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Electronic Supplementary Information for

Classifying the chemical bonds involving the noble-gas atoms

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Data S1 CCSD(T)/aug-cc-pVTZ cartesian coordinates (a_0) of the species included in the NgBC47 data set

HeH^+

He	0.000000	0.000000	0.000000
H	1.466427	0.000000	0.000000

NeH^+

Ne	0.000000	0.000000	0.000000
H	1.874608	0.000000	0.000000

ArH^+

Ar	0.000000	0.000000	0.000000
H	2.422629	0.000000	0.000000

KrH^+

Kr	0.000000	0.000000	0.000000
H	2.675853	0.000000	0.000000

XeH^+

Xe	0.000000	0.000000	0.000000
H	3.014113	0.000000	0.000000

H-He-F

He	0.000000	0.000000	0.000000
H	-1.532568	0.000000	0.000000
F	2.673962	0.000000	0.000000

H-Ar-F

Ar	0.000000	0.000000	0.000000
H	-2.511446	0.000000	0.000000
F	3.739768	0.000000	0.000000

H-Kr-F

Kr	0.000000	0.000000	0.000000
H	-2.791126	0.000000	0.000000
F	3.858821	0.000000	0.000000

H-Xe-F

Xe	0.000000	0.000000	0.000000
H	-3.142615	0.000000	0.000000
F	3.998660	0.000000	0.000000

He-H-F

He	0.000000	0.000000	0.000000
H	4.207475	0.000000	0.000000
F	5.947913	0.000000	0.000000

Ne-H-F

Ne	0.000000	0.000000	0.000000
H	4.221648	0.000000	0.000000
F	5.962086	0.000000	0.000000

Ar-H-F

Ar	0.000000	0.000000	0.000000
H	4.735654	0.000000	0.000000
F	6.477982	0.000000	0.000000

Kr-H-F

Kr	0.000000	0.000000	0.000000
H	4.790456	0.000000	0.000000
F	6.534673	0.000000	0.000000

Xe-H-F

Xe	0.000000	0.000000	0.000000
H	5.058797	0.000000	0.000000
F	6.804904	0.000000	0.000000

HeAr

He	0.000000	0.000000	0.000000
Ar	6.621411	0.000000	0.000000

NeAr

Ne	0.000000	0.000000	0.000000
Ar	6.631049	0.000000	0.000000

ArAr

Ar	0.000000	0.000000	0.000000
Ar	7.201935	0.000000	0.000000

KrAr

Kr	0.000000	0.000000	0.000000
Ar	7.332137	0.000000	0.000000

XeAr

Xe	0.000000	0.000000	0.000000
Ar	7.732759	0.000000	0.000000

$HeNa^+$

He	0.000000	0.000000	0.000000
Na	4.566145	0.000000	0.000000

$NeNa^+$

Ne	0.000000	0.000000	0.000000
Na	4.831652	0.000000	0.000000

$ArNa^+$

Ar	0.000000	0.000000	0.000000
Na	5.421624	0.000000	0.000000

$KrNa^+$

Kr	0.000000	0.000000	0.000000
Na	5.613054	0.000000	0.000000

$XeNa^+$

Xe	0.000000	0.000000	0.000000
Na	5.904827	0.000000	0.000000

HeF^-

He	0.000000	0.000000	0.000000
F	6.157106	0.000000	0.000000

NeF^-

Ne	0.000000	0.000000	0.000000
F	6.060163	0.000000	0.000000

ArF^-

Ar	0.000000	0.000000	0.000000
F	5.706973	0.000000	0.000000

KrF^-

Kr	0.000000	0.000000	0.000000
F	5.704327	0.000000	0.000000

XeF^-

Xe	0.000000	0.000000	0.000000
F	5.589999	0.000000	0.000000

He-Be-O

He	0.000000	0.000000	0.000000
Be	2.879943	0.000000	0.000000
O	5.408397	0.000000	0.000000

Ne-Be-O

Ne	0.000000	0.000000	0.000000
Be	3.399617	0.000000	0.000000
O	5.931850	0.000000	0.000000

Ar-Be-O

Ar	0.000000	0.000000	0.000000
Be	3.917402	0.000000	0.000000
O	6.451525	0.000000	0.000000

Kr-Be-O

Kr	0.000000	0.000000	0.000000
Be	4.159287	0.000000	0.000000
O	6.695299	0.000000	0.000000

Xe-Be-O

Xe	0.000000	0.000000	0.000000
Be	4.478651	0.000000	0.000000
O	7.018443	0.000000	0.000000

He-Cu-F

He	0.000000	0.000000	0.000000
Cu	3.224440	0.000000	0.000000
F	6.545067	0.000000	0.000000

Ne-Cu-F

Ne	0.000000	0.000000	0.000000
Cu	4.230530	0.000000	0.000000
F	7.565897	0.000000	0.000000

Ar-Cu-F

Ar	0.000000	0.000000	0.000000
Cu	4.292702	0.000000	0.000000
F	7.623155	0.000000	0.000000

Kr-Cu-F

Kr	0.000000	0.000000	0.000000
Cu	4.438778	0.000000	0.000000
F	7.770932	0.000000	0.000000

Xe-Cu-F

Xe	0.000000	0.000000	0.000000
Cu	4.669135	0.000000	0.000000
F	8.009415	0.000000	0.000000

F-He-O$^-$

He	0.000000	0.000000	0.000000
F	-3.072695	0.000000	0.000000
O	2.097596	0.000000	0.000000

F-Kr-O$^-$

Kr	0.000000	0.000000	0.000000
F	-4.268891	0.000000	0.000000
O	3.503552	0.000000	0.000000

F-Xe-O$^-$

Xe	0.000000	0.000000	0.000000
F	-4.386054	0.000000	0.000000
O	3.717091	0.000000	0.000000

He-H-OH$_2^+$

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.853254
He	-0.308213	0.000000	5.210218
H	0.791098	-1.527508	-0.679294
H	0.791098	1.527508	-0.679294

Ne-H-OH_2^+

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.856467
Ne	-0.262991	0.000000	5.377234
H	0.791015	-1.526284	-0.680598
H	0.791015	1.526284	-0.680598

Ar-H-OH_2^+

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.878199
Ar	-0.198941	0.000000	5.755919
H	0.795577	-1.521921	-0.679921
H	0.795577	1.521921	-0.679921

Kr-H-OH_2^+

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.889159
Kr	-0.181731	0.000000	5.978270
H	0.800080	-1.520117	-0.677125
H	0.800080	1.520117	-0.677125

Xe-H-OH_2^+

O	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.906356
Xe	-0.167024	0.000000	6.261240
H	0.807408	-1.517389	-0.672471
H	0.807408	1.517389	-0.672471

Data S2 Cartesian coordinates (a_0) of the exemplary species taken from the literature

$HHeNH_3^+$ [CCSD(T)/aVTZ, taken from Ref. 1)

He	0.000000	0.000000	0.000000
N	3.569693	0.000000	0.000000
H	-1.451310	0.000000	0.000000
H	4.313098	0.000000	1.774297
H	4.313098	-1.536586	-0.887148
H	4.313098	1.536586	-0.887148

$HeBO^+$ [CCSD(T)/6-311++G(2df,2pd), taken from Ref. 2)

He	0.000000	0.000000	0.000000
B	2.350819	0.000000	0.000000
O	4.601483	0.000000	0.000000

$HeO(LiF)_2$ [CCSD(T)/6-311++G(d,p), taken from Ref. 3)

