Supplementary Information (SI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2026

How Fluorination Collapses Inversion Barriers and Increases Electrophilicity in Bicyclo[1.1.0]butanes

Supporting Information

Bruno A. Piscelli, Caio E. D. V. P. Nascimento, Rodrigo A. Cormanich*

Universidade Estadual de Campinas, Instituto de Química, Departamento de Química Orgânica, PO Box 6154 – 13083-970 – Campinas, São Paulo, Brazil.

*E-mail: cormanich@unicamp.br

Table of Contents

Table S1. Benchmark calculations done at several DFT levels and using DLPNO-CCSD(T) level as the benchmark for the inversion barrier of BCB, 1-FBCB and 2-FBCB. R, TS and P indicate the "reactants", transition states and "products", respectively. Energies are given in kcal mol^{-1}. 3

Figure S1. Displacement vectors corresponding to the imaginary modes for all conformational transition states investigated for the BCB derivatives. 6

Table S2. NBO analysis relative energies (in kcal mol^{-1}) obtained at the B3LYP/6-311+G** level for several fluoro-bicyclobutane derivatives. Compounds that may exhibit *cis-trans* isomerism were also calculated. $\Delta E^{\ddagger}_{T}$ is the electronic, $\Delta E^{\ddagger}_{L}$ the Lewis, and $\Delta E^{\ddagger}_{NL}$ the non-Lewis energy contributions to the inversion barrier. 7

Table S3. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for BCB(Min). 8

Table S4. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for BCB(TS). 9

Table S5. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for 1-FBCB(Min). 10

Table S6. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for 1-FBCB(TS). 11

Table S7. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for 2-FBCB(Min). 12

Table S8. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for 2-FBCB(TS). 13

Table S9. Experimental conversion rates (Baran *et al*[7]) and calculated LUMO (au), $\Delta H^{\ddagger}(TS_N)$ (kcal mol^{-1}) and $\Delta G^{\ddagger}(TS_N)$ (kcal mol^{-1}) for the for the reaction of dibenzylamine with sulfonylated BCBs. 14

Optimised Cartesian Coordinates 15

Table S1. Benchmark calculations done at several DFT levels and using DLPNO-CCSD(T) level as the benchmark for the inversion barrier of **BCB**, **1-FBCB** and **2-FBCB**. R, TS and P indicate the "reactants", transition states and "products", respectively. Energies are given in kcal mol^{-1}.

		BCB				1F-BCB				2F-BCB		
		ΔE	**ΔH**	**ΔG**		**ΔE**	**ΔH**	**ΔG**		**ΔE**	**ΔH**	**ΔG**
DLPNO-CCSD(T)/CBS	**R**	**0.00**	**-**	**-**	**R**	**0.00**	**-**	**-**	**R**	**0.00**	**-**	**-**
	TS	**64.14**	**-**	**-**	**TS**	**49.70**	**-**	**-**	**TS**	**50.69**	**-**	**-**
	P	**0.00**	**-**	**-**	**P**	**0.00**	**-**	**-**	**P**	**-3.28**	**-**	**-**
B3LYP/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	73.97	71.8	71.75	**TS**	54.04	52.34	52.18	**TS**	51.75	50.12	49.96
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.11	-2.84	-2.77
B3LYP/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	74.63	72.43	72.38	**TS**	54.02	52.29	52.17	**TS**	52.86	51.22	51.09
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.06	-2.77	-2.70
B3LYP-D3/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	74.09	71.87	71.80	**TS**	54.23	52.52	52.33	**TS**	51.81	50.12	49.94
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.14	-2.87	-2.79
B3LYP-D3/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	74.76	72.51	72.45	**TS**	54.21	52.46	52.32	**TS**	52.94	51.24	51.1
	P	-0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.09	-2.8	-2.72
BHandH/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	88.73	86.59	86.55	**TS**	66.47	64.75	64.75	**TS**	66.91	65.27	65.26
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-2.89	-2.59	-2.51
BHandH/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	89.21	87.00	86.97	**TS**	65.99	64.22	64.24	**TS**	67.87	66.18	66.18
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-2.81	-2.50	-2.41
M06-L/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	80.36	78.25	78.21	**TS**	57.48	55.87	55.86	**TS**	59.88	58.16	57.98
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-2.79	-2.52	-2.43

Table S1: (continuation).

		BCB				1F-BCB				2F-BCB		
		ΔE	**ΔH**	**ΔG**		**ΔE**	**ΔH**	**ΔG**		**ΔE**	**ΔH**	**ΔG**
M06-L/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	80.63	78.5	78.47	**TS**	57.33	55.73	55.74	**TS**	60.93	59.28	59.17
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-2.82	-2.51	-2.4
PBE0/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	79.83	77.69	77.65	**TS**	58.23	56.54	56.51	**TS**	58.64	56.99	56.93
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-2.95	-2.67	-2.59
PBE0/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	80.31	78.11	78.09	**TS**	57.96	56.23	56.23	**TS**	59.61	57.93	57.89
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-2.89	-2.6	-2.52
M06-2X/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	86.07	84.03	84.01	**TS**	63.86	62.26	62.35	**TS**	65.61	63.94	63.93
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.02	-2.73	-2.64
M06-2X/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	86.09	84.02	84.01	**TS**	63.16	61.53	61.63	**TS**	65.78	64.1	64.09
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.01	-2.72	-2.62
CAM-B3LYP/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	80.69	78.6	78.55	**TS**	60.04	58.38	58.3	**TS**	58.05	56.43	56.31
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	0.00	0.01	0.00
CAM-B3LYP/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	81.15	79.02	78.98	**TS**	59.72	58.02	57.98	**TS**	58.97	57.31	57.21
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	0.00	0.00	0.00
CAM-B3LYP-D3/6-311+G**	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	80.71	78.6	78.55	**TS**	60.09	58.42	58.33	**TS**	58.05	56.4	56.28
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	-3.11	-2.84	-2.76

Table S1: (continuation).

		BCB				1F-BCB				2F-BCB		
		ΔE	**ΔH**	**ΔG**		**ΔE**	**ΔH**	**ΔG**		**ΔE**	**ΔH**	**ΔG**
CAM-B3LYP-D3/aug-cc-pVTZ	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00	**R**	0.00	0.00	0.00
	TS	81.17	79.02	78.98	**TS**	59.77	58.07	58.02	**TS**	58.97	57.3	57.2
	P	0.00	0.00	0.00	**P**	0.00	0.00	0.00	**P**	0.00	0.00	0.00

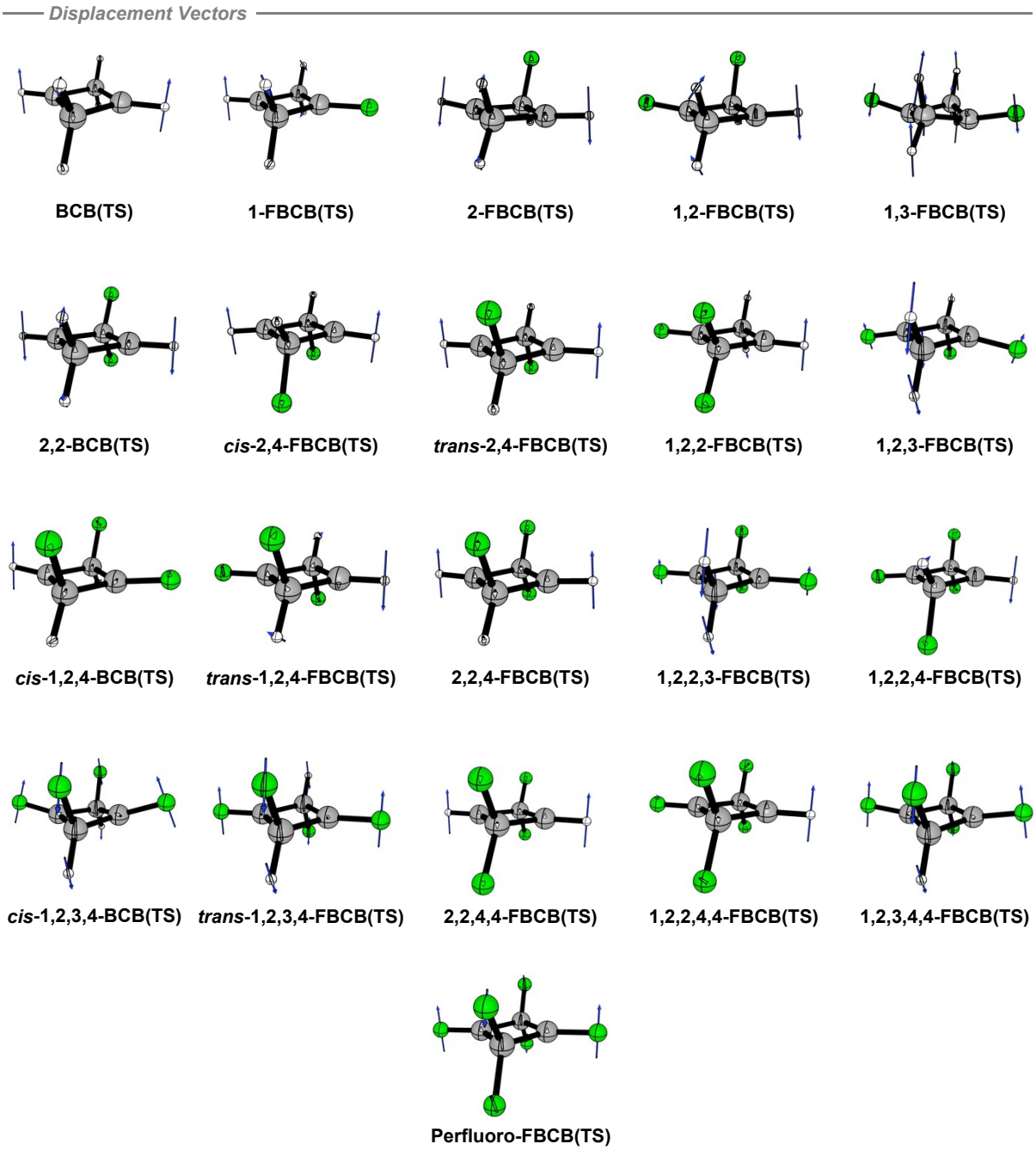


Figure S1. Displacement vectors corresponding to the imaginary modes for all conformational transition states investigated for the BCB derivatives. Calculations at the B3LYP/6-311+G** level.

Table S2. NBO analysis relative energies (in kcal mol^{-1}) obtained at the B3LYP/6-311+G** level for several fluoro-bicyclobutane derivatives. Compounds that may exhibit *cis-trans* isomerism were also calculated. $\Delta E^{\ddagger}_{T}$ is the electronic, $\Delta E^{\ddagger}_{L}$ the Lewis, and $\Delta E^{\ddagger}_{NL}$ the non-Lewis energy contributions to the inversion barrier.

	Compound	$\Delta E_T^{\ddagger}$ (kcal mol^{-1})	$\Delta E_L^{\ddagger}$ (kcal mol^{-1})	$\Delta E_{NL}^{\ddagger}$ (kcal mol^{-1})
F=0	**BCB**	73.9	56.5	17.4
F=1	**1-FBCB**	54.1	88.8	-34.7
	2-FBCB	51.7	57.5	-5.8
F=2	**1,2-FBCB**	38.8	77.4	-38.6
	1,3-FBCB	36.5	90.3	-53.8
	2,2-FBCB	46.9	43.9	3.0
	***cis*-2,4-FBCB**	36.6	50.2	-13.6
	***trans*-2,4-FBCB**	40.9	44.5	-3.6
F=3	**1,2,2-FBCB**	30.8	68.0	-37.2
	1,2,3-FBCB	25.0	83.7	-58.7
	***cis*-1,2,4-FBCB**	27.5	58.4	-30.9
	***trans*-1,2,4-FBCB**	25.3	65.5	-40.2
	2,2,4-FBCB	32.7	44.0	-11.3
F=4	**1,2,2,3-FBCB**	16.9	74.4	-57.5
	1,2,2,4-FBCB	17.3	61.5	-44.2
	***cis*-1,2,3,4-FBCB**	5.4	63.7	-58.3
	***trans*-1,2,3,4-FBCB**	11.8	69.8	-58.0
	2,2,4,4-FBCB	27.4	34.6	-7.2
F=5	**1,2,2,4,4-FBCB**	14.3	52.6	-38.3
	1,2,3,4,4-FBCB	4.7	59.6	-54.9
F=6	**Perfluoro-BCB**	3.6	48.7	-45.1

Table S3. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for **BCB(Min)**.

