Supporting Information

Unveiling the conformations and van der Waals interactions between rare-gas and bicyclic aromatic: Rotational spectroscopy of benzofuran complexes with Argon and Krypton

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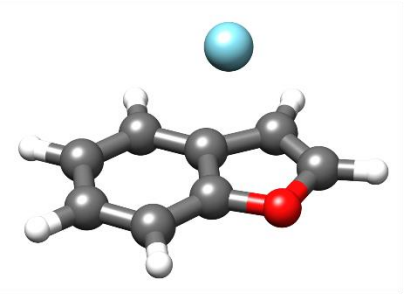
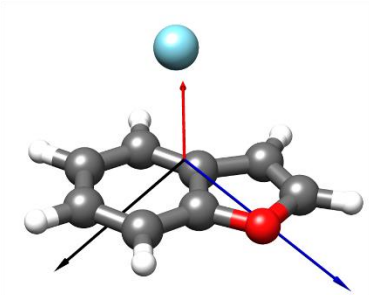
Figure S1. Shapes and geometries of the three conformations of **BF-Ar** obtained with the MP2/6-311++G(d,p) calculations.



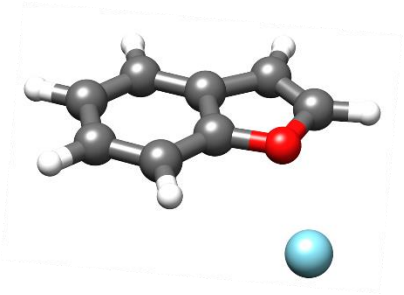
BF-Ar_I

r(Ar···C5) = 3.351 Å
a(Ar···C5C4) = 85.5°
d(Ar···C5C4O1) = 81.9°



BF-Ar_II

r(Ar···C5) = 3.437 Å
a(Ar···C5C4) = 81.7°
d(Ar···C5C4O1) = 95.2°



BF-Ar_III

r(Ar···C5) = 4.041 Å
a(Ar···C5C4) = 162.0°
d(Ar···C5C4O1) = 3.9°

Figure S2. Shape and geometry the BF-Ar complex calculated at different levels of theory combined with the def2-TZVP basis set.

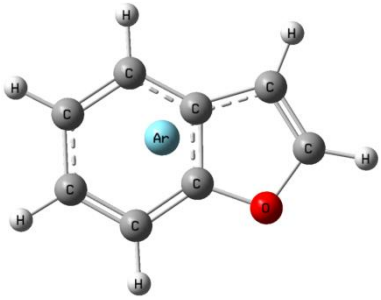
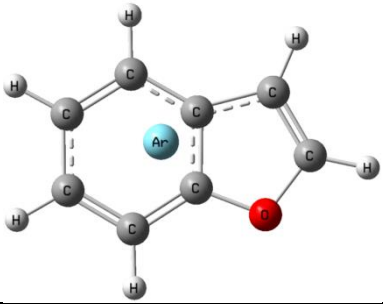
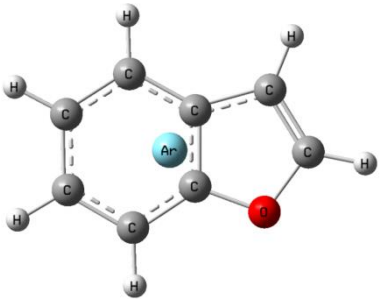
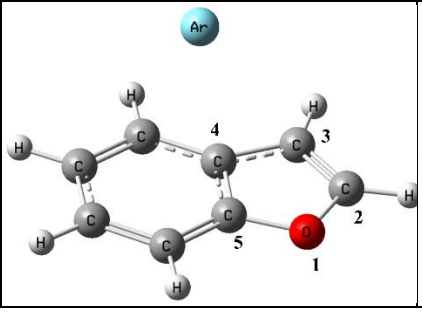
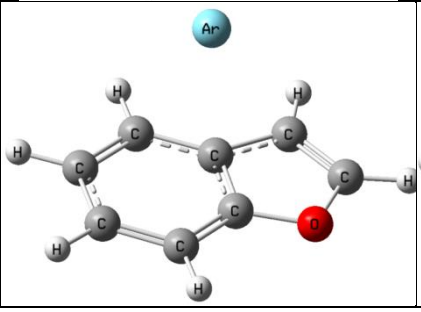
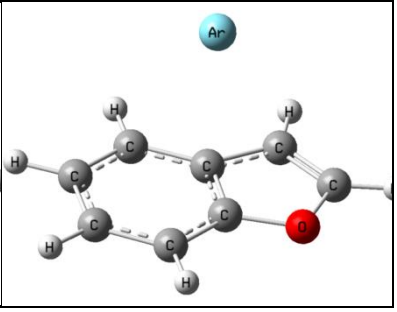
	B3LYP-D3(BJ)	ωB97XD	B97D
Top view			
Side view			

Figure S3. Shapes and geometries of the two conformations of **BF-Kr** obtained with the MP2/6-311++G(d,p) calculations.