He	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.174697
Li	3.950470	0.000000	1.765194
F	3.853506	0.000000	-1.294059
Li	-3.950470	0.000000	1.765194
F	-3.853506	0.000000	-1.294059

$FNeBN^-$ [CCSD(T)/aVTZ, taken from Ref. 4)

F	0.000000	0.000000	0.000000
Ne	4.225428	0.000000	0.000000
B	7.197967	0.000000	0.000000
N	9.601698	0.000000	0.000000

$ArOH^+$ ($^1A'$) [CCSD(T)/cc-pVQZ, taken from Ref. 5]

Ar	0.000000	0.000000	0.000000
O	0.000000	0.000000	3.269226
H	1.842407	0.000000	3.594092

$ArOH^+$ ($^3\Sigma^-$) [CCSD(T)/cc-pVQZ, taken from Ref. 5]

O	0.000000	0.000000	0.000000
H	2.040904	0.000000	0.000000
Ar	5.423514	0.000000	0.000000

$FArCH_3$ [MP2/6-311++G(3df,3pd), taken from Ref. 6]

Ar	0.000000	0.000000	0.000000
C	3.505442	0.000000	0.000000
H	4.044979	0.000000	1.972215
H	4.044979	-1.707988	-0.986107
H	4.044979	1.707988	-0.986107
F	-3.788901	0.000000	0.000000

$HArBeCl_3$ (MP2/def2-TZVP, taken from Ref. 7)

Cl	-0.524973	5.294200	0.000000
Cl	3.302134	0.130797	0.000000
Cl	-2.970767	-0.570905	0.000000
Be	0.000000	1.779368	0.000000
Ar	0.080803	-4.629852	0.000000
H	1.836865	-6.299737	0.000000

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Table S1 CCSD T1 diagnostic and largest excitation amplitude (in parenthesis) calculated with the specified basis set.

	Basis set	He	Ne	Ar	Kr	Xe
NgH^+	aug-cc-pVTZ	0.0054 (0.0375)	0.0075 (0.025)	0.0044 (0.0425)	0.0041 (0.0571)	0.0049 (0.0768)
H-Ng-F	aug-cc-pVTZ	0.0310 (0.0698)		0.0227 (0.0513)	0.0157 (0.0495)	0.0137 (0.0535)
Ng-HF	aug-cc-pVTZ	0.0092 (0.0308)	0.0091 (0.0278)	0.0075 (0.0232)	0.0063 (0.0261)	0.0064 (0.0208)
NgAr	aug-cc-pVTZ	0.0019 (0.0375)	0.0056 (0.0283)	0.0020 (0.0160)	0.0025 (0.0220)	0.0026 (0.0220)
$NgNa^+$	aug-cc-pVTZ	0.0018 (0.0212)	0.0076 (0.0258)	0.0022 (0.0201)	0.0028 (0.0185)	0.0030 (0.0162)
NgF^-	aug-cc-pVTZ	0.0184 (0.0391)	0.0155 (0.0305)	0.0147 (0.0355)	0.0118 (0.0333)	0.0118 (0.0350)
Ng-BeO	aug-cc-pVTZ	0.0272 (0.0316)	0.0224 (0.0366)	0.0215 (0.0338)	0.0172 (0.0399)	0.0175 (0.0328)
Ng-CuF	aug-cc-pVTZ	0.0307 (0.0767)	0.0301 (0.0807)	0.0273 (0.0684)	0.0230 (0.0698)	0.0228 (0.0659)
$F\text{-}Ng\text{-}O^-$	aug-cc-pVTZ	0.0270 (0.0512)		0.0292 (0.0756)	0.0219 (0.0713)	0.0190 (0.0547)
$Ng\text{-}H\text{-}OH_2^+$	aug-cc-pVTZ	0.0058 (0.0188)	0.0074 (0.0161)	0.0055 (0.0232)	0.0049 (0.0178)	0.0054 (0.0191)
$HHeNH_3^+$	aug-cc-pVTZ	0.0117 (0.0309)				
$HeBO^+$	6-311++G(2df,2pd)	0.0236 (0.0640)				
$HeO(LiF)_2$	6-311++G(d,p)	0.0205 (0.0411)				
$FNeBN^-$	aug-cc-pVTZ	0.0245 (0.0543)				
$ArOH^+$ ($^1A'$)	cc-pVQZ	0.0162 (0.0903)				
$ArOH^+$ ($^3\Sigma^-$)	cc-pVQZ	0.0072 (0.0341)				
$FArCH_3$	6-311++G(3df,3pd)	0.0242 (00648)				
$HArBeCl_3$	def2-TZVP	0.0087 (0.0439)				

Table S2 CCSD(T)/aug-cc-pVTZ and CCSD/aug-cc-pVTZ optimized bond distances of the species included in the NgBC47 reference set.

	CCSD(T)	CCSD	Δ^a	$\Delta(\%)^b$
HeH^+	1.4664	1.4464	-0.0200	-1.36
NeH^+	1.8746	1.8697	-0.0049	-0.26
ArH^+	2.4226	2.4192	-0.0034	-0.14
KrH^+	2.6759	2.6719	-0.0040	-0.15
XeH^+	3.0141	3.0158	0.0017	0.056
H-He-F	1.5326/2.6740	1.4763/2.6774	-0.0563/0.0034	-3.67/0.13
H-Ar-F	2.5114/3.7398	2.4767/3.7764	-0.0347/0.0366	-1.38/0.97
H-Kr-F	2.7911/3.8588	2.7564/3.8537	-0.0347/-0.0051	-1.24/-0.13
H-Xe-F	3.1426/3.9987	3.1252/3.9911	-0.0174/-0.0076	-0.55/-0.19
He-HF	4.2075/1.7404	4.2092/1.7353	0.0017/-0.0051	0.040/-0.29
Ne-HF	4.2216/1.7404	4.2844/1.7353	0.0628/-0.0051	1.49/-0.29
Ar-HF	4.7357/1.7423	4.8277/1.7365	0.0920/-0.0058	1.94/-0.33
Kr-HF	4.7905/1.7442	4.8693/1.7378	0.0788/-0.0064	1.64/-0.37
Xe-HF	5.0588/1.7461	5.1899/1.7391	0.1311/-0.0070	2.59/-0.40
HeAr	6.6214	6.7053	0.0839	1.27
NeAr	6.6310	6.7422	0.1112	1.68
ArAr	7.2019	7.3308	0.1289	1.79
KrAr	7.3321	7.5119	0.1798	2.45
XeAr	7.7328	7.9061	0.1733	2.24
$HeNa^+$	4.5661	4.5661	0	0
$NeNa^+$	4.8317	4.8317	0	0
$ArNa^+$	5.4216	5.4216	0	0
$KrNa^+$	5.6131	5.6131	0	0
$XeNa^+$	5.9048	5.9271	0.0223	0.38
HeF^-	6.1571	6.1571	0	0
NeF^-	6.0602	6.0602	0	0
ArF^-	5.7070	5.7797	0.0727	1.27
KrF^-	5.7043	5.7253	0.0210	0.37
XeF^-	5.5900	5.6401	0.0501	0.90
He-Be-O	2.8799/2.5285	2.8826/2.5065	0.0027/-0.0220	0.094/-0.88
Ne-Be-O	3.3996/2.5322	3.3828/2.5092	-0.0168/-0.0230	-0.49/-0.92
Ar-Be-O	3.9174/2.5341	3.9218/2.5133	0.0044/-0.0208	0.11/-0.83
Kr-Be-O	4.1593/2.5360	4.1663/2.5152	0.0070/-0.0208	0.17/-0.83
Xe-Be-O	4.4787/2.5398	4.4934/2.5179	0.0147/-0.0219	0.33/-0.87
He-Cu-F	3.2244/3.3206	3.2919/3.3352	0.0675/0.0146	2.09/0.44
Ne-Cu-F	4.2305/3.3354	4.3660/3.3526	0.1355/0.0172	3.20/0.51
Ar-Cu-F	4.2927/3.3305	4.3558/3.3456	0.0631/0.0151	1.47/0.45
Kr-Cu-F	4.4388/3.3322	4.4941/3.3477	0.0553/0.0155	1.25/0.46
Xe-Cu-F	4.6691/3.3403	4.7300/3.3539	0.0609/0.0136	1.30/0.41
$F\text{-}He\text{-}O^-$	3.0727/2.0976	3.1347/2.0566	0.0620/-0.0410	2.02/-1.99
$F\text{-}Kr\text{-}O^-$	4.2689/3.5036	4.3175/3.4514	0.0486/-0.0522	1.14/-1.51
$F\text{-}Xe\text{-}O^-$	4.3861/3.7171	4.3776/3.6585	-0.0085/-0.0586	-0.19/-1.60
$He\text{-}H\text{-}OH_2^+$	3.3711/1.8533	3.4023/1.8487	0.0312/-0.0046	0.93/-0.25
$Ne\text{-}H\text{-}OH_2^+$	3.5306/1.8565	3.5756/1.8512	0.0450/-0.0053	1.27/-0.29
$Ar\text{-}H\text{-}OH_2^+$	3.8828/1.8782	3.9301/1.8705	0.0473/-0.0077	1.22/-0.41
$Kr\text{-}H\text{-}OH_2^+$	4.0931/1.8892	4.0850/1.8824	-0.0081/-0.0068	-0.20/-0.36
$Xe\text{-}H\text{-}OH_2^+$	4.3581/1.9094	4.3743/1.8965	0.0162/-0.0129	0.37/-0.68

