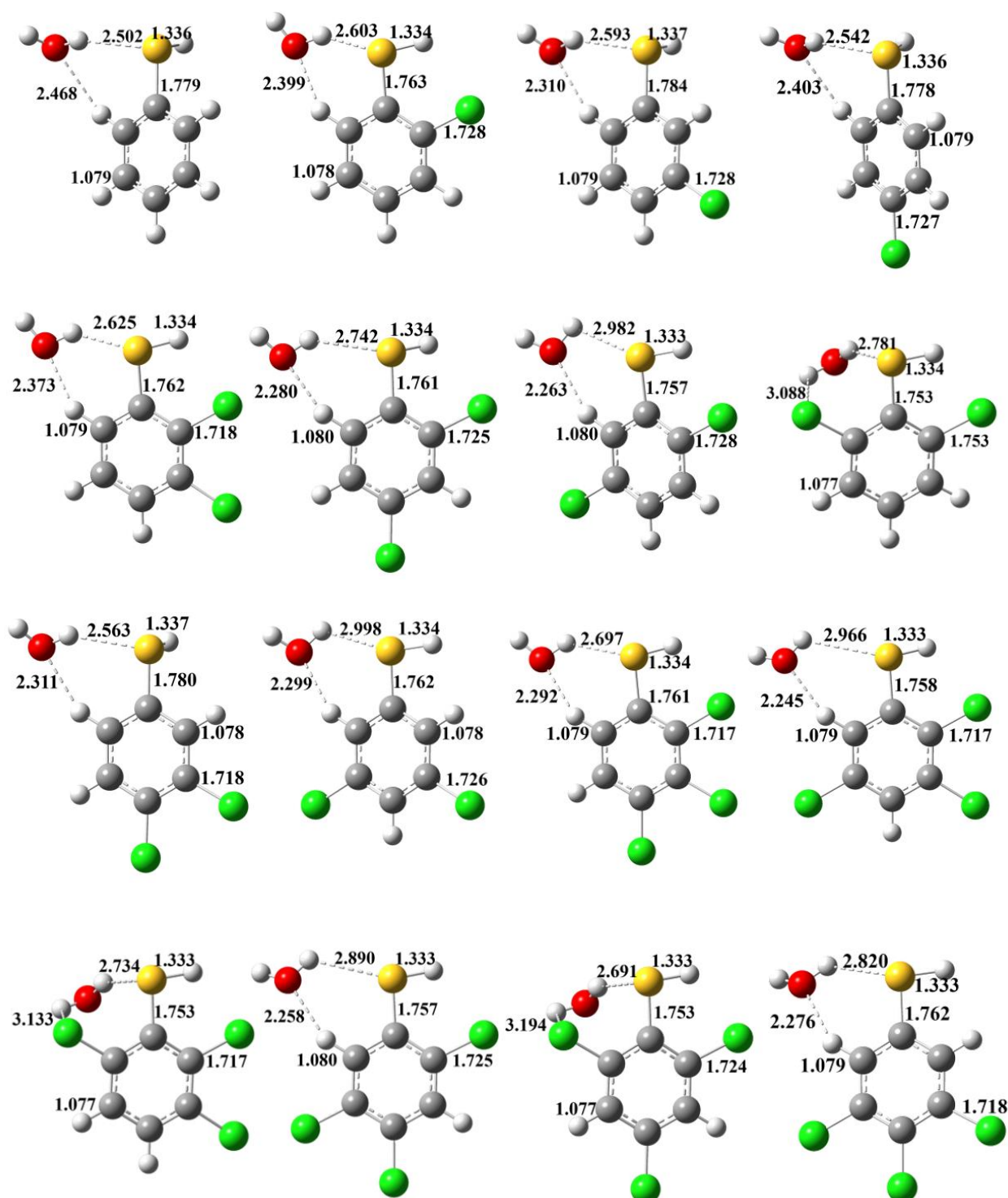


Effect of Water Molecule on the Complete Series Reactions of Chlorothiobenzenes with $\text{H}\cdot\text{OH}$: a Theoretical Study

Yanan Han, Siyuan Zheng, Zhuochao Teng, Mohammad Hassan Hadizadeh, Qi Zhang, Fei Xu and Yanhui Sun



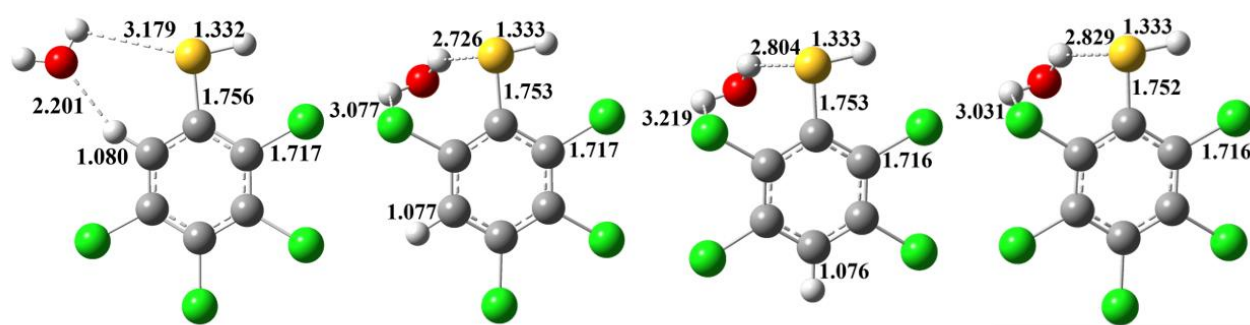


Figure S1. Structures of the hydrated reactants CTB-H₂O. Distances are in angstrom.

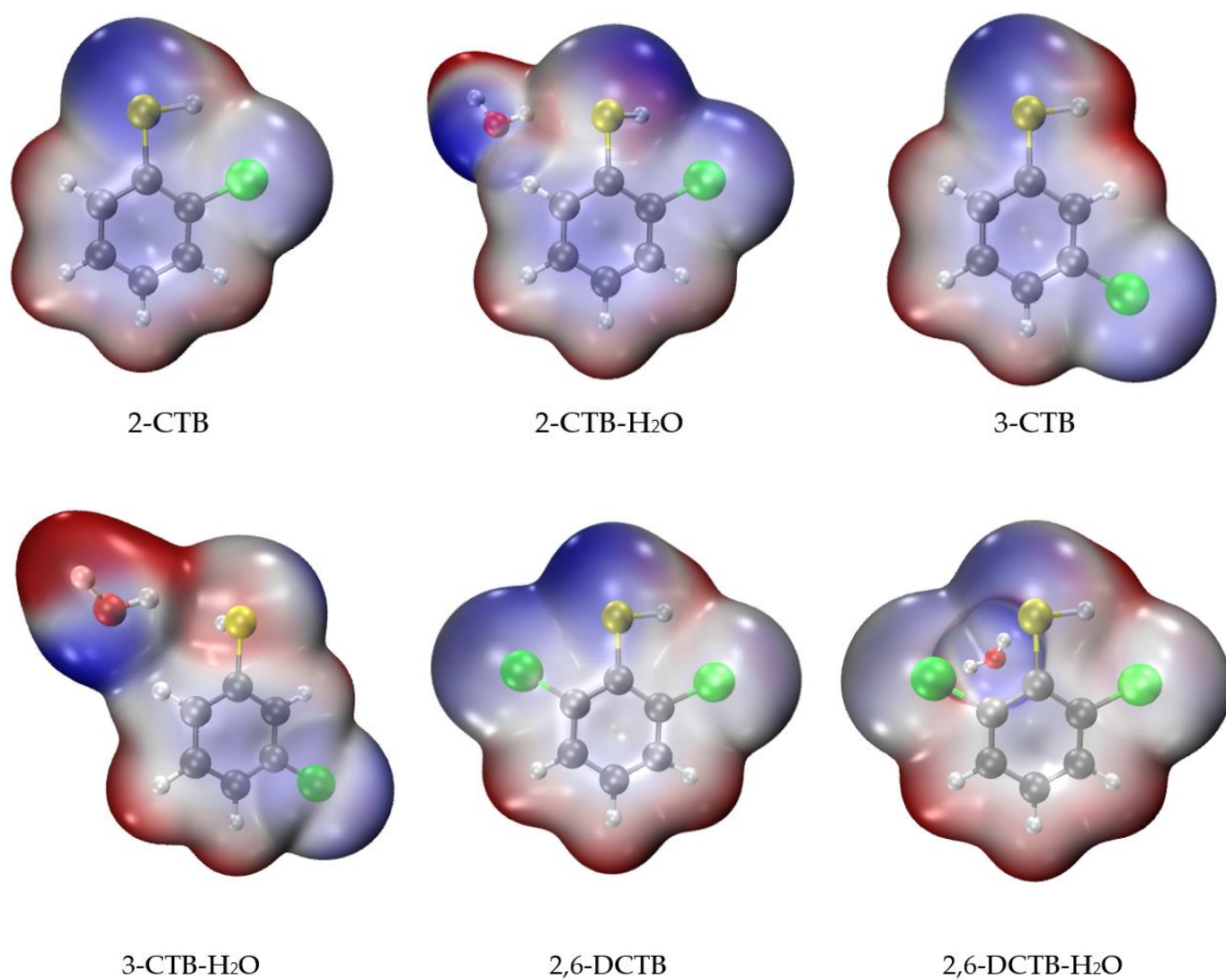
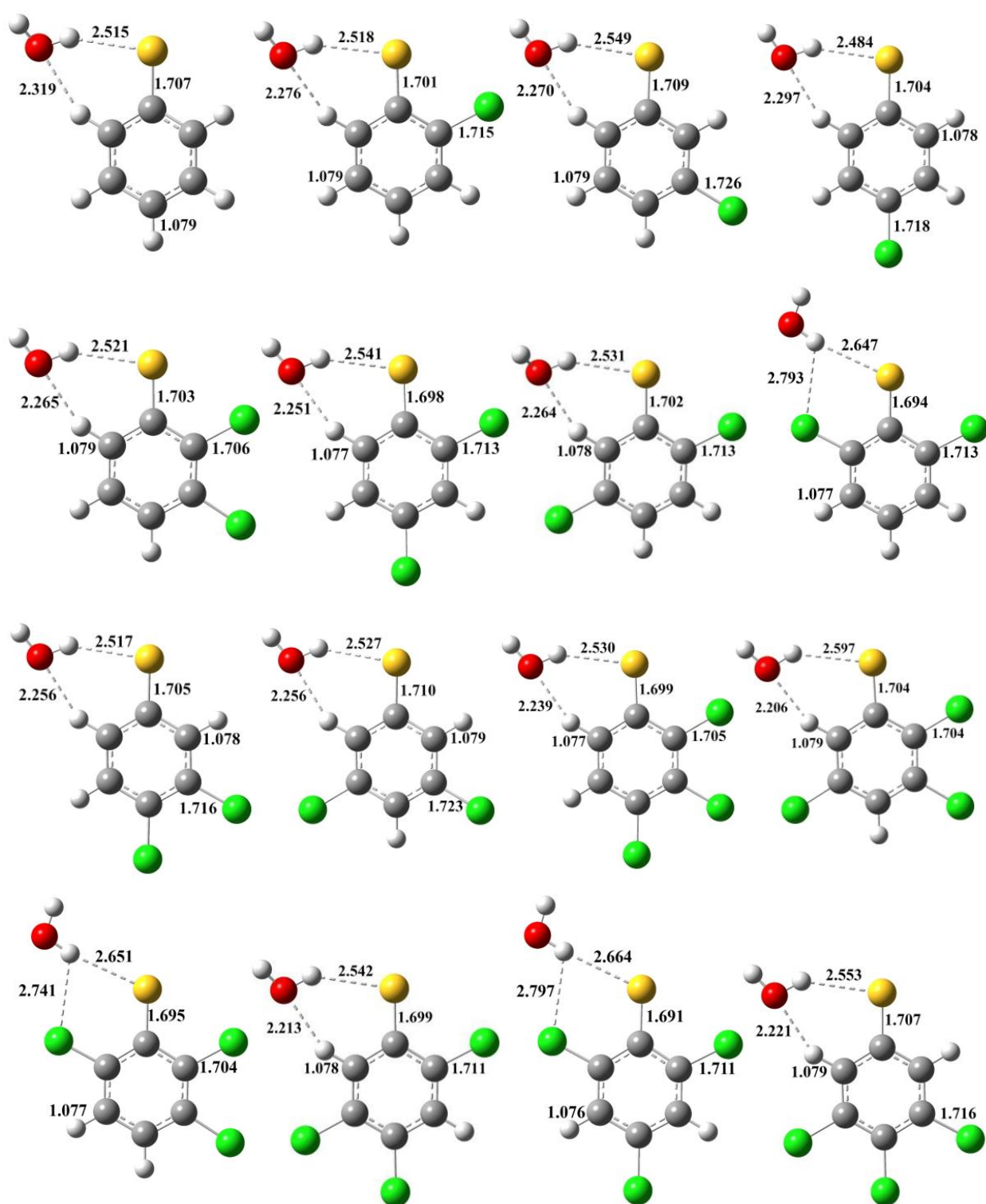


Figure S2. Electron density from total SCF density of 2-CTB, 3-CTB, 2,6-DCTB, 2-CTB-H₂O, 3-CTB-H₂O and 2,6-DCTB-H₂O at MPWB1K/6-311+G(3df,2p) level (positive region in blue; negative region in red).



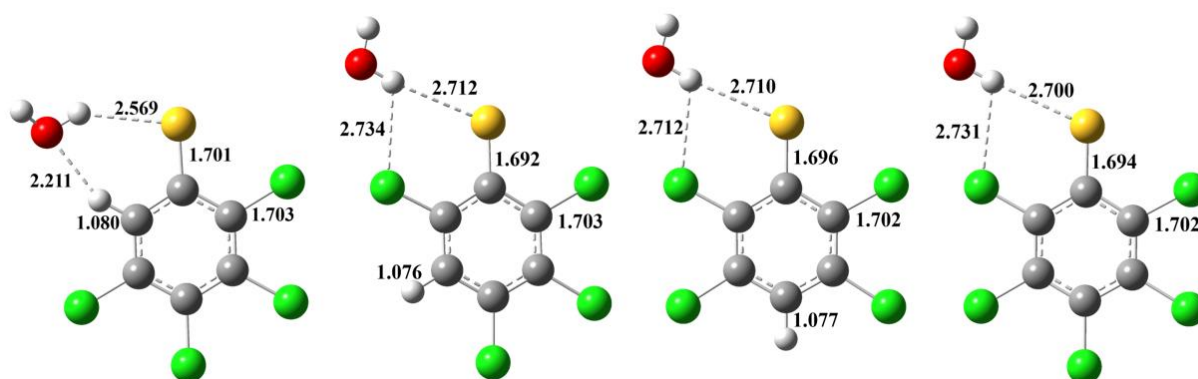
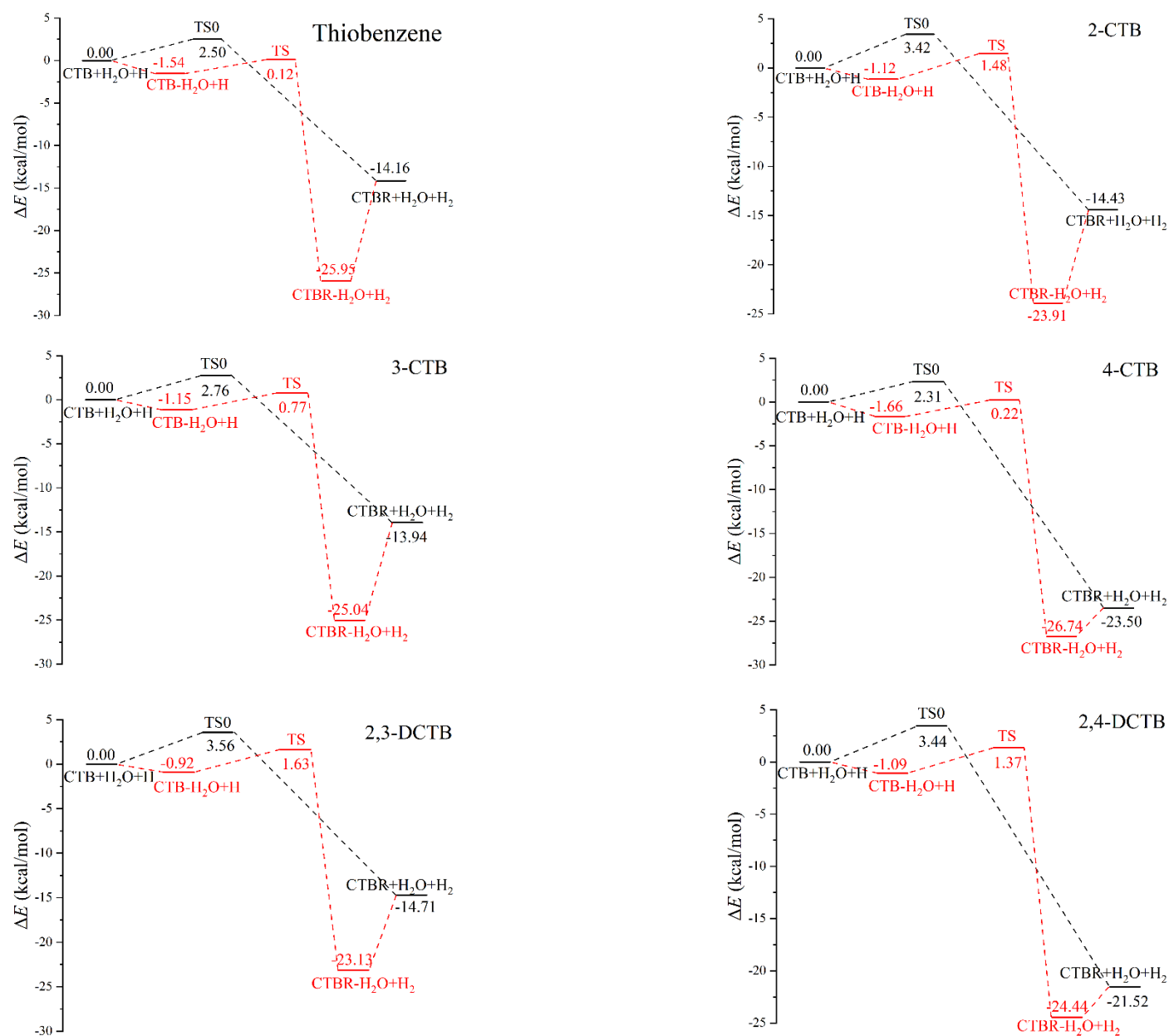
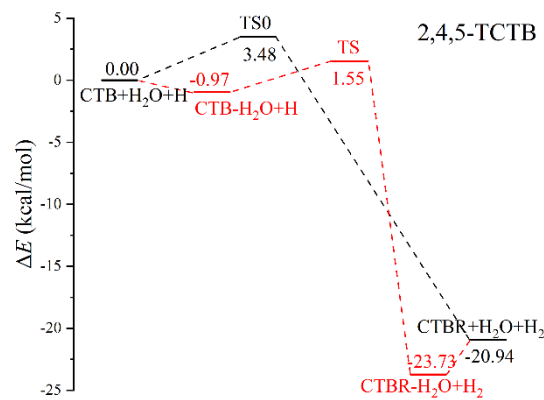
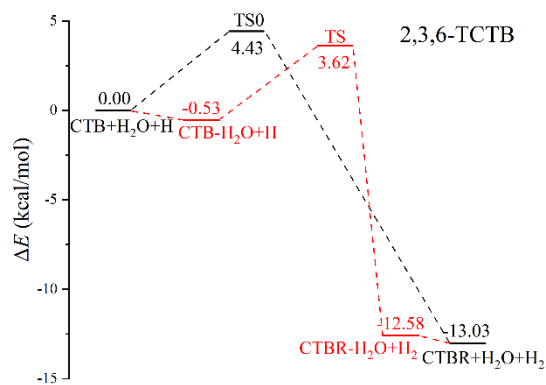
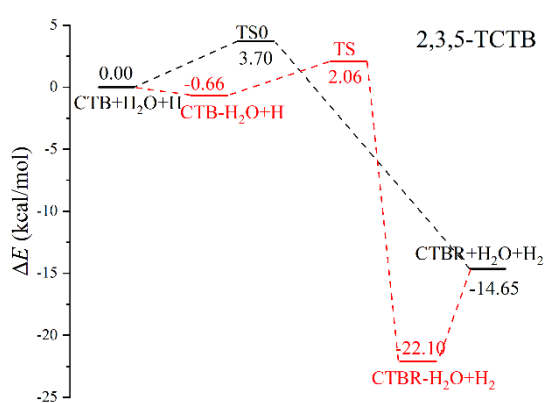
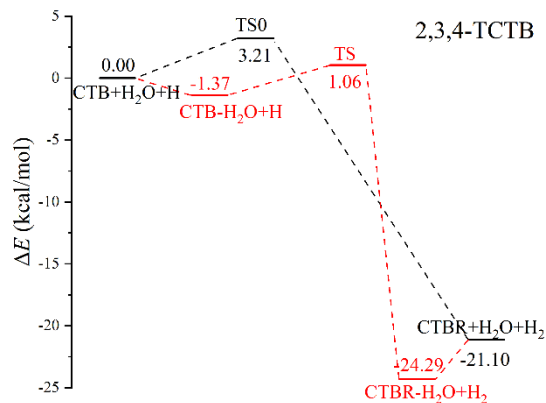
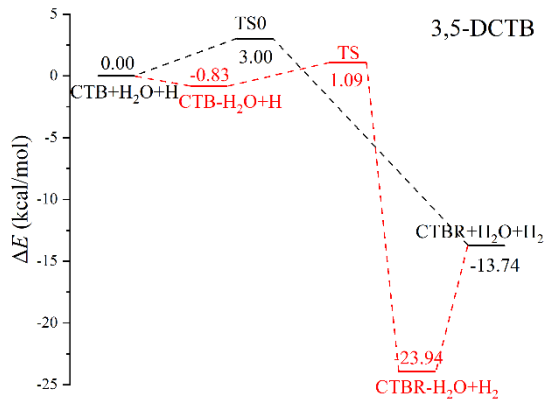
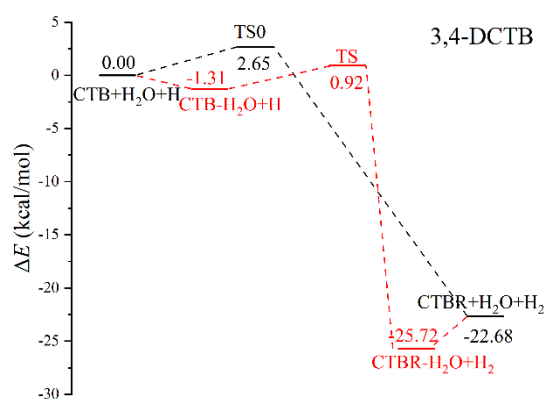
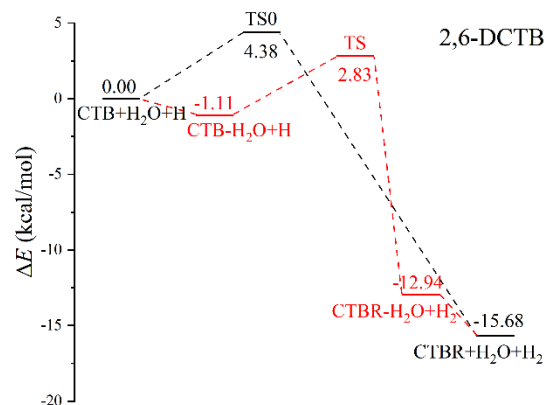
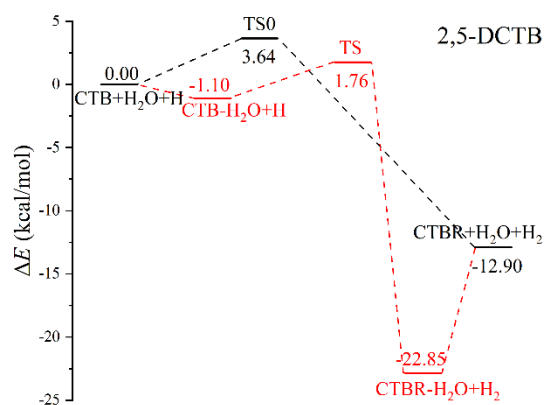


