |
| H | -2.515017 | 1.193629 | 1.238494 |
| H | -2.468860 | -2.066098 | -1.655019 |
| Mn | 1.881916 | -0.260643 | -0.348720 |
| Mn | -0.220512 | 1.251564 | -0.001427 |
| O | 3.478194 | -0.168584 | -0.284828 |
| H | -0.247748 | -2.388593 | 1.936912 |
| H | -0.425743 | 0.214734 | 2.355067 |
| O | -3.777054 | 0.000965 | -0.723058 |
| H | 0.752650 | -2.375116 | 1.878277 |
| 19 | | | |
| **T8-9** | | | |
| C | 0.904213 | 1.451263 | 0.690156 |
| C | 0.308822 | 2.356919 | -0.289057 |
| C | -1.023539 | 2.375092 | -0.542809 |
| C | -1.969546 | 1.386546 | 0.072127 |
| C | -1.372701 | 0.576454 | 1.214091 |
| C | 0.031311 | 0.597555 | 1.450208 |
| O | -2.196500 | 0.307173 | -0.896414 |
| O | 0.183600 | -1.166829 | -1.122392 |
| H | -1.440500 | 3.073072 | -1.272401 |
| H | -2.946742 | 1.829449 | 0.328211 |
| H | 0.430650 | 0.083006 | 2.328823 |
| H | 1.874665 | 1.707464 | 1.125022 |

| | | | | |
|---|---|---|---|---|
| H | 0.977276 | 3.048454 | -0.807069 | |
| H | -2.043277 | 0.199423 | 1.990834 | |
| Mn | -1.195530 | -0.949192 | -0.106903 | |
| Mn | 1.453522 | -0.325447 | -0.212289 | |
| O | -1.914143 | -2.229003 | 0.445644 | |
| O | 3.061819 | 0.043229 | -0.692010 | |
| O | 2.793570 | -0.771804 | 0.854935 | |
| 19 | | | | |
| **T9-10** | | | | |
| C | 0.776496 | 1.097397 | 0.715792 | |
| C | 0.408177 | 2.232993 | -0.109170 | |
| C | -0.892401 | 2.500890 | -0.385745 | |
| C | -1.941305 | 1.487952 | -0.032620 | |
| C | -1.597991 | 0.646553 | 1.191574 | |
| C | -0.219670 | 0.436825 | 1.469101 | |
| O | -1.927221 | 0.445665 | -1.093777 | |
| O | 2.477237 | 0.228107 | -1.443367 | |
| O | 0.428846 | -1.477529 | -0.427408 | |
| H | -1.190498 | 3.384931 | -0.953491 | |
| H | 0.074182 | -0.300550 | 2.223937 | |
| H | 1.977386 | 0.665130 | 1.363957 | |
| H | 1.208009 | 2.873173 | -0.490889 | |
| Mn | -1.256998 | -0.907157 | -0.169218 | |
| Mn | 1.788193 | -0.407051 | -0.180000 | |
| O | 2.623789 | -0.392912 | 1.291457 | |
| O | -2.253590 | -2.107174 | 0.121881 | |
| H | -2.962190 | 1.893391 | 0.004738 | |
| H | -2.379089 | 0.354227 | 1.898321 | |

**Table S10.** Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis of structures A1, A2, A3, B1, B2, B3

| Cấu hình | Donor NBO (i) | Type | Acceptor NBO (j) | Type | E(2)-kcal.mol-1 | E(j)-E(i) (au) | F(i,j) (au) |
|---|---|---|---|---|---|---|---|
| A1 | C 3 - C 4 | π | LP*( 5) | Mn 14 | 21.41 | 0.65 | 0.159 |
| | C 3 - C 4 | π | LP*( 2) | Mn 14 | 14.1 | 0.31 | 0.085 |
| | C 3 - C 4 | σ | LP*( 5) | Mn 14 | 7.53 | 1.02 | 0.113 |
| | C 3 - C 4 | π* | LP*( 3) | Mn 14 | 7.06 | 0.18 | 0.07 |
| | C 3 - H 9 | σ | LP*( 5) | Mn 14 | 3.34 | 0.87 | 0.07 |
| | C 4 - H 15 | σ | LP*( 5) | Mn 14 | 3.34 | 0.87 | 0.07 |
| | | | | | | | |
| A2 | C 4 | LP ( 1) | O 13 -Mn 14 | BD*( 3) | 9.78 | 0.07 | 0.037 |
| | C 1 | LP*( 1) | Mn 14 | LP*( 2) | 9.42 | 0.64 | 0.12 |
| | C 2 - C 3 | π | O 13 -Mn 14 | BD*( 3) | 9.23 | 0.18 | 0.054 |
| | C 5 - C 6 | π | Mn 14 | LP*( 2) | 9.08 | 0.75 | 0.106 |
| | C 4 | LP ( 1) | Mn 14 | LP*( 2) | 9.03 | 0.64 | 0.118 |
| | C 4 | LP ( 1) | Mn 14 | LP*( 5) | 8.19 | 0.61 | 0.121 |
| | C 1 | LP*( 1) | Mn 14 | LP*( 5) | 8.13 | 0.61 | 0.12 |
| | C 1 - C 2 | σ | Mn 14 | LP*( 5) | 7 | 1.1 | 0.112 |
| | C 3 - C 4 | σ | Mn 14 | LP*( 5) | 6.94 | 1.1 | 0.112 |
| | C 4 - C 5 | σ | Mn 14 | LP*( 5) | 6.73 | 1.1 | 0.11 |
| | C 1 - C 6 | σ | Mn 14 | LP*( 5) | 6.57 | 1.1 | 0.109 |
| | | | | | | | |
| A3 | C 2 - C 3 | σ | C 4 - O 14 | σ* | 3.09 | 0.71 | 0.051 |
| | C 5 - C 6 | σ | C 1 - O 15 | σ* | 3.09 | 0.71 | 0.051 |
| | C 6 - H 11 | σ | C 4 - C 5 | σ* | 2.47 | 0.81 | 0.057 |
| | C 1 - C 2 | σ | C 3 - H 8 | σ* | 1.62 | 0.96 | 0.05 |
| | C 1 - C 6 | σ | C 5 - H 12 | σ* | 1.62 | 0.96 | 0.05 |
| | C 3 - C 4 | σ | C 2 - H 9 | σ* | 1.62 | 0.96 | 0.05 |
| | C 4 - C 5 | σ | C 6 - H 11 | σ* | 1.62 | 0.96 | 0.05 |
| | C 1 - O 15 | σ | Mn 13 | LP*( 2) | 1.41 | 0.79 | 0.042 |
| | C 4 - O 14 | σ | Mn 13 | LP*( 2) | 1.41 | 0.79 | 0.042 |
| | | | | | | | |
| | | | | | | | |
| B1 | C 4 | LP ( 1) | σ* | C 5 -Mn 16 | 48.03 | 0.1 | 0.126 |
| | C1 | LP ( 1) | σ* | C 6 -Mn 17 | 35.94 | 0.49 | 0.197 |
| | C 2 | LP ( 1) | σ* | C 1 -Mn 17 | 34.16 | 0.07 | 0.071 |
| | C 4 -Mn 16 | σ | σ* | C 5 -Mn 16 | 33.02 | 0.57 | 0.178 |
| | C 6 | LP ( 1) | LP*( 1) | Mn 17 | 27.17 | 0.23 | 0.118 |
| | C 5 -Mn 16 | σ* | RY*( 6) | Mn 17 | 26.28 | 0.06 | 0.14 |
| | C 1 -Mn 17 | σ* | LP*( 1) | Mn 17 | 24.22 | 0.13 | 0.101 |
| | | | | | | | |
| B2 | C 2-C 3 | π | Mn 13 | LP*( 4) | 13.08 | 0.07 | 0.052 |
| | C 2-C 3 | π | Mn 13 | LP*( 5) | 12.65 | 0.27 | 0.07 |
| | C 3 | LP*( 1) | Mn 13 | LP*( 3) | 7.71 | 0.37 | 0.09 |
| | C 2 - C 3 | σ | Mn 13 | LP*( 2) | 7.09 | 0.83 | 0.099 |
| | C 3 | LP*( 1) | Mn 13 | LP*( 2) | 6.97 | 0.38 | 0.086 |
| | C 2 - H 12 | σ | Mn 13 | LP*( 2) | 4.35 | 0.68 | 0.07 |
| | C 2 | LP ( 1) | Mn 13 - O 15 | σ* | 4.24 | 0.29 | 0.055 |
| | C 3 - H 11 | σ | Mn 13 | LP*( 3) | 3.77 | 0.68 | 0.065 |
| | C 1 - C 2 | σ | Mn 13 | LP*( 2) | 3.18 | 0.84 | 0.067 |
| | C 2 | CR ( 1) | Mn 13 | LP*( 2) | 3.13 | 9.98 | 0.23 |
| | C 2 | LP ( 1) | Mn 13 - O 16 | BD*( 3) | 3.04 | 0.32 | 0.05 |
| | | | | | | | |
| B3 | C 1 - H 17 | σ | C 1 - O 8 | π | 17.93 | 0.86 | 0.069 |
| | C 2 | LP ( 1) | Mn 15 | LP*( 3) | 16.32 | 0.76 | 0.062 |
| | C 2 - H 11 | σ | Mn 15 | LP*( 4) | 3.07 | 0.5 | 0.049 |
| | C 1 - C 2 | σ | Mn 15 | LP*( 3) | 2.74 | 0.71 | 0.056 |

