Supporting Information

A (TD-)DFT Study on Photo-NHC Catalysis: Photoenolization/Diels-Alder Reaction of Acid Fluorides Catalyzed by *N*-Heterocyclic Carbenes

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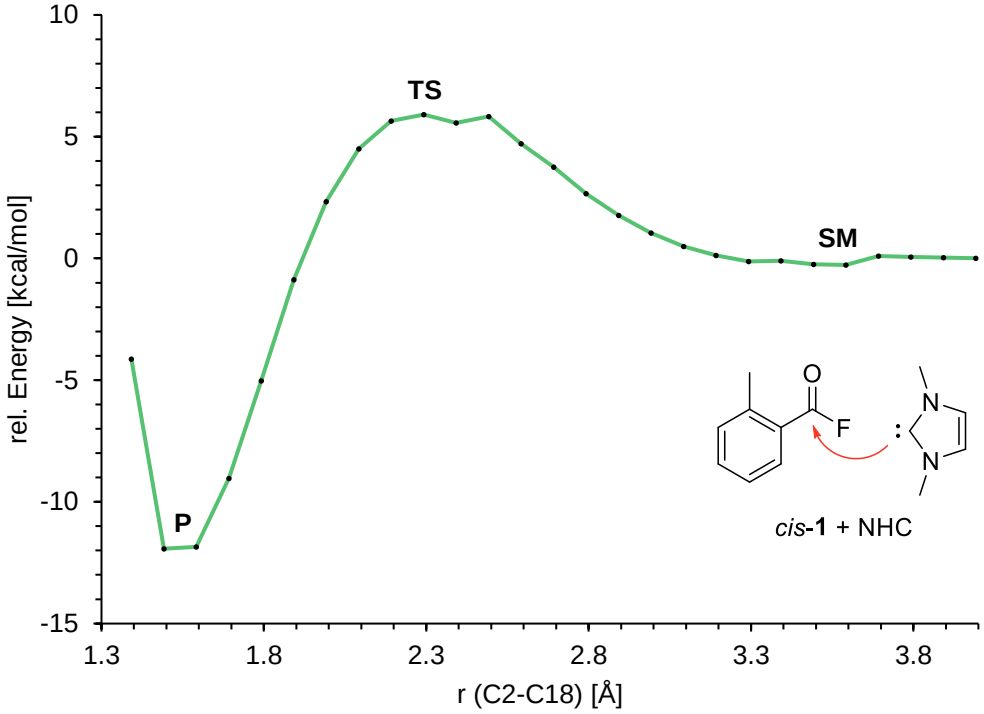
1. (TD-)DFT Calculations

1.1 Formation of **A** from **1** and NHC



Species	r (C2-C18) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.59	–788.568402	0.00	0
TS	2.28	–788.548651	12.4	1 (–184 cm^{-1})
P	1.54	–788.572122	–2.33	0

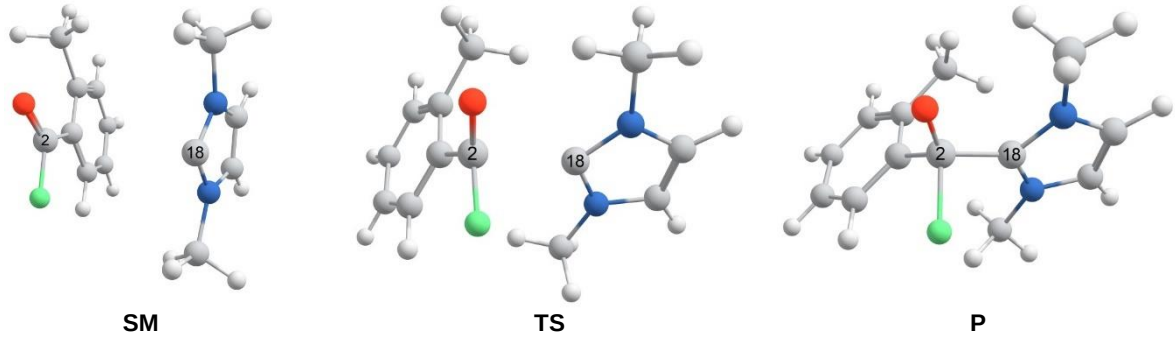
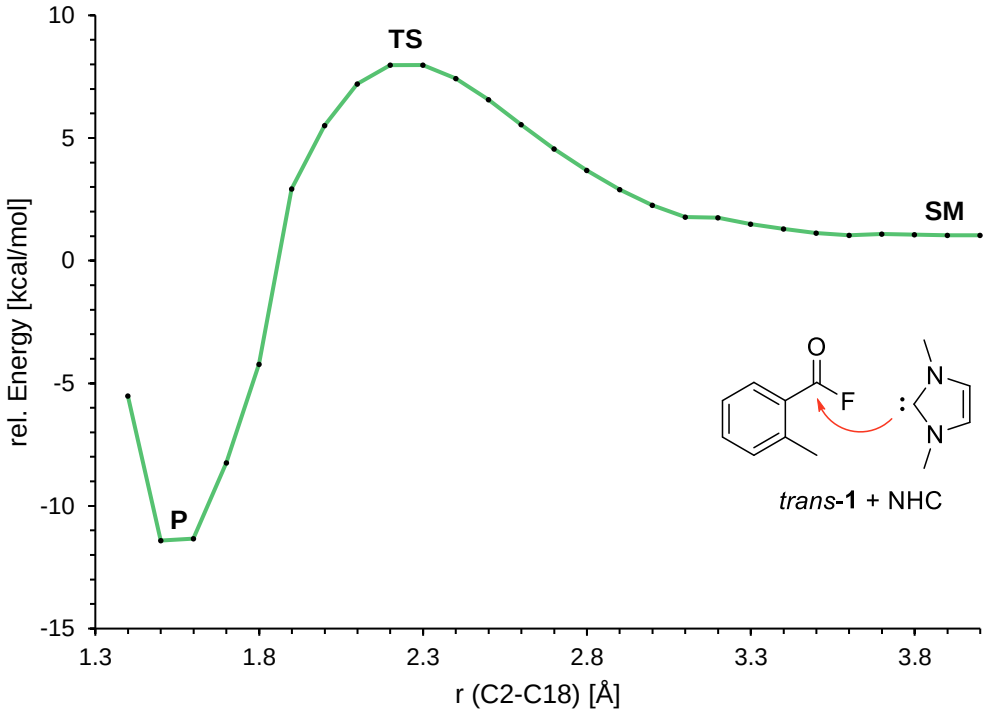


Figure S1. Relaxed PES scan of the nucleophilic addition of NHC on *cis*-**1** along the C2-C18 coordinate and the Gibbs free energies (298 K) and geometries of the involved species (CAM-B3LYP).



Species	r (C2-C18) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.92	–788.567354	0.00	0
TS	2.27	–788.547667	13.0	1 (–186 cm^{-1})
P	1.54	–788.571550	–1.98	0

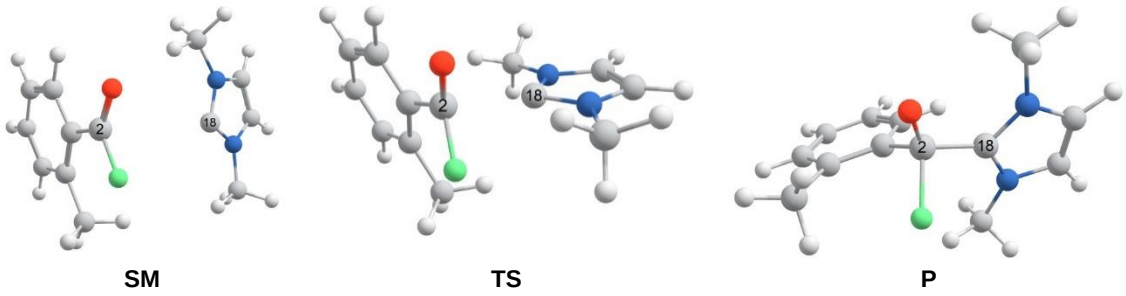


Figure S2. Relaxed PES scan of the nucleophilic addition of the NHC on *trans*-**1** along the C2-C18 coordinate and the Gibbs free energies (298 K) and geometries of the involved species (CAM-B3LYP).

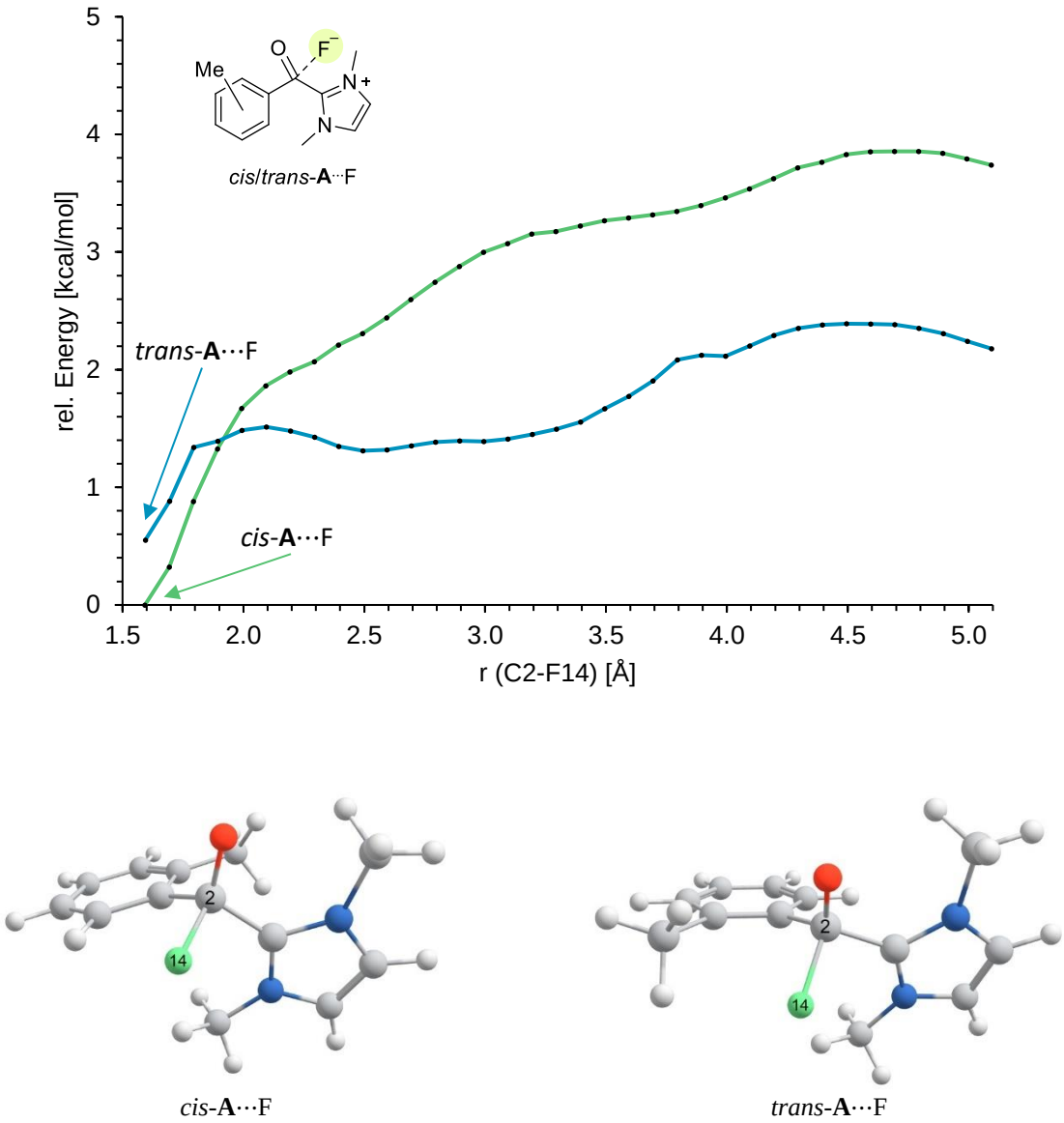
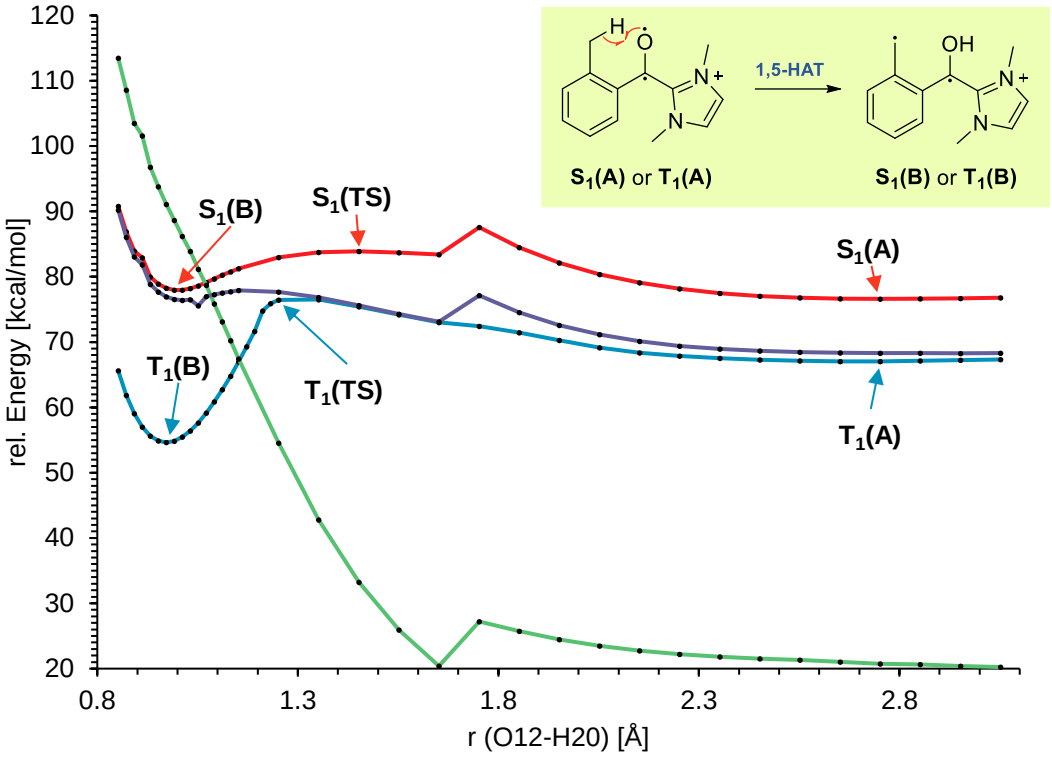


Figure S3. Relaxed PES scans for the fluoride elimination of *cis*-**A**···F (green) and *trans*-**A**···F (blue) along the C2-F14 coordinate (CAM-B3LYP).