Figure S3. Structures of the hydrated products CTBR-H₂O_s. Distances are in angstrom.





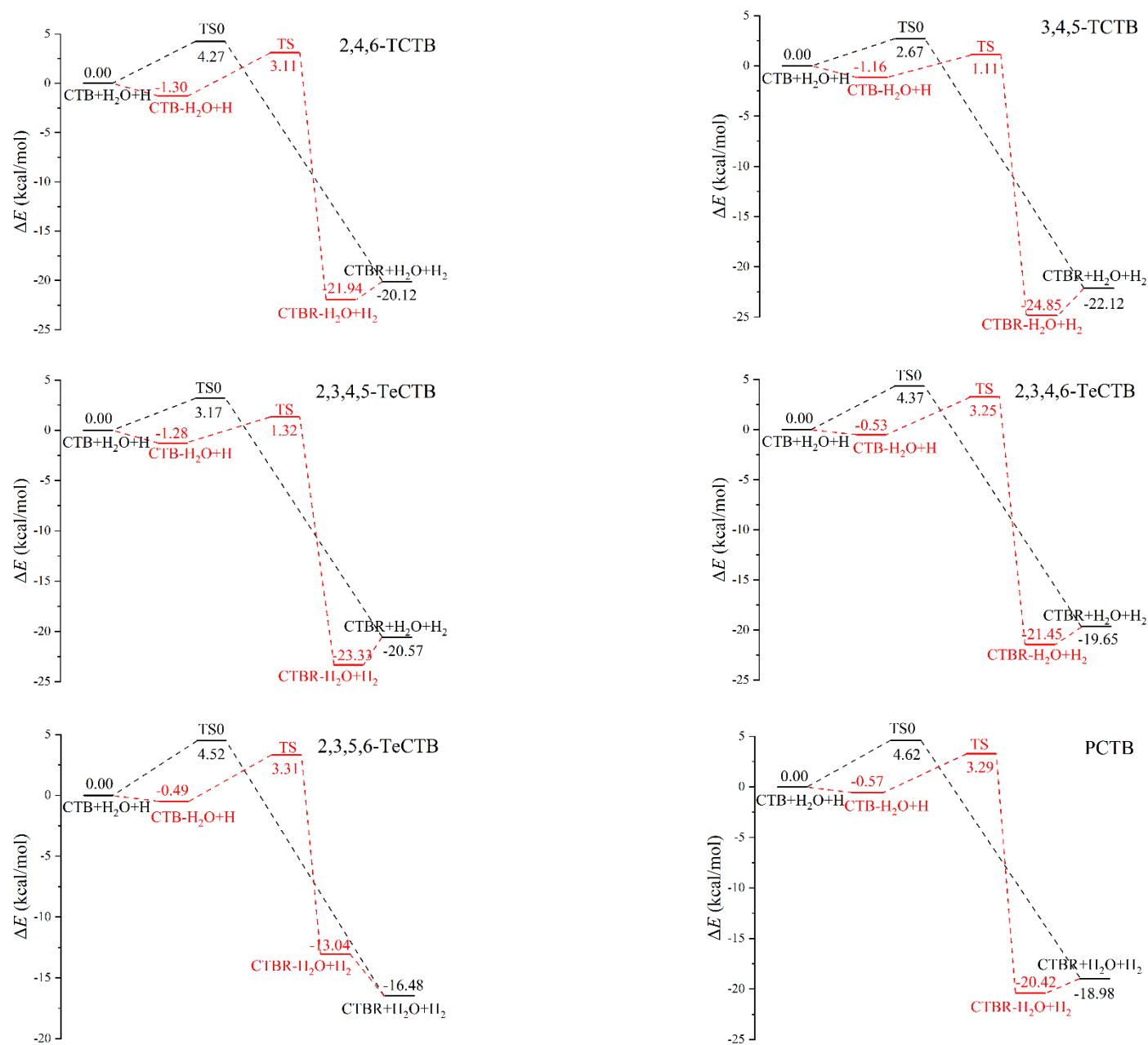
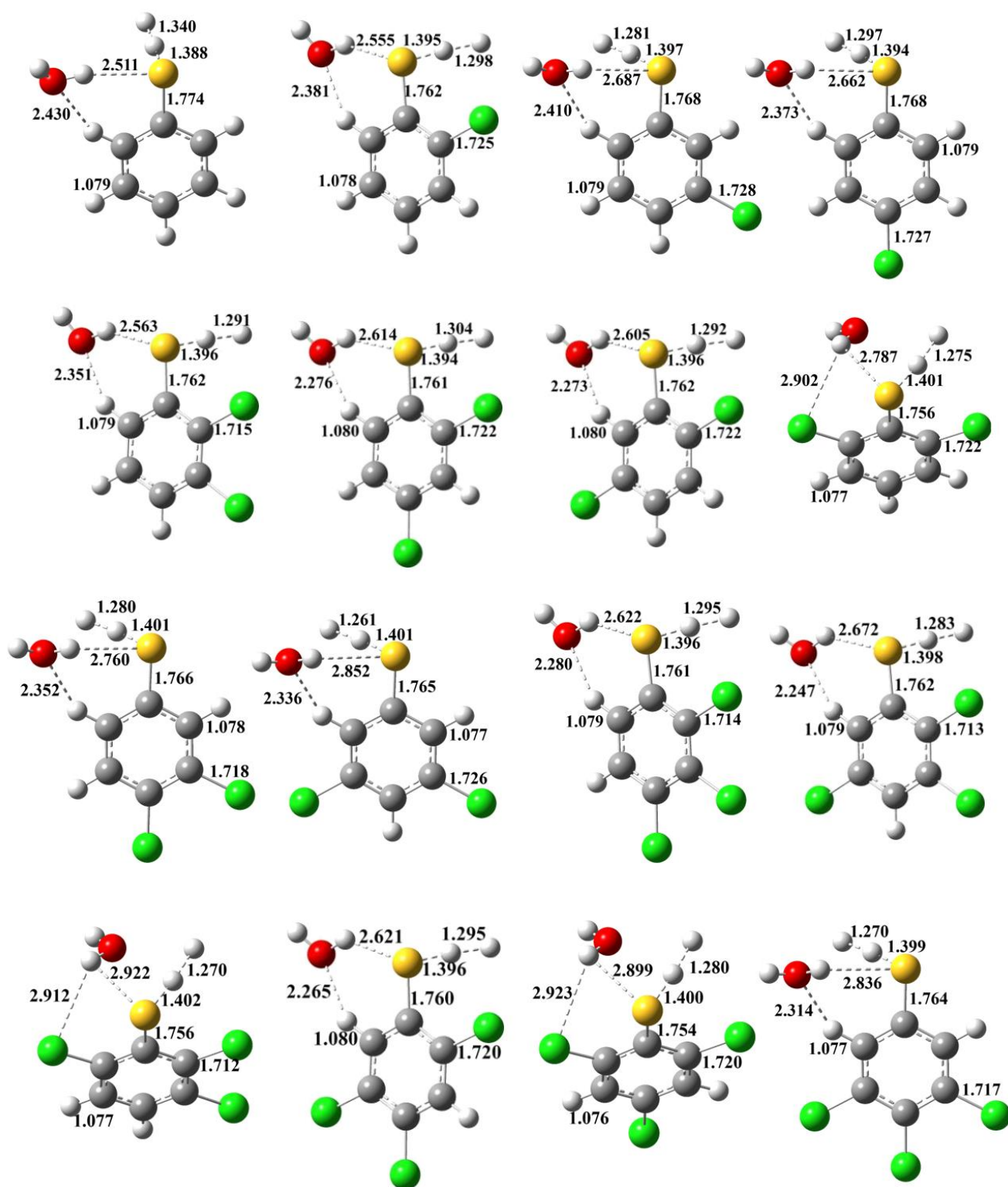


Figure S4. The schematic energy profiles of the H abstraction from CTBs by H atom with and without the aid of water. ΔE and ΔH is calculated at 0 K.



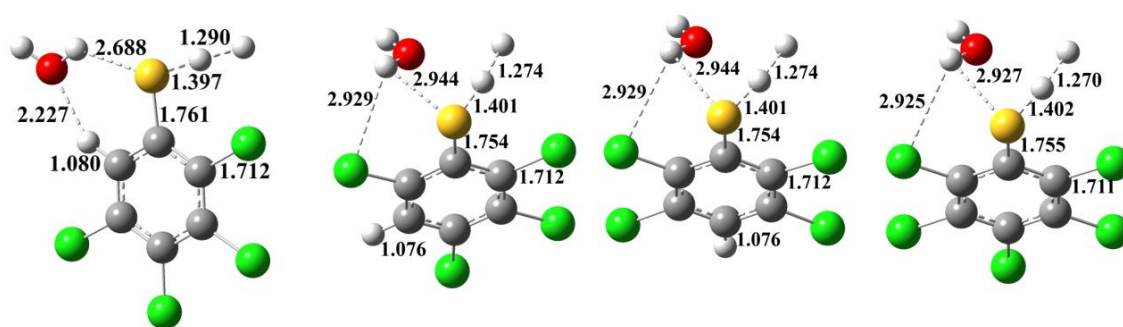
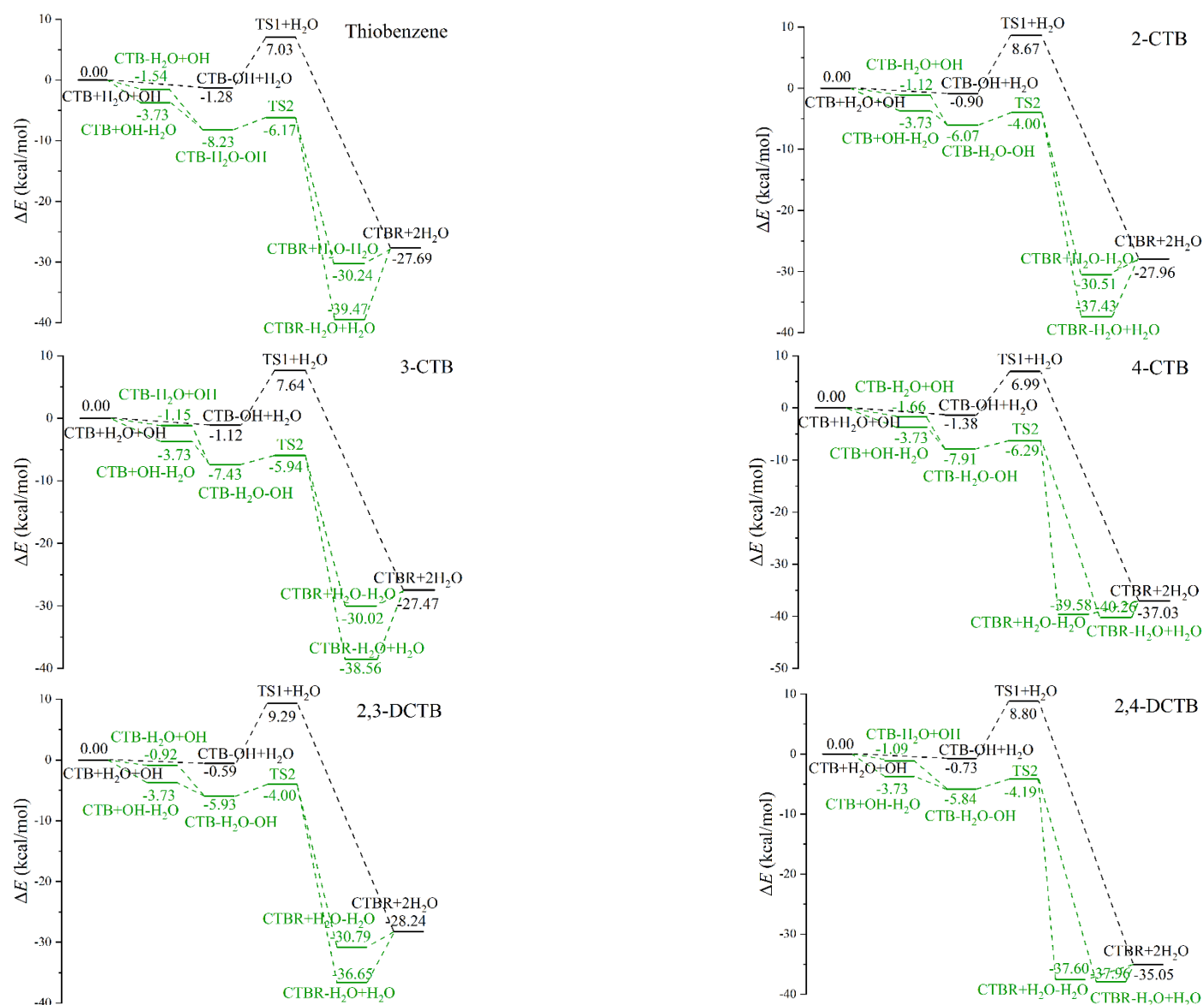
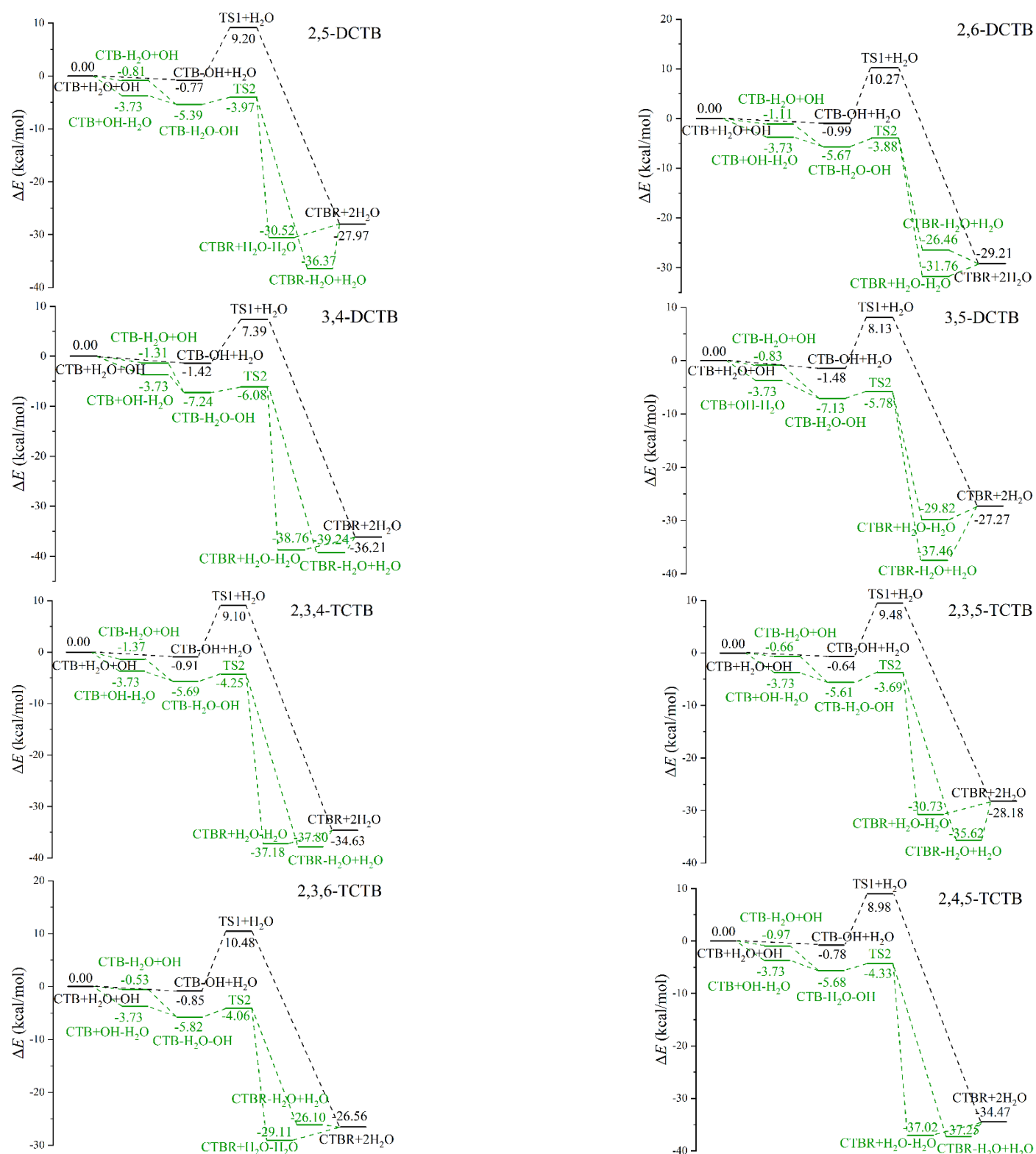


Figure S5. Structures of the CTB-H₂O-H transition states for H abstraction from CTBs by H atom. Distances are in angstrom.