NLMO (i)	NLMO (j)	$S_{(i,j)}$	$\Delta E_{(i,j)}$
σ_{C1-C2}	σ_{C3-C4}	0.1246	4.19
σ_{C1-C2}	σ_{C3-H7}	-0.0455	1.58
σ_{C1-C2}	σ_{C4-H5}	0.1049	1.59
σ_{C1-C2}	σ_{C4-H6}	-0.1099	4.36
σ_{C1-C3}	σ_{C2-H8}	-0.0777	3.58
σ_{C1-C3}	σ_{C2-H9}	0.0992	2.69
σ_{C1-C3}	σ_{C4-H5}	-0.0777	3.58
σ_{C1-C3}	σ_{C4-H6}	0.0992	2.69
σ_{C1-C4}	σ_{C2-C3}	0.1246	4.19
σ_{C1-C4}	σ_{C2-H8}	0.1049	1.59
σ_{C1-C4}	σ_{C2-H9}	-0.1099	4.36
σ_{C1-C4}	σ_{C3-H7}	-0.0455	1.58
σ_{C1-H10}	σ_{C2-C3}	-0.0455	1.58
σ_{C1-H10}	σ_{C2-H8}	-0.0600	1.31
σ_{C1-H10}	σ_{C2-H9}	0.0684	1.03
σ_{C1-H10}	σ_{C3-C4}	-0.0455	1.58
σ_{C1-H10}	σ_{C4-H5}	-0.0600	1.31
σ_{C1-H10}	σ_{C4-H6}	0.0684	1.03
σ_{C2-C3}	σ_{C4-H5}	0.1049	1.59
σ_{C2-C3}	σ_{C4-H6}	-0.1099	4.36
σ_{C2-H8}	σ_{C3-C4}	0.1049	1.59
σ_{C2-H8}	σ_{C3-H7}	-0.0600	1.31
σ_{C2-H8}	σ_{C4-H5}	0.0897	0.92
σ_{C2-H9}	σ_{C3-C4}	-0.1099	4.36
σ_{C2-H9}	σ_{C3-H7}	0.0684	1.03
σ_{C3-H7}	σ_{C4-H5}	-0.0600	1.31
σ_{C3-H7}	σ_{C4-H6}	0.0684	1.03

Table S4. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for **BCB(TS)**.

NLMO (i)	NLMO (j)	$S_{(i,j)}$	$\Delta E_{(i,j)}$
σ_{C1-C2}	σ_{C3-C4}	0.2884	24.08
σ_{C1-C2}	σ_{C3-H7}	-0.0951	4.21
σ_{C1-C2}	σ_{C4-H5}	-0.0453	0.93
σ_{C1-C2}	σ_{C4-H6}	-0.0453	0.93
σ_{C1-C3}	σ_{C2-H8}	0.2396	17.19
σ_{C1-C3}	σ_{C2-H9}	-0.2396	17.19
σ_{C1-C3}	σ_{C4-H5}	0.2396	17.19
σ_{C1-C3}	σ_{C4-H6}	-0.2396	17.19
σ_{C1-C4}	σ_{C2-C3}	0.2884	24.08
σ_{C1-C4}	σ_{C2-H8}	-0.0453	0.93
σ_{C1-C4}	σ_{C2-H9}	-0.0453	0.93
σ_{C1-C4}	σ_{C3-H7}	-0.0951	4.21
σ_{C1-H0}	σ_{C2-C3}	-0.0951	4.21
σ_{C1-H0}	σ_{C3-C4}	-0.0951	4.21
σ_{C2-C3}	σ_{C4-H5}	-0.0453	0.93
σ_{C2-C3}	σ_{C4-H6}	-0.0453	0.93
σ_{C2-H8}	σ_{C3-C4}	-0.0453	0.93
σ_{C2-H9}	σ_{C3-C4}	-0.0453	0.93

Table S5. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for **1-FBCB(Min)**.

NLMO (i)	NLMO (j)	$S_{(i,j)}$	$\Delta E_{(i,j)}$
n_{F10}	σ_{C2-C3}	-0.0497	-0.78
n_{F10}	σ_{C3-C4}	-0.0497	-0.78
n_{F10}	σ_{C1-C2}	-0.1284	6.86
n_{F10}	σ_{C1-C4}	0.1283	6.84
n_{F10}	σ_{C1-C2}	-0.0531	1.68
n_{F10}	σ_{C1-C3}	0.1631	12.00
n_{F10}	σ_{C1-C4}	-0.0532	1.68
σ_{C1-C2}	σ_{C3-C4}	0.1168	3.42
σ_{C1-C2}	σ_{C3-H6}	-0.0365	1.23
σ_{C1-C2}	σ_{C4-H5}	-0.1020	3.81
σ_{C1-C2}	σ_{C4-H8}	0.0961	1.35
σ_{C1-C3}	σ_{C2-H7}	-0.0850	4.11
σ_{C1-C3}	σ_{C2-H9}	0.1104	3.63
σ_{C1-C3}	σ_{C4-H5}	0.1105	3.63
σ_{C1-C3}	σ_{C4-H8}	-0.0850	4.11
σ_{C1-C4}	σ_{C2-C3}	0.1170	3.45
σ_{C1-C4}	σ_{C2-H7}	0.0962	1.36
σ_{C1-C4}	σ_{C2-H9}	-0.1019	3.80
σ_{C1-C4}	σ_{C3-H6}	-0.0366	1.23
σ_{C1-F10}	σ_{C2-C3}	-0.0737	1.66
σ_{C1-F10}	σ_{C2-H7}	-0.0665	1.03
σ_{C1-F10}	σ_{C3-C4}	-0.0737	1.66
σ_{C1-F10}	σ_{C4-H8}	-0.0665	1.03
σ_{C2-C3}	σ_{C4-H5}	-0.1154	4.58
σ_{C2-C3}	σ_{C4-H8}	0.0950	1.47
σ_{C2-H7}	σ_{C3-C4}	0.0950	1.47
σ_{C2-H7}	σ_{C3-H6}	-0.0594	1.15
σ_{C2-H7}	σ_{C4-H8}	0.0716	0.55
σ_{C2-H9}	σ_{C3-C4}	-0.1154	4.58
σ_{C2-H9}	σ_{C3-H6}	0.0731	1.16
σ_{C3-H6}	σ_{C4-H5}	0.0731	1.16
σ_{C3-H6}	σ_{C4-H8}	-0.0594	1.16

Table S6. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for **1-FBCB(TS)**.

NLMO (i)	NLMO (j)	$S_{(i,j)}$	$\Delta E_{(i,j)}$
n_{F10}	σ_{C2-C3}	-0.0673	-1.18
n_{F10}	σ_{C3-C4}	-0.0673	-1.18
n_{F10}	σ_{C1-C2}	0.1431	8.44
n_{F10}	σ_{C1-C4}	-0.1431	8.44
n_{F10}	σ_{C1-C3}	0.1492	12.03
σ_{C1-C2}	σ_{C3-C4}	0.2570	21.23
σ_{C1-C2}	σ_{C3-H6}	-0.0809	3.62
σ_{C1-C2}	σ_{C4-H5}	-0.0508	0.98
σ_{C1-C2}	σ_{C4-H8}	-0.0508	0.98
σ_{C1-C3}	σ_{C2-H7}	0.2359	17.27
σ_{C1-C3}	σ_{C2-H9}	-0.2358	17.26
σ_{C1-C3}	σ_{C4-H5}	-0.2358	17.26
σ_{C1-C3}	σ_{C4-H8}	0.2359	17.27
σ_{C1-C4}	σ_{C2-C3}	0.2570	21.22
σ_{C1-C4}	σ_{C2-H7}	-0.0508	0.98
σ_{C1-C4}	σ_{C2-H9}	-0.0508	0.98
σ_{C1-C4}	σ_{C3-H6}	-0.0809	3.62
σ_{C1-F0}	σ_{C2-C3}	-0.1215	3.50
σ_{C1-F0}	σ_{C3-C4}	-0.1215	3.50
σ_{C2-C3}	σ_{C4-H5}	-0.0443	0.88
σ_{C2-C3}	σ_{C4-H8}	-0.0443	0.88
σ_{C2-H7}	σ_{C3-C4}	-0.0443	0.88
σ_{C2-H9}	σ_{C3-C4}	-0.0443	0.88

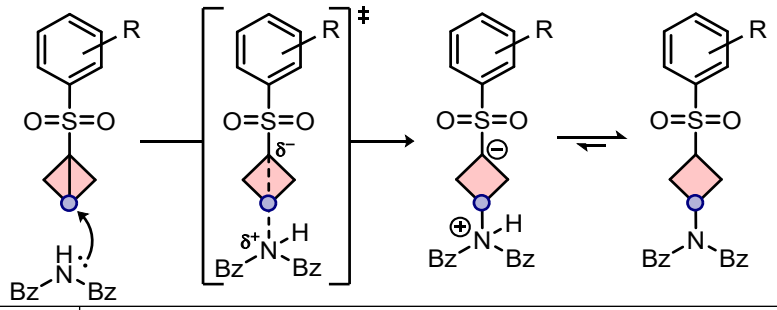
Table S7. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for **2-FBCB(Min)**.

NLMO (i)	NLMO (j)	$S_{(i,j)}$	$\Delta E_{(i,j)}$
n_{F10}	σ_{C1-C2}	-0.0898	2.16
n_{F10}	σ_{C1-C3}	-0.0815	0.78
n_{F10}	σ_{C2-C3}	-0.0898	2.16
n_{F10}	σ_{C2-H7}	0.1201	7.46
n_{F10}	σ_{C1-C2}	-0.1286	7.36
n_{F10}	σ_{C2-C3}	0.1287	7.36
σ_{C1-C2}	σ_{C3-C4}	0.1345	4.76
σ_{C1-C2}	σ_{C3-H6}	-0.0391	1.30
σ_{C1-C2}	σ_{C4-H5}	-0.1114	4.45
σ_{C1-C2}	σ_{C4-H8}	0.1011	1.47
σ_{C1-C3}	σ_{C2-H7}	-0.0792	3.89
σ_{C1-C3}	σ_{C2-F1}	0.1014	3.09
σ_{C1-C3}	σ_{C4-H5}	0.1025	3.21
σ_{C1-C3}	σ_{C4-H8}	-0.0875	4.21
σ_{C1-C4}	σ_{C2-C3}	0.1345	4.76
σ_{C1-C4}	σ_{C2-H7}	0.0779	0.70
σ_{C1-C4}	σ_{C2-F1}	-0.1022	2.94
σ_{C1-C4}	σ_{C3-H6}	-0.0501	1.80
σ_{C1-H9}	σ_{C2-C3}	-0.0391	1.30
σ_{C1-H9}	σ_{C2-H7}	-0.0465	0.82
σ_{C1-H9}	σ_{C3-C4}	-0.0501	1.80
σ_{C1-H9}	σ_{C4-H5}	0.0633	0.99
σ_{C1-H9}	σ_{C4-H8}	-0.0588	1.24
σ_{C2-C3}	σ_{C4-H5}	-0.1114	4.45
σ_{C2-C3}	σ_{C4-H8}	0.1011	1.47
σ_{C2-H7}	σ_{C3-C4}	0.0779	0.70
σ_{C2-H7}	σ_{C3-H6}	-0.0465	0.82
σ_{C2-H7}	σ_{C4-H8}	0.0702	0.58
σ_{C2-F0}	σ_{C3-C4}	-0.1022	2.94
σ_{C3-H6}	σ_{C4-H5}	0.0633	0.99
σ_{C3-H6}	σ_{C4-H8}	-0.0588	1.24

Table S8. Pairwise steric exchange energies $\Delta E_{(i,j)}$ (kcal mol^{-1}) and associated pre-NLMO overlaps S(i,j) (au) for interactions between NLMOs (i, j) as obtained by Natural Steric analysis at the B3LYP/6-311+G** level for **2-FBCB(TS)**.