[a] Δ = CCSD-CCSD(T). [b] $\Delta(\%) = [\Delta/\text{CCSD(T)}*100]$.

Table S3 CCSD/aug-cc-pVTZ properties of the (3,+1) HCP and the (3,-1) BCP of ArH^+ and H-Ar-F calculated at the CCSD(T)/aug-cc-VTZ and CCSD/aug-cc-pVTZ optimized geometries

				H-Ar-F			
		ArH^+ (2.4226/2.4192)[a]		Ar-H (2.5114/2.4767)		Ar-F (3.7398/3.7764)	
		HCP	BCP	HCP	BCP	HCP	BCP
R(Ng)[b]	CCSD(T)	1.7069	1.9224	1.7360	1.8517	1.9147	1.9099
	CCSD	1.7047	1.9203	1.7177	1.8348	1.9324	1.9282
$\rho(\boldsymbol{r})$[c]	CCSD(T)	0.2450	0.2327	0.2295	0.2255	0.0976	0.0976
	CCSD	0.2461	0.2338	0.2393	0.2350	0.0930	0.0930
sign(λ_2)×$\rho(\boldsymbol{r})$[d]	CCSD(T)	-0.2450	-0.2327	-0.2295	-0.2255	-0.0976	-0.0976
	CCSD	-0.2461	-0.2338	-0.2393	-0.2350	-0.0930	-0.0930
$\nabla^2\rho(\boldsymbol{r})$[e]	CCSD(T)	-0.6722	-1.1874	-0.5049	-0.6409	0.3479	0.3476
	CCSD	-0.6780	-1.1981	-0.5567	-0.7107	0.3389	0.3387
$H(\boldsymbol{r})$[f]	CCSD(T)	-0.2392	-0.3375	-0.2045	-0.2230	-0.0218	-0.0219
	CCSD	-0.2411	-0.3405	-0.2205	-0.2426	-0.0189	-0.0189
$G(\boldsymbol{r})$[g]	CCSD(T)	0.0712	0.0407	0.0782	0.0628	0.1088	0.1088
	CCSD	0.0716	0.0409	0.0813	0.0649	0.1036	0.1036
$V(\boldsymbol{r})$[h]	CCSD(T)	-0.3104	-0.3782	-0.2827	-0.2858	-0.1307	-0.1306
	CCSD	-0.3128	-0.3814	-0.3018	-0.3074	-0.1225	-0.1224

[a] CCSD(T)/CCSD bond distance (a_0). [b] Distance (a_0) of the HCP/BCP from Ng. [c] Electron density ($e\ a_0^{-3}$) at the HCP/BCP. [d] sign(λ_2) = sign of the second eigenvalue of the Hessian matrix of $\rho(\boldsymbol{r})$ at the HCP/BCP. [e] Laplacian of the electron density ($e\ a_0^{-5}$) at the HCP/BCP. [f] Energy density (hartree a_0^{-3}) at the HCP/BCP. [g] Kinetic energy density (hartree a_0^{-3}) at the HCP/BCP. [h] Potential energy density (hartree a_0^{-3}) at the HCP/BCP.

Table S4 CCSD/aVTZ properties of the non-covalent Ar-X interactions included in the NgBC47 reference set calculated at the CCSD(T)/aug-cc-VTZ and CCSD/aug-cc-pVTZ optimized geometries. ρ_s(ave) and $N(\Omega_s)$ are, respectively, the average electron density ($e\ a_0^{-3}$) and the total electronic charge (me) over the volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP. H_s(ave/max/min) are the average, maximum and minimum value of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over Ω_s

		type	Ω_s	$N(\Omega_s)$	ρ_s(ave)	H_s(ave/max/min)
ArAr	CCSD(T)	*n*Cov(*C*)	0.0877	0.23	0.0026	0.0007/0.0007/0.0006
	CCSD	*n*Cov(*C*)	0.0780	0.18	0.0023	0.0006/0.0006/0.0005
Ar-HF	CCSD(T)	*n*Cov(*C*)	0.0763	0.64	0.0084	0.0015/0.0016/0.0014
	CCSD	*n*Cov(*C*)	0.0700	0.52	0.0075	0.0015/0.0016/0.0014
ArF^-	CCSD(T)	*n*Cov(*C*)	0.1818	1.62	0.0089	0.0015/0.0018/0.0013
	CCSD	*n*Cov(*C*)	0.1755	1.45	0.0082	0.0014/0.0017/0.0012
$ArNa^+$	CCSD(T)	*n*Cov(*C*)	0.0488	0.35	0.0072	0.0031/0.0036/0.0027
	CCSD	*n*Cov(*C*)	0.0488	0.35	0.0072	0.0031/0.0036/0.0027
Ar-H-OH_2^+	CCSD(T)	*p*Cov(*A*/H^-)	0.1540	4.14	0.0269	-0.0034/-0.0017/-0.0065
	CCSD	*p*Cov(*A*/H^-)	0.1478	3.75	0.0253	-0.0027/-0.0013/-0.0056
Ar-BeO	CCSD(T)	*p*Cov(*B*/$H^{+/-}$)	0.0856	2.62	0.0306	0.0015/0.0098/-0.0044
	CCSD	*p*Cov(*B*/$H^{+/-}$)	0.0856	2.60	0.0304	0.0015/0.0097/-0.0044
Ar-CuF	CCSD(T)	*p*Cov(*A*/H^-)	0.4607	22.6	0.0490	-0.0095/-0.0061/-0.0148
	CCSD	*p*Cov(*A*/H^-)	0.4440	20.3	0.0458	-0.0082/-0.0053/-0.0127

