Supplementary Material

**A DFT study of the chemical reactivity of thiobencarb and its oxidized derivatives in aqueous phase.**

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Table IS. xyz coordinates of thiobencarb optimized at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase employing the PCM solvation model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | x | y | z |
| H | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.00000000 | 0.00000000 | 1.08215012 |
| C | 0.01955886 | 0.00000000 | 3.85784491 |
| C | -1.11635737 | 0.46081044 | 1.77364562 |
| C | 1.12047642 | -0.45708648 | 1.75880177 |
| C | 1.11524823 | -0.45327124 | 3.14310956 |
| C | -1.09206808 | 0.45499948 | 3.16525814 |
| H | 1.98488356 | -0.80860486 | 1.21478815 |
| H | -1.95033699 | 0.81092947 | 3.72029904 |
| H | 0.03155678 | -0.00061677 | 4.93785464 |
| Cl | 2.52500093 | -1.02970077 | 4.00801831 |
| C | -2.33104817 | 0.93833994 | 1.02860532 |
| H | -2.07088766 | 1.31157456 | 0.04279811 |
| H | -2.85431261 | 1.71773274 | 1.57501386 |
| S | -3.46644692 | -0.47784272 | 0.8189588 |
| C | -4.7496949 | 0.33564665 | -0.1632449 |
| O | -4.63082049 | 1.50468968 | -0.49179816 |
| N | -5.79645533 | -0.44100483 | -0.49443651 |
| C | -6.8589914 | 0.13249874 | -1.31807131 |
| H | -7.26217279 | -0.67308936 | -1.93134012 |
| H | -6.41413548 | 0.86260495 | -1.9892733 |
| C | -7.96161992 | 0.77201278 | -0.4866548 |
| H | -8.40356021 | 0.05030302 | 0.2011689 |
| H | -8.75209736 | 1.14589339 | -1.13736444 |
| H | -7.56946535 | 1.60652775 | 0.09362932 |
| C | -5.95098551 | -1.83049753 | -0.07986993 |
| H | -5.44003753 | -1.97977984 | 0.86984761 |
| H | -7.01058844 | -1.98969306 | 0.1218172 |
| C | -5.45408966 | -2.82399018 | -1.12087262 |
| H | -5.98588814 | -2.70043301 | -2.06451023 |
| H | -5.61717308 | -3.84333066 | -0.77191393 |
| H | -4.38866514 | -2.68957169 | -1.30657985 |

Table IIS. xyz coordinates of dechlorinated thiobencarb optimized at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase employing the PCM solvation model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | x | y | z |
| H | -2.653064 | 0.320674 | -2.127341 |
| C | -3.147256 | 0.171998 | -1.175446 |
| C | -4.419002 | -0.212583 | 1.258197 |
| C | -2.483928 | -0.506055 | -0.15617 |
| C | -4.434899 | 0.652568 | -0.982777 |
| C | -5.0733 | 0.462301 | 0.235728 |
| C | -3.132263 | -0.694399 | 1.061984 |
| H | -4.940247 | 1.171945 | -1.785802 |
| H | -2.626528 | -1.222323 | 1.860985 |
| H | -4.911438 | -0.366996 | 2.208727 |
| C | -1.08526 | -1.015696 | -0.36702 |
| H | -0.878772 | -1.190437 | -1.418555 |
| H | -0.906257 | -1.934468 | 0.184442 |
| S | 0.08908 | 0.250333 | 0.232736 |
| C | 1.63297 | -0.525657 | -0.300932 |
| O | 1.617085 | -1.586755 | -0.903688 |
| N | 2.754481 | 0.151968 | 0.002827 |
| C | 4.037271 | -0.403687 | -0.424267 |
| H | 4.71329 | 0.434067 | -0.592861 |
| H | 3.892589 | -0.904882 | -1.377933 |
| C | 4.623292 | -1.364854 | 0.600224 |
| H | 4.78036 | -0.86817 | 1.55819 |
| H | 5.58379 | -1.744749 | 0.252148 |
| H | 3.953308 | -2.209913 | 0.754452 |
| C | 2.782152 | 1.409139 | 0.741276 |
| H | 1.942972 | 1.438721 | 1.434398 |
| H | 3.680628 | 1.397446 | 1.358712 |
| C | 2.778441 | 2.633028 | -0.164485 |
| H | 3.627252 | 2.615111 | -0.848357 |
| H | 2.843299 | 3.541732 | 0.433524 |
| H | 1.862702 | 2.6736 | -0.753889 |
| H | -6.076521 | 0.836947 | 0.38722 |