NLMO (i)	NLMO (j)	$S_{(i,j)}$	$\Delta E_{(i,j)}$
n_{F10}	σ_{C1-C2}	-0.0760	1.29
n_{F10}	σ_{C1-C3}	0.0621	1.74
n_{F10}	σ_{C2-C3}	-0.0760	1.29
n_{F10}	σ_{C2-H7}	0.1190	5.77
n_{F10}	σ_{C1-C2}	0.1132	4.32
n_{F10}	σ_{C2-C3}	-0.1132	4.32
σ_{C1-C2}	σ_{C3-C4}	0.2927	24.69
σ_{C1-C2}	σ_{C3-H6}	-0.0956	4.35
σ_{C1-C2}	σ_{C4-H5}	-0.0427	0.93
σ_{C1-C2}	σ_{C4-H8}	-0.0371	0.68
σ_{C1-C3}	σ_{C2-H7}	0.1539	7.20
σ_{C1-C3}	σ_{C2-F10}	-0.2734	20.46
σ_{C1-C3}	σ_{C4-H5}	-0.1989	13.34
σ_{C1-C3}	σ_{C4-H8}	0.2340	15.71
σ_{C1-C4}	σ_{C2-C3}	0.2927	24.69
σ_{C1-C4}	σ_{C2-H7}	-0.0806	2.57
σ_{C1-C4}	σ_{C3-H6}	-0.0921	3.97
σ_{C1-H9}	σ_{C2-C3}	-0.0956	4.35
σ_{C1-H9}	σ_{C3-C4}	-0.0921	3.97
σ_{C2-C3}	σ_{C4-H5}	-0.0427	0.93
σ_{C2-C3}	σ_{C4-H8}	-0.0371	0.68
σ_{C2-H7}	σ_{C3-C4}	-0.0806	2.57

Table S9. Experimental conversion rates (Baran *et al*[7]) and calculated LUMO (au), $\Delta H^{\ddagger}(TS_N)$ (kcal mol^{-1}) and $\Delta G^{\ddagger}(TS_N)$ (kcal mol^{-1}) for the for the reaction of dibenzylamine with sulfonylated BCBs.



R	Conversion (24h)	LUMO	$\Delta H^{\ddagger}(TS_N)$	$\Delta G^{\ddagger}(TS_N)$
4-OMe	16%	-0.04601	14.9	27.9
4-Me	10%	-0.05423	15.2	27.9
4-F	40%	-0.06053	13.7	26.1
4-Cl	59%	-0.06800	13.4	25.5
4-CF_3	79%	-0.07850	12.6	24.8
3,5-diF	87%	-0.07090	12.0	24.3

Optimised Cartesian Coordinates

Ring Inversion Barriers (B3LYP/6-311+G)**

BCB(Min)

Electronic Energy = -155.991199645 au
Enthalpy = -155.900644 au
Gibbs Free Energy = -155.930772 au
Lowest Harmonic Vibrational Frequency (LHVF) = 425.22 cm-1

C	-0.000002	0.746299	-0.317785
C	1.137408	0.000056	0.313321
C	-0.000002	-0.746420	-0.317519
C	-1.137405	0.000056	0.313333
H	-2.083256	-0.000041	-0.221489
H	-1.236908	0.000285	1.400136
H	-0.000006	-1.428825	-1.152419
H	2.083253	-0.000041	-0.221512
H	1.236924	0.000285	1.400123
H	-0.000006	1.428396	-1.152938

BCB(TS)

Electronic Energy = -155.873328674 au
Enthalpy = -155.786216 au
Gibbs Free Energy = -155.816431 au
Lowest Harmonic Vibrational Frequency (LHVF) = 694.03*i* cm-1

C	0.000000	0.955553	0.000001
C	1.172525	-0.000000	-0.000000
C	-0.000000	-0.955552	0.000000
C	-1.172525	-0.000000	-0.000001
H	-1.835860	-0.000000	-0.886546
H	-1.835861	0.000000	0.886545
H	-0.000000	-2.047449	0.000001
H	1.835861	-0.000001	-0.886546
H	1.835861	-0.000000	0.886546
H	-0.000001	2.047450	-0.000000

1-FBCB(Min)

Electronic Energy = -255.250011409 au
Enthalpy = -255.166585 au
Gibbs Free Energy = -255.199086 au
Lowest Harmonic Vibrational Frequency (LHVF) = 320.45 cm-1

C	-0.865204	0.000008	0.683710
C	-0.616470	-1.154963	-0.272260
C	0.306248	-0.000003	-0.197672
C	-0.616447	1.154969	-0.272263
H	-0.261190	2.072702	0.188701
H	-0.261235	-2.072706	0.188697
H	-1.257394	-1.302599	-1.143126
H	-0.970471	0.000018	1.755857
F	1.639878	-0.000011	0.055990
H	-1.257368	1.302626	-1.143132

1-FBCB(TS)

Electronic Energy = -255.163887944 au
Enthalpy = -255.083166 au
Gibbs Free Energy = -255.115925 au
Lowest Harmonic Vibrational Frequency (LHVF) = 385.11*i* cm-1

C	1.408330	-0.000081	-0.000365
C	0.462478	1.192461	0.000194
C	-0.412680	0.000019	-0.000108
C	0.462269	-1.192503	0.000117
H	0.428010	-1.844401	0.893572
H	0.428297	1.844339	0.893674
H	0.428309	1.844878	-0.892871
H	2.494342	-0.000189	0.000021
F	-1.747728	0.000063	-0.000086
H	0.428218	-1.844566	-0.892649

2-FBCB(Min)

Electronic Energy = -255.263599043 au
Enthalpy = -255.179699 au
Gibbs Free Energy = -255.211975 au
Lowest Harmonic Vibrational Frequency (LHVF) = 264.57 cm-1

C	0.593366	-0.389673	-0.764474
C	1.213375	0.744616	0.000221
C	0.594129	-0.389725	0.764039
C	-0.654575	-0.529411	0.000253
H	-1.173568	-1.481838	0.001234
H	1.055132	-1.079134	1.455307
H	2.298972	0.792562	-0.000061
H	0.722522	1.712563	0.000295
H	1.054026	-1.077747	-1.457386
F	-1.603873	0.502084	0.000042

2-FBCB(TS)

Electronic Energy = -255.176164985 au
Enthalpy = -255.095295 au
Gibbs Free Energy = -255.127948 au
Lowest Harmonic Vibrational Frequency (LHVF) = 518.30*i* cm-1

C	-0.462735	0.965142	0.166215
C	-1.546485	0.000001	-0.292784
C	-0.462738	-0.965143	0.166215
C	0.551395	0.000001	0.546008
H	1.126059	0.000000	1.472229
H	-0.390663	-2.047846	0.073973
H	-2.482545	0.000003	0.280818
H	-1.805189	0.000002	-1.362900
H	-0.390657	2.047844	0.073972
F	1.718485	-0.000001	-0.450223

1,2-FBCB(Min)

Electronic Energy = -354.522383983 au
Enthalpy = -354.445709 au
Gibbs Free Energy = -354.480364 au
Lowest Harmonic Vibrational Frequency (LHVF) = 235.15 cm-1

C	0.034911	0.743947	0.868628
C	-0.501056	1.279216	-0.450091
C	-0.563979	-0.172576	-0.168220

1,2-FBCB(TS)

Electronic Energy = -354.460627666 au
Enthalpy = -354.386135 au
Gibbs Free Energy = -354.420584 au
Lowest Harmonic Vibrational Frequency (LHVF) = 261.18*i* cm-1

C	0.300808	1.363278	0.160222
C	-1.132544	1.064355	-0.281841
C	-0.602032	-0.261314	0.153933

C	0.760467	-0.447794	0.377474	C	0.762703	0.034660	0.528742
H	0.874177	-1.289854	1.052249	H	1.235994	-0.245139	1.470890
H	-1.448382	1.808048	-0.384527	H	-1.945956	1.490691	0.318896
H	0.183468	1.665246	-1.199812	H	-1.382698	1.173106	-1.348566
H	-0.252932	1.005802	1.874975	H	0.881227	2.272049	0.038291
F	-1.659333	-0.965434	-0.160397	F	-1.177215	-1.437007	0.015068
F	1.910623	-0.324121	-0.407339	F	1.759195	-0.551502	-0.442385
1,3-FBCB(Min) Electronic Energy = -354.502390266 au Enthalpy = -354.425783 au Gibbs Free Energy = -354.460775 au Lowest Harmonic Vibrational Frequency (LHVF) = 137.38 cm-1				**1,3-FBCB(TS)** Electronic Energy = -354.444182815 au Enthalpy = -354.369719 au Gibbs Free Energy = -354.403631 au Lowest Harmonic Vibrational Frequency (LHVF) = 175.02*i* cm-1			
C	0.727749	0.000001	0.133134	C	0.897300	-0.000002	0.199190
C	-0.000004	-1.165857	0.735335	C	0.000000	1.181144	-0.013728
C	-0.727767	0.000001	0.133145	C	-0.897300	-0.000001	0.199191
C	-0.000004	1.165868	0.735320	C	-0.000000	-1.181150	-0.013715
H	-0.000022	2.061066	0.116808	H	-0.000001	-1.968482	0.746128
H	-0.000022	-2.061070	0.116852	H	0.000001	1.968459	0.746132
H	0.000031	-1.354313	1.810726	H	-0.000001	1.646411	-1.026336
F	-1.708259	-0.000006	-0.793153	F	-2.201601	0.000006	-0.092509
F	1.708274	-0.000006	-0.793147	F	2.201601	0.000006	-0.092509
H	0.000032	1.354355	1.810712	H	-0.000000	-1.646432	-1.026389
2,2-FBCB(Min) Electronic Energy = -354.534295152 au Enthalpy = -354.457944 au Gibbs Free Energy = -354.492098 au Lowest Harmonic Vibrational Frequency (LHVF) = 245.30 cm-1				**2,2-FBCB(TS)** Electronic Energy = -354.459495726 au Enthalpy = -354.385856 au Gibbs Free Energy = -354.420058 au Lowest Harmonic Vibrational Frequency (LHVF) = 494.19*i* cm-1			
C	0.698679	-0.425707	0.776190	C	-0.679026	0.000918	0.975292
C	1.759256	0.295690	-0.000010	C	-1.850772	-0.000173	0.000004
C	0.698654	-0.425591	-0.776268	C	-0.679036	0.001017	-0.975296
C	-0.463852	0.008053	0.000021	C	0.385967	0.000182	0.000003
H	1.780371	1.381684	0.000051	H	-2.494030	-0.890455	-0.000037
H	2.740171	-0.170257	-0.000061	H	-2.495702	0.888865	0.000052
H	0.780093	-1.255621	1.461172	H	-0.637597	-0.000155	2.062390
H	0.780010	-1.255430	-1.461383	H	-0.637614	0.000093	-2.062394
F	-0.912052	1.302718	0.000135	F	1.288194	-1.087565	-0.000053
F	-1.558734	-0.793278	-0.000066	F	1.289822	1.086452	0.000050
***cis*-2,4-FBCB(Min)** Electronic Energy = -354.530224670 au Enthalpy = -354.453272 au Gibbs Free Energy = -354.487615 au Lowest Harmonic Vibrational Frequency (LHVF) = 177.45 cm-1				***cis*-2,4-FBCB(TS)** Electronic Energy = -354.464809647 au Enthalpy = -354.390551 au Gibbs Free Energy = -354.425068 au Lowest Harmonic Vibrational Frequency (LHVF) = 420.20*i* cm-1			
C	-0.000000	-0.846433	0.782293	C	-0.000003	0.489145	0.970150
C	-1.128561	-0.306098	0.000049	C	1.112091	0.454121	-0.000033
C	-0.000000	-0.846508	-0.782306	C	-0.000003	0.489005	-0.970218
C	1.128572	-0.306059	0.000049	C	-1.112088	0.454093	-0.000033
H	-2.061907	-0.861705	0.000035	H	1.914731	1.192692	-0.000086
H	0.000009	-1.668412	1.485051	H	-0.000007	0.381766	2.052879
H	0.000008	-1.668291	-1.485275	H	-0.000006	0.381466	-2.052932
F	1.419130	1.049477	-0.000020	F	-1.841294	-0.803713	0.000057
F	-1.419139	1.049489	-0.000020	F	1.841298	-0.803715	0.000058
H	2.061902	-0.861699	0.000035	H	-1.914745	1.192737	-0.000083
***trans*-2,4-FBCB(Min)** Electronic Energy = -354.530596512 au Enthalpy = -354.453922 au Gibbs Free Energy = -354.488426 au Lowest Harmonic Vibrational Frequency (LHVF) =				***trans*-2,4-FBCB(TS)** Electronic Energy = -354.465455469 au Enthalpy = -354.391228 au Gibbs Free Energy = -354.425779 au Lowest Harmonic Vibrational Frequency (LHVF) =			