1.2 Photoenolization of **A**



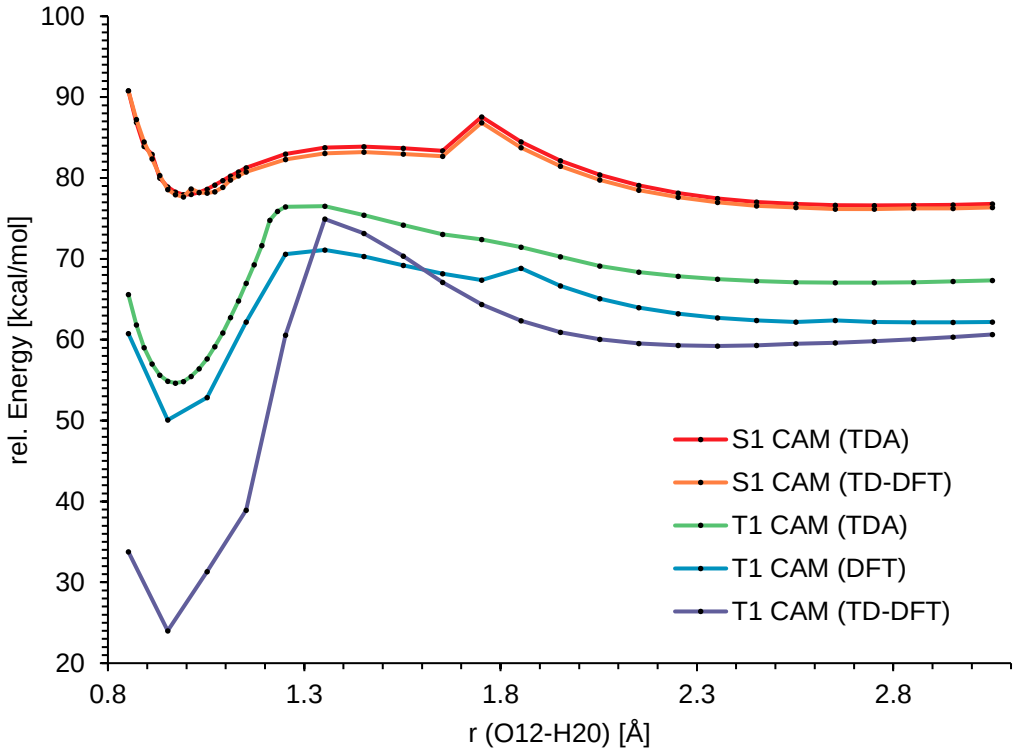
Species	r (O12-H20) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
A	2.65	–688.562228	0.00	0
S_1(A)	2.72	–688.442785	75.0	0
S_1(TS)	1.43	–688.430696	82.5	1 (–494 cm^{-1})
S_1(B)	1.00	–688.430059	82.9	0
T_1(A)	2.72	–688.458081	65.4	0
T_1(TS)	1.29	–688.443702	74.4	1 (–1402 cm^{-1})
T_1(B)	0.97	–688.477034	53.5	0

Calculated SOCMEs of selected S_1 geometries

r (O12-H20) [Å]	Root		<T|H_{SO}|S> (Re, Im) [cm^{-1}] Z	X	Y	$\sqrt{Z^2+X^2+Y^2}$
2.72, **S_1(A)**	T_1	S_0	(0.00, 29.2)	(0.00, 19.8)	(-0.00, 25.7)	43.6
	T_1	S_1	(0.00, 1.39)	(0.00, -0.15)	(-0.00, -0.26)	1.4
1.43, **S_1(TS)**	T_1	S_0	(0.00, -35.2)	(0.00, 4.79)	(-0.00, 0.76)	36
	T_1	S_1	(0.00, -1.99)	(0.00, 0.24)	(-0.00, -0.26)	2.0
1.00, **S_1(B)**	T_1	S_0 (former S_1)	(0.00, 8.61)	(0.00, -6.41)	(-0.00, -1.75)	10.9
	T_1	S_1 (former S_0)	(0.00, -0.17)	(0.00, 0.24)	(-0.00, -0.29)	0.41

Figure S4: Relaxed PES scans of the photoenolization of **A** along the O12-H20 coordinate. Shown are the S_1 (red) and T_1 (blue) surfaces and the singlet ground state (green) and triplet energies (violet) of the S_1 geometries as well as the calculated Gibbs Free energies (298 K) and SOCMEs ((TDA-)CAM-B3LYP).

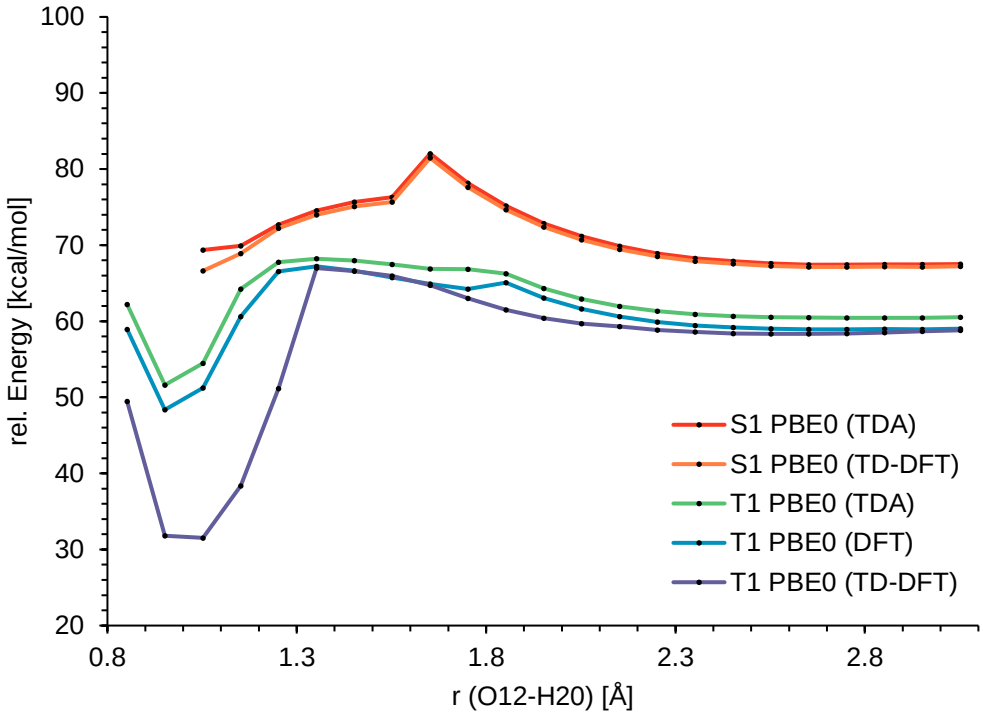
Comparison of frameworks for the calculation of excited PES with CAM-B3LYP



Species	r (O12-H20) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
A [DFT]	2.65	–688.424773	0.00	0
S_1(A) [TDA]	2.72	–688.442785	75.0	0
S_1(TS) [TDA]	1.43	–688.430696	82.5	1 (–494 cm^{-1})
S_1(B) [TDA]	1.00	–688.430059	82.9	0
T_1(A) [TDA]	2.72	–688.458081	65.4	0
T_1(TS) [TDA]	1.29	–688.443702	74.4	1 (–1402 cm^{-1})
T_1(B) [TDA]	0.97	–688.477034	53.5	0
T_1(A) [DFT]	2.63	–688.331457	57.3	0
T_1(TS) [DFT]	1.32	–688.319377	66.1	1 (– 1197 cm^{-1})
T_1(B) [DFT]	0.97	–688.349288	47.4	0

Figure S5: Relaxed PES scans of the photoenolization of **A** along the O12-H20 coordinate with the CAM-B3LYP functional. Shown are the S_1 (red, orange) and T_1 (blue, indigo, violet) surfaces as well as the calculated Gibbs Free energies (298 K) of the involved species.

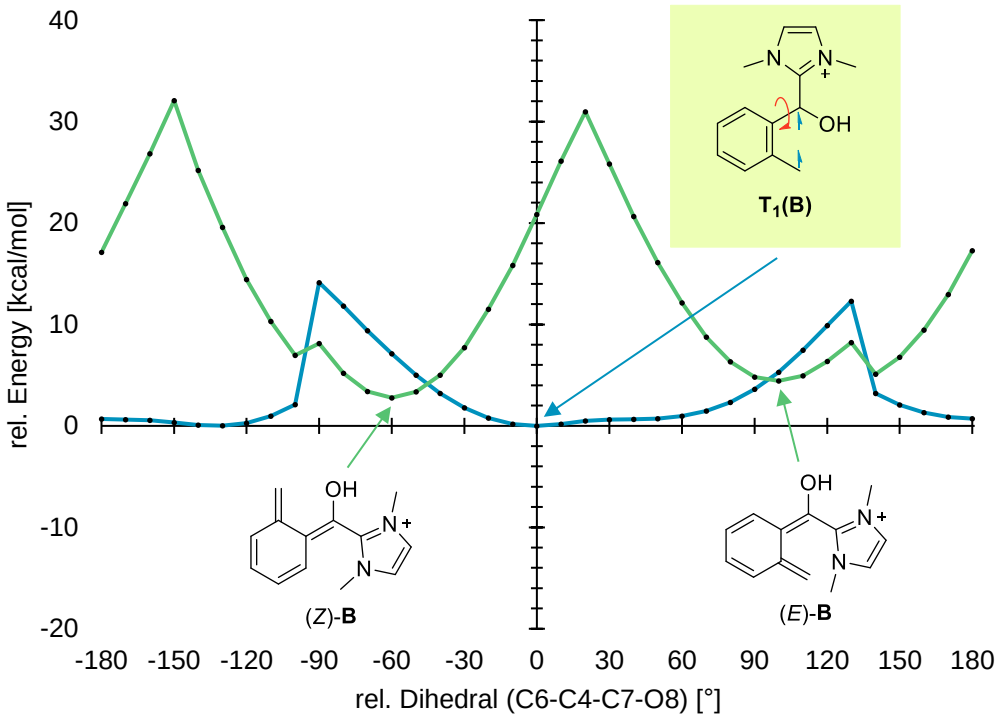
Comparison of frameworks for the calculation of excited PES with the PBE0 functional



Species	r (O12-H20) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
A [DFT]	2.65	–687.993354	0.00	0
S_1(A) [TDA]	2.69	–687.889094	65.4	0
S_1(TS) [TDA]		*not determined*		
S_1(B) [TDA]		*not determined*		
T_1(A) [TDA]	2.85	–687.900839	58.1	0
T_1(TS) [TDA]	1.36	–687.889923	64.9	1 (–757 cm^{-1})
T_1(B) [TDA]	0.97	–687.913357	50.2	0
T_1(A) [DFT]	2.75	–687.905183	55.3	0
T_1(TS) [DFT]	1.34	–687.893364	62.7	1 (–1038 cm^{-1})
T_1(B) [DFT]	0.97	–687.920313	45.8	0

Figure S6: Relaxed PES scans of the photoenolization of **A** along the O12-H20 coordinate with the PBE0 functional. Shown are the excited singlet (red, orange) and triplet surfaces (blue, indigo, violet) as well as the calculated Gibbs Free energies (298 K) of most of the involved species.

1.3 Triplet rotation of **T_1(B)**



Species	absolute Dihedral (C6-C4-C7-O8) [°]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
A	24	–688.562228	0.00	0
S_1(B)	11	–688.430059	82.9	0
T_1(B)	60	–688.477034	53.5	0
(*Z*)-**B**	5	–688.503627	36.8	0
(*E*)-**B**	–167	–688.500747	38.6	0

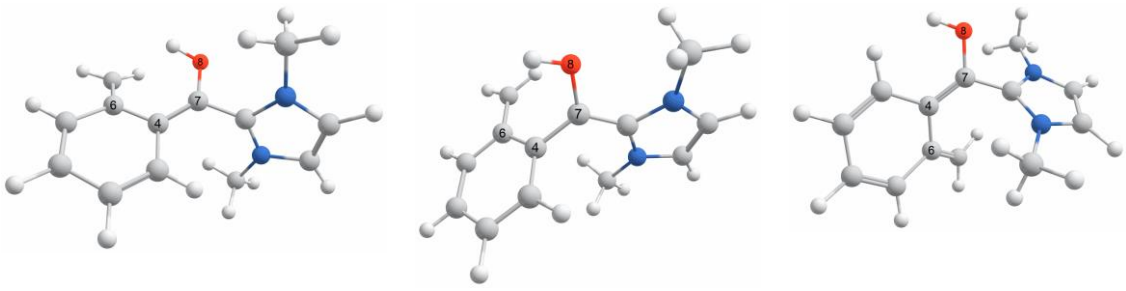


Figure S7. Relaxed PES scan of the dihedral (C6-C4-C7-C8) representing rotation around the C-C bond in **T_1(B)** (relative dihedral set to 0° for the optimized **T_1(B)** geometry). Shown are the T_1 surface (blue) and the corresponding "hot" S_0 surface (green). The *o*-QDMs (*Z*)-**B** and (*E*)-**B** were obtained after optimization in the respective minimum well of the singlet surface ((TDA-)CAM-B3LYP).