Table IIIS. xyz coordinates of thiobencarb sulfone optimized at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase employing the PCM solvation model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | x | y | z |
| H | 1.946046 | -2.322063 | -0.281924 |
| C | 2.36446 | -1.327573 | -0.353296 |
| C | 3.446827 | 1.225333 | -0.534644 |
| C | 1.534819 | -0.244415 | -0.628186 |
| C | 3.725158 | -1.146268 | -0.168473 |
| C | 4.250928 | 0.131634 | -0.261454 |
| C | 2.086623 | 1.02982 | -0.713979 |
| H | 4.367758 | -1.988008 | 0.043206 |
| H | 1.4531 | 1.879898 | -0.928697 |
| H | 3.874988 | 2.213847 | -0.609559 |
| Cl | 5.969379 | 0.368047 | -0.034787 |
| C | 0.060273 | -0.445832 | -0.80228 |
| H | -0.185527 | -1.417626 | -1.226185 |
| H | -0.398542 | 0.338359 | -1.400553 |
| S | -0.764896 | -0.41311 | 0.807667 |
| C | -2.567973 | -0.764724 | 0.341801 |
| O | -2.891209 | -1.922288 | 0.481555 |
| N | -3.328018 | 0.229078 | -0.107131 |
| C | -4.710358 | -0.113039 | -0.474283 |
| H | -5.305758 | 0.787183 | -0.336728 |
| H | -5.073042 | -0.861902 | 0.224873 |
| C | -4.812359 | -0.613784 | -1.906555 |
| H | -4.44112 | 0.131576 | -2.610045 |
| H | -5.854464 | -0.819751 | -2.148176 |
| H | -4.241239 | -1.532015 | -2.035983 |
| C | -2.942506 | 1.630805 | -0.299227 |
| H | -1.87151 | 1.709859 | -0.443909 |
| H | -3.410266 | 1.951189 | -1.229689 |
| C | -3.379849 | 2.515261 | 0.857099 |
| H | -4.454998 | 2.448297 | 1.022137 |
| H | -3.136703 | 3.554021 | 0.636611 |
| H | -2.865806 | 2.223822 | 1.771097 |
| O | -0.60302 | 0.894563 | 1.414035 |
| O | -0.34129 | -1.573599 | 1.558536 |

Table IVS. xyz coordinates of dechlorinated thiobencarb sulfone optimized at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase employing the PCM solvation model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | x | y | z |
| H | 2.796354 | -2.172223 | -0.410744 |
| C | 3.147173 | -1.148787 | -0.431248 |
| C | 4.045589 | 1.476884 | -0.487755 |
| C | 2.24039 | -0.113042 | -0.638764 |
| C | 4.495005 | -0.873045 | -0.254062 |
| C | 4.946284 | 0.44024 | -0.28099 |
| C | 2.697895 | 1.20169 | -0.664844 |
| H | 5.193984 | -1.68319 | -0.097563 |
| H | 1.99643 | 2.009648 | -0.826505 |
| H | 4.393069 | 2.500645 | -0.513901 |
| C | 0.779279 | -0.404444 | -0.805908 |
| H | 0.588763 | -1.389724 | -1.226976 |
| H | 0.270767 | 0.349623 | -1.403265 |
| S | -0.042129 | -0.416865 | 0.806043 |
| C | -1.838743 | -0.805017 | 0.347816 |
| O | -2.143195 | -1.967089 | 0.494431 |
| N | -2.618927 | 0.173605 | -0.10151 |
| C | -3.996278 | -0.194632 | -0.461708 |
| H | -4.606928 | 0.695978 | -0.328374 |
| H | -4.344152 | -0.944774 | 0.243546 |
| C | -4.094906 | -0.706373 | -1.890396 |
| H | -3.736046 | 0.039691 | -2.599541 |
| H | -5.134598 | -0.928541 | -2.128058 |
| H | -3.510902 | -1.617035 | -2.015518 |
| C | -2.260224 | 1.580967 | -0.304376 |
| H | -1.191052 | 1.680545 | -0.448611 |
| H | -2.73288 | 1.884724 | -1.238048 |
| C | -2.714553 | 2.467393 | 0.843813 |
| H | -3.788399 | 2.383077 | 1.009065 |
| H | -2.489501 | 3.508244 | 0.613961 |
| H | -2.19554 | 2.193382 | 1.760391 |
| O | 0.080228 | 0.886525 | 1.431196 |
| O | 0.415256 | -1.574458 | 1.5416 |
| H | 5.997402 | 0.653712 | -0.143246 |

