SUPPORTING INFORMATION FOR

Asymmetric Bifurcated Halogen Bonds

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Table S1: Selected geometric properties of all m- complexes of BrF dihalogen molecule. ΔE is the interaction energy, α is the angle between the dihalogen molecule and the aromatic ring, d(Br···O_m) and d(Br···O_p) are the XB lengths. The ratio between the calculated values and the sum of the vdW radii (3.37 Å) is given as percentage.

Complex	ΔE /kcal.mol^{-1}	α /degrees	d(Br···O_m)/ Å	%d(Br···O_m)	d(Br···O_p)/ Å	%d(Br···O_p)
m-COO^-	-14.79	55.7	2.448	72.6	3.293	97.7
m-O^-	-18.89	54.7	2.335	69.3	3.316	98.4
m-PO_3H^-	-13.88	41.1	2.496	74.1	3.207	95.2
m-S^-	-16.04	57.3	2.419	71.8	3.305	98.1
m-SO_2^-	-13.97	38.0	2.505	74.3	3.187	94.6
m-SO_3^-	-12.65	18.4	2.584	76.7	3.087	91.6
m-Br	-8.13	13.0	2.747	81.5	3.028	89.9
m-C_2H_3	-8.57	13.2	2.728	80.9	3.041	90.2
m-CF_3	-7.98	10.9	2.743	81.4	3.033	90.0
m-CH_3	-8.79	12.1	2.732	81.1	3.021	89.6
m-CHO	-8.01	12.6	2.738	81.2	3.045	90.4
m-Cl	-8.16	13.6	2.757	81.8	3.017	89.5
m-CN	-7.70	11.3	2.761	81.9	3.028	89.9
m-COOH	-8.16	11.8	2.737	82.3	3.002	89.1
m-F	-8.28	13.5	2.772	82.3	2.997	88.9
m-H	-8.72	14.7	2.724	80.8	3.032	90.0
m-NH_2	-8.82	7.8	2.750	81.6	2.999	89.0
m-NO_2	-7.57	12.5	2.747	81.5	3.051	90.5
m-OCH_3	-8.69	12.2	2.743	81.4	3.014	89.4
m-OCHO	-8.28	18.5	2.720	80.7	3.075	91.2
m-OH	-8.62	13.6	2.744	81.4	3.014	89.4
m-SCH_3	-8.52	16.8	2.739	81.3	3.032	90.0
m-SH	-8.38	11.1	2.748	81.5	3.019	89.6
m-SO_2Cl	-7.45	3.1	2.867	85.1	2.923	86.7
m-SO_3H	-7.66	17.0	2.744	81.4	3.059	90.8
m-$CH_2NH_3^+$	-5.08	4.2	2.867	85.1	2.993	88.8

m-$N(CH_3)_3^+$	-5.38	70.3	2.705	80.3	3.304	98.0
m-NH_3^+	-4.61	48.7	2.758	81.8	3.219	95.5
m-$S(CH_3)_2^+$	-4.71	3.2	2.934	87.4	2.938	87.2

Table S2: Selected geometric properties of all p- complexes of BrF dihalogen molecule. ΔE is the interaction energy, α is the angle between the dihalogen molecule and the aromatic ring, d(Br···O_m) and d(Br···O_p) are the XB lengths. The ratio between the calculated values and the sum of the vdW radii (3.37 Å) is given as percentage.

Complex	ΔE /kcal.mol^{-1}	α /degrees	d(Br···O_m)/ Å	%d(Br···O_m)	d(Br···O_p)/ Å	%d(Br···O_p)
p-COO^-	-14.36	57.7	3.312	98.3	2.451	72.7
p-O^-	-20.24	37.8	4.658	138.2	2.282	67.7
p-PO_3H^-	-13.61	54.2	3.328	98.8	2.465	73.1
p-S^-	-17.14	56.6	3.430	101.8	2.367	70.2
p-SO_2^-	-12.63	5.5	3.009	89.3	2.650	78.6
p-SO_3^-	-12.15	3.9	2.986	88.6	2.686	79.7
p-Br	-8.21	12.7	3.033	90.0	2.746	81.5
p-C_2H_3	-8.60	14.4	3.030	89.9	2.737	81.2
p-CF_3	-7.94	11.6	3.004	89.1	2.775	82.3
p-CH_3	-8.85	13.7	3.041	90.2	2.713	80.5
p-CHO	-7.96	13.2	2.967	88.0	2.808	83.3
p-Cl	-8.26	13.5	3.036	90.1	2.743	81.4
p-CN	-7.61	11.2	2.985	88.6	2.801	83.1
p-COOH	-8.32	60.0	3.287	97.5	2.614	77.6
p-F	-8.41	12.2	3.050	98.3	2.720	72.7
p-H	-8.71	14.7	3.035	90.1	2.732	81.1
p-NH_2	-9.11	8.6	3.046	90.4	2.708	80.4
p-NO_2	-7.52	13.0	2.962	87.9	2.827	83.9
p-OCH_3	-8.89	12.7	3.048	90.4	2.715	80.6
p-OCHO	-8.37	3.2	3.028	89.9	2.745	81.5
p-OH	-8.84	14.5	3.058	90.7	2.710	80.4
p-SCH_3	-8.66	17.0	3.052	90.6	2.719	80.7
p-SH	-8.52	13.5	3.041	90.2	2.731	81.0
p-SO_2Cl	-7.34	46.9	3.231	95.9	2.673	79.3
p-SO_3H	-7.55	41.0	3.184	94.5	2.698	80.1
p-$CH_2NH_3^+$	-5.12	16.8	2.987	88.6	2.869	85.1
p-$N(CH_3)_3^+$	-4.95	11.9	3.011	89.3	2.854	84.7
p-NH_3^+	-4.58	48.7	3.003	89.1	2.875	85.3

p-$S(CH_3)_2^+$	−4.70	4.9	2.945	87.4	2.927	86.9

Table S3: Selected quantities from the AIM analysis for bond critical points between the halogen and oxygens in respective m− complexes of BrF molecule. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{LCP}$, energy density H^{LCP}. DI is delocalization index between the two atoms.

