Electronic Supplementary Information

# Does the Photoredox Reaction Effect the Photorelease of Anthraquinone Protected Benzaldehyde? A Time-Resolved Spectroscopic Study

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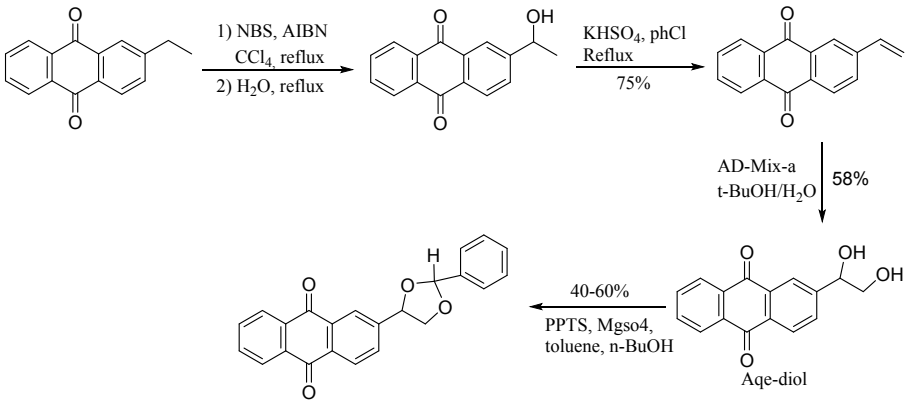



**Scheme S1.** The synthetic route of the compound **1**.

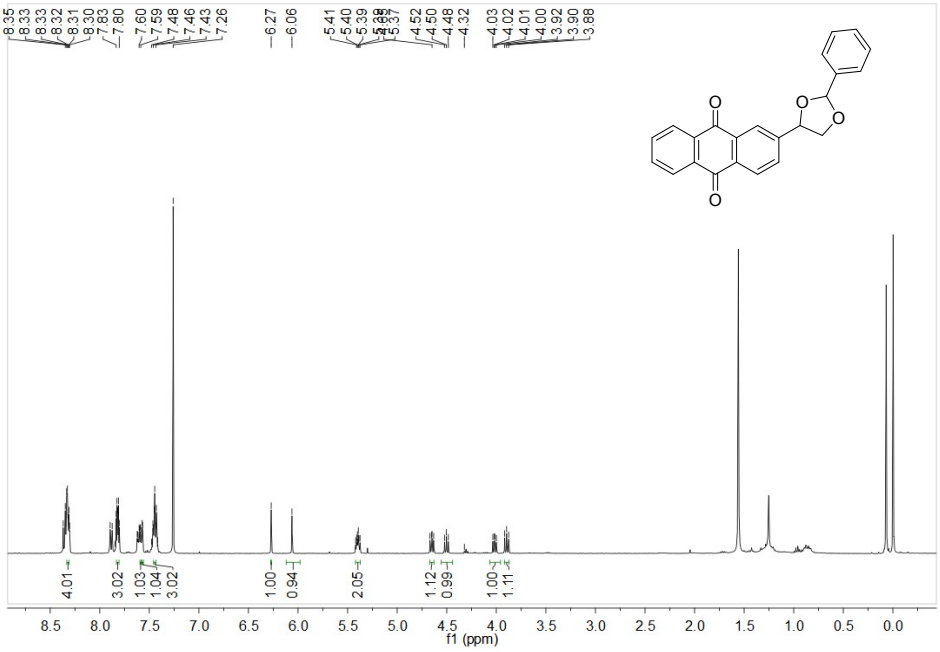



**Fig. S1** The $^1$H NMR spectra of **1** in $CDCl_3$.

$^1$H NMR ($CDCl_3$, 400 MHz): δ 3.87-3.91 (t, 1H, J=8.2 HZ), 3.99-4.04 (q, 1H, J=8.4, 7.7 HZ), 4.47-4.52 (t, 1H,J=7.8 HZ), 4.62-4.67 (q, 1H, J=8.4, 6.5 HZ), 5.36-5.42 (m, 1H,), 6.06 (s, 1H,), 6.27 (s, 1H), 7.42-7.46 (m, 3H), 7.56-7.61 (m, 2H), 7.80-7.83 (m, 3H), 8.31-8.33 (m, 4H)

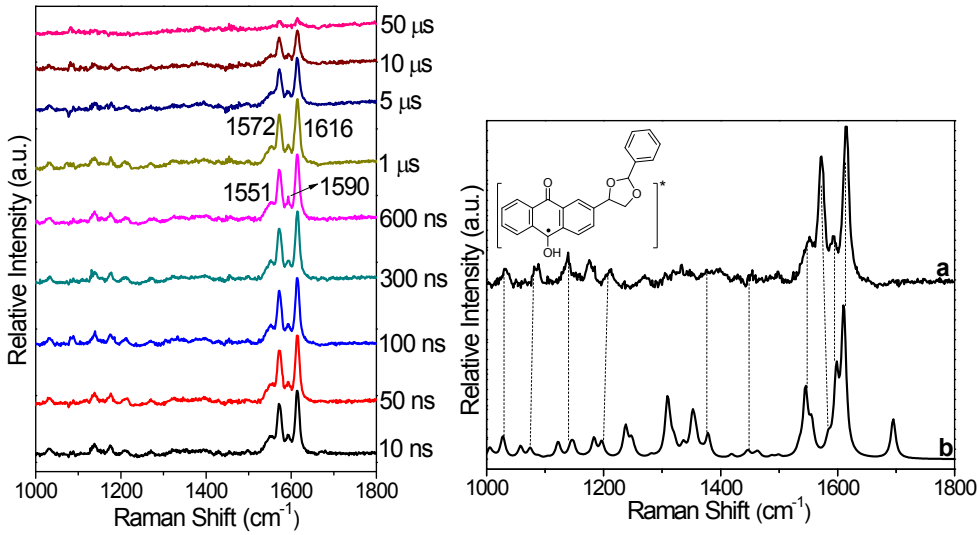



**Fig. S2** (Left) the ns-TR$^3$ spectra of **1** in IPA obtained at various time delays upon 266 nm irradiation and a 368.9 nm laser probe. (Right) Comparison of (a) the ns-TR$^3$ spectrum recorded at 50 ns with (b) the calculated normal Raman spectrum of the ketyl radical species of Aqe-diol (the scale factor is 1.0 and the half-width is 8 cm$^{-1}$) with its chemical structure shown in the figure.

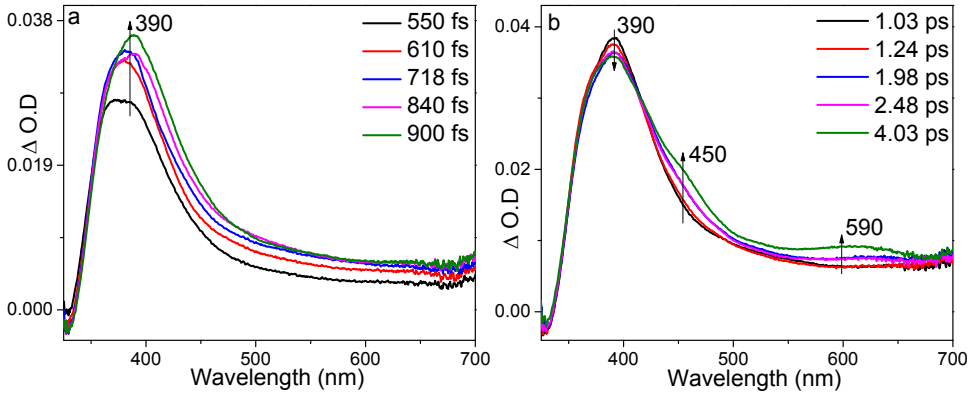



**Fig. S3** Fs-TA results acquired after 355 nm photoexcitation of **1** in ACN-PBS (1:1, v: v).

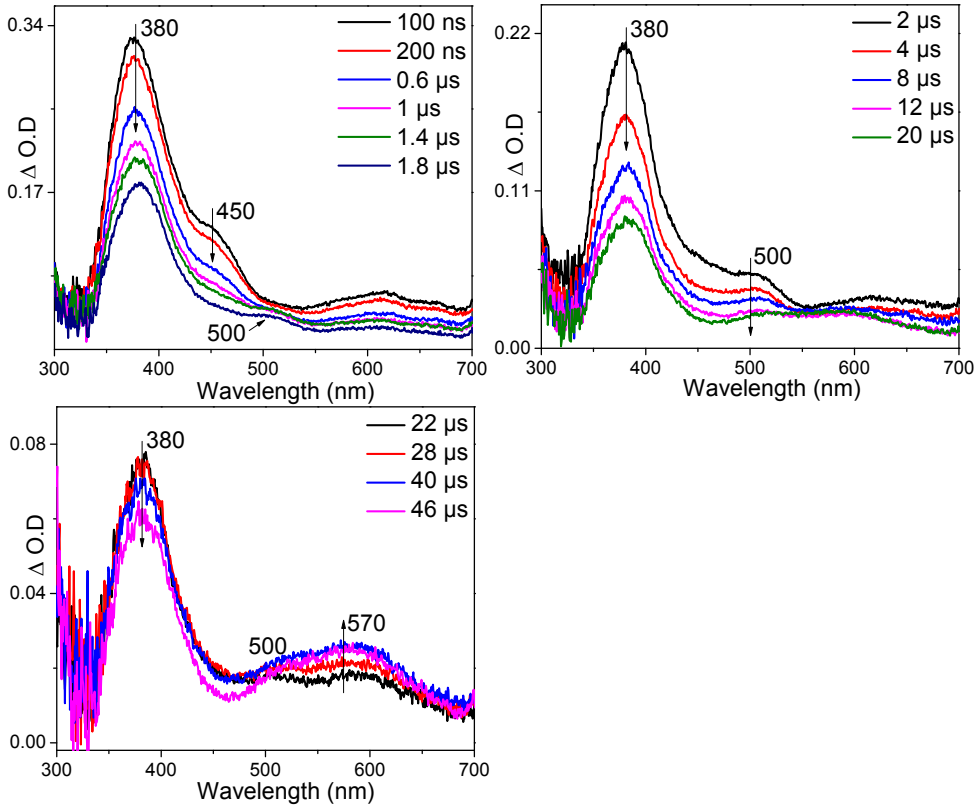



**Fig. S4** Ns-TA results acquired after 355 nm photoexcitation of **1** in ACN-PBS (9:1, v: v) under deoxygenated condition.