Table S5 Dependence on $s(\boldsymbol{r})$ of the CCSD/aVTZ properties of the non-covalent (nCov) and partially-covalent (pCov) Ar-X interactions included in the NgBC47 reference set. ρ_s(ave) and $N(\Omega_s)$ are, respectively, the average electron density ($e\ a_0^{-3}$) and the total electronic charge (me) over the volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ isosurface at around the BCP. H_s(ave/max/min) are the average, maximum and minimum value of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over Ω_s

	$s(\boldsymbol{r})$	type	Ω_s	$N(\Omega_s)$	ρ_s(ave)	H_s(ave/max/min)
Ar-Ar	0.3	nCov(C)	0.0385	0.10	0.0026	0.0007/0.0007/0.0007
	0.4	nCov(C)	0.0877	0.23	0.0026	0.0007/0.0007/0.0006
	0.5	nCov(C)	0.1691	0.43	0.0025	0.0007/0.0007/0.0006
Ar-HF	0.3	nCov(C)	0.0301	0.26	0.0085	0.0015/0.0016/0.0015
	0.4	nCov(C)	0.0763	0.64	0.0084	0.0015/0.0016/0.0014
	0.5	nCov(C)	0.1464	1.20	0.0082	0.0015/0.0016/0.0014
Ar-F^-	0.3	nCov(C)	0.0778	0.71	0.0091	0.0015/0.0017/0.0014
	0.4	nCov(C)	0.1818	1.62	0.0089	0.0015/0.0018/0.0013
	0.5	nCov(C)	0.3521	3.03	0.0086	0.0014/0.0019/0.0012
Ar-Na^+	0.3	nCov(C)	0.0200	0.15	0.0074	0.0031/0.0036/0.0029
	0.4	nCov(C)	0.0488	0.35	0.0072	0.0031/0.0036/0.0027
	0.5	nCov(C)	0.0946	0.67	0.0071	0.0030/0.0039/0.0026
Ar-H-OH_2^+	0.3	pCov(A/H^-)	0.0641	1.77	0.0276	-0.0038/-0.0027/-0.0057
	0.4	pCov(A/H^-)	0.1540	4.14	0.0269	-0.0034/-0.0017/-0.0065
	0.5	pCov(A/H^-)	0.3060	8.01	0.0262	-0.0029/-0.0007/-0.0069
Ar-BeO	0.3	pCov(B/$H^{+/-}$)	0.0322	1.01	0.0315	0.0018/0.0066/-0.0028
	0.4	pCov(B/$H^{+/-}$)	0.0856	2.62	0.0306	0.0015/0.0098/-0.0044
	0.5	pCov(B/$H^{+/-}$)	0.1885	5.51	0.0292	0.0005/0.0104/-0.0069
Ar-CuF	0.3	pCov(A/H^-)	0.1900	9.92	0.0522	-0.0104/-0.0080/-0.0135
	0.4	pCov(A/H^-)	0.4607	22.6	0.0490	-0.0095/-0.0061/-0.0148
	0.5	pCov(A/H^-)	0.9220	43.2	0.0468	-0.0087/-0.0043/-0.0174

Section S1 Bonds classification and computational level

Our proposed bonds classification is, in principle, applicable to any Ng compound. The study of medium and large-size species demands, however, computational levels lower than the CCSD/aVTZ. To help a judicious choice, we repeated the bonding analysis of the NgH^+ and of all the non-covalent species included in the NgBC47 reference set at the MP2 and B3LYP levels of theory, using both the aVDZ and the aVTZ. The obtained results, given in Tables S6-S13, are best compared in Tables S14-S19.

As shown in Table S14, all the four employed methods predict the correct topology of the $H(\boldsymbol{r})$ of the covalent Ng-H^+ bonds, with a HCP falling on the bond axis, and values of ρ(BCP) that are, generally, in very good agreement with the benchmark CCSD/aVTZ. Best overall performing is the MP2/aVTZ, but the B3LYP/aVTZ is as well producing comparably-good results. Both these levels are, therefore, expectedly effective in describing Ng-X bonds of covalent character. On the other hand, the use of the aVDZ suffers of certain defaillances, including the lack of location of the BCP of HeH^+ and NeH^+, and some minor, but non-negligible deviations from the CCSD/aVTZ computed parameters.

As shown in Table S15, with the single exception of Xe-F^-, predicted as pCov(C,$H^{+/-}$) at the MP2/aVDZ level of theory, the MP2/aVnZ and B3LYP/aVnZ (n = D, T) correctly predict the nCov(C) type of the various Ng-Ar, Ng-HF, Ng-F^-, and Ng-Na^+ contacts. They also well reproduce the corresponding CCSD/aVTZ ρ_s(ave), the quantitative agreement being excellent for the MP2/aVTZ, but still very high for the other methods. The MP2/aVTZ is also best performing in reproducing the CCSD/aVTZ values of Ω_s, $N(\Omega_s)$, and H_s(ave/max/min) (see Tables S17 and S18). As for the Ng-H-OH_2^+, Ng-BeO, Ng-CuF, and F-Ng-O^-, the data quoted in Table S16 unravel certain differences in the performance of the various methods. Thus, the four computational levels correctly predict the C type of the Ng-H bonds of He-H-OH_2^+ and Ne-H-OH_2^+, but, used with the aVDZ, both the MP2 and the B3LYP fail to predict the covalent contribution to the Ne-H bond,

correctly assigned, instead, as pCov(C/$H^{+/-}$) with the aVTZ. This major inadequacy of the smaller basis set is even more evident for Ar-H-OH_2^+ and Kr-H-OH_2^+, whose Ng-H contacts are assigned, respectively, as nCov(C) and pCov(C/$H^{+/-}$), rather than pCov(A/H^-). In any case, both the MP2/aVDZ and the B3LYP/aVDZ correctly predict the pCov(A/H^-) type of the Xe-H-OH_2^+ bond.

All the four MP2/aVnZ and B3LYP/aVnZ (*n* = D, T) well describe the various Ng-BeO and Ng-CuF bonds. The nCov(C) type of the He-BeO bond, actually at the onset of nCov(B), is, indeed, assigned as nCov(B) at the MP2/aVTZ, and the MP2/aVDZ slightly underestimates the role of covalency in the He-CuF [pCov(A/$H^{-/+}$) rather than pCov(A/H^-)]. On the other hand, both the MP2/aVDZ and the B3LYP/aVDZ correctly predict the nCov(C) type of the Ne-CuF bond, assigned, instead, as pCov(C/$H^{+/-}$) at the MP2/aVTZ and the B3LYP/aVTZ. This single best performance of the smaller basis set is, however, probably fortuitous, and likely mirrors its general tendency to underestimate the role of covalency (*vide supra*). This is also a likely partial limitation of the B3LYP. One notes, in fact, that the bond type of the F-NgO^-, generally well predicted also at the MP2/aVDZ level of theory, is not invariably correctly assigned at the B3LYP/aVDZ (C rather than A, or H^+ rather than or $H^{+/-}$).