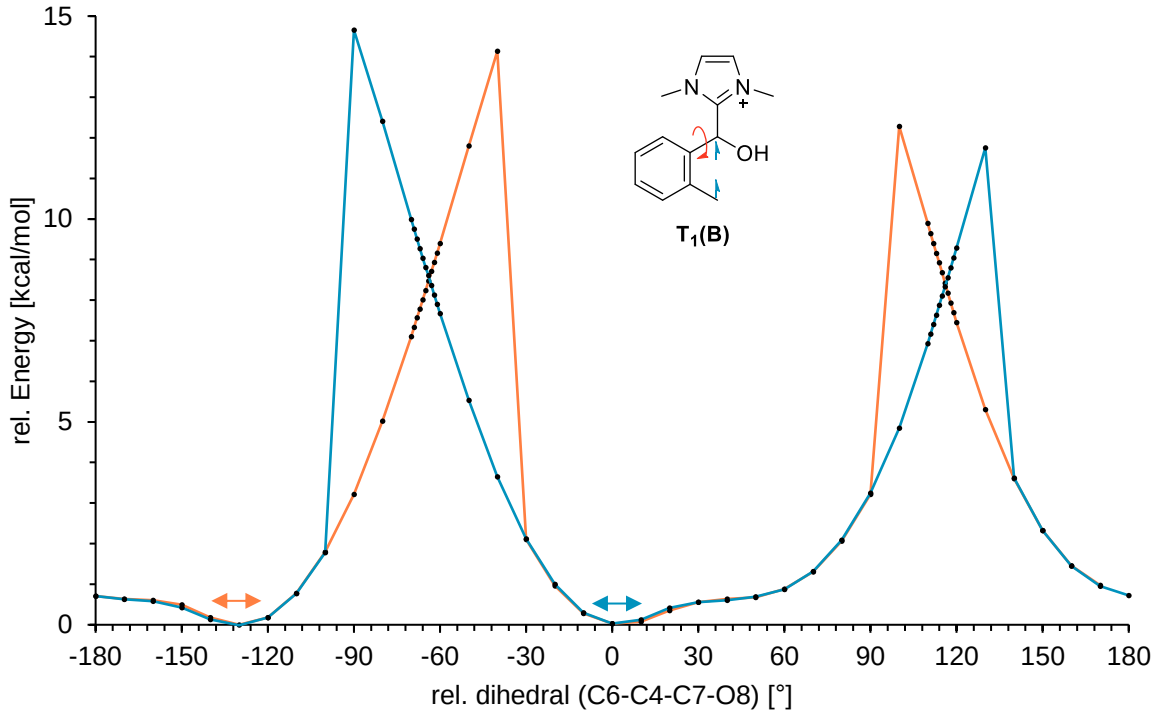
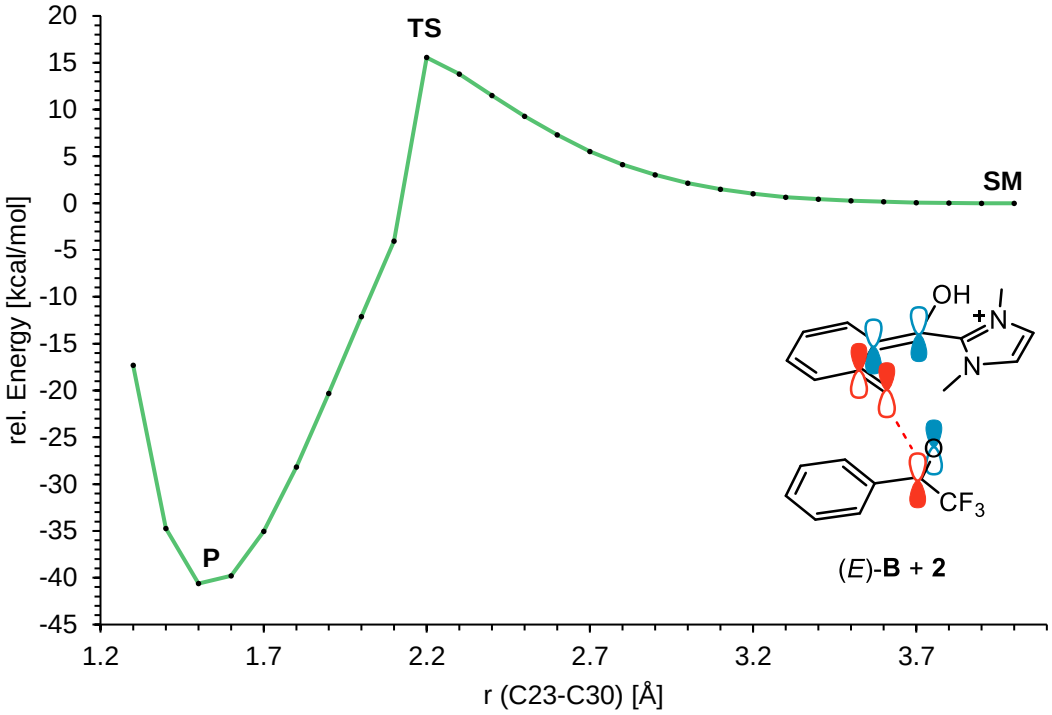


Figure S8. Relaxed PES scans of the dihedral (C6-C4-C7-C8) representing rotation around the C-C bond in **T_1(B)** (relative dihedral set to 0° for the optimized **T_1(B)** geometry). Shown are the T_1 surfaces (orange and blue) obtained from the two minima of **T_1(B)** (double arrows) as starting point.

1.4 Cycloaddition of (*E*)-**B** with **2**



Species	r (C23-C30) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.96	–1370.959441	0.00	0
TS	2.20	–1370.924717	21.8	1 (–287 cm^{-1})
P	1.54	–1371.004072	–28.1	0

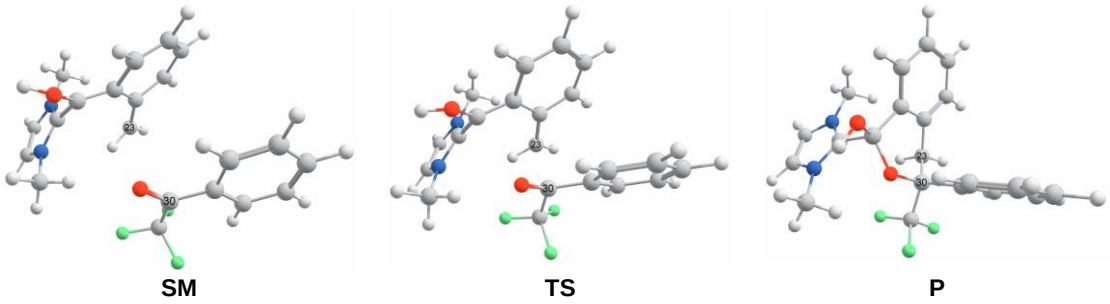
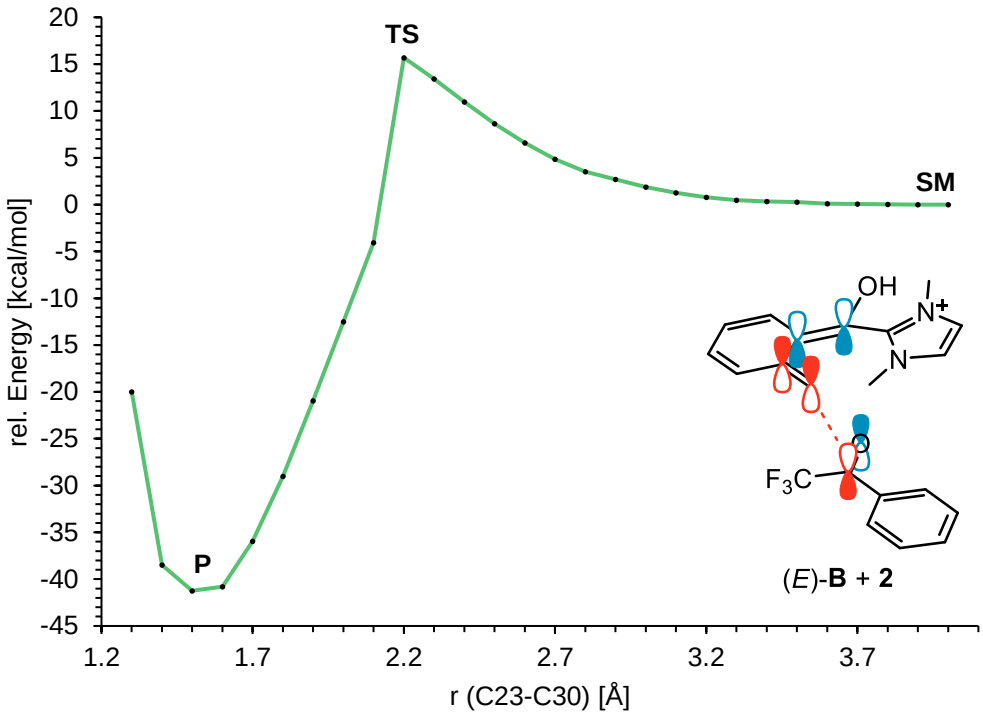


Figure S9. Relaxed PES scan of the (*E*)-**B** *endo* cycloaddition with ketone **2** along the C23-C30 coordinate and the Gibbs free energies (298 K) and geometries of the involved species (CAM-B3LYP).



Species	r (C23-C30) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.96	–1370.957778	1.04	0
TS	2.16	–-1370.919725	24.9	1 (–223 cm^{-1})
P	1.53	–-1371.005696	–29.0	0

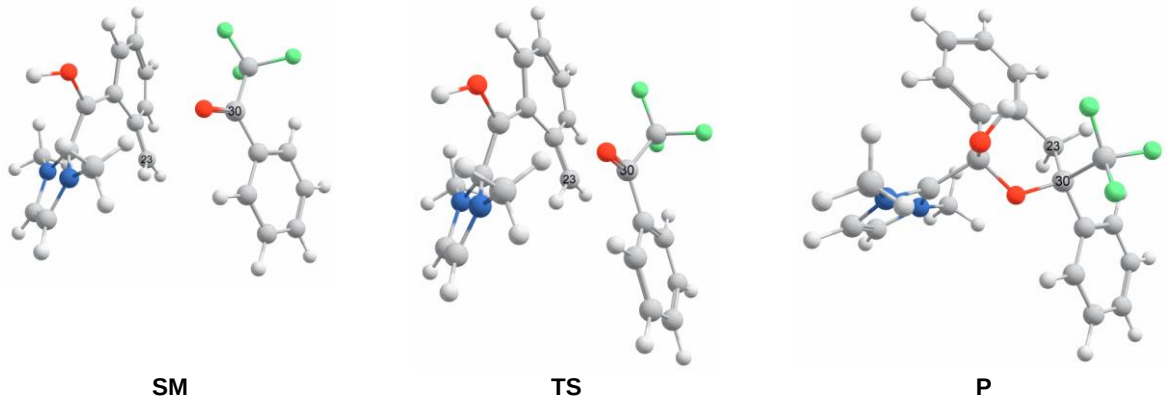
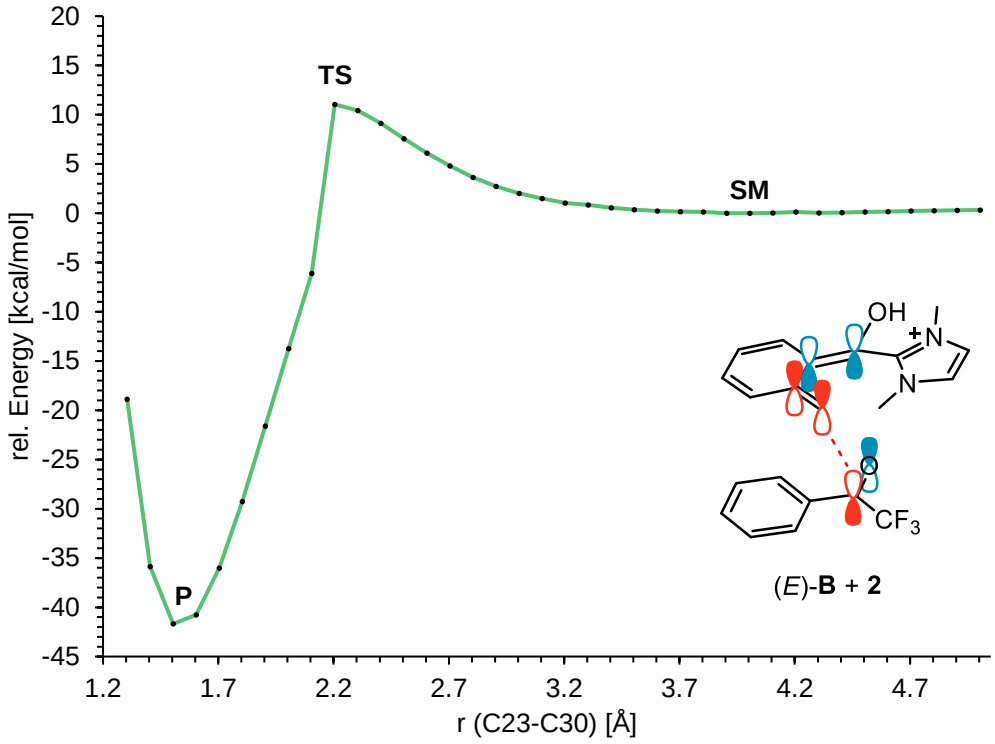


Figure S10. Relaxed PES scan of the (E)-**B** *exo* cycloaddition with ketone **2** along the C23-C30 coordinate and the Gibbs free energies (298 K) and geometries of the involved species (CAM-B3LYP).