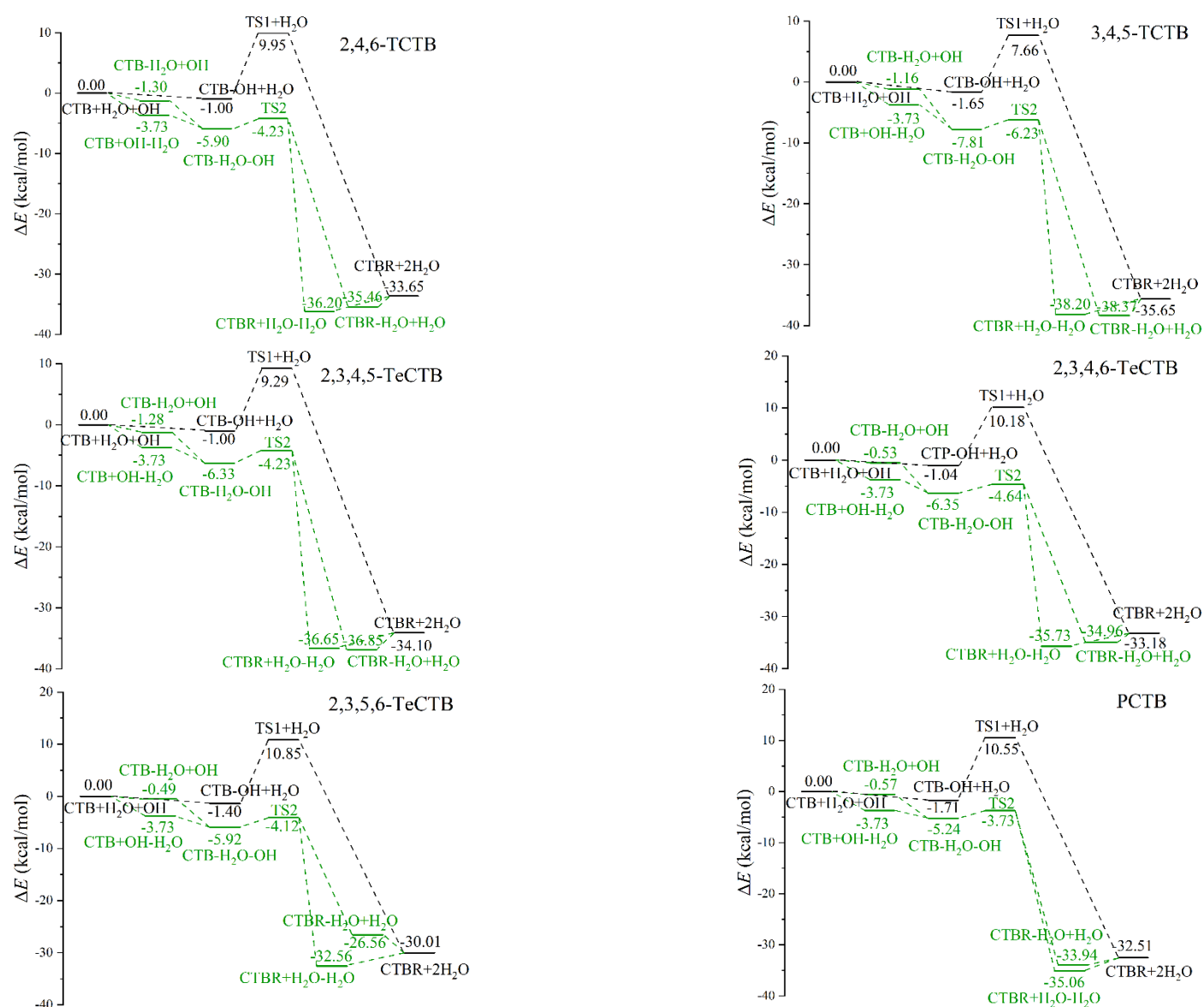
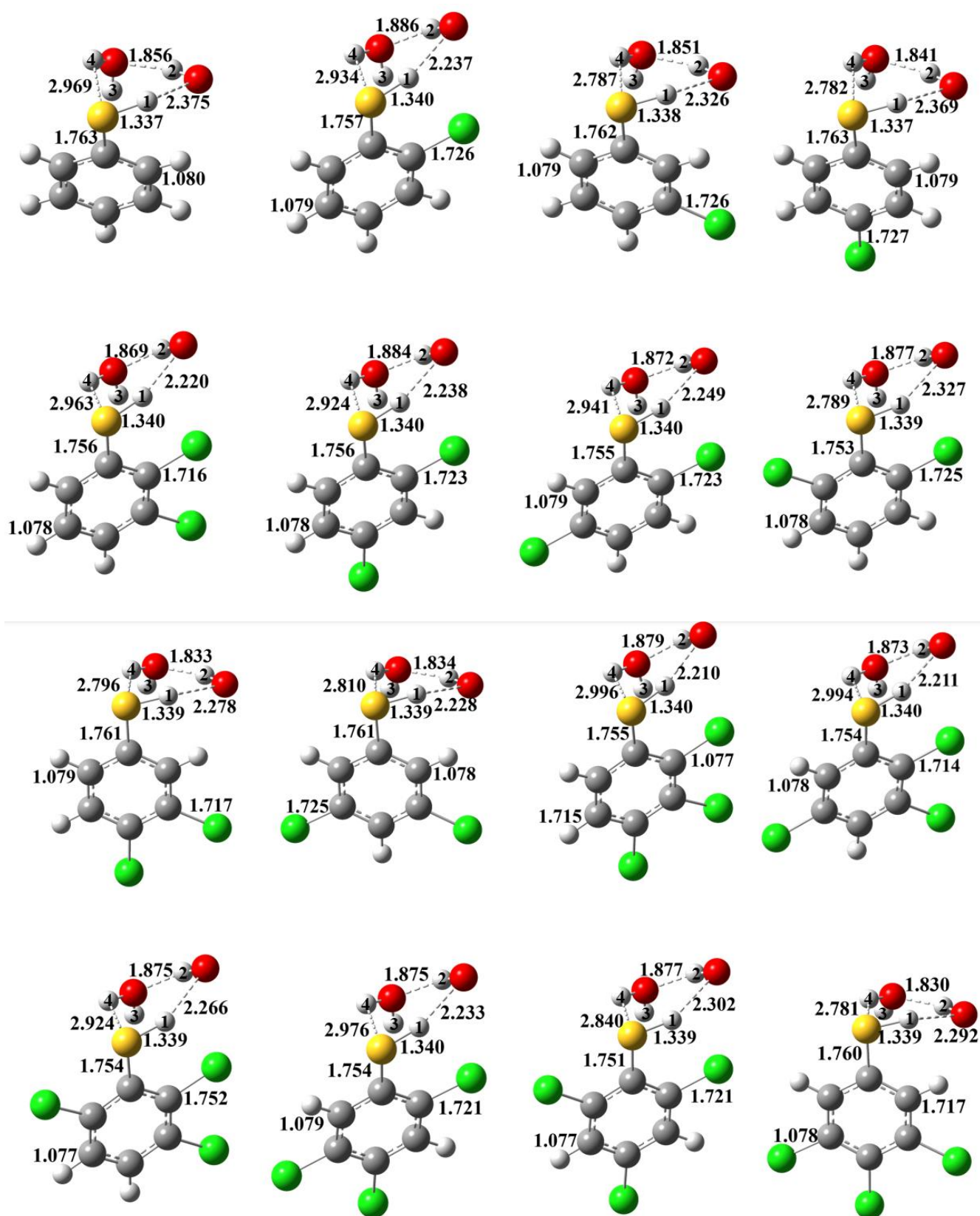


Figure S6. The schematic energy profiles of the H abstraction from CTBs by OH radicals in hydrated and non-hydrated cases. ΔE and ΔH is calculated at 0 K.



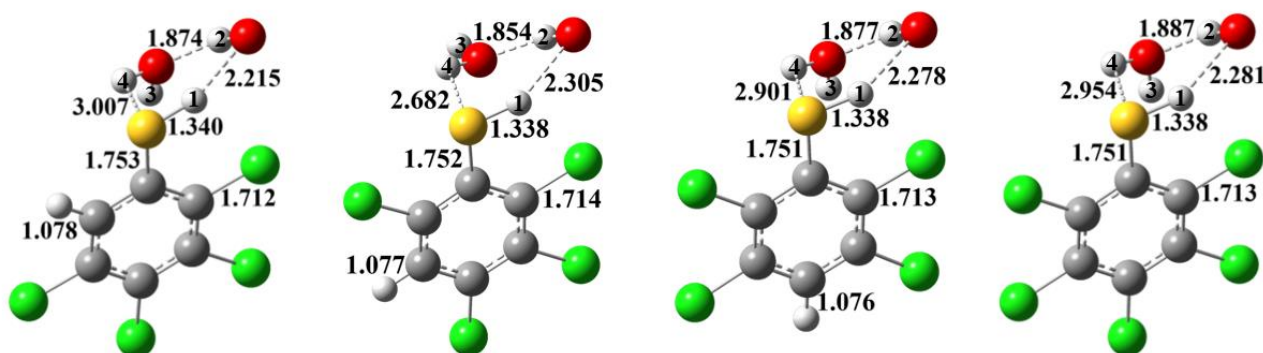
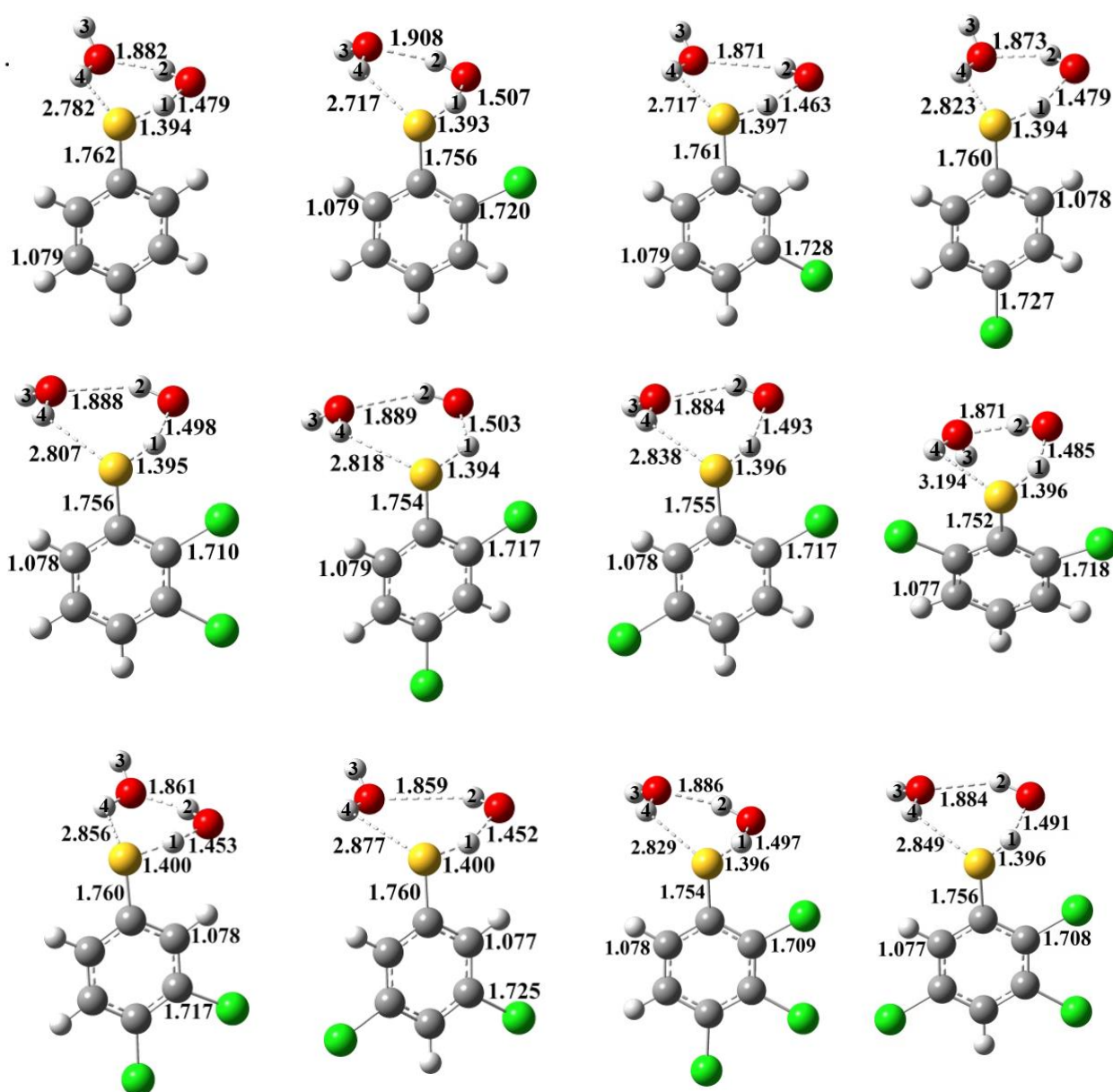


Figure S7. Structures of the CTB-H₂O-OH pre-reactive intermediates of the H abstraction from CTBs by $\cdot\text{OH}$ radical. Distances are in angstrom.



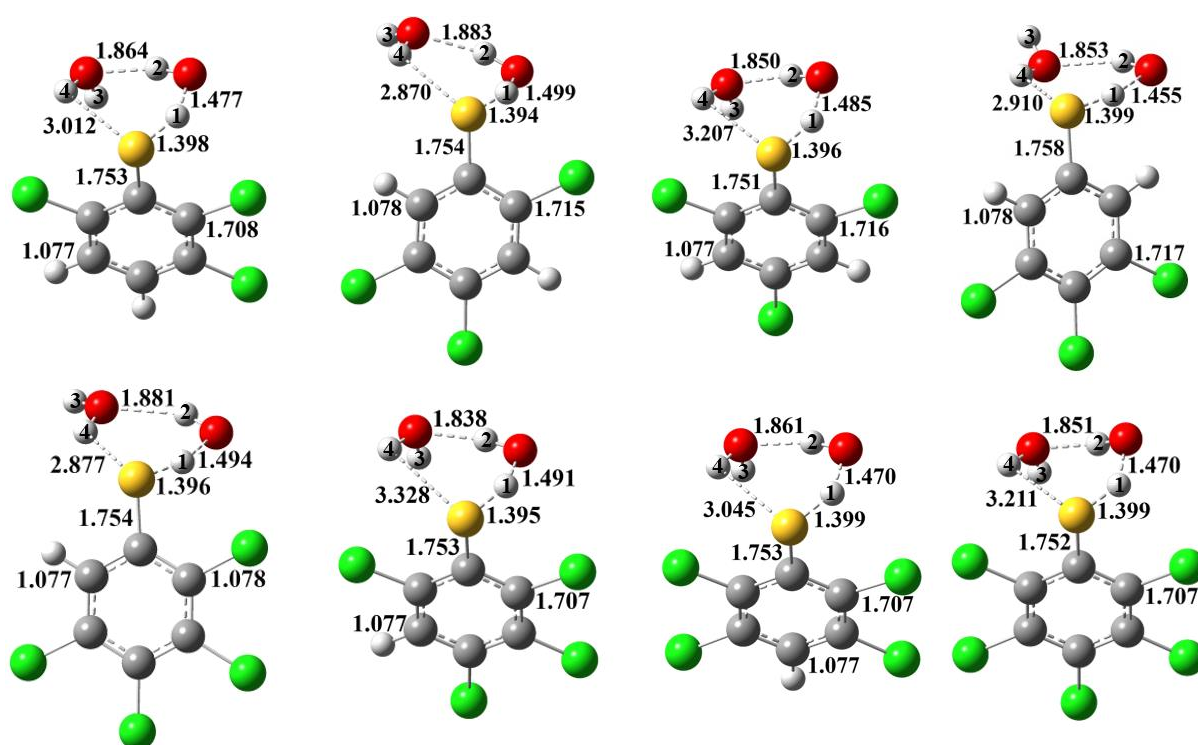


Figure S8. Structures of the CTB-H₂O-OH transition states of the H abstraction from CTBs by ·OH radical. Distances are in angstrom.

Table S1. Potential barriers ΔE and reaction heats ΔH (in kcal mol⁻¹) of the H abstraction from CBs by H atom in hydrated and non-hydrated cases. ΔE and ΔH are calculated at 0 K.