Table VS. xyz coordinates of thiobencarb sulfoxide optimized at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase employing the PCM solvation model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | x | y | z |
| H | 1.90487 | -2.206 | 0.823432 |
| C | 2.336176 | -1.341053 | 0.336558 |
| C | 3.459838 | 0.868304 | -0.913749 |
| C | 1.520624 | -0.472423 | -0.3848 |
| C | 3.699438 | -1.118049 | 0.437834 |
| C | 4.246388 | -0.010648 | -0.189783 |
| C | 2.096312 | 0.632049 | -1.004755 |
| H | 4.327474 | -1.795806 | 0.99698 |
| H | 1.47713 | 1.314586 | -1.570918 |
| H | 3.902245 | 1.725764 | -1.399059 |
| Cl | 5.968429 | 0.278603 | -0.069115 |
| C | 0.04427 | -0.703873 | -0.459115 |
| H | -0.212995 | -1.760926 | -0.444288 |
| H | -0.404037 | -0.222023 | -1.325876 |
| S | -0.766001 | 0.026973 | 1.029965 |
| C | -2.446594 | -0.677468 | 0.56894 |
| O | -2.526467 | -1.844442 | 0.910336 |
| N | -3.397994 | 0.047754 | -0.005481 |
| C | -4.69742 | -0.59563 | -0.229722 |
| H | -5.450412 | 0.190378 | -0.209676 |
| H | -4.893287 | -1.264984 | 0.604294 |
| C | -4.74204 | -1.353823 | -1.547985 |
| H | -4.549805 | -0.6886 | -2.390032 |
| H | -5.726067 | -1.800453 | -1.686163 |
| H | -3.997662 | -2.148789 | -1.556255 |
| C | -3.226844 | 1.400319 | -0.543571 |
| H | -2.174559 | 1.580187 | -0.730732 |
| H | -3.737771 | 1.419793 | -1.506254 |
| C | -3.784435 | 2.46923 | 0.382332 |
| H | -4.84363 | 2.309655 | 0.584466 |
| H | -3.673457 | 3.449207 | -0.080991 |
| H | -3.243156 | 2.470509 | 1.327188 |
| O | -0.618594 | 1.512416 | 0.912748 |

Table VIS. xyz coordinates of dechlorinated thiobencarb sulfoxide optimized at the wB97XD/6-311++G(2d,2p) level of theory in the aqueous phase employing the PCM solvation model.

|  |  |  |  |
| --- | --- | --- | --- |
| Atom | x | y | z |
| H | -2.696743 | -2.068128 | -0.807369 |
| C | -3.115689 | -1.199194 | -0.31547 |
| C | -4.194267 | 1.020344 | 0.950702 |
| C | -2.283381 | -0.352677 | 0.414637 |
| C | -4.474081 | -0.93912 | -0.411372 |
| C | -5.016474 | 0.173256 | 0.220606 |
| C | -2.833723 | 0.759648 | 1.044975 |
| H | -5.110152 | -1.604056 | -0.979548 |
| H | -2.195288 | 1.420645 | 1.61654 |
| H | -4.611179 | 1.886505 | 1.446315 |
| C | -0.81161 | -0.619207 | 0.486543 |
| H | -0.580249 | -1.682639 | 0.48431 |
| H | -0.346675 | -0.137862 | 1.344991 |
| S | 0.010712 | 0.069342 | -1.014687 |
| C | 1.669895 | -0.695377 | -0.573841 |
| O | 1.709058 | -1.862291 | -0.92297 |
| N | 2.650402 | -0.005653 | -0.00397 |
| C | 3.93191 | -0.690116 | 0.200264 |
| H | 4.707124 | 0.074003 | 0.181768 |
| H | 4.099924 | -1.355113 | -0.643347 |
| C | 3.967295 | -1.464941 | 1.509107 |
| H | 3.796937 | -0.805433 | 2.36034 |
| H | 4.94159 | -1.935905 | 1.635109 |
| H | 3.204601 | -2.242277 | 1.513493 |
| C | 2.526502 | 1.346656 | 0.547458 |
| H | 1.482752 | 1.554694 | 0.752422 |
| H | 3.051778 | 1.34278 | 1.502609 |
| C | 3.100107 | 2.407399 | -0.3779 |
| H | 4.152288 | 2.222173 | -0.594386 |
| H | 3.02024 | 3.386576 | 0.093501 |
| H | 2.546266 | 2.429087 | -1.315188 |
| H | -6.076152 | 0.375696 | 0.145248 |
| O | -0.07283 | 1.560957 | -0.908065 |

|  |  |  |
| --- | --- | --- |
| 1. TB | 1. TBS | 1. TBSu |
|  |  |  |
| 1. DTB | 1. DTBS | 1. DTBSu |
|  |  |  |

Figure 1S. Mapping of the electrostatic potentials evaluated at the wB97XD/6-311++G(2d,2p) level of theory employing the PCM solvation model, onto a density isosurface (value =0.002 e/a.u.3) for a) TB, b) TBS, c) TBSu, d) DTB, e) DTBS and f) DTBSu.

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