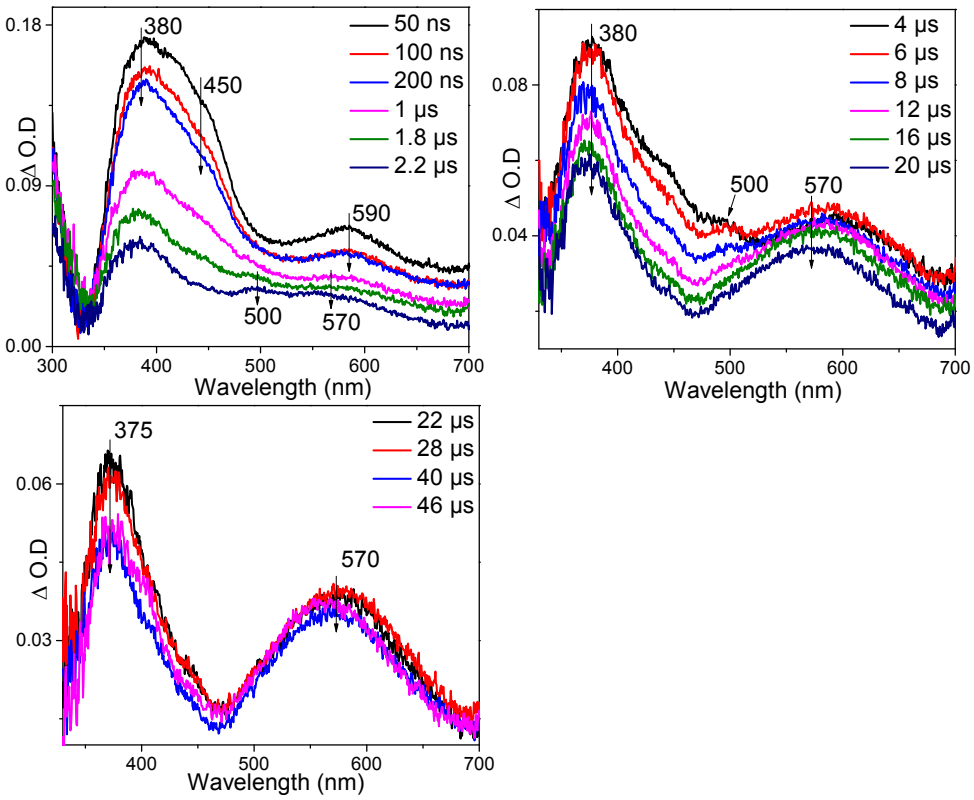



**Fig. S5** Ns-TA results acquired after 355 nm photoexcitation of **1** in ACN-PBS (1:9, v: v) under deoxygenated condition.

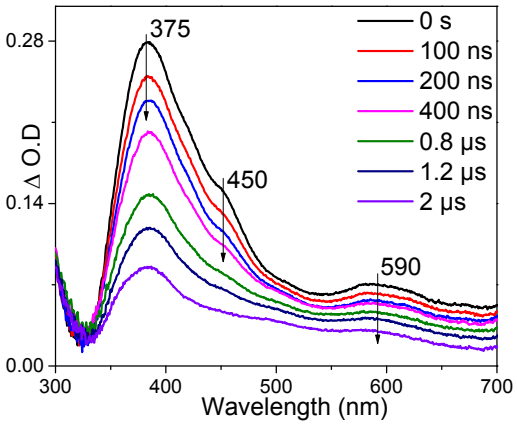



**Fig. S6** Ns-TA results acquired after 355 nm photoexcitation of **1** in ACN-PBS (1:1, v: v) under aerated condition.

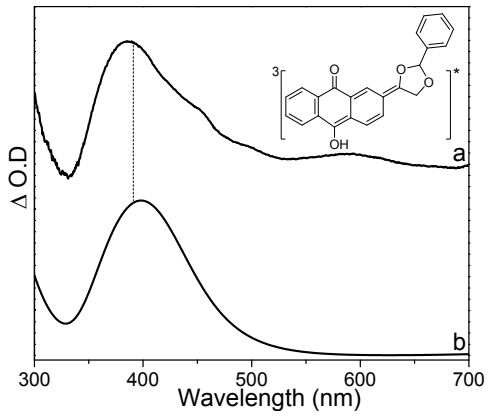



**Fig. S7** Comparison of (a) the 200 ns experimental ns-TA spectrum of **1** in ACN-PBS (1:1, v: v) with (b) the calculated normal UV-vis spectrum of the **2** (the scale factor is 1.0 and the half-width is 2000 cm-1) with its chemical structure shown in the figure.

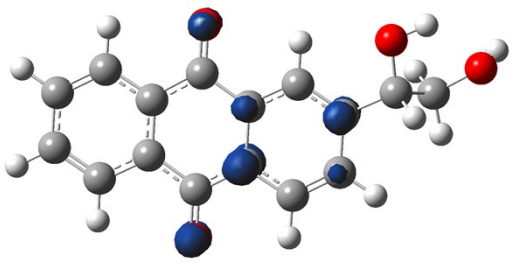


**Fig. S8** Visualized spin density (isovalue = 0.02) plots for the triplet state of Aqe-diol calculated at the uB3LYP/6-311G(d, p) level of theory.

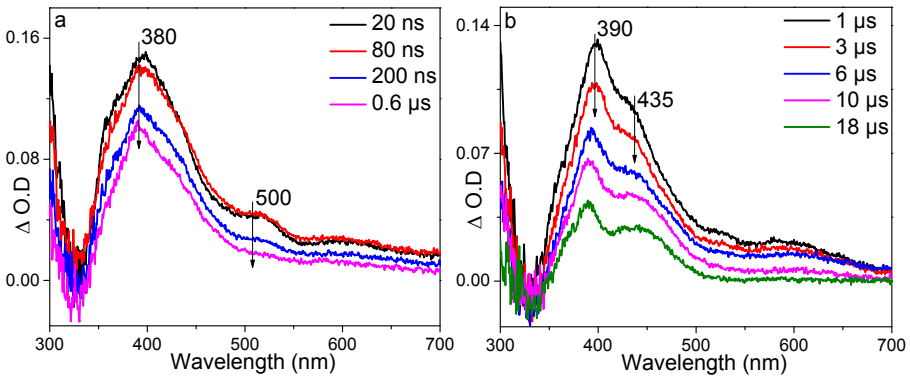



**Fig. S9** Ns-TA results acquired after 355 nm photoexcitation of Aqe-diol in ACN-PBS (9:1, v: v).

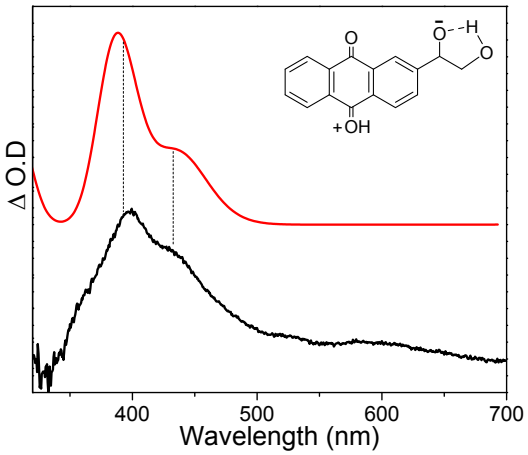
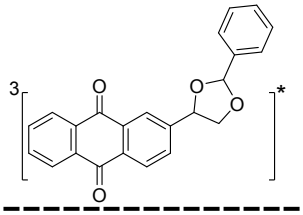



**Fig. S10** Comparison of (black) the ns-TA spectrum of Aqe-diol in ACN-PBS (9:1, v: v) at 1 µs to (red) the computed UV-vis spectrum for the Aqe-diol zwitterion (utilizing a 1.0 scale factor with a 1500 $cm^{-1}$ half-width).

Cartesian coordinates, total energies, and vibrational zero-point energies for the optimized geometry for the compounds and intermediates considered in this paper are given.

Triplet state of compound **1**:



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.9899 | 0.839734 | 0.275959 |
| 2 | 6 | 0 | -5.807612 | 1.526944 | 0.067233 |
| 3 | 6 | 0 | -4.572149 | 0.85821 | 0.05994 |
| 4 | 6 | 0 | -4.55714 | -0.545965 | 0.270199 |
| 5 | 6 | 0 | -5.772626 | -1.239203 | 0.483755 |
| 6 | 6 | 0 | -6.968311 | -0.55081 | 0.485085 |
| 7 | 6 | 0 | -3.33423 | 1.617946 | -0.163032 |
| 8 | 6 | 0 | -3.296638 | -1.238242 | 0.2623 |
| 9 | 6 | 0 | -2.058206 | -0.548254 | 0.029431 |
| 10 | 6 | 0 | -2.080571 | 0.854831 | -0.175839 |
| 11 | 6 | 0 | -0.859843 | 1.516732 | -0.395067 |
| 12 | 1 | 0 | -0.881297 | 2.589 | -0.548043 |
| 13 | 6 | 0 | 0.358994 | -0.570362 | -0.216843 |
| 14 | 6 | 0 | -0.825352 | -1.243345 | 0.012054 |
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| 16 | 1 | 0 | -5.809155 | 2.597937 | -0.095649 |
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| 18 | 1 | 0 | -7.896029 | -1.087584 | 0.648179 |
| 19 | 1 | 0 | -0.814649 | -2.314328 | 0.180128 |
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| 21 | 1 | 0 | 1.522314 | -2.323423 | 0.174987 |
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| 23 | 8 | 0 | 2.690853 | -0.631579 | 0.425051 |
| 24 | 8 | 0 | 3.660832 | -1.2211 | -1.525912 |
| 25 | 6 | 0 | 2.259043 | -1.492863 | -1.700552 |
| 26 | 1 | 0 | 1.855966 | -0.767293 | -2.409141 |
| 27 | 1 | 0 | 2.108271 | -2.504752 | -2.085083 |
| 28 | 6 | 0 | 0.336002 | 0.827874 | -0.417725 |
| 29 | 8 | 0 | -3.277793 | -2.52444 | 0.477026 |
| 30 | 8 | 0 | -3.347869 | 2.850428 | -0.333745 |
| 31 | 1 | 0 | 1.263828 | 1.36065 | -0.585097 |
| 32 | 6 | 0 | 5.049843 | -0.201437 | 0.177674 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 6 | 0 | 5.112774 | 1.063489 | -0.415642 |
| 34 | 6 | 0 | 6.043848 | -0.592956 | 1.075271 |
| 35 | 6 | 0 | 6.161895 | 1.925739 | -0.110418 |
| 36 | 1 | 0 | 4.346756 | 1.364609 | -1.1208 |
| 37 | 6 | 0 | 7.094426 | 0.271879 | 1.382442 |
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| 39 | 6 | 0 | 7.153928 | 1.531655 | 0.789994 |
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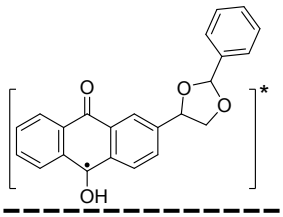
Sum of electronic and zero-point Energies= -1186.878498