Overall, the tests performed on the NgBC47 reference set suggest that both the MP2/aVTZ and the B3LYP/aVTZ well describe the types of the Ng-X bonds. If possible, we recommend the former, that *i*) furnishes bond indices in excellent quantitative agreement with the CCSD/aVTZ benchmark data, and *ii*) avoids the sometimes underestimated role of covalency suffered by the B3LYP. The smaller aVDZ basis set should be used with caution, as it seemingly underestimates the role of covalency [especially for interactions of type A, and ρ_s(ave) higher than 0.010 - 0.015 $e\ a_0^{-3}$], and could be also not generally adequate in describing weak interactions of type C.

Table S6 MP2/aVTZ properties of the (3,+1) HCP and the (3,-1) BCP of the NgH^+

	HeH^+ (1.4664)[a]		NeH^+ (1.8746)		ArH^+ (2.4226)		KrH^+ (2.6759)		XeH^+ (3.0141)	
	HCP	BCP	HCP	BCP	HCP	BCP	HCP	BCP	HCP	BCP
R(Ng)[b]	0.9283	1.2851	1.2704	1.6797	1.7090	1.9346	1.8888	2.0106	1.9659	2.0763
$\rho(\boldsymbol{r})$[c]	0.2695	0.2027	0.3074	0.2118	0.2431	0.2300	0.2098	0.2070	0.1724	0.1711
sign(λ_2)×$\rho(\boldsymbol{r})$[d]	-0.2695	-0.2027	-0.3074	-0.2118	-0.2431	-0.2300	-0.2098	-0.2070	-0.1724	-0.1711
$\nabla^2\rho(\boldsymbol{r})$[e]	-1.0070	-3.4373	-0.3101	-3.0538	-0.6644	-1.2165	-0.5810	-0.6904	-0.3080	-0.3888
$H(\boldsymbol{r})$[f]	-0.3269	-0.8620	-0.3255	-0.8001	-0.2360	-0.3429	-0.1972	-0.2120	-0.1442	-0.1460
$G(\boldsymbol{r})$[g]	0.0751	0.0026	0.2480	0.0366	0.0699	0.0388	0.0519	0.0394	0.0672	0.0488
$V(\boldsymbol{r})$[h]	-0.4020	-0.8646	-0.5735	-0.8367	-0.3059	-0.3817	-0.2491	-0.2514	-0.2114	-0.1948

[a] CCSD(T)/aVTZ bond distance (a_0). [b] Distance (a_0) of the HCP/BCP from Ng. [c] Electron density ($e\ a_0^{-3}$) at the HCP/BCP. [d] sign(λ_2) = sign of the second eigenvalue of the Hessian matrix of $\rho(\boldsymbol{r})$. [e] Laplacian of the electron density ($e\ a_0^{-5}$) at the HCP/BCP. [f] Energy density (hartree a_0^{-3}) at the HCP/BCP. [g] Kinetic energy density (hartree a_0^{-3}) at the HCP/BCP. [h] Potential energy density (hartree a_0^{-3}) at the HCP/BCP.

Table S7 MP2/aVDZ properties of the (3,+1) HCP and the (3,-1) BCP of the NgH^+

	HeH^+ (1.4664)[a]	NeH^+ (1.8746)	ArH^+ (2.4226)		KrH^+ (2.6759)		XeH^+ (3.0141)	
	HCP[b]	HCP	HCP	BCP	HCP	BCP	HCP	BCP
R(Ng)[c]	1.0268	1.4062	1.6653	1.9754	1.7761	2.0340	1.9229	2.0070
$\rho(\boldsymbol{r})$[d]	0.2248	0.2251	0.2433	0.2204	0.2110	0.2031	0.1653	0.1645
sign(λ_2)×$\rho(\boldsymbol{r})$[e]	-0.2248	-0.22151	-0.2433	-0.2204	-0.2110	-0.2031	-0.1653	-0.164
$\nabla^2\rho(\boldsymbol{r})$[f]	-0.8610	-0.1184	-0.6953	-0.9411	-0.4968	-0.7705	-0.1906	-0.2681
$H(\boldsymbol{r})$[g]	-0.2595	-0.1546	-0.2483	-0.2671	-0.1920	-0.2264	-0.1218	-0.1238
$G(\boldsymbol{r})$[h]	0.0442	0.1250	0.0744	0.0318	0.0677	0.0337	0.0741	0.0569
$V(\boldsymbol{r})$[i]	-0.3037	-0.2796	-0.3227	-0.2989	-0.2597	-0.2601	-0.1959	-0.1807

[a] CCSD(T)/aVTZ bond distance (a_0). [b] BCP not located at this computational level. [c] Distance (a_0) of the HCP/BCP from Ng. [d] Electron density ($e\ a_0^{-3}$) at the HCP/BCP. [e] sign(λ_2) = sign of the second eigenvalue of the Hessian matrix of $\rho(\boldsymbol{r})$. [f] Laplacian of the electron density ($e\ a_0^{-5}$) at the HCP/BCP. [g] Energy density (hartree a_0^{-3}) at the HCP/BCP. [h] Kinetic energy density (hartree a_0^{-3}) at the HCP/BCP. [i] Potential energy density (hartree a_0^{-3}) at the HCP/BCP.

Table S8 B3LYP/aVTZ properties of the (3,+1) HCP and the (3,-1) BCP of the NgH^+

	HeH^+ (1.4664)[a]		NeH^+ (1.8746)		ArH^+ (2.4226)		KrH^+ (2.6759)		XeH^+ (3.0141)	
	HCP	BCP	HCP	BCP	HCP	BCP	HCP	BCP	HCP	BCP
R(Ng)[b]	0.9151	1.2623	1.2511	1.6641	1.6998	1.9027	1.8813	1.9863	1.9796	2.0682
$\rho(\boldsymbol{r})$[c]	0.2747	0.2093	0.3181	0.2188	0.2453	0.2337	0.2110	0.2088	0.1722	0.1713
sign(λ_2)×$\rho(\boldsymbol{r})$[d]	-0.2747	-0.2093	-0.3181	-0.2188	-0.2453	-0.2337	-0.2110	-0.2088	-0.1722	-0.1713
$\nabla^2\rho(\boldsymbol{r})$[e]	-1.0067	-2.8732	-0.2575	-2.7417	-0.6635	-1.1259	-0.5750	-0.6629	-0.3074	-0.3717
$H(\boldsymbol{r})$[f]	-0.3210	-0.7183	-0.3172	-0.7203	-0.2300	-0.3173	-0.1915	-0.2023	-0.1383	-0.1397
$G(\boldsymbol{r})$[g]	0.0692	0.0000	0.2529	0.0349	0.0641	0.0358	0.0477	0.0365	0.0615	0.0467
$V(\boldsymbol{r})$[h]	-0.3902	-0.7183	-0.5701	-0.7552	-0.2941	-0.3531	-0.2392	-0.2388	-0.1998	-0.1864

[a] CCSD(T)/aVTZ bond distance (a_0). [b] Distance (a_0) of the HCP/BCP from Ng. [c] Electron density ($e\ a_0^{-3}$) at the HCP/BCP. [d] sign(λ_2) = sign of the second eigenvalue of the Hessian matrix of $\rho(\boldsymbol{r})$. [e] Laplacian of the electron density ($e\ a_0^{-5}$) at the HCP/BCP. [f] Energy density (hartree a_0^{-3}) at the HCP/BCP. [g] Kinetic energy density (hartree a_0^{-3}) at the HCP/BCP. [h] Potential energy density (hartree a_0^{-3}) at the HCP/BCP.