CBs	non-hydrated ^a		hydrated ^b		$\Delta E - \Delta E_{H_2O}$
	ΔE	ΔH	ΔE_{H_2O}	ΔH_{H_2O}	
Phenol	11.73	-13.98	7.92	-13.98	3.21
2-CB	13.80	-12.01	11.34	-12.01	2.46
3-CB	12.51	-12.93	10.10	-12.93	2.41
4-CB	11.41	-15.17	9.00	-15.17	2.41
2,3-DCB	14.49	-11.24	11.82	-11.24	2.67
2,4-DCB	13.58	-13.22	11.09	-13.22	2.49
2,5-DCB	14.44	-11.15	12.25	-11.15	2.19
2,6-DCB	13.33	-13.33	11.69	-13.33	1.64
3,4-DCB	12.01	-14.17	9.66	-14.17	2.35
3,5-DCB	12.99	-11.80	10.82	-11.80	2.17
2,3,4-TCB	14.17	-12.56	11.46	-12.56	2.71
2,3,5-TCB	14.92	-10.41	12.37	-10.41	2.55
2,3,6-TCB	13.88	-12.81	12.30	-12.81	1.58
2,4,5-TCB	13.96	-12.55	11.64	-12.55	2.32
2,4,6-TCB	12.81	-14.62	11.41	-14.62	1.40
3,4,5-TCB	12.40	-13.14	10.39	-13.14	2.01
2,3,4,5-TeCB	14.21	-11.77	12.08	-11.77	2.13
2,3,4,6-TeCB	13.60	-14.21	12.12	-14.21	1.48
2,3,5,6-TeCB	14.11	-12.34	12.79	-12.34	1.32
PCB	13.68	-13.54	12.41	-13.54	1.27

^a Potential barriers and reaction heats for H abstraction from CBs by H atom in non-hydrated cases. The values are from Reference 33.

^b Potential barriers and reaction heats for H abstraction from CBs by H atom in hydrated cases. The values are from Reference 31.

Table S2. Potential barriers ΔE (in kcal mol⁻¹) and reaction heats ΔH of the H abstraction from CBs by $\cdot\text{OH}$ radical in hydrated and non-hydrated cases. ΔE and ΔH are calculated at 0 K.

CBs	non-hydrated ^a		hydrated ^b		$\Delta E - \Delta E_{H_2O}$
	ΔE	ΔH	ΔE_{H_2O}	ΔH_{H_2O}	
Phenol	−0.20	−28.88	−4.49	−28.88	4.29
2-CB	3.20	−26.91	−1.62	−26.91	4.82
3-CB	0.20	−27.83	−3.95	−27.83	4.15
4-CB	−0.80	−30.07	−4.83	−30.07	4.03
2,3-DCB	3.60	−26.14	−0.98	−26.14	4.58
2,4-DCB	2.80	−28.12	−1.83	−28.12	4.63
2,5-DCB	3.50	−26.05	−1.13	−26.05	4.63
2,6-DCB	2.80	−28.23	−3.27	−28.23	6.07
3,4-DCB	−0.40	−29.07	−4.24	−29.07	3.84
3,5-DCB	0.60	−26.70	−3.54	−26.70	4.14
2,3,4-TCB	3.30	−27.46	−1.47	−27.46	4.77
2,3,5-TCB	3.90	−25.31	−0.82	−25.31	4.72
2,3,6-TCB	3.40	−27.71	−2.85	−27.71	6.25
2,4,5-TCB	3.20	−27.45	−1.70	−27.45	4.90
2,4,6-TCB	2.70	−29.52	−3.63	−29.52	6.33
3,4,5-TCB	0.00	−28.03	−3.94	−28.03	3.94
2,3,4,5-TeCB	3.50	−26.67	−1.42	−26.67	4.92
2,3,4,6-TeCB	3.20	−29.10	−3.14	−29.10	6.34
2,3,5,6-TeCB	3.70	−27.23	−2.70	−27.23	6.40
PCB	3.20	−28.44	−3.13	−28.44	6.33

^a Potential barriers and reaction heats for H abstraction from CBs by OH radical in non-hydrated cases. The values are from Reference 34.

^b Potential barriers and reaction heats for H abstraction from CBs by OH radical in non-hydrated cases. The values are from Reference 31.

Table S3. Cartesian coordinates of the hydrated reactants CTB-H₂O_s.

TBe			
0 1			
C	1.34004500	1.57054000	0.22243600
C	0.13557400	0.89020300	0.26375500
C	0.12027900	−0.48448400	0.06810300
C	1.29952600	−1.16536300	−0.19433900
C	2.49743400	−0.47333900	−0.25327600
C	2.52025400	0.89354300	−0.03828300
H	−1.71041000	−1.19000300	1.36987600
O	−3.16839700	1.45550400	−0.21810600
H	−2.88240200	0.56039500	−0.41194300
H	−3.74224000	1.71914700	−0.93190500
H	1.27626400	−2.23359000	−0.34312600
H	−0.78824600	1.42309700	0.43226400
H	3.45475700	1.43169600	−0.07717900
S	−1.40650000	−1.39829400	0.08576700
H	1.35175700	2.63767000	0.38266800
H	3.41303300	−1.00633800	−0.45846000
2-CTB			
0 1			
C	−0.18483300	2.36329900	−0.16477100
C	−0.84952100	1.15495100	−0.23634000
C	−0.15398700	−0.04576000	−0.14094700
C	1.22489500	0.00011400	0.04028900
C	1.88968000	1.20971600	0.13344700
C	1.18592000	2.39345200	0.02349300
H	−0.34042400	−2.30070100	0.47622500
H	−1.92308200	1.13406800	−0.34876700
O	−3.95046900	0.12967200	0.44945100
H	−3.35450500	−0.61787000	0.50558400
H	−4.81386800	−0.22673300	0.25975700
H	−0.74520600	3.28157500	−0.24099200
Cl	2.15171400	−1.45284300	0.16862300
H	2.95707900	1.21024600	0.28417800
S	−1.07116200	−1.53798800	−0.33873400
H	1.71029400	3.33353600	0.09053400
3-CTB			
0 1			
C	0.14751400	1.90605100	0.08422500
C	−0.88502300	0.98318200	0.07320100
C	−0.58540300	−0.37043000	0.03612000
C	0.73272900	−0.79871200	−0.01780300
C	1.74590900	0.14168200	−0.00622500
C	1.46676700	1.49493900	0.04861500
H	−2.04031900	−1.72867100	1.30278900
O	−4.19189200	0.97549300	−0.06669300

H	−3.84428300	0.09893200	−0.24057400
H	−4.96644900	1.07547700	−0.61272900
H	0.96400300	−1.85017600	−0.06835200
H	−1.91181900	1.31460900	0.09007700
Cl	3.38888100	−0.38948300	−0.06629300
H	2.27451300	2.20894400	0.05403900
S	−1.88794000	−1.58762900	−0.01834700
H	−0.07940600	2.95994600	0.12001800

4-CTB

0 1

C	0.85315900	1.05815200	0.21043700
C	−0.48093100	0.69506700	0.22607200
C	−0.83993100	−0.63545400	0.05781900
C	0.13996700	−1.59338100	−0.15254600
C	1.47525600	−1.23332200	−0.18558200
C	1.82057600	0.09140800	0.00280000
H	−2.79950700	−0.90287100	1.33314800
O	−3.49420600	2.09653300	−0.17042300
H	−3.51474400	1.17036100	−0.41755500
H	−4.05477100	2.55883100	−0.78730200
S	−2.54640900	−1.13418800	0.04167600
H	−1.24101200	1.45024300	0.35853200
H	−0.14136000	−2.62616000	−0.28479500
H	1.14071300	2.08791100	0.34736400
Cl	3.48571200	0.54797400	−0.02695900
H	2.24118500	−1.97395400	−0.34852200

2,3-DCTB

0 1

C	−0.30320700	2.26470900	−0.24073300
C	−1.20957100	1.22367800	−0.25989500
C	−0.77029200	−0.08981600	−0.16284600
C	0.59463400	−0.34951900	−0.03526000
C	1.49333400	0.71092000	0.00602900
C	1.04736100	2.01479200	−0.10383800
H	−1.39780300	−2.24936700	0.50288500
H	−2.26767100	1.42368900	−0.33044100
O	−4.41541700	0.88460900	0.52202000
H	−4.04255300	0.00646300	0.59954900
H	−5.36081500	0.77563300	0.46858400
H	−0.65562200	3.28097300	−0.31605700
Cl	1.16924200	−1.96426100	0.08218200
S	−1.98653600	−1.35834100	−0.29628900
H	1.76485600	2.81796800	−0.07407000
Cl	3.18099100	0.43206400	0.18212800

2,4-DCTB

0 1

C	−0.92072000	−1.54473200	−0.15726500
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C	0.41853000	−1.21289500	−0.18772700
C	0.83520300	0.11112800	−0.10567400
C	−0.13707600	1.09873500	0.01848800
C	−1.48169000	0.77920100	0.07183900
C	−1.86362700	−0.54313500	−0.02427500
H	2.59126100	1.52050800	0.53240600
H	1.15868100	−1.99600500	−0.25885000
O	3.16838300	−2.89687500	0.33083800
H	3.51007500	−2.02219400	0.51174100
H	3.92102100	−3.45421100	0.15299100
H	−1.22891800	−2.57514200	−0.22067200
Cl	0.29711700	2.76513900	0.12690900
H	−2.21664500	1.55921200	0.17853100
Cl	−3.54134900	−0.94003300	0.03062900
S	2.56035500	0.43663800	−0.24458200

2,5-DCTB

0 1			
C	1.46175700	−0.92546400	−0.03836100
C	0.81868400	0.29214700	−0.12002300
C	−0.57108500	0.34574400	−0.08706400
C	−1.28353700	−0.84274900	0.04348300
C	−0.62345400	−2.05354300	0.14678600
C	0.75426000	−2.10561500	0.09879900
H	−2.45134700	1.65636800	0.36243900
H	1.38950100	1.20611000	−0.19014300
O	1.63199800	3.41145800	0.37734800
H	0.70452300	3.55843300	0.55520700
H	2.01522700	4.26376100	0.18916200
Cl	−3.00969500	−0.85296500	0.09019100
H	−1.19866100	−2.95856600	0.25561600
S	−1.31957900	1.92549600	−0.28902700
H	1.27231100	−3.04746600	0.17038100
Cl	3.18534000	−0.97299800	−0.09011700

2,6-DCTB

0 1			
C	−0.67877700	2.11225900	0.01049300
C	−0.87806900	0.78946900	−0.32447900
C	0.15891900	−0.14236500	−0.33946100
C	1.42460900	0.32706300	0.01086400
C	1.64003200	1.64864400	0.35298600
C	0.58816200	2.54174800	0.35313900
H	1.00197800	−2.27628300	−0.54026800
O	−1.78981800	−1.32449800	2.47365300
H	−1.45882200	−1.79575800	1.71074200
H	−2.50938000	−0.78985500	2.14796300
Cl	2.78809100	−0.73313200	0.02847700
Cl	−2.47105300	0.27571600	−0.75017500

H	−1.51580600	2.79064700	0.00326900
H	2.63564300	1.96378600	0.61821800
H	0.75600600	3.57229400	0.62066800
S	−0.21937400	−1.79710500	−0.77888700
3,4-DCTB			
0 1			
C	0.07780200	1.51174100	−0.00029800
C	−1.14530200	0.86962100	−0.00427200
C	−1.18839200	−0.51639300	−0.00408700
C	−0.01175500	−1.24708800	−0.01845600
C	1.21112500	−0.60070700	−0.00405200
C	1.25732000	0.78804900	0.00327200
H	−2.82780000	−1.66197600	1.24015000
H	−2.05876400	1.44466600	−0.00603300
O	−4.36162500	1.63067200	0.05546400
H	−4.27057800	0.68396100	−0.06430700
H	−5.13558300	1.89571400	−0.43408000
S	−2.74543900	−1.37595400	−0.06278800
Cl	2.64841500	−1.54190100	−0.00945500
Cl	2.75268800	1.63084000	0.01146800
H	−0.03718600	−2.32424100	−0.04420500
H	0.12639900	2.58848200	0.00250800
3,5-DCTB			
0 1			
C	0.08994800	1.31343500	−0.03476600
C	−0.87796100	0.32850700	−0.05628400
C	−0.47473500	−0.99957600	−0.04822600
C	0.87295800	−1.32838600	−0.01493500
C	1.80739200	−0.31202800	0.02049500
C	1.44022600	1.01909200	0.00708100
H	−0.95419400	−3.25764600	0.24802700
O	−4.16263600	0.13545300	0.21886700
H	−4.20950900	−0.72797200	0.62358300
H	−4.96538800	0.24166500	−0.28473200
H	1.20236800	−2.35454400	−0.02041900
H	−1.92624800	0.58330200	−0.06813200
Cl	3.48491900	−0.71648700	0.07229600
H	2.17955600	1.80103800	0.03026900
Cl	−0.39821100	2.96827800	−0.04818700
S	−1.72790600	−2.23601100	−0.12059800
2,3,4-TCTB			
0 1			
C	−0.07013600	−1.89608200	−0.17127700
C	1.14112400	−1.24215400	−0.18895400
C	1.19744200	0.14340500	−0.12129500
C	0.00925200	0.86359700	−0.02422700

C	−1.21890900	0.20432000	0.01749000
C	−1.24847500	−1.18246100	−0.06432100
H	2.54240200	1.94491000	0.53632100
H	2.05788400	−1.80978800	−0.23810600
O	4.23575800	−2.11448400	0.40822900
H	4.31415500	−1.17318000	0.55851500
H	5.12193400	−2.45226800	0.31169500
Cl	0.04233000	2.57837100	0.05303000
H	−0.10933100	−2.97147800	−0.22305000
Cl	−2.67393400	1.09208700	0.15688800
Cl	−2.73471800	−2.04081900	−0.02694100
S	2.78453500	0.89562700	−0.25039400

2,3,5-TCTB

0 1

C	−0.81932700	1.50048700	−0.06608600
C	−1.26702500	0.19822300	−0.10164300
C	−0.34886800	−0.84394600	−0.08027900
C	1.01595000	−0.56188600	−0.01709400
C	1.43661200	0.76303500	0.03767000
C	0.52603400	1.80051400	0.00768300
H	0.02861600	−3.11531000	0.30779800
O	−4.14228800	−1.26697600	0.28875200
H	−3.81759600	−2.06662300	0.69717500
H	−5.02464900	−1.12604400	0.62154600
S	−1.01869900	−2.46481100	−0.19856400
H	−2.32388200	−0.01919400	−0.12870700
Cl	−1.96190900	2.79042900	−0.09592500
Cl	3.10685400	1.15237800	0.13356600
Cl	2.17543200	−1.82862500	0.00014800
H	0.86833500	2.82030900	0.04527900

2,3,6-TCTB

0 1

C	0.34399400	−2.09298300	−0.18554900
C	1.07505200	−0.94073500	−0.38023700
C	0.47977300	0.31830700	−0.37591200
C	−0.90086100	0.38329700	−0.16591900
C	−1.63642900	−0.77890400	0.03290600
C	−1.01515000	−2.01265200	0.02227200
H	0.56300400	2.62248100	−0.43389400
O	2.39071800	0.50237900	2.64485500
H	2.35953600	1.08954000	1.89104300
H	2.93406500	−0.23243900	2.37212300
Cl	−1.70923900	1.89801600	−0.14968800
Cl	2.77452700	−1.07040600	−0.64277100
H	0.84282700	−3.04776000	−0.19688000
H	−1.60213100	−2.90206500	0.17793500
Cl	−3.33193000	−0.71995400	0.29147900
S	1.51447500	1.71019300	−0.63361700

2,4,5-TCTB			
0 1			
C	1.14177300	0.66834700	−0.06904700
C	−0.20625200	0.96488200	−0.10787200
C	−1.16481100	−0.03945500	−0.07251200
C	−0.73018100	−1.35865300	0.01342600
C	0.61637000	−1.65903500	0.07156300
C	1.56048700	−0.65257900	0.02402800
H	−3.37543900	−0.64543000	0.33968100
H	−0.52086900	1.99708900	−0.15016500
O	−2.00904700	3.64344000	0.26761400
H	−2.76442800	3.20687600	0.65575900
H	−2.01638400	4.54293300	0.58382000
Cl	−1.84607700	−2.67328800	0.06004100
H	0.93435900	−2.68543200	0.14512000
Cl	2.27272600	1.95812700	−0.12155900
S	−2.84681600	0.44961200	−0.20689800
Cl	3.22393100	−1.06709800	0.08726700
2,4,6-TCTB			
0 1			
C	−1.12918200	−1.28283400	−0.26925700
C	0.20883500	−0.99327900	−0.43038200
C	0.71544100	0.30225000	−0.34728300
C	−0.20740800	1.31304500	−0.08167700
C	−1.55282300	1.05027800	0.08999600
C	−2.00417600	−0.24910400	−0.00638300
H	2.44091700	1.82279600	−0.22252000
O	2.14308100	−1.15675600	2.54517900
H	2.55306900	−0.77141800	1.77180800
H	2.02916000	−2.08135900	2.34154600
Cl	0.29526500	2.95762800	0.04493200
Cl	1.28804900	−2.29789400	−0.75763300
Cl	−3.67951500	−0.58399300	0.20006000
H	−1.47759500	−2.29865100	−0.34447900
H	−2.23531700	1.85693800	0.29641200
S	2.43727600	0.53725100	−0.57621100
3,4,5-TCTB			
0 1			
C	0.07353400	1.05822500	−0.09506800
C	−1.15882000	0.43607500	−0.13739400
C	−1.22727000	−0.94743700	−0.10797800
C	−0.06399400	−1.69498600	−0.03083900
C	1.16083900	−1.05978600	0.02964100
C	1.25509200	0.32756300	−0.00761500
H	−2.44633700	−2.89442000	0.25862200
O	−4.26136600	1.18756600	0.37763000

H	−4.48058000	0.34427100	0.76890900
H	−4.86059100	1.82988100	0.74826500
S	−2.81427100	−1.70531500	−0.21959200
Cl	2.77297800	1.10969800	0.05713700
H	−2.05865400	1.03122000	−0.17192100
H	−0.08839600	−2.77241500	−0.02086700
Cl	0.11251900	2.77476400	−0.13609100
Cl	2.57435700	−2.02987000	0.13806800

2,3,4,5-TeCTB

0 1			
C	−0.03600600	1.44424000	−0.03527100
C	−1.20304000	0.71337500	−0.04048600
C	−1.17048600	−0.67332900	−0.03002500
C	0.06308400	−1.31881800	−0.00886800
C	1.24260000	−0.57843900	0.01497200
C	1.20186500	0.81235700	−0.00304700
H	−2.30785100	−2.67559700	0.33226400
O	−4.33306400	1.48513100	0.12466400
H	−4.80604200	0.81053900	0.60608300
H	−4.89106500	2.25856300	0.11887300
Cl	0.14587600	−3.03415500	−0.00780600
Cl	2.75136900	−1.38209600	0.05685200
Cl	2.64716800	1.72352000	0.01685300
H	−2.15372400	1.22537800	−0.04405800
Cl	−0.14224500	3.15675100	−0.05374000
S	−2.72511000	−1.48653700	−0.10005200

2,3,4,6-TeCTB

0 1			
C	−0.14324900	−1.74331600	−0.28679000
C	0.99449800	−0.98226200	−0.41904000
C	0.96629900	0.40793400	−0.36272400
C	−0.27483000	1.01380500	−0.16350700
C	−1.43778300	0.25894300	−0.02284500
C	−1.36040600	−1.12643900	−0.08657800
H	1.99971100	2.46897200	−0.27614500
O	2.65183100	−0.40147800	2.63116000
H	2.91681000	0.18161800	1.92125000
H	2.87357700	−1.28042700	2.33432400
Cl	−0.39140000	2.72474400	−0.08877500
Cl	2.49290400	−1.79332100	−0.67521500
H	−0.08597800	−2.81721500	−0.33736500
S	2.48761200	1.25854200	−0.54546000
Cl	−2.94215500	1.02725300	0.22295000
Cl	−2.75862700	−2.10278100	0.07544700

2,3,5,6-TeCTB

0 1

C	−0.88921400	1.38798200	−0.14391000
C	−1.08534200	0.03171600	−0.34260700
C	−0.00490000	−0.85045200	−0.35200000
C	1.28021400	−0.33871600	−0.16776600
C	1.46182700	1.02497600	0.02854900
C	0.38415500	1.88421700	0.04079800
H	0.87041100	−2.98158700	−0.38568500
O	−1.51078000	−1.52646900	2.64876200
H	−1.48931600	−2.17867400	1.95045200
H	−2.37026300	−1.11657500	2.59390400
Cl	2.64689700	−1.37615300	−0.17764900
Cl	−2.66803900	−0.59021600	−0.56813000
Cl	−2.20583900	2.48513900	−0.12384000
Cl	3.02768900	1.68473200	0.25783400
H	0.53668800	2.93840000	0.19500400
S	−0.37211000	−2.54673000	−0.59511300

PTCB

0 1

C	−0.88921400	1.38798200	−0.14391000
C	−1.08534200	0.03171600	−0.34260700
C	−0.00490000	−0.85045200	−0.35200000
C	1.28021400	−0.33871600	−0.16776600
C	1.46182700	1.02497600	0.02854900
C	0.38415500	1.88421700	0.04079800
H	0.87041100	−2.98158700	−0.38568500
O	−1.51078000	−1.52646900	2.64876200
H	−1.48931600	−2.17867400	1.95045200
H	−2.37026300	−1.11657500	2.59390400
Cl	2.64689700	−1.37615300	−0.17764900
Cl	−2.66803900	−0.59021600	−0.56813000
Cl	−2.20583900	2.48513900	−0.12384000
Cl	3.02768900	1.68473200	0.25783400
H	0.53668800	2.93840000	0.19500400
S	−0.37211000	−2.54673000	−0.59511300

Table S4. Cartesian coordinates of the hydrated CTB-H₂O-H transition states for H abstraction from CTBs by H atom.