Sum of electronic and thermal Free Energies= -1186.932600

Ketyl radical species of compound **1**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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| 4 | 6 | 0 | -4.555573 | -0.535919 | 0.135579 |
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| 6 | 6 | 0 | -6.976117 | -0.496018 | 0.155116 |
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| 10 | 6 | 0 | -2.039634 | 0.856774 | -0.068564 |
| 11 | 6 | 0 | -0.783048 | 1.509723 | -0.153978 |
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| 13 | 6 | 0 | 0.387988 | -0.594186 | 0.097891 |
| 14 | 6 | 0 | -0.830982 | -1.24792 | 0.197392 |
| 15 | 1 | 0 | -7.890011 | 1.44602 | -0.087239 |
| 16 | 1 | 0 | -5.742096 | 2.64819 | -0.26504 |
| 17 | 1 | 0 | -5.767975 | -2.272313 | 0.37237 |
| 18 | 1 | 0 | -7.922431 | -1.018728 | 0.232755 |
| 19 | 1 | 0 | -0.885495 | -2.320347 | 0.349795 |
| 20 | 6 | 0 | 1.675362 | -1.372445 | 0.13483 |
| 21 | 1 | 0 | 1.550245 | -2.265066 | 0.763577 |
| 22 | 6 | 0 | 3.932346 | -1.204837 | 0.20303 |
| 23 | 8 | 0 | 2.740897 | -0.571133 | 0.644321 |
| 24 | 8 | 0 | 3.647873 | -1.743721 | -1.082612 |
| 25 | 6 | 0 | 2.229054 | -1.784801 | -1.24803 |
| 26 | 1 | 0 | 1.928182 | -1.072262 | -2.022154 |
| 27 | 1 | 0 | 1.917228 | -2.790665 | -1.539161 |
| 28 | 6 | 0 | 0.397827 | 0.80445 | -0.076871 |
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| 30 | 8 | 0 | -3.344346 | 2.894044 | -0.320758 |
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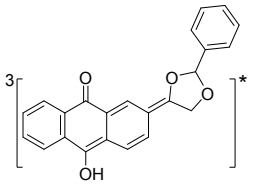
| 32 | 6 | 0 | 5.066485 | -0.20946 | 0.176503 |
| 33 | 6 | 0 | 5.585823 | 0.267 | -1.026096 |
| 34 | 6 | 0 | 5.589343 | 0.254016 | 1.386296 |
| 35 | 6 | 0 | 6.616792 | 1.204953 | -1.018343 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 1 | 0 | 5.18471 | -0.11101 | -1.957401 |
| 37 | 6 | 0 | 6.61363 | 1.195711 | 1.393053 |
| 38 | 1 | 0 | 5.187475 | -0.117925 | 2.322989 |
| 39 | 6 | 0 | 7.130112 | 1.672866 | 0.188741 |
| 40 | 1 | 0 | 7.02064 | 1.567951 | -1.956972 |
| 41 | 1 | 0 | 7.011842 | 1.554317 | 2.335603 |
| 42 | 1 | 0 | 7.932896 | 2.401725 | 0.192916 |
| 43 | 1 | 0 | 4.166869 | -2.03801 | 0.885457 |
| 44 | 1 | 0 | -2.458579 | 3.264336 | -0.388655 |

Sum of electronic and zero-point Energies= -1187.513914

Sum of electronic and thermal Free Energies= -1187.568200

Triplet state of compound **2**:




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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| 4 | 6 | 0 | -2.68362 | -2.58482 | -0.23309 |
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| 6 | 1 | 0 | -2.65838 | -3.18328 | -1.1549 |
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| 8 | 6 | 0 | 0.399421 | -2.50146 | 0.100474 |
| 9 | 6 | 0 | 0.335718 | -0.10181 | -0.28379 |
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| 12 | 6 | 0 | 1.732065 | -0.0381 | -0.14726 |
| 13 | 1 | 0 | -0.20339 | 0.813795 | -0.4807 |
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| 17 | 6 | 0 | 3.900881 | -1.15432 | 0.237795 |
| 18 | 6 | 0 | 3.856105 | 1.278904 | -0.11012 |
| 19 | 6 | 0 | 4.593217 | 0.081221 | 0.138456 |
| 20 | 6 | 0 | 4.555886 | 2.497363 | -0.20676 |
| 21 | 6 | 0 | 6.003394 | 0.152653 | 0.278819 |
| 22 | 6 | 0 | 5.928759 | 2.543863 | -0.06437 |
| 23 | 1 | 0 | 3.991043 | 3.40123 | -0.39683 |
| 24 | 6 | 0 | 6.657096 | 1.361077 | 0.180401 |
| 25 | 1 | 0 | 6.562066 | -0.75473 | 0.466154 |
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| 27 | 1 | 0 | 7.734259 | 1.403339 | 0.291168 |
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| 31 | 6 | 0 | -4.91765 | 0.510074 | 1.192317 |
| 32 | 6 | 0 | -6.55338 | 1.958569 | -0.54598 |
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| | | | | | |
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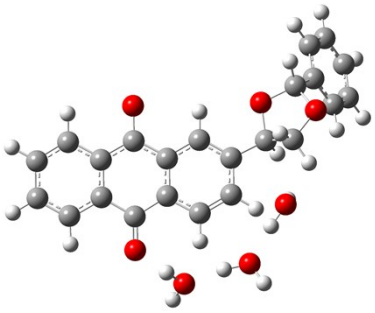
| 36 | 6 | 0 | -6.62433 | 2.180341 | 0.827624 |
| 37 | 1 | 0 | -7.1885 | 2.519135 | -1.22212 |
| 38 | 1 | 0 | -5.86137 | 1.627331 | 2.765009 |
| 39 | 1 | 0 | -7.3158 | 2.915604 | 1.223391 |
| 40 | 1 | 0 | -4.00508 | -0.8462 | -1.82408 |
| 41 | 8 | 0 | 4.658997 | -2.2445 | 0.460657 |
| 42 | 8 | 0 | 1.752227 | 2.308351 | -0.4952 |
| 43 | 1 | 0 | 4.135043 | -3.05632 | 0.474139 |

Sum of electronic and zero-point Energies= -1186.909960

Sum of electronic and thermal Free Energies= -1186.962744

$RC_1$



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
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| 2 | 6 | 0 | 5.460928 | -1.81882 | 0.016024 |
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| 6 | 6 | 0 | 4.917031 | -4.17296 | 0.066679 |
| 7 | 6 | 0 | 3.696263 | -0.07219 | -0.07105 |
| 8 | 6 | 0 | 1.741134 | -2.1966 | -0.05335 |
| 9 | 6 | 0 | 1.294277 | -0.83078 | -0.0967 |
| 10 | 6 | 0 | 2.259008 | 0.21087 | -0.10543 |
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| 14 | 6 | 0 | -0.08652 | -0.52231 | -0.13423 |
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| 17 | 1 | 0 | 2.836925 | -4.67843 | 0.03461 |
| 18 | 1 | 0 | 5.239848 | -5.20712 | 0.100588 |
| 19 | 1 | 0 | -0.81907 | -1.31922 | -0.14212 |
| 20 | 6 | 0 | -1.97744 | 1.153882 | -0.19917 |
| 21 | 6 | 0 | -3.75671 | -0.05463 | 0.69015 |
| 22 | 8 | 0 | -2.8267 | 0.016567 | -0.40483 |
| 23 | 8 | 0 | -3.83633 | 1.261855 | 1.197281 |
| 24 | 6 | 0 | -2.49877 | 1.753004 | 1.12947 |
| 25 | 1 | 0 | -2.52458 | 2.841393 | 1.130831 |
| 26 | 1 | 0 | -1.91104 | 1.392208 | 1.982095 |
| 27 | 6 | 0 | 0.446337 | 1.829292 | -0.18379 |
| 28 | 8 | 0 | 0.858995 | -3.15379 | -0.04756 |
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| | | | | | |
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| 33 | 6 | 0 | -5.62366 | -1.73874 | 0.70014 |
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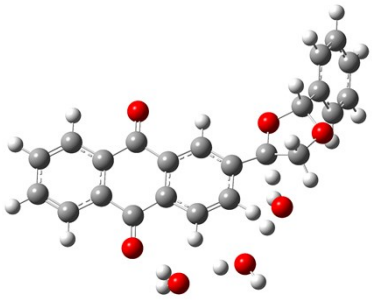
| 35 | 1 | 0 | -5.42909 | 1.141756 | -1.08615 |
| 36 | 6 | 0 | -6.86708 | -2.19445 | 0.258797 |
| 37 | 1 | 0 | -5.05749 | -2.31812 | 1.422178 |
| 38 | 6 | 0 | -7.59244 | -1.44776 | -0.66682 |
| 39 | 1 | 0 | -7.63709 | 0.33827 | -1.87173 |
| 40 | 1 | 0 | -7.26595 | -3.12876 | 0.637994 |
| 41 | 1 | 0 | -8.55898 | -1.79914 | -1.01111 |
| 42 | 1 | 0 | -3.34726 | -0.72722 | 1.457062 |
| 43 | 1 | 0 | -2.15156 | 1.857838 | -1.01924 |
| 44 | 8 | 0 | 0.434365 | 5.231463 | -0.4542 |
| 45 | 1 | 0 | 1.301902 | 5.160278 | -0.00658 |
| 46 | 1 | 0 | 0.62812 | 4.993563 | -1.36803 |
| 47 | 8 | 0 | 2.919883 | 5.002319 | 0.810271 |
| 48 | 1 | 0 | 3.602942 | 4.506301 | 0.307563 |
| 49 | 1 | 0 | 2.860406 | 4.545636 | 1.657795 |
| 50 | 8 | 0 | 4.76544 | 3.527595 | -0.60199 |
| 51 | 1 | 0 | 4.696486 | 2.573346 | -0.38933 |
| 52 | 1 | 0 | 4.612968 | 3.576783 | -1.55388 |