Complex	ρ^{LCP}_{Br-Om}	ρ^{LCP}_{Br-Op}	$\nabla^2\rho^{LCP}_{Br-Om}$	$\nabla^2\rho^{LCP}_{Br-Op}$	H^{LCP}_{Br-Om}	H^{LCP}_{Br-Op}	DI_{Br-Om}	DI_{Br-Op}
m-COO^-	0.0383	0.0081	0.1224	0.0299	−0.0022	0.0014	0.2804	0.0539
m-O^-	0.0504	0.0084	0.1360	0.0310	−0.0070	0.0013	0.3590	0.0445
m-PO_3H^-	0.0336	0.0095	0.1161	0.0347	−0.0005	0.0015	0.2494	0.0645
m-S^-	0.0412	0.0079	0.1259	0.0294	−0.0032	0.0013	0.2996	0.0527
m-SO_2^-	0.0328	0.0099	0.1145	0.0360	−0.0003	0.0015	0.2439	0.0670
m-SO_3^-	0.0267	0.0114	0.1018	0.0428	0.0012	0.0017	0.1992	0.0787
m-Br	0.0187	0.0122	0.0763	0.0468	0.0020	0.0017	0.1369	0.0847
m-C_2H_3	0.0195	0.0120	0.0792	0.0458	0.0020	0.0017	0.1434	0.0831
m-CF_3	0.0187	0.0122	0.0769	0.0467	0.0020	0.0017	0.1376	0.0839
m-CH_3	0.0193	0.0125	0.0785	0.0476	0.0020	0.0017	0.1418	0.0864
m-CHO	0.0190	0.0119	0.0778	0.0454	0.0020	0.0017	0.1396	0.0817
m-Cl	0.0185	0.0124	0.0750	0.0475	0.0020	0.0018	0.1348	0.0862
m-CN	0.0183	0.0121	0.0746	0.0465	0.0020	0.0017	0.1328	0.0838
m-COOH	0.0191	0.0118	0.0779	0.0452	0.0020	0.0017	0.1401	0.0813
m-F	0.0181	0.0127	0.0730	0.0489	0.0020	0.0018	0.1309	0.0893
m-H	0.0196	0.0123	0.0797	0.0468	0.0020	0.0017	0.1445	0.0848
m-NH_2	0.0187	0.0129	0.0759	0.0494	0.0020	0.0018	0.1364	0.0897
m-NO_2	0.0186	0.0117	0.0765	0.0449	0.0020	0.0017	0.1364	0.0806
m-OCH_3	0.0190	0.0126	0.0770	0.0481	0.0020	0.0018	0.1387	0.0875
m-OCHO	0.0198	0.0113	0.0803	0.0429	0.0020	0.0017	0.1455	0.0789
m-OH	0.0189	0.0126	0.0766	0.0481	0.0020	0.0018	0.1382	0.0876
m-SCH_3	0.0192	0.0121	0.0776	0.0463	0.0019	0.0017	0.1406	0.0847
m-SH	0.0187	0.0124	0.0762	0.0476	0.0020	0.0018	0.1368	0.0863
m-SO_2Cl	0.0152	0.0141	0.0610	0.0555	0.0020	0.0019	0.1087	0.0983
m-SO_3H	0.0188	0.0115	0.0769	0.0441	0.0020	0.0017	0.1380	0.0797
m-$CH_2NH_3^+$	0.0147	0.0125	0.0608	0.0492	0.0020	0.0018	0.1053	0.0867
m-$N(CH_3)_3^+$	0.0195	0.0072	0.0950	0.0301	0.0013	0.0012	N/A[a]	N/A[a]

m−NH_3^+	0.0171	0.0083	0.0841	0.0346	0.0017	0.0013	0.0908	0.0463
m−$S(CH_3)_2^+$	0.0134	0.0134	0.0540	0.0537	0.0019	0.0019	0.0943	0.0932
[a] These quantities were not computed using Promega integration algorithm.								

Table S4: Selected quantities from the AIM analysis for bond critical points between the halogen and oxygens in respective p- complexes of BrF molecule. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{LCP}$, energy density H^{LCP}. DI is delocalization index between the two atoms.

Complex	ρ^{LCP}_{Br-Om}	ρ^{LCP}_{Br-Op}	$\nabla^2\rho^{LCP}_{Br-Om}$	$\nabla^2\rho^{LCP}_{Br-Op}$	H^{LCP}_{Br-Om}	H^{LCP}_{Br-Op}	DI_{Br-Om}	DI_{Br-Op}
p-COO^-	0.0079	0.0380	0.0289	0.1226	0.0013	-0.0020	0.0521	0.2775
p-O^-	N/A[a]	0.0575	N/A[a]	0.1420	N/A[a]	-0.0105	N/A[a]	0.4112
p-PO_3H^-	0.0075	0.0366	0.0276	0.1211	0.0013	-0.0015	0.0504	0.2678
p-S^-	N/A[a]	0.0470	N/A[a]	0.1318	N/A[a]	-0.0055	N/A[a]	0.3391
p-SO_2^-	0.0128	0.0232	0.0487	0.0910	0.0017	0.0016	0.0895	0.1715
p-SO_3^-	0.0133	0.0216	0.0506	0.0853	0.0018	0.0018	0.0928	0.1589
p-Br	0.0120	0.0189	0.0460	0.0766	0.0017	0.0020	0.0837	0.1377
p-C_2H_3	0.0122	0.0193	0.0464	0.0778	0.0017	0.0020	0.0849	0.1408
p-CF_3	0.0125	0.0180	0.0482	0.0727	0.0018	0.0020	0.0874	0.1296
p-CH_3	0.0121	0.0200	0.0461	0.0813	0.0017	0.0019	0.0835	0.1479
p-CHO	0.0134	0.0169	0.0517	0.0681	0.0018	0.0020	0.0936	0.1216
p-Cl	0.0120	0.0190	0.0458	0.0771	0.0017	0.0020	0.0835	0.1387
p-CN	0.0129	0.0172	0.0498	0.0693	0.0018	0.0020	0.0900	0.1230
p-COOH	0.0080	0.0259	0.0291	0.0980	0.0013	0.0011	0.0543	0.1882
p-F	0.0119	0.0196	0.0454	0.0803	0.0017	0.0020	0.0819	0.1452
p-H	0.0123	0.0196	0.0469	0.0796	0.0017	0.0020	0.0849	0.1444
p-NH_2	0.0118	0.0203	0.0452	0.0823	0.0017	0.0019	0.0820	0.1497
p-NO_2	0.0134	0.0163	0.0520	0.0658	0.0018	0.0020	0.0939	0.1169
p-OCH_3	0.0118	0.0201	0.0450	0.0811	0.0017	0.0019	0.0820	0.1476
p-OCHO	0.0121	0.0188	0.0465	0.0768	0.0017	0.0020	0.0842	0.1375
p-OH	0.0116	0.0203	0.0441	0.0819	0.0017	0.0019	0.0805	0.1494
p-SCH_3	0.0118	0.0199	0.0447	0.0805	0.0017	0.0019	0.0818	0.1467
p-SH	0.0119	0.0195	0.0455	0.0788	0.0017	0.0020	0.0828	0.1426
p-SO_2Cl	0.0082	0.0201	0.0338	0.1003	0.0012	0.0014	0.0468	0.1076
p-SO_3H	0.0089	0.0191	0.0367	0.0943	0.0013	0.0015	N/A[b]	N/A[b]
p-$CH_2NH_3^+$	0.0127	0.0150	0.0495	0.0609	0.0018	0.0020	0.0879	0.1061
p-$N(CH_3)_3^+$	0.0122	0.0151	0.0475	0.0625	0.0018	0.0020	0.0843	0.1085

p-NH_3^+	0.0124	0.0145	0.0484	0.0598	0.0018	0.0020	0.0853	0.1034
p-$S(CH_3)_2^+$	0.0134	0.0134	0.0534	0.0544	0.0019	0.0019	0.0932	0.0943

[a] LCP does not exist.
[b] These quantities were not computed using Promega integration algorithm.