Species	r (C23-C30) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.96	–1370.959298	0.25	0
TS	2.17	–1370.922073	23.6	1 (–386 cm^{-1})
P	1.54	–1371.004250	–28.0	0

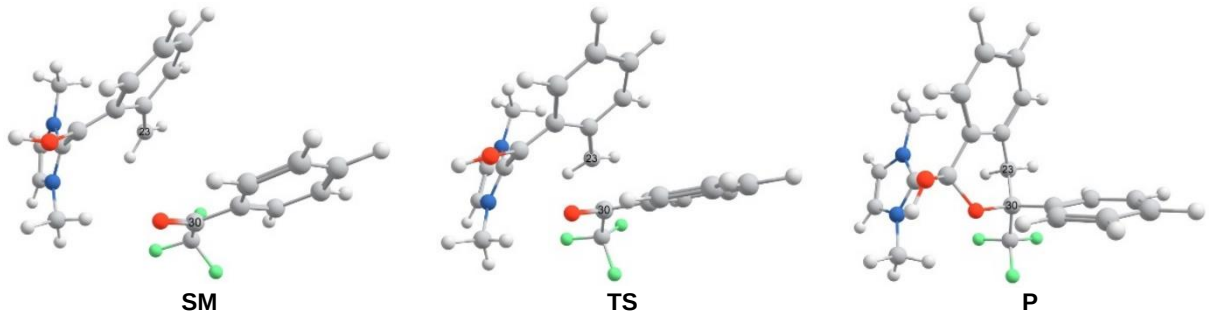
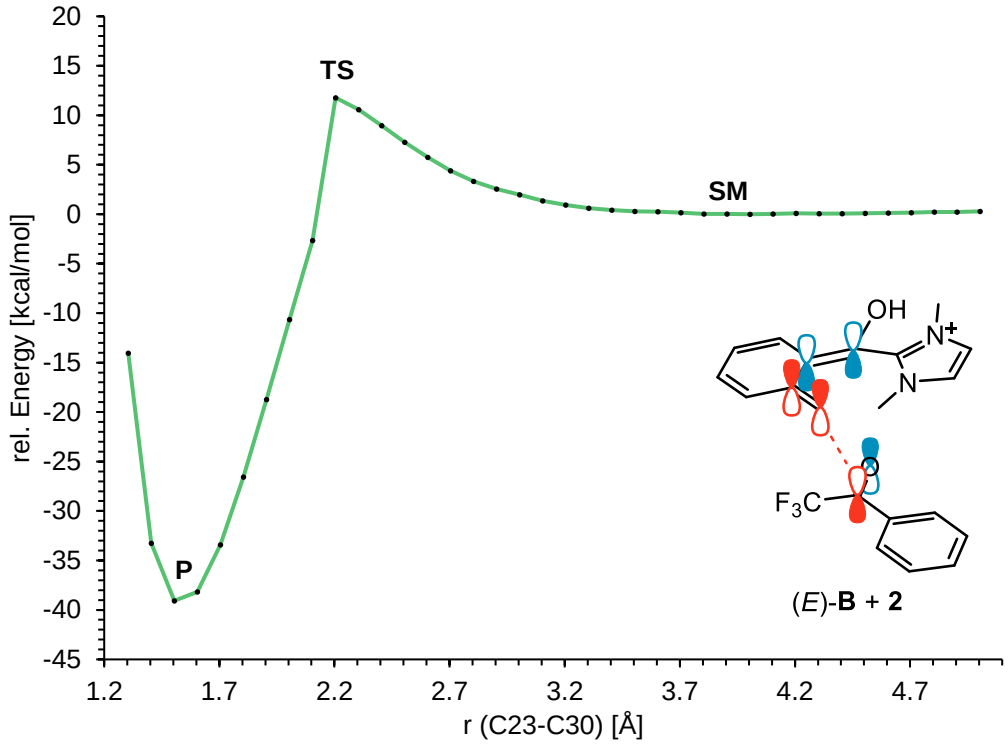


Figure S11. Relaxed PES scan of the (*E*)-**B** *endo* cycloaddition with ketone **2** along the C23-C30 coordinate and the Gibbs free energies (298 K) and geometries of the involved species (PBE0).



Species	r (C23-C30) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.98	–1370.959703	0.00	0
TS	2.12	–1370.919551	25.2	1 (–407 cm^{-1})
P	1.54	–1370.999640	–25.1	0

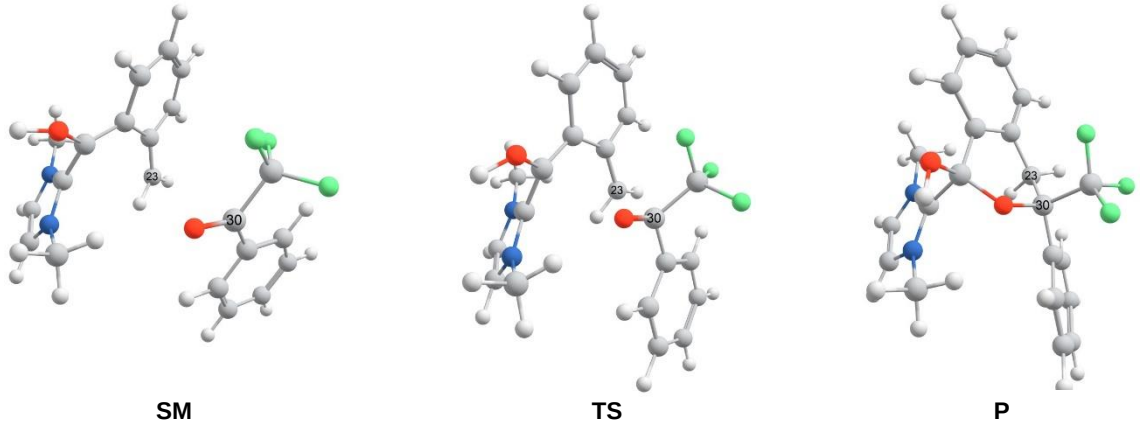
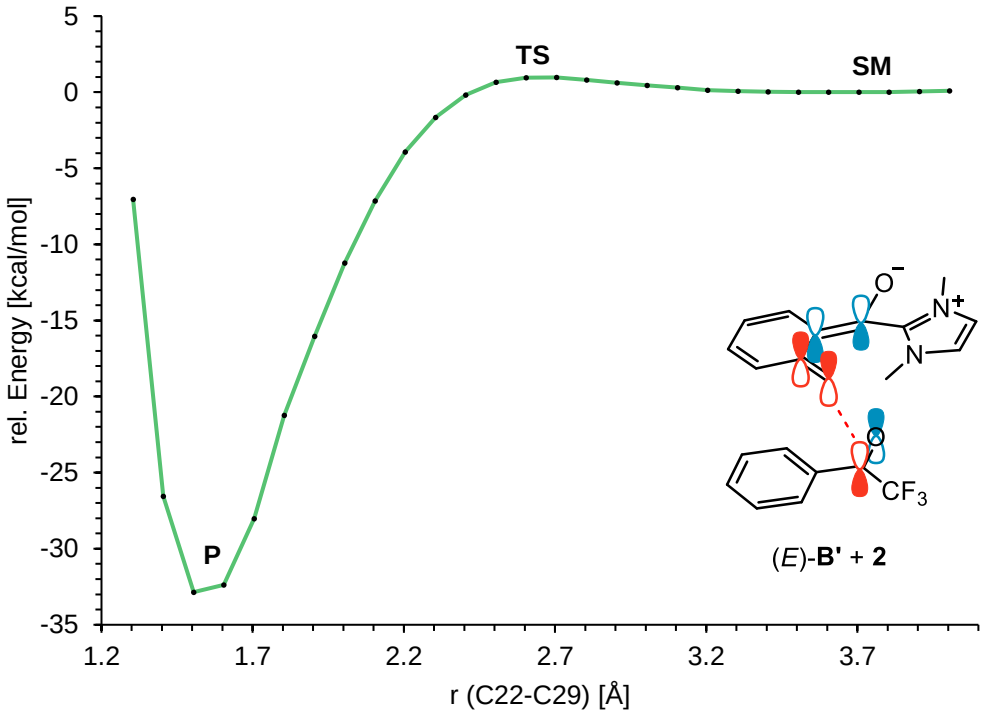


Figure S12. Relaxed PES scan of the (E)-**B** *exo* cycloaddition with ketone **2** along the C23-C30 coordinate and the Gibbs free energies (298 K) and geometries of the involved species (PBE0).

1.5 Cycloaddition of (*E*)-**B′** with **2**



Species	r (C22-C29) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.69	–1370.527297	1.15	0
TS	2.62	–1370.520784	5.24	1 (–101 cm^{-1})
P	1.54	–1370.564028	–21.9	0

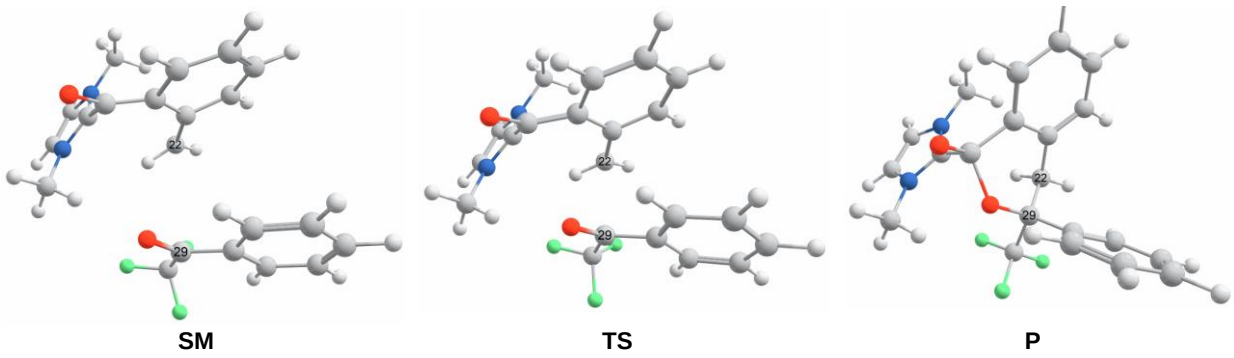
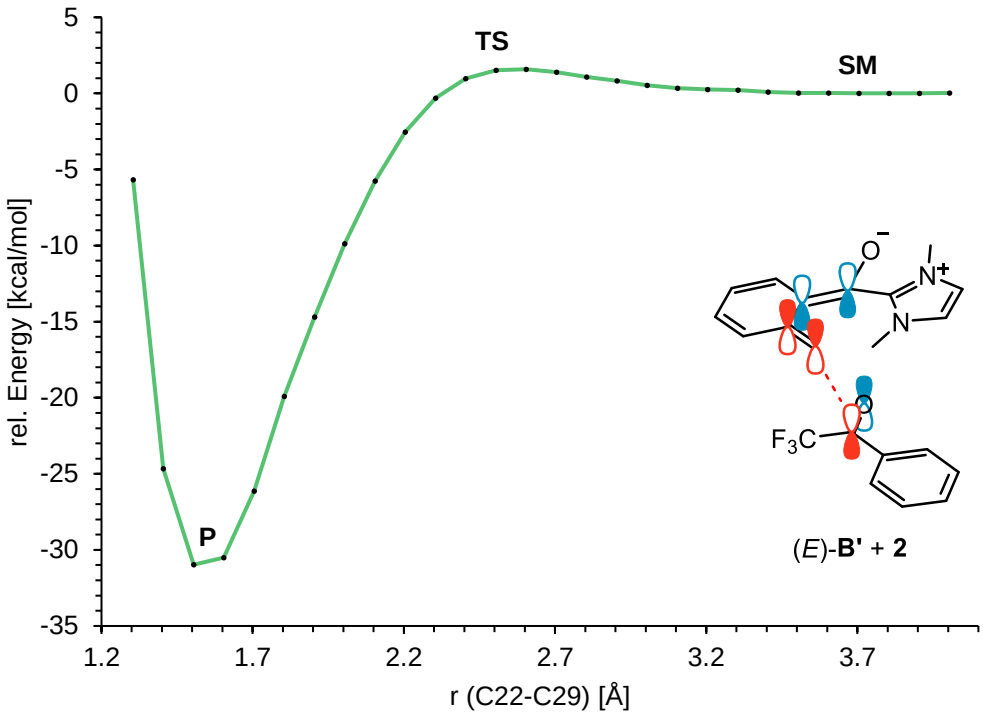


Figure S13. Relaxed PES scan of the (E)-**B′** *endo* cycloaddition with ketone **2** along the C22-C29 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.



Species	r (C22-C29) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.72	–1370.529132	0.00	0
TS	2.56	–1370.519400	6.11	1 (–133 cm^{-1})
P	1.54	–1370.560522	–19.7	0

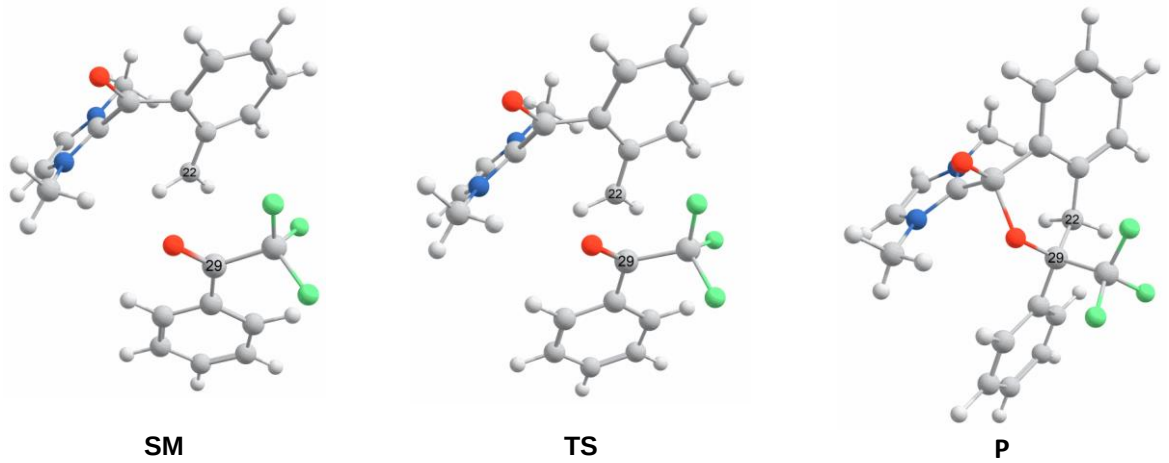
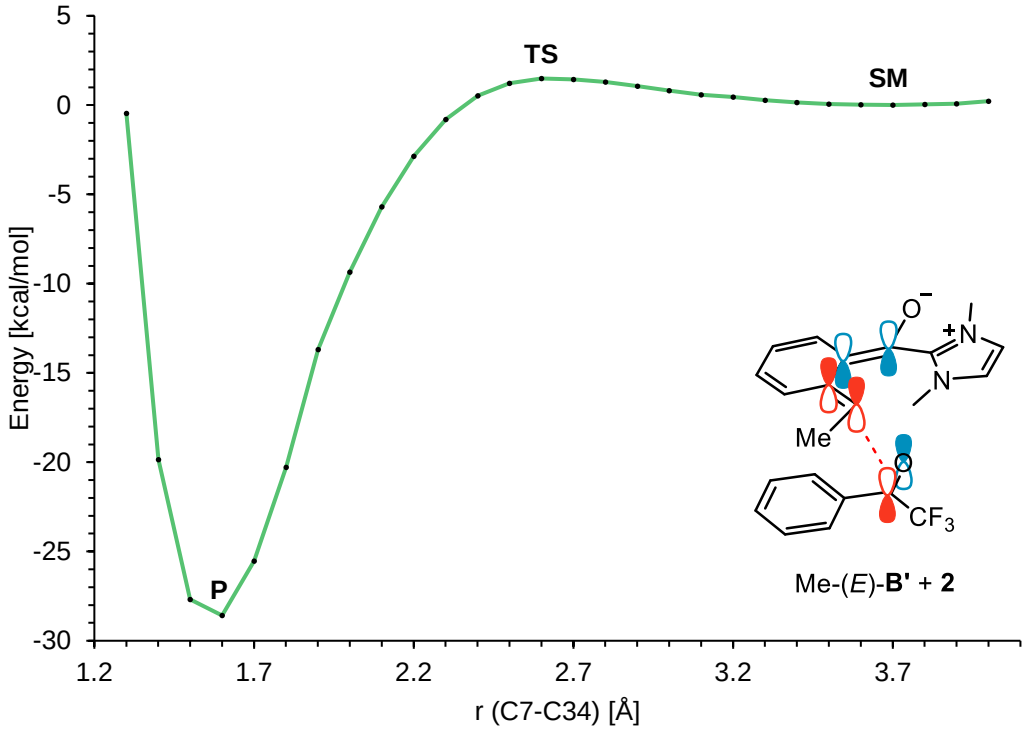
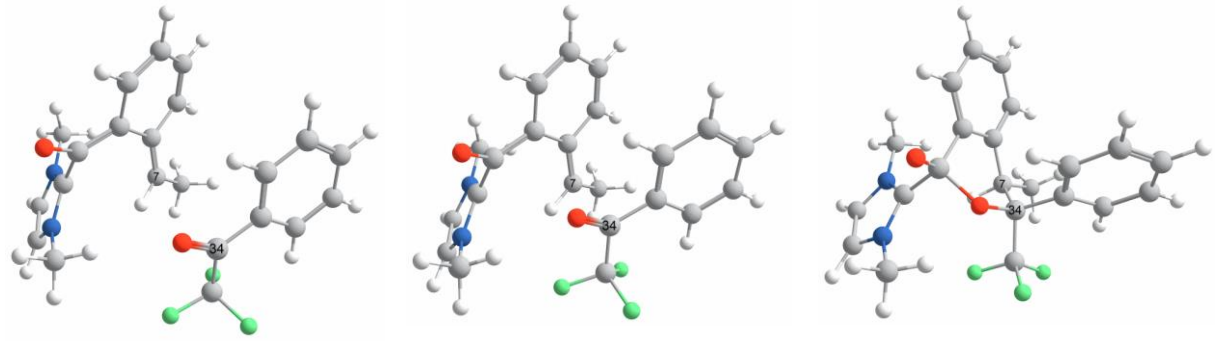


Figure S14. Relaxed PES scan of the (E)-**B′** *exo* cycloaddition with ketone **2** along the C22-C29 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.