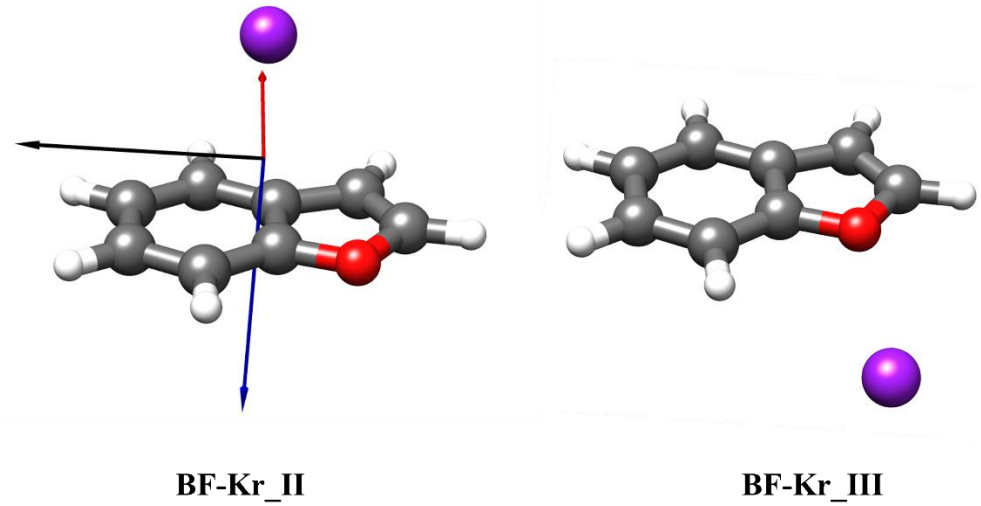


Figure S4. Shape and geometry of the BF-Kr complex calculated at different levels of theory combined with the def2-TZVP basis set.

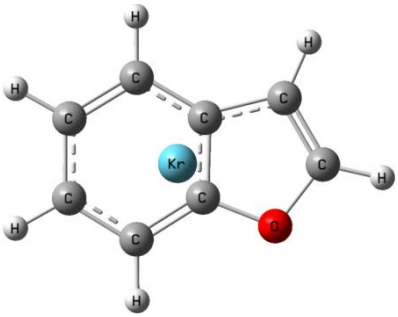
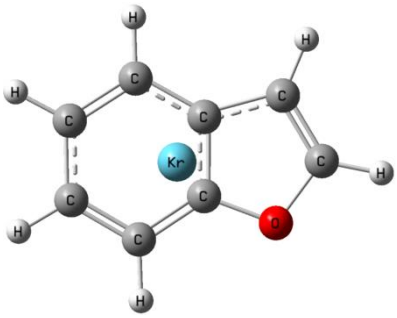
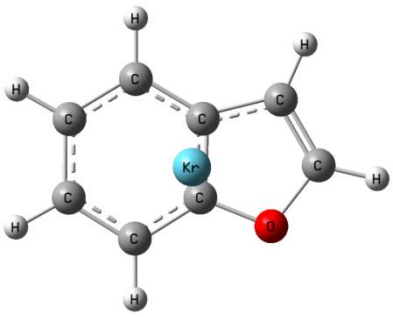
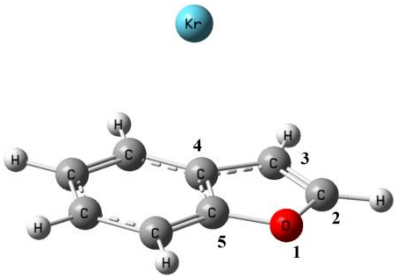
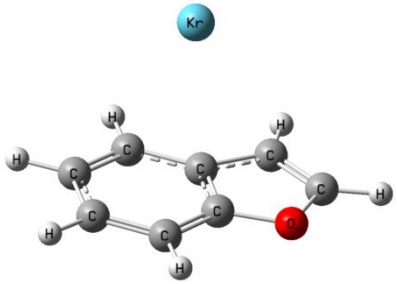
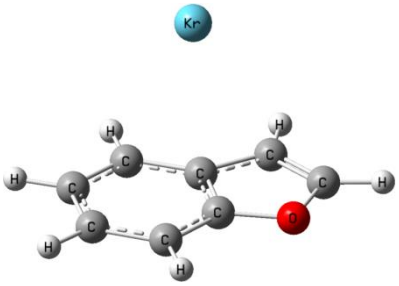
	B3LYP-D3(BJ)	ωB97XD	B97D
Top view			
Side view			

Table S1. Theoretical spectroscopic parameters of the three conformations of the BF-Ar complex calculated at the MP2/6-311++G(d,p) level.