180.13 cm-1				423.33*i* cm-1			
C	0.042796	0.519593	0.776990	C	-0.000004	0.971583	0.000040
C	-1.198495	0.461247	0.000095	C	0.979401	-0.000000	0.518075
C	0.042794	0.519959	-0.776911	C	-0.000005	-0.971580	0.000040
C	0.840443	-0.467307	-0.000062	C	-0.979366	-0.000000	-0.518067
H	0.397046	1.245289	1.493662	H	0.000010	2.059114	-0.000022
H	0.396615	1.245205	-1.494295	H	0.000008	-2.059111	-0.000021
F	2.202962	-0.236120	0.000064	F	-2.216194	-0.000001	0.257124
H	0.647026	-1.534446	-0.000738	H	-1.349407	-0.000000	-1.544845
H	-1.857996	1.321468	0.000384	H	1.349487	-0.000000	1.544836
F	-1.974954	-0.705931	-0.000028	F	2.216166	-0.000001	-0.257177
1,2,2-FBCB(Min)				**1,2,2-FBCB(TS)**			
Electronic Energy = -453.789331106 au				Electronic Energy = -453.740279176 au			
Enthalpy = -453.720134 au				Enthalpy = -453.672947 au			
Gibbs Free Energy = -453.756669 au				Gibbs Free Energy = -453.709028 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 200.28 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 240.65*i* cm-1			
C	0.288185	-0.598771	0.998027	C	-0.043415	1.416521	0.002377
C	-0.680220	-0.039205	0.045050	C	0.599357	0.126722	0.000455
C	0.735611	0.145272	-0.265361	C	-0.774739	-0.320532	0.001758
C	1.274136	-1.202274	0.014667	C	-1.512107	0.981158	-0.000260
H	0.398557	-0.396390	2.051859	H	0.396019	2.407885	-0.000304
H	0.993966	-2.054802	-0.598608	H	-2.106096	1.206102	-0.896385
F	-1.525179	-0.807387	-0.708538	F	1.419186	-0.233546	-1.086085
F	-1.372524	1.054103	0.439310	F	1.422048	-0.235576	1.083807
F	1.408656	1.290706	-0.461064	F	-1.262894	-1.535791	-0.000224
H	2.302624	-1.215738	0.365079	H	-2.109562	1.207006	0.893230
1,2,3-FBCB(Min)				**1,2,3-FBCB(TS)**			
Electronic Energy = -453.774869568 au				Electronic Energy = -453.735096079 au			
Enthalpy = -453.705116 au				Enthalpy = -453.667061 au			
Gibbs Free Energy = -453.742253 au				Gibbs Free Energy = -453.703439 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 145.71 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 117.15*i* cm-1			
C	0.257490	0.752736	-0.063358	C	0.903694	-0.357204	0.181535
C	-0.875307	-0.000053	0.486113	C	0.000001	0.715669	0.549015
C	0.257514	-0.752768	-0.063394	C	-0.903695	-0.357199	0.181530
C	0.565253	0.000021	-1.323733	C	-0.000002	-1.487305	-0.223675
H	1.618692	0.000072	-1.597748	H	-0.000008	-2.387220	0.403269
F	-2.135658	-0.000082	-0.120073	F	0.000005	1.852722	-0.422096
F	0.971901	-1.739695	0.503519	F	-2.198380	-0.269773	-0.052338
H	-0.124100	0.000029	-2.164684	H	0.000001	-1.776211	-1.287324
H	-0.995894	-0.000051	1.566106	H	-0.000001	1.261120	1.494568
F	0.971712	1.739815	0.503504	F	2.198378	-0.269778	-0.052338
***cis*-1,2,4-FBCB(Min)**				***cis*-1,2,4-FBCB(TS)**			
Electronic Energy = -453.775392318 au				Electronic Energy = -453.745089866 au			
Enthalpy = -453.706060 au				Enthalpy = -453.677207 au			
Gibbs Free Energy = -453.743004 au				Gibbs Free Energy = -453.713456 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 159.14 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 178.60*i* cm-1			
C	-0.000012	-0.932452	-0.458455	C	0.000000	-1.227292	-0.565124
C	1.139384	-0.528072	0.420184	C	-1.134546	-0.289329	-0.444917
C	0.000020	0.391401	0.290499	C	0.000000	0.635641	-0.348359
C	-1.139372	-0.528010	0.420153	C	1.134547	-0.289329	-0.444916
H	-1.448778	-1.039279	1.330433	H	1.906249	-0.189980	-1.209609
F	2.261604	-0.125904	-0.278359	F	-1.897995	-0.411450	0.775889
F	0.000051	1.690580	-0.023122	F	0.000000	1.902203	-0.020338
H	1.448799	-1.039341	1.330445	H	-1.906249	-0.189981	-1.209610
F	-2.261664	-0.125882	-0.278331	F	1.897995	-0.411451	0.775889
H	-0.000058	-1.287734	-1.476856	H	-0.000000	-2.311896	-0.543845
***trans*-1,2,4-FBCB(Min)**				***trans*-1,2,4-FBCB(TS)**			

Electronic Energy = -453.785864433 au
Enthalpy = -453.716334 au
Gibbs Free Energy = -453.753177 au
Lowest Harmonic Vibrational Frequency (LHVF) = 162.35 cm-1

C	0.101453	-0.552737	0.923657
C	-0.710243	-0.749000	-0.323744
C	-0.049858	0.558864	-0.127506
C	1.260946	0.155947	0.349665
F	-2.072137	-0.727236	-0.115372
F	-0.620365	1.772295	-0.147198
H	-0.467144	-1.455172	-1.111734
H	-0.200286	-0.707300	1.948390
H	1.805660	0.840028	0.991608
F	2.164501	-0.506836	-0.488618

Electronic Energy = -453.745563097 au
Enthalpy = -453.677702 au
Gibbs Free Energy = -453.714021 au
Lowest Harmonic Vibrational Frequency (LHVF) = 194.70*i* cm-1

C	0.000026	-1.288020	0.000060
C	-1.007168	-0.339983	-0.511348
C	-0.000012	0.591988	0.000020
C	1.007228	-0.339927	0.511344
F	-2.236149	-0.323243	0.258265
F	-0.000074	1.900078	0.000010
H	-1.367112	-0.327450	-1.542040
H	0.000025	-2.372451	0.000091
H	1.367215	-0.327329	1.542019
F	2.236159	-0.323181	-0.258333

2,2,4-FBCB(Min)
Electronic Energy = -453.798585462 au
Enthalpy = -453.729539 au
Gibbs Free Energy = -453.765918 au
Lowest Harmonic Vibrational Frequency (LHVF) = 157.30 cm-1

C	-0.275709	-0.325265	-0.790738
C	0.907665	-0.005514	-0.000050
C	-0.275746	-0.325468	0.790771
C	-1.273726	0.441990	0.000036
F	1.475362	1.240851	0.000060
H	-0.443159	-1.118673	-1.503580
H	-1.347200	1.524804	0.000172
F	-2.537282	-0.113093	-0.000032
F	1.921761	-0.905707	-0.000038
H	-0.443123	-1.119050	1.503377

2,2,4-FBCB(TS)
Electronic Energy = -453.746440771 au
Enthalpy = -453.679650 au
Gibbs Free Energy = -453.715878 au
Lowest Harmonic Vibrational Frequency (LHVF) = 373.61*i* cm-1

C	-0.245555	-0.276125	0.981720
C	0.798199	0.016165	-0.000000
C	-0.245551	-0.276123	-0.981718
C	-1.319215	-0.549374	-0.000002
F	1.917428	-0.816402	0.000000
H	-0.249847	-0.219928	2.066853
H	-1.890985	-1.478024	-0.000005
F	-2.343869	0.467771	-0.000001
F	1.366818	1.285367	0.000000
H	-0.249838	-0.219932	-2.066851

1,2,2,3-FBCB(Min)
Electronic Energy = -553.038861739 au
Enthalpy = -552.976476 au
Gibbs Free Energy = -553.015500 au
Lowest Harmonic Vibrational Frequency (LHVF) = 145.93 cm-1

C	-0.486589	-0.766016	0.118889
C	0.765121	-0.000051	0.090786
C	-0.486563	0.765979	0.118764
C	-1.279424	0.000078	1.131224
F	1.443455	-0.000105	-1.078367
H	-2.349536	0.000119	0.930988
F	1.691111	0.000014	1.098336
H	-1.016120	0.000162	2.186917
F	-0.884398	1.767815	-0.669791
F	-0.884569	-1.767749	-0.669720

1,2,2,3-FBCB(TS)
Electronic Energy = -553.011968486 au
Enthalpy = -552.950985 au
Gibbs Free Energy = -552.989091 au
Lowest Harmonic Vibrational Frequency (LHVF) = 110.82*i* cm-1

C	0.917684	0.516921	-0.000042
C	0.000002	-0.595673	0.000163
C	-0.917688	0.516918	-0.000052
C	-0.000004	1.710474	0.000477
F	-0.000002	-1.489293	1.083710
H	-0.000012	2.341886	0.899561
F	0.000009	-1.489458	-1.083380
H	0.000016	2.342523	-0.898155
F	-2.229830	0.512913	-0.000427
F	2.229827	0.512921	-0.000423

1,2,2,4-FBCB(Min)
Electronic Energy = -553.050483972 au
Enthalpy = -552.988498 au
Gibbs Free Energy = -553.027260 au
Lowest Harmonic Vibrational Frequency (LHVF) = 139.95 cm-1

C	0.151733	-0.569046	0.875405
C	-0.997646	-0.177204	0.056589
C	0.264673	0.433399	-0.330486
C	1.178368	-0.719742	-0.205720
F	-1.915800	0.630191	0.635936
F	-1.679152	-1.058381	-0.738398
H	1.229031	-1.554073	-0.899595

1,2,2,4-FBCB(TS)
Electronic Energy = -553.022930046 au
Enthalpy = -552.962419 au
Gibbs Free Energy = -553.000367 au
Lowest Harmonic Vibrational Frequency (LHVF) = 156.45*i* cm-1

C	0.128800	-1.239110	-0.347129
C	-0.876396	-0.244047	0.011496
C	0.262300	0.653696	-0.177190
C	1.287409	-0.336874	-0.542692
F	-1.468116	-0.303583	1.263931
F	-1.967609	-0.081884	-0.834974
H	1.840590	-0.281295	-1.481403