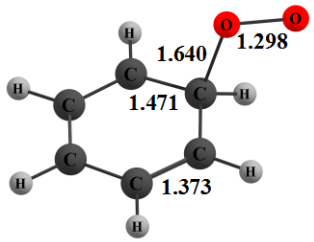
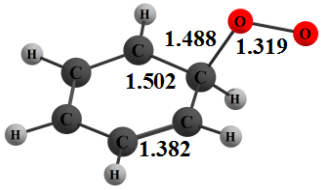
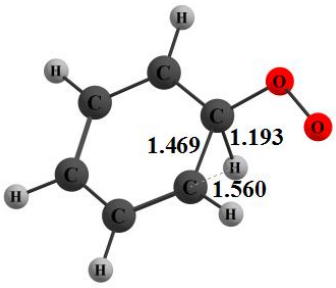
**Table S11.** Theoretical predictions of detailed energies of reactants and intermediates, transition states, and products in the oxidation reaction of the $C_6H_6$ and $Mn_2O_3$ cluster by the method PBE/6-311++g(d,p) (H, C, O)/LandL2DZ (Mn). ZPE energies are reported unscaled

| Species | Single point energy (a.u) | ZPE (a.u) | Etotal (au) | Erelative ($kcal.mol^{-1}$) |
|---|---|---|---|---|
| $C_6H_6$ | -231.9948881 | 0.0975380 | -231.897350 | |
| $O_2$ | -150.2295138 | 0.0035290 | -150.225985 | |
| $Mn_2O_3$ | -433.3495628 | 0.0092550 | -433.340308 | |

| | | | | |
|---|---|---|---|---|
| $H_2$ | -1.1658574 | 0.0098350 | -1.156022 | |
| hydroquinone | -382.3492791 | 0.1048390 | -382.244440 | |
| p-benzoquinone | -381.1178449 | 0.0819440 | -381.035901 | |
| catechol | -382.3531811 | 0.1051620 | -382.248019 | |
| o-benzoquinone | -381.1066674 | 0.0819050 | -381.024762 | |
| I16 | -814.5516306 | 0.0932920 | -814.536859 | |
| I33 | -814.5281548 | 0.0934940 | -814.536859 | |
| I34 | -814.5769315 | 0.0938350 | -814.536859 | |
| T33/34 | -814.49109455 | 0.092151 | -814.536859 | |
| I25 | -814.56763340 | 0.093741 | -814.536859 | |
| I17 | -814.55298028 | 0.092946 | -814.536859 | |
| $Mn_2O_3+C_6H_6$ | -665.34445089 | 0.106793 | -665.237658 | 0.00 |
| I1 | -665.41575774 | 0.107918 | -665.307840 | -44.04 |
| I2 | -665.39288121 | 0.107979 | -665.284902 | -29.65 |
| I3 | -665.39540081 | 0.10495800 | -665.290443 | -33.12 |
| I4 | -665.38332734 | 0.107233 | -665.276094 | -24.12 |
| I5 | -665.38431648 | 0.105339 | -665.278977 | -25.93 |
| I6 | -665.38236470 | 0.107042 | -665.275323 | -23.64 |
| I7 | -665.39392634 | 0.108440 | -665.285486 | -30.01 |
| T1/2 | -665.37556228 | 0.107021 | -665.268541 | -19.38 |
| T1/3 | -665.35199879 | 0.10230600 | -665.249693 | -7.55 |
| T1/5 | -665.34724324 | 0.101724 | -665.245519 | -4.93 |
| T2/7 | -665.36676236 | 0.106430 | -665.260332 | -14.23 |
| T3/4 | -665.36106411 | 0.105005 | -665.256059 | -11.55 |
| T5/6 | -665.32837194 | 0.104003 | -665.224369 | 8.34 |
| $I7+O_2$ | -815.62344012 | 0.111969 | -815.511471 | 0.00 |
| I8 | -815.69710340 | 0.11413200 | -815.582971 | -44.87 |
| I9 | -815.75573928 | 0.116584 | -815.639155 | -80.12 |
| I10 | -815.74170337 | 0.114277 | -815.627426 | -72.76 |
| I11 | -815.79645445 | 0.114568 | -815.681886 | -106.94 |
| I12 | -815.79826610 | 0.114591 | -815.683675 | -108.06 |
| I13 | -815.72432238 | 0.111632 | -815.612690 | -63.52 |
| I14 | -815.73275877 | 0.114504 | -815.618255 | -67.01 |
| I15 | -815.72880681 | 0.112064 | -815.616743 | -66.06 |
| I16 | -815.74674734 | 0.116115 | -815.630632 | -74.77 |
| I17 | -814.55298028 | 0.092946 | -814.460034 | 659.79 |
| T8/9 | -815.66214072 | 0.113950 | -815.548191 | -23.04 |
| T9/10 | -815.68630212 | 0.109725 | -815.576577 | -40.85 |

| | | | | |
|---|---|---|---|---|
| T10/11 | -815.68265808 | 0.112329 | -815.570329 | -36.93 |
| T11/12 | -815.75227518 | 0.113166 | -815.639109 | -80.09 |
| T12/13 | -815.70414637 | 0.11021100 | -815.593935 | -51.75 |
| T13/14 | -815.71202914 | 0.111296 | -815.600733 | -56.01 |
| T14/15 | -815.69419175 | 0.109609 | -815.584583 | -45.88 |
| T15/16 | -815.70230463 | 0.111387 | -815.590918 | -49.85 |
| T16/17 | -815.64810807 | 0.104643 | -815.543465 | -20.08 |
| PR1 | -815.63326516 | 0.101034 | -815.532231 | -13.03 |
| I2+$O_2$ | -815.62239499 | 0.111508 | -815.510887 | 0.00 |
| I18 | -815.69256893 | 0.11483900 | -815.577730 | -41.94 |
| I19 | -815.74175172 | 0.11605700 | -815.562628 | -32.47 |
| I20 | -815.73822655 | 0.113714 | -815.558790 | -30.06 |
| I21 | -815.73649615 | 0.115766 | -815.620730 | -68.93 |
| I22 | -815.75826667 | 0.114534 | -815.643733 | -83.36 |
| I23 | -815.72538958 | 0.112245 | -815.613145 | -64.17 |
| I24 | -815.74674729 | 0.116115 | -815.630632 | -75.14 |
| I25+$H_2$ | -815.73349084 | 0.103576 | -815.629915 | -74.69 |
| T18/19 | -815.68447945 | 0.113774 | -815.570705 | -37.54 |
| T19/20 | -815.67802063 | 0.108980 | -815.569041 | -36.49 |
| T20/21 | -815.69083423 | 0.113243 | -815.577591 | -41.86 |
| T21/22 | -815.72273166 | 0.112091 | -815.610641 | -62.60 |
| T22/23 | -815.68058222 | 0.10841400 | -815.572168 | -38.45 |
| T23/24 | -815.71117240 | 0.110497 | -815.600675 | -56.34 |
| T24/25 | -815.64799090 | 0.10464300 | -815.543348 | -20.37 |
| PR2 | -815.63326516 | 0.101034 | -815.532231 | -13.39 |
| I4+$O_2$ | -815.61284112 | 0.110762 | -815.502079 | 0.00 |
| I26 | -815.71150299 | 0.113873 | -815.597630 | -59.96 |
| I27 | -815.70830652 | 0.113694 | -815.577278 | -47.19 |
| I28 | -815.78185285 | 0.114591 | -815.568516 | -41.69 |
| I29 | -815.75488792 | 0.115052 | -815.639836 | -86.44 |
| I30 | -815.76598297 | 0.115691 | -815.650292 | -93.01 |
| I31 | -815.77165060 | 0.116361 | -815.655290 | -96.14 |
| I32 | -815.77967045 | 0.114812 | -815.664858 | -102.15 |
| I33+$H_2$ | -815.69401226 | 0.103329 | -815.590683 | -55.60 |
| I34+$H_2$ | -815.74278891 | 0.103670 | -815.639119 | -85.99 |
| T26/27 | -815.70635905 | 0.110380 | -815.595979 | -58.92 |
| T26/31 | -815.65926961 | 0.113067 | -815.546203 | -27.69 |
| T27/28 | -815.69533858 | 0.111670 | -815.583669 | -51.20 |

| | | | | |
|---|---|---|---|---|
| T28/29 | -815.69948142 | 0.109362 | -815.590119 | -55.25 |
| T29/30 | -815.70179405 | 0.113747 | -815.588047 | -53.95 |
| T31/32 | -815.76745069 | 0.111685 | -815.655766 | -96.44 |
| T31/33 | -815.67478976 | 0.106530 | -815.568260 | -41.53 |
| T32/33 | -815.66596753 | 0.105103 | -815.5608645 | -36.89 |
| T33/34+$H_2$ | -815.65695199 | 0.101986 | -815.5549660 | -33.19 |
| PR4 | -815.62208765 | 0.100995 | -815.5210927 | -11.93 |
| PR3 | -815.70274395 | 0.114417 | -815.5883270 | -54.12 |
| I6+$O_2$ | -815.61187848 | 0.110571 | -815.5013075 | 0.00 |
| I35 | -815.70790882 | 0.113939 | -815.5939698 | -58.15 |
| I36 | -815.76565888 | 0.115544 | -815.5969370 | -60.01 |
| I37 | -815.78194739 | 0.114482 | -815.5609690 | -37.44 |
| I38 | -815.75257278 | 0.115637 | -815.6369358 | -85.11 |
| T35/36 | -815.67560542 | 0.112822 | -815.5627834 | -38.58 |
| T36/37 | -815.70500752 | 0.109885 | -815.5951225 | -58.87 |
| T37/38 | -815.70456684 | 0.114260 | -815.5903068 | -55.85 |
| PR1 | -815.70274395 | 0.114417 | -815.5883270 | -54.61 |
| I1+$O_2$ | -815.64527152 | 0.111447 | -815.5338245 | 0.00 |
| I39 | -815.69371054 | 0.114681 | -815.5790295 | -28.37 |
| I40 | -815.75549522 | 0.114911 | -815.6405842 | -66.99 |
| I41 | -815.69194829 | 0.110692 | -815.5812563 | -29.76 |
| I42 | -815.75448750 | 0.115623 | -815.6388645 | -65.91 |
| I43 | -815.69531705 | 0.113011 | -815.5823061 | -30.42 |
| I44 | -815.76227097 | 0.115897 | -815.6463740 | -70.63 |
| T39/40 | -815.68391526 | 0.113157 | -815.5707583 | -23.18 |
| T40/41 | -815.68415018 | 0.107951 | -815.5761992 | -26.59 |
| T41/42 | -815.68485819 | 0.111555 | -815.5733032 | -24.77 |
| T42/43 | -815.68450310 | 0.109179 | -815.5753241 | -26.04 |
| T43/44 | -815.68454967 | 0.112466 | -815.5720837 | -24.01 |
| PR1 | -815.69884190 | 0.114094 | -815.5847479 | -31.95 |

