Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. *83* (9) S288–S293 (2018) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

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

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J. Serb. Chem. Soc. *83* (9) (2018) 981–993

TABLE S-I. The *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

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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 S-II. The *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 S-III. The *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 S-IV. The *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 S-V. The *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 S-VI. The *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

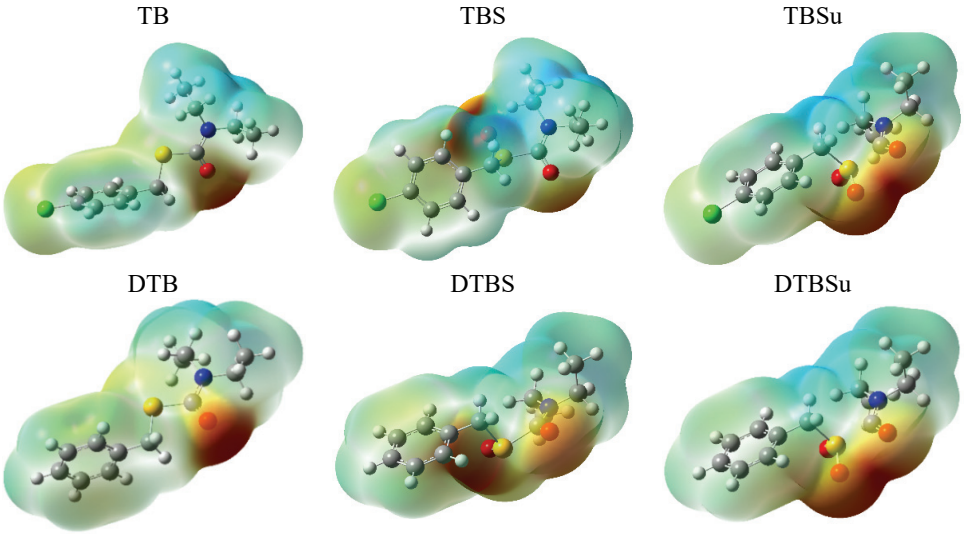

Fig. S-1. Mapping of the electrostatic potentials evaluated at the wB97XD/6-311++G(2d,2p) level of theory employing the PCM solvation model, onto a density isosurface (value = 0.002 e/a.u.^{3}) for a) TB, b) TBS, c) TBSu, d) DTB, e) DTBS and f) DTBSu.