Sum of electronic and zero-point Energies= -1416.213301

Sum of electronic and thermal Free Energies= -1416.281714

$TS_1$



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.644447 | 1.68517 | 0.56385 |
| 2 | 6 | 0 | 5.95535 | 0.534795 | 0.238583 |
| 3 | 6 | 0 | 4.561405 | 0.563214 | 0.0097 |
| 4 | 6 | 0 | 3.865584 | 1.799621 | 0.133116 |
| 5 | 6 | 0 | 4.592581 | 2.959503 | 0.473291 |
| 6 | 6 | 0 | 5.95672 | 2.91066 | 0.681305 |
| 7 | 6 | 0 | 3.86409 | -0.66961 | -0.32963 |
| 8 | 6 | 0 | 2.411289 | 1.897514 | -0.05274 |
| 9 | 6 | 0 | 1.724326 | 0.662412 | -0.42911 |
| 10 | 6 | 0 | 2.452613 | -0.55999 | -0.64948 |
| 11 | 6 | 0 | 1.760892 | -1.69748 | -1.14543 |
| 12 | 1 | 0 | 2.331635 | -2.5844 | -1.38565 |
| 13 | 6 | 0 | -0.34553 | -0.51224 | -0.93053 |
| 14 | 6 | 0 | 0.330756 | 0.642887 | -0.53514 |
| 15 | 1 | 0 | 7.71542 | 1.648621 | 0.730846 |
| 16 | 1 | 0 | 6.467655 | -0.41549 | 0.149312 |
| 17 | 1 | 0 | 4.046693 | 3.890602 | 0.566703 |
| 18 | 1 | 0 | 6.500905 | 3.813116 | 0.93748 |
| 19 | 1 | 0 | -0.21883 | 1.544129 | -0.29722 |
| 20 | 6 | 0 | -1.79759 | -0.64694 | -0.85681 |
| 21 | 6 | 0 | -3.81498 | 0.450517 | -1.12551 |
| 22 | 8 | 0 | -2.50999 | 0.466322 | -0.45166 |
| 23 | 8 | 0 | -3.95558 | -0.86256 | -1.59996 |
| 24 | 6 | 0 | -2.64809 | -1.28489 | -1.97258 |
| 25 | 1 | 0 | -2.62028 | -2.37127 | -1.99427 |
| 26 | 1 | 0 | -2.35598 | -0.8737 | -2.94734 |
| 27 | 6 | 0 | 0.403024 | -1.6903 | -1.27523 |
| 28 | 8 | 0 | 1.791956 | 2.970287 | 0.110135 |
| 29 | 8 | 0 | 4.443073 | -1.7973 | -0.33568 |
| 30 | 1 | 0 | -0.11933 | -2.58003 | -1.60478 |
| 31 | 6 | 0 | -4.91618 | 0.82969 | -0.17876 |
| 32 | 6 | 0 | -5.29865 | -0.03906 | 0.849112 |

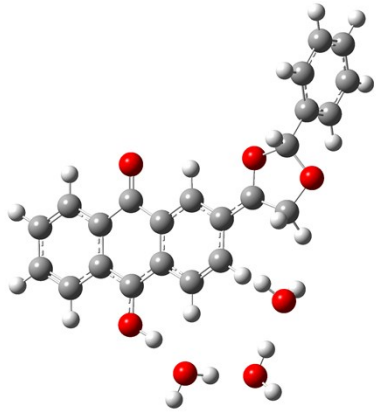
| | | | | | |
|---|---|---|---|---|---|
| 33 | 6 | 0 | -5.55209 | 2.06386 | -0.31814 |
| 34 | 6 | 0 | -6.31081 | 0.330376 | 1.729479 |
| 35 | 1 | 0 | -4.80915 | -1.00016 | 0.953994 |
| 36 | 6 | 0 | -6.56593 | 2.432941 | 0.565937 |
| 37 | 1 | 0 | -5.25549 | 2.733498 | -1.11854 |
| 38 | 6 | 0 | -6.94511 | 1.566906 | 1.58945 |
| 39 | 1 | 0 | -6.60668 | -0.34456 | 2.524764 |
| 40 | 1 | 0 | -7.05848 | 3.39206 | 0.452721 |
| 41 | 1 | 0 | -7.73422 | 1.851485 | 2.276624 |
| 42 | 1 | 0 | -3.72496 | 1.166964 | -1.95093 |
| 43 | 1 | 0 | -1.86121 | -1.45501 | 0.056092 |
| 44 | 8 | 0 | -1.98235 | -2.51401 | 1.18291 |
| 45 | 1 | 0 | -1.11209 | -3.00219 | 1.23971 |
| 46 | 1 | 0 | -2.05839 | -2.00695 | 2.005656 |
| 47 | 8 | 0 | 0.259943 | -3.92164 | 1.375592 |
| 48 | 1 | 0 | 1.208232 | -3.67321 | 1.289118 |
| 49 | 1 | 0 | 0.19247 | -4.7986 | 0.980092 |
| 50 | 8 | 0 | 2.985208 | -3.58108 | 1.244166 |
| 51 | 1 | 0 | 3.496361 | -3.03024 | 0.612662 |
| 52 | 1 | 0 | 3.348941 | -3.36223 | 2.110522 |

Sum of electronic and zero-point Energies= -1416.206785

Sum of electronic and thermal Free Energies= -1416.269455

The imaginary frequency: -177.73

$PC_1$

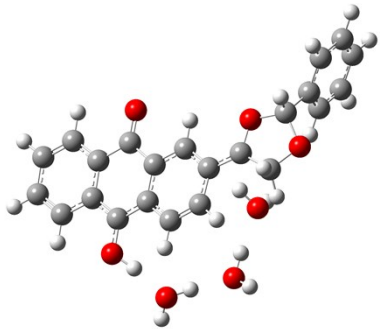


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.094248 | -2.65459 | -0.41901 |
| 2 | 6 | 0 | 5.577788 | -1.4069 | -0.14702 |
| 3 | 6 | 0 | 4.179012 | -1.21837 | 0.008994 |
| 4 | 6 | 0 | 3.311016 | -2.34334 | -0.13004 |
| 5 | 6 | 0 | 3.870328 | -3.60547 | -0.41133 |
| 6 | 6 | 0 | 5.234331 | -3.7664 | -0.55214 |
| 7 | 6 | 0 | 3.636323 | 0.069243 | 0.290762 |
| 8 | 6 | 0 | 1.86091 | -2.2101 | 0.001662 |
| 9 | 6 | 0 | 1.342285 | -0.8707 | 0.315579 |
| 10 | 6 | 0 | 2.217555 | 0.238831 | 0.476817 |
| 11 | 6 | 0 | 1.649273 | 1.491971 | 0.839354 |
| 12 | 1 | 0 | 2.285667 | 2.349157 | 1.015621 |
| 13 | 6 | 0 | -0.60296 | 0.550399 | 0.79182 |
| 14 | 6 | 0 | -0.04437 | -0.70143 | 0.468599 |
| 15 | 1 | 0 | 7.16482 | -2.78373 | -0.53255 |
| 16 | 1 | 0 | 6.234933 | -0.55294 | -0.04669 |
| 17 | 1 | 0 | 3.195339 | -4.44633 | -0.51483 |
| 18 | 1 | 0 | 5.647499 | -4.7457 | -0.7669 |
| 19 | 1 | 0 | -0.67801 | -1.56653 | 0.330891 |
| 20 | 6 | 0 | -1.99391 | 0.750161 | 0.923366 |
| 21 | 6 | 0 | -4.19568 | 0.232841 | 1.074337 |
| 22 | 8 | 0 | -2.8614 | -0.27354 | 0.737827 |
| 23 | 8 | 0 | -4.10809 | 1.619205 | 0.875164 |
| 24 | 6 | 0 | -2.7718 | 1.991971 | 1.244612 |
| 25 | 1 | 0 | -2.47939 | 2.861839 | 0.653726 |
| 26 | 1 | 0 | -2.72312 | 2.253508 | 2.312297 |
| 27 | 6 | 0 | 0.293698 | 1.645923 | 0.990222 |
| 28 | 8 | 0 | 1.093625 | -3.18517 | -0.13605 |
| 29 | 8 | 0 | 4.511475 | 1.067157 | 0.384128 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 1 | 0 | -0.09689 | 2.61609 | 1.276104 |
| 31 | 6 | 0 | -5.23811 | -0.39892 | 0.198897 |
| 32 | 6 | 0 | -5.32556 | -0.06212 | -1.15585 |
| 33 | 6 | 0 | -6.11386 | -1.34244 | 0.737189 |
| 34 | 6 | 0 | -6.28402 | -0.66802 | -1.96238 |
| 35 | 1 | 0 | -4.64955 | 0.676345 | -1.57059 |
| 36 | 6 | 0 | -7.07351 | -1.95039 | -0.07246 |
| 37 | 1 | 0 | -6.04577 | -1.59861 | 1.789335 |
| 38 | 6 | 0 | -7.15857 | -1.61364 | -1.42188 |
| 39 | 1 | 0 | -6.35143 | -0.4042 | -3.01197 |
| 40 | 1 | 0 | -7.75277 | -2.68186 | 0.350695 |
| 41 | 1 | 0 | -7.9051 | -2.08371 | -2.0526 |
| 42 | 1 | 0 | -4.35588 | -0.00965 | 2.131965 |
| 43 | 1 | 0 | 0.451405 | 2.709102 | -1.36234 |
| 44 | 8 | 0 | 0.371643 | 3.574207 | -1.78771 |
| 45 | 1 | 0 | 1.918508 | 4.435502 | -1.6902 |
| 46 | 1 | 0 | 0.058716 | 3.384646 | -2.68181 |
| 47 | 8 | 0 | 2.773092 | 4.895665 | -1.54123 |
| 48 | 1 | 0 | 3.59845 | 4.10921 | -0.27609 |
| 49 | 1 | 0 | 2.526641 | 5.786112 | -1.26173 |
| 50 | 8 | 0 | 3.994833 | 3.632869 | 0.496813 |
| 51 | 1 | 0 | 4.158322 | 2.000216 | 0.412948 |
| 52 | 1 | 0 | 4.809666 | 4.09735 | 0.722482 |

Sum of electronic and zero-point Energies= -1416.254868
Sum of electronic and thermal Free Energies= -1416.321181