1.6 Cycloaddition of Me-(*E*)-**B′** with **2**

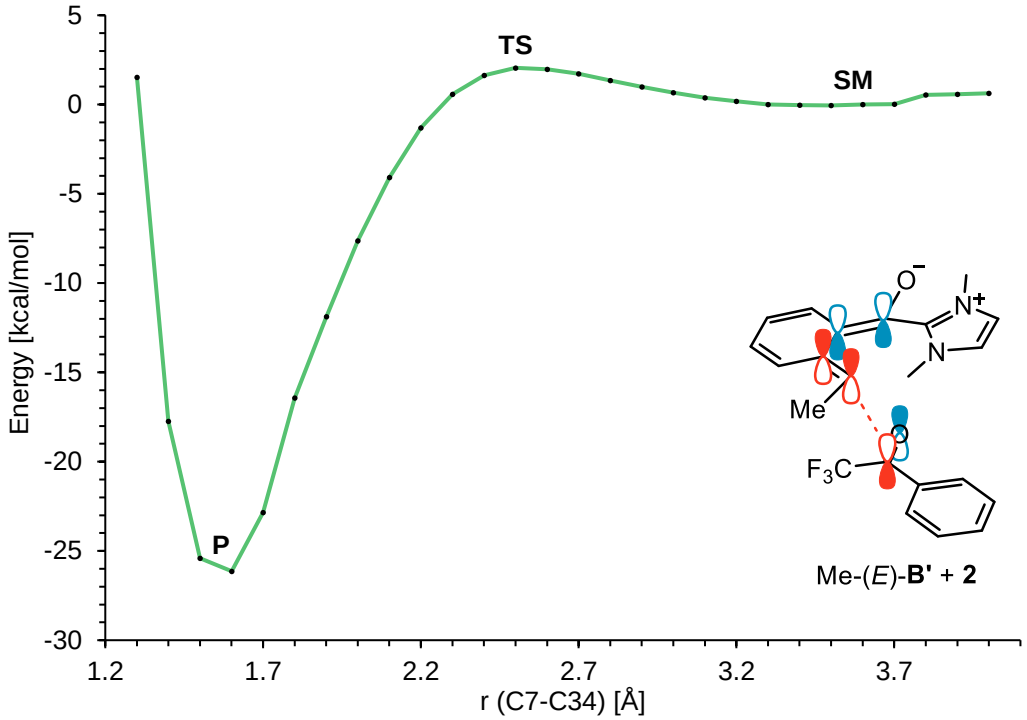


Species	r (C7-C34) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.70	–1409.799626	0.11	0
TS	2.65	–1409.786976	8.05	1 (–81 cm^{-1})
P	1.57	–1409.820805	–13.2	0



SM **TS** **P**

Figure S15. Relaxed PES scan of the Me-(*E*)-**B′** *endo* cycloaddition with ketone **2** along the C7-C34 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.



Species	r (C7-C34) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.57	–1409.799802	0.00	0
TS	2.55	–1409.788179	7.29	1 (–128 cm^{-1})
P	1.56	–1409.824518	–15.5	0

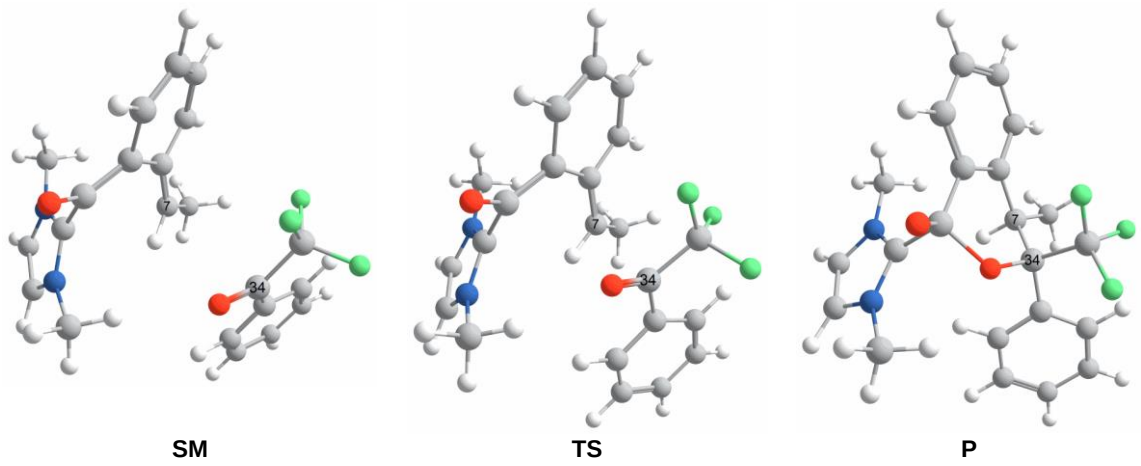
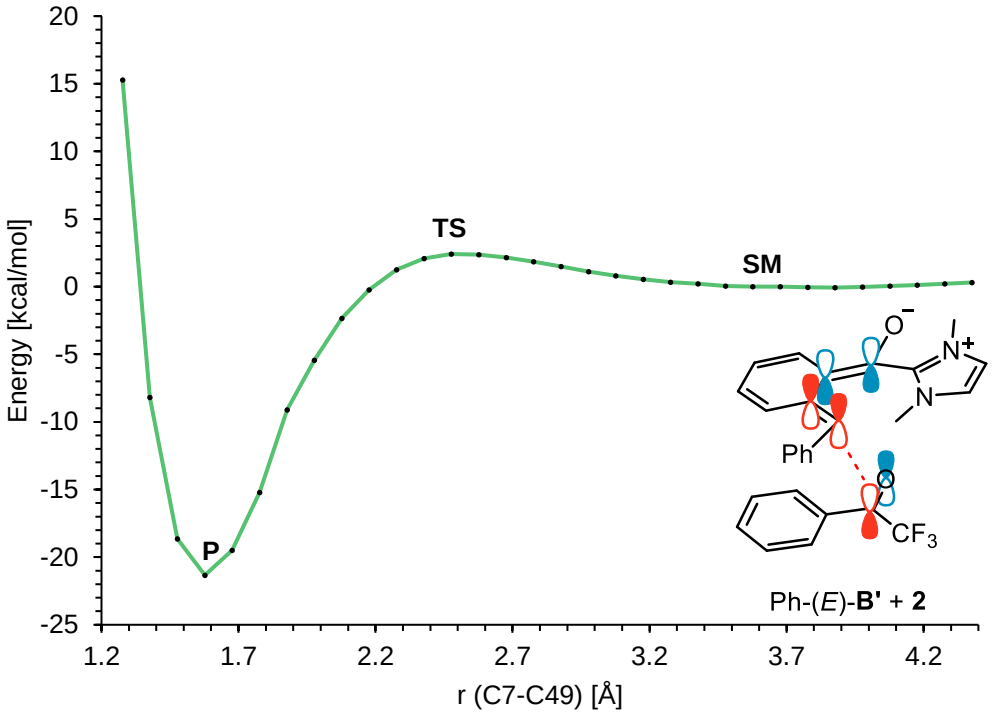


Figure S16. Relaxed PES scan of the Me-(*E*)-**B′** *exo* cycloaddition with ketone **2** along the C7-C34 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.

1.7 Cycloaddition of Ph-(*E*)-**B′** with **2**



Species	r (C7-C49) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.58	–1601.427024	1.24	0
TS	2.52	–1601.408834	12.7	1 (–115 cm^{-1})
P	1.58	–1601.435316	–3.96	0

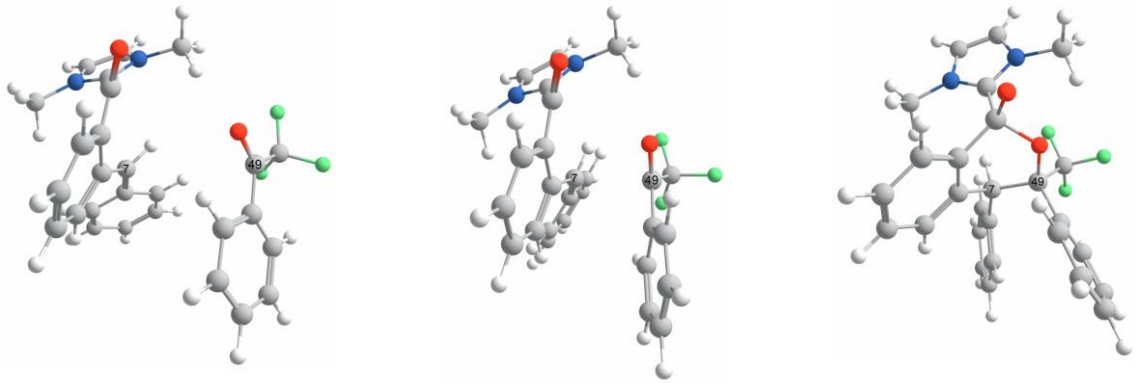
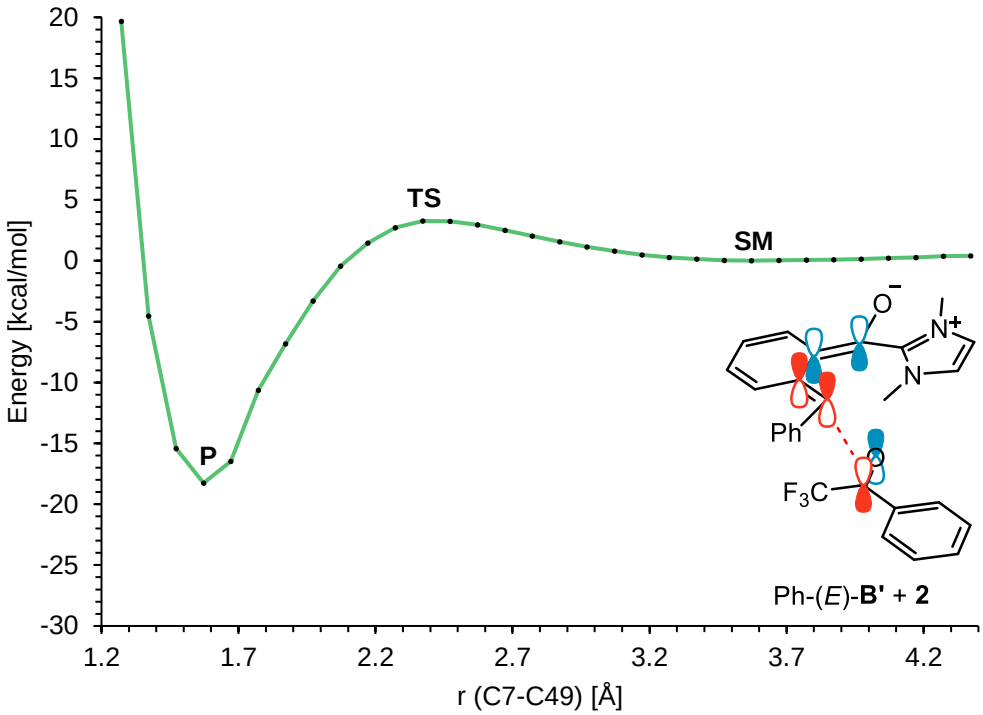


Figure S17. Relaxed PES scan of the Ph-(*E*)-**B′** *endo* cycloaddition with ketone **2** along the C7-C49 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.



