Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for "Theoretical study of the mechanism of the solvent dependency of ESIPT in HBT"

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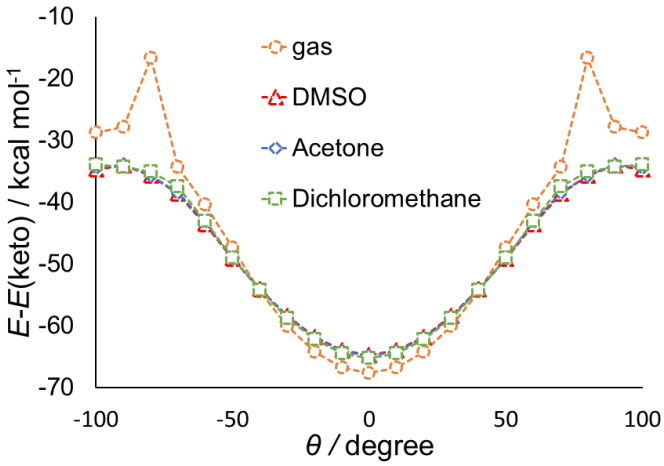

Figure S1. Calculated S_0 energy profiles along C=C twisting at the ωB97X-D/6-31G(d,p) level.

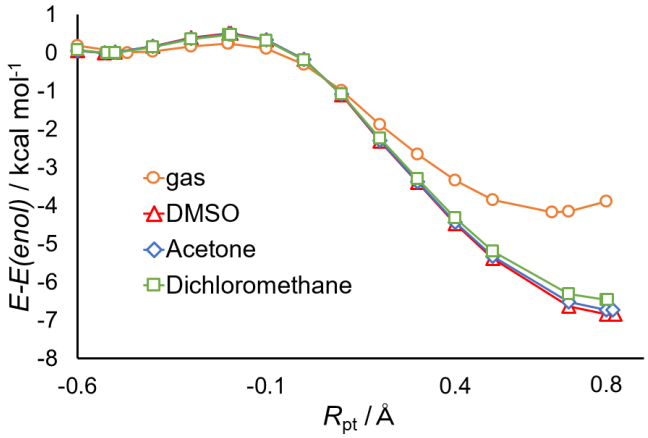

Figure S2. Calculated S_1 energy profiles along ESIPT in the gas phase and in solutions at the M11/6-31G(d,p) level.

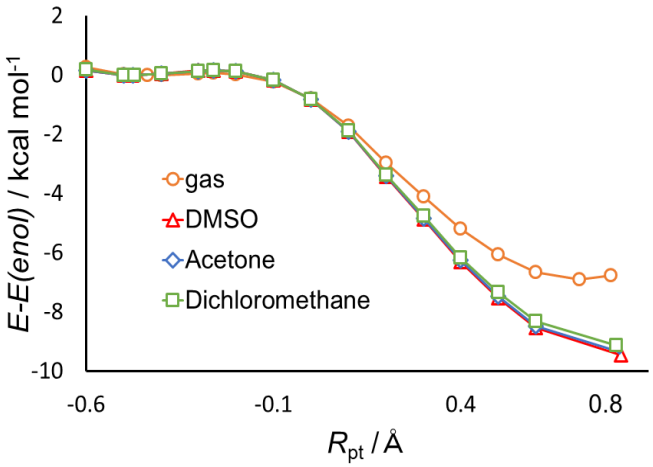

Figure S3. Calculated S_1 energy profiles along ESIPT in the gas phase and in solutions at the EOM-CCSD/6-31G(d,p) level.

Table S1. Calculated activation energies of ESIPT ΔE_{pt} (in kcal/mol).

Calculation level	gas	DMSO	Acetone	CH_2Cl_2
ωB97X-D/6-31G(d)	0.53	1.16	1.18	1.13
M11/6-31G(d,p)	0.24	0.51	0.50	0.47
EOM-CCSD/6-31G(d,p)	0.08	0.17	0.17	0.16

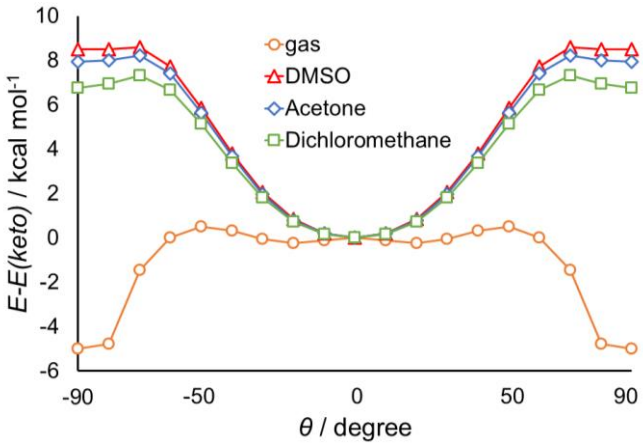

Figure S4. Calculated S_1 energy profiles along C=C twisting at the M11/6-31G(d,p) level.