TBe			
O 2			
C	1.35787300	1.59462100	0.16812500
C	0.15326800	0.91327400	0.13386700
C	0.15112700	−0.46642600	−0.02820700
C	1.34905200	−1.15298600	−0.17561200
C	2.54837100	−0.46301100	−0.14738200
C	2.55380000	0.91059600	0.02758800
H	−1.59013600	−1.46749000	1.25937800
O	−3.18413000	1.51618900	−0.11711900
H	−2.91496700	0.61086600	−0.28635200
H	−3.84199800	1.73137900	−0.77226200
H	−1.72179400	−1.51601800	2.59195000
S	−1.37616800	−1.36521200	−0.10821000
H	−0.77974300	1.44815100	0.22721400
H	1.33423800	−2.22323400	−0.31002400
H	3.47741200	−0.99991500	−0.26159300
H	3.48933800	1.44801700	0.05067800
H	1.35843700	2.66570900	0.29903900
2-CTB			
O 2			
C	−0.14569400	2.40819000	−0.06579600
C	−0.83324000	1.21197700	−0.14426600
C	−0.15335600	−0.00137800	−0.11880300
C	1.23480600	0.01698600	0.00374200
C	1.92256800	1.21247600	0.10456800
C	1.23193400	2.40899300	0.06215900
H	−0.58301700	−2.15995400	0.79053000
H	−1.91020000	1.20975400	−0.21529300
O	−3.99295300	0.17810600	0.30250100
H	−3.37946000	−0.55639000	0.24736700
H	−4.84099100	−0.15469900	0.02239000
H	−0.14370800	−2.66055900	1.90465300
H	−0.69227900	3.33752800	−0.09020300
H	1.77429700	3.33864900	0.13416000
Cl	2.13793300	−1.45219000	0.04818200
S	−1.07270900	−1.48936700	−0.33063800
H	2.99536300	1.19444400	0.20787700
3-CTB			
O 2			
C	0.23289400	1.91783500	0.19487900
C	−0.82074600	1.02272800	0.17920400
C	−0.55683400	−0.33805600	0.08409700
C	0.75015300	−0.79360700	−0.01092900
C	1.78365900	0.12493900	−0.02142500

C	1.54231100	1.48078400	0.08738700
H	−2.57133400	−1.01419300	1.11815300
O	−4.11877400	0.87194000	−0.37765400
H	−3.78573000	0.11861700	−0.86502500
H	−4.87044100	1.20462500	−0.86076000
H	−3.11847900	−0.43897000	2.12392800
S	−1.86210600	−1.52978000	0.03075900
H	−1.84085600	1.37184900	0.23163000
H	0.96176000	−1.84899400	−0.06600100
H	2.36463100	2.17727200	0.08757800
H	0.03205500	2.97469800	0.27823300
Cl	3.41080400	−0.44304000	−0.15281900
4-CTB			
0 2			
C	0.88475900	1.06517500	0.14254300
C	−0.44796800	0.69924100	0.13435400
C	−0.80108700	−0.63936300	0.01280200
C	0.18905000	−1.60258000	−0.11697100
C	1.52338800	−1.23799900	−0.13596900
C	1.86083000	0.09487200	0.00038700
H	−2.88160300	−0.48639100	1.13277600
O	−3.48270500	2.01261700	−0.20288700
H	−3.54448300	1.20379400	−0.71118800
H	−4.03568600	2.65662300	−0.63714200
H	−3.11226500	0.19312700	2.21306800
S	−2.49446500	−1.14640500	−0.03281000
H	−1.21527300	1.45458700	0.21829800
H	−0.08324300	−2.64333300	−0.19631900
Cl	3.52532200	0.55703000	−0.00583600
H	1.16619900	2.10059100	0.24615900
H	2.29513400	−1.98302600	−0.24126100
2,3-DCTB			
0 2			
C	−0.25967500	2.30680400	−0.11732500
C	−1.18119400	1.27809400	−0.15659700
C	−0.75721100	−0.04374000	−0.13118500
C	0.60865800	−0.32821100	−0.04868600
C	1.52230200	0.71746400	0.01187500
C	1.08918600	2.03074700	−0.02859600
H	−1.60158000	−2.05820500	0.82161900
H	−2.23770300	1.49322300	−0.19639500
O	−4.45543500	0.93725000	0.35216500
H	−4.03861500	0.07577100	0.30398700
H	−5.37680800	0.80700500	0.14583400
H	−1.25244800	−2.62980600	1.92560200
H	−0.59822400	3.33025500	−0.13995600
H	1.81894300	2.82240400	0.01550100

Cl	1.16051600	−1.95141600	−0.01508500
Cl	3.21077100	0.41500500	0.12782300
S	−1.96964800	−1.31166300	−0.29918500
2,4-DCTB			
O 2			
C	−0.99357100	−1.54961400	−0.10149100
C	0.35457000	−1.25334900	−0.14011800
C	0.80456100	0.06192000	−0.10872400
C	−0.14200800	1.08122900	−0.02170000
C	−1.49403800	0.79882900	0.03946400
C	−1.90782000	−0.51794500	−0.00894400
H	2.67177200	1.16616900	0.86716600
H	1.07413300	−2.05686300	−0.18461000
O	3.11100300	−2.97199600	0.25330300
H	3.37543900	−2.05146600	0.24143400
H	3.87336000	−3.48101900	−0.00787700
H	2.71732400	1.82367100	1.99204100
H	−1.33000100	−2.57270200	−0.12817400
Cl	0.34222200	2.73294700	0.02847500
H	−2.21058200	1.59919800	0.11543100
Cl	−3.59450200	−0.86788900	0.05525000
S	2.53119600	0.36978600	−0.26850600
2,5-DCTB			
O 2			
C	1.53328300	−0.87760000	−0.01781300
C	0.83898100	0.31358400	−0.09391100
C	−0.55184700	0.30420500	−0.09314100
C	−1.21816900	−0.91604100	0.00474000
C	−0.50878900	−2.09860900	0.10466000
C	0.87164200	−2.08657700	0.08547100
H	−2.24015100	1.72357300	0.79897600
H	1.37248200	1.25123200	−0.14049500
O	1.52347000	3.47957400	0.28000800
H	0.56736200	3.45680200	0.23499200
H	1.79597100	4.32725600	−0.06016000
H	−2.91002300	1.57125900	1.89367300
S	−1.39744700	1.83476900	−0.30855900
H	−1.04431000	−3.03025400	0.18755100
Cl	−2.93906800	−0.98786300	0.01536500
H	1.42792900	−3.00696200	0.15321300
Cl	3.25739400	−0.85446500	−0.03365400
2,6-DCTB			
O 2			
C	−0.79551200	2.12291300	0.13206600
C	−0.95611200	0.80697500	−0.25645800
C	0.11870900	−0.07958300	−0.33940900

C	1.37676300	0.43181400	−0.01142500
C	1.55066900	1.74046500	0.39734300
C	0.46178900	2.58598200	0.46460600
H	0.59382500	−2.32380600	0.16038700
O	−1.45291800	−1.69076600	2.20652100
H	−1.81934300	−1.71872700	1.32359200
H	−2.04202400	−1.14313600	2.71843800
H	1.08341400	−2.79858400	1.23716900
Cl	2.77461900	−0.56988100	−0.10610600
Cl	−2.55404200	0.28029700	−0.64795100
S	−0.12236300	−1.73020500	−0.88701100
H	−1.65631200	2.76940900	0.17564500
H	0.59410300	3.61015100	0.77474300
H	2.53984100	2.08563900	0.64866700

3,4-DCTBO₂

C	0.13201900	1.51307600	0.13380600
C	−1.09640000	0.88650300	0.13182800
C	−1.15856300	−0.50056600	0.06947400
C	0.01018800	−1.23973500	−0.00484300
C	1.23987500	−0.60389100	−0.03151400
C	1.30465400	0.77983800	0.04514000
H	−3.28293200	−0.66588800	1.09006900
H	−2.00482100	1.46894400	0.17062500
O	−4.30189300	1.50582200	−0.33133100
H	−4.24681000	0.72984900	−0.88779800
H	−4.96990300	2.07147000	−0.70995400
H	−3.68158300	0.02264500	2.09282100
S	−2.69877500	−1.36350800	0.02959300
H	−0.02399400	−2.31666500	−0.03408500
Cl	2.66370900	−1.55921600	−0.13806600
H	0.19420600	2.58782600	0.19021800
Cl	2.80810000	1.60980500	0.03229700

3,5-DCTBO₂

C	0.19576300	1.33291300	0.06908900
C	−0.83165000	0.41140600	0.10790700
C	−0.51219100	−0.94053500	0.09229100
C	0.80987600	−1.35421400	0.02015600
C	1.80697900	−0.39931800	−0.04678500
C	1.52267900	0.95171200	−0.01581500
H	−2.57517200	−1.54213200	1.06898800
O	−4.04694400	0.15752900	−0.45381700
H	−3.82197400	−0.56108700	−1.04284400
H	−4.73956100	0.65778600	−0.87785200
H	−3.17862300	−0.89268600	1.96532500
S	−1.77310000	−2.17569100	0.11080600

H	−1.86097300	0.73430700	0.13531100
H	1.06091500	−2.40197600	0.02732200
H	2.30950400	1.68541400	−0.05534300
Cl	3.45297100	−0.90761800	−0.14858200
Cl	−0.18224700	3.01699600	0.10597500
2,3,4-TCTB			
O 2			
C	−0.13151800	−1.92304700	−0.10554100
C	1.09352200	−1.29278700	−0.13266800
C	1.17595300	0.09278600	−0.11191000
C	0.00030200	0.84122000	−0.04902300
C	−1.24006300	0.20829700	0.00297200
C	−1.29446100	−1.18114400	−0.03413600
H	2.67128000	1.67525300	0.85070600
O	4.20822700	−2.21818900	0.28830400
H	4.23724900	−1.26111900	0.28675600
H	5.08692700	−2.52128700	0.07714600
H	2.54536600	2.33747300	1.95611100
S	2.76417000	0.83773500	−0.26231800
Cl	0.07474700	2.55312100	−0.02247100
H	1.99871600	−1.87961000	−0.15994900
Cl	−2.67873600	1.12675200	0.09871700
Cl	−2.79961500	−2.00237100	0.01701700
H	−0.19323600	−2.99845200	−0.12375000
2,3,5-TCTB			
O 2			
C	−0.82288400	1.54427300	−0.04683100
C	−1.27856700	0.24208900	−0.09130600
C	−0.36337500	−0.80133400	−0.09755100
C	1.00606800	−0.53040600	−0.04070600
C	1.43464200	0.78998100	0.02911200
C	0.52477800	1.83066800	0.01909900
H	−0.30835400	−3.00721900	0.80153700
O	−4.13962300	−1.23588900	0.32574100
H	−3.56242600	−1.99860300	0.30877200
H	−5.00103400	−1.53308700	0.04596600
H	0.26047900	−3.42991700	1.87119000
S	−0.99227900	−2.43733100	−0.27628700
Cl	2.14717500	−1.80802700	−0.05228000
H	−2.33755200	0.03426300	−0.10783800
Cl	3.10581800	1.17345900	0.11627400
H	0.87322100	2.84832400	0.06645800
Cl	−1.95504400	2.84157000	−0.05236600
2,3,6-TCTB			
O 2			
C	0.31434600	−2.15678100	−0.05433600

C	1.07926600	−1.03487500	−0.30566400
C	0.51179500	0.23491500	−0.39187300
C	−0.87360100	0.34037500	−0.21264500
C	−1.63918100	−0.78618800	0.05991100
C	−1.04348100	−2.03126600	0.13333200
H	1.05341300	2.41929400	0.28603500
O	2.11996300	0.90532600	2.40639400
H	2.71301100	0.64190600	1.70431600
H	2.37409900	0.40317300	3.17592800
H	0.70884700	3.02365000	1.34871800
Cl	−1.63593800	1.86882600	−0.33142400
Cl	2.77936200	−1.25767400	−0.50201600
S	1.51466400	1.62463300	−0.77262200
H	0.78809400	−3.12261100	0.00152000
Cl	−3.33605400	−0.67602800	0.29717300
H	−1.65193100	−2.89632900	0.33846700
2,4,5-TCTB			
O 2			
C	1.19366500	0.66302600	−0.05463900
C	−0.15059300	0.98476700	−0.09720600
C	−1.12429400	−0.00447600	−0.09155300
C	−0.71722200	−1.33578000	−0.02364700
C	0.62183400	−1.66154800	0.04353500
C	1.58272100	−0.66771900	0.02017900
H	−3.29183900	−0.21799000	0.85387200
O	−1.92170100	3.69015700	0.28637800
H	−2.61048000	3.02613600	0.26065100
H	−2.31756300	4.51249300	0.01128000
H	−3.61880400	−0.81995300	1.95330000
S	−2.81131500	0.46627500	−0.26367300
Cl	−1.86333200	−2.61863200	−0.00868000
H	−0.44277700	2.02396200	−0.12386600
H	0.92339700	−2.69366700	0.10393000
Cl	3.23561000	−1.11533000	0.09150200
Cl	2.34984300	1.92912300	−0.07761200
2,4,6-TCTB			
O 2			
C	−1.27160500	−1.23776800	−0.20385900
C	0.08627100	−1.07689100	−0.39524700
C	0.70467400	0.17438200	−0.37793500
C	−0.12893200	1.27297300	−0.15609100
C	−1.48703700	1.13932700	0.05762100
C	−2.04723000	−0.12083300	0.02706100
H	2.69102400	1.09954300	0.45931200
O	2.18896400	−0.86338700	2.39568800
H	2.43523000	−1.39866600	1.64279700
H	1.95308400	−1.47050800	3.09196700

H	2.85709200	1.67198600	1.59176600
Cl	0.51553300	2.86747900	−0.13510800
Cl	1.01436900	−2.50682800	−0.65825900
S	2.42483200	0.33331400	−0.68205900
H	−1.71018600	−2.22054200	−0.22833600
H	−2.09548700	2.00965300	0.23414100
Cl	−3.74029200	−0.30327100	0.27845400

3,4,5-TCTB

O 2			
C	0.12260700	1.06543200	0.07362300
C	−1.11778400	0.45902400	0.09327500
C	−1.20299100	−0.92462900	0.07596800
C	−0.04938600	−1.68811000	0.01895400
C	1.18580700	−1.07002100	−0.03181700
C	1.29503000	0.31615500	0.00316800
H	−3.33978100	−0.97114300	1.07743000
O	−4.26283100	1.14302400	−0.41727300
H	−4.28753400	0.38388200	−0.99792700
H	−4.82069700	1.81063600	−0.80821000
H	−3.73202000	−0.21294500	2.01737500
S	−2.76044300	−1.75338400	0.07211900
H	−2.01119800	1.06469000	0.11032600
H	−0.10038800	−2.76432300	0.02324200
Cl	2.82312800	1.07817600	−0.03877800
Cl	0.18589800	2.78179300	0.11597900
Cl	2.58871800	−2.05690800	−0.11467000

2,3,4,5-TeCTB

O 2			
C	0.20819000	1.47184600	−0.05756200
C	−1.05891200	0.92520300	−0.08782700
C	−1.23280800	−0.44880500	−0.09119500
C	−0.11407400	−1.28052600	−0.04566400
C	1.16213500	−0.72961800	0.01099300
C	1.33029500	0.65435900	−0.00341900
H	−2.84074400	−1.92955700	0.84843200
O	−4.05133600	2.08064800	0.29899900
H	−4.28049800	1.15219000	0.28729000
H	−4.84025800	2.56622300	0.07426100
H	−2.76351000	−2.61834400	1.93568800
S	−2.87168600	−1.07194200	−0.25358700
Cl	−0.30880900	−2.98162800	−0.05000400
H	−1.91797800	1.57894000	−0.09748000
Cl	2.53111500	−1.75007600	0.08337900
Cl	2.89684300	1.32962100	0.05157300
Cl	0.36506900	3.17865100	−0.06934400

2,3,4,6-TeCTB

0 2			
C	−0.28335400	−1.78961700	−0.22188700
C	0.91267400	−1.12612900	−0.38417200
C	0.98813400	0.26508000	−0.39051500
C	−0.20783500	0.97027100	−0.22640600
C	−1.42359100	0.31635800	−0.04079800
C	−1.44759300	−1.07268000	−0.04457200
H	2.41827000	1.92631500	0.44737400
O	2.51940800	−0.06995700	2.45870300
H	3.04461400	−0.49796300	1.78430900
H	2.58280200	−0.61626800	3.23752800
H	2.32968600	2.54172500	1.55881600
Cl	−0.18896500	2.68178900	−0.25145000
Cl	2.33098600	−2.08591300	−0.57092000
S	2.52557700	1.06749000	−0.65454200
H	−0.31087400	−2.86575100	−0.22239500
Cl	−2.91196000	−1.93756200	0.16965100
Cl	−2.86886100	1.20122000	0.17316100

2,3,5,6-TeCTB

0 2			
C	−0.97634500	1.40973100	−0.07320900
C	−1.13256700	0.05245400	−0.31764500
C	−0.01740100	−0.78629200	−0.38441900
C	1.25315200	−0.23019300	−0.20951400
C	1.39169500	1.12753000	0.04910300
C	0.28151500	1.94232000	0.11315900
H	0.55907100	−2.94543500	0.32414300
O	−1.12660000	−2.06742500	2.38744700
H	−1.76003000	−2.24360500	1.69330200
H	−1.63083900	−1.80956800	3.15450500
H	1.14118400	−3.28760900	1.39669600
Cl	2.64928500	−1.21342700	−0.31703500
Cl	2.93435300	1.84047900	0.28125900
Cl	−2.32453500	2.46721300	0.01517500
Cl	−2.71082300	−0.58743800	−0.52359000
S	−0.23843200	−2.49241800	−0.73678800
H	0.39726800	2.99495600	0.30678300

PCTB

0 2			
C	−0.57332500	−1.33599600	−0.16216800
C	0.75373800	−0.96820700	−0.34477400
C	1.13625000	0.37221900	−0.37843700
C	0.14496900	1.34327800	−0.23337100
C	−1.18403300	0.98765900	−0.03360600
C	−1.54470000	−0.35461200	0.00021500
H	2.90529300	1.68333100	0.42736300
O	2.55506700	−0.25588300	2.47543400

H	2.99693400	−0.78244600	1.81106300
H	2.48531900	−0.80444200	3.25222700
H	2.96377600	2.33012500	1.51896600
Cl	0.55738400	3.00175900	−0.30610400
Cl	−2.37950300	2.19229100	0.15536800
Cl	−3.17583400	−0.79550600	0.23660600
Cl	−1.01567800	−2.98511500	−0.12365100
Cl	1.93792600	−2.19600700	−0.52096600
S	2.81860900	0.79114300	−0.65009800

Table S5. Cartesian coordinates of the hydrated products CTBR-H₂O_s.