| | | |
|---|---|---|
|  |  |  |
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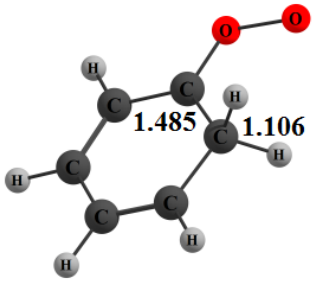
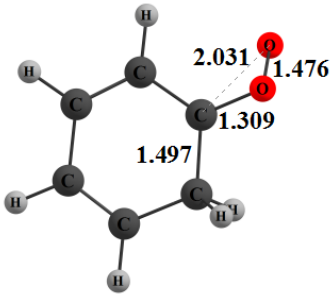
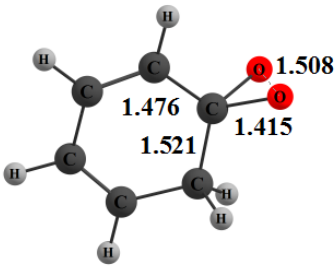
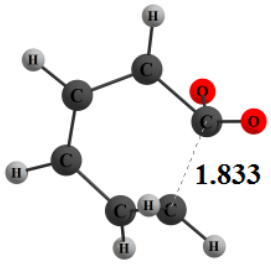
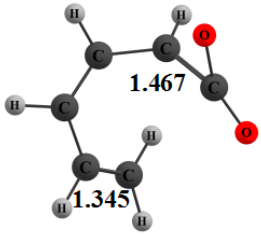
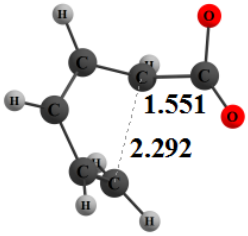
|  |  |  |
| **I2g, 14.41** | **T2g/3g, 47.60** | **I3g, 12.36** |
|  |  |  |
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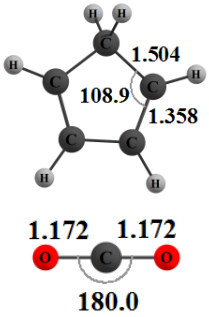
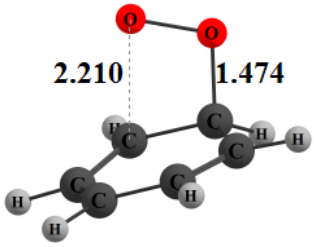
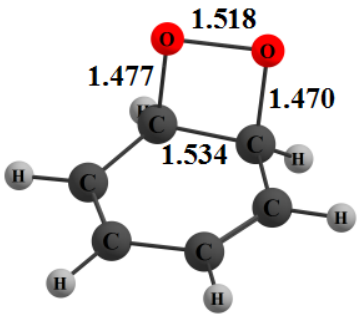
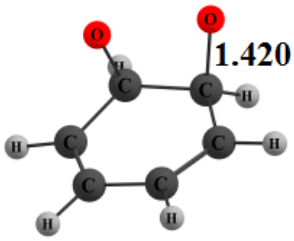
|  | | |
| **PR1g, -76.77** | | |
|  |  |  |
| **T0g/5g, 53.01** | **I5g, 28.40** | **T5g/6g, 47.20** |

| | | |
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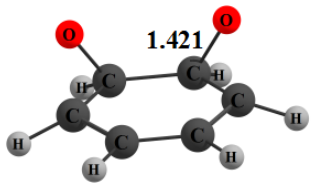
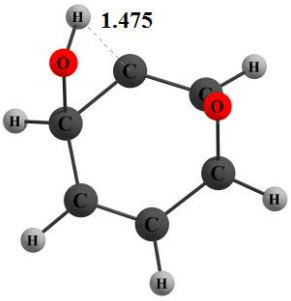
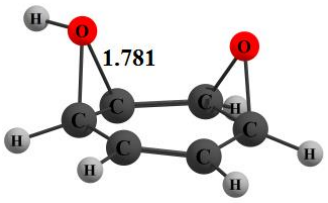
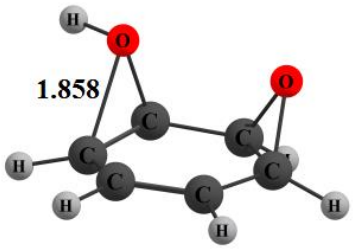
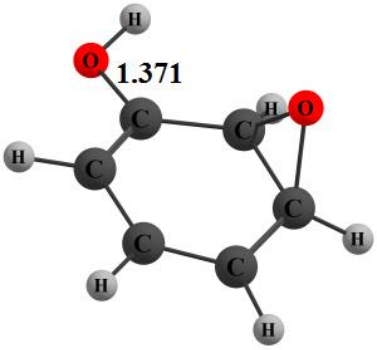
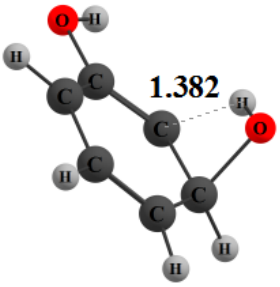
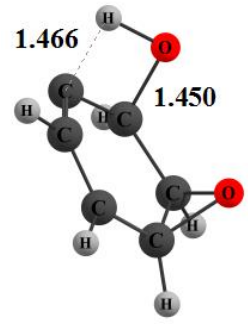
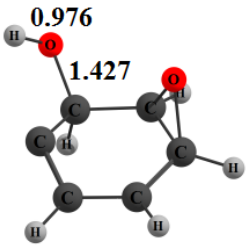
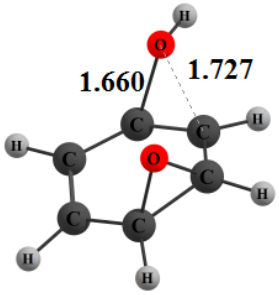
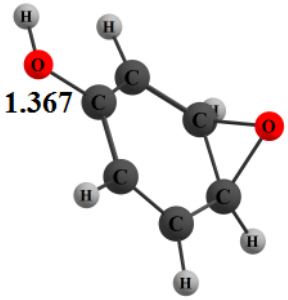
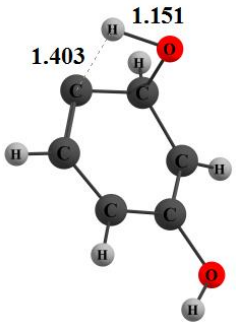
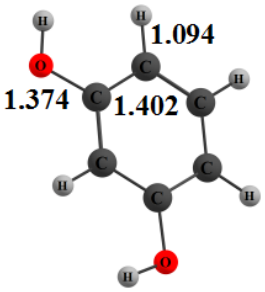
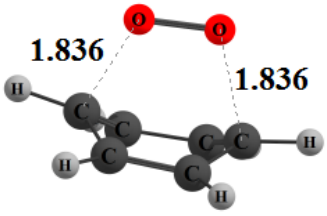
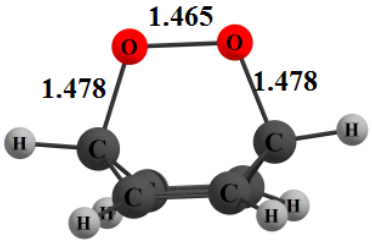
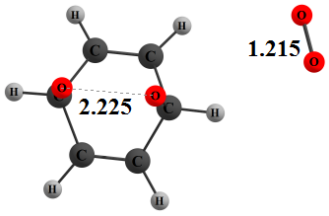
|  |  |  |
| **I6g, -11.34** | **T6g/7g, 52.86** | **I7g, 51.58** |
|  |  |  |
| **T7g/8g, 56.52** | **I8g, -33.73** | **T8gP2g, 22.57** |
|  |  |  |
| **T6g/9g, 49.08** | **I9g, 35.01** | **T9g/10g, 57.84** |
|  |  |  |
| **I10g, -34.27** | **T10gP2g, 26.83** | **PR2g, -77.92** |
|  |  |  |
| **T0/11g, 35.86** | **I11g, 28.0** | **T11g/COM, 21.91** |