Table S5: Selected geometric properties of all m- complexes of ClF dihalogen molecule. ΔE is the interaction energy, α is the angle between the dihalogen molecule and the aromatic ring, d(Cl···O_m) and d(Cl···O_p) are the XB lengths. The ratio between the calculated values and the sum of the vdW radii (3.27 Å) is given as percentage.

Complex	ΔE /kcal.mol^{-1}	α /degrees	d(Br···O_m)/ Å	%d(Br···O_m)	d(Br···O_p)/ Å	%d(Br···O_p)
m-COO^-	-10.82	49.7	2.432	74.4	3.191	97.6
m-O^-	-13.86	54.3	2.328	71.2	3.265	99.8
m-PO_3H^-	-10.38	47.4	2.445	74.8	3.187	97.5
m-S^-	-11.72	52.8	2.408	73.6	3.205	98.0
m-SO_2^-	-10.65	49.8	2.433	74.4	3.199	97.8
m-SO_3^-	-9.88	45.3	2.463	75.3	3.179	97.2
m-Br	-6.05	26.2	2.641	80.8	3.118	95.4
m-C_2H_3	-6.36	23.2	2.631	80.5	3.111	95.1
m-CF_3	-5.88	22.7	2.656	81.2	3.105	95.0
m-CH_3	-6.51	24.2	2.627	80.3	3.109	95.1
m-CHO	-5.98	24.1	2.642	80.8	3.112	95.2
m-Cl	-6.08	26.9	2.639	80.7	3.120	95.4
m-CN	-5.72	24.7	2.655	81.2	3.116	95.3
m-COOH	-6.28	38.6	2.590	79.2	3.178	97.2
m-F	-6.13	27.0	2.640	80.7	3.119	95.4
m-H	-6.51	27.7	2.618	80.1	3.121	95.4
m-NH_2	-6.51	21.9	2.637	80.6	3.100	94.8
m-NO_2	-5.65	24.0	2.656	81.2	3.117	95.3
m-OCH_3	-6.40	22.2	2.639	80.7	3.103	94.9
m-OCHO	-6.11	23.1	2.645	80.9	3.110	95.1
m-OH	-6.38	25.6	2.634	80.6	3.112	95.2
m-SCH_3	-6.31	22.8	2.640	80.7	3.104	94.9
m-SH	-6.22	24.9	2.640	80.7	3.111	95.1
m-SO_2Cl	-5.51	23.2	2.665	81.5	3.114	95.2
m-SO_3H	-5.72	22.3	2.656	81.2	3.112	95.2
m-$CH_2NH_3^+$	-4.79	79.3	2.631	80.5	3.306	101.1
m-$N(CH_3)_3^+$	-4.27	78.6	2.660	81.3	3.272	100.1
m-NH_3^+	-3.95	79.2	2.679	81.9	3.268	99.9

m-$S(CH_3)_2^+$	−4.21	79.7	2.668	81.6	3.277	100.2

Table S6: Selected geometric properties of all p- complexes of ClF dihalogen molecule. ΔE is the interaction energy, α is the angle between the dihalogen molecule and the aromatic ring, d(Cl···O_m) and d(Cl···O_p) are the XB lengths. The ratio between the calculated values and the sum of the vdW radii (3.27 Å) is given as percentage.

Complex	ΔE /kcal.mol^{-1}	α /degrees	d(Br···O_m)/ Å	%d(Br···O_m)	d(Br···O_p)/ Å	%d(Br···O_p)
p-COO^-	-10.33	54.8	3.268	99.9	2.445	74.8
p-O^-	-14.96	30.8	4.723	144.4	2.245	68.7
p-PO_3H^-	-9.96	57.5	3.258	99.6	2.454	75.0
p-S^-	-12.46	61.9	3.418	104.5	2.354	72.0
p-SO_2^-	-10.28	54.9	3.246	97.8	2.430	74.4
p-SO_3^-	-9.56	51.7	3.243	99.2	2.742	83.9
p-Br	-6.48	57.2	3.250	99.4	2.561	78.3
p-C_2H_3	-6.83	63.3	3.253	99.5	2.531	77.4
p-CF_3	-6.18	63.3	3.219	98.4	2.572	78.7
p-CH_3	-7.09	63.7	3.274	100.1	2.520	77.1
p-CHO	-6.15	65.0	3.240	99.1	2.566	78.5
p-Cl	-6.59	64.1	3.254	99.5	2.551	78.0
p-CN	-5.89	64.1	3.256	99.6	2.580	78.9
p-COOH	-5.89	24.2	3.103	94.9	2.678	81.9
p-F	-6.79	65.2	3.287	100.5	2.527	77.3
p-H	-6.91	64.2	3.267	99.9	2.532	77.4
p-NH_2	-7.50	60.5	3.279	100.3	2.512	76.8
p-NO_2	-5.65	48.3	3.098	94.7	2.693	82.4
p-OCH_3	-7.23	64.6	3.289	100.6	2.511	76.8
p-OCHO	-6.72	64.3	3.271	100.0	2.537	77.6
p-OH	-7.19	65.7	3.295	100.8	2.513	76.9
p-SCH_3	-6.93	64.3	3.246	99.3	2.532	77.4
p-SH	-6.81	64.0	3.279	100.3	2.528	77.3
p-SO_2Cl	-5.56	46.2	3.251	99.4	2.597	79.4
p-SO_3H	-5.68	44.7	3.186	97.4	2.627	80.3
p-$CH_2NH_3^+$	-4.26	77.0	3.236	99.0	2.667	81.5
p-$N(CH_3)_3^+$	-4.34	76.3	3.251	99.4	2.657	81.3
p-NH_3^+	-3.50	7.4	3.037	92.9	2.799	85.6

p-$S(CH_3)_2^+$	−3.99	76.1	3.246	99.3	2.679	81.9

Table S7: Selected quantities from the AIM analysis for bond critical points between the halogen and oxygens in respective m− complexes of ClF molecule. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{LCP}$, energy density H^{LCP}. DI is delocalization index between the two atoms.