F	0.578957	1.718591	-0.473884	F	0.373099	1.933437	0.031238
F	2.448499	-0.370231	0.196352	F	2.315837	-0.481262	0.449112
H	0.295666	-0.531889	1.944813	H	0.067827	-2.321071	-0.369282
***cis*-1,2,3,4-FBCB(Min)**				***cis*-1,2,3,4-FBCB(TS)**			
Electronic Energy = -553.024155576 au				Electronic Energy = -553.015594128 au			
Enthalpy = -552.961568 au				Enthalpy = -552.954266 au			
Gibbs Free Energy = -553.000941 au				Gibbs Free Energy = -552.992398 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 123.02 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 71.79*i* cm-1			
C	0.000000	-0.763530	0.149740	C	-0.000024	0.903833	-0.369325
C	1.145915	-0.000001	0.698618	C	1.154616	0.000031	-0.457024
C	-0.000001	0.763529	0.149745	C	0.000024	-0.903834	-0.369325
C	-1.145917	-0.000004	0.698616	C	-1.154617	-0.000031	-0.457023
F	2.245237	0.000002	-0.141084	F	1.993741	0.000054	0.705573
H	-1.492817	-0.000008	1.732105	H	-1.863538	-0.000050	-1.287337
F	-0.000001	1.849261	-0.616936	F	0.000059	-2.165990	-0.011636
F	-2.245237	-0.000001	-0.141088	F	-1.993741	-0.000053	0.705573
H	1.492813	-0.000005	1.732109	H	1.863538	0.000050	-1.287338
F	0.000003	-1.849256	-0.616950	F	-0.000058	2.165990	-0.011636
***trans*-1,2,3,4-FBCB(Min)**				***trans*-1,2,3,4-FBCB(TS)**			
Electronic Energy = -553.036313990 au				Electronic Energy = -553.017439854 au			
Enthalpy = -552.973628 au				Enthalpy = -552.956060 au			
Gibbs Free Energy = -553.012930 au				Gibbs Free Energy = -552.994234 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 131.47 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 81.75*i* cm-1			
C	0.045216	0.772500	-0.153215	C	-0.000075	0.916216	-0.000404
C	1.282214	0.000003	-0.254890	C	-1.025400	-0.000006	0.507436
C	0.045220	-0.772498	-0.153216	C	-0.000065	-0.916216	-0.000404
C	-0.706490	-0.000001	0.876861	C	1.025596	0.000006	-0.507507
F	2.236426	0.000004	0.769219	F	-2.249568	-0.000013	-0.258847
F	-0.377666	-1.817382	-0.864709	F	0.000110	-2.226318	-0.000115
H	1.792121	0.000003	-1.214713	H	-1.379011	-0.000009	1.541186
F	-0.377677	1.817380	-0.864710	F	0.000084	2.226319	-0.000115
F	-2.068828	-0.000004	0.668775	F	2.249240	0.000012	0.259644
H	-0.499360	-0.000001	1.944287	H	1.379884	0.000009	-1.541010
2,2,4,4-FBCB(Min)				**2,2,4,4-FBCB(TS)**			
Electronic Energy = -553.069795634 au				Electronic Energy = -553.026065837 au			
Enthalpy = -553.008196 au				Enthalpy = -552.966815 au			
Gibbs Free Energy = -553.046276 au				Gibbs Free Energy = -553.004736 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 143.13 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 326.01*i* cm-1			
C	-0.000037	-0.537181	0.811478	C	-0.000001	0.000185	0.991078
C	1.107944	-0.020253	-0.000001	C	-1.082091	0.000032	-0.000000
C	-0.000038	-0.537165	-0.811493	C	0.000001	0.000184	-0.991079
C	-1.107913	-0.020022	-0.000001	C	1.082092	0.000036	0.000002
F	2.244333	-0.761943	-0.000015	F	-1.943806	1.086035	-0.000002
H	-0.000149	-1.357718	1.514832	H	-0.000002	0.000279	2.076809
H	-0.000150	-1.357691	-1.514882	H	0.000002	0.000287	-2.076809
F	-2.244348	-0.761927	-0.000014	F	1.943810	1.086032	0.000002
F	-1.476286	1.284324	0.000023	F	1.943504	-1.086211	-0.000002
F	1.476364	1.284339	0.000022	F	-1.943508	-1.086209	0.000001
1,2,2,4,4-FBCB(Min)				**1,2,2,4,4-FBCB(TS)**			
Electronic Energy = -652.321878863 au				Electronic Energy = -652.299126866 au			
Enthalpy = -652.267383 au				Enthalpy = -652.246065 au			
Gibbs Free Energy = -652.307901 au				Gibbs Free Energy = -652.285671 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 124.47 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 127.51*i* cm-1			
C	0.000000	-0.165631	1.061479	C	-0.000000	-1.229484	0.000563
C	-1.121977	-0.226988	0.111648	C	-1.103992	-0.267036	0.000049
C	-0.000000	0.568524	-0.391656	C	0.000000	0.700679	-0.000118

C	1.121977	-0.226988	0.111648	C	1.103992	-0.267037	0.000048
F	-2.226941	0.472604	0.460224	F	-1.961741	-0.257356	1.084276
H	-0.000000	0.162611	2.091331	H	-0.000000	-2.312865	0.001251
F	2.226941	0.472604	0.460224	F	1.961739	-0.257357	1.084277
F	1.538333	-1.378553	-0.471273	F	1.961530	-0.258083	-1.084338
F	-1.538334	-1.378553	-0.471273	F	-1.961529	-0.258083	-1.084339
F	0.000000	1.827885	-0.805685	F	0.000000	1.996449	-0.000377
1,2,3,4,4-FBCB(Min)				**1,2,3,4,4-FBCB(TS)**			
Electronic Energy = -652.298675343 au				Electronic Energy = -652.291239405 au			
Enthalpy = -652.243441 au				Enthalpy = -652.237141 au			
Gibbs Free Energy = -652.284772 au				Gibbs Free Energy = -652.277000 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 103.04 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 65.01*i* cm-1			
C	0.179830	-0.796908	0.000504	C	-0.189239	0.926933	-0.197155
C	1.156771	-0.000001	-0.787147	C	-1.287514	0.000001	-0.526177
C	0.179830	0.796909	0.000501	C	-0.189240	-0.926934	-0.197155
C	-1.031728	0.000001	-0.166544	C	0.916052	-0.000000	0.017205
F	-1.787088	-0.000001	-1.311247	F	1.972903	-0.000001	-0.883874
F	-1.901300	0.000002	0.871893	F	1.555718	-0.000000	1.242114
F	2.417303	-0.000001	-0.224687	F	-2.350102	0.000001	0.426457
F	0.404560	1.862181	0.753541	F	-0.239554	-2.217185	-0.008317
F	0.404558	-1.862182	0.753542	F	-0.239552	2.217185	-0.008317
H	1.249478	-0.000002	-1.871268	H	-1.795070	0.000001	-1.492870
Perfluoro-FBCB(Min)				**Perfluoro-FBCB(TS)**			
Electronic Energy = -751.570549088 au				Electronic Energy = -751.564752544 au			
Enthalpy = -751.522826 au				Enthalpy = -751.518010 au			
Gibbs Free Energy = -751.566145 au				Gibbs Free Energy = -751.559555 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 77.20 cm-1				Lowest Harmonic Vibrational Frequency (LHVF) = 50.20*i* cm-1			
C	0.000004	0.845405	-0.165799	C	0.000000	0.944617	-0.000151
C	-1.129625	-0.000004	0.238463	C	1.120577	-0.000000	0.000144
C	0.000002	-0.845442	-0.165735	C	-0.000001	-0.944612	-0.000156
C	1.129615	-0.000005	0.238505	C	-1.120575	-0.000001	0.000143
F	2.190148	-0.000017	-0.607022	F	-1.974904	-0.000005	1.083315
F	1.639452	0.000052	1.501151	F	-1.975333	0.000004	-1.082668
F	-1.639507	0.000050	1.501089	F	1.975333	0.000001	-1.082668
F	0.000015	-1.908096	-0.942499	F	-0.000001	-2.243792	-0.000642
F	0.000021	1.908053	-0.942571	F	-0.000001	2.243792	-0.000637
F	-2.190125	-0.000010	-0.607104	F	1.974906	-0.000003	1.083314
Dibenzylamine Attack to Sulfonylated BCBs [SMD(DMSO)/B3LYP/6-311+G]**							
4-OMe (TS_N)				**4-Me (TS_N)**			
Electronic Energy = -1647.734603 au				Electronic Energy = -1572.502521 au			
Enthalpy = -1647.240686 au				Enthalpy = -1572.014626 au			
Gibbs Free Energy = -1647.333649 au				Gibbs Free Energy = -1572.105808 au			
Lowest Harmonic Vibrational Frequency (LHVF) = 375.24*i* cm^{-1}				Lowest Harmonic Vibrational Frequency (LHVF) = 385.17*i* cm^{-1}			
C	1.304318	1.084685	-2.371821	C	-1.145497	-2.772507	0.018316
C	0.239870	-0.010147	-2.596353	C	-0.286131	-2.254423	-1.153004
C	0.087017	0.393013	-1.174146	C	-0.026937	-1.312554	-0.032936
C	0.480071	1.821039	-1.298664	C	-0.194690	-2.245950	1.111365
H	-0.262850	2.498033	-1.728443	H	0.628732	-2.932451	1.321350
H	0.988769	2.273970	-0.450445	H	-0.610249	-1.830311	2.028027
H	0.600519	-0.201434	-0.428701	H	-0.598928	-0.393723	-0.012861
H	-0.547274	0.308818	-3.284742	H	0.518223	-2.942490	-1.421996
H	0.557998	-1.031256	-2.797619	H	-0.776323	-1.848583	-2.036519
S	2.979023	0.709150	-2.148654	S	-2.858236	-2.575840	0.090974
O	3.407097	-0.124068	-3.300922	O	-3.426115	-3.136859	-1.161283
O	3.690991	1.987169	-1.893932	O	-3.314214	-3.133074	1.389808
C	3.307389	-0.309132	-0.682910	C	-3.403653	-0.840896	0.114215
C	3.557369	0.297553	0.545978	C	-3.497182	-0.158259	1.330002

C	3.248231	-1.705112	-0.772152
C	3.752163	-0.476654	1.690146
H	3.618073	1.376419	0.616670
C	3.441266	-2.480266	0.361091
H	3.068244	-2.183044	-1.727138
C	3.692396	-1.872520	1.601431
N	-1.793096	-0.003327	-0.383760
H	-2.393695	0.614258	-0.926332
C	-2.108553	-1.412570	-0.709504
H	-1.460374	-2.044051	-0.097713
H	-1.832103	-1.566266	-1.754986
C	-1.894958	0.320218	1.057221
H	-2.818286	-0.107163	1.466596
H	-1.058104	-0.167064	1.563760
C	-1.875812	1.807402	1.331079
C	-2.909800	2.630708	0.865294
C	-0.847828	2.382705	2.084406
C	-2.908532	3.997656	1.136960
H	-3.724746	2.199841	0.291136
C	-0.848045	3.749868	2.365435
H	-0.042306	1.756717	2.454165
C	-1.876583	4.561761	1.889310
H	-3.716054	4.621080	0.768314
H	-0.043410	4.179272	2.952661
H	-1.877097	5.624805	2.104293
C	-3.559977	-1.800213	-0.506258
C	-3.947998	-2.613111	0.564036
C	-4.543169	-1.343071	-1.394443
C	-5.287926	-2.960054	0.747494
H	-3.196645	-2.981755	1.255152
C	-5.881725	-1.684988	-1.212538
H	-4.256919	-0.720106	-2.236699
C	-6.258212	-2.494906	-0.138891
H	-5.571475	-3.592821	1.581721
H	-6.630094	-1.325913	-1.910917
H	-7.299463	-2.764053	0.001454
H	3.409118	-3.562262	0.301899
H	3.954889	0.015690	2.631654
O	3.869918	-2.715089	2.651148
C	4.144374	-2.154629	3.941173
H	4.249550	-3.003824	4.614805
H	5.074894	-1.579678	3.932668
H	3.320020	-1.520830	4.280965