TBe			
O 2			
C	−1.20563300	1.61567000	0.01142500
C	−0.04084100	0.87971500	0.01470100
C	−0.09505300	−0.52706700	0.00493400
C	−1.35284400	−1.15933100	−0.00668400
C	−2.50909700	−0.41249000	−0.00945500
C	−2.43804600	0.97584000	−0.00043100
O	3.23670600	1.35888800	−0.05994500
H	2.98221100	0.43309000	−0.03511100
H	4.10952000	1.41315400	0.31865500
H	0.91928400	1.37227700	0.02486100
H	−3.46887200	−0.90506600	−0.01884800
S	1.33156000	−1.46457200	0.00639600
H	−1.38805900	−2.23737300	−0.01414600
H	−1.15718800	2.69332000	0.01790600
H	−3.34642500	1.55862800	−0.00302800
2-CTBR			
O 2			
C	0.26709300	2.33152600	0.00091400
C	0.90581100	1.11459000	0.00146800
C	0.18087500	−0.09616400	0.00087100
C	−1.23233300	−0.00900100	−0.00005300
C	−1.86771300	1.21475600	−0.00058900
C	−1.12040600	2.38194300	−0.00012500
H	−2.94484600	1.25034200	−0.00136300
H	−1.62978400	3.33314800	−0.00061800
H	1.98369500	1.06584100	0.00246800
O	4.00310800	0.01684300	−0.00527400
H	3.36318100	−0.69894500	−0.00205600
H	4.86747000	−0.38345000	0.02145800
Cl	−2.20007400	−1.42500000	−0.00066100
H	0.84508900	3.24171800	0.00126500
S	1.00572700	−1.58401800	0.00108500
3-CTBR			

0 2			
C	−0.08340800	1.88637200	0.00206000
C	0.93433500	0.95692700	0.00234300
C	0.62831900	−0.41569300	0.00131200
C	−0.71848500	−0.82068100	0.00012400
C	−1.71331500	0.12773100	−0.00013300
C	−1.40999900	1.48367100	0.00082300
H	−2.20881500	2.20768800	0.00056700
H	1.96593600	1.27223800	0.00348800
O	4.20332300	0.89020400	−0.00660500
H	3.85456900	−0.00382500	−0.00432400
H	5.15327200	0.81882700	0.01801600
H	0.15081000	2.93914200	0.00278500
H	−0.95754200	−1.87148500	−0.00065300
Cl	−3.36628700	−0.36808200	−0.00157400
S	1.86358600	−1.59604900	0.00128400

4-CTBR

0 2			
C	−0.78692000	1.07744900	0.00093300
C	0.53565700	0.69905400	0.00106400
C	0.88970100	−0.66398500	0.00037000
C	−0.13853900	−1.62571700	−0.00046700
C	−1.46000000	−1.24997600	−0.00056900
C	−1.77661200	0.10308800	0.00019800
H	0.12980300	−2.67022200	−0.00105500
H	1.31161400	1.44935000	0.00174900
O	3.53036200	2.04560700	−0.00339200
H	3.57092100	1.08598900	−0.00183100
H	4.42931400	2.36120200	0.01580800
H	−1.06051700	2.11994500	0.00138900
H	−2.24751000	−1.98572600	−0.00124100
Cl	−3.42704900	0.57990500	−0.00016500
S	2.51897500	−1.16395400	0.00037200

2,3-DCTBR

0 2			
C	0.38068300	2.24500100	0.01158700
C	1.26469000	1.19177300	0.01426600
C	0.80595300	−0.13927800	0.00877800
C	−0.59411500	−0.37250500	0.00246400
C	−1.46731500	0.70296300	0.00023800
C	−0.98178000	2.00408200	0.00471900
H	2.32896500	1.36849500	0.02084600
O	4.51612500	0.78123800	−0.05703900
H	4.06162600	−0.06376700	−0.03250100
H	5.41175000	0.62202800	0.22723200
Cl	−1.20407100	−1.96548300	−0.00313100

H	−1.68839400	2.81819200	0.00249600
S	1.93177600	−1.41678000	0.00958600
Cl	−3.16924100	0.47267600	−0.00758800
H	0.74624700	3.25911200	0.01477400
2,4-DCTBR			
0 2			
C	0.85183200	−1.57977200	0.01099600
C	−0.47279800	−1.21981600	0.01465000
C	−0.87940600	0.13133600	0.00824900
C	0.14279500	1.11130200	0.00000800
C	1.47396300	0.75847900	−0.00325600
C	1.81907700	−0.58363200	0.00219400
H	−1.23511700	−1.98355000	0.02286000
O	−3.34627200	−2.77283000	−0.05701900
H	−3.48885400	−1.82418700	−0.03068200
H	−4.15071200	−3.18299900	0.24777800
Cl	−0.23711800	2.78145800	−0.00707800
S	−2.52999200	0.53122600	0.01076000
H	1.14293700	−2.61698900	0.01487300
H	2.23704200	1.51824700	−0.01003000
Cl	3.48017600	−1.01292200	−0.00220700
2,5-DCTBR			
0 2			
C	−1.42121000	−0.94355400	0.00324500
C	−0.82517600	0.29377700	0.01200500
C	0.58004800	0.41116800	0.00811500
C	1.34342100	−0.77946000	−0.00205400
C	0.72473000	−2.01242600	−0.01056800
C	−0.65496000	−2.10187600	−0.00743500
H	−1.42536800	1.19110800	0.02006800
O	−1.73750400	3.43135300	−0.08240100
H	−0.78061200	3.38772200	−0.03258600
H	−2.00147000	4.23902100	0.34920700
Cl	3.05558500	−0.73629600	−0.00593100
H	1.32493600	−2.90735300	−0.01912000
H	−1.13720900	−3.06593700	−0.01388700
Cl	−3.13888400	−1.07152900	0.00797700
S	1.30342000	1.95199100	0.01880500
2,6-DCTBR			
0 2			
C	0.48034900	2.27919700	0.00003800
C	−0.30295000	1.14597800	−0.00001600
C	0.26177900	−0.15749600	−0.00000500
C	1.68063500	−0.22058300	0.00003000
C	2.46214600	0.91303500	0.00008200
C	1.85901900	2.15939500	0.00009900

O	−4.25420700	−1.14684000	0.00010900
H	−3.29676400	−1.12050800	−0.00020500
H	−4.49234500	−2.06953800	0.00105100
Cl	2.48073000	−1.73521300	−0.00000400
H	3.53501300	0.81775000	0.00010600
H	2.47103700	3.04763200	0.00013000
H	0.00929500	3.24788500	0.00003000
Cl	−2.00113300	1.35339000	−0.00010100
S	−0.68697500	−1.56091600	−0.00009800

3,4-DCTBR

O 2			
C	−0.01301400	1.50241900	0.00195100
C	1.19574900	0.85045600	0.00237400
C	1.23731400	−0.55615200	0.00137500
C	0.02602300	−1.26776300	0.00019300
C	−1.18140700	−0.60938900	−0.00016000
C	−1.20502700	0.78714200	0.00075200
O	4.36958600	1.53357500	−0.00934500
H	4.25247900	0.58093000	−0.00514900
H	5.30694700	1.69967500	0.03542700
H	−0.05443900	2.57937500	0.00255400
H	0.04601900	−2.34524500	−0.00055700
H	2.11647600	1.41354500	0.00354500
Cl	−2.63540100	−1.52110200	−0.00169700
Cl	−2.68196700	1.64617500	0.00026100
S	2.71332800	−1.41021200	0.00152700

3,5-DCTBR

O 2			
C	−0.05348700	1.30493900	0.00119500
C	0.91802400	0.32849500	0.00229400
C	0.52527100	−1.02056900	0.00187200
C	−0.84008100	−1.35183000	0.00047600
C	−1.77919100	−0.34750900	−0.00061300
C	−1.40388300	0.98770100	−0.00023400
O	4.14783600	0.02062300	−0.01231500
H	3.78163000	−0.86562500	−0.00494100
H	5.09589700	−0.06658800	0.02981500
H	−1.13810700	−2.38693300	0.00019400
H	1.96490600	0.59100500	0.00334800
Cl	−3.45683800	−0.74037600	−0.00242300
H	−2.14863600	1.76607800	−0.00106400
Cl	0.40381800	2.96531100	0.00178300
S	1.68519000	−2.27713600	0.00325800

2,3,4-TCTBR

O 2			
C	−0.00509300	−1.90043000	0.00005800

C	−1.19713800	−1.22533500	0.00007300
C	−1.24064100	0.18196600	−0.00001800
C	−0.00869500	0.88426800	−0.00010400
C	1.19908400	0.20016200	−0.00005400
C	1.19076600	−1.19733700	0.00000300
H	−2.12683200	−1.77289400	0.00019900
O	−4.35527900	−1.98825500	−0.00109900
H	−4.26504700	−1.03300000	−0.00054000
H	−5.28854900	−2.18125300	0.00442300
Cl	−0.00230100	2.58881000	0.00008200
H	0.01894100	−2.97737200	0.00013500
Cl	2.68351400	1.04664900	0.00006400
Cl	2.65372500	−2.07892800	0.00013100
S	−2.73874500	0.98436000	0.00000900

2,3,5-TCTBR

O 2			
C	0.85043100	1.47668500	0.00030700
C	1.29469500	0.17664700	0.00053700
C	0.37177400	−0.88499800	0.00042600
C	−1.01546100	−0.58983300	0.00008400
C	−1.42918600	0.73325500	−0.00014500
C	−0.50347100	1.76535700	−0.00001500
O	4.14801300	−1.32191100	−0.00310700
H	3.50684700	−2.03379100	−0.00085800
H	5.01373600	−1.72028900	0.00707800
H	2.35161200	−0.04078100	0.00071400
Cl	−2.16795000	−1.84450100	−0.00007900
Cl	−3.09387900	1.14739300	−0.00056300
H	−0.84676000	2.78642600	−0.00018400
Cl	1.97849100	2.77532500	0.00045900
S	0.94965700	−2.48804000	0.00087800

2,3,6-TCTBR

O 2			
C	0.10532100	2.15359600	0.00007900
C	−0.78556200	1.10218400	0.00023500
C	−0.34145000	−0.24446400	0.00023400
C	1.06703800	−0.46156300	0.00001400
C	1.94720500	0.60532800	−0.00010700
C	1.46189600	1.90562800	−0.00007600
O	−4.92261500	−0.69613800	−0.00185700
H	−3.97189700	−0.81179400	0.00110500
H	−5.29710100	−1.57237600	0.00394700
H	2.16376600	2.72353900	−0.00018400
H	−0.26346800	3.16552300	0.00006900
Cl	1.67937400	−2.05162300	−0.00002400
Cl	3.64621400	0.37271500	−0.00030000
Cl	−2.45360000	1.47051600	0.00034200

S	−1.42505400	−1.54733600	0.00046000
2,4,5-TCTBR			
0 2			
C	1.12185900	0.68135500	−0.01153600
C	−0.21752800	0.98948400	−0.02007500
C	−1.20868400	−0.01093700	−0.01378300
C	−0.77314100	−1.35726900	0.00080400
C	0.56722600	−1.66591200	0.00935600
C	1.51900700	−0.65717400	0.00277800
O	−2.00511200	3.66356000	0.07896200
H	−2.63519900	2.94379500	0.01343400
H	−2.47940300	4.46916900	−0.10699600
H	−0.52180500	2.02545000	−0.02996100
Cl	−1.89180100	−2.65197500	0.00876200
H	0.88648400	−2.69432200	0.02086700
Cl	3.16938000	−1.09120600	0.01475100
Cl	2.27607000	1.94772800	−0.01957900
S	−2.85460200	0.41205300	−0.02507500
2,4,6-TCTBR			
0 2			
C	0.95111800	−1.49800700	−0.00046800
C	−0.28803700	−0.89934300	−0.00102300
C	−0.44999600	0.51251300	−0.00081300
C	0.75219800	1.26964300	0.00010400
C	1.99514700	0.68173300	0.00078100
C	2.08295300	−0.70034400	0.00044200
O	−4.81857900	−0.96898100	0.00384800
H	−4.02303100	−0.43613800	0.00638700
H	−5.54857500	−0.35646000	0.00720300
Cl	0.69865900	2.97990700	0.00037700
H	2.88483900	1.28769000	0.00151100
H	1.03650000	−2.57110200	−0.00073800
Cl	−1.65463100	−1.92356200	−0.00210200
Cl	3.62775000	−1.43932300	0.00116200
S	−1.96760200	1.25883200	−0.00185700
3,4,5-TCTBR			
0 2			
C	−0.00093800	1.05176700	−0.00010800
C	1.20611200	0.39171700	−0.00038900
C	1.23847400	−1.01150700	−0.00021400
C	0.02815600	−1.72076200	0.00014700
C	−1.17214400	−1.05302400	0.00046000
C	−1.20892700	0.34581000	0.00052800
O	4.34288600	1.08583400	−0.00043300
H	4.30658200	0.12783600	−0.00040900
H	5.26297300	1.33412400	0.00462800

H	2.12578700	0.95720300	−0.00078600
H	0.04248800	−2.79789200	0.00009200
Cl	−2.62594400	−1.96416500	0.00066500
Cl	−2.69515200	1.17126700	0.00033500
Cl	−0.00037700	2.76650100	−0.00054500
S	2.71498200	−1.86770000	−0.00064600
2,3,4,5-TeCTBR			
O 2			
C	0.04946100	1.45578700	0.00775100
C	1.22193400	0.74265100	0.01248700
C	1.21998700	−0.66190100	0.00974500
C	−0.02798300	−1.33149500	0.00285800
C	−1.21032300	−0.60785000	−0.00155100
C	−1.17889300	0.79207100	0.00094100
O	4.36696700	1.44087700	−0.08438100
H	4.32486900	0.48474500	−0.03247700
H	5.19825600	1.70605600	0.29911700
H	2.16526500	1.26823600	0.01760000
Cl	−0.08020300	−3.03381100	−0.00016300
Cl	−2.62972400	1.67737900	−0.00409400
Cl	0.11729600	3.16729700	0.01149500
S	2.69823000	−1.50331800	0.01526000
Cl	−2.71565700	−1.41489600	−0.00998900
2,3,4,6-TeCTBR			
O 2			
C	−0.22502900	−1.74284100	−0.00147400
C	0.88951600	−0.93998800	−0.00261200
C	0.78992500	0.47414500	−0.00229700
C	−0.52517700	1.01862200	−0.00053700
C	−1.65163900	0.21095200	0.00063000
C	−1.48708200	−1.17587900	0.00011500
O	5.35474500	−0.31806300	0.01200100
H	4.48347700	0.07815200	0.00111500
H	5.97620400	0.40434300	0.00542400
Cl	−0.73344700	2.70859100	0.00005000
Cl	2.41319600	−1.70760500	−0.00396900
Cl	−3.22152000	0.88046700	0.00264100
H	−0.12239600	−2.81442000	−0.00172200
Cl	−2.83619400	−2.21918400	0.00146700
S	2.15669300	1.47173700	−0.00418800
2,3,5,6-TeCTBR			
O 2			
C	−0.00952200	1.69056500	−0.00005000
C	0.79822900	0.56560900	−0.00023900
C	0.21734800	−0.73198600	−0.00026200
C	−1.20083100	−0.83210300	−0.00004300

C	−1.98135700	0.31068800	0.00014800
C	−1.38577700	1.55950300	0.00014100
O	4.78970300	−1.52103200	0.00145700
H	3.83601800	−1.60112200	0.00006900
H	5.13239100	−2.41027200	0.00001200
Cl	−1.95392500	−2.35793100	−0.00003600
Cl	2.48723800	0.75145200	−0.00039300
Cl	−3.69334700	0.24106600	0.00039800
H	−2.00316300	2.44225400	0.00029000
Cl	0.64469800	3.27371700	−0.00003400
S	1.17808100	−2.12983900	−0.00056800
PCTBR			
O 2			
C	0.23317200	−1.38370700	−0.00026800
C	−0.90016100	−0.58786900	−0.00045600
C	−0.80426800	0.82847700	−0.00045500
C	0.49668000	1.39683100	−0.00017800
C	1.62871800	0.60076300	0.00004100
C	1.49759500	−0.79024100	−0.00002600
O	−5.35032900	−0.00651100	0.00222100
H	−4.50556500	0.44346900	0.00130000
H	−6.01706100	0.67434400	−0.00164700
Cl	0.68195800	3.08829400	0.00004400
Cl	3.18593900	1.29787900	0.00048900
Cl	2.88755500	−1.76610500	0.00029800
Cl	0.10208400	−3.08424700	−0.00019600
Cl	−2.42797200	−1.32977600	−0.00042100
S	−2.18048400	1.81537300	−0.00081400

Table S6. Cartesian coordinates of the hydrated CTB-H₂O-OH pre-reactive intermediates for H abstraction from CTBs by OH radical.