Species	r (C7-C49) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.57	–1601.429004	0.00	0
TS	2.43	–1601.410209	11.8	1 (–149 cm^{-1})
P	1.57	–1601.439610	–6.66	0

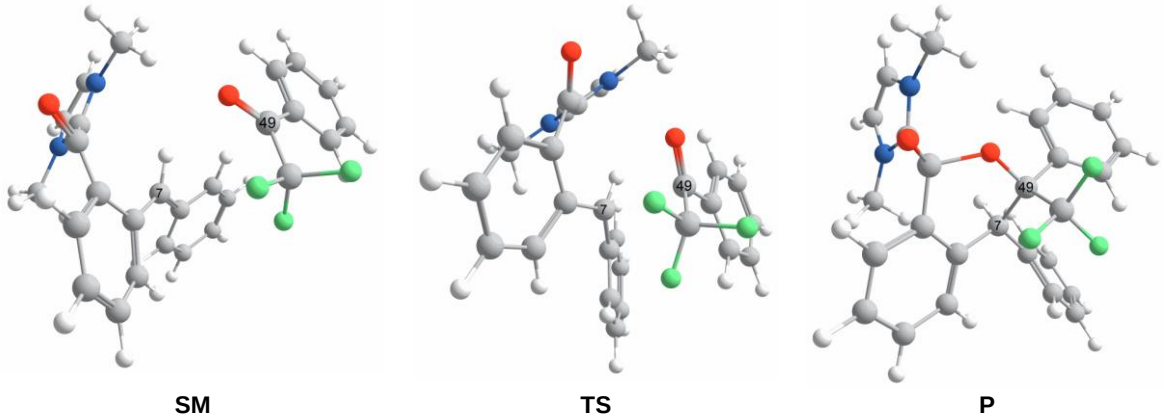
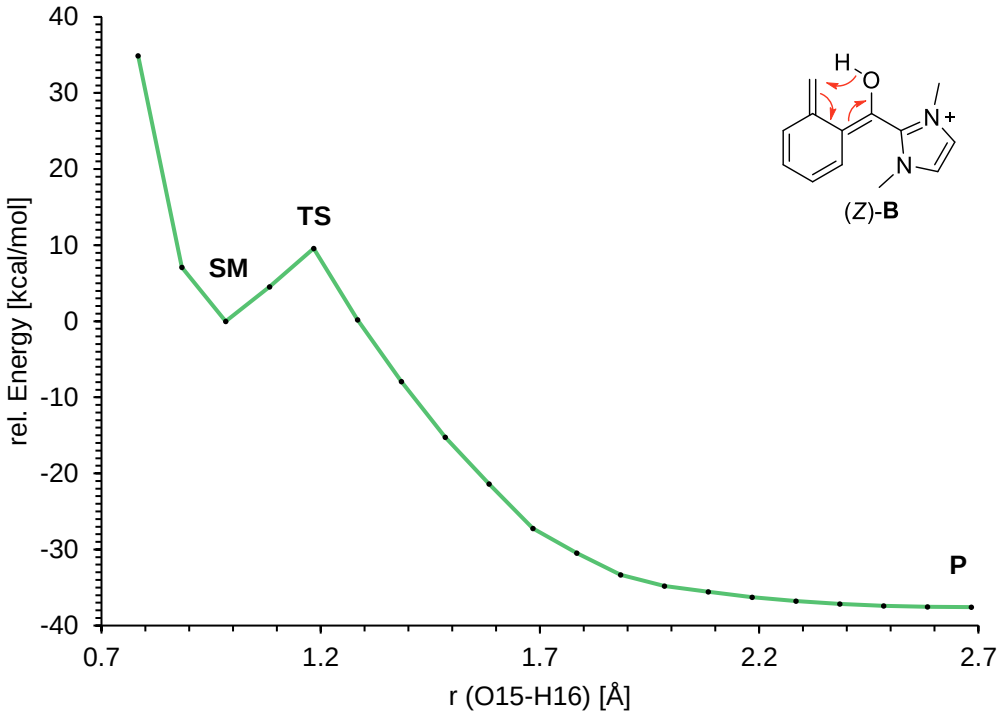


Figure S18. Relaxed PES scan of the Ph-(*E*)-**B′** *exo* cycloaddition with ketone **2** along the C7-C49 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.

1.8 Sigmatropic rearrangement of (*Z*)-**B** and cycloaddition with **2**



Species	r (O15-H16) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	0.98	–688.365434	0.00	0
TS	1.16	–688.352710	7.98	1 (–1621 cm^{-1})
P	2.68	–688.425063	–37.4	0

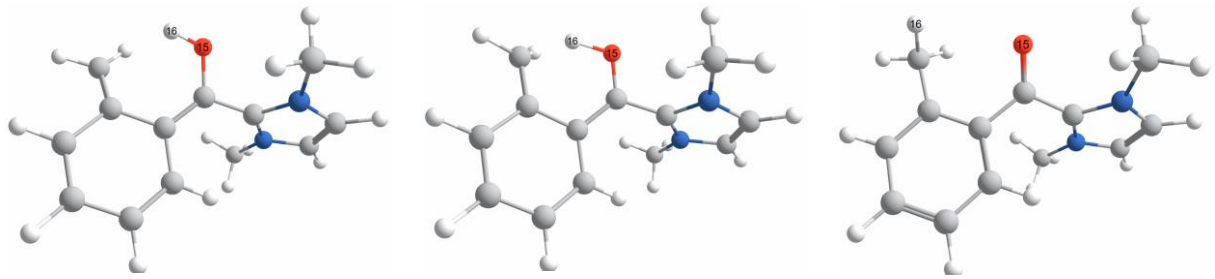
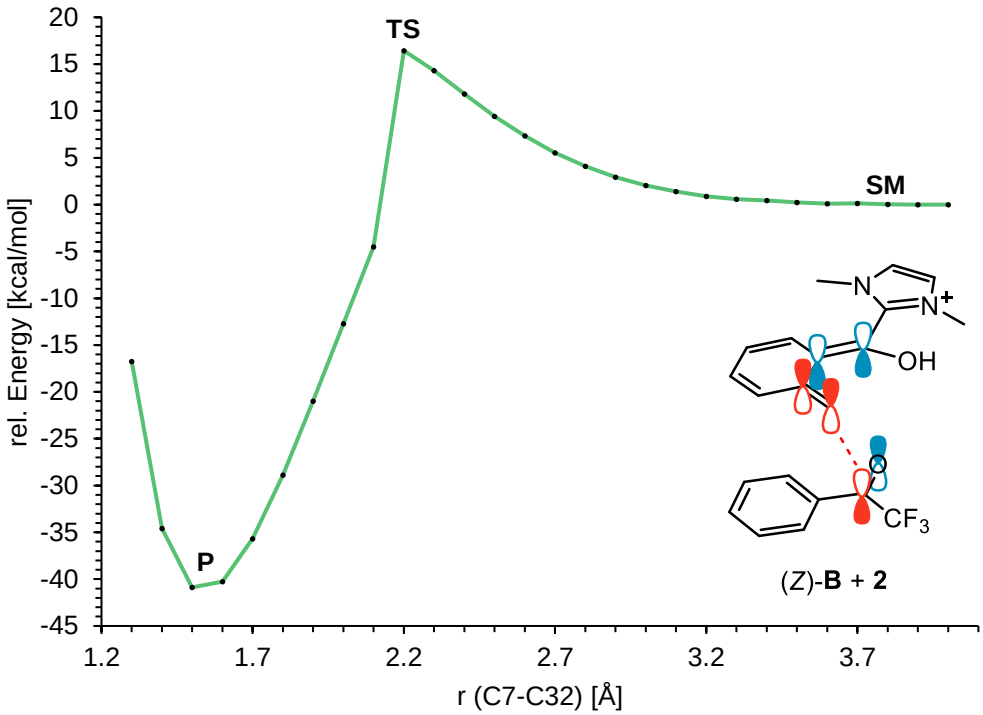


Figure S19. Relaxed PES scan of the 1,5-sigmatropic rearrangement of (*Z*)-**B** along the O15-H16 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.



Species	r (C7-C32) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.82	–1370.658694	0.00	0
TS	2.11	–1370.620416	24.0	1 (–425 cm^{-1})
P	1.54	–1370.707848	–30.8	0

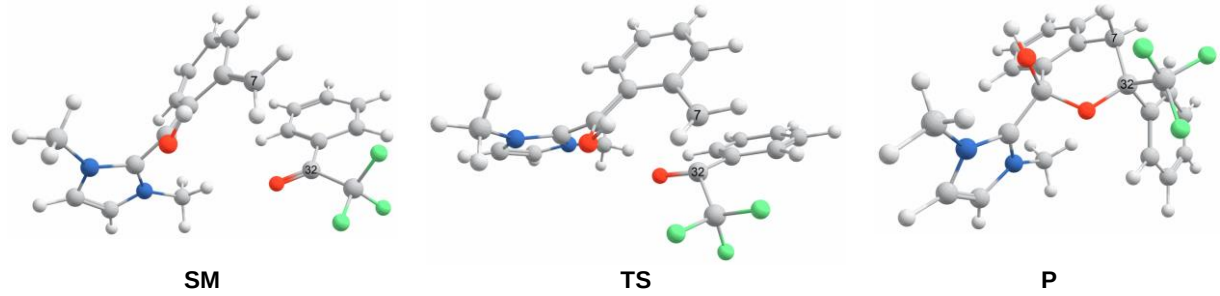
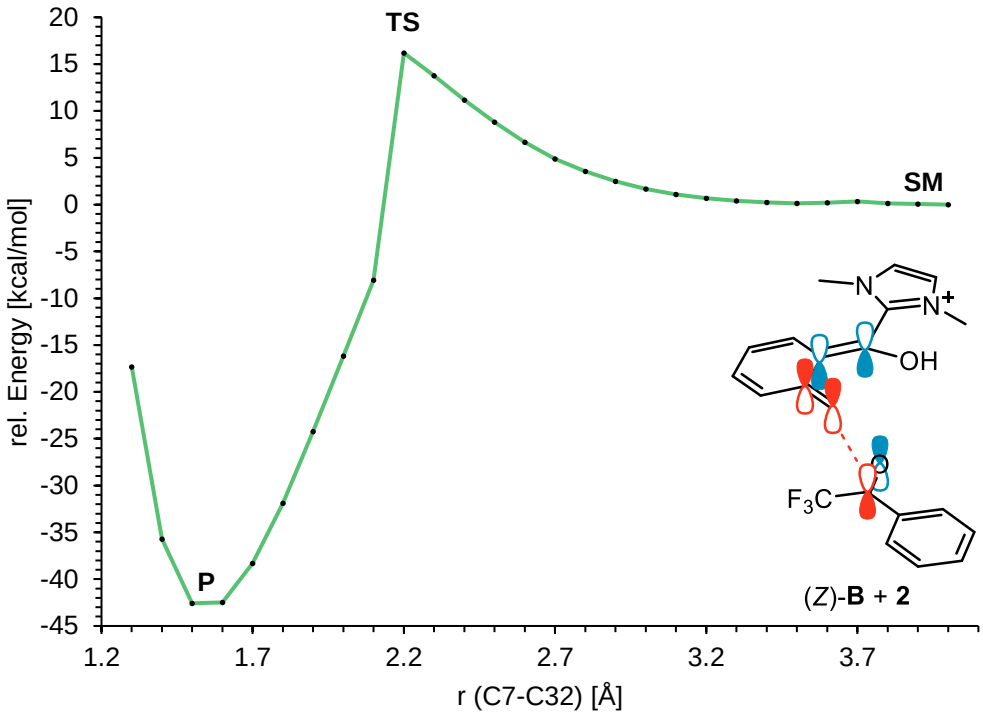


Figure S20. Relaxed PES scan of the (*Z*)-**B** *endo* cycloaddition with ketone **2** along the C7-C32 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.



Species	r (C7-C32) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	3.96	–1370.659701	0.00	0
TS	2.13	–1370.621403	24.0	1 (–438 cm^{-1})
P	1.55	–1370.710865	–32.1	0

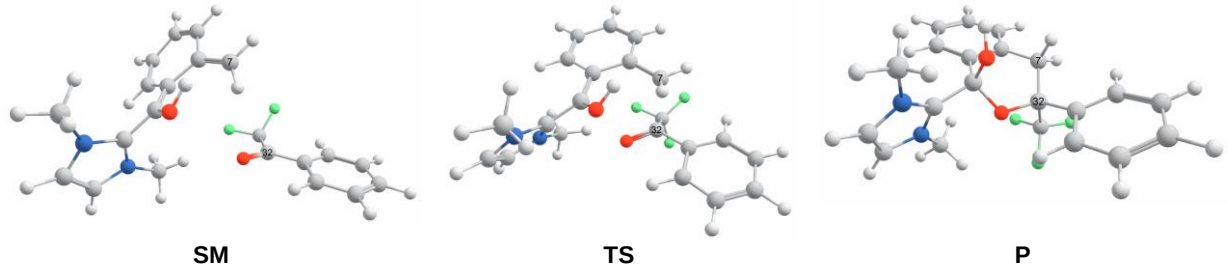
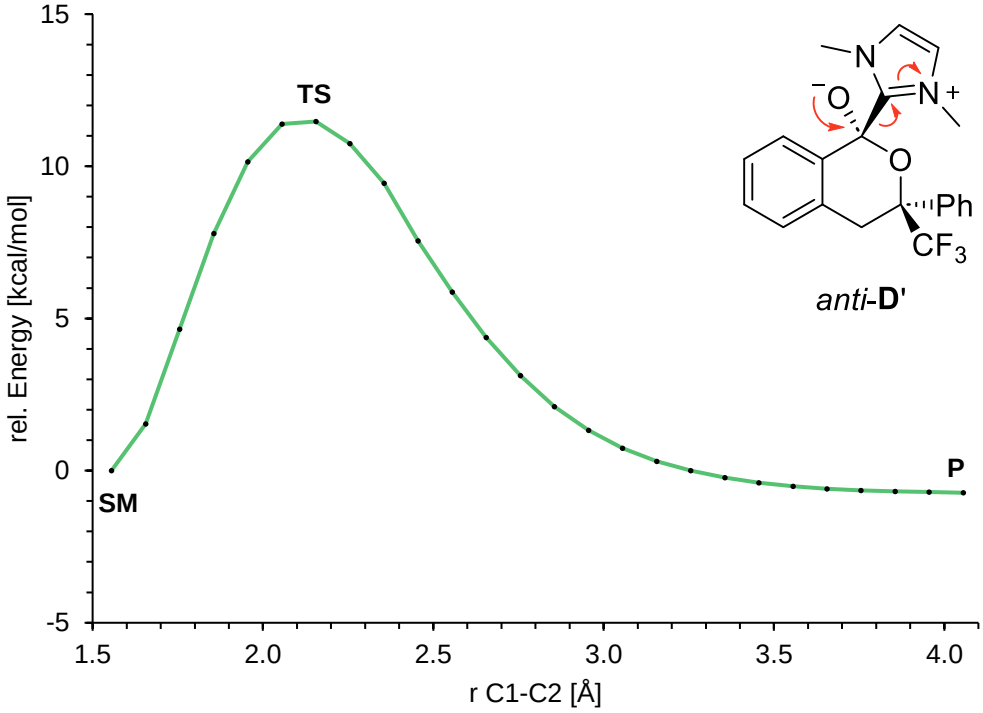


Figure S21. Relaxed PES scan of the (*Z*)-**B** *exo* cycloaddition with ketone **2** along the C7-C32 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.