Complex	ρ^{LCP}_{Br-Om}	ρ^{LCP}_{Br-Op}	$\nabla^2\rho^{LCP}_{Br-Om}$	$\nabla^2\rho^{LCP}_{Br-Op}$	H^{LCP}_{Br-Om}	H^{LCP}_{Br-Op}	DI_{Br-Om}	DI_{Br-Op}
m-COO^-	0.0338	0.0080	0.1273	0.0323	0.0004	0.0017	0.2308	0.0504
m-O^-	0.0442	0.0075	0.1459	0.0305	−0.0026	0.0016	0.2962	0.0362
m-PO_3H^-	0.0326	0.0080	0.1250	0.0324	0.0007	0.0017	0.2227	0.0508
m-S^-	0.0360	0.0079	0.1315	0.0316	−0.0002	0.0016	0.2451	0.0491
m-SO_2^-	0.0336	0.0079	0.1271	0.0318	0.0004	0.0017	0.2296	0.0496
m-SO_3^-	0.0310	0.0081	0.1215	0.0329	0.0010	0.0017	0.2122	0.0517
m-Br	0.0198	0.0086	0.0881	0.0356	0.0026	0.0018	0.1356	0.0567
m-C_2H_3	0.0203	0.0087	0.0898	0.0362	0.0025	0.0019	0.1387	0.0574
m-CF_3	0.0191	0.0088	0.0856	0.0365	0.0026	0.0019	0.1308	0.0575
m-CH_3	0.0205	0.0088	0.0906	0.0363	0.0025	0.0019	0.1403	0.0578
m-CHO	0.0198	0.0086	0.0880	0.0358	0.0026	0.0018	0.1353	0.0564
m-Cl	0.0199	0.0086	0.0884	0.0354	0.0025	0.0018	0.1364	0.0565
m-CN	0.0192	0.0086	0.0857	0.0357	0.0026	0.0018	0.1311	0.0564
m-COOH	0.0226	0.0078	0.0976	0.0318	0.0023	0.0017	0.1541	0.0508
m-F	0.0199	0.0086	0.0883	0.0355	0.0025	0.0018	0.1361	0.0569
m-H	0.0210	0.0086	0.0921	0.0355	0.0025	0.0018	0.1436	0.0565
m-NH_2	0.0200	0.0089	0.0887	0.0370	0.0026	0.0019	0.1367	0.0591
m-NO_2	0.0191	0.0086	0.0855	0.0356	0.0026	0.0018	0.1305	0.0561
m-OCH_3	0.0199	0.0089	0.0885	0.0367	0.0026	0.0019	0.1362	0.0586
m-OCHO	0.0196	0.0087	0.0873	0.0361	0.0026	0.0019	0.1340	0.0575
m-OH	0.0202	0.0088	0.0893	0.0361	0.0025	0.0018	0.1379	0.0578
m-SCH_3	0.0198	0.0088	0.0882	0.0366	0.0026	0.0019	0.1357	0.0582
m-SH	0.0199	0.0087	0.0883	0.0361	0.0026	0.0019	0.1361	0.0576
m-SO_2Cl	0.0187	0.0086	0.0839	0.0358	0.0026	0.0018	0.1276	0.0562
m-SO_3H	0.0190	0.0086	0.0855	0.0360	0.0026	0.0019	0.1303	0.0565
m-$CH_2NH_3^+$	0.0213	0.0064	0.0922	0.0260	0.0023	0.0014	0.1407	0.0378
m-$N(CH_3)_3^+$	0.0199	0.0068	0.0871	0.0275	0.0024	0.0015	0.1309	0.0410

m-NH_3^+	0.0191	0.0069	0.0840	0.0276	0.0024	0.0015	0.1253	0.0414
m-$S(CH_3)_2^+$	0.0197	0.0068	0.0859	0.0273	0.0024	0.0015	0.1293	0.0404

Table S8: Selected quantities from the AIM analysis for bond critical points between the halogen and oxygens in respective p- complexes of ClF molecule. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{BCP}$, energy density H^{BCP}. DI is delocalization index between the two atoms.

Complex	ρ^{LCP}_{Br-Om}	ρ^{LCP}_{Br-Op}	$\nabla^2\rho^{LCP}_{Br-Om}$	$\nabla^2\rho^{LCP}_{Br-Op}$	H^{LCP}_{Br-Om}	H^{LCP}_{Br-Op}	DI_{Br-Om}	DI_{Br-Op}
p-COO^-	0.0068	0.0329	0.0273	0.1249	0.0015	0.0005	0.0428	0.2240
p-O^-	N/A[a]	0.0541	N/A[a]	0.1607	N/A[a]	−0.0061	N/A[a]	0.3621
p-PO_3H^-	0.0062	0.0274	0.0286	0.1484	0.0014	0.0006	0.0338	0.1346
p-S^-	N/A[a]	0.0418	N/A[a]	0.1408	N/A[a]	−0.0020	N/A[a]	0.2825
p-SO_2^-	0.0071	0.0339	0.0289	0.1282	0.0016	0.0003	0.0448	0.2302
p-SO_3^-	0.0071	0.0306	0.0284	0.1198	0.0015	0.0010	0.0450	0.2085
p-Br	0.0069	0.0247	0.0278	0.1034	0.0015	0.0020	0.0439	0.1669
p-C_2H_3	0.0070	0.0266	0.0284	0.1096	0.0015	0.0017	0.0436	0.1791
p-CF_3	0.0075	0.0241	0.0302	0.1017	0.0016	0.0020	0.0468	0.1627
p-CH_3	0.0067	0.0274	0.0269	0.1117	0.0015	0.0015	0.0414	0.1839
p-CHO	0.0072	0.0245	0.0289	0.1029	0.0016	0.0020	0.0448	0.1644
p-Cl	0.0065	0.0234	0.0286	0.1190	0.0009	0.0013	0.0344	0.1148
p-CN	0.0069	0.0238	0.0276	0.1003	0.0015	0.0020	0.0431	0.1592
p-COOH	0.0087	0.0184	0.0361	0.0818	0.0019	0.0026	0.0577	0.1248
p-F	0.0065	0.0270	0.0263	0.1106	0.0015	0.0016	0.0401	0.1811
p-H	0.0068	0.0266	0.0273	0.1094	0.0015	0.0017	0.0420	0.1788
p-NH_2	0.0066	0.0279	0.0266	0.1128	0.0015	0.0015	0.0410	0.1887
p-NO_2	0.0074	0.0214	0.0299	0.0923	0.0016	0.0023	0.0484	0.1443
p-OCH_3	0.0065	0.0281	0.0263	0.1136	0.0014	0.0015	0.0399	0.1885
p-OCHO	0.0067	0.0263	0.0270	0.1085	0.0015	0.0017	0.0417	0.1770
p-OH	0.0064	0.0279	0.0260	0.1132	0.0014	0.0015	0.0393	0.1875
p-SCH_3	0.0068	0.0267	0.0274	0.1092	0.0015	0.0017	0.0423	0.1792
p-SH	0.0066	0.0269	0.0266	0.1103	0.0015	0.0016	0.0409	0.1803
p-SO_2Cl	0.0125	0.0132	0.0499	0.0531	0.0019	0.0020	0.0867	0.0905
p-SO_3H	0.0077	0.0209	0.0309	0.0910	0.0017	0.0024	0.0500	0.1417
p-$CH_2NH_3^+$	0.0074	0.0196	0.0296	0.0857	0.0016	0.0024	0.0444	0.1294
p-$N(CH_3)_3^+$	0.0072	0.0200	0.0289	0.0874	0.0015	0.0024	0.0431	0.1327