TBe			
O 2			
C	1.53060200	−1.07282200	−1.00824100
C	0.32868700	−0.39220800	−1.10103400
C	0.09685500	0.71952700	−0.29854500
C	1.08936000	1.15229100	0.57366200
C	2.29500000	0.47593800	0.64597400
C	2.51850700	−0.64498700	−0.13686900
H	−2.15431200	0.60350900	−0.84733900
O	−1.15238800	−1.17895800	1.93880600
H	−1.39464300	−0.25401100	1.99221300
H	−0.20627500	−1.17819100	1.79363500
O	−2.25630400	−1.75426500	−0.58192800
H	−1.93756500	−1.71370000	0.34451500

S	−1.43022500	1.59944700	−0.32637000
H	3.05786700	0.82284200	1.32603500
H	3.45448500	−1.17694500	−0.07164000
H	0.91507000	2.01325700	1.20176300
H	−0.42819300	−0.72732700	−1.79405000
H	1.69263200	−1.94124000	−1.62792400
2-CTB			
0 2			
C	1.62940200	−1.45647700	0.07246200
C	0.53478000	−0.70756800	−0.32836800
C	0.59057700	0.68427200	−0.36381100
C	1.79057400	1.29319300	−0.00054400
C	2.88846100	0.55006400	0.38210700
C	2.80903700	−0.83177100	0.42573400
H	−1.73499500	0.88502800	−0.71676700
O	−1.49341200	0.31109500	2.25411900
H	−1.14866400	1.15768000	1.97133300
H	−0.73861800	−0.27172500	2.31111800
O	−3.38778200	−0.27598800	0.24360800
H	−2.87544900	−0.18505200	1.07125700
Cl	−0.89972500	−1.55374400	−0.78044500
S	−0.71698400	1.74291000	−0.87066900
H	1.85049200	2.37090100	−0.02016100
H	3.80315200	1.05299300	0.65368500
H	1.54543300	−2.53126800	0.09084100
H	3.65828200	−1.42260900	0.72967100
3-CTB			
0 2			
C	1.57036000	0.07606200	−0.11630800
C	0.31678800	−0.19319500	−0.63414300
C	−0.69211500	0.75094300	−0.48678100
C	−0.42796800	1.95136500	0.16175100
C	0.83819700	2.20212000	0.65809200
C	1.84941900	1.26613900	0.53027700
H	−2.20773800	−0.85139500	−1.20834100
O	−1.95619500	−0.83189600	2.11156300
H	−2.42668900	−0.17761500	1.59304700
H	−1.17067600	−0.39233000	2.43167100
O	−1.41755200	−2.64526500	0.04339100
H	−1.59275400	−2.16404900	0.87943100
S	−2.31664800	0.47887200	−1.11337800
H	−1.21059800	2.68587500	0.27574800
H	1.03930400	3.13787600	1.15626500
H	2.83663000	1.45271000	0.91923200
H	0.13696600	−1.12474000	−1.14711100
Cl	2.81904800	−1.10185800	−0.29428600

4-CTB

0 2

C	1.07941400	−0.66583500	−0.92043100
C	−0.24379400	−0.28190000	−1.04028000
C	−0.73143800	0.79570900	−0.31099300
C	0.13041300	1.49334300	0.52630800
C	1.45775500	1.12265000	0.63661500
C	1.92490900	0.03884400	−0.08414500
H	−2.88129200	0.19540600	−0.95091800
O	−2.09669600	−1.24735400	1.93560600
H	−2.33401600	−0.32556100	1.82476400
H	−1.17144400	−1.25349700	2.17257900
O	−2.60145100	−2.13910100	−0.66314300
H	−2.46044000	−2.00504000	0.29791000
S	−2.40968800	1.32547600	−0.41301000
H	−0.23396500	2.33391900	1.09757500
H	2.12522000	1.66882800	1.28338400
H	−0.89284500	−0.82657100	−1.70892600
Cl	3.57836400	−0.43610200	0.06186300
H	1.45323300	−1.50659500	−1.48202700

2,3-DCTB

0 2

C	1.71852000	−0.10198100	0.01664900
C	0.37825500	−0.04289100	−0.35770500
C	−0.29059400	1.18302700	−0.33700600
C	0.41054800	2.32216200	0.04627100
C	1.74235500	2.25280500	0.39783800
C	2.40207900	1.03963000	0.39038800
H	−2.38801200	0.15353600	−0.69023800
O	−1.84772200	−0.36768900	2.26678900
H	−1.85054500	0.55677600	2.02150600
H	−0.94067100	−0.59215600	2.46359000
O	−3.22518800	−1.69602900	0.20728100
H	−2.82146900	−1.39449900	1.04523200
S	−1.96481800	1.41906000	−0.81125600
H	−0.10666700	3.26891200	0.06633100
H	2.26855600	3.14816700	0.68825800
Cl	−0.43440300	−1.47394500	−0.84242500
Cl	2.56690500	−1.59759900	0.01798000
H	3.43966100	0.96378200	0.66981300

2,4-DCTB

0 2

C	1.26797700	0.87569900	0.30564300
C	−0.01565900	0.39700500	0.50849200
C	−0.31639100	−0.95541500	0.36120200
C	0.72788200	−1.81163800	0.01931400
C	2.01451400	−1.35431300	−0.16994900

C	2.27685200	−0.00352400	−0.02967800
H	−2.63750100	−0.57191900	0.49862300
O	−1.94205200	0.23916600	−2.32361700
H	−1.84182400	−0.69436100	−2.13968700
H	−1.06077000	0.60692500	−2.31906700
O	−3.84586000	1.07460400	−0.41616600
H	−3.27595800	0.95214100	−1.20075900
Cl	−1.23276600	1.53429300	0.94727400
S	−1.89493800	−1.68187500	0.61174500
H	0.51916700	−2.86356200	−0.10260000
H	2.80642800	−2.03649800	−0.43167000
H	1.47162300	1.92705300	0.42297500
Cl	3.87453600	0.59471700	−0.27478100
2,5-DCTB			
O 2			
C	−0.64976500	1.81162300	0.01501600
C	0.32071500	0.89535300	−0.35418000
C	0.00190200	−0.45155100	−0.51926400
C	−1.31915300	−0.84175800	−0.31474600
C	−2.27918900	0.08266100	0.03779100
C	−1.95674400	1.41657500	0.21190200
H	2.26533600	−1.06272600	−0.72252000
O	1.88539900	−0.66208000	2.28152000
H	1.37666500	−1.38151100	1.90904000
H	1.27173700	0.05752800	2.41392400
O	4.02141200	−0.33535300	0.48053000
H	3.42342700	−0.37931800	1.25295300
S	1.12601600	−1.70937500	−1.00332700
H	−1.59282300	−1.87848100	−0.43126900
Cl	1.92556600	1.47113800	−0.60407300
H	−2.71305900	2.13038600	0.49252300
Cl	−3.90418400	−0.44055700	0.27742200
H	−0.37212000	2.84628100	0.13614900
2,6-DCTB			
O 2			
C	−0.31911300	2.32291900	0.09321300
C	0.29236100	1.14578800	−0.29961700
C	−0.40300600	−0.06509400	−0.34439400
C	−1.75228000	−0.01991300	0.01477600
C	−2.37617300	1.14870200	0.40223900
C	−1.65407800	2.32529400	0.44441200
H	1.55310100	−1.21188500	−0.87122700
O	1.75822200	−0.84250900	2.19031200
H	1.03825800	−1.37563800	1.85220800
H	1.38370000	0.00910400	2.40467600
O	3.65497900	−1.06231100	0.11606700
H	3.17125000	−0.96904100	0.96060700

Cl	1.95754500	1.22427400	−0.74307400
S	0.27598200	−1.60936100	−0.81991800
H	−3.42029100	1.12426600	0.66727800
H	0.26090300	3.23103200	0.10995000
H	−2.13162800	3.24350400	0.74578000
Cl	−2.68124400	−1.47187300	−0.02547800
3,4-DCTB			
O 2			
C	−0.96363100	0.46601000	−0.33624600
C	0.38002200	0.31424100	−0.63527400
C	0.99575800	−0.91843800	−0.48150300
C	0.24736700	−2.00274100	−0.03849200
C	−1.09230500	−1.84871200	0.24815300
C	−1.70953400	−0.61692700	0.10791800
H	3.01239000	0.12088000	−0.99312000
O	2.71808400	0.59238500	2.19371300
H	2.81113900	−0.27973900	1.80901100
H	1.94050800	0.56846400	2.74645600
O	2.90184800	2.20004600	−0.06770800
H	2.88286100	1.80388200	0.82851400
S	2.70099900	−1.17200000	−0.83895900
H	−1.67622900	−2.68831700	0.58910800
H	0.70971400	−2.97033900	0.08110400
H	0.93043600	1.16939800	−0.99551100
Cl	−1.67715600	2.01484400	−0.53569500
Cl	−3.37768600	−0.46615500	0.48642400
3,5-DCTB			
O 2			
C	−0.48985300	1.41444500	−0.22256300
C	0.60386400	0.66899500	−0.62074700
C	0.48646500	−0.71343400	−0.68440600
C	−0.71720300	−1.32854900	−0.36427700
C	−1.79102300	−0.54796700	0.01623300
C	−1.69974400	0.82851300	0.09984500
H	2.77943800	−0.81862900	−1.02326400
O	2.29889200	−1.01874000	2.21281400
H	2.04578100	−1.72491400	1.61755500
H	1.51808400	−0.78717600	2.71047800
O	3.51764700	0.76511100	0.45347300
H	3.17634500	0.23802600	1.20616100
S	1.82462500	−1.74308400	−1.18357900
Cl	−0.34699000	3.12986700	−0.13614500
H	1.52460400	1.16429100	−0.88372700
H	−0.82132300	−2.40060100	−0.41176300
Cl	−3.28600700	−1.31278100	0.40937400
H	−2.54331400	1.42488100	0.40212500

2,3,4-TCTB			
0 2			
C	1.14110400	−0.42048300	−0.18410000
C	−0.20449000	−0.15033900	−0.44434300
C	−0.68565700	1.15796600	−0.41611900
C	0.21297600	2.18499700	−0.14662800
C	1.54334600	1.92861900	0.08852300
C	2.01335200	0.62822600	0.07813200
H	−2.93839300	0.45281100	−0.53103300
O	−2.18776300	−0.09696600	2.36747100
H	−2.13354000	0.82956600	2.13674700
H	−1.28966600	−0.42084800	2.39125000
O	−3.94623000	−1.23086100	0.48490000
H	−3.43827700	−0.98614500	1.28365300
S	−2.34282900	1.63484600	−0.74167300
H	−0.14579700	3.20208100	−0.12042000
H	2.22886700	2.73424900	0.29309500
Cl	3.67532600	0.34468600	0.39704400
Cl	−1.26431400	−1.45037700	−0.80076200
Cl	1.71547200	−2.03081200	−0.19970900
2,3,5-TCTB			
0 2			
C	−0.69712500	1.32690100	−0.08428500
C	0.33959700	0.45581200	−0.40779100
C	0.08106500	−0.91375500	−0.50019900
C	−1.21153900	−1.37540900	−0.27776500
C	−2.22299700	−0.48998000	0.02471200
C	−1.98082100	0.86464800	0.13169500
H	2.37862000	−1.41770100	−0.67644000
O	2.00300700	−0.85443700	2.33521000
H	1.42321400	−1.53979500	2.00589200
H	1.44307300	−0.13697900	2.62316000
O	4.08501300	−0.58975900	0.45892800
H	3.50727600	−0.60745700	1.24714200
S	1.27106900	−2.13065800	−0.92528500
Cl	1.91260000	1.06997200	−0.69883300
Cl	−0.41593200	3.01532600	0.05073100
Cl	−3.81725800	−1.08450800	0.28928900
H	−1.42196400	−2.43075700	−0.34241400
H	−2.77054800	1.55405200	0.37574000
2,3,6-TCTB			
0 2			
C	−1.01998800	−1.58286100	0.03353300
C	−0.62246000	−0.30131000	−0.33367200
C	0.73406800	0.04752700	−0.33862200
C	1.65277600	−0.94123500	0.01488700
C	1.25575800	−2.21401600	0.36842600

C	−0.08331800	−2.53671100	0.38265200
H	0.19167000	2.27002300	−0.80558600
O	−0.36527500	2.17761100	2.21046500
H	0.55203600	1.99363500	2.01230600
H	−0.73584700	1.37949200	2.57940100
O	−1.39565600	3.64808300	0.03934300
H	−1.18014600	3.24908200	0.90482000
S	1.36348500	1.62365000	−0.77264900
H	1.99968000	−2.94713900	0.63259900
Cl	−2.68068900	−2.01993200	0.05665200
Cl	−1.81174200	0.84466000	−0.79518600
Cl	3.33677100	−0.57957700	0.01019000
H	−0.41050200	−3.52496700	0.65899600

2,4,5-TCTB

0 2

C	0.55009600	−1.36872400	−0.27700000
C	−0.60998700	−0.65132300	−0.50044600
C	−0.60193900	0.74245300	−0.48865100
C	0.61322500	1.37718500	−0.26086700
C	1.77938500	0.66774800	−0.05415100
C	1.74979900	−0.72107400	−0.05443100
H	−2.94872200	0.86439500	−0.53096800
O	−2.29555100	0.16248100	2.36087300
H	−1.97184000	1.02490400	2.10359600
H	−1.53125300	−0.40824800	2.40468900
O	−4.42471000	−0.36970800	0.60150600
H	−3.80913800	−0.30432100	1.35821300
S	−1.99284300	1.77107400	−0.77726700
Cl	−2.05721300	−1.53431000	−0.79494700
Cl	3.16464100	−1.65154800	0.21147400
Cl	3.23665500	1.53040000	0.21554400
H	0.65381800	2.45477900	−0.24176200
H	0.52182000	−2.44569200	−0.28845700

2,4,6-TCTB

0 2

C	1.09910000	−1.44715000	−0.25873300
C	−0.12712200	−0.84336500	−0.46881000
C	−0.29936000	0.53952400	−0.37880300
C	0.84375500	1.28466300	−0.08037300
C	2.07913800	0.70632600	0.12737900
C	2.19581500	−0.66565800	0.03891700
H	−2.59261600	0.30943200	−0.67896600
O	−2.30240100	−0.41318800	2.28049500
H	−2.01862500	0.47074700	2.04895000
H	−1.52072800	−0.89530600	2.53955800
O	−4.10660700	−1.15473800	0.25134100
H	−3.61020200	−1.02997500	1.08371400

S	−1.80789600	1.39319100	−0.62868500
H	2.93265700	1.32232900	0.35392500
Cl	−1.44824400	−1.87474700	−0.86434500
Cl	0.72590100	2.99877100	0.03194800
H	1.19068500	−2.51701600	−0.33931000
Cl	3.72641700	−1.40954800	0.29821600
3,4,5-TCTB			
O 2			
C	−0.42582800	1.11098900	−0.34059800
C	0.83894500	0.65560000	−0.66213800
C	1.10032400	−0.70559900	−0.67366900
C	0.08314800	−1.59987200	−0.37784100
C	−1.18005400	−1.13487600	−0.06991300
C	−1.45900100	0.22803900	−0.04102100
H	3.34449600	−0.19745600	−0.95822100
O	3.04046100	−0.37458300	2.25649000
H	2.89230700	−1.13311200	1.69110500
H	2.35313700	−0.37811700	2.91814500
O	3.64282800	1.61372500	0.41369400
H	3.49549100	1.04950800	1.20114300
S	2.68565500	−1.35698600	−1.07271000
H	0.26043800	−2.66328500	−0.38421900
H	1.60629900	1.37328200	−0.90391300
Cl	−0.70005400	2.80440900	−0.32981400
Cl	−3.02065500	0.79833200	0.35050700
Cl	−2.40483100	−2.28379100	0.28689100
2,3,4,5-TeCTB			
O 2			
C	−0.57068400	1.01548300	−0.19309700
C	0.64055400	0.37531700	−0.44984000
C	0.70217100	−1.01634400	−0.49799500
C	−0.46587000	−1.73824500	−0.29778200
C	−1.66701500	−1.10739500	−0.06094400
C	−1.73684500	0.27957900	0.00045600
H	3.05826000	−1.00952000	−0.60567900
O	2.52865800	−0.46709900	2.37213900
H	2.07395100	−1.25808500	2.08746700
H	1.88678300	0.08276400	2.81478500
O	4.52803700	0.21144000	0.51561400
H	3.97009400	0.07661100	1.30597800
S	2.14155700	−1.95895900	−0.83615700
Cl	2.05126500	1.30989900	−0.71148600
Cl	−0.62839200	2.72217100	−0.12292000
Cl	−3.21993200	1.06584700	0.31241500
Cl	−3.06651000	−2.07073400	0.16887300
H	−0.44075300	−2.81564900	−0.32783400

2,3,4,6-TeCTB			
0 2			
C	1.44833500	−0.79193100	−0.03499700
C	0.08850800	−0.65656800	−0.31140200
C	−0.51893100	0.59961800	−0.37784800
C	0.28910500	1.71139600	−0.14884700
C	1.63223200	1.59407300	0.12716100
C	2.21488400	0.34515900	0.18410500
H	−2.57042100	−0.40108500	−0.86797500
O	−4.11590700	−0.11127900	1.91150300
H	−3.52344000	0.56468600	1.57989900
H	−4.11489100	−0.05776700	2.86341600
O	−4.04463800	−2.01254600	−0.12973700
H	−4.20797100	−1.50018500	0.68671300
S	−2.21019000	0.88129000	−0.73672300
Cl	−0.84523400	−2.06981700	−0.57050700
Cl	2.16712800	−2.33929400	0.03532400
Cl	−0.39407300	3.28956200	−0.20894400
H	2.22802100	2.47454100	0.29724500
Cl	3.89049200	0.23715500	0.52913300
2,3,5,6-TeCTB			
0 2			
C	−0.05902300	1.75689800	−0.08772700
C	0.68504300	0.61881500	−0.37800900
C	0.06230400	−0.63277900	−0.41476700
C	−1.31326000	−0.70215100	−0.17207600
C	−2.04071900	0.44439700	0.10799400
C	−1.41405800	1.67228200	0.15340000
H	2.12944900	−1.65792300	−0.73240600
O	2.18785500	−1.15686900	2.31479100
H	1.45441200	−1.70867500	2.04615000
H	1.81658300	−0.35953100	2.68465200
O	4.14057000	−1.36052700	0.29565100
H	3.63817300	−1.26555400	1.12807700
S	0.88159600	−2.14085900	−0.76425700
Cl	2.35995200	0.77097500	−0.70295400
Cl	0.67741700	3.30507000	−0.02959400
Cl	−2.09356000	−2.22565300	−0.22850700
Cl	−3.72692400	0.37775700	0.40776800
H	−1.98031400	2.56131200	0.37109000
PTCB			
0 2			
C	−0.42967600	1.39368700	−0.19242100
C	0.71530100	0.63523100	−0.41826700
C	0.66410900	−0.75942900	−0.41309200
C	−0.57368700	−1.36717400	−0.19658400
C	−1.72273300	−0.62031700	0.02084100

C	−1.65171400	0.76872200	0.02820800
H	2.97773300	−0.85750100	−0.65175400
O	2.80223600	−0.24477000	2.37544000
H	2.41093800	−1.09139400	2.16347300
H	2.08022200	0.37103000	2.48161900
O	4.69677600	0.26467700	0.34244000
H	4.20287300	0.16671700	1.18011600
S	2.03901700	−1.81128500	−0.67712700
Cl	2.19529800	1.44456400	−0.71838700
Cl	−0.34200700	3.09912100	−0.19687600
Cl	−3.05736300	1.69681700	0.30295900
Cl	−0.65659700	−3.07711000	−0.20445600
Cl	−3.21566600	−1.40291300	0.28413900

Table S7. Cartesian coordinates of the hydrated CTB-H₂O-OH transition states for H abstraction from CTBs by OH radical.