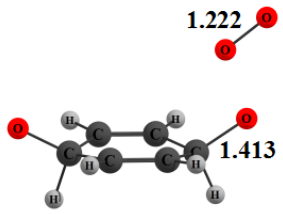
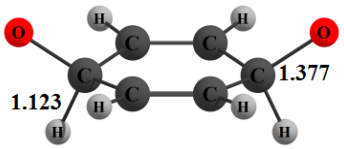
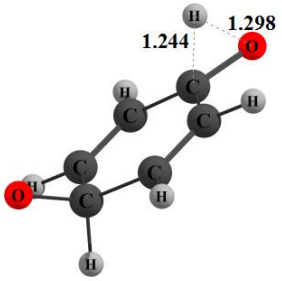
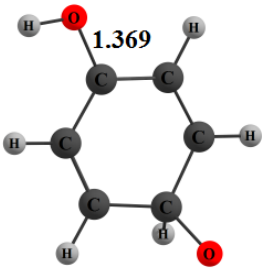
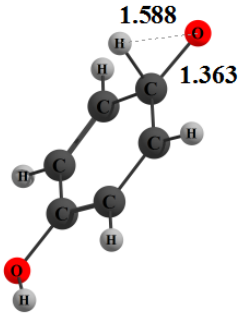
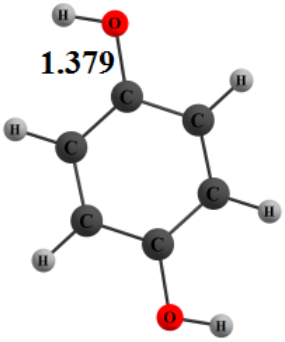
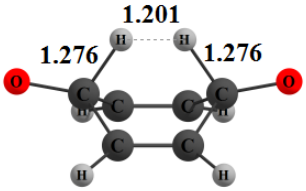
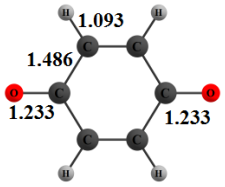
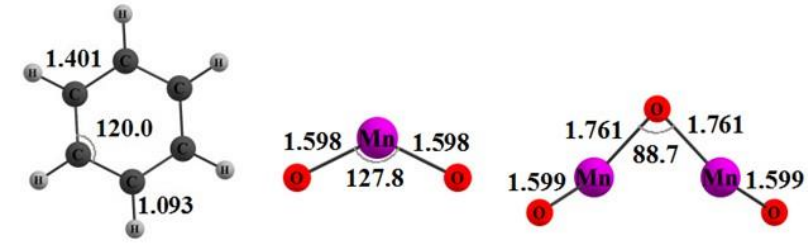
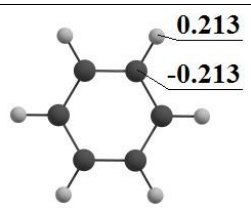
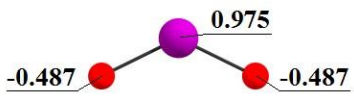
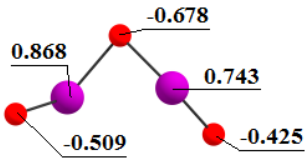
| | | |
|---|---|---|
|  |  |  |
| **COM, 6.41** | **I12g, 39.20** | **T12g/13g, 51.59** |
|  |  |  |
| **I13g, 3.63** | **T13gP4g, 27.14** | **PR4g, -75.99** |
|  |  +$H_2$ | |
| **T12gP3g, 49.56** | **PR3g, -43.04** | |

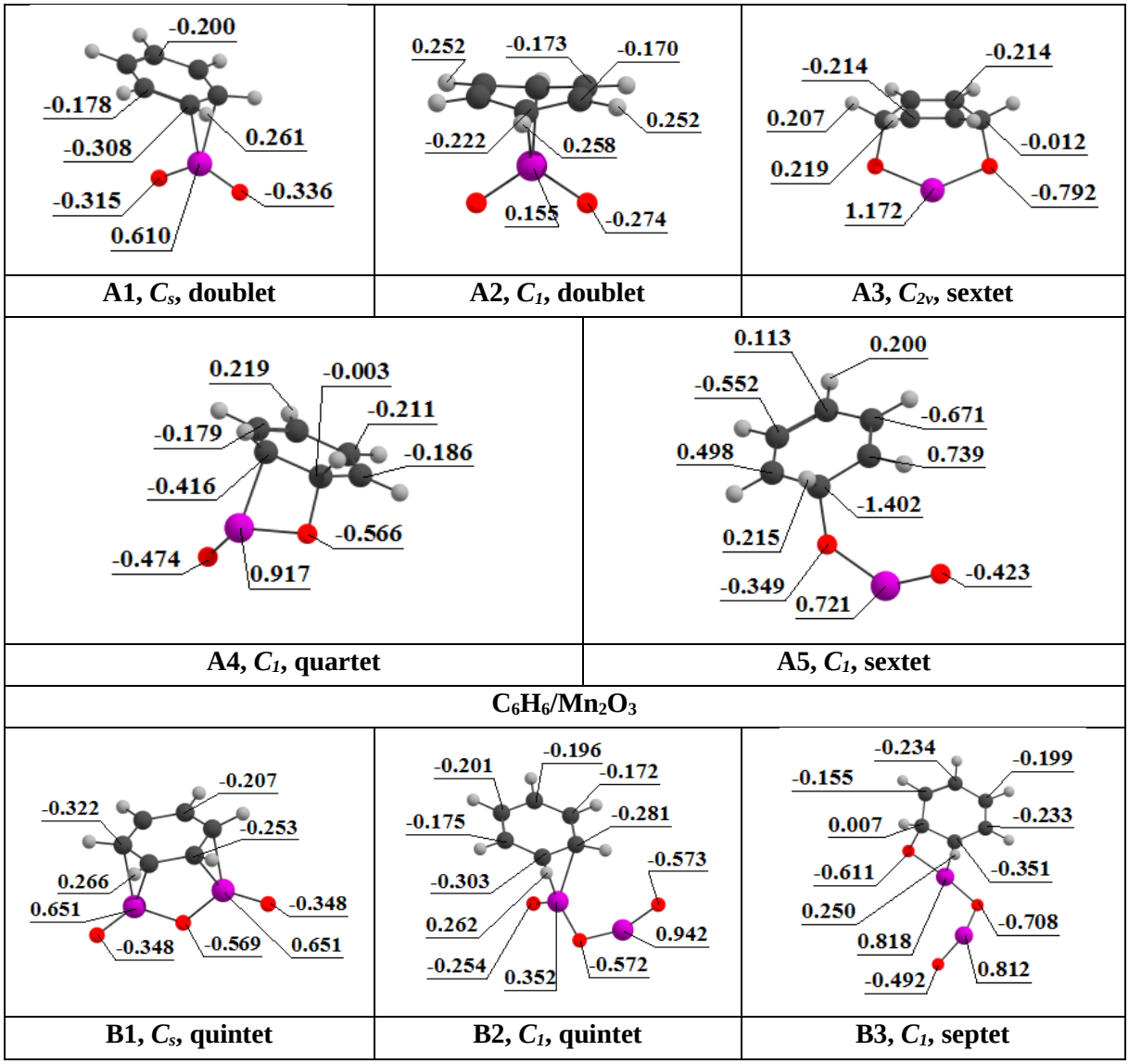
**Figure S1.** Optimized geometries of the intermediates and transition states of the $C_6H_6$ + $O_2$ reaction in the gas phase.




$C_6H_6$, $D_{6h}$, singlet $MnO_2$, $C_{2v}$, quartet $Mn_2O_3$, $C_2$, septet

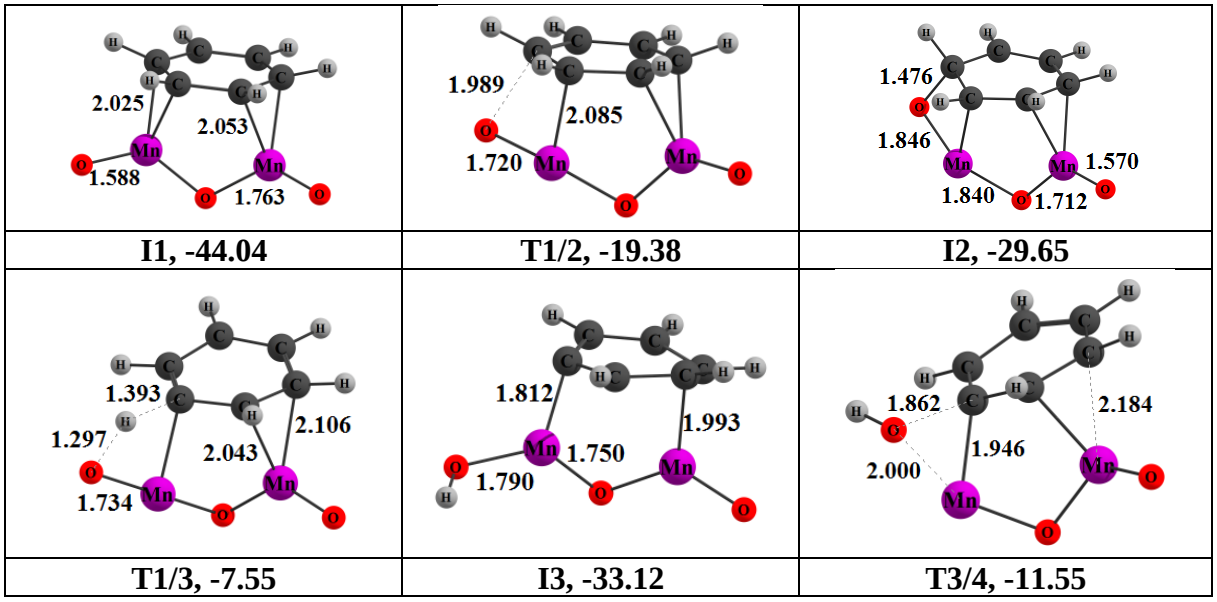
**Figure S2.** The structures, point group symmetry, and the spin multiplicity of $MnO_x$ and $C_6H_6$

| $C_6H_6/MnO_2$ | | |
|---|---|---|
|  |  |  |
| **$C_6H_6$, $D_{6h}$, singlet** | **$MnO_2$, $C_{2v}$, quartet** | **$Mn_2O_3$, $C_1$, septet** |