$RC_2$

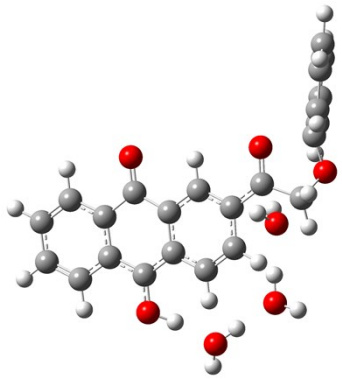


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.35011 | -2.00224 | 0.519448 |
| 2 | 6 | 0 | -5.7284 | -0.79821 | 0.27117 |
| 3 | 6 | 0 | -4.33599 | -0.7444 | -0.00054 |
| 4 | 6 | 0 | -3.58029 | -1.95686 | 0.009573 |
| 5 | 6 | 0 | -4.24516 | -3.17012 | 0.272577 |
| 6 | 6 | 0 | -5.60412 | -3.20081 | 0.518002 |
| 7 | 6 | 0 | -3.68139 | 0.492484 | -0.25878 |
| 8 | 6 | 0 | -2.13339 | -1.95976 | -0.21644 |
| 9 | 6 | 0 | -1.50751 | -0.66697 | -0.52988 |
| 10 | 6 | 0 | -2.28325 | 0.521136 | -0.59969 |
| 11 | 6 | 0 | -1.64706 | 1.717264 | -1.03051 |
| 12 | 1 | 0 | -2.22582 | 2.62246 | -1.1539 |
| 13 | 6 | 0 | 0.51211 | 0.591439 | -1.13674 |
| 14 | 6 | 0 | -0.12556 | -0.61522 | -0.77971 |
| 15 | 1 | 0 | -7.41559 | -2.03009 | 0.718493 |
| 16 | 1 | 0 | -6.29569 | 0.123648 | 0.275723 |
| 17 | 1 | 0 | -3.65643 | -4.0794 | 0.279135 |
| 18 | 1 | 0 | -6.09997 | -4.14487 | 0.714885 |
| 19 | 1 | 0 | 0.442401 | -1.53106 | -0.69275 |
| 20 | 6 | 0 | 1.910342 | 0.682022 | -1.31073 |
| 21 | 6 | 0 | 4.089742 | 0.030753 | -1.25075 |
| 22 | 8 | 0 | 2.698837 | -0.39456 | -1.07793 |
| 23 | 8 | 0 | 4.058008 | 1.430078 | -1.12813 |
| 24 | 6 | 0 | 2.783162 | 1.855174 | -1.63473 |
| 25 | 1 | 0 | 2.498125 | 2.775254 | -1.12328 |
| 26 | 1 | 0 | 2.841983 | 2.049146 | -2.7163 |
| 27 | 6 | 0 | -0.30282 | 1.754802 | -1.29544 |
| 28 | 8 | 0 | -1.46033 | -3.00904 | -0.16225 |
| 29 | 8 | 0 | -4.41664 | 1.602632 | -0.19614 |
| 30 | 1 | 0 | 0.145891 | 2.687837 | -1.61527 |
| 31 | 6 | 0 | 4.961117 | -0.59145 | -0.19798 |

| | | | | | |
|---|---|---|---|---|---|
| 32 | 6 | 0 | 4.757187 | -0.28228 | 1.15165 |
| 33 | 6 | 0 | 5.972418 | -1.47984 | -0.56189 |
| 34 | 6 | 0 | 5.563467 | -0.86153 | 2.125885 |
| 35 | 1 | 0 | 3.96853 | 0.40679 | 1.432221 |
| 36 | 6 | 0 | 6.78197 | -2.05894 | 0.416326 |
| 37 | 1 | 0 | 6.127432 | -1.7169 | -1.60926 |
| 38 | 6 | 0 | 6.577831 | -1.75002 | 1.759252 |
| 39 | 1 | 0 | 5.403781 | -0.62221 | 3.171341 |
| 40 | 1 | 0 | 7.568633 | -2.74736 | 0.128714 |
| 41 | 1 | 0 | 7.205711 | -2.19895 | 2.521021 |
| 42 | 1 | 0 | 4.38533 | -0.27803 | -2.26065 |
| 43 | 1 | 0 | 0.653667 | 1.106448 | 1.459667 |
| 44 | 8 | 0 | 0.899864 | 1.882053 | 1.982152 |
| 45 | 1 | 0 | -0.34532 | 3.182328 | 1.911398 |
| 46 | 1 | 0 | 1.085949 | 1.538235 | 2.865571 |
| 47 | 8 | 0 | -0.9484 | 3.952529 | 1.852156 |
| 48 | 1 | 0 | -2.46007 | 3.842616 | 1.049585 |
| 49 | 1 | 0 | -0.41418 | 4.652294 | 1.457472 |
| 50 | 8 | 0 | -3.31632 | 3.854764 | 0.55495 |
| 51 | 1 | 0 | -3.90268 | 2.430377 | 0.040236 |
| 52 | 1 | 0 | -3.93765 | 4.345225 | 1.106783 |

Sum of electronic and zero-point Energies= -1416.254082
Sum of electronic and thermal Free Energies= -1416.319060

$TS_2$



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.178531 | -1.9146 | -0.668 |
| 2 | 6 | 0 | 5.541141 | -0.71125 | -0.45135 |
| 3 | 6 | 0 | 4.18 | -0.6747 | -0.05378 |
| 4 | 6 | 0 | 3.473507 | -1.90416 | 0.101052 |
| 5 | 6 | 0 | 4.149747 | -3.11541 | -0.13198 |
| 6 | 6 | 0 | 5.480446 | -3.12873 | -0.5059 |
| 7 | 6 | 0 | 3.510538 | 0.565407 | 0.171322 |
| 8 | 6 | 0 | 2.054821 | -1.92861 | 0.474594 |
| 9 | 6 | 0 | 1.417085 | -0.62864 | 0.741648 |
| 10 | 6 | 0 | 2.150949 | 0.58697 | 0.631685 |
| 11 | 6 | 0 | 1.506154 | 1.793632 | 1.010293 |
| 12 | 1 | 0 | 2.052536 | 2.726896 | 0.995139 |
| 13 | 6 | 0 | -0.58201 | 0.610995 | 1.427385 |
| 14 | 6 | 0 | 0.068417 | -0.59413 | 1.120211 |
| 15 | 1 | 0 | 7.220926 | -1.92728 | -0.9662 |
| 16 | 1 | 0 | 6.073652 | 0.222124 | -0.57978 |
| 17 | 1 | 0 | 3.594801 | -4.03795 | -0.01196 |
| 18 | 1 | 0 | 5.987778 | -4.07117 | -0.67918 |
| 19 | 1 | 0 | -0.47502 | -1.52787 | 1.170035 |
| 20 | 6 | 0 | -1.98575 | 0.620085 | 1.778359 |
| 21 | 6 | 0 | -4.38087 | 0.275748 | 1.163142 |
| 22 | 8 | 0 | -2.69987 | -0.44896 | 1.779332 |
| 23 | 8 | 0 | -3.91069 | 1.501924 | 0.919105 |
| 24 | 6 | 0 | -2.84841 | 1.845778 | 1.871357 |
| 25 | 1 | 0 | -2.40684 | 2.777514 | 1.531057 |
| 26 | 1 | 0 | -3.29568 | 1.972663 | 2.864201 |
| 27 | 6 | 0 | 0.188953 | 1.806385 | 1.403186 |
| 28 | 8 | 0 | 1.420692 | -2.99458 | 0.573269 |
| 29 | 8 | 0 | 4.212902 | 1.67929 | -0.03816 |
| 30 | 1 | 0 | -0.26057 | 2.7486 | 1.691665 |

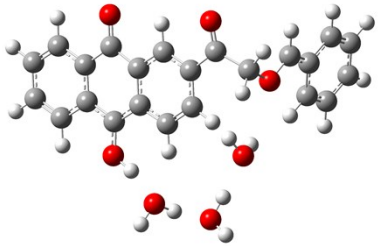
| | | | | | |
|---|---|---|---|---|---|
| 31 | 6 | 0 | -4.83115 | -0.49962 | 0.023854 |
| 32 | 6 | 0 | -4.34507 | -0.24439 | -1.27341 |
| 33 | 6 | 0 | -5.75006 | -1.54578 | 0.221881 |
| 34 | 6 | 0 | -4.77701 | -1.01967 | -2.34127 |
| 35 | 1 | 0 | -3.62246 | 0.548382 | -1.42605 |
| 36 | 6 | 0 | -6.17728 | -2.31628 | -0.85328 |
| 37 | 1 | 0 | -6.12523 | -1.74381 | 1.22031 |
| 38 | 6 | 0 | -5.69433 | -2.05538 | -2.13744 |
| 39 | 1 | 0 | -4.39864 | -0.82133 | -3.33797 |
| 40 | 1 | 0 | -6.88866 | -3.11873 | -0.69332 |
| 41 | 1 | 0 | -6.0287 | -2.65633 | -2.97565 |
| 42 | 1 | 0 | -4.86151 | 0.107218 | 2.124197 |
| 43 | 1 | 0 | -0.77444 | 1.051897 | -1.23483 |
| 44 | 8 | 0 | -0.98842 | 1.66597 | -1.95087 |
| 45 | 1 | 0 | 0.146775 | 3.050836 | -2.06298 |
| 46 | 1 | 0 | -1.05846 | 1.112459 | -2.73958 |
| 47 | 8 | 0 | 0.706792 | 3.854139 | -2.0994 |
| 48 | 1 | 0 | 2.198477 | 3.857394 | -1.27204 |
| 49 | 1 | 0 | 0.138816 | 4.565759 | -1.78013 |
| 50 | 8 | 0 | 3.044367 | 3.905745 | -0.76059 |
| 51 | 1 | 0 | 3.669665 | 2.491561 | -0.25965 |
| 52 | 1 | 0 | 3.656363 | 4.420983 | -1.30014 |

Sum of electronic and zero-point Energies= -1416.239394

Sum of electronic and thermal Free Energies= -1416.303466

The imaginary frequency: -460.15

$PC_2$

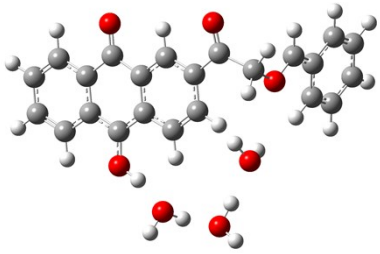


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.222507 | 0.306813 | -1.61965 |
| 2 | 6 | 0 | 5.210889 | 0.919145 | -0.90407 |
| 3 | 6 | 0 | 4.070182 | 0.187173 | -0.4984 |
| 4 | 6 | 0 | 3.985674 | -1.18794 | -0.84191 |
| 5 | 6 | 0 | 5.025126 | -1.7868 | -1.56889 |
| 6 | 6 | 0 | 6.134178 | -1.05417 | -1.95665 |
| 7 | 6 | 0 | 3.015866 | 0.82326 | 0.247851 |
| 8 | 6 | 0 | 2.820698 | -1.99732 | -0.44636 |
| 9 | 6 | 0 | 1.764105 | -1.30353 | 0.317289 |
| 10 | 6 | 0 | 1.865632 | 0.083298 | 0.656658 |
| 11 | 6 | 0 | 0.799016 | 0.665669 | 1.393029 |
| 12 | 1 | 0 | 0.849489 | 1.701371 | 1.701533 |
| 13 | 6 | 0 | -0.40211 | -1.44595 | 1.425241 |
| 14 | 6 | 0 | 0.64519 | -2.03169 | 0.715173 |
| 15 | 1 | 0 | 7.090264 | 0.882415 | -1.92195 |
| 16 | 1 | 0 | 5.282406 | 1.967161 | -0.64636 |
| 17 | 1 | 0 | 4.935228 | -2.83715 | -1.81746 |
| 18 | 1 | 0 | 6.931636 | -1.52773 | -2.51765 |
| 19 | 1 | 0 | 0.595079 | -3.08183 | 0.457956 |
| 20 | 6 | 0 | -1.54624 | -2.29943 | 1.836529 |
| 21 | 6 | 0 | -4.16225 | -1.31532 | 0.48961 |
| 22 | 8 | 0 | -1.51092 | -3.51547 | 1.73624 |
| 23 | 8 | 0 | -3.39821 | -0.73191 | 1.448207 |
| 24 | 6 | 0 | -2.80773 | -1.63211 | 2.398718 |
| 25 | 1 | 0 | -2.57454 | -1.03646 | 3.282228 |
| 26 | 1 | 0 | -3.51476 | -2.41862 | 2.670518 |
| 27 | 6 | 0 | -0.30644 | -0.07377 | 1.754989 |
| 28 | 8 | 0 | 2.730356 | -3.19522 | -0.73755 |
| 29 | 8 | 0 | 3.205695 | 2.115019 | 0.502057 |
| 30 | 1 | 0 | -1.09568 | 0.413935 | 2.312266 |
| 31 | 6 | 0 | -4.69046 | -0.54324 | -0.56077 |
| 32 | 6 | 0 | -4.4114 | 0.844765 | -0.71452 |
| 33 | 6 | 0 | -5.54325 | -1.16001 | -1.5218 |