p-NH_3^+	0.0094	0.0140	0.0405	0.0639	0.0020	0.0025	0.0617	0.0929
p-$S(CH_3)_2^+$	0.0072	0.0190	0.0291	0.0836	0.0016	0.0024	0.0439	0.1257
[a] LCP does not exist.								

Table S9: Selected geometric properties of all m- complexes of BrCl dihalogen molecule. ΔE is the interaction energy, α is the angle between the dihalogen molecule and the aromatic ring, d(Br···O_m) and d(Br···O_p) are the XB lengths. The ratio between the calculated values and the sum of the vdW radii (3.37 Å) is given as percentage.

Complex	ΔE /kcal.mol^{-1}	α /degrees	d(Br···O_m)/ Å	%d(Br···O_m)	d(Br···O_p)/ Å	%d(Br···O_p)
m-COO^-	-9.58	6.5	2.771	82.2	3.006	89.2
m-O^-	-13.02	50.8	2.517	74.7	3.257	96.6
m-PO_3H^-	-9.25	12.3	2.757	81.8	3.046	90.4
m-S^-	-10.87	47.1	2.613	77.5	3.222	95.6
m-SO_2^-	-9.59	43.3	2.671	79.3	3.203	95.0
m-SO_3^-	-9.08	44.8	2.682	79.6	3.221	95.6
m-Br	-5.81	67.0	2.791	82.8	3.292	97.7
m-C_2H_3	-6.19	68.9	2.778	82.4	3.292	97.7
m-CF_3	-5.76	4.6	2.913	86.4	3.020	89.6
m-CH_3	-6.37	6.1	2.924	86.8	2.971	88.2
m-CHO	-5.79	6.1	2.939	87.2	2.992	88.8
m-Cl	-5.83	66.5	2.788	82.7	3.294	97.7
m-CN	-5.56	4.7	2.913	86.4	3.034	90.0
m-COOH	-5.94	3.7	2.958	87.8	2.959	87.8
m-F	-5.90	64.0	2.791	82.8	3.269	97.0
m-H	-6.30	5.6	2.908	86.3	2.993	88.8
m-NH_2	-6.39	65.8	2.761	81.9	3.286	97.5
m-NO_2	-5.47	5.9	2.931	87.0	3.024	89.7
m-OCH_3	-6.27	32.4	2.862	84.9	3.089	91.7
m-OCHO	-5.93	39.0	2.837	84.2	3.176	94.2
m-OH	-6.19	69.3	2.788	82.7	3.279	97.3
m-SH	-6.04	31.8	2.865	85.0	3.108	92.2
m-SO_2Cl	-5.45	8.0	2.960	87.8	2.979	88.4
m-SO_3H	-5.57	12.6	2.898	86.0	3.055	90.7
m-$CH_2NH_3^+$	-4.25	80.4	2.943	87.3	3.167	94.0
m-$N(CH_3)_3^+$	-3.84	36.7	2.950	87.5	3.184	94.5
m-NH_3^+	-4.08	86.1	2.925	86.8	3.308	98.2

m-$S(CH_3)_2^+$	-4.18	81.6	2.895	85.9	3.331	98.8

Table S10: Selected geometric properties of all p- complexes of BrCl dihalogen molecule. ΔE is the interaction energy, α is the angle between the dihalogen molecule and the aromatic ring, d(Br···O_m) and d(Br···O_p) are the XB lengths. The ratio between the calculated values and the sum of the vdW radii (3.37 Å) is given as percentage.

Complex	ΔE /kcal.mol^{-1}	α /degrees	d(Br···O_m)	%d(Br···O_m)	d(Br···O_p)	%d(Br···O_p)
p-COO^-	-9.61	53.5	3.281	97.4	2.636	78.2
p-O^-	-14.91	60.1	3.593	106.6	2.453	72.8
p-PO_3H^-	-9.21	9.2	2.918	86.6	2.874	85.3
p-S^-	-11.43	49.9	3.280	97.3	2.583	76.6
p-SO_2^-	-9.59	2.2	2.948	87.5	2.839	84.2
p-SO_3^-	-8.97	9.9	2.929	86.9	2.872	85.2
p-Br	-5.95	4.7	3.016	89.5	2.911	86.4
p-C_2H_3	-6.25	8.1	2.996	88.9	2.910	86.4
p-CF_3	-5.77	5.6	2.981	88.5	2.943	87.3
p-CH_3	-6.37	5.6	3.016	89.5	2.889	85.7
p-CHO	-5.82	5.7	2.976	88.3	2.948	87.5
p-Cl	-5.97	6.3	3.020	89.6	2.906	86.2
p-CN	-5.58	11.4	2.974	88.2	2.968	88.1
p-COOH	-5.90	17.1	2.966	88.0	2.957	87.7
p-F	-6.03	4.6	3.046	90.4	2.887	85.7
p-H	-6.29	5.6	2.987	88.6	2.913	86.4
p-NH_2	-6.54	2.9	3.049	90.5	2.861	84.9
p-NO_2	-5.50	5.8	2.983	88.5	2.957	87.7
p-OCH_3	-6.37	4.8	3.047	90.4	2.868	85.1
p-OCHO	-6.03	0.6	3.037	90.1	2.891	85.8
p-OH	-6.33	7.4	3.048	90.4	2.870	85.2
p-SCH_3	-6.27	9.4	3.013	89.4	2.898	86.0
p-SH	-6.16	6.7	3.026	89.8	2.893	85.8
p-SO_2Cl	-5.45	8.6	2.987	88.6	2.953	87.6
p-SO_3H	-5.55	9.6	2.977	88.3	2.962	87.9
p-$CH_2NH_3^+$	-4.02	0.8	3.039	90.2	2.993	88.8
p-$N(CH_3)_3^+$	-3.86	1.1	3.126	92.8	2.969	88.1
p-NH_3^+	-3.64	0.3	3.124	92.7	2.985	88.6

p-$S(CH_3)_2^+$	-3.76	21.6	3.061	90.8	2.995	88.9

Table S11: Selected quantities from the AIM analysis for bond critical points between the halogen and oxygens in respective m- complexes of BrCl molecule. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{LCP}$, energy density H^{LCP}. DI is delocalization index between two atoms.