	BF-Ar_I	**BF-Ar_II**	**BF-Ar_III**
A/MHz	1302	1163	1801
B/MHz	979	1064	617
C/MHz	775	777	460
Δ_J/kHz	3.02	6.33	0.25
Δ_{JK}/kHz	−2.87	−9.79	2.18
Δ_K/kHz	0.35	3.91	0.43
δ_J/kHz	−1.14	−0.29	−0.09
δ_K/kHz	−1.23	2.77	−0.03
μ_a/D	0.04	0.09	0.55
μ_b/D	0.31	0.24	0.57
μ_c/D	0.69	0.71	0.00
ΔE_0/cm^{-1}	0	17	490

Table S2. Theoretical spectroscopic parameters of the BF-Ar complex calculated at different levels of theory combined with the def2-TZVP basis set.

	B3LYP-D3(BJ)	ωB97XD	B97D
A/MHz	1227	1236	1166
B/MHz	993	945	993
C/MHz	760	733	739
Δ_J/kHz	6.07	4.69	5.95
Δ_{JK}/kHz	−8.96	−15.93	−8.87
Δ_K/kHz	3.40	11.49	3.39
δ_J/kHz	−1.17	0.79	−0.81
δ_K/kHz	−2.84	−10.39	−1.27
μ_a/D	0.12	0.13	0.03
μ_b/D	0.23	0.26	0.29
μ_c/D	0.69	0.64	0.64

Table S3. The MP2/6-311++G(d,p)) calculated spectroscopic parameters of the BF-Kr complex

	BF-Kr_II	**BF-Kr_III**
A /MHz	1163	1789
B/MHz	690	373
C/MHz	557	308
Δ_J /kHz	0.41	0.16
Δ_{JK}/kHz	18.39	1.56
Δ_K/kHz	−18.45	1.19
δ_J/kHz	0.08	0.03
δ_K/kHz	8.69	1.30
μ_a/D	0.10	0.61
μ_b/D	0.23	0.56
μ_c/D	0.71	0.02
ΔE_0/cm^{-1}	0	597

Table S4. Theoretical spectroscopic parameters of the BF-Kr complex calculated at different levels of theory combined with the def2-TZVP basis set.

	B3LYP-D3(BJ)	ωB97XD	B97XD
A/MHz	1186	1203	1164
B/MHz	664	631	645
C/MHz	543	523	527
Δ_J /kHz	0.49	0.49	0.12
Δ_{JK}/kHz	8.89	2.71	10.89
Δ_K/kHz	−7.69	−2.01	−10.72
δ_J/kHz	−0.22	−0.14	0.07
δ_K/kHz	−0.12	−0.04	−0.12
μ_a/D	0.25	0.15	0.09
μ_b/D	0.69	0.25	0.27
μ_c/D	0.13	0.64	0.63

Table S5. Partial r_0 structure of **BF-Ar_I** derived from strfit based on the RI-SCS-MP2/aug-cc-pVDZ calculated geometry.

Bond lengths/Å[a]		Angles/°		Dihedral angles/°	
C2O1	1.3843				
C3C2	1.3727	C3C2O1	112.38		
C4C3	1.4529	C4C3C2	105.75	C4C3C2O1	0.10
C5C4	1.4147	C5C4C3	105.47	C5C4C3C2	-0.14
C6C5	1.4038	C6C5C4	123.87	C6C5C4C2	179.66
C7C6	1.4046	C7C6C5	116.11	C7C6C5C4	-0.20
C8C7	1.4227	C8C7C6	121.44	C8C7C6C5	0.09
C9C8	1.4025	C9C8C7	121.38	C9C8C7C6	0.04
H10C2	1.0884	H10C2C3	132.50	H10C2C3C4	179.88
H11C3	1.0893	H11C3C4	128.36	H11C3C4C5	179.91
H12C9	1.0945	H12C9C8	120.87	H12C9C8C7	179.96
H13C8	1.0947	H13C8C7	119.01	H13C8C7C6	-179.94
H14C7	1.0946	H14C7C7	119.26	H14C7C7C5	-179.90
H15C6	1.0932	H15C6C5	121.67	H15C6C5C4	-179.94
Ar16C5	**3.433(21)**	Ar16C5C4	86.54	**Ar16C5C4O1**	**86.4(8)**

[a] The parameters in bold have been modified to reproduce the experimental values of rotational constants, uncertainties (in parentheses) are given in units of the last digit.