1.9 Dissociation of *anti*/*syn*-**D**'



Species	r (C1-C2) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	1.56	–1370.564028	0.00	0
TS	2.12	–1370.549461	9.14	1 (–240 cm^{-1})
P	4.06	–1370.577266	–8.31	0

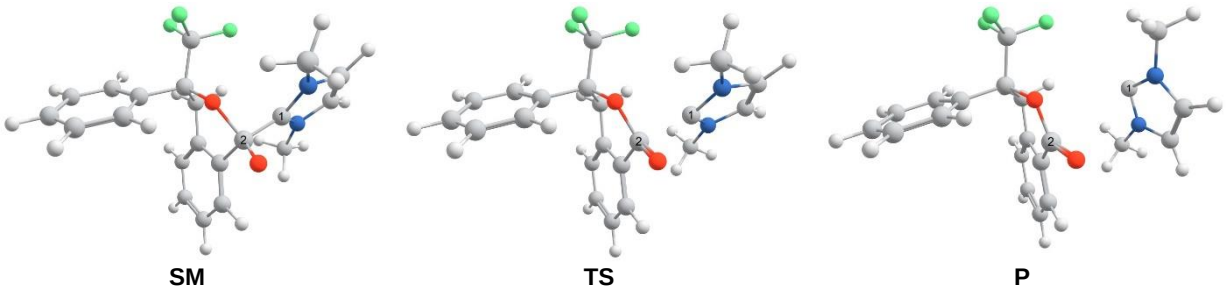
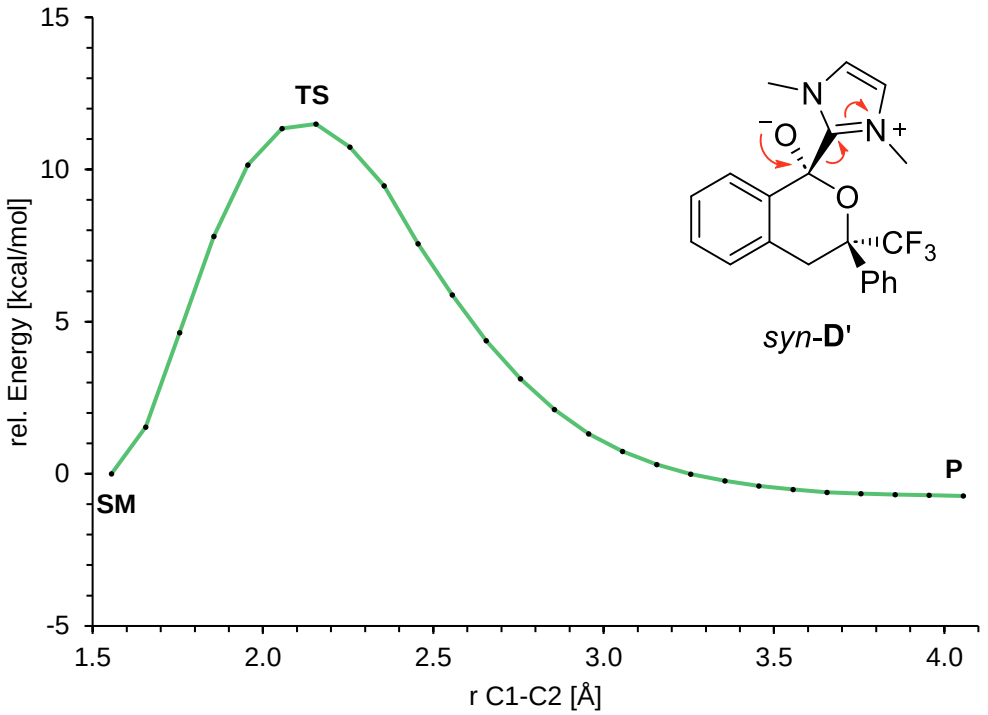


Figure S22. Relaxed PES scan of the dissociation of *anti*-**D**' along the C1-C2 coordinate and the Gibbs free energies (298 K) and geometries of the involved species.



Species	r (C1-C2) [Å]	Gibbs Free Energy [Eh]	rel. Gibbs Free Energy [kcal/mol]	Imaginary Frequencies
SM	1.56	–1370.560522	2.20	0
TS	2.11	–1370.547155	10.6	1 (–240 cm^{-1})
P	4.06	–1370.574745	–6.73	0

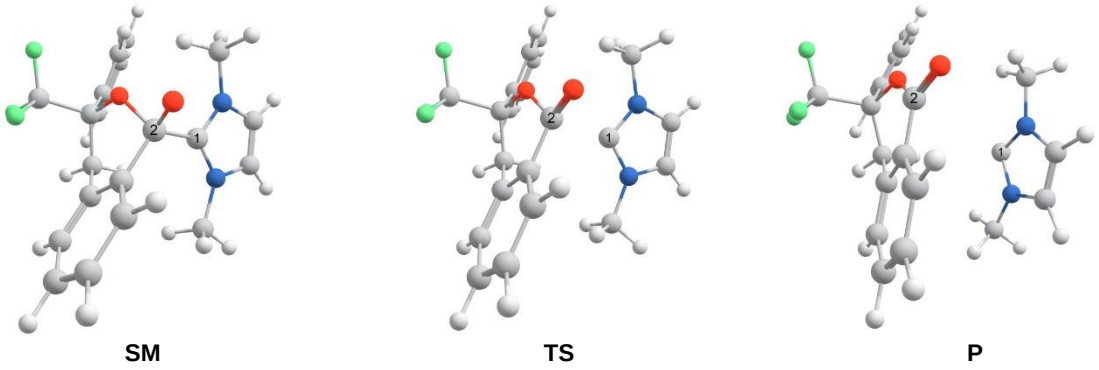


Figure S23. Relaxed PES scan of the dissociation of *syn*-**D**' along the C1-C2 coordinate and the calculated Gibbs free energies (298 K) and geometries of the involved species.

1.10 Calculated UV-Vis spectra

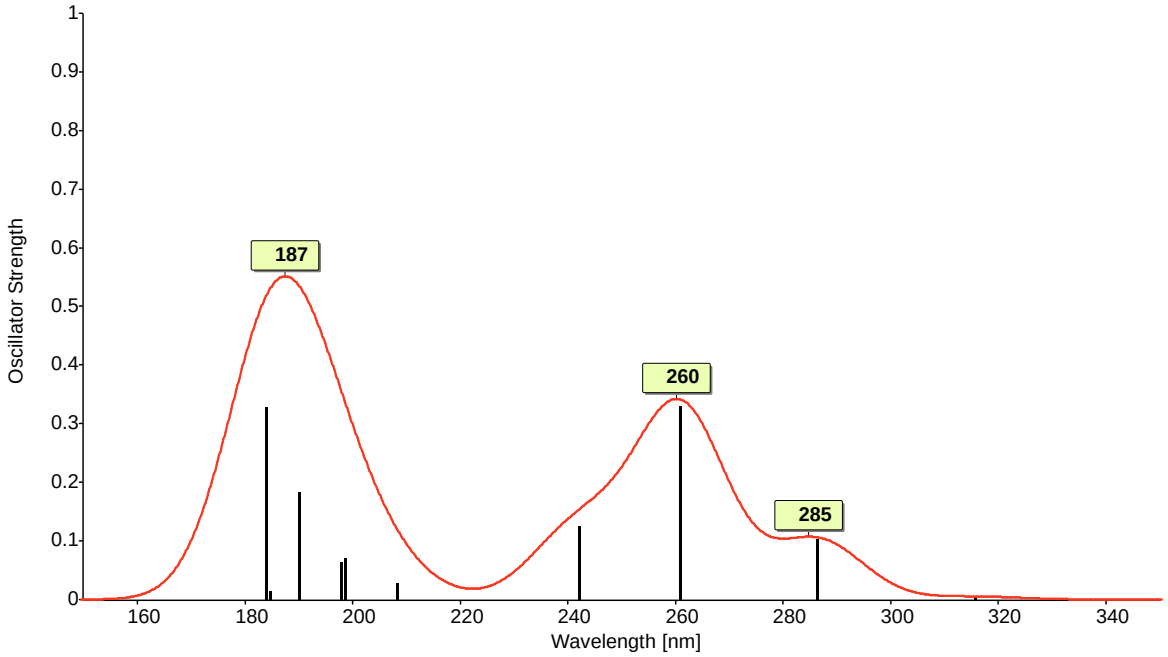


Figure S24. Calculated UV-Vis Spectrum of acyl azolium **A** at the TD-DFT level (CAM-B3LYP/6-311+G(d), PCM(CH_3CN); nstates=10, Gaussian line broadening with FWHM = 20).

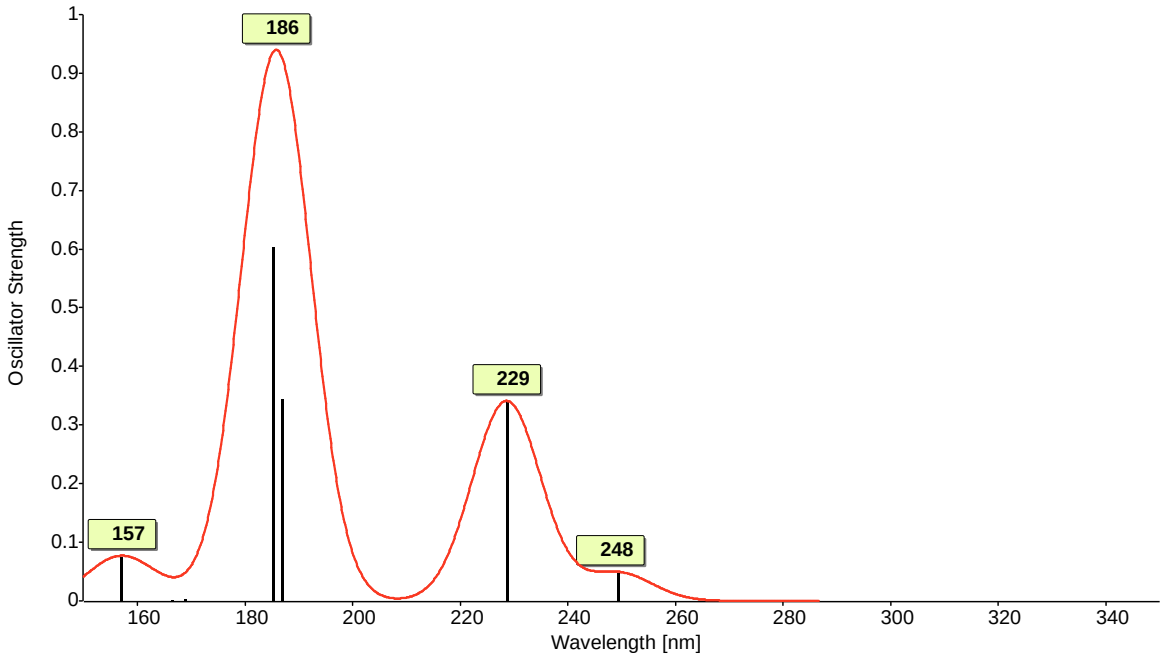


Figure S25. Calculated UV-Vis Spectrum of *ortho*-toluoyl fluoride **1** at the TD-DFT level of theory (CAM-B3LYP/6-311+G(d), PCM(CH_3CN); nstates=10, Gaussian line broadening with FWHM = 20).

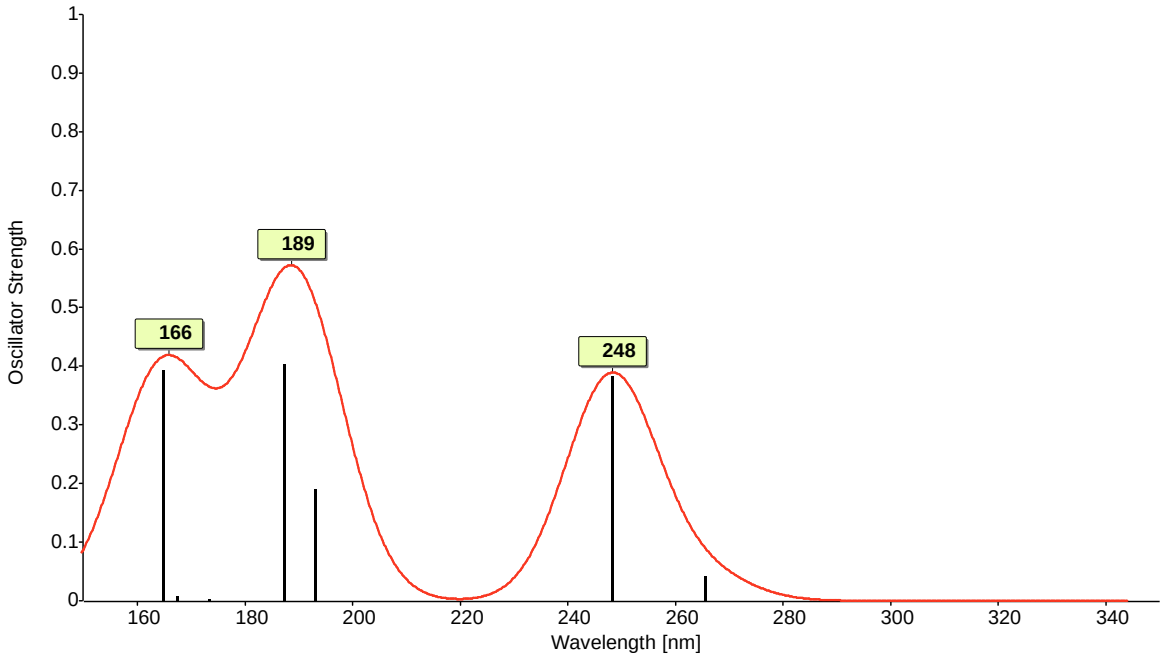


Figure S26. Calculated UV-Vis Spectrum of ketone **2** (dienophile) at the TD-DFT level of theory (CAM-B3LYP/6-311+G(d), PCM(CH_3CN); nstates=10, Gaussian line broadening with FWHM = 20).