Table S9 B3LYP/aVDZ properties of the (3,+1) HCP and the (3,-1) BCP of the NgH^+

	HeH^+ (1.4664)[a]	NeH^+ (1.8746)	ArH^+ (2.4226)		KrH^+ (2.6759)		XeH^+ (3.0141)	
	HCP[b]	HCP	HCP	BCP	HCP	BCP	HCP	BCP
R(Ng)[c]	1.0229	1.4037	1.6596	1.9667	1.7794	2.0281	1.9423	2.0222
$\rho(\boldsymbol{r})$[d]	0.2271	0.2277	0.2458	0.2228	0.2127	0.2046	0.1670	0.1662
sign(λ_2)×$\rho(\boldsymbol{r})$[e]	-0.2271	-0.2277	-0.2458	-0.2228	-0.2127	-0.2046	-0.1670	-0.1662
$\nabla^2\rho(\boldsymbol{r})$[f]	-0.8746	-0.1280	-0.6975	-0.9410	-0.4984	-0.7697	-0.2087	-0.2797
$H(\boldsymbol{r})$[g]	-0.2575	-0.1499	-0.2453	-0.2637	-0.1898	-0.2237	-0.1211	-0.1233
$G(\boldsymbol{r})$[h]	0.0389	0.1179	0.0710	0.0285	0.0651	0.0313	0.0689	0.0534
$V(\boldsymbol{r})$[i]	-0.2964	-0.2678	-0.3163	-0.2922	-0.2549	-0.2550	-0.1900	-0.1767

[a] CCSD(T)/aVTZ bond distance (a_0). [b] BCP not located at this computational level. [c] Distance (a_0) of the HCP/BCP from Ng. [d] Electron density ($e\ a_0^{-3}$) at the HCP/BCP. [e] sign(λ_2) = sign of the second eigenvalue of the Hessian matrix of $\rho(\boldsymbol{r})$. [f] Laplacian of the electron density ($e\ a_0^{-5}$) at the HCP/BCP. [g] Energy density (hartree a_0^{-3}) at the HCP/BCP. [h] Kinetic energy density (hartree a_0^{-3}) at the HCP/BCP. [i] Potential energy density (hartree a_0^{-3}) at the HCP/BCP.

Table S10 MP2/aVTZ properties at the CCSD(T)/aVTZ geometries of the non-covalent Ng-X interactions included in the NgBC47 reference set. ρ_s(ave) and $N(\Omega_s)$ are, respectively, the average electron density ($e\ a_0^{-3}$) and the total electronic charge (me) over the volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP. H_s(ave/max/min) are the average, maximum and minimum value of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over Ω_s

		type	Ω_s	$N(\Omega_s)$	ρ_s(ave)	H_s(ave/max/min)
Ng-Ar	He	nCov(C)	0.0225	0.027	0.0012	0.0004/0.0005/0.0004
	Ne	nCov(C)	0.0370	0.081	0.0022	0.0006/0.0007/0.0006
	Ar	nCov(C)	0.0906	0.24	0.0026	0.0007/0.0007/0.0006
	Kr	nCov(C)	0.1156	0.35	0.0030	0.0008/0.0008/0.0007
	Xe	nCov(C)	0.1452	0.42	0.0029	0.0006/0.0007/0.0006
Ng-HF	He	nCov(C)	0.0196	0.071	0.0036	0.0014/0.0015/0.0014
	Ne	nCov(C)	0.0365	0.24	0.0066	0.0014/0.0015/0.0013
	Ar	nCov(C)	0.0768	0.65	0.0085	0.0015/0.0016/0.0014
	Kr	nCov(C)	0.1155	1.28	0.0111	0.0009/0.0011/0.0006
	Xe	nCov(C)	0.1734	2.03	0.0117	0.0004/0.0006/0.0001
Ng-F^-	He	nCov(C)	0.0322	0.055	0.0017	0.0006/0.0006/0.0005
	Ne	nCov(C)	0.0659	0.22	0.0033	0.0005/0.0006/0.0005
	Ar	nCov(C)	0.1978	1.78	0.0090	0.0014/0.0017/0.0012
	Kr	nCov(C)	0.2693	3.07	0.0114	0.0013/0.0015/0.0011
	Xe	nCov(C)	0.4288	6.95	0.0162	0.0012/0.0019/0.0009
Ng-Na^+	He	nCov(C)	0.0110	0.048	0.0044	0.0029/0.0031/0.0028
	Ne	nCov(C)	0.0210	0.13	0.0060	0.0029/0.0033/0.0026
	Ar	nCov(C)	0.0492	0.35	0.0072	0.0031/0.0036/0.0027
	Kr	nCov(C)	0.0683	0.56	0.0082	0.0028/0.0034/0.0023
	Xe	nCov(C)	0.1174	1.04	0.0089	0.0023/0.0032/0.0015
Ng-HOH_2^+	He	nCov(C)	0.0331	0.39	0.0118	0.0019/0.0023/0.0014
	Ne	pCov(C/$H^{+/-}$)	0.0564	0.97	0.0172	0.0012/0.0026/-0.0006
	Ar	pCov(A/H^-)	0.1592	4.31	0.0271	-0.0035/-0.0018/-0.0067
	Kr	pCov(A/H^-)	0.2404	6.80	0.0283	-0.0047/-0.0027/-0.0084
	Xe	pCov(A/H^-)	0.4000	11.9	0.0297	-0.0056/-0.0033/-0.0103
Ng-BeO	He	nCov(B)	0.0222	0.61	0.0276	0.0117/0.0173/0.0075
	Ne	nCov(C)	0.0301	0.67	0.0222	0.0106/0.0150/0.0079
	Ar	pCov(B/$H^{+/-}$)	0.0905	2.72	0.0301	0.0016/0.0101/-0.0042
	Kr	pCov(B/$H^{-/+}$)	0.1522	4.63	0.0304	-0.0023/0.0056/-0.0082
	Xe	pCov(B/$H^{-/+}$)	0.3067	9.42	0.0307	-0.0064/0.0035/-0.0134
Ng-CuF	He	pCov(A/H^-)	0.1496	8.44	0.0564	-0.0062/-0.0048/-0.0089
	Ne	pCov(C/$H^{+/-}$)	0.1598	3.64	0.0228	0.0007/0.0027/-0.0005
	Ar	pCov(A/H^-)	0.5151	25.3	0.0491	-0.0101/-0.0065/-0.0151
	Kr	pCov(A/H^-)	0.8258	43.4	0.0525	-0.0131/-0.0083/-0.0210
	Xe	pCov(A/H^-)	1.4893	81.8	0.0549	-0.0161/-0.0088/-0.0401
F-NgO^-	He	pCov(A/$H^{-/+}$)	0.1273	9.01	0.0708	-0.0007/0.0033/-0.0091
	Kr	pCov(A/$H^{-/+}$)	0.5381	27.8	0.0517	-0.0028/0.0007/-0.0119
	Xe	pCov(A/H^-)	0.7911	42.6	0.0538	-0.0072/-0.0011/-0.0235