Table S6. Partial r_0 structure of **BF-Kr_I** derived from strfit based on the RI-SCS-MP2/aug-cc-pVDZ calculated geometry.

Bond lengths/Å[a]		Angles/°		Dihedral angles/°	
C2O1	1.3719				
C3C2	1.3503	C3C2O1	112.10		
C4C3	1.4408	C4C3C2	106.16	C4C3C2O1	0.06
C5C4	1.4030	C5C4C3	105.43	C5C4C3C2	-0.03
C6C5	1.3827	C6C5C4	123.64	C6C5C4C2	179.21
C7C6	1.3886	C7C6C5	116.45	C7C6C5C4	-0.08
C8C7	1.4019	C8C7C6	121.29	C8C7C6C5	0.06
C9C8	1.3858	C9C8C7	121.33	C9C8C7C6	0.03
H10C2	1.0759	H10C2C3	132.61	H10C2C3C4	-179.97
H11C3	1.0768	H11C3C4	127.64	H11C3C4C5	-179.87
H12C9	1.0821	H12C9C8	120.74	H12C9C8C7	-179.74
H13C8	1.0820	H13C8C7	119.11	H13C8C7C6	-179.86
H14C7	1.0818	H14C7C7	119.32	H14C7C7C5	-179.80
H15C6	1.0810	H15C6C5	121.43	H15C6C5C4	-179.69
Kr16C5	**3.670(5)** [a]	Kr16C5C4	79.81	**Kr16C5C4O1**	**95.8(14)**

[a] The parameters in bold have been modified to reproduce the experimental values of rotational constants, uncertainties (in parentheses) are given in units of the last digit.

Table S7. Partial r_e^{SE} structure of **BF-Ar_I** derived from strfit based on the r_e^{SE} geometry of benzofuran.

Bond lengths/Å[a]		Angles/°		Dihedral angles/°	
C2C1	1.4036				
C3C2	1.3860	C3C2C1	121.29		
C4C1	1.3875	C4C1C2	121.41	C4C1C2C3	0.00
H5C1	1.0802	H5C1C2	119.35	H5C1C2C3	180.00
H6C2	1.0803	H6C2C1	119.09	H6C2C1H5	0.00
H7C3	1.0805	H7C3C2	120.74	H7C3C2H6	0.00
H8C4	1.0794	H8C4C1	122.14	H8C4C1H5	0.00
C9C3	1.3995	C9C3C2	118.29	C9C3C2C1	0.00
C10C4	1.3848	C10C4C1	116.25	C10C4C1C2	0.00
C11C9	1.4399	C11C9C3	135.61	C11C9C3C2	180.00
O12C10	1.3651	O12C10C4	125.72	O12C10C4C1	180.00
H13C11	1.0752	H13C11C9	127.88	H13C11C9C3	0.00
C14C11	1.3515	C14C11C9	105.77	C14C11C9C3	180.00
H15C14	1.0742	H15C14O12	115.20	H15C14O12C10	180.00
Ar16O10	**3.453(8)**	Ar16O10C9	86.55	**Ar16O10C9O12**	**87.2(3)**

[a] The parameters in bold have been modified to reproduce the experimental values of rotational constants, uncertainties (in parentheses) are given in units of the last digit.

Table S8. Partial r_e^{SE} structure of **BF-Kr_I** derived from strfit based on the r_e^{SE} geometry of benzofuran.

Bond lengths/Å[a]		Angles/°		Dihedral angles/°	
C2C1	1.4036				
C3C2	1.3860	C3C2C1	121.29		
C4C1	1.3875	C4C1C2	121.41	C4C1C2C3	0.00
H5C1	1.0802	H5C1C2	119.35	H5C1C2C3	180.00
H6C2	1.0803	H6C2C1	119.09	H6C2C1H5	0.00
H7C3	1.0805	H7C3C2	120.74	H7C3C2H6	0.00
H8C4	1.0794	H8C4C1	122.14	H8C4C1H5	0.00
C9C3	1.3995	C9C3C2	118.29	C9C3C2C1	0.00
C10C4	1.3848	C10C4C1	116.25	C10C4C1C2	0.00
C11C9	1.4399	C11C9C3	135.61	C11C9C3C2	180.00
O12C10	1.3651	O12C10C4	125.72	O12C10C4C1	180.00
H13C11	1.0752	H13C11C9	127.88	H13C11C9C3	0.00
C14C11	1.3515	C14C11C9	105.77	C14C11C9C3	180.00
H15C14	1.0742	H15C14O12	115.20	H15C14O12C10	180.00
Kr16O10	**3.53403(9)**	**Kr16O10C9**	**88.480(8)**	**Kr16O10C9O12**	**90.866(6)**

[a] The parameters in bold have been modified to reproduce the experimental values of rotational constants, uncertainties (in parentheses) are given in units of the last digit.