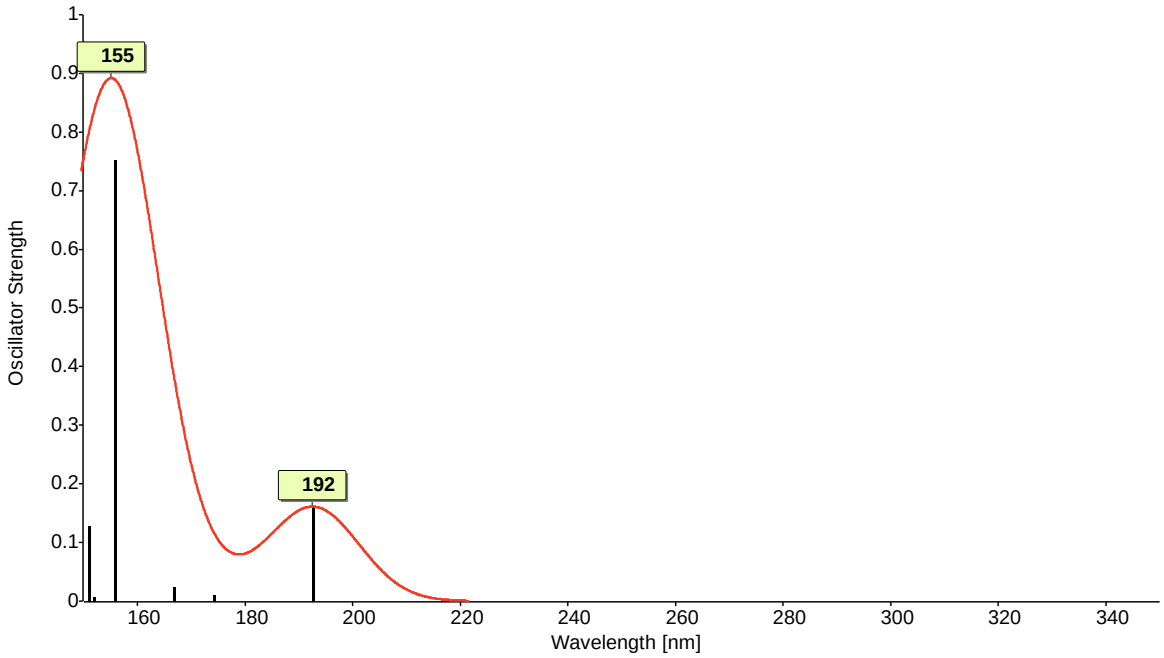


Figure S27. Calculated UV-Vis Spectrum of 1,3-dimethyl-1*H*-imidazol-3-ium (precatalyst) at the TD-DFT level of theory (CAM-B3LYP/6-311+G(d), PCM(CH_3CN); nstates=10, Gaussian line broadening with FWHM = 20).

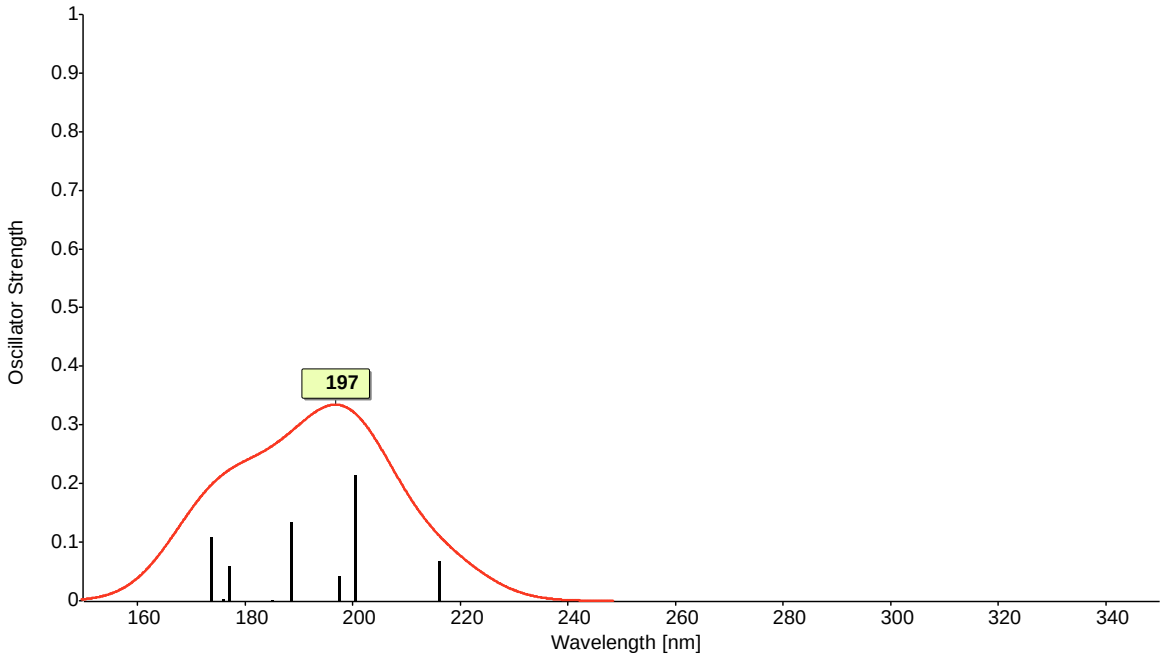
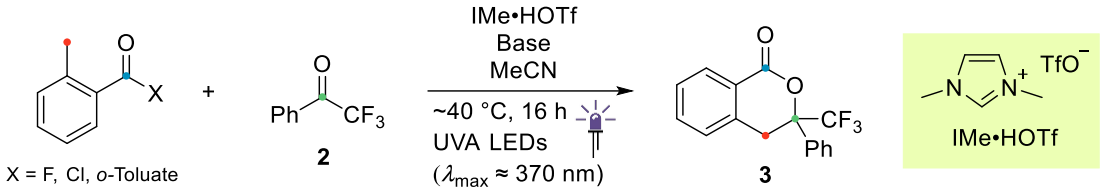


Figure S28. Calculated UV-Vis Spectrum of 1,3-dimethyl-1*H*-imidazolylidene (catalyst) at the TD-DFT level (CAM-B3LYP/6-311+G(d), PCM(CH_3CN); nstates=10, Gaussian line broadening with FWHM = 20).

2. Catalytic Test Reactions



Entry	Starting Material	Dienophile	NHC•HX	Base	Solvent	NMR Yield
1	*o*-Toluoyl fluoride **1** 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	Na_2CO_3 2 equiv	MeCN 0.1 M	18%
2	*o*-Toluoyl fluoride **1** 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	K_2CO_3 2 equiv	MeCN 0.1 M	6%
3	*o*-Toluoyl fluoride **1** 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	Rb_2CO_3 2 equiv	MeCN 0.1 M	62%
4	*o*-Toluoyl fluoride **1** 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	Cs_2CO_3 2 equiv	MeCN 0.1 M	88%
5	*o*-Toluoyl fluoride **1** 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	$CsHCO_3$ 2 equiv	MeCN 0.1 M	6%
6	*o*-Toluoyl fluoride **1** 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	CsOPiv 2 equiv	MeCN 0.1 M	10%
7	*o*-Toluoyl chloride 3 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	Cs_2CO_3 2 equiv	MeCN 0.1 M	17%
8	*o*-Toluic anhydride 1.5 equiv	**2** 1 equiv	IMe•HOTf 0.2 equiv	Cs_2CO_3 2 equiv	MeCN 0.1 M	5%

Figure S29. Catalytic test reactions (0.1 mmol scale).

3. Crystallographic data

3.1 *ortho*-Toluoyl 1,3-dimethylimidazolium triflate **4**

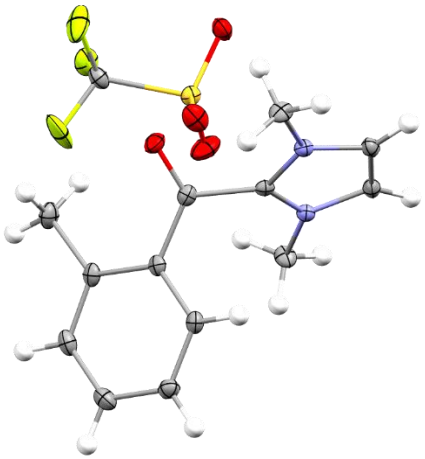


Figure S30. Crystal structure of ortho-Toluoyl 1,3-dimethylimidazolium triflate (thermal ellipsoids at 50% probability).

Table S1. Crystal data of *ortho*-toluoyl 1,3-dimethylimidazolium triflate.

CCDC Deposition Number	2169961
Sum formula	$C_{14}\ H_{15}\ F_3\ N_2\ O_4\ S$
Formula weight /g mol^{-1}	364.34
Temperature /K	100(2)
Crystal system	monoclinic
Space group	C 2/c
Cell dimensions /Å or °	a = 25.7587(4) α = 90 b = 7.7074(10) β = 92.5083(6) c = 16.1440(3) γ = 90
Volume /$Å^3$	3202.04(9)
Z	8
Density /g cm^{-3}	1.512
μ /mm^{-1}	0.256
F(000)	1504.0
Crystal size /mm^{-3}	0.85 x 0.30 x 0.16
Radiation /Å	0.71073 (MoKα)
Θ range for data collection /°	2.526 to 26.397
Reflections collected	11352
Independent reflections	3262 [R_{int} = 0.0245, R_{sigma} = 0.0236]
Data/restraints/parameters	3262/0/221
Goodness-of-fit on F^2	S = 1.059
Final R indexes [I > 2σ(I)]	R1 = 0.0357, wR2 = 0.0890
Final R indexes [all data]	R1 = 0.0390, wR2 = 0.0912
Largest diff. peak and hole/e $Å^{-3}$	0.40 and –0.40

3.2 Major diastereomer in the PEDA reaction of *ortho*-ethylbenzoyl fluoride

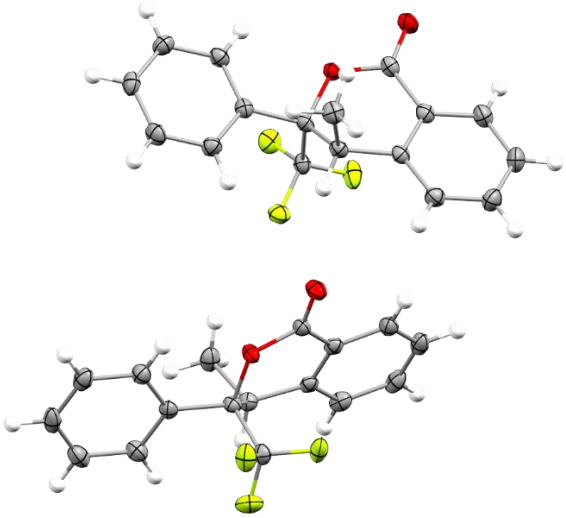


Figure S31. Crystal structure of (3*S*,4*R*)- and (3*R*,4*S*)-4-methyl-3-phenyl-3-(trifluoromethyl)isochroman-1-one (thermal ellipsoids at 50% probability).

Table S2. Crystal data of (3*S*,4*R*)- and (3*R*,4*S*)-4-methyl-3-phenyl-3-(trifluoromethyl)isochroman-1-one

CCDC Deposition Number	2169962
Sum formula	$C_{17}\ H_{13}\ F_3\ O_2$
Formula weight /g mol^{-1}	306.27
Temperature /K	100(2)
Crystal system	triclinic
Space group	P $\bar{1}$
Cell dimensions /Å or °	a = 9.2422(7) α = 87.244(2) b = 11.4334(7) β = 72.344(2) c = 14.3847(12) γ = 78.9480(10)
Volume /Å^3	1421.48(18)
Z	4
Density /g cm^{-3}	1.431
μ /mm^{-1}	1.024
F(000)	632.0
Crystal size /mm^{-3}	0.50 x 0.43 x 0.40
Radiation /Å	1.54178 (CuKα)
Θ range for data collection /°	3.224 to 68.309
Reflections collected	27657
Independent reflections	5070 [R_{int} = 0.0295, R_{sigma} = 0.0251]
Data/restraints/parameters	5070/0/400
Goodness-of-fit on F^2	S = 1.100
Final R indexes [I > 2σ(I)]	R1 = 0.0362, wR2 = 0.0903
Final R indexes [all data]	R1 = 0.0370, wR2 = 0.0909
Largest diff. peak and hole/e$^-$Å^{-3}	0.34 and –0.22

3.3 Major diastereomer in the PEDA reaction of *ortho*-benzylbenzoyl fluoride

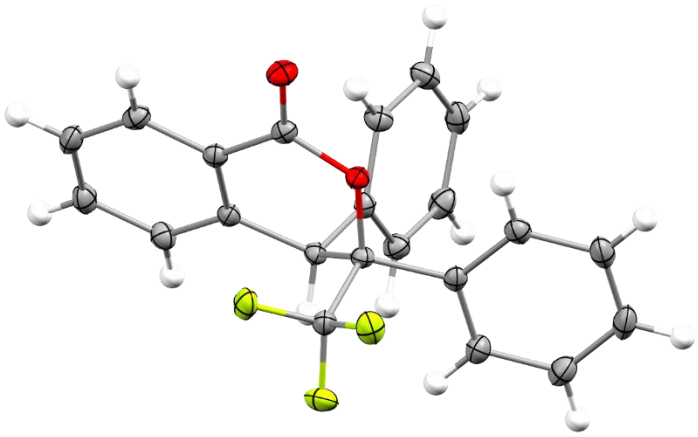


Figure S32. Crystal structure of (3*S*,4*R*)-3,4-diphenyl-3-(trifluoro-methyl)isochroman-1-one (thermal ellipsoids at 50% probability).

Table S3. Crystal data of (3*S*,4*R*)-3,4-diphenyl-3-(trifluoro-methyl)isochroman-1-one

CCDC Deposition Number	2169963
Sum formula	C_{22} H_{15} F_3 O_2
Formula weight /g mol^{-1}	368.34
Temperature /K	100(2)
Crystal system	monoclinic
Space group	P 2_1/n
Cell dimensions /Å or °	a = 9.6916(2) α = 90 b = 13.1235(2) β = 97.0695(7) c = 13.3856(2) γ = 90
Volume /$Å^3$	1689.54(5)
Z	4
Density /g cm^{-3}	1.448
μ /mm^{-1}	0.114
F(000)	760.0
Crystal size /mm^{-3}	0.28 x 0.15 x 0.15
Radiation /Å	0.71073 (MoKα)
Θ range for data collection /°	2.181 to 26.395
Reflections collected	30837
Unique reflections	3458 [R_{int} = 0.0324, R_{sigma} = 0.0152]
Data/restraints/parameters	3458/0/244
Goodness-of-fit on F^2	S = 1.066
Final R indexes [I > 2σ(I)]	R1 = 0.0326, wR2 = 0.0796
Final R indexes [all data]	R1 = 0.0355, wR2 = 0.0818
Largest diff. peak and hole/$e^-Å^{-3}$	0.39 and –0.26