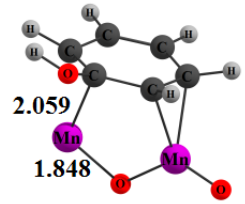
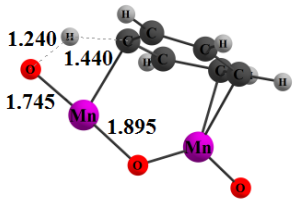
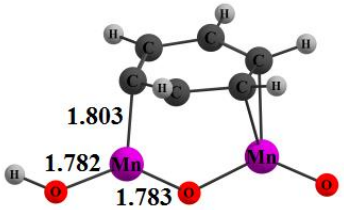
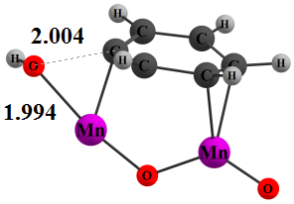
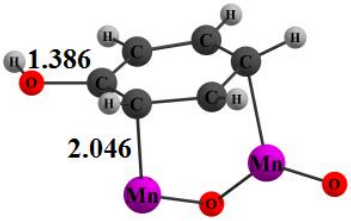
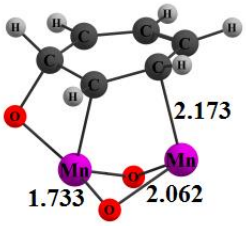
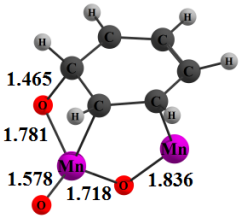
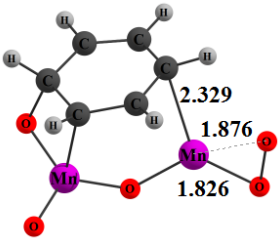
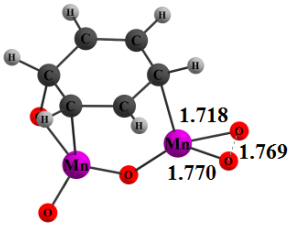
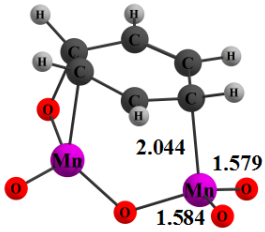
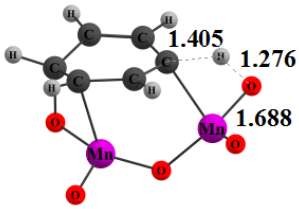
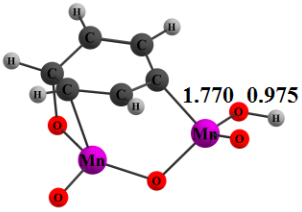
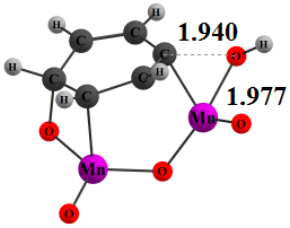
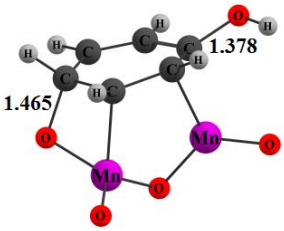
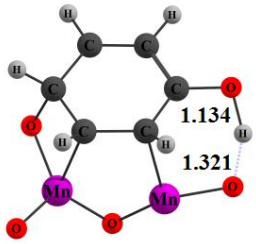
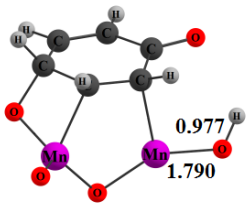
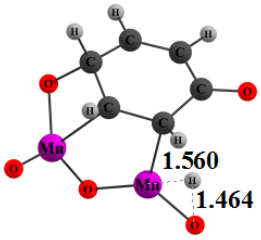
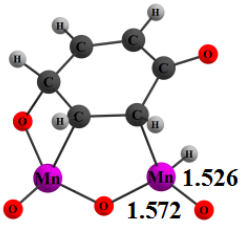


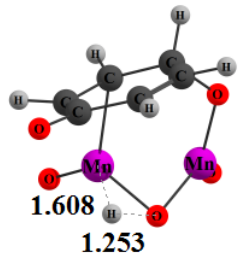
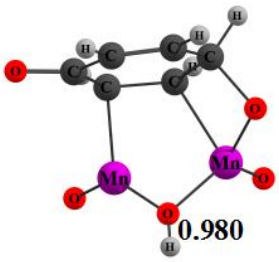
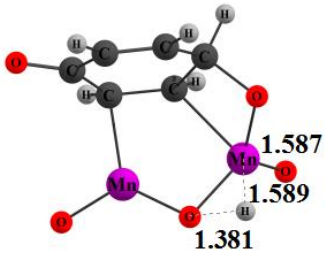
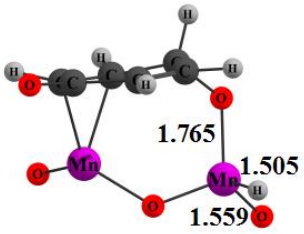
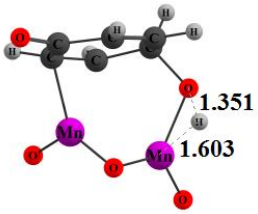
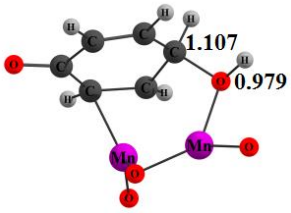
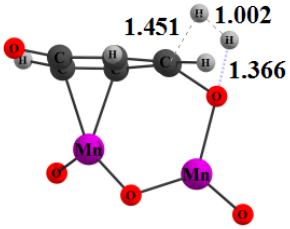
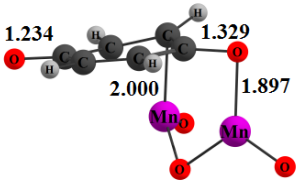
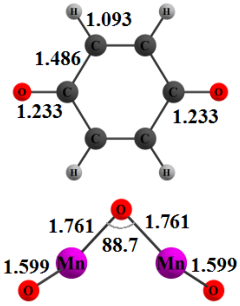
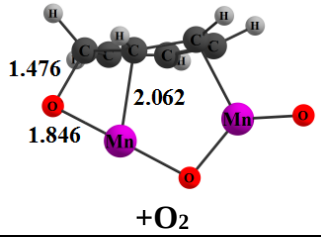
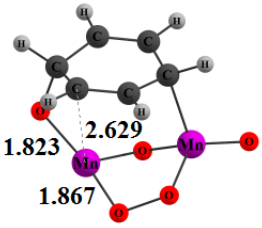
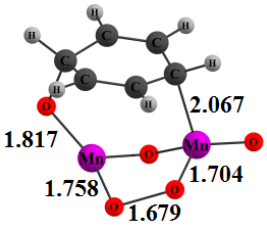
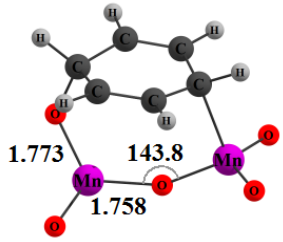
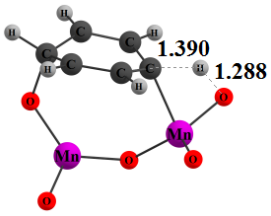
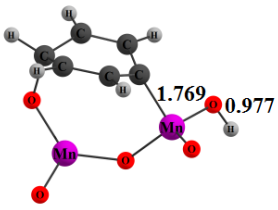
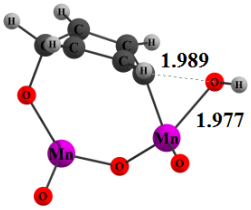
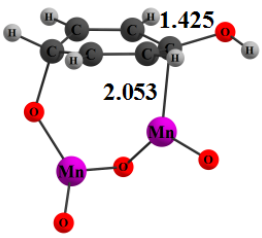
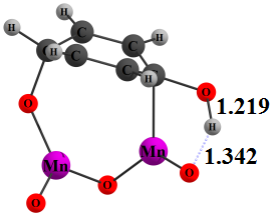

| A1, $C_s$, doublet | A2, $C_1$, doublet | A3, $C_{2v}$, sextet |
|---|---|---|
| A4, $C_1$, quartet | A5, $C_1$, sextet | |
| $C_6H_6/Mn_2O_3$ | | |
| B1, $C_s$, quintet | B2, $C_1$, quintet | B3, $C_1$, septet |

**Figure S3.** The comparison of the atomic charges of the $C_6H_6/MnO_2$ and $C_6H_6/Mn_2O_3$ systems obtained by NPA analysis. The unit of the charge is one electron charge e




| I1, -44.04 | T1/2, -19.38 | I2, -29.65 |
|---|---|---|
| T1/3, -7.55 | I3, -33.12 | T3/4, -11.55 |

| | | |
|---|---|---|
|  |  |  |
| **I4, -24.12** | **T1/5, -4.93** | **I5, -25.93** |
|  |  |  |
| **T5/6, 8.34** | **I6, -23.64** | **T2/7, -14.23** |
|  |  |  |
| **I7, -30.01** | **I8, -44.87** | **T8/9, -23.04** |
|  |  |  |
| **I9, -80.12** | **T9/10, -37.02** | **I10, -71.13** |
|  |  |  |
| **T10/11, -34.40** | **I11, -83.92** | **T11/12, -80.09** |
|  |  |  |
| **I12, -108.06** | **T12/13, -51.75** | **I13, -63.52** |

| | | |
|---|---|---|
|  |  |  |
| **T13/14, -56.01** | **I14, -67.01** | **T14/15, -45.88** |
|  |  |  |
| **I15, -66.06** | **T15/16, -49.85** | **I16, -74.48** |
|  |  |  |
| **T16/17, -20.06** | **I17 + $H_2$, -65.63** | **PR1, -13.03** |
|  |  |  |
| **I2+$O_2$, 0.00** | **I18, -41.94** | **T18/19, -37.54** |
|  |  |  |
| **I19, -72.04** | **T19/20, -36.49** | **I20, -71.30** |
|  |  |  |
| **T20/21, -41.86** | **I21, -68.93** | **T21/22, -62.60** |

