

## Supplementary Information

### Solvent Effects on the ESIPT Mechanism of 3-(Benzo[d]thiazol-2-yl)Triphenylen-2-ol: A DFT Investigation

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#### (a)HTpT-enol form with B3LYP/def2-TZVP in Toluene

N	-3.29708300	-1.12712200	0.00003600
C	-4.57693800	-0.61696900	0.00013600
C	-4.64068900	0.79217600	0.00022500
S	-3.02973100	1.44777600	0.00018600
C	-2.38403900	-0.19330100	0.00003100
C	-0.96094200	-0.47230100	-0.00008400
C	-0.49527100	-1.81418200	-0.00043500
O	-1.33060800	-2.86599000	-0.00067800
H	-2.25831700	-2.51701500	-0.00039700
C	-5.85941000	1.46194100	0.00033400
H	-5.90315400	2.54242500	0.00041300
C	-7.02038800	0.70345700	0.00034500
H	-7.98025800	1.20239700	0.00043000
C	-6.96816600	-0.69605200	0.00025400
H	-7.89004800	-1.26208700	0.00026700
C	-5.75608100	-1.36419300	0.00015100
H	-5.70559900	-2.44454900	0.00008200
C	0.86624700	-2.05389700	-0.00050800
H	1.16797300	-3.08931200	-0.00074500
C	1.81021100	-1.02126100	-0.00026000
C	3.24310700	-1.30026800	-0.00012600
C	3.73082100	-2.62030300	-0.00007300
H	3.03989300	-3.44894800	-0.00025200
C	5.08025500	-2.89491600	0.00025700
H	5.42367100	-3.92097600	0.00029300
C	5.99708000	-1.84241800	0.00061900
H	7.06042100	-2.04344200	0.00098600
C	5.54431400	-0.54121600	0.00054100
H	6.27485800	0.25270200	0.00094300
C	4.17150000	-0.23275000	0.00009100
C	3.70116200	1.15158100	-0.00011500
C	4.60030900	2.23379800	-0.00045200
H	5.66357000	2.05058700	-0.00077800
C	4.16477600	3.54079900	-0.00051100
H	4.88279500	4.35029400	-0.00079100
C	2.79540100	3.81061200	-0.00024400
H	2.43862400	4.83227700	-0.00026000
C	1.89451100	2.76839800	-0.00003200
H	0.84156900	3.00636600	0.00006900
C	2.31426900	1.42539100	-0.00000700
C	1.35648600	0.32315600	-0.00000600
C	-0.01999900	0.54913800	0.00012400
H	-0.38701000	1.56412100	0.00040900

**(b)HTpT-keto form with B3LYP/def2-TZVP in Toluene**

N	3.32852400	-1.09154400	-0.00087000
C	4.61317800	-0.63915700	-0.00065800
C	4.67525100	0.76783000	0.00047600
S	3.05949200	1.45216900	0.00148800
C	2.35847500	-0.14472200	0.00035400
C	0.96169500	-0.43721700	0.00020700
C	0.50991300	-1.82985500	0.00042100
O	1.33133000	-2.78867300	0.00086900
H	2.98689900	-2.06331400	-0.00102100
C	5.88955200	1.43416600	0.00077100
H	5.93002700	2.51736800	0.00164200
C	7.05784800	0.67516500	-0.00004700
H	8.01923600	1.17562900	0.00016000
C	6.99981400	-0.72053200	-0.00111600
H	7.92153400	-1.29207400	-0.00169100
C	5.78835900	-1.39521600	-0.00142500
H	5.74453800	-2.47830100	-0.00221000
C	-0.89043300	-2.04498100	0.00018200
H	-1.18170500	-3.08744600	0.00040000
C	-1.85153500	-1.02108500	-0.00004900
C	-3.27137300	-1.30282900	-0.00012200
C	-3.75843200	-2.62618700	-0.00028700
H	-3.06377900	-3.45598000	-0.00044800
C	-5.10712300	-2.89862900	-0.00030500
H	-5.45004700	-3.92778200	-0.00046400
C	-6.03177700	-1.84729500	-0.00013300
H	-7.09648000	-2.05361800	-0.00013400
C	-5.58278800	-0.54582900	-0.00000100
H	-6.31663200	0.24983900	0.00007400
C	-4.20897700	-0.23663100	-0.00000700
C	-3.73722300	1.13309100	-0.00000300
C	-4.62471200	2.22229500	0.00025900
H	-5.69250000	2.04743800	0.00063900
C	-4.17772400	3.52533800	0.00004600
H	-4.89219800	4.34131100	0.00026600
C	-2.80086500	3.79320900	-0.00049100
H	-2.44373900	4.81719200	-0.00076200
C	-1.90546100	2.75472300	-0.00065900
H	-0.84967800	2.99021700	-0.00112300
C	-2.33272600	1.40050300	-0.00031600
C	-1.39952300	0.31808800	-0.00018400
C	0.01368500	0.55759200	-0.00017200
H	0.35975900	1.58399800	-0.00043900