Table S9. Ground-state rotational constants and the corresponding vibrational corrections calculated at the B3LYP-D3(BJ)/def2-TZVP level. Values in MHz.

Isotopologue	A_0	B_0	C_0	A_0-A_e	B_0-B_e	C_0-C_e
BF-Ar_I	1271.123	958.323	756.769	−10.826	−3.064	−4.547
BF-Kr_I (^{84}Kr)	1199.854	668.504	550.558	−6.875	−0.239	−0.918
BF-Kr_I (^{86}Kr)	1199.177	661.415	545.613	−6.883	−0.223	−0.897

Table S10. Experimental transition frequencies of the observed parent species of the BF-Ar complex.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ /MHz
3	3	1	2	2	1	7056.2744	0.00177
4	4	0	3	3	0	9449.3942	−0.00114
4	4	1	3	3	1	9476.6941	0.00160
5	5	0	4	4	0	11903.5253	0.00186
5	5	1	4	4	1	11911.2617	0.00277
6	6	0	5	5	0	14346.0399	−0.00264
6	6	1	5	5	1	14347.9718	0.00010
7	7	0	6	6	0	16780.7327	−0.00310
7	7	1	6	6	1	16781.1792	−0.00230
4	3	1	3	2	1	8710.4639	−0.00630
4	3	2	3	2	2	8947.5756	−0.00084
5	4	1	4	3	1	11165.0271	−0.00437
5	4	2	4	3	2	11305.0661	0.00049
6	5	1	5	4	1	13648.2442	0.00049
6	5	2	5	4	2	13705.0596	0.00192
7	6	1	6	5	1	16108.5125	0.00192
7	6	2	6	5	2	16126.7353	0.00286
4	2	2	3	1	2	8362.8096	−0.00218
4	2	3	3	1	3	8711.6685	0.00065
5	3	2	4	2	2	10532.1159	−0.00288
5	3	3	4	2	3	10924.9606	0.00025
6	4	2	5	3	2	12864.0371	0.00074
6	4	3	5	3	3	13197.8189	0.00126
7	5	2	6	4	2	15333.3355	0.00794
7	5	3	6	4	3	15533.2393	−0.00354
4	1	3	3	0	3	8535.1021	0.00257
5	1	4	4	0	4	10769.6468	0.00023
6	1	5	5	0	5	12973.2573	0.00050
7	1	6	6	0	6	15157.6200	−0.00357
5	2	3	4	1	3	10496.1723	0.00184
5	2	4	4	1	4	10837.4349	0.00239
6	2	4	5	1	4	12745.5704	0.00145
6	2	5	5	1	5	12994.5885	−0.00193
7	2	5	6	1	5	15002.4506	0.00994
7	2	6	6	1	6	15163.6201	−0.00761
6	3	3	5	2	3	12507.7118	0.00119
6	3	4	5	2	4	12983.5842	0.00239

7	3	4	6	2	4	14655.4403	−0.00306
7	3	5	6	2	5	15102.4102	0.00084
7	4	3	6	3	3	14661.8283	0.00081
7	4	4	6	3	4	15171.4064	−0.00716
8	4	4	7	3	4	16630.7820	−0.00758
8	3	5	7	2	5	16925.4905	0.00443
8	5	3	7	4	3	17000.4524	0.00356
8	3	6	7	2	6	17254.8315	0.00339
8	6	2	7	5	2	17830.6651	0.00600
8	6	3	7	5	3	17916.8976	−0.00666
8	8	0	7	7	0	19208.3675	0.01455
8	8	1	7	7	1	19208.4401	−0.01062
8	7	1	7	6	1	18548.6377	−0.00313
8	7	2	7	6	2	18553.7403	−0.00224