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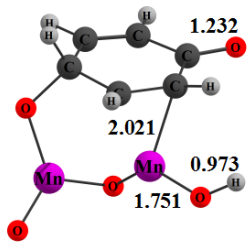
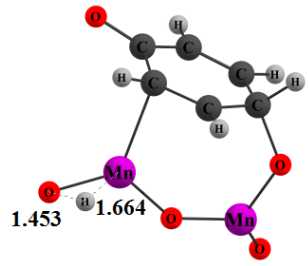
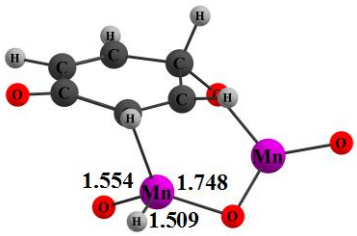
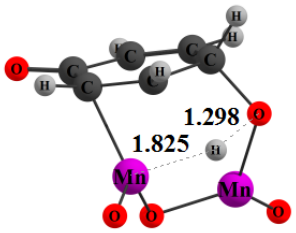
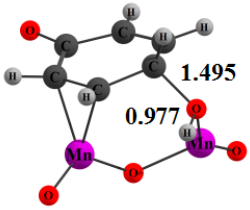
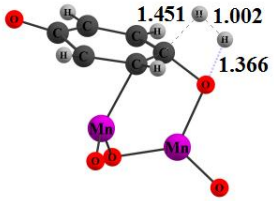
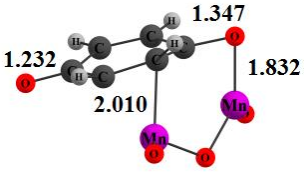
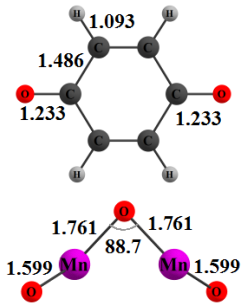
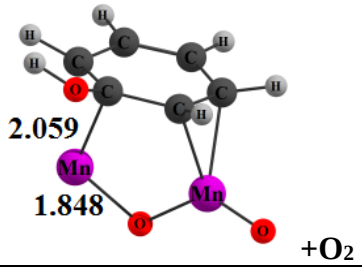
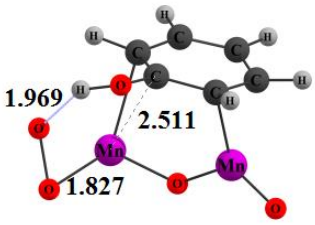
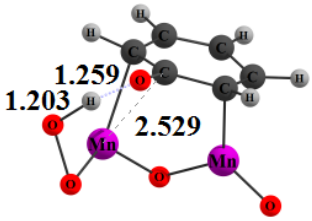
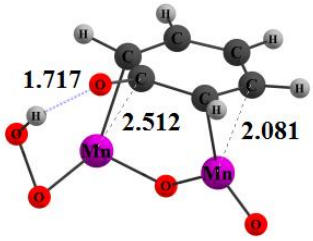
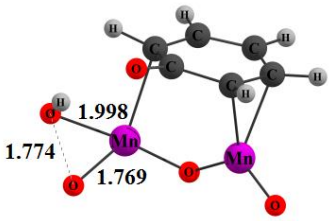
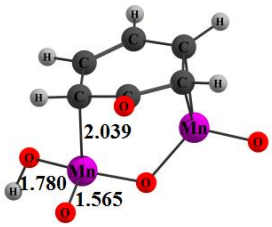
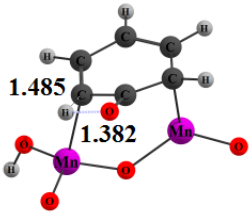
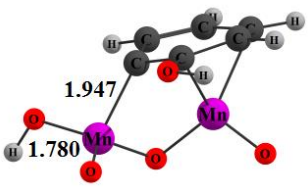
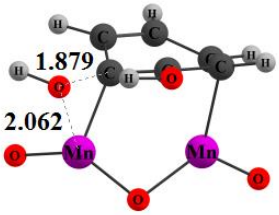
|  |  |  |
| **I22, -83.36** | **T22/23, -38.45** | **I23, -64.17** |
|  |  |  |
| **T23/24, -56.34** | **I24, -74.78** | **T24/25, -20.37** |
|  |  $H_2$ | |
| **I25+$H_2$, -74.69** | **PR1, -13.39** | |
|  +$O_2$ |  |  |
| **I4+$O_2$, 0.00** | **I26, -59.96** | **T26/27, -58.92** |
|  |  |  |
| **I27, -58.07** | **T27/28, -51.20** | **I28, -103.65** |
|  |  |  |
| **T28/29, -55.25** | **I29, -86.44** | **T29/30, -53.95** |

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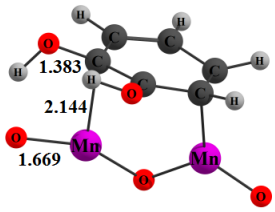
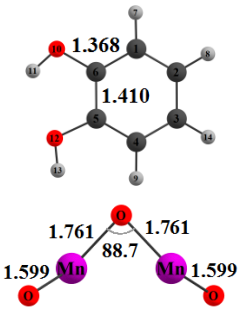
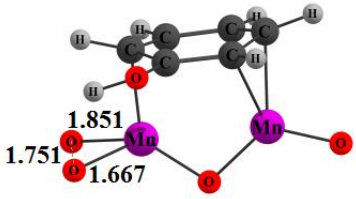
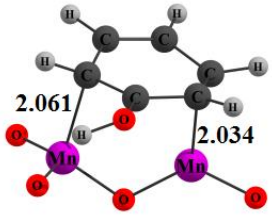
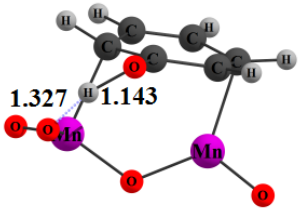
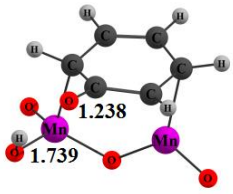
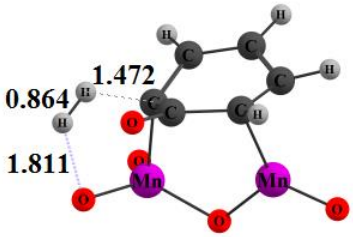
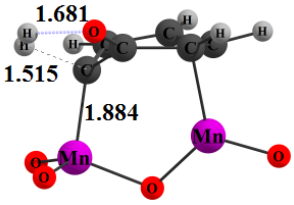
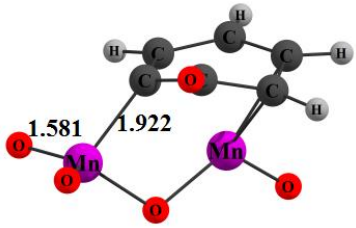
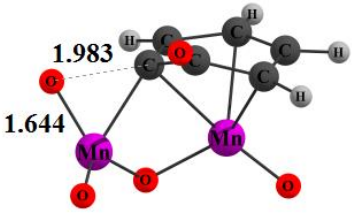
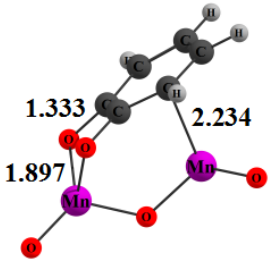
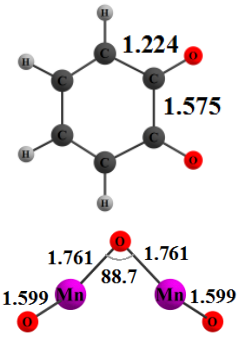
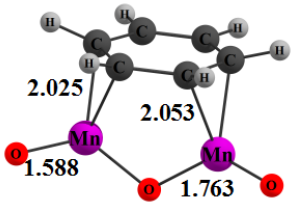
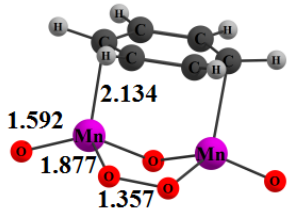
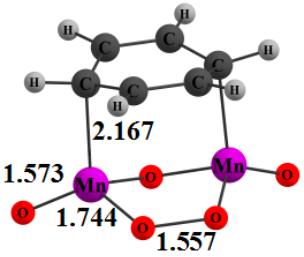
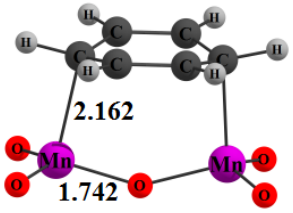
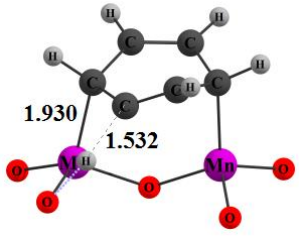
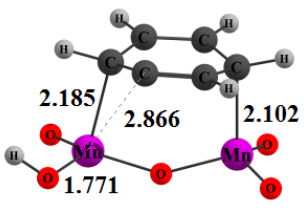
|  |  |  |
| **I30, -93.01** | **PR2, -54.12** | **T26/31, -27.69** |
|  |  |  |
| **I31, -96.14** | **T31/32, -96.44** | **I32, -102.15** |
|  |  |  |
| **T32/33, -36.89** | **T31/33, -41.53** | **I33+$H_2$, -55.60** |
|  |  |  |
| **T33/34+$H_2$,** | **I34+$H_2$, -85.99** | **PR3, -11.93** |
|  |  |  |
| **I1+$O_2$, 0.00** | **I39, -28.37** | **T39/40, -23.18** |
|  |  |  |
| **I40, -66.99** | **T40/41, -26.59** | **I41, -29.76** |