| | | | | | |
|---|---|---|---|---|---|
| 34 | 6 | 0 | -4.95995 | 1.560049 | -1.76809 |
| 35 | 1 | 0 | -3.75612 | 1.339648 | -0.00963 |
| 36 | 6 | 0 | -6.08068 | -0.42843 | -2.56624 |
| 37 | 1 | 0 | -5.76857 | -2.21709 | -1.42417 |
| 38 | 6 | 0 | -5.7985 | 0.938921 | -2.70193 |
| 39 | 1 | 0 | -4.73327 | 2.616825 | -1.86731 |
| 40 | 1 | 0 | -6.72772 | -0.91971 | -3.28546 |
| 41 | 1 | 0 | -6.2232 | 1.507333 | -3.52134 |
| 42 | 1 | 0 | -4.37739 | -2.37259 | 0.597544 |
| 43 | 1 | 0 | -1.24174 | 2.121176 | -0.18923 |
| 44 | 8 | 0 | -1.66035 | 2.965726 | -0.40605 |
| 45 | 1 | 0 | -0.73663 | 4.373802 | 0.151085 |
| 46 | 1 | 0 | -1.86661 | 2.90332 | -1.34799 |
| 47 | 8 | 0 | -0.18852 | 5.083038 | 0.549694 |
| 48 | 1 | 0 | 1.033176 | 4.279634 | 1.408465 |
| 49 | 1 | 0 | -0.78185 | 5.542555 | 1.156834 |
| 50 | 8 | 0 | 1.677513 | 3.709289 | 1.900235 |
| 51 | 1 | 0 | 2.516267 | 2.605977 | 1.031796 |
| 52 | 1 | 0 | 2.219786 | 4.295851 | 2.440823 |

Sum of electronic and zero-point Energies= -1416.265156
Sum of electronic and thermal Free Energies= -1416.332436

$RC_3$

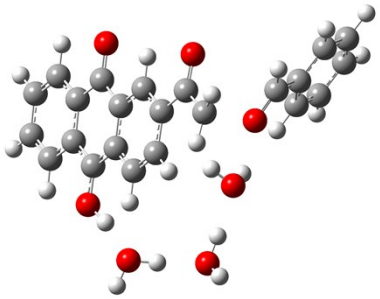


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.223294 | 0.314978 | 1.619025 |
| 2 | 6 | 0 | -5.210297 | 0.924985 | 0.903419 |
| 3 | 6 | 0 | -4.071001 | 0.190558 | 0.498216 |
| 4 | 6 | 0 | -3.989363 | -1.184595 | 0.842292 |
| 5 | 6 | 0 | -5.030237 | -1.78111 | 1.569164 |
| 6 | 6 | 0 | -6.137863 | -1.046072 | 1.956447 |
| 7 | 6 | 0 | -3.015039 | 0.824234 | -0.247882 |
| 8 | 6 | 0 | -2.826055 | -1.99659 | 0.447089 |
| 9 | 6 | 0 | -1.767022 | -1.304746 | -0.314946 |
| 10 | 6 | 0 | -1.865589 | 0.082127 | -0.654726 |
| 11 | 6 | 0 | -0.796563 | 0.662413 | -1.389362 |
| 12 | 1 | 0 | -0.845048 | 1.697843 | -1.699155 |
| 13 | 6 | 0 | 0.40089 | -1.451128 | -1.419074 |
| 14 | 6 | 0 | -0.648718 | -2.034921 | -0.71088 |
| 15 | 1 | 0 | -7.089908 | 0.892497 | 1.920984 |
| 16 | 1 | 0 | -5.279622 | 1.973062 | 0.645425 |
| 17 | 1 | 0 | -4.942627 | -2.831571 | 1.818028 |
| 18 | 1 | 0 | -6.936382 | -1.517813 | 2.517466 |
| 19 | 1 | 0 | -0.600856 | -3.085056 | -0.45333 |
| 20 | 6 | 0 | 1.544504 | -2.306071 | -1.828464 |
| 21 | 6 | 0 | 4.164235 | -1.31644 | -0.487971 |
| 22 | 8 | 0 | 1.508618 | -3.521842 | -1.725364 |
| 23 | 8 | 0 | 3.395812 | -0.736925 | -1.44532 |
| 24 | 6 | 0 | 2.805921 | -1.640612 | -2.392839 |
| 25 | 1 | 0 | 2.572426 | -1.047881 | -3.278388 |
| 26 | 1 | 0 | 3.513152 | -2.427852 | -2.661672 |
| 27 | 6 | 0 | 0.308475 | -0.07884 | -1.748892 |
| 28 | 8 | 0 | -2.73823 | -3.194637 | 0.738452 |
| 29 | 8 | 0 | -3.201224 | 2.116439 | -0.502061 |
| 30 | 1 | 0 | 1.099899 | 0.406836 | -2.304922 |
| 31 | 6 | 0 | 4.69387 | -0.541039 | 0.5593 |
| 32 | 6 | 0 | 4.413854 | 0.847075 | 0.710218 |
| 33 | 6 | 0 | 5.550268 | -1.154356 | 1.51935 |

| | | | | | |
|---|---|---|---|---|---|
| 34 | 6 | 0 | 4.965221 | 1.56566 | 1.76012 |
| 35 | 1 | 0 | 3.756271 | 1.339447 | 0.005616 |
| 36 | 6 | 0 | 6.089866 | -0.419652 | 2.560415 |
| 37 | 1 | 0 | 5.776685 | -2.211383 | 1.423553 |
| 38 | 6 | 0 | 5.806882 | 0.947769 | 2.693293 |
| 39 | 1 | 0 | 4.738463 | 2.622598 | 1.856981 |
| 40 | 1 | 0 | 6.739551 | -0.908494 | 3.2789 |
| 41 | 1 | 0 | 6.233666 | 1.518723 | 3.509795 |
| 42 | 1 | 0 | 4.381306 | -2.373516 | -0.594322 |
| 43 | 1 | 0 | 1.237511 | 2.115545 | 0.213095 |
| 44 | 8 | 0 | 1.659491 | 2.964043 | 0.407752 |
| 45 | 1 | 0 | 0.731376 | 4.367027 | -0.153796 |
| 46 | 1 | 0 | 1.890632 | 2.914106 | 1.344622 |
| 47 | 8 | 0 | 0.183896 | 5.074708 | -0.555855 |
| 48 | 1 | 0 | -1.033497 | 4.270399 | -1.421143 |
| 49 | 1 | 0 | 0.77872 | 5.531943 | -1.163253 |
| 50 | 8 | 0 | -1.678112 | 3.702498 | -1.915645 |
| 51 | 1 | 0 | -2.512975 | 2.604301 | -1.036759 |
| 52 | 1 | 0 | -2.228413 | 4.293223 | -2.443271 |

Sum of electronic and zero-point Energies= -1416.265136
Sum of electronic and thermal Free Energies= -1416.332454

$TS_3$

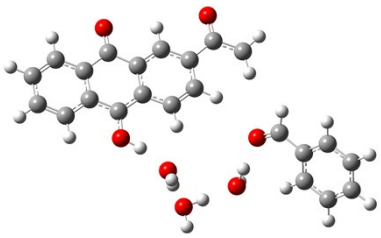


| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.184528 | -1.216152 | 1.243016 |
| 2 | 6 | 0 | -5.382774 | -0.169606 | 0.83184 |
| 3 | 6 | 0 | -4.093428 | -0.414108 | 0.299263 |
| 4 | 6 | 0 | -3.636914 | -1.757373 | 0.204125 |
| 5 | 6 | 0 | -4.470804 | -2.802458 | 0.632277 |
| 6 | 6 | 0 | -5.730245 | -2.54348 | 1.143973 |
| 7 | 6 | 0 | -3.25642 | 0.670241 | -0.129241 |
| 8 | 6 | 0 | -2.300184 | -2.070553 | -0.326219 |
| 9 | 6 | 0 | -1.48684 | -0.92792 | -0.781146 |
| 10 | 6 | 0 | -1.970788 | 0.41389 | -0.699495 |
| 11 | 6 | 0 | -1.142068 | 1.447912 | -1.208527 |
| 12 | 1 | 0 | -1.481961 | 2.474861 | -1.197178 |
| 13 | 6 | 0 | 0.598526 | -0.151504 | -1.787156 |
| 14 | 6 | 0 | -0.216689 | -1.174368 | -1.309121 |
| 15 | 1 | 0 | -7.170339 | -1.011967 | 1.645857 |
| 16 | 1 | 0 | -5.733107 | 0.850774 | 0.911319 |
| 17 | 1 | 0 | -4.098958 | -3.816563 | 0.551351 |
| 18 | 1 | 0 | -6.364858 | -3.359792 | 1.46963 |
| 19 | 1 | 0 | 0.137002 | -2.196078 | -1.3473 |
| 20 | 6 | 0 | 1.946355 | -0.50648 | -2.321513 |
| 21 | 6 | 0 | 4.701561 | 0.007539 | -1.056396 |
| 22 | 8 | 0 | 2.374768 | -1.670229 | -2.232643 |
| 23 | 8 | 0 | 3.898278 | 0.917291 | -1.422034 |
| 24 | 6 | 0 | 2.820952 | 0.518384 | -2.867268 |
| 25 | 1 | 0 | 2.459835 | 1.516803 | -3.06806 |
| 26 | 1 | 0 | 3.588794 | 0.156117 | -3.54062 |
| 27 | 6 | 0 | 0.101662 | 1.172826 | -1.736882 |
| 28 | 8 | 0 | -1.881922 | -3.234619 | -0.393498 |
| 29 | 8 | 0 | -3.768932 | 1.890616 | 0.0231 |
| 30 | 1 | 0 | 0.693931 | 1.998241 | -2.110637 |
| 31 | 6 | 0 | 4.846089 | -0.406485 | 0.319622 |
| 32 | 6 | 0 | 4.04268 | 0.133144 | 1.346603 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 6 | 0 | 5.83616 | -1.355047 | 0.648008 |
| 34 | 6 | 0 | 4.224501 | -0.278747 | 2.658663 |
| 35 | 1 | 0 | 3.283603 | 0.866599 | 1.101765 |
| 36 | 6 | 0 | 6.014551 | -1.756008 | 1.96568 |
| 37 | 1 | 0 | 6.456053 | -1.770081 | -0.139875 |
| 38 | 6 | 0 | 5.209427 | -1.221294 | 2.97458 |
| 39 | 1 | 0 | 3.60098 | 0.13367 | 3.444301 |
| 40 | 1 | 0 | 6.777051 | -2.486995 | 2.210002 |
| 41 | 1 | 0 | 5.347711 | -1.536198 | 4.002806 |
| 42 | 1 | 0 | 5.319823 | -0.495749 | -1.807405 |
| 43 | 1 | 0 | 0.662093 | 1.608378 | 0.90681 |
| 44 | 8 | 0 | 1.018241 | 2.207578 | 1.577555 |
| 45 | 1 | 0 | 0.124289 | 3.754783 | 1.584773 |
| 46 | 1 | 0 | 0.987501 | 1.704254 | 2.401893 |
| 47 | 8 | 0 | -0.389601 | 4.586223 | 1.508628 |
| 48 | 1 | 0 | -1.729203 | 4.344051 | 0.489351 |
| 49 | 1 | 0 | 0.222267 | 5.221424 | 1.11659 |
| 50 | 8 | 0 | -2.45949 | 4.155258 | -0.152619 |
| 51 | 1 | 0 | -3.150813 | 2.667929 | -0.079702 |
| 52 | 1 | 0 | -3.087122 | 4.884478 | -0.081693 |