Table S11. Experimental transition frequencies of the observed species of BF-^{84}Kr.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ /MHz
3	3	0	2	2	0	6501.8764	−0.00002
3	3	1	2	2	1	6520.3926	0.00047
4	4	0	3	3	0	8871.8424	0.00043
4	4	1	3	3	1	8873.7906	−0.00158
5	5	0	4	4	0	11233.7288	0.00138
5	5	1	4	4	1	11233.8944	−0.00048
6	6	0	5	5	0	13594.2741	−0.00074
6	6	1	5	5	1	13594.2881	0.00039
7	7	0	6	6	0	15954.2558	0.00131
7	7	1	6	6	1	15954.2558	0.00039
8	8	0	7	7	0	18313.7177	−0.00010
8	8	1	7	7	1	18313.7177	−0.00016
4	3	1	3	2	1	7676.3583	−0.00013
4	3	2	3	2	2	7761.5261	−0.00003
5	4	1	4	3	1	10074.4905	−0.00006
5	4	2	4	3	2	10087.5781	0.00001
6	5	1	5	4	1	12440.2082	−0.00020
6	5	2	5	4	2	12441.6755	0.00024
7	6	1	6	5	1	14798.9838	−0.00025
7	6	2	6	5	2	14799.1219	−0.00107
8	7	1	7	6	1	17155.8974	0.00541
8	7	2	7	6	2	17155.8974	−0.00640
5	3	2	4	2	2	8811.3993	−0.00036
5	3	3	4	2	3	9034.2815	0.00036
6	4	2	5	3	2	11258.3951	0.00007
6	4	3	5	3	3	11307.4953	0.00016
7	5	2	6	4	2	13640.9369	0.00057
7	5	3	6	4	3	13648.0021	−0.00039
8	6	2	7	5	2	16000.8433	0.00082
8	6	3	7	5	3	16001.6561	0.00054
4	2	2	3	1	2	6457.9155	−0.00148
4	2	3	3	1	3	6936.0283	0.00202
4	1	3	3	0	3	6077.8085	0.00024
5	1	4	4	0	4	7668.5654	−0.00122
6	1	5	5	0	5	9344.3893	0.00156
5	2	3	4	1	3	7722.0903	−0.00098
5	2	4	4	1	4	8385.7413	−0.00022
6	2	4	5	1	4	9076.8338	−0.00078
6	2	5	5	1	5	9888.6294	−0.00027

7	2	5	6	1	5	10537.0804	0.00114
7	2	6	6	1	6	11437.6193	0.00083
8	2	6	7	1	6	12111.4776	−0.00048
8	2	5	7	1	5	13132.5363	−0.00156
6	3	3	5	2	3	9922.4814	0.00004
6	3	4	5	2	4	10349.1301	0.00083
7	3	4	6	2	4	11051.9405	0.00146
7	3	5	6	2	5	11713.8324	−0.00033
7	4	3	6	3	3	12407.6820	0.00019
7	4	4	6	3	4	12541.1637	−0.00159
8	4	4	7	3	4	13511.1080	−0.00004
8	3	5	7	2	5	12247.2095	0.00130
8	5	3	7	4	3	14829.4091	−0.00047
8	4	5	7	3	5	13798.9187	0.00122
8	3	6	7	2	6	13132.5363	−0.00156
7	1	7	6	1	6	7839.4995	0.00110
7	0	7	6	0	6	7865.3078	−0.00243
7	1	7	6	0	6	7890.0843	0.00102

Table S12. Experimental transition frequencies of the observed species of BF-^{86}Kr.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{obs}/MHz	$\Delta\nu_{obs-calc}$ /MHz
3	3	0	2	2	0	6495.8407	0.00028
4	4	0	3	3	0	8865.4093	−0.00020
4	4	1	3	3	1	8867.2109	0.00040
5	5	0	4	4	0	11227.1985	0.00012
5	5	1	4	4	1	11227.3477	−0.00048
6	6	0	5	5	0	13587.7158	−0.00211
6	6	1	5	5	1	13587.7311	0.00203
7	7	0	6	6	0	15947.6856	0.00049
7	7	1	6	6	1	15947.6856	−0.00028
5	4	1	4	3	1	10055.8499	−0.00010
5	4	2	4	3	2	10067.9594	−0.00007
6	5	1	5	4	1	12421.0935	−0.00041
6	5	2	5	4	2	12422.4083	0.00054

Table S13. NBO stabilization energy contributions (≥ 0.21 kJ/mol) for the isomer **BF-Ar_I** of the BF-Ar complex calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

Donor NBO	Acceptor NBO	$E^{(2)}$ [kJ·mol^{-1}]
From BF to Ar		
C8=C9	Ar10	0.38
C8–H14	Ar10	0.25
C6–H16	Ar10	0.29
C6–H16	Ar10	0.33
C4=C5	Ar10	0.21
C4=C5	Ar10	0.25
C3=C4	Ar10	0.25
C3–H12	Ar10	0.41
C3–H12	Ar10	0.46
From Ar to BF		
Ar10	C4=C5	0.25
Sum		3.10

Table S14. NBO stabilization energy contributions (≥ 0.21 kJ/mol) for the isomer **BF-Kr_I** of the BF-Kr complex calculated at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

Donor NBO	Acceptor NBO	$E^{(2)}$ [kJ·mol^{-1}]
From BF to Ar		
C8=C9	Kr10	0.38
C8=C9	Kr10	0.25
C8–H14	Kr10	0.25
C6–H16	Kr10	0.25
C6–H16	Kr10	0.29
C4=C5	Kr10	0.21
C3–H12	Kr10	0.33
C3–H12	Kr10	0.21
C3–H12	Kr10	0.54
From Ar to BF		
Kr10	C4=C5	0.25
Sum		2.97

Table S15. The output of the SAPT2+δMP2/aug-cc-pVDZ level of calculation for the isomer **BF-Ar_I** of the BF-Ar complex.