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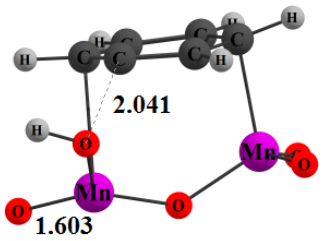
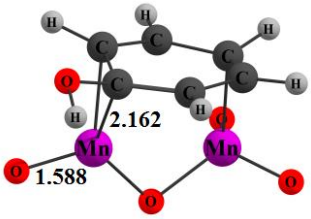
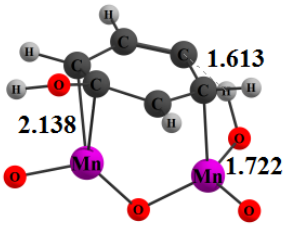
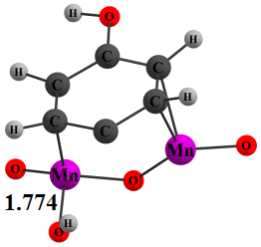
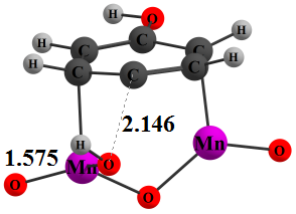
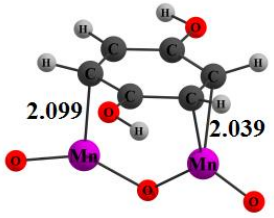
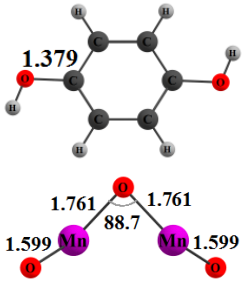
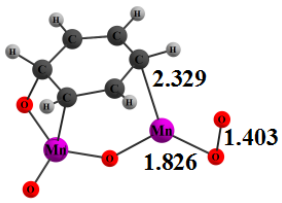
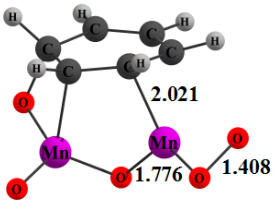
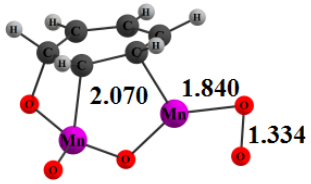
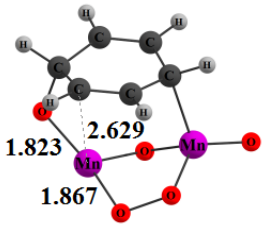
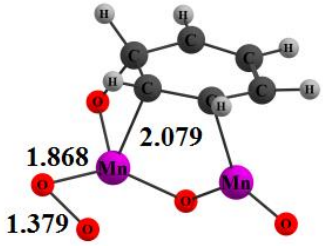
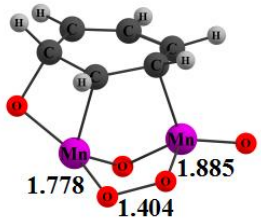
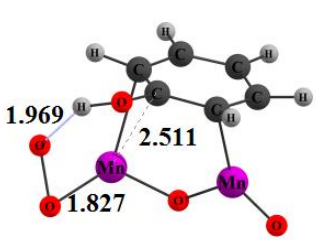
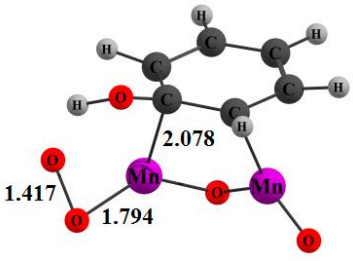
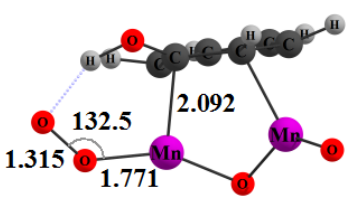
|  |  |  |
| **T41/42, -24.77** | **I42, -65.91** | **T42/43, -26.04** |
|  |  |  |
| **I43, -30.42** | **T43/44, -24.01** | **I44, -70.63** |
|  | | |
| **PR4, -31.95** | | |

**Figure S4.** Optimized geometries (length is in Å and angle is in degree) of the reactants, transition states, and intermediates of the $C_6H_6 + O_2$ reaction assisted by the $Mn_2O_3$ cluster at the PBE/6-311++G(d,p)/LanL2DZ level. (Energy values in parenthesis are in kcal.mol$^{-1}$)

| **I7 + $O_2$** | | |
|---|---|---|
|  |  |  |
| **I8a, -44.87** | **I8b, -35.35** | **I8c, -31.65** |
|  |  |  |
| **I18a, -41.94** | **I18b, -32.47** | **I18c, -30.06** |
|  |  |  |

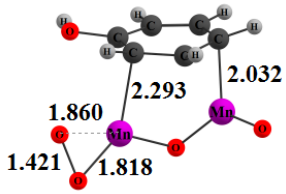
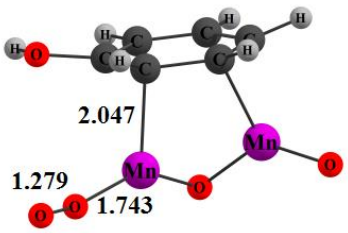
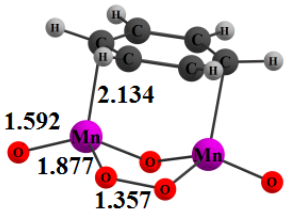
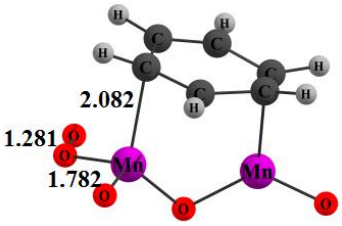
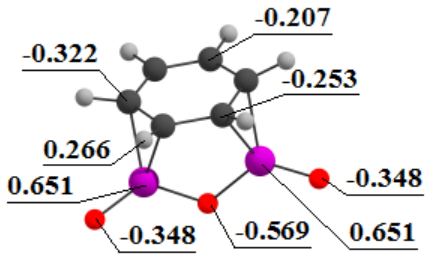
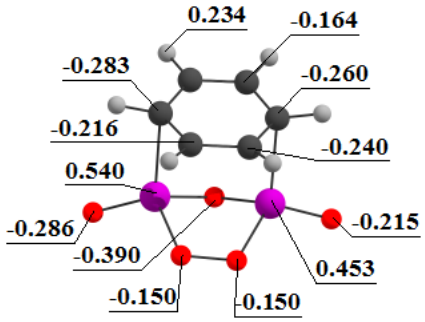
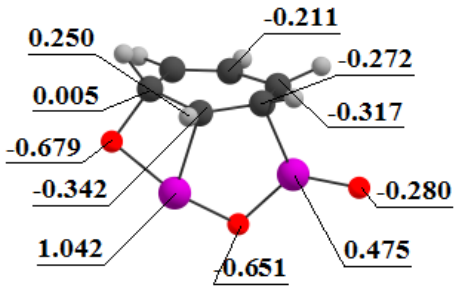
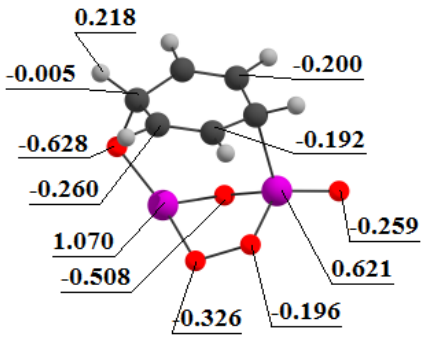
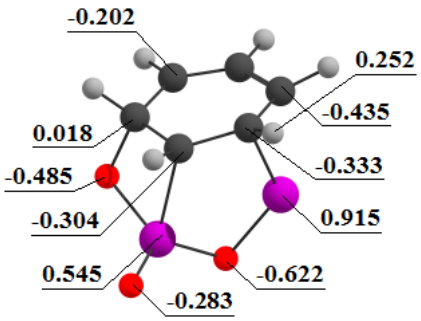
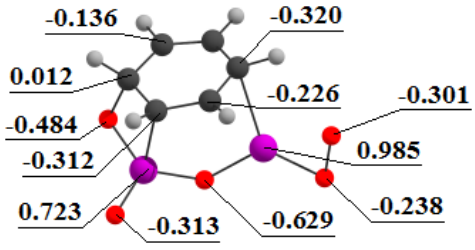
| I26a, -59.96 | I26b, -47.19 | I26c, -41.69 |
|---|---|---|
|  |  | |
| **I35a, -58.15** | **I35b, -37.44** | |
|  |  | |
| **I39b, -28.37** | **I39b, -14.80** | |