Sum of electronic and zero-point Energies= -1416.244502
Sum of electronic and thermal Free Energies= -1416.312608
The imaginary frequency: -646.83

$PC_3$



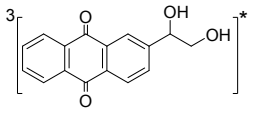
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 6.484394 | -2.413483 | -0.648644 |
| 2 | 6 | 0 | 5.103545 | -2.415027 | -0.613176 |
| 3 | 6 | 0 | 4.385493 | -1.214723 | -0.392274 |
| 4 | 6 | 0 | 5.114385 | -0.009389 | -0.203598 |
| 5 | 6 | 0 | 6.517225 | -0.035308 | -0.242369 |
| 6 | 6 | 0 | 7.200949 | -1.218289 | -0.462795 |
| 7 | 6 | 0 | 2.948677 | -1.213001 | -0.356134 |
| 8 | 6 | 0 | 4.421633 | 1.267362 | 0.035577 |
| 9 | 6 | 0 | 2.947834 | 1.224269 | 0.050316 |
| 10 | 6 | 0 | 2.228838 | 0.003958 | -0.149974 |
| 11 | 6 | 0 | 0.811075 | 0.063202 | -0.138532 |
| 12 | 1 | 0 | 0.225786 | -0.831832 | -0.304623 |
| 13 | 6 | 0 | 0.855232 | 2.456208 | 0.284037 |
| 14 | 6 | 0 | 2.246271 | 2.412771 | 0.260457 |
| 15 | 1 | 0 | 7.018256 | -3.341533 | -0.820667 |
| 16 | 1 | 0 | 4.555221 | -3.336563 | -0.755287 |
| 17 | 1 | 0 | 7.048466 | 0.897022 | -0.094906 |
| 18 | 1 | 0 | 8.284599 | -1.224909 | -0.491504 |
| 19 | 1 | 0 | 2.810509 | 3.323939 | 0.408771 |
| 20 | 6 | 0 | 0.187738 | 3.775829 | 0.513412 |
| 21 | 6 | 0 | -4.241852 | 0.635214 | -0.552199 |
| 22 | 8 | 0 | 0.873245 | 4.811714 | 0.612977 |
| 23 | 8 | 0 | -3.36612 | 0.224399 | 0.198519 |
| 24 | 6 | 0 | -1.238759 | 3.867316 | 0.628956 |
| 25 | 1 | 0 | -1.902639 | 3.014785 | 0.590356 |
| 26 | 1 | 0 | -1.664119 | 4.851901 | 0.780669 |
| 27 | 6 | 0 | 0.145397 | 1.251174 | 0.076378 |
| 28 | 8 | 0 | 5.044156 | 2.323042 | 0.211814 |
| 29 | 8 | 0 | 2.375229 | -2.402162 | -0.534613 |
| 30 | 1 | 0 | -0.937445 | 1.234647 | 0.077319 |
| 31 | 6 | 0 | -5.635992 | 0.176073 | -0.581849 |
| 32 | 6 | 0 | -6.113535 | -0.813877 | 0.293594 |
| 33 | 6 | 0 | -6.50275 | 0.757438 | -1.518596 |
| 34 | 6 | 0 | -7.441722 | -1.210624 | 0.225037 |

| | | | | | |
|---|---|---|---|---|---|
| 35 | 1 | 0 | -5.444016 | -1.264694 | 1.01663 |
| 36 | 6 | 0 | -7.833136 | 0.355958 | -1.583608 |
| 37 | 1 | 0 | -6.125652 | 1.521704 | -2.190208 |
| 38 | 6 | 0 | -8.300973 | -0.627104 | -0.711902 |
| 39 | 1 | 0 | -7.814262 | -1.973643 | 0.898781 |
| 40 | 1 | 0 | -8.50264 | 0.805094 | -2.307878 |
| 41 | 1 | 0 | -9.337548 | -0.941746 | -0.760165 |
| 42 | 1 | 0 | -3.998323 | 1.423515 | -1.284877 |
| 43 | 1 | 0 | -3.289245 | -1.053791 | 1.496825 |
| 44 | 8 | 0 | -3.288202 | -1.748533 | 2.184016 |
| 45 | 1 | 0 | -2.091139 | -2.998484 | 2.005157 |
| 46 | 1 | 0 | -3.316382 | -1.277775 | 3.025946 |
| 47 | 8 | 0 | -1.411529 | -3.690749 | 1.840897 |
| 48 | 1 | 0 | -0.614072 | -3.28347 | 0.420138 |
| 49 | 1 | 0 | -1.90299 | -4.518134 | 1.771752 |
| 50 | 8 | 0 | -0.177642 | -2.958427 | -0.409313 |
| 51 | 1 | 0 | 1.384407 | -2.469082 | -0.449981 |
| 52 | 1 | 0 | -0.519689 | -3.486897 | -1.139307 |

Sum of electronic and zero-point Energies= -1416.273403

Sum of electronic and thermal Free Energies= -1416.342941

Triplet state of Aqe-diol

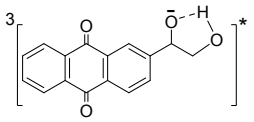



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 5.108907 | -0.004501 | -0.222787 |
| 2 | 6 | 0 | 4.099337 | 0.935877 | -0.14014 |
| 3 | 6 | 0 | 2.750623 | 0.540524 | -0.04812 |
| 4 | 6 | 0 | 2.435437 | -0.842684 | -0.0395 |
| 5 | 6 | 0 | 3.479849 | -1.784129 | -0.125279 |
| 6 | 6 | 0 | 4.796933 | -1.376396 | -0.215468 |
| 7 | 6 | 0 | 1.710226 | 1.57415 | 0.035892 |
| 8 | 6 | 0 | 1.048485 | -1.328584 | 0.058549 |
| 9 | 6 | 0 | 0.003906 | -0.314817 | 0.143824 |
| 10 | 6 | 0 | 0.340643 | 1.128227 | 0.130395 |
| 11 | 6 | 0 | -0.718406 | 2.086764 | 0.211701 |
| 12 | 1 | 0 | -0.452891 | 3.135434 | 0.205039 |
| 13 | 6 | 0 | -2.346467 | 0.256677 | 0.306768 |
| 14 | 6 | 0 | -1.331112 | -0.691485 | 0.232599 |
| 15 | 1 | 0 | 6.142791 | 0.314527 | -0.293715 |
| 16 | 1 | 0 | 4.323646 | 1.995356 | -0.145033 |
| 17 | 1 | 0 | 3.220527 | -2.83565 | -0.117289 |
| 18 | 1 | 0 | 5.590859 | -2.111992 | -0.280549 |
| 19 | 1 | 0 | -1.576486 | -1.744209 | 0.247113 |
| 20 | 6 | 0 | -3.779711 | -0.124638 | 0.419713 |
| 21 | 6 | 0 | -2.010016 | 1.683161 | 0.291177 |
| 22 | 8 | 0 | 0.771677 | -2.544336 | 0.06739 |
| 23 | 8 | 0 | 1.981228 | 2.802714 | 0.033054 |
| 24 | 1 | 0 | -2.815134 | 2.405626 | 0.354899 |
| 25 | 6 | 0 | -4.569898 | 0.204193 | -0.871218 |
| 26 | 1 | 0 | -4.561017 | 1.280972 | -1.061109 |
| 27 | 1 | 0 | -4.110567 | -0.32124 | -1.713684 |
| 28 | 8 | 0 | -3.923049 | -1.492748 | 0.725067 |
| 29 | 1 | 0 | -4.843141 | -1.707025 | 0.506516 |
| 30 | 8 | 0 | -5.896903 | -0.266851 | -0.632553 |
| 31 | 1 | 0 | -6.270571 | -0.552231 | -1.474365 |
| 32 | 1 | 0 | -4.224065 | 0.496168 | 1.219874 |