TBe			
0 2			
C	−2.03746600	1.41321200	0.14793300
C	−0.80142200	1.05885300	−0.36153300
C	−0.44523200	−0.28195400	−0.43007900
C	−1.33023500	−1.25619600	0.01557000
C	−2.56943300	−0.89065100	0.50948400
C	−2.92780600	0.44443300	0.57999500
H	1.73776600	0.41729300	−1.12782600
O	2.91432100	−0.29467600	1.76228800
H	3.73218100	−0.70669900	2.02897600
H	2.38038500	−0.97584300	1.35151300
O	2.48774000	1.45911400	−0.39262400
H	2.76264000	1.04210300	0.44685000
S	1.09054600	−0.81680700	−1.10834200
H	−1.05171300	−2.29850000	−0.02717900
H	−0.10841600	1.81769400	−0.68906900
H	−3.25251400	−1.65464000	0.84760800
H	−3.89158700	0.72847600	0.97246600
H	−2.30439800	2.45733900	0.20461000
2-CTB			
0 2			
C	2.43293400	0.11859400	−0.56456700
C	1.22420500	0.52664800	−0.02832500
C	0.30967500	−0.40727600	0.45633000
C	0.65417100	−1.75432300	0.40271200
C	1.86933400	−2.16346500	−0.10999700
C	2.75836100	−1.22385200	−0.60195900
H	−1.63790000	0.98166100	0.28752900
O	−3.72850000	−1.23487100	−0.68749700
H	−3.12584900	−1.47788400	0.01673900
H	−3.79957600	−1.98757600	−1.26880500
O	−2.32830200	1.19822700	−1.03493900
H	−2.94600100	0.44866200	−1.12771900
Cl	0.88070500	2.21098300	0.02545500
S	−1.21162100	0.03301600	1.21455900
H	−0.04952000	−2.48339600	0.77373800
H	2.11440800	−3.21349500	−0.13504700
H	3.11484500	0.86319600	−0.94203700
H	3.70589100	−1.53094500	−1.01575100
3-CTB			
0 2			
C	1.80952900	−0.21254900	0.04167500
C	0.50568600	−0.29630300	−0.40727300

C	−0.29039600	0.84047100	−0.36715500
C	0.22252600	2.03500600	0.12331400
C	1.53306600	2.09190900	0.55757400
C	2.34094300	0.96939900	0.52350800
H	−2.09033900	−0.52466700	−1.18134800
O	−3.39012900	−0.78899600	1.72488700
H	−4.27211100	−0.81279400	2.08713900
H	−3.20845500	0.11973600	1.48474200
O	−2.33414200	−1.86168800	−0.64024900
H	−2.75046600	−1.71904600	0.23235300
S	−1.95064700	0.84626000	−0.95403300
H	−0.39898000	2.91639500	0.16075300
H	0.11331800	−1.23375800	−0.76631600
H	1.93045600	3.02189300	0.93342100
Cl	2.79946900	−1.62788400	−0.00345300
H	3.36199300	1.00399000	0.86552800
4-CTB			
O 2			
C	1.37360500	−0.98348300	−0.58673200
C	0.05263700	−0.65987300	−0.83135400
C	−0.45114600	0.56905900	−0.42587600
C	0.38290100	1.46771200	0.22748500
C	1.70826300	1.15269000	0.46010700
C	2.19609900	−0.07428400	0.05274200
H	−2.61680200	−0.18551900	−1.10567800
O	−3.54010100	−0.59573000	1.92881100
H	−4.35482200	−0.46208600	2.40647400
H	−3.17386700	0.27075100	1.75033000
O	−3.11677200	−1.51257900	−0.68698400
H	−3.35500600	−1.41825400	0.25586200
S	−2.11120400	1.06150400	−0.74274000
H	−0.00018900	2.42228700	0.55491100
H	−0.58978100	−1.37353400	−1.32201600
H	2.35652200	1.85267400	0.96163100
Cl	3.84879500	−0.47733600	0.35075100
H	1.76451500	−1.94013400	−0.89329000
2,3-CTB			
O 2			
C	1.90284600	0.38577600	0.19479900
C	0.72424500	−0.20302600	−0.25113200
C	−0.37531900	0.60684900	−0.54925200
C	−0.26087100	1.98430300	−0.41261100
C	0.92226700	2.55809100	0.00704700
C	2.00368000	1.75985600	0.32017700
H	−2.03171200	−1.11721000	−0.33115800
O	−4.36003300	0.51759800	1.14410600
H	−3.93468600	0.99525000	0.43183600

H	−4.52650900	1.14456500	1.84332400
O	−2.49167700	−1.58351300	1.01621600
H	−3.22595600	−0.98769800	1.25938300
Cl	0.62903900	−1.90023100	−0.43963600
S	−1.88282800	−0.02727800	−1.18869100
H	−1.11458700	2.60225300	−0.64133100
H	0.99934100	3.62926300	0.10395400
H	2.93165600	2.18664600	0.66333400
Cl	3.27333100	−0.57273400	0.58981100

2,4-CTB

O 2

C	1.67037200	0.79374400	−0.23157000
C	0.34215400	0.91271700	0.13574000
C	−0.36230600	−0.17575300	0.64845500
C	0.31811100	−1.37912100	0.79918500
C	1.64932200	−1.50854500	0.46048100
C	2.314703w00	−0.41552000	−0.06257000
H	−2.54425900	0.65264100	0.12803100
O	−3.77825700	−2.12805000	−0.98404400
H	−3.28865200	−2.20750200	−0.16530000
H	−3.52190000	−2.86205000	−1.53661900
O	−3.09200600	0.59202400	−1.27018700
H	−3.44585300	−0.31109300	−1.38132500
Cl	−0.41529000	2.44130600	−0.05900100
S	−2.02726400	−0.08437000	1.19240800
H	−0.21369200	−2.23088500	1.19361600
H	2.16280000	−2.44707300	0.58791600
H	2.19412800	1.64322200	−0.63656600
Cl	3.97185700	−0.55685100	−0.51351400

2,5-CTB

O 2

C	−1.12692200	−1.85758700	−0.58629000
C	0.05594100	−1.39566000	−0.03711000
C	0.12908700	−0.11059300	0.49832300
C	−1.01326800	0.68221000	0.48504600
C	−2.19271500	0.20074600	−0.04345600
C	−2.25885300	−1.06669500	−0.59010500
H	2.50462800	0.10266100	0.33546600
O	2.60791900	3.12989200	−0.78203500
H	2.00656800	3.01733400	−0.04598000
H	2.17949200	3.70852800	−1.40777700
O	3.13049300	0.37120900	−0.99342100
H	3.09555600	1.34001000	−1.11118300
Cl	1.42041600	−2.43808700	−0.02683200
S	1.56473700	0.54111500	1.26937700
H	−0.97474400	1.67991500	0.89111300
H	−3.18104900	−1.43106600	−1.01160800

H	−1.15809200	−2.85045900	−1.00449000
Cl	−3.59542100	1.20584600	−0.03848300
2,6-CTB			
O 2			
C	1.17544500	2.08814100	0.60582500
C	1.23219500	0.85532300	−0.01686300
C	0.07593100	0.18873300	−0.43822400
C	−1.13677600	0.84849900	−0.22261900
C	−1.20685900	2.08800000	0.38287400
C	−0.04438300	2.70408300	0.80277400
H	1.02765200	−1.95537600	−0.37329200
O	−1.44298000	−1.93662200	1.92207700
H	−1.96578300	−1.74328300	1.14364800
H	−1.52193000	−1.17508000	2.49175500
O	1.10171700	−2.67854100	0.92156900
H	0.25464200	−2.50363700	1.37627000
Cl	2.78219100	0.15816700	−0.26997700
S	0.11542500	−1.36389600	−1.24920200
H	−2.16744700	2.55665800	0.51922500
H	2.09206600	2.55932400	0.91982900
H	−0.08923300	3.67027300	1.27934800
Cl	−2.62454300	0.11819100	−0.71833600
3,4-CTB			
O 2			
C	−1.14989300	0.54223800	−0.18056800
C	0.19877400	0.42671100	−0.46902100
C	0.81033300	−0.81599000	−0.44018100
C	0.06423200	−1.94128600	−0.11198500
C	−1.27966400	−1.81930000	0.17064100
C	−1.89859900	−0.58154800	0.14088100
H	2.84709900	0.29438800	−1.07123300
O	3.98947400	0.48187900	1.89305500
H	4.82970100	0.42559600	2.34083300
H	3.71667200	−0.41204800	1.68690400
O	3.18706400	1.60245700	−0.53719600
H	3.54832400	1.43287100	0.35539100
S	2.51310200	−1.04231100	−0.82523300
H	0.52800600	−2.91499700	−0.08331800
H	0.76515400	1.31392200	−0.70126300
H	−1.86425800	−2.68959500	0.42126900
Cl	−3.57330200	−0.47398300	0.50592300
Cl	−1.86574100	2.10264200	−0.22653000
3,5-CTB			
O 2			
C	−0.95185300	1.35635100	−0.04177300
C	0.28535000	0.86411800	−0.40845300

C	0.44323800	−0.50864500	−0.53860700
C	−0.62177700	−1.36685900	−0.29704100
C	−1.84315200	−0.83310900	0.06232000
C	−2.03267200	0.52864600	0.19792300
H	2.74142600	−0.07227400	−1.08033200
O	3.81138300	−0.71855600	1.84567100
H	4.57203400	−1.10960500	2.26776000
H	3.26237200	−1.43553100	1.52893000
O	3.49807400	0.94643600	−0.37391000
H	3.75485000	0.53653500	0.47590900
S	1.96715700	−1.23734300	−1.03267800
H	−0.50818400	−2.43475100	−0.39069500
H	1.11165400	1.53516400	−0.57421500
Cl	−1.15882200	3.06070900	0.12408400
H	−2.98930500	0.93135000	0.48287600
Cl	−3.16881500	−1.89714800	0.35781700

2,3,4-TCTB

0 2

C	−1.43722900	0.31694400	0.01769900
C	−0.11429500	0.60022600	−0.32054500
C	0.76357100	−0.42973300	−0.66065500
C	0.28854000	−1.73401900	−0.68057300
C	−1.02292600	−2.01890000	−0.37537000
C	−1.88494800	−0.99942900	−0.01854700
H	2.77303700	0.78733200	−0.19029800
O	4.50969200	−1.51352200	1.23526500
H	4.04271600	−1.82047600	0.45831900
H	4.48449100	−2.21886300	1.87684000
O	3.22185900	0.98886900	1.22374000
H	3.76870200	0.20906300	1.43906600
Cl	0.43206100	2.21965800	−0.31701500
S	2.42355500	−0.15588300	−1.15769300
H	−1.38664600	−3.03272200	−0.39702200
H	0.96330400	−2.53387600	−0.94027300
Cl	−2.50330100	1.57770900	0.45730500
Cl	−3.50706500	−1.39205100	0.37926000

2,3,5-TCTB

0 2

C	1.56750900	−0.82691300	0.17347600
C	0.24928000	−0.93670000	−0.25670700
C	−0.45869100	0.22413200	−0.57875000
C	0.16520500	1.45951900	−0.47887600
C	1.48014500	1.53898300	−0.07069200
C	2.18857000	0.40524700	0.26619500
H	−2.63977800	−0.72088100	−0.30151700
O	−4.13078700	1.73047100	1.13804100
H	−3.59273600	2.02371000	0.40313300

H	−4.08299600	2.40586700	1.80990200
O	−3.16874200	−0.91258700	1.07904600
H	−3.61904400	−0.07510700	1.30197300
S	−2.10062400	0.20129500	−1.20039300
H	3.21089800	0.46792000	0.59790700
H	−0.38037300	2.35642100	−0.72050600
Cl	2.24403700	3.07933400	0.04224700
Cl	2.47665300	−2.22023800	0.59443600
Cl	−0.48785800	−2.47129200	−0.39839900

2,3,6-TCTB

O 2			
C	−1.83748600	−0.74808100	0.19338100
C	−0.98683800	0.23936000	−0.28881600
C	0.36930500	−0.04034300	−0.51414600
C	0.81099800	−1.34058800	−0.27182800
C	−0.04111300	−2.32502700	0.18859300
C	−1.36343500	−2.02511100	0.42870500
H	1.06729500	2.19327000	−0.28164500
O	2.87231900	0.66674600	2.02445900
H	2.61025000	−0.05306800	2.59308900
H	3.15774800	0.27220300	1.20028600
O	1.20520400	2.73126800	1.08661800
H	1.77883900	2.10681200	1.57298100
Cl	−1.60659700	1.79705400	−0.61765800
S	1.47926300	1.16586200	−1.13567500
H	0.33559600	−3.31961400	0.36032300
H	−2.03931300	−2.77937500	0.79591000
Cl	2.46107200	−1.77280400	−0.54465300
Cl	−3.49608600	−0.42539100	0.49324700

2,4,5-TCTB

O 2			
C	1.04216600	−1.48005100	0.21077800
C	−0.26045500	−1.25540300	−0.18764700
C	−0.66933400	0.01570000	−0.58966600
C	0.27305300	1.03399800	−0.59541200
C	1.58413500	0.81104400	−0.22239100
C	1.97066000	−0.45595900	0.19271000
H	−2.99979000	−0.32529500	−0.20489900
O	−3.80120800	2.48674900	1.13383200
H	−3.23319700	2.60662600	0.37325400
H	−3.56883700	3.16016000	1.76815100
O	−3.51395600	−0.31062600	1.20282000
H	−3.73848700	0.62175200	1.38679900
Cl	−1.35378400	−2.57682100	−0.17490900
S	−2.28320900	0.38104600	−1.17017100
H	−0.01948900	2.02655800	−0.89706300
H	1.34258300	−2.46416700	0.52909700

Cl	3.57848600	−0.78561700	0.68652200
Cl	2.69462200	2.11847600	−0.26314500
2,4,6-TCTB			
O 2			
C	−1.56055200	1.24145000	0.06154800
C	−0.22152700	1.25689700	−0.27872800
C	0.49100200	0.08330200	−0.55048200
C	−0.23427300	−1.10867400	−0.48995000
C	−1.57695700	−1.14931600	−0.16991500
C	−2.22751200	0.03487700	0.11129700
H	2.59848200	0.94521300	0.01620400
O	2.04881400	−1.51118900	2.19981600
H	2.10022800	−2.04027500	1.40420400
H	1.17512400	−1.64770300	2.55849000
O	2.99500900	1.02326200	1.44545200
H	2.71251800	0.18129900	1.85488100
Cl	0.55298700	2.78528500	−0.36305900
S	2.18379500	0.08101600	−0.99929300
H	−2.10136000	−2.08910100	−0.13986600
Cl	0.53777000	−2.61788600	−0.82038000
H	−2.07364000	2.16423000	0.27210800
Cl	−3.89803500	0.00567700	0.52213900
3,4,5-TCTB			
O 2			
C	−0.64959300	1.14505700	−0.19014700
C	0.65248400	0.80346500	−0.49943400
C	1.00937800	−0.53224200	−0.58706800
C	0.05859900	−1.51463500	−0.35816600
C	−1.24174300	−1.16108000	−0.05786600
C	−1.62183600	0.17399300	0.03401300
H	3.25157400	0.20272600	−0.99224200
O	4.18360800	−0.32065500	2.00655800
H	4.94796000	−0.58136700	2.51401000
H	3.78712400	−1.11893400	1.65903400
O	3.81697900	1.30463900	−0.22794000
H	4.06152300	0.92380600	0.63913000
S	2.63414100	−1.05232800	−1.01223100
H	0.31477800	−2.56014400	−0.41463100
H	1.38139900	1.58204500	−0.65231600
Cl	−1.04383900	2.81270500	−0.08668200
Cl	−2.38198500	−2.41729100	0.20968900
Cl	−3.22941400	0.60634500	0.41615600
2,3,4,5-TeCTB			
O 2			
C	1.07706900	−0.97787600	0.02888400
C	−0.26767000	−0.97093300	−0.33071300

C	−0.90574200	0.23586300	−0.61795900
C	−0.17665200	1.41154500	−0.55934900
C	1.16122200	1.40534000	−0.22811400
C	1.80276800	0.21204600	0.07751400
H	−3.12867000	−0.54128500	−0.21442000
O	−4.42991900	1.96821200	1.28648500
H	−3.90395000	2.26157400	0.54324600
H	−4.38374900	2.64936400	1.95260000
O	−3.55769300	−0.70111800	1.20812300
H	−3.96816100	0.15190400	1.44831700
Cl	−1.13183700	−2.44096200	−0.42117500
S	−2.57666900	0.34410200	−1.14126700
Cl	3.45434600	0.20487200	0.50847400
Cl	1.85428100	−2.45330100	0.39825500
H	−0.65862500	2.35086100	−0.77334700
Cl	2.00113900	2.90052600	−0.18405800

2,3,4,6-TeCTB

O 2

C	−1.59262100	0.36030700	−0.01763300
C	−0.35709400	0.89798600	−0.37020600
C	0.75782200	0.08041000	−0.59582300
C	0.56982900	−1.29643700	−0.50166400
C	−0.65097000	−1.84536000	−0.17426700
C	−1.72692500	−1.02031700	0.07704900
H	2.35707800	1.69753600	−0.02898600
O	3.36545000	−0.61284200	2.24969600
H	2.82033900	−1.14696200	2.82255200
H	3.51384400	−1.12328400	1.45460900
O	2.43975600	1.90832800	1.44425300
H	2.79505700	1.08369900	1.83387900
Cl	−0.20510100	2.59008400	−0.53409400
S	2.32339900	0.73375300	−1.03715800
Cl	1.86908900	−2.39249000	−0.79958600
Cl	−2.93048700	1.37732700	0.27810900
Cl	−3.22381500	−1.73732200	0.50063800
H	−0.76726300	−2.91364900	−0.10999600

2,3,5,6-TeCTB

O 2

C	−1.32365800	−1.37766200	0.11730100
C	−1.26159700	−0.05401800	−0.30010400
C	−0.01925200	0.54380100	−0.54390000
C	1.13792900	−0.22721100	−0.39765900
C	1.05677000	−1.55303900	0.00518600
C	−0.17140200	−2.12132600	0.26789700
H	−0.79652600	2.72449900	−0.14921500
O	1.62728600	2.39105400	2.07034200
H	2.08675600	2.21317400	1.24959500

H	1.89928800	1.71814300	2.68934300
O	−0.95617900	3.14317200	1.25050000
H	−0.10890200	2.94640200	1.69657600
Cl	−2.70599000	0.82527600	−0.52978700
S	0.11841800	2.20933600	−1.07418100
H	−0.23207000	−3.14852200	0.58454700
Cl	2.46073800	−2.51891200	0.19759000
Cl	2.67881000	0.46266900	−0.71849500
Cl	−2.82325300	−2.14198400	0.44227900
PCTB			
O 2			
C	−1.08323300	1.23731500	−0.03723100
C	0.26836700	1.23857400	−0.36323600
C	0.95937400	0.04114900	−0.56895800
C	0.24468300	−1.15381400	−0.46923600
C	−1.10908000	−1.16637300	−0.15908300
C	−1.77421600	0.03397200	0.06402000
H	3.05621400	0.97628500	−0.07956600
O	2.59607600	−1.32679500	2.39899200
H	1.83360600	−1.55975000	2.92315500
H	2.54672200	−1.86651100	1.60957200
O	3.60682700	1.04181500	1.28225000
H	3.16545400	0.32006500	1.77338500
Cl	1.08061600	2.73151000	−0.52657500
S	2.65675200	0.00102100	−1.00010400
Cl	1.05356300	−2.64590800	−0.72807900
Cl	−1.90775100	2.70883600	0.22353100
Cl	−1.95411200	−2.64594100	−0.03995000
Cl	−3.43517600	0.02847200	0.45504500