C	-3.693749	-0.185453	-1.081960
C	-3.885425	1.177934	1.339356
H	-3.286002	-0.671296	2.260166
C	-4.083299	1.153219	-1.055864
H	-3.634819	-0.718644	-2.022709
C	-4.186841	1.856441	0.149559
N	1.831480	-0.366546	-0.096753
H	1.919627	-0.004729	0.850956
C	2.868199	-1.398574	-0.329540
H	2.767201	-1.741287	-1.360913
H	2.633064	-2.239810	0.325587
C	1.858911	0.745539	-1.074656
H	2.898107	1.008891	-1.303562
H	1.403002	0.383299	-1.999925
C	1.136871	1.978938	-0.581677
C	1.639676	2.705128	0.506839
C	-0.018531	2.439761	-1.220171
C	0.998431	3.860505	0.948799
H	2.543527	2.369041	1.006005
C	-0.658071	3.601888	-0.785025
H	-0.416458	1.889981	-2.066825
C	-0.152895	4.313728	0.301751
H	1.401352	4.411860	1.791593
H	-1.550733	3.948091	-1.294381
H	-0.649271	5.216223	0.641457
C	4.289967	-0.936146	-0.072516
C	5.193751	-0.760754	-1.125465
C	4.723934	-0.680682	1.235433
C	6.501500	-0.336787	-0.880689
H	4.874114	-0.962047	-2.142992
C	6.027167	-0.254537	1.483203
H	4.037385	-0.821412	2.065192
C	6.920687	-0.080947	0.423876
H	7.190236	-0.207442	-1.708726
H	6.348466	-0.064818	2.501784
H	7.936381	0.247295	0.616143
H	-4.315773	1.655998	-1.989163
H	-3.963564	1.700843	2.287525
C	-4.628643	3.296912	0.177948
H	-5.635512	3.387138	0.600564
H	-3.964165	3.903129	0.800272
H	-4.648867	3.726837	-0.825526

4-F (TS_N)

Electronic Energy = -1632.443994 au
Enthalpy = -1631.992519 au
Gibbs Free Energy = -1632.081693 au
Lowest Harmonic Vibrational Frequency (LHVF) = 371.51*i* cm^{-1}

C	1.666602	0.291192	-2.275847
C	0.557709	-0.780386	-2.289264
C	0.322057	0.017552	-1.058176
C	0.807185	1.336197	-1.541352
H	0.144590	1.885387	-2.215113
H	1.273074	1.994733	-0.811905
H	0.730269	-0.358978	-0.128664
H	-0.149400	-0.638479	-3.110541
H	0.825578	-1.827793	-2.165594
S	3.292341	-0.062909	-1.814147
O	3.764508	-1.192954	-2.651342

4-Cl (TS_N)

Electronic Energy = -1992.799002 au
Enthalpy = -1992.348476 au
Gibbs Free Energy = -1992.439408 au
Lowest Harmonic Vibrational Frequency (LHVF) = 370.60*i* cm^{-1}

C	1.372085	1.321807	-2.190873
C	0.342635	0.226948	-2.533851
C	0.139507	0.529652	-1.093515
C	0.494636	1.972245	-1.106738
H	-0.249090	2.657182	-1.521453
H	0.962639	2.379655	-0.213578
H	0.633982	-0.104399	-0.368559
H	-0.428241	0.579057	-3.224075
H	0.691709	-0.770276	-2.793866
S	3.046959	0.978697	-1.953458
O	3.535795	0.253931	-3.151426

O	4.054744	1.209481	-1.837166
C	3.438174	-0.660456	-0.099608
C	3.609317	0.257138	0.939078
C	3.317187	-2.025874	0.168098
C	3.658224	-0.189623	2.257770
H	3.719626	1.312121	0.723469
C	3.364528	-2.481212	1.483779
H	3.201718	-2.733560	-0.642786
C	3.530944	-1.548666	2.495050
N	-1.652314	-0.063482	-0.368271
H	-2.160300	0.440974	-1.092396
C	-2.053105	-1.487922	-0.382870
H	-1.493563	-1.994412	0.406940
H	-1.725578	-1.900006	-1.339907
C	-1.834483	0.599520	0.942064
H	-2.834335	0.376214	1.334182
H	-1.109097	0.163967	1.633703
C	-1.652708	2.099402	0.875103
C	-2.533110	2.891771	0.126421
C	-0.625422	2.727007	1.586586
C	-2.381815	4.276502	0.081436
H	-3.346168	2.423805	-0.420721
C	-0.476259	4.114278	1.550624
H	0.061691	2.126380	2.173729
C	-1.351891	4.892580	0.794791
H	-3.071447	4.875220	-0.503884
H	0.325291	4.584702	2.109982
H	-1.235864	5.970466	0.763366
C	-3.539214	-1.732479	-0.207985
C	-4.051738	-2.244956	0.988524
C	-4.428927	-1.444524	-1.251845
C	-5.422308	-2.461757	1.142984
H	-3.373872	-2.480365	1.802873
C	-5.797785	-1.656926	-1.100108
H	-4.045887	-1.056495	-2.191019
C	-6.298757	-2.166332	0.099824
H	-5.803049	-2.861279	2.076854
H	-6.472803	-1.432361	-1.919030
H	-7.363608	-2.335439	0.217541
H	3.281777	-3.535153	1.720359
H	3.798436	0.498782	3.082397
F	3.579025	-1.990209	3.784225

O	3.717550	2.241286	-1.558957
C	3.347784	-0.160681	-0.564239
C	3.339108	-1.538853	-0.785429
C	3.520570	0.350240	0.723012
C	3.500272	-2.414602	0.285724
H	3.222123	-1.931844	-1.787406
C	3.682628	-0.519492	1.798821
H	3.543697	1.419699	0.889261
C	3.665380	-1.890968	1.564443
N	-1.773036	0.027382	-0.393592
H	-2.376831	0.641443	-0.936490
C	-2.010299	-1.378339	-0.789465
H	-1.352828	-2.006275	-0.183776
H	-1.693204	-1.472799	-1.830590
C	-1.946750	0.284713	1.052870
H	-2.869639	-0.191905	1.405622
H	-1.114058	-0.193573	1.574805
C	-1.993081	1.758555	1.388829
C	-1.030794	2.331190	2.226305
C	-3.023916	2.570051	0.896415
C	-1.091774	3.684306	2.563267
H	-0.229066	1.714017	2.618495
C	-3.082899	3.923428	1.224034
H	-3.789606	2.141056	0.256814
C	-2.115960	4.485165	2.059858
H	-0.337592	4.111468	3.215529
H	-3.886997	4.537808	0.833357
H	-2.163437	5.537512	2.317933
C	-3.447070	-1.842951	-0.652457
C	-4.424509	-1.385050	-1.546424
C	-3.827367	-2.727803	0.362033
C	-5.750291	-1.796366	-1.424374
H	-4.143687	-0.706179	-2.346229
C	-5.154291	-3.144360	0.485447
H	-3.080087	-3.097011	1.057278
C	-6.119310	-2.677886	-0.405959
H	-6.494148	-1.435301	-2.126546
H	-5.431946	-3.831832	1.277282
H	-7.150392	-3.001000	-0.312181
H	3.824480	-0.131331	2.799653
H	3.502436	-3.484938	0.121580
Cl	3.866186	-2.996383	2.926134

4-CF_3 (TS_N)

Electronic Energy = -1870.324377 au
Enthalpy = -1869.857814 au
Gibbs Free Energy = -1869.954718 au
Lowest Harmonic Vibrational Frequency (LHVF) = 369.25*i* cm^{-1}

C	-0.621087	-2.236203	-1.976101
C	0.266340	-1.102169	-2.522230
C	0.376195	-1.025302	-1.041934
C	0.239293	-2.469526	-0.723050
H	1.109379	-3.100176	-0.921926
H	-0.243203	-2.732033	0.215168
H	-0.265076	-0.326589	-0.519933
H	1.140401	-1.475740	-3.061604
H	-0.196904	-0.262075	-3.035653
S	-2.341231	-2.139975	-1.931132
O	-2.820106	-1.863018	-3.306369
O	-2.847791	-3.341133	-1.225490

3,5-DiF (TS_N)

Electronic Energy = -1731.710095 au
Enthalpy = -1731.266292 au
Gibbs Free Energy = -1731.357659 au
Lowest Harmonic Vibrational Frequency (LHVF) = 362.69*i* cm^{-1}

C	1.490925	0.052572	-2.385103
C	0.399912	-1.026639	-2.250095
C	0.177310	-0.078812	-1.127752
C	0.625124	1.174263	-1.787223
H	-0.057043	1.613852	-2.519011
H	1.089148	1.932028	-1.160702
H	0.598702	-0.326017	-0.161869
H	-0.319737	-0.996110	-3.071665
H	0.684488	-2.045944	-1.997958
S	3.130746	-0.209182	-1.929983
O	3.616706	-1.419754	-2.631969
O	3.865147	1.065632	-2.103084

C	-2.941405	-0.728822	-0.942218
C	-3.159446	-0.889924	0.428262
C	-3.123890	0.511356	-1.553284
C	-3.564282	0.199521	1.190065
H	-3.031128	-1.859346	0.892227
C	-3.527269	1.602916	-0.788363
H	-2.970324	0.624545	-2.618648
C	-3.746306	1.444372	0.579768
N	2.135262	-0.074791	-0.379915
H	2.865047	-0.713919	-0.688836
C	2.238349	1.195579	-1.130547
H	1.440628	1.852686	-0.776366
H	2.036111	0.962436	-2.178477
C	2.184206	0.088055	1.089920
H	3.015556	0.749777	1.362648
H	1.259865	0.584622	1.396085
C	2.337084	-1.225228	1.824554
C	3.499654	-1.993543	1.676513
C	1.338771	-1.680651	2.691426
C	3.653592	-3.193346	2.368743
H	4.293223	-1.648803	1.020176
C	1.493096	-2.877711	3.392443
H	0.434793	-1.094297	2.819933
C	2.649431	-3.639462	3.230012
H	4.559660	-3.776091	2.241896
H	0.708818	-3.214988	4.061659
H	2.770212	-4.571264	3.771723
C	3.578660	1.895768	-1.016571
C	4.708159	1.364902	-1.654002
C	3.717723	3.074808	-0.276934
C	5.947243	1.993556	-1.548136
H	4.615051	0.455595	-2.240478
C	4.956924	3.709513	-0.171747
H	2.850139	3.501373	0.216542
C	6.075179	3.168942	-0.804787
H	6.811308	1.571281	-2.049958
H	5.046856	4.624145	0.404516
H	7.038609	3.660484	-0.724203
H	-3.677480	2.563942	-1.263257
H	-3.744790	0.076260	2.251644
C	-4.170285	2.607893	1.426815
F	-4.479771	3.706503	0.703702
F	-5.260635	2.324468	2.186982
F	-3.198071	2.988224	2.303296
C	3.313722	-0.605983	-0.155239
C	3.239572	-1.937612	0.254490
C	3.456819	0.435134	0.762584
C	3.308359	-2.192977	1.613458
H	3.147526	-2.749213	-0.454799
C	3.517842	0.100393	2.104472
H	3.532982	1.467334	0.448139
C	3.446962	-1.202252	2.572701
H	3.504021	-1.433799	3.628447
F	3.663517	1.098631	3.015882
F	3.245910	-3.484132	2.034624
N	-1.802012	-0.085839	-0.384804
H	-2.318392	0.382432	-1.126973
C	-2.229766	-1.498772	-0.296910
H	-1.655616	-1.967528	0.505669
H	-1.940668	-1.977121	-1.235383
C	-1.935442	0.665386	0.882950
H	-2.928118	0.491259	1.316052
H	-1.199510	0.261728	1.582969
C	-1.725378	2.152527	0.706840
C	-2.630720	2.913677	-0.044396
C	-0.644002	2.800845	1.311502
C	-2.451134	4.287246	-0.197538
H	-3.484941	2.429789	-0.508705
C	-0.465627	4.177630	1.167007
H	0.062980	2.225531	1.900309
C	-1.366585	4.923986	0.408708
H	-3.160817	4.861658	-0.783262
H	0.377985	4.664524	1.644418
H	-1.228064	5.993454	0.293009
C	-3.714254	-1.701031	-0.061248
C	-4.633567	-1.436052	-1.085420
C	-4.195359	-2.149840	1.173171
C	-6.000536	-1.609609	-0.877766
H	-4.275381	-1.096361	-2.052787
C	-5.564122	-2.327683	1.383763
H	-3.494374	-2.365254	1.973429
C	-6.469993	-2.056283	0.359418
H	-6.699061	-1.403857	-1.681788
H	-5.920500	-2.677880	2.346621
H	-7.533521	-2.194933	0.520805