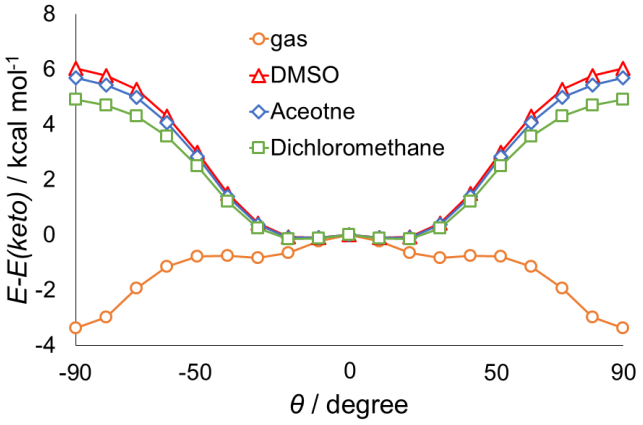

Figure S5. Calculated S_1 energy profiles along C=C twisting at the EOM-CCSD/6-31G(d,p) level.

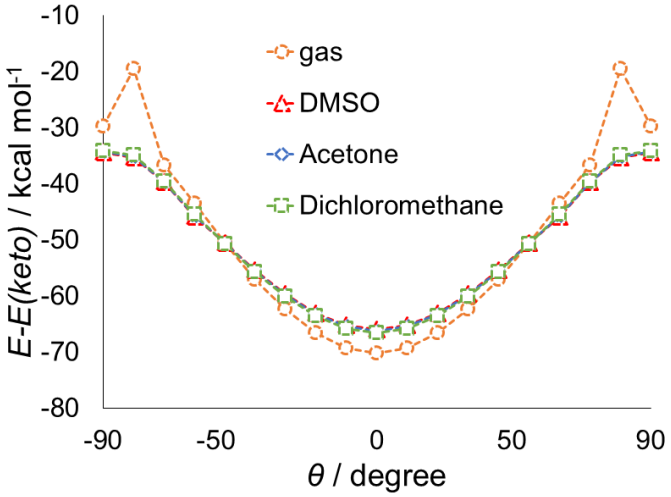

Figure S6. Calculated S_0 energy profiles along C=C twisting at the M11/6-31G(d,p) level.

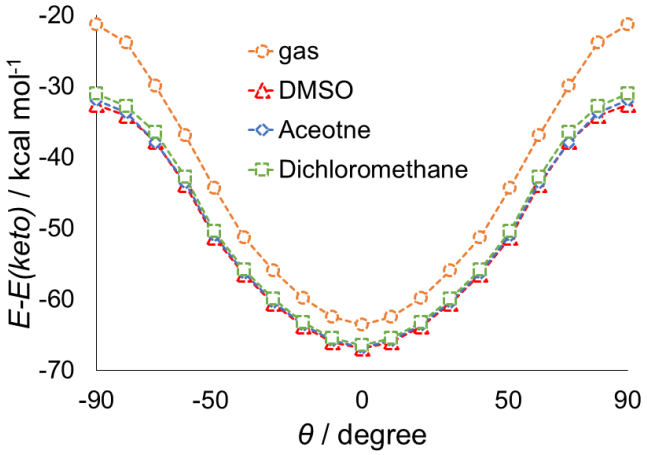

Figure S7. Calculated S_0 energy profiles along C=C twisting at the EOM-CCSD/6-31G(d,p) level.

Table S2. Calculated activation energies of C=C twisting ΔE_{tw} (in kcal/mol).

Calculation level	gas	DMSO	Acetone	CH_2Cl_2
ωB97X-D/6-31G(d)	No barrier	4.56	4.21	3.45
M11/6-31G(d,p)	0.50	8.59	8.20	7.31
EOM-CCSD/6-31G(d,p)	No barrier	6.04	5.70	4.90

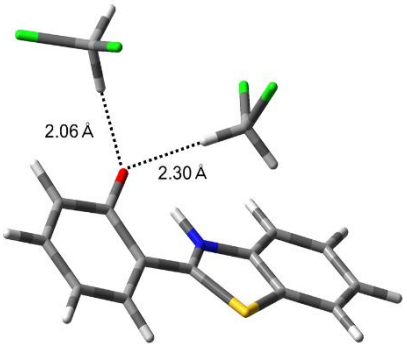

Figure S8. Optimized geometry of complex between the keto HBT and two CH_2Cl_2 molecules at the PCM-ωB97X-D/6-31G(d,p) level.

Table S3. Calculated interaction energies E_{int} between the keto HBT and one or two CH_2Cl_2 molecules in the S_1 state and $S_1 \rightarrow S_0$ transition energies $\Delta E_{1\rightarrow 0}$ of the complexes (in kcal/mol).

	one CH_2Cl_2		two CH_2Cl_2	
Calculation level	E_{int}	$\Delta E_{1\rightarrow 0}$	E_{int}	$\Delta E_{1\rightarrow 0}$
ωB97X-D/6-31G(d,p)	−18.35	22.32	−27.43	20.66
ωB97X-D/6-311G(d,p)	−17.56	24.71	−29.03	23.58
PCM-ωB97X-D/6-31G(d,p)	−7.04	63.75	−7.46	62.74
PCM-ωB97X-D/6-311G(d,p)	−7.46	63.73	−12.34	63.03