Complex	ρ^{LCP}_{Br-Om}	ρ^{LCP}_{Br-Op}	$\nabla^2\rho^{LCP}_{Br-Om}$	$\nabla^2\rho^{LCP}_{Br-Op}$	H^{LCP}_{Br-Om}	H^{LCP}_{Br-Op}	DI_{Br-Om}	DI_{Br-Op}
m-COO^-	0.0189	0.0128	0.0743	0.0493	0.0020	0.0019	0.1341	0.0885
m-O^-	0.0342	0.0091	0.1129	0.0333	-0.0006	0.0014	0.2399	0.0517
m-PO_3H^-	0.0195	0.0119	0.0764	0.0456	0.0020	0.0018	0.1380	0.0825
m-S^-	0.0275	0.0091	0.0977	0.0331	0.0009	0.0015	0.1954	0.0631
m-SO_2^-	0.0240	0.0094	0.0888	0.0342	0.0015	0.0015	0.1708	0.0646
m-SO_3^-	0.0234	0.0090	0.0873	0.0329	0.0015	0.0015	0.1663	0.0624
m-Br	0.0182	0.0075	0.0788	0.0298	0.0011	0.0013	N/A[a]	N/A[a]
m-C_2H_3	0.0188	0.0074	0.0807	0.0297	0.0010	0.0013	0.1008	0.0464
m-CF_3	0.0142	0.0119	0.0573	0.0469	0.0020	0.0019	0.0983	0.0824
m-CH_3	0.0141	0.0130	0.0563	0.0515	0.0020	0.0019	0.0975	0.0904
m-CHO	0.0137	0.0124	0.0546	0.0494	0.0020	0.0019	0.0945	0.0857
m-Cl	0.0183	0.0074	0.0789	0.0295	0.0011	0.0013	0.0992	0.0465
m-CN	0.0141	0.0116	0.0572	0.0457	0.0020	0.0018	0.0979	0.0802
m-COOH	0.0133	0.0132	0.0527	0.0525	0.0019	0.0020	0.0919	0.0905
m-F	0.0182	0.0077	0.0785	0.0309	0.0011	0.0013	0.0991	0.0487
m-H	0.0144	0.0126	0.0579	0.0495	0.0020	0.0019	0.1000	0.0871
m-NH_2	0.0192	0.0075	0.0834	0.0299	0.0009	0.0013	0.1042	0.0476
m-NO_2	0.0137	0.0117	0.0553	0.0465	0.0020	0.0019	0.0951	0.0809
m-OCH_3	0.0159	0.0110	0.0629	0.0415	0.0020	0.0017	0.1107	0.0768
m-OCHO	0.0167	0.0094	0.0662	0.0351	0.0020	0.0016	0.1165	0.0662
m-OH	0.0184	0.0077	0.0790	0.0304	0.0010	0.0013	0.0988	0.0479
m-SH	0.0157	0.0106	0.0625	0.0400	0.0020	0.0017	0.1098	0.0741
m-SO_2Cl	0.0130	0.0129	0.0521	0.0510	0.0020	0.0019	0.0899	0.0876
m-SO_3H	0.0132	0.0126	0.0527	0.0500	0.0020	0.0019	0.0915	0.0866
m-$CH_2NH_3^+$	0.0149	0.0076	0.0629	0.0305	0.0013	0.0013	N/A[a]	N/A[a]
m-$N(CH_3)_3^+$	0.0132	0.0090	0.0533	0.0342	0.0020	0.0016	0.0909	0.0631
m-NH_3^+	0.0136	0.0067	0.0567	0.0275	0.0014	0.0012	0.0700	0.0384

m-$S(CH_3)_2^+$	0.0154	0.0075	0.0613	0.0275	0.0020	0.0013	0.1015	0.0484
[a] These quantities were not computed using Promega integration algorithm.								

Table S12: Selected quantities from the AIM analysis for bond critical points between the halogen and oxygens in respective p– complexes of BrCl molecule. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{LCP}$, energy density H^{LCP}. DI is delocalization index between two atoms.

Complex	ρ^{LCP}_{Br-Om}	ρ^{LCP}_{Br-Op}	$\nabla^2\rho^{LCP}_{Br-Om}$	$\nabla^2\rho^{LCP}_{Br-Op}$	H^{LCP}_{Br-Om}	H^{LCP}_{Br-Op}	DI_{Br-Om}	DI_{Br-Op}
p-COO^-	0.0081	0.0262	0.0293	0.0945	0.0014	0.0011	0.0560	0.1841
p-O^-	N/A[a]	0.0411	N/A[a]	0.1179	N/A[a]	−0.0029	N/A[a]	0.2920
p-PO_3H^-	0.0147	0.0158	0.0570	0.0617	0.0019	0.0020	0.1032	0.1102
p-S^-	0.0082	0.0298	0.0297	0.1014	0.0014	0.0004	0.0565	0.2117
p-SO_2^-	0.0139	0.0167	0.0539	0.0660	0.0019	0.0020	0.0973	0.1168
p-SO_3^-	0.0144	0.0157	0.0559	0.0619	0.0019	0.0020	0.1004	0.1097
p-Br	0.0120	0.0142	0.0473	0.0574	0.0019	0.0020	0.0834	0.0988
p-C_2H_3	0.0126	0.0143	0.0493	0.0576	0.0019	0.0020	0.0870	0.0996
p-CF_3	0.0127	0.0136	0.0504	0.0543	0.0019	0.0020	0.0880	0.0934
p-CH_3	0.0121	0.0149	0.0474	0.0600	0.0019	0.0020	0.0839	0.1039
p-CHO	0.0129	0.0134	0.0510	0.0536	0.0019	0.0020	0.0891	0.0921
p-Cl	0.0120	0.0144	0.0470	0.0580	0.0018	0.0020	0.0829	0.1000
p-CN	0.0128	0.0130	0.0510	0.0517	0.0019	0.0019	0.0888	0.0894
p-COOH	0.0131	0.0133	0.0519	0.0529	0.0019	0.0019	0.0911	0.0917
p-F	0.0114	0.0149	0.0447	0.0601	0.0018	0.0021	0.0793	0.1036
p-H	0.0127	0.0143	0.0500	0.0574	0.0019	0.0020	0.0878	0.0992
p-NH_2	0.0115	0.0156	0.0446	0.0631	0.0018	0.0021	0.0795	0.1094
p-NO_2	0.0127	0.0131	0.0503	0.0527	0.0019	0.0020	0.0877	0.0901
p-OCH_3	0.0115	0.0154	0.0447	0.0623	0.0018	0.0021	0.0796	0.1078
p-OCHO	0.0116	0.0148	0.0455	0.0597	0.0018	0.0021	0.0806	0.1027
p-OH	0.0115	0.0154	0.0447	0.0621	0.0018	0.0021	0.0795	0.1075
p-SCH_3	0.0122	0.0146	0.0478	0.0589	0.0018	0.0020	0.0845	0.1020
p-SH	0.0119	0.0148	0.0465	0.0595	0.0018	0.0020	0.0823	0.1027
p-SO_2Cl	0.0125	0.0132	0.0499	0.0531	0.0019	0.0020	0.0867	0.0905
p-SO_3H	0.0128	0.0131	0.0508	0.0523	0.0019	0.0020	0.0885	0.0898
p-$CH_2NH_3^+$	0.0113	0.0121	0.0451	0.0492	0.0018	0.0019	0.0776	0.0830
p-$N(CH_3)_3^+$	0.0096	0.0125	0.0380	0.0512	0.0017	0.0020	0.0669	0.0860
p-NH_3^+	0.0096	0.0121	0.0381	0.0497	0.0017	0.0020	0.0667	0.0832