Dibenzylamine Attack to Fluorinated BCBs [SMD(DMSO)/B3LYP/6-311+G]**

BCB (TS_N)

Electronic Energy = -753.382855 au
Enthalpy = -753.022283 au
Gibbs Free Energy = -753.087795 au
Lowest Harmonic Vibrational Frequency (LHVF) = 383.86*i* cm^{-1}

C	-5.081634	0.002662	0.376115
C	-3.958627	1.101306	0.316262
C	-3.241210	-0.044303	-0.318756
C	-3.969478	-1.106671	0.436642
H	-4.137454	-2.062968	-0.062307
H	-3.596628	-1.270917	1.453818
H	-3.338578	-0.102503	-1.400279
H	-4.118224	1.999173	-0.283725
H	-3.583763	1.371665	1.309708

1-FBCB ($TS1_N$)

Electronic Energy = -852.654606 au
Enthalpy = -852.301758 au
Gibbs Free Energy = -852.368893 au
Lowest Harmonic Vibrational Frequency (LHVF) = 354.20*i* cm^{-1}

C	2.361165	3.280251	1.030130
C	2.497628	1.773364	0.617026
C	1.168706	2.073475	0.020920
C	0.793506	3.173314	0.948416
H	0.220491	3.995910	0.516756
H	0.323826	2.823628	1.872175
H	3.280483	1.474115	-0.081165
H	2.449245	1.073705	1.455841
H	2.705907	3.899014	0.195143

H	-5.581244	-0.048062	-0.600128
N	-1.389845	-0.046429	-0.212313
H	-1.254174	0.017411	0.796089
C	-0.884070	-1.351887	-0.709667
H	-0.949251	-1.326429	-1.798219
H	-1.592410	-2.103918	-0.351516
C	-0.863136	1.174801	-0.875706
H	-0.820912	0.970585	-1.946283
H	-1.615235	1.953372	-0.717200
C	0.476713	1.676187	-0.378057
C	1.558963	1.806724	-1.253453
C	0.637819	2.073990	0.955619
C	2.778712	2.318350	-0.807652
H	1.446395	1.508187	-2.290657
C	1.856592	2.576998	1.405715
H	-0.196130	1.993444	1.646543
C	2.932037	2.701923	0.523806
H	3.607794	2.414062	-1.500564
H	1.965179	2.879069	2.441860
H	3.879717	3.097500	0.872583
C	0.513952	-1.737576	-0.274164
C	1.530664	-1.912123	-1.217874
C	0.799222	-1.978357	1.076296
C	2.808327	-2.312259	-0.823447
H	1.320705	-1.736305	-2.267982
C	2.075476	-2.370631	1.473992
H	0.016847	-1.861298	1.820325
C	3.085039	-2.539310	0.523794
H	3.585571	-2.444156	-1.568565
H	2.281017	-2.552785	2.523362
H	4.077531	-2.849067	0.832532

N	-0.096325	0.669214	-0.140264
H	-0.139733	0.329746	0.820578
C	-1.416663	1.255212	-0.508671
H	-1.380245	1.495578	-1.571648
H	-1.510938	2.190284	0.047000
C	0.334790	-0.433241	-1.043975
H	-0.534655	-1.063367	-1.255886
H	0.648144	0.022355	-1.984421
C	1.441897	-1.288540	-0.471744
C	2.658273	-1.418495	-1.148826
C	1.251709	-2.005571	0.716822
C	3.666307	-2.244548	-0.650109
H	2.817354	-0.870526	-2.071756
C	2.260348	-2.823802	1.221987
H	0.308210	-1.929807	1.249082
C	3.471587	-2.946298	0.538804
H	4.603433	-2.335380	-1.188639
H	2.098242	-3.371189	2.144242
H	4.255255	-3.586127	0.929568
C	-2.593505	0.354334	-0.205052
C	-3.004581	0.152715	1.119538
C	-3.295402	-0.283939	-1.233220
C	-4.086578	-0.675891	1.409154
H	-2.477700	0.652150	1.927060
C	-4.382271	-1.111342	-0.945769
H	-2.993772	-0.127258	-2.263819
C	-4.778455	-1.311268	0.375802
H	-4.395104	-0.820035	2.438973
H	-4.917813	-1.597430	-1.754085
H	-5.623378	-1.952959	0.600688
F	1.205139	2.432746	-1.310138

1-FBCB (TS2$_N$)

Electronic Energy = -852.656219 au
Enthalpy = -852.303699 au
Gibbs Free Energy = -852.373955 au
Lowest Harmonic Vibrational Frequency (LHVF) = 334.09*i* cm^{-1}

C	2.624514	-3.279223	0.212122
C	1.883534	-2.573528	-0.988584
C	1.530149	-1.690406	0.141852
C	1.579525	-2.685901	1.232636
H	1.927001	-2.349948	2.209231
H	0.737104	-3.371278	1.323948
H	2.478424	-2.151822	-1.797884
H	1.104750	-3.234310	-1.368776
H	-0.190919	-0.113893	0.932681
N	-0.107789	-0.490852	-0.010211
C	0.092714	0.607947	-0.984276
H	-0.868620	1.084806	-1.206040
H	0.459629	0.158630	-1.910690
C	-1.268257	-1.362020	-0.302648
H	-1.159159	-1.720565	-1.327968
H	-1.190257	-2.223823	0.363948
C	-2.617098	-0.695073	-0.121816
C	-3.399113	-0.335980	-1.224794
C	-3.104421	-0.425624	1.164397
C	-4.638382	0.282926	-1.049863
H	-3.038559	-0.546553	-2.226630
C	-4.339578	0.194374	1.342463
H	-2.514678	-0.708038	2.031530

2-FBCB (TS$_N$)

Electronic Energy = -951.930541 au
Enthalpy = -951.585739 au
Gibbs Free Energy = -951.656327 au
Lowest Harmonic Vibrational Frequency (LHVF) = 230.92*i* cm^{-1}

C	2.858975	-2.579585	-1.048319
C	2.676233	-1.068516	-0.665503
C	1.447526	-1.615503	-0.041881
C	1.312718	-2.827712	-0.883959
H	0.976229	-3.737535	-0.388418
H	0.795731	-2.670048	-1.829029
H	3.399357	-0.603862	0.002729
H	2.502141	-0.460551	-1.551588
H	-0.292087	-0.119872	-0.896771
N	-0.211407	-0.435502	0.068381
C	-1.358119	-1.314475	0.402180
H	-1.256513	-1.601107	1.450371
H	-1.252810	-2.216752	-0.204537
C	-0.053389	0.723518	0.979006
H	-1.031733	1.191170	1.137769
H	0.284416	0.337711	1.943039
C	0.916027	1.760521	0.458787
C	0.629479	2.482352	-0.707627
C	2.096534	2.044493	1.152267
C	1.509760	3.456053	-1.175626
H	-0.290161	2.284615	-1.250480
C	2.975699	3.025323	0.690879
H	2.328570	1.495447	2.059014

C	-5.110515	0.551506	0.234022
H	-5.232795	0.553352	-1.916040
H	-4.704321	0.392613	2.344647
H	-6.073382	1.031261	0.372098
C	1.066179	1.650273	-0.482750
C	2.341916	1.773482	-1.042629
C	0.696508	2.522935	0.549514
C	3.232283	2.743955	-0.580374
H	2.639375	1.108360	-1.846658
C	1.585684	3.488690	1.017554
H	-0.295213	2.449135	0.985515
C	2.857564	3.601675	0.453018
H	4.217221	2.827877	-1.026911
H	1.284317	4.156995	1.816987
H	3.548833	4.355314	0.814217
F	3.925782	-2.624555	0.422861
H	2.214498	-0.861194	0.279464

C	2.686564	3.730834	-0.476388
H	1.274048	4.005618	-2.080619
H	3.886348	3.234643	1.241825
H	3.370043	4.491407	-0.837871
C	-2.716869	-0.690291	0.158111
C	-3.184147	-0.503204	-1.149856
C	-3.528151	-0.291656	1.225786
C	-4.429547	0.076306	-1.383941
H	-2.570866	-0.817950	-1.989027
C	-4.777972	0.285693	0.994340
H	-3.181874	-0.438524	2.243836
C	-5.230394	0.473323	-0.310880
H	-4.778940	0.211701	-2.401888
H	-5.395808	0.587446	1.833310
H	-6.201256	0.921408	-0.492459
F	1.569860	-1.876478	1.292049
F	3.533413	-3.240335	0.066603

3-FBCB (TS1$_N$)

Electronic Energy = -1051.193599 au
Enthalpy = -1050.855652 au
Gibbs Free Energy = -1050.929174 au
Lowest Harmonic Vibrational Frequency (LHVF) = 188.96*i* cm^{-1}

C	3.064308	-2.177823	-0.961309
C	2.712013	-0.677135	-0.712827
C	1.545464	-1.295025	-0.037136
C	1.545618	-2.561070	-0.824367
H	3.378158	-0.102376	-0.071906
H	2.487344	-0.149712	-1.637578
H	-0.382823	0.055398	-0.934420
C	-1.360193	-1.212089	0.363939
H	-1.225495	-1.510825	1.405418
N	-0.291101	-0.240124	0.035782
H	-1.193726	-2.091424	-0.262124
C	-0.246169	0.938190	0.930381
H	-1.254964	1.354971	1.036534
H	0.067145	0.589860	1.916965
C	0.689653	2.017951	0.435594
C	1.829550	2.365485	1.167219
C	0.413277	2.712084	-0.749926
C	2.677996	3.381908	0.725490
H	2.053879	1.838080	2.088671
C	1.263100	3.721579	-1.198142
H	-0.475425	2.465358	-1.323330
C	2.399028	4.060069	-0.460321
H	3.556840	3.640409	1.306400
H	1.035092	4.249277	-2.118048
H	3.058329	4.848732	-0.806236
C	-2.768322	-0.694227	0.146477
C	-3.263736	-0.524155	-1.153152
C	-3.594917	-0.374018	1.228520
C	-4.552979	-0.039664	-1.365414
H	-2.637846	-0.778458	-2.003485
C	-4.888050	0.108676	1.019353
H	-3.225968	-0.507221	2.240505
C	-5.369237	0.279095	-0.278004
H	-4.923853	0.082611	-2.377429
H	-5.517050	0.350825	1.869309
H	-6.373978	0.653055	-0.442255
F	1.685212	-1.478745	1.295341

3-FBCB (TS2$_N$)

Electronic Energy = -1051.203868 au
Enthalpy = -1050.865811 au
Gibbs Free Energy = -1050.940241 au
Lowest Harmonic Vibrational Frequency (LHVF) = 240.79*i* cm^{-1}