**Figure S5.** The structures and relative energy (kcal.mol$^{-1}$) of interaction configuration when $O_2$ interact with I7, I2, I4, I6, and I1

| | |
|---|---|
|  |  |
| I1 | I39 |
|  |  |
| I2 | I18 |
|  |  |
| I7 | I8 |

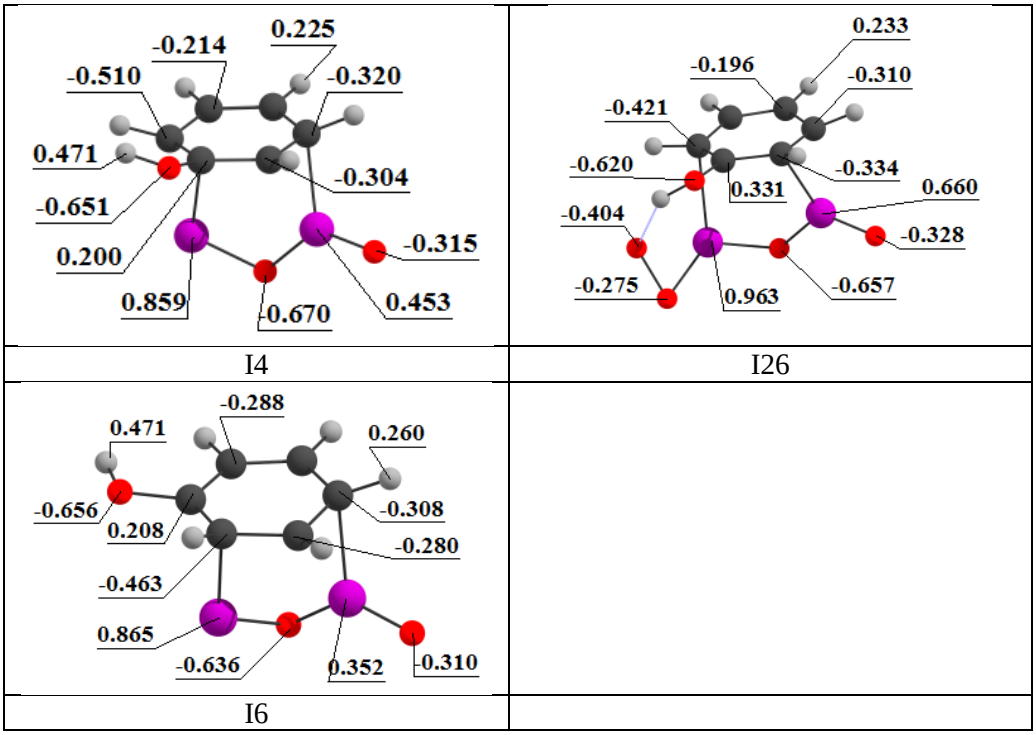



**Figure S6.** Atomic charges obtained by NPA analysis of the structures of transition states, intermediates and products appeared in the paths plotted in Fig. 6. The unit of the charge is one electron charge e

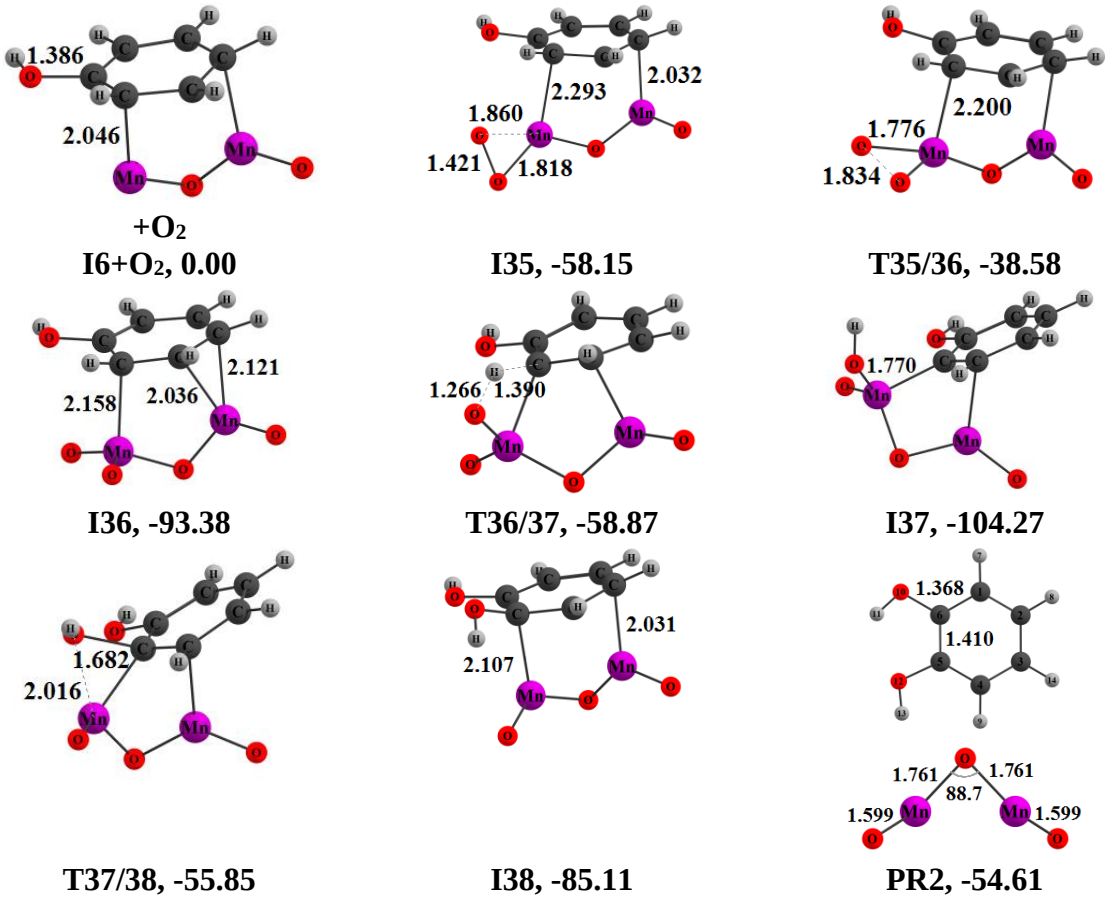



**Figure S7.** Optimized geometries (length is in Å and angle is in degree) of the reactants, transition states and intermediates of I6 + $O_2$ pathways at the PBE/6-311++G(d,p)/LanL2DZ level. (Energy values in parenthesis are in kcal.mol$^{-1}$)

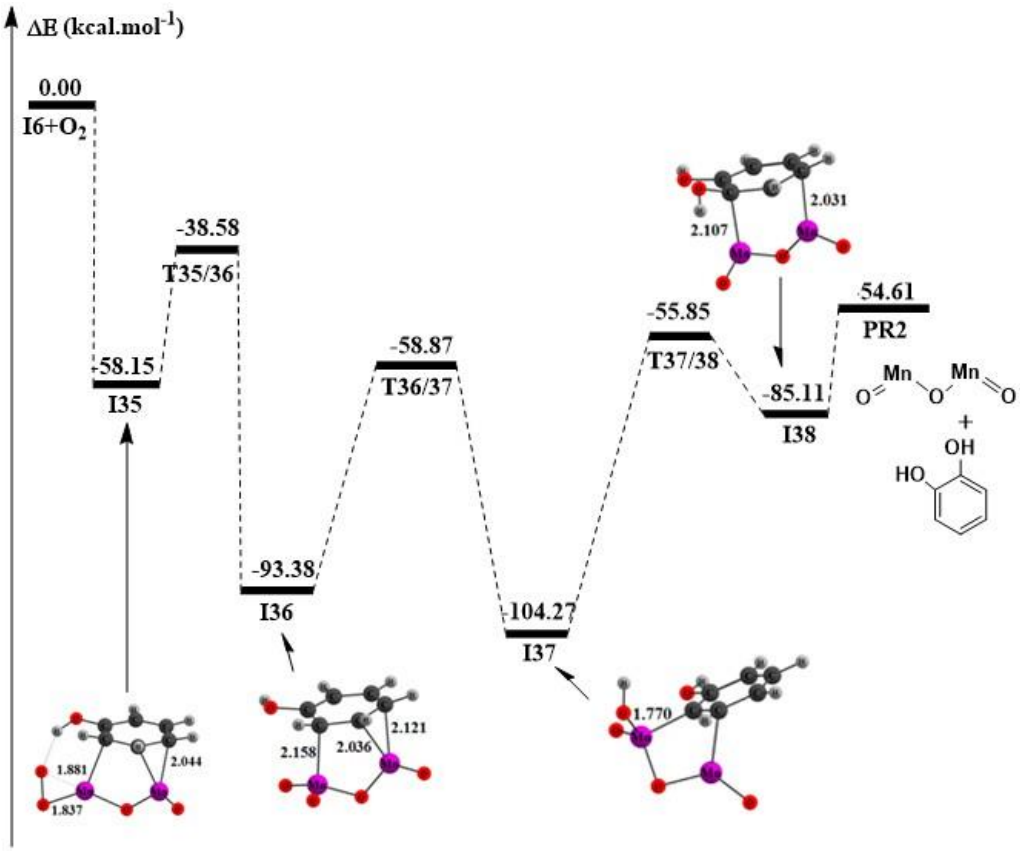



**Figure S8.** Profile of potential energy profile for the subsequent reaction pathways of I6 with $O_2$ at the PBE/6-311++G(d,p)/LanL2DZ level

### 3.3.2. Subsequent reactions of intermediates with triplet $O_2$

***Subsequent reactions of I6 with $O_2$***

The following paragraphs displayed in italics are only reported in the SI file.

*Similar to I4, the preferential adsorption site of $O_2$ when interacting with I6 is an unsaturated Mn site, leading to form I35 which lies 58.15 kcal.mol$^{-1}$ under the reactants. From I35, I36 is born corresponding to the cleavage O-O bond via T36/37 with a barrier height of 19.57 kcal.mol$^{-1}$. As compared to I35, I36 is more stable as its relative energy is lower than I35 by 35.23 kcal.mol$^{-1}$. After the T36/37, the migration H atom attaches the C site to the O atom forming the structure of I38. In T37/38, the Mn-O bond is stretched to 2.016 Å from 1.770 Å in oxide (see Fig. 12) leading to form I38 which lies at 85.11 kcal.mol$^{-1}$ below the reactants and is similar to the geometry of I30. Finally, the catechol molecule in I38 is free from the surface of the oxide with an endothermicity of 38.88 kcal.mol$^{-1}$. The $Mn_2O_3$ molecule comes back to the initial state for the next catalytic cycle.*