Sum of electronic and zero-point Energies= -917.758602

Sum of electronic and thermal Free Energies= -917.804454

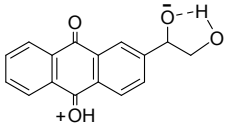
Triplet state of IM1



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 5.064945 | -0.072442 | -0.251879 |
| 2 | 6 | 0 | 4.074118 | 0.885726 | -0.180555 |
| 3 | 6 | 0 | 2.712377 | 0.526363 | -0.066142 |
| 4 | 6 | 0 | 2.367735 | -0.856168 | -0.024111 |
| 5 | 6 | 0 | 3.400541 | -1.81776 | -0.09978 |
| 6 | 6 | 0 | 4.723728 | -1.441529 | -0.210971 |
| 7 | 6 | 0 | 1.697295 | 1.574058 | 0.004949 |
| 8 | 6 | 0 | 0.981668 | -1.299991 | 0.096272 |
| 9 | 6 | 0 | -0.032552 | -0.252658 | 0.173162 |
| 10 | 6 | 0 | 0.312435 | 1.130248 | 0.125776 |
| 11 | 6 | 0 | -0.722701 | 2.089079 | 0.199135 |
| 12 | 1 | 0 | -0.450147 | 3.136817 | 0.162766 |
| 13 | 6 | 0 | -2.387721 | 0.339469 | 0.376027 |
| 14 | 6 | 0 | -1.391383 | -0.612958 | 0.29668 |
| 15 | 1 | 0 | 6.104592 | 0.223783 | -0.339194 |
| 16 | 1 | 0 | 4.319611 | 1.940378 | -0.211228 |
| 17 | 1 | 0 | 3.122945 | -2.864359 | -0.066833 |
| 18 | 1 | 0 | 5.501896 | -2.194935 | -0.266927 |
| 19 | 1 | 0 | -1.640392 | -1.666065 | 0.337692 |
| 20 | 6 | 0 | -3.842858 | -0.054906 | 0.489407 |
| 21 | 6 | 0 | -2.042667 | 1.709825 | 0.315563 |
| 22 | 8 | 0 | 0.67679 | -2.522951 | 0.13225 |
| 23 | 8 | 0 | 2.001405 | 2.797076 | -0.035034 |
| 24 | 1 | 0 | -2.824866 | 2.460602 | 0.370539 |
| 25 | 6 | 0 | -4.454031 | -0.188237 | -1.011016 |
| 26 | 1 | 0 | -4.213447 | 0.749949 | -1.508805 |
| 27 | 1 | 0 | -3.930987 | -1.021686 | -1.486177 |
| 28 | 8 | 0 | -4.118239 | -1.217408 | 1.089215 |
| 29 | 8 | 0 | -5.840379 | -0.339494 | -1.012217 |
| 30 | 1 | 0 | -4.453071 | 0.769005 | 0.899326 |
| 31 | 1 | 0 | -6.058315 | -1.219974 | -0.679978 |

Sum of electronic and zero-point Energies= -917.412592
Sum of electronic and thermal Free Energies= -917.458268

Ground state of Aqe-diol zwitterion

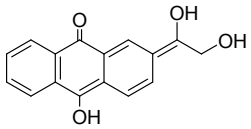



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 5.093138 | 0.059423 | -0.116835 |
| 2 | 6 | 0 | 4.048301 | 0.973124 | -0.083755 |
| 3 | 6 | 0 | 2.723263 | 0.520638 | -0.02842 |
| 4 | 6 | 0 | 2.46225 | -0.868695 | -0.007632 |
| 5 | 6 | 0 | 3.520257 | -1.768297 | -0.042357 |
| 6 | 6 | 0 | 4.831593 | -1.309638 | -0.096123 |
| 7 | 6 | 0 | 1.615306 | 1.461773 | 0.005557 |
| 8 | 6 | 0 | 1.071621 | -1.361898 | 0.047957 |
| 9 | 6 | 0 | -0.020018 | -0.353834 | 0.083221 |
| 10 | 6 | 0 | 0.274479 | 1.049312 | 0.058568 |
| 11 | 6 | 0 | -0.810117 | 1.963607 | 0.085398 |
| 12 | 1 | 0 | -0.624513 | 3.031134 | 0.055169 |
| 13 | 6 | 0 | -2.399802 | 0.134612 | 0.153022 |
| 14 | 6 | 0 | -1.317164 | -0.776469 | 0.134502 |
| 15 | 1 | 0 | 6.113713 | 0.409656 | -0.159206 |
| 16 | 1 | 0 | 4.248433 | 2.031242 | -0.100844 |
| 17 | 1 | 0 | 3.301652 | -2.8247 | -0.026907 |
| 18 | 1 | 0 | 5.650337 | -2.013504 | -0.122175 |
| 19 | 1 | 0 | -1.522219 | -1.833518 | 0.154786 |
| 20 | 6 | 0 | -3.765416 | -0.380343 | 0.257611 |
| 21 | 6 | 0 | -2.107232 | 1.524375 | 0.132242 |
| 22 | 8 | 0 | 0.843428 | -2.48485 | 0.063192 |
| 23 | 8 | 0 | 1.976383 | 2.722794 | -0.013943 |
| 24 | 1 | 0 | -2.912882 | 2.249057 | 0.145617 |
| 25 | 6 | 0 | -4.916101 | 0.544489 | -0.236794 |
| 26 | 1 | 0 | -5.092668 | 1.348396 | 0.485967 |
| 27 | 1 | 0 | -4.679039 | 1.00293 | -1.210997 |
| 28 | 8 | 0 | -4.027866 | -1.674363 | -0.027066 |
| 29 | 8 | 0 | -6.05677 | -0.289728 | -0.343992 |
| 30 | 1 | 0 | -3.756291 | -0.239651 | 1.405887 |
| 31 | 1 | 0 | 1.227858 | 3.340627 | 0.012638 |
| 32 | 1 | 0 | -5.661916 | -1.165577 | -0.142431 |

Sum of electronic and zero-point Energies= -917.775279

Sum of electronic and thermal Free Energies= -917.819046

Ground state of Aqe-diol xylylene

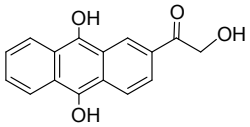



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.101223 | 0.052231 | -0.007825 |
| 2 | 6 | 0 | -4.063382 | 0.966793 | -0.006903 |
| 3 | 6 | 0 | -2.718189 | 0.534025 | -0.005528 |
| 4 | 6 | 0 | -2.456469 | -0.863585 | -0.004953 |
| 5 | 6 | 0 | -3.52963 | -1.770951 | -0.00619 |
| 6 | 6 | 0 | -4.839619 | -1.327146 | -0.007554 |
| 7 | 6 | 0 | -1.630628 | 1.479411 | -0.004234 |
| 8 | 6 | 0 | -1.077989 | -1.371266 | -0.002617 |
| 9 | 6 | 0 | -0.008776 | -0.358249 | 0.001554 |
| 10 | 6 | 0 | -0.317627 | 1.06852 | -0.001107 |
| 11 | 6 | 0 | 0.808119 | 1.978094 | -0.000472 |
| 12 | 1 | 0 | 0.632639 | 3.048776 | -0.006049 |
| 13 | 6 | 0 | 2.396895 | 0.125738 | 0.015156 |
| 14 | 6 | 0 | 1.297122 | -0.779808 | 0.010313 |
| 15 | 1 | 0 | -6.12583 | 0.406935 | -0.008739 |
| 16 | 1 | 0 | -4.278602 | 2.026599 | -0.00707 |
| 17 | 1 | 0 | -3.306538 | -2.8306 | -0.005855 |
| 18 | 1 | 0 | -5.658299 | -2.037032 | -0.008258 |
| 19 | 1 | 0 | 1.488785 | -1.845088 | 0.014926 |
| 20 | 6 | 0 | 3.699753 | -0.340989 | 0.036771 |
| 21 | 6 | 0 | 2.08995 | 1.542155 | 0.006198 |
| 22 | 8 | 0 | -0.832087 | -2.594583 | -0.003776 |
| 23 | 8 | 0 | -2.023315 | 2.80152 | -0.005904 |
| 24 | 1 | 0 | 2.895231 | 2.26626 | 0.008656 |
| 25 | 6 | 0 | 4.930892 | 0.53999 | 0.085209 |
| 26 | 1 | 0 | 4.87787 | 1.319627 | -0.677711 |
| 27 | 1 | 0 | 4.981801 | 1.026441 | 1.063409 |
| 28 | 8 | 0 | 3.951376 | -1.648939 | 0.055864 |
| 29 | 8 | 0 | 6.109298 | -0.249772 | -0.057627 |
| 30 | 1 | 0 | 6.30187 | -0.336237 | -1.000454 |
| 31 | 1 | 0 | -1.253689 | 3.382531 | -0.000483 |
| 32 | 1 | 0 | 4.927389 | -1.743797 | 0.072271 |

Sum of electronic and zero-point Energies= -917.824088

Sum of electronic and thermal Free Energies= -917.867613

Ground state of ($\alpha$-hydroxy ketone)-$AQH_2$




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -5.059944 | 0.112731 | -0.000445 |
| 2 | 6 | 0 | -4.033385 | 1.018777 | -0.000439 |
| 3 | 6 | 0 | -2.669914 | 0.593827 | -0.000165 |
| 4 | 6 | 0 | -2.401313 | -0.82315 | -0.000051 |
| 5 | 6 | 0 | -3.500347 | -1.73396 | 0.000001 |
| 6 | 6 | 0 | -4.791579 | -1.281822 | -0.000148 |
| 7 | 6 | 0 | -1.589451 | 1.499823 | 0.000071 |
| 8 | 6 | 0 | -1.072473 | -1.286137 | 0.000043 |
| 9 | 6 | 0 | 0.005426 | -0.378591 | 0.000404 |
| 10 | 6 | 0 | -0.266546 | 1.041566 | 0.000379 |
| 11 | 6 | 0 | 0.838971 | 1.948313 | 0.000522 |
| 12 | 1 | 0 | 0.635919 | 3.010676 | 0.00055 |
| 13 | 6 | 0 | 2.404683 | 0.097598 | 0.000581 |
| 14 | 6 | 0 | 1.360177 | -0.800854 | 0.000605 |
| 15 | 1 | 0 | -6.086089 | 0.461221 | -0.000625 |
| 16 | 1 | 0 | -4.278071 | 2.075269 | -0.000591 |
| 17 | 1 | 0 | -3.293604 | -2.795748 | 0.000251 |
| 18 | 1 | 0 | -5.615179 | -1.986187 | -0.000003 |
| 19 | 1 | 0 | 1.613368 | -1.854995 | 0.000663 |
| 20 | 6 | 0 | 3.787885 | -0.425689 | 0.0003 |
| 21 | 6 | 0 | 2.127375 | 1.501767 | 0.000537 |
| 22 | 8 | 0 | -0.902761 | -2.644068 | -0.000607 |
| 23 | 8 | 0 | -1.765714 | 2.863114 | 0.000145 |
| 24 | 1 | 0 | 2.938965 | 2.217989 | 0.000592 |
| 25 | 6 | 0 | 4.953228 | 0.546594 | -0.000662 |
| 26 | 1 | 0 | 4.872365 | 1.191782 | -0.884197 |
| 27 | 1 | 0 | 4.873516 | 1.191878 | 0.88295 |
| 28 | 8 | 0 | 4.041328 | -1.628611 | 0.000863 |
| 29 | 8 | 0 | 6.189464 | -0.142899 | -0.001552 |
| 30 | 1 | 0 | 0.03316 | -2.877134 | 0.00198 |
| 31 | 1 | 0 | -2.703637 | 3.086181 | -0.001395 |
| 32 | 1 | 0 | 5.95399 | -1.085981 | -0.00017 |

Sum of electronic and zero-point Energies= -917.841441

Sum of electronic and thermal Free Energies= -917.885692