Electrostatics	-1.61273449 [mEh]	-1.01200617 [kcal/mol]	-4.23423382 [kJ/mol]
Elst10,r	-1.47801587 [mEh]	-0.92746896 [kcal/mol]	-3.88053013 [kJ/mol]
Elst12,r	-0.13471862 [mEh]	-0.08453721 [kcal/mol]	-0.35370369 [kJ/mol]
Exchange	4.26864836 [mEh]	2.67861729 [kcal/mol]	11.20733473 [kJ/mol]
Exch10	3.91880060 [mEh]	2.45908450 [kcal/mol]	10.28880955 [kJ/mol]
Exch10(S^2)	3.91141035 [mEh]	2.45444705 [kcal/mol]	10.26940645 [kJ/mol]
Exch11(S^2)	0.09340453 [mEh]	0.05861223 [kcal/mol]	0.24523357 [kJ/mol]
Exch12(S^2)	0.25644323 [mEh]	0.16092055 [kcal/mol]	0.67329160 [kJ/mol]
Induction	-0.24935690 [mEh]	-0.15647382 [kcal/mol]	-0.65468646 [kJ/mol]
Ind20,r	-2.09737508 [mEh]	-1.31612273 [kcal/mol]	-5.50665750 [kJ/mol]
Ind22	-0.11465154 [mEh]	-0.07194493 [kcal/mol]	-0.30101758 [kJ/mol]
Exch-Ind20,r	2.03734135 [mEh]	1.27845100 [kcal/mol]	5.34903898 [kJ/mol]
Exch-Ind22	0.11136984 [mEh]	0.06988563 [kcal/mol]	0.29240147 [kJ/mol]
delta HF,r (2)	-0.23077160 [mEh]	-0.14481137 [kcal/mol]	-0.60589076 [kJ/mol]
delta MP2,r (2)	0.04473013 [mEh]	0.02806858 [kcal/mol]	0.11743893 [kJ/mol]
Dispersion	-4.16093339 [mEh]	-2.61102512 [kcal/mol]	-10.92452912 [kJ/mol]
Disp20	-5.17255736 [mEh]	-3.24582874 [kcal/mol]	-13.58054747 [kJ/mol]
Disp21	1.54252761 [mEh]	0.96795069 [kcal/mol]	4.04990569 [kJ/mol]
Disp22 (SDQ)	-0.19019214 [mEh]	-0.11934737 [kcal/mol]	-0.49934939 [kJ/mol]
Disp22 (T)	-0.75488413 [mEh]	-0.47369694 [kcal/mol]	-1.98194800 [kJ/mol]
Est. Disp22 (T)	-0.80040885 [mEh]	-0.50226414 [kcal/mol]	-2.10147315 [kJ/mol]
Exch-Disp20	0.45969734 [mEh]	0.28846443 [kcal/mol]	1.20693519 [kJ/mol]
Total HF	2.14997940 [mEh]	1.34913244 [kcal/mol]	5.64477014 [kJ/mol]
Total SAPT0	-2.56288062 [mEh]	-1.60823187 [kcal/mol]	-6.72884214 [kJ/mol]
Total SAPT2	-2.35103318 [mEh]	-1.47529559 [kcal/mol]	-6.17263676 [kJ/mol]
Total SAPT2+	-1.79910655 [mEh]	-1.12895641 [kcal/mol]	-4.72355361 [kJ/mol]

Total SAPT2+dMP2	-1.75437643 [mEh]	-1.10088783 [kcal/mol]	-4.60611468 [kJ/mol]
Special recipe for scaled SAPT0 (see Manual):			
Electrostatics sSAPT0	-1.47801587 [mEh]	-0.92746896 [kcal/mol]	-3.88053013 [kJ/mol]
Exchange sSAPT0	3.91880060 [mEh]	2.45908450 [kcal/mol]	10.28880955 [kJ/mol]
Induction sSAPT0	-0.27923539 [mEh]	-0.17522285 [kcal/mol]	-0.73313241 [kJ/mol]
Dispersion sSAPT0	-4.71024942 [mEh]	-2.95572614 [kcal/mol]	-12.36675816 [kJ/mol]
Total sSAPT0	-2.54870008 [mEh]	-1.59933345 [kcal/mol]	-6.69161115 [kJ/mol]

Table S16. The output of the SAPT2+δMP2/aug-cc-pVDZ level of calculation for the isomer **BF-Kr_I** of the BF-Ar complex.