p-$S(CH_3)_2^+$	0.0109	0.0122	0.0432	0.0490	0.0018	0.0019	0.0757	0.0834

[a] LCP does not exist.

Table S13: Selected quantities from the AIM analysis for bond critical points between the aromatic carbon and oxygens in respective monomers. The electron density ρ^{LCP}, the Laplacian of the electron density $\nabla^2\rho^{LCP}$. DI is delocalization index between two atoms.

Substituent	ρ^{LCP}_{Cb-Om}	ρ^{LCP}_{Cb-Op}	$\nabla^2\rho^{LCP}_{Cb-Om}$	$\nabla^2\rho^{LCP}_{Cb-Op}$	DI_{Cb-Om}	DI_{Cb-Op}
COO^-	0.2812	0.2796	−0.4441	−0.4269	0.8893	0.8867
O^-	0.2736	0.2650	−0.4237	−0.4019	0.8759	0.8746
PO_3H^-	0.2834	0.2813	−0.4460	−0.4300	0.8920	0.8888
S^-	0.2778	0.2730	−0.4308	−0.4168	0.8831	0.8808
SO_2^-	0.2828	0.2803	−0.4468	−0.4306	0.8912	0.8877
SO_3^-	0.2848	0.2824	−0.4495	−0.4339	0.8933	0.8902
Br	0.2964	0.2952	−0.4618	−0.4616	0.9122	0.9104
C_2H_3	0.2934	0.2940	−0.4592	−0.4505	0.9073	0.9086
CF_3	0.2967	0.2976	−0.4653	−0.4545	0.9123	0.9136
CH_3	0.2926	0.2918	−0.4534	−0.4570	0.9063	0.9050
CHO	0.2955	0.2988	−0.4679	−0.4423	0.9106	0.9166
Cl	0.2963	0.2948	−0.4622	−0.4623	0.9119	0.9098
CN	0.2981	0.2996	−0.4687	−0.4494	0.9147	0.9174
COOH	0.2962	0.2984	−0.4690	−0.4428	0.9114	0.9155
F	0.2966	0.2928	−0.4611	−0.4693	0.9121	0.9070
H	0.2931	0.2931	−0.4558	−0.4558	0.9068	0.9069
NH_2	0.2934	0.2890	−0.4530	−0.4640	0.9064	0.9022
NO_2	0.2990	0.3011	−0.4743	−0.4449	0.9162	0.9201
OCH_3	0.2949	0.2906	−0.4573	−0.4641	0.9087	0.9040
OCHO	0.2958	0.2940	−0.4630	−0.4636	0.9111	0.9086
OH	0.2953	0.2904	−0.4572	−0.4669	0.9095	0.9041
SCH_3	0.2949	0.2926	−0.4578	−0.4586	0.9091	0.9067
SH	0.2953	0.2931	−0.4582	−0.4608	0.9100	0.9076
SO_2Cl	0.3002	0.3021	−0.4730	−0.4461	0.9180	0.9219
SO_3H	0.2991	0.3002	−0.4710	−0.4486	0.9162	0.9183
$CH_2NH_3^+$	0.3067	0.3099	−0.4669	−0.4543	0.9309	0.9363
$N(CH_3)_3^+$	0.3082	0.3106	−0.4662	−0.4633	0.9323	0.9363
NH_3^+	0.3118	0.3127	−0.4658	−0.4646	0.9392	0.9412

$S(CH_3)_2^+$	0.3094	0.3137	−0.4775	−0.4427	0.9353	0.9441

Table S14: Contributions to the total M06-2X/TZ2P interaction energies (ΔE^{Int}) of selected BrF complexes calculated using ADF software. See Methods section for explanation of the respective contributions. Angles are reported in degrees, energies in kcal.mol^{-1}.

Complex	Angle	ΔE^{Elstat}	ΔE^{Kin}	$\Delta E^{Coulomb}$	ΔE^{XC}	ΔE^{Int}
m-COO^-	– [a]	– [a]	– [a]	– [a]	– [a]	– [a]
	55.7	-21.65	48.03	-16.27	-24.64	-14.53
p-COO^-	– [a]	– [a]	– [a]	– [a]	– [a]	– [a]
	57.7	-20.96	47.16	-15.99	-24.21	-14.00
m-SO_2^-	38.0	-19.50	41.01	-12.35	-23.09	-13.93
	52.4	-20.70	46.12	-15.26	-24.26	-14.10
p-SO_2^-	5.5	-16.07	19.75	2.71	-19.21	-12.81
	54.0	-20.07	43.26	-13.48	-23.39	-13.67
m-Br	13.0	-11.02	20.03	-0.36	-16.67	-8.02
	57.5	-12.45	25.62	-3.27	-18.35	-8.47
p-Br	12.7	-11.09	19.51	0.00	-16.48	-8.06
	60.0	-12.76	25.70	-3.10	-18.42	-8.58
m-C_2H_3	13.2	-11.61	15.95	3.54	-16.42	-8.54
	61.2	-13.47	28.07	-4.42	-19.25	-9.06
p-C_2H_3	14.4	-11.56	6.46	11.25	-14.79	-8.63
	61.4	-13.37	28.33	-4.89	-19.13	-9.06
m-NH_3^+	48.7	-6.48	6.63	6.90	-11.51	-4.46
	77.4	-6.45	5.16	8.80	-12.22	-4.70
p-NH_3^+	48.7	-6.82	6.74	7.11	-11.51	-4.48
	74.1	-6.84	6.31	8.25	-12.61	-4.89
m-$N(CH_3)_3^+$	– [a]	– [a]	– [a]	– [a]	– [a]	– [a]
	70.3	-7.27	8.07	7.06	-13.00	-5.14
p-$N(CH_3)_3^+$	11.9	-7.34	8.18	6.42	-12.14	-4.87
	74.5	-7.53	-4.88	18.71	-11.78	-5.49

Table S15: Contributions to the total M06-2X/TZ2P interaction energies (ΔE^{Int}) of selected BrF complexes calculated using ADF software. ΔE^{Pauli} is the Pauli repulsion term, ΔE^{Elstat} is the electrostatic term, and $\Delta E^{Orbital}$ defines the stabilizing orbital interactions. Black and red numbers represent the complexes closer to 'in plane' and 'perpendicular' geometries, respectively. Angles are reported in degrees, energies in kcal.mol^{-1}.