C	2.837692	-2.552773	-0.202373
C	1.686575	-2.612964	-1.156736
C	1.762088	-1.252349	-0.527311
C	2.468085	-1.531341	0.709752
H	1.947383	-2.624690	-2.218269
H	0.843423	-3.264970	-0.933609
H	-0.385008	0.091430	-1.144009
C	-1.242697	-1.413306	-0.048804
H	-1.012263	-1.928950	0.886501
N	-0.227925	-0.355130	-0.242753
H	-1.112156	-2.129064	-0.862897
C	-0.232186	0.669322	0.826101
H	-1.263018	0.951521	1.075394
H	0.204012	0.216013	1.719377
C	0.535455	1.918238	0.452346
C	0.088669	2.743257	-0.588763
C	1.686834	2.290884	1.153121
C	0.781977	3.903800	-0.927526
H	-0.811480	2.478797	-1.135872
C	2.379913	3.456622	0.821793
H	2.042403	1.666406	1.966088
C	1.931858	4.264505	-0.222314
H	0.421672	4.530347	-1.736526
H	3.270053	3.730444	1.378186
H	2.470454	5.169134	-0.483061
C	-2.686150	-0.940718	-0.033034
C	-3.446448	-0.975127	1.140453
C	-3.284845	-0.461464	-1.206008
C	-4.773239	-0.539567	1.146223
H	-2.997709	-1.347911	2.055936
C	-4.607607	-0.022958	-1.204183
H	-2.711650	-0.435793	-2.128246
C	-5.356486	-0.060349	-0.025785
H	-5.348285	-0.573693	2.065477
H	-5.056885	0.341947	-2.121734
H	-6.386817	0.278418	-0.023946
F	2.128930	-0.189697	-1.288918

F	3.767978	-2.691188	0.178495
F	1.214914	-3.713891	-0.142667
H	1.020684	-2.532265	-1.776219

F	4.113273	-2.929513	-0.501262
F	1.659435	-1.897200	1.968346
H	3.189685	-0.818057	1.095275

4-FBCB (TS1$_N$)

Electronic Energy = -1150.474129 au
Enthalpy = -1150.143142 au
Gibbs Free Energy = -1150.221313 au
Lowest Harmonic Vibrational Frequency (LHVF) = 116.08i cm^{-1}

C	-2.016229	-2.077180	1.018036
C	-2.461327	-0.768809	0.579830
C	-1.773418	-1.270138	-0.617012
C	-1.630912	-2.675915	-0.238191
H	-2.171140	0.158271	1.066451
H	0.432323	-0.052589	0.733101
C	1.508142	-1.171930	-0.610075
H	1.459474	-1.360274	-1.685572
H	1.260580	-2.104378	-0.097174
N	0.449200	-0.199187	-0.274147
C	0.580468	1.096671	-0.969543
H	1.606745	1.478584	-0.883557
H	0.388998	0.923734	-2.031750
C	-0.376660	2.136796	-0.432033
C	-1.480078	2.559476	-1.180471
C	-0.164982	2.705802	0.831207
C	-2.355651	3.524241	-0.679277
H	-1.653854	2.134084	-2.163278
C	-1.041186	3.664130	1.337994
H	0.695372	2.400537	1.419397
C	-2.140852	4.076312	0.582917
H	-3.204928	3.842027	-1.274721
H	-0.862215	4.094801	2.317423
H	-2.821182	4.824873	0.974346
C	2.919517	-0.757703	-0.227301
C	3.301562	-0.713240	1.120166
C	3.860927	-0.411189	-1.202025
C	4.590231	-0.326835	1.483904
H	2.585669	-0.987124	1.889714
C	5.154054	-0.026214	-0.842154
H	3.581261	-0.445781	-2.250395
C	5.521281	0.018949	0.502001
H	4.870838	-0.301243	2.531514
H	5.871707	0.238194	-1.611506
H	6.525306	0.317078	0.783899
F	-1.728003	-0.756061	-1.828821
F	-1.999614	-2.594336	2.240251
F	-2.658428	-3.608855	-0.864997
H	-0.716888	-3.241368	-0.394084
F	-3.943042	-0.599023	0.436611

4-FBCB (TS2$_N$)

Electronic Energy = -1150.485479 au
Enthalpy = -1150.154236 au
Gibbs Free Energy = -1150.229398 au
Lowest Harmonic Vibrational Frequency (LHVF) = 219.16i cm^{-1}

C	-2.724238	-2.328077	-0.335537
C	-1.392716	-2.760009	-0.005550
C	-1.506034	-1.409156	0.584917
C	-2.625127	-0.892382	-0.232655
H	-1.219609	-3.612245	0.647962
F	-0.428918	-2.944909	-1.106813
H	0.366755	-0.102113	-0.684431
C	0.367731	1.040401	1.039397
H	1.378766	1.463654	1.008132
N	0.352789	-0.257602	0.321712
H	0.133423	0.835580	2.086250
C	1.481685	-1.136572	0.708524
H	1.452459	-1.248782	1.794565
H	1.294705	-2.115253	0.264483
C	2.849512	-0.642208	0.275691
C	3.207737	-0.656161	-1.079238
C	3.777051	-0.168590	1.209466
C	4.459108	-0.201033	-1.490142
H	2.502959	-1.029622	-1.816281
C	5.033164	0.284979	0.801876
H	3.516556	-0.157617	2.263123
C	5.376404	0.271925	-0.549212
H	4.721675	-0.220997	-2.542491
H	5.740600	0.648519	1.539557
H	6.351524	0.623874	-0.868076
C	-0.603779	2.051241	0.475459
C	-0.318132	2.711087	-0.726962
C	-1.787902	2.365931	1.149434
C	-1.202180	3.652953	-1.249887
H	0.604240	2.488004	-1.254777
C	-2.673114	3.312717	0.631583
H	-2.017744	1.870114	2.086961
C	-2.384167	3.955963	-0.571345
H	-0.966543	4.155414	-2.181964
H	-3.586294	3.547220	1.168206
H	-3.071045	4.691858	-0.975211
F	-1.464549	-1.227045	1.916370
F	-3.851424	-3.075874	-0.356561
F	-2.285719	-0.134635	-1.436689
H	-3.406488	-0.310259	0.250335

5-FBCB (TS1$_N$)

Electronic Energy = -1249.753879 au
Enthalpy = -1249.430182 au
Gibbs Free Energy = -1249.508315 au
Lowest Harmonic Vibrational Frequency (LHVF) = 139.48i cm^{-1}

C	-2.691360	-2.285872	-0.397125
C	-1.354129	-2.729595	-0.081641
C	-1.469272	-1.415205	0.572641
C	-2.564451	-0.851553	-0.243322
H	-1.203167	-3.610360	0.539044

5-FBCB (TS2$_N$)

Electronic Energy = -1249.752161 au
Enthalpy = -1249.428384 au
Gibbs Free Energy = -1249.506033 au
Lowest Harmonic Vibrational Frequency (LHVF) = 93.35i cm^{-1}

C	4.151298	-0.410738	-0.372022
C	3.195655	-1.413741	0.052390
C	2.741954	-0.148280	0.640359
C	3.354560	0.799747	-0.302748
F	2.363136	-2.039981	-0.943063

F	-0.404428	-2.859330	-1.171929
H	0.593297	-0.070445	-0.738534
C	0.631632	1.074455	0.976803
H	1.651788	1.477811	0.931456
N	0.563089	-0.222119	0.267422
H	0.406325	0.884967	2.029291
C	1.644413	-1.151683	0.660189
H	1.589205	-1.282882	1.743672
H	1.425264	-2.115069	0.196310
C	3.045572	-0.715775	0.268262
C	3.437250	-0.729335	-1.077385
C	3.969240	-0.292058	1.229623
C	4.716712	-0.323625	-1.452339
H	2.735984	-1.064034	-1.836179
C	5.253097	0.112881	0.858518
H	3.683164	-0.281532	2.276753
C	5.629405	0.100049	-0.483795
H	5.004565	-0.343535	-2.498105
H	5.956407	0.438431	1.617629
H	6.626186	0.413768	-0.774407
C	-0.324258	2.104804	0.421673
C	-1.466758	2.483746	1.133316
C	-0.067526	2.717060	-0.812537
C	-2.337966	3.448267	0.624046
H	-1.674406	2.024058	2.094252
C	-0.938674	3.675002	-1.327622
H	0.823056	2.444786	-1.371139
C	-2.078261	4.043469	-0.609590
H	-3.218580	3.732042	1.190500
H	-0.725664	4.139537	-2.284543
H	-2.754694	4.792170	-1.007569
F	-1.357428	-1.216269	1.880592
F	-3.820569	-3.000699	-0.447102
F	-2.308189	-0.010213	-1.322432
F	-3.561424	-0.204051	0.445463
H	3.516494	-2.210029	0.720414
H	0.296931	-0.170959	-0.706527
C	-0.142827	1.331255	0.642786
H	0.583961	2.028719	0.213553
N	0.317350	-0.022171	0.298057
H	-0.079810	1.432765	1.728953
C	-0.308742	-1.147421	1.010895
H	0.398405	-1.983667	0.976801
H	-0.411757	-0.859186	2.059386
C	-1.647878	-1.643283	0.486260
C	-1.755806	-2.148613	-0.816236
C	-2.784498	-1.648800	1.300448
C	-2.970221	-2.636555	-1.294782
H	-0.882251	-2.163116	-1.461471
C	-4.002611	-2.140911	0.827005
H	-2.716922	-1.265231	2.313692
C	-4.099769	-2.633983	-0.473324
H	-3.035112	-3.023843	-2.306170
H	-4.873892	-2.136012	1.473511
H	-5.045034	-3.015346	-0.844096
C	-1.532832	1.746727	0.182958
C	-1.858708	1.770801	-1.179479
C	-2.497734	2.157696	1.107579
C	-3.118911	2.186265	-1.604559
H	-1.120215	1.462902	-1.913836
C	-3.760702	2.579242	0.686348
H	-2.259440	2.148435	2.166778
C	-4.075701	2.592703	-0.671412
H	-3.354121	2.198621	-2.663625
H	-4.496453	2.894225	1.418850
H	-5.056061	2.918406	-1.002028
F	2.555572	0.086875	1.930591
F	5.479434	-0.507457	-0.461999
F	3.945550	1.908067	0.248655
F	2.655714	1.302036	-1.395893

Perfluoro-FBCB (TS_N)

Electronic Energy = -1349.018381 au

Enthalpy = -1348.702155 au

Gibbs Free Energy = -1348.781774 au

Lowest Harmonic Vibrational Frequency (LHVF) = 88.99*i* cm^{-1}

C	2.931469	-1.788268	-0.606747
C	2.620002	-0.397825	-0.333283
C	1.659654	-1.103561	0.534511
C	1.726557	-2.425232	-0.115085
F	3.587111	0.339680	0.311576
F	2.182014	0.448434	-1.339103
H	-0.732788	0.085371	-0.825443
C	-1.667777	-1.180903	0.497896
H	-1.577210	-1.396229	1.565927
N	-0.698388	-0.115191	0.171465
H	-1.357920	-2.075002	-0.045945
C	-0.913980	1.126657	0.941942
H	-1.965790	1.439000	0.885077
H	-0.700898	0.906078	1.991366
C	-0.040981	2.265385	0.467411
C	-0.333953	2.929058	-0.731631
C	1.063898	2.687036	1.213994
C	0.464863	3.980088	-1.178397
H	-1.196765	2.623733	-1.316129

C	1.862460	3.743749	0.773257	
H	1.298937	2.187929	2.148610	
C	1.567274	4.390536	-0.426066	
H	0.224205	4.483534	-2.108746	
H	2.714433	4.059254	1.366130	
H	2.187268	5.211140	-0.770645	
C	-3.117464	-0.868949	0.164379	
C	-3.531877	-0.785408	-1.171860	
C	-4.063734	-0.656660	1.172285	
C	-4.856357	-0.492413	-1.491534	
H	-2.812165	-0.954227	-1.967665	
C	-5.392656	-0.365921	0.856782	
H	-3.759007	-0.721569	2.212233	
C	-5.792052	-0.281407	-0.476259	
H	-5.160961	-0.434777	-2.531179	
H	-6.113145	-0.204982	1.651748	
H	-6.823670	-0.055908	-0.723922	
F	1.466652	-0.888650	1.812867	
F	4.102510	-2.332042	-0.886833	
F	0.727733	-2.841069	-0.987831	
F	1.884216	-3.504441	0.724742	