Table S11 MP2/aVDZ properties at the CCSD(T)/aVTZ geometries of the non-covalent Ng-X interactions included in the NgBC47 reference set. ρ_s(ave) and $N(\Omega_s)$ are, respectively, the average electron density ($e\ a_0^{-3}$) and the total electronic charge (me) over the volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP. H_s(ave/max/min) are the average, maximum and minimum value of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over Ω_s

		type	Ω_s	$N(\Omega_s)$	ρ_s(ave)	H_s(ave/max/min)
Ng-Ar	He	nCov(C)	0.0201	0.028	0.0014	0.0004/0.0004/0.0004
	Ne	nCov(C)	0.0260	0.055	0.0021	0.0009/0.00090/0.0008
	Ar	nCov(C)	0.1036	0.30	0.0029	0.0005/0.0005/0.0004
	Kr	nCov(C)	0.1448	0.49	0.0034	0.0005/0.0005/0.0004
	Xe	nCov(C)	0.1914	0.61	0.0032	0.0004/0.0004/0.0004
Ng-HF	He	nCov(C)	0.0335	0.12	0.0037	0.0007/0.0007/0.0006
	Ne	nCov(C)	0.0414	0.27	0.0065	0.0019/0.0022/0.0017
	Ar	nCov(C)	0.1264	1.0	0.0079	0.0014/0.0020/0.0011
	Kr	nCov(C)	0.1828	1.83	0.0100	0.0015/0.0024/0.0010
	Xe	nCov(C)	0.2515	2.64	0.0105	0.0012/0.0024/0.0082
Ng-F^-	He	nCov(C)	0.0339	0.058	0.0017	0.0006/0.0006/0.0005
	Ne	nCov(C)	0.0365	0.11	0.0030	0.0012/0.0012/0.0012
	Ar	nCov(C)	0.1926	1.81	0.0094	0.0014/0.0019/0.0009
	Kr	nCov(C)	0.2749	3.22	0.0117	0.0012/0.0018/0.0006
	Xe	pCov(C/$H^{+/-}$)	0.4092	6.75	0.0165	0.0006/0.0011/-0.0002
Ng-Na^+	He	nCov(C)	0.0163	0.077	0.0047	0.0020/0.0022/0.0019
	Ne	nCov(C)	0.0160	0.094	0.0059	0.0033/0.0036/0.0030
	Ar	nCov(C)	0.0594	0.43	0.0072	0.0024/0.0030/0.0021
	Kr	nCov(C)	0.0857	0.69	0.0080	0.0023/0.0030/0.0018
	Xe	nCov(C)	0.1284	1.07	0.0083	0.0020/0.0029/0.0015
Ng-HOH_2^+	He	nCov(C)	0.0496	0.54	0.0108	0.0034/0.0041/0.0029
	Ne	nCov(C)	0.0609	1.04	0.0170	0.0031/0.0045/0.0018
	Ar	nCov(C)	0.1676	4.12	0.0246	0.0024/0.0026/0.0018
	Kr	pCov(C/$H^{+/-}$)	0.2516	6.44	0.0256	0.0007/0.0011/-0.0003
	Xe	pCov(A/H^-)	0.4148	11.3	0.0273	-0.0015/-0.0005/-0.0037
Ng-BeO	He	nCov(C)	0.0213	0.51	0.0240	0.0159/0.0204/0.0130
	Ne	nCov(C)	0.0258	0.57	0.0220	$0.0084/0.0131/0.0048_5$
	Ar	pCov(B/$H^{+/-}$)	0.1201	3.28	0.0273	$0.0028/0.0118/-0.0011_5$
	Kr	pCov(B/$H^{-/+}$)	0.2266	6.30	0.0278	-0.0018/0.0085/-0.0064
	Xe	pCov(B/$H^{-/+}$)	0.4627	13.3	0.0287	-0.0064/0.0055/-0.0120
Ng-CuF	He	pCov(A/$H^{-/+}$)	0.1329	7.40	0.0557	-0.0011/0.0008/-0.0037
	Ne	nCov(C)	0.1744	4.17	0.0239	-0.0029/-0.0026/-0.0031
	Ar	pCov(A/H^-)	0.4891	23.7	0.0484	-0.0082/-0.0048/-0.0125
	Kr	pCov(A/H^-)	0.7647	40.1	0.0524	-0.0123/-0.0070/-0.0209
	Xe	pCov(A/H^-)	1.4965	84.4	0.0564	-0.0179/-0.0088/-0.0538
F-NgO^-	He	pCov(A/$H^{-/+}$)	0.1395	9.29	0.0666	0.0047/0.0096/-0.0059
	Kr	pCov(A/$H^{-/+}$)	0.6206	31.5	0.0507	-0.0046/0.0005/-0.0161
	Xe	pCov(A/H^-)	0.9793	51.5	0.0526	-0.0099/-0.0038/-0.0267

Table S12 B3LYP/aVTZ properties at the CCSD(T)/aVTZ geometries of the non-covalent Ng-X interactions included in the NgBC47 reference set. ρ_s(ave) and $N(\Omega_s)$ are, respectively, the average electron density ($e\ a_0^{-3}$) and the total electronic charge (me) over the volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP. H_s(ave/max/min) are the average, maximum and minimum value of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over Ω_s

		type	Ω_s	$N(\Omega_s)$	ρ_s(ave)	H_s(ave/max/min)
Ng-Ar	He	nCov(C)	0.0259	0.034	0.0013	0.0004/0.0005/0.0004
	Ne	nCov(C)	0.0411	0.095	0.0023	0.0006/0.0006/0.0006
	Ar	nCov(C)	0.1026	0.28	0.0027	0.0007/0.0007/0.0006
	Kr	nCov(C)	0.1305	0.40	0.0031	0.0008/0.0008/0.0007
	Xe	nCov(C)	0.1600	0.48	0.0030	0.0006/0.0007/0.0006
Ng-HF	He	nCov(C)	0.0233	0.093	0.0040	0.0014/0.0015/0.0014
	Ne	nCov(C)	0.0411	0.29	0.0071	0.0014/0.0015/0.0013
	Ar	nCov(C)	0.0843	0.75	0.0089	0.0015/0.0016/0.0013
	Kr	nCov(C)	0.1246	1.45	0.0116	0.0009/0.0011/0.0005
	Xe	nCov(C)	0.1889	2.30	0.0122	0.0005/0.0007/0.0001
Ng-F^-	He	nCov(C)	0.0423	0.080	0.0019	0.0005/0.0006/0.0005
	Ne	nCov(C)	0.0754	0.26	0.0034	0.0005/0.0005/0.0004
	Ar	nCov(C)	0.2091	1.88	0.0090	0.0015/0.0018/0.0013
	Kr	nCov(C)	0.2833	3.20	0.0113	0.0013/0.0017/0.0012
	Xe	nCov(C)	0.4322	6.96	0.0161	0.0014/0.0022/0.0011
Ng-Na^+	He	nCov(C)	0.0158	0.077	0.0049	0.0029/0.0031/0.0027
	Ne	nCov(C)	0.0265	0.17	0.0065	0.0028/0.0033/0.0024
	Ar	nCov(C)	0.0633	0.49	0.0078	0.0029/0.0035/0.0025
	Kr	nCov(C)	0.0904	0.80	0.0088	0.0026/0.0033/0.0020
	Xe	nCov(C)	0.1506	1.43	0.0095	0.0020/0.0031/0.0012
Ng-HOH_2^+	He	nCov(C)	0.0380	0.48	0.0127	0.0017/0.0021/0.0009
	Ne	pCov(C/$H^{+/-}$)	0.0616	1.11	0.0181	0.0011/0.0028/-0.0010
	Ar	pCov(A/H^-)	0.1705	4.81	0.0282	-0.0033/-0.0014/-0.0070
	Kr	pCov(A/H^-)	0.2590	7.61	0.0294	-0.0044/-0.0024/-0.0088
	Xe	pCov(A/H^-)	0.4238	12.9	0.0305	-0.0050/-0.0028/-0.0106
Ng-BeO	He	nCov(C)	0.0289	0.86	0.0296	0.0091/0.0154/0.0047
	Ne	nCov(C)	0.0386	0.92	0.0238	0.0091/0.0064/0.01400
	Ar	pCov(B/$H^{-/+}$)	0.1186	3.77	0.0318	-0.0004/0.0082/-0.0060
	Kr	pCov(B/$H^{-/+}$)	0.1990	6.41	0.0322	-0.0046/0.0038/-0.0104
	Xe	pCov(B/$H^{-/+}$)	0.4211	13.7	0.0325	-0.0082/0.0013/-0.0146
Ng-CuF	He	pCov(A/H^-)	0.1593	9.29	0.0583	-0.0059/-0.0042/-0.0100
	Ne	pCov(C/$H^{+/-}$)	0.1717	4.03	0.0235	0.0012/0.0032/-0.00004
	Ar	pCov(A/H^-)	0.5278	26.3	0.0499	-0.0092/-0.0058/-0.013
	Kr	pCov(A/H^-)	0.8306	43.9	0.0529	-0.0117/-0.0073/-0.0187
	Xe	pCov(A/H^-)	1.3737	74.2	0.0540	-0.0140/-0.0076/-0.0316
F-NgO^-	He	pCov(A/$H^{-/+}$)	0.1320	9.50	0.0720	0.0011/0.0050/-0.0082
	Kr	pCov(A/$H^{-/+}$)	0.5016	25.9	0.0516	-0.0004/0.0024/-0.0079
	Xe	pCov(A/H^-)	0.7136	38.2	0.0536	-0.0048/0.0005/-0.0197