Complex	Angle	ΔE^{Pauli}	ΔE^{Elstat}	$\Delta E^{Orbital}$	ΔE^{Int}
m-COO^-	_ [a]	_ [a]	_ [a]	_ [a]	_ [a]
	55.7	21.42	-21.65	-14.30	-14.53
p-COO^-	_ [a]	_ [a]	_ [a]	_ [a]	_ [a]
	57.7	20.93	-20.96	-13.97	-14.00
m-SO_2^-	38.0	17.85	-19.50	-12.28	-13.93
	52.4	20.20	-20.70	-13.60	-14.10
p-SO_2^-	5.5	12.00	-16.07	-8.74	-12.81
	54.0	19.66	-20.07	-13.26	-13.67
m-Br	13.0	8.35	-11.02	-5.35	-8.02
	57.5	11.61	-12.45	-7.62	-8.47
p-Br	12.7	8.37	-11.09	-5.34	-8.06
	60.0	12.14	-12.76	-7.96	-8.58
m-C_2H_3	13.2	8.81	-11.61	-5.74	-8.54
	61.2	12.78	-13.47	-8.38	-9.06
p-C_2H_3	14.4	8.69	-11.56	-5.77	-8.63
	61.4	12.65	-13.37	-8.34	-9.06
m-NH_3^+	48.7	6.38	-6.48	-4.37	-4.46
	77.4	6.78	-6.45	-5.04	-4.70
p-NH_3^+	48.7	5.83	-6.82	-3.50	-4.48
	74.1	7.12	-6.84	-5.17	-4.89
m-$N(CH_3)_3^+$	_ [a]	_ [a]	_ [a]	_ [a]	_ [a]
	70.3	7.41	-7.27	-5.28	-5.14
p-$N(CH_3)_3^+$	11.9	6.11	-7.34	-3.65	-4.87
	74.5	7.58	-7.53	-5.54	-5.49

[a] Not available.

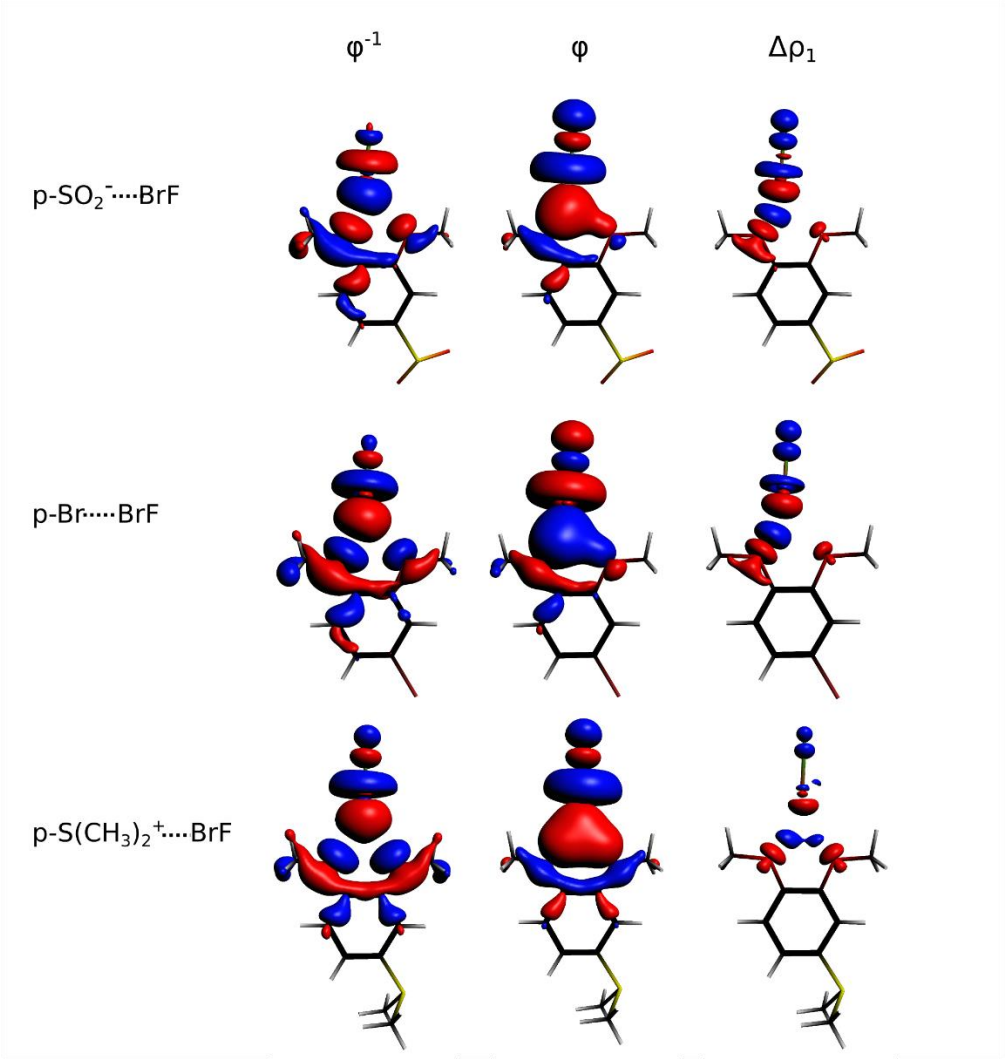

Figure S1: Visualization of largest NOCV contributions to $\Delta\rho$ for p-SO_2^-···BrF, p-Br···BrF, and p-$S(CH_3)_2^+$···BrF. Left: antibonding orbital ϕ_{-1}, center: bonding orbital ϕ_1, right: $\Delta\rho_1$ contribution to the total EDD. Isosurfaces for orbitals at 0.03 a.u.; $\Delta\rho_1$: isosurface at 0.001 a.u.; Red - charge depletion, blue - charge concentration.