Electrostatics	-2.36766197 [mEh]	-1.48573032 [kcal/mol]	-6.21629565 [kJ/mol]
Elst10,r	-2.19487277 [mEh]	-1.37730346 [kcal/mol]	-5.76263767 [kJ/mol]
Elst12,r	-0.17278920 [mEh]	-0.10842686 [kcal/mol]	-0.45365798 [kJ/mol]
Exchange	5.93646377 [mEh]	3.72518726 [kcal/mol]	15.58618348 [kJ/mol]
Exch10	5.43042872 [mEh]	3.40764547 [kcal/mol]	14.25758865 [kJ/mol]
Exch10(S^2)	5.41427838 [mEh]	3.39751097 [kcal/mol]	14.21518592 [kJ/mol]
Exch11(S^2)	0.18069230 [mEh]	0.11338613 [kcal/mol]	0.47440756 [kJ/mol]
Exch12(S^2)	0.32534275 [mEh]	0.20415566 [kcal/mol]	0.85418727 [kJ/mol]
Induction	-0.37062977 [mEh]	-0.23257369 [kcal/mol]	-0.97308832 [kJ/mol]
Ind20,r	-3.84264938 [mEh]	-2.41129889 [kcal/mol]	-10.08887455 [kJ/mol]
Ind22	-0.20152197 [mEh]	-0.12645695 [kcal/mol]	-0.52909587 [kJ/mol]
Exch-Ind20,r	3.71042575 [mEh]	2.32832731 [kcal/mol]	9.74172147 [kJ/mol]
Exch-Ind22	0.19458770 [mEh]	0.12210563 [kcal/mol]	0.51088994 [kJ/mol]
delta HF,r (2)	-0.29988228 [mEh]	-0.18817897 [kcal/mol]	-0.78734083 [kJ/mol]
delta MP2,r (2)	0.06841041 [mEh]	0.04292818 [kcal/mol]	0.17961150 [kJ/mol]
Dispersion	-5.32764759 [mEh]	-3.34314934 [kcal/mol]	-13.98773683 [kJ/mol]
Disp20	-6.80543074 [mEh]	-4.27047226 [kcal/mol]	-17.86765595 [kJ/mol]
Disp21	2.12658488 [mEh]	1.33445216 [kcal/mol]	5.58334783 [kJ/mol]
Disp22 (SDQ)	-0.29397124 [mEh]	-0.18446974 [kcal/mol]	-0.77182139 [kJ/mol]
Disp22 (T)	-1.00205135 [mEh]	-0.62879672 [kcal/mol]	-2.63088546 [kJ/mol]
Est. Disp22 (T)	-1.06082953 [mEh]	-0.66568058 [kcal/mol]	-2.78520754 [kJ/mol]
Exch-Disp20	0.70599904 [mEh]	0.44302109 [kcal/mol]	1.85360023 [kJ/mol]
Total HF	2.80345004 [mEh]	1.75919146 [kcal/mol]	7.36045707 [kJ/mol]
Total SAPT0	-3.29598166 [mEh]	-2.06825971 [kcal/mol]	-8.65359865 [kJ/mol]
Total SAPT2	-2.96967008 [mEh]	-1.86349611 [kcal/mol]	-7.79686772 [kJ/mol]
Total SAPT2+	-2.19788597 [mEh]	-1.37919427 [kcal/mol]	-5.77054882 [kJ/mol]
Total SAPT2+dMP2	-2.12947556 [mEh]	-1.33626609 [kcal/mol]	-5.59093732 [kJ/mol]

Special recipe for scaled SAPT0 (see Manual):			
Electrostatics sSAPT0	-2.19487277 [mEh]	-1.37730346 [kcal/mol]	-5.76263767 [kJ/mol]
Exchange sSAPT0	5.43042872 [mEh]	3.40764547 [kcal/mol]	14.25758865 [kJ/mol]
Induction sSAPT0	-0.39880308 [mEh]	-0.25025271 [kcal/mol]	-1.04705733 [kJ/mol]
Dispersion sSAPT0	-6.09309502 [mEh]	-3.82347485 [kcal/mol]	-15.99741878 [kJ/mol]
Total sSAPT0	-3.25634215 [mEh]	-2.04338555 [kcal/mol]	-8.54952514 [kJ/mol]