Table S13 B3LYP/aVDZ properties at the CCSD(T)/aVTZ geometries of the non-covalent Ng-X interactions included in the NgBC47 reference set. ρ_s(ave) and $N(\Omega_s)$ are, respectively, the average electron density ($e\ a_0^{-3}$) and the total electronic charge (me) over the volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP. H_s(ave/max/min) are the average, maximum and minimum value of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over Ω_s

		type	Ω_s	$N(\Omega_s)$	ρ_s(ave)	H_s(ave/max/min)
Ng-Ar	He	nCov(C)	0.0252	0.035	0.0014	0.0004/0.0004/0.0004
	Ne	nCov(C)	0.0295	0.062	0.0021	0.0008/0.0008/0.0008
	Ar	nCov(C)	0.1097	0.32	0.0029	0.0005/0.0005/0.0004
	Kr	nCov(C)	0.1551	0.53	0.0034	0.0005/0.0005/0.0004
	Xe	nCov(C)	0.2005	0.62	0.0031	0.0004/0.0004/0.0004
Ng-HF	He	nCov(C)	0.0389	0.16	0.0040	0.0006/0.0007/0.0006
	Ne	nCov(C)	0.0477	0.33	0.0069	0.0017/0.0021/0.0015
	Ar	nCov(C)	0.1351	1.12	0.0083	0.0013/0.0019/0.0010
	Kr	nCov(C)	0.1993	2.09	0.0105	0.0013/0.0023/0.0009
	Xe	nCov(C)	0.2636	2.90	0.0110	0.0011/0.0020/0.0008
Ng-F^-	He	nCov(C)	0.0414	0.075	0.0018	0.0005/0.0005/0.0005
	Ne	nCov(C)	0.0460	0.15	0.0032	0.0011/0.0012/0.0011
	Ar	nCov(C)	0.1977	1.84	0.0093	0.0014/0.0020/0.0009
	Kr	nCov(C)	0.2805	3.23	0.0115	0.0013/0.0020/0.0007
	Xe	nCov(C)	0.4071	6.64	0.0163	0.0008/0.0012/0.0002
Ng-Na^+	He	nCov(C)	0.0196	0.098	0.0050	0.0020/0.0022/0.0018
	Ne	nCov(C)	0.0188	0.11	0.0061	0.0032/0.0036/0.0029
	Ar	nCov(C)	0.0671	0.50	0.0074	0.0024/0.0030/0.0020
	Kr	nCov(C)	0.1012	0.83	0.0082	0.0022/0.0030/0.0017
	Xe	nCov(C)	0.1538	1.31	0.0085	0.0020/0.0029/0.0015
Ng-HOH_2^+	He	nCov(C)	0.0553	0.64	0.0116	0.0032/0.0038/0.0027
	Ne	nCov(C)	0.0700	1.25	0.0179	0.0026/0.0040/0.0012
	Ar	nCov(C)	0.1769	4.56	0.0258	0.0023/0.0025/0.0019
	Kr	pCov(C/$H^{+/-}$)	0.2676	7.17	0.0268	0.0006/0.0010/-0.0002
	Xe	pCov(A/H^-)	0.4248	12.0	0.0283	-0.0015/-0.0006/-0.0037
Ng-BeO	He	nCov(C)	0.0277	0.72	0.0260	0.0139/0.0189/0.0110
	Ne	nCov(C)	0.0362	0.85	0.0234	0.0062/0.0117/0.0027
	Ar	pCov(B/$H^{+/-}$)	0.1439	4.14	0.0288	0.0010/0.0090/-0.0028
	Kr	pCov(B/$H^{-/+}$)	0.2633	7.74	0.0294	-0.0034/0.0072/-0.0074
	Xe	pCov(B/$H^{-/+}$)	0.5226	15.9	0.0304	-0.0076/0.0042/-0.0124
Ng-CuF	He	pCov(A/H^-)	0.1333	7.69	0.0577	-0.0010/0.0014/-0.0045
	Ne	nCov(C)	0.1885	4.60	0.0244	-0.0025/-0.0023/0.0027
	Ar	pCov(A/H^-)	0.4777	23.5	0.0492	-0.0070/-0.0038/-0.0114
	Kr	pCov(A/H^-)	0.7218	38.0	0.0526	-0.0106/-0.0056/-0.0180
	Xe	pCov(A/H^-)	1.2807	69.8	0.0545	-0.0148/-0.0074/-0.0356
F-NgO^-	He	pCov(C/$H^{+/-}$)	0.1322	8.94	0.0676	0.0087/0.0145/-0.0019
	Kr	pCov(C/$H^{-/+}$)	0.5521	28.0	0.0507	-0.0017/0.0045/-0.0136
	Xe	pCov(C/H^-)	0.8572	45.2	0.0527	-0.0074/-0.0002/-0.0237

Table S14 Properties of the Cov bonds of the NgH^+ at the CCSD(T)/aVTZ geometries

		R(HCP)[a]	ρ(HCP)[b]	H(HCP)[c]	R(BCP)[d]	ρ(BCP)[e]	H(BCP)[f]
He	CCSD/aVTZ	0.9254	0.2716	-0.3308	1.2781	0.2058	-0.8175
	MP2/aVTZ	0.9283	0.2695	-0.3269	1.2851	0.2027	-0.8620
	B3LYP/aVTZ	0.9151	0.2747	-0.3209	1.2623	0.2093	-0.7183
	MP2/aVDZ[g]	1.0268	0.2248	-0.2595			
	B3LYP/aVDZ[g]	1.0229	0.2271	-0.2575			
Ne	CCSD/aVTZ	1.2712	0.3085	-0.3304	1.6802	0.2131	-0.8106
	MP2/aVTZ	1.2704	0.3074	-0.3255	1.6797	0.2118	-0.8001
	B3LYP/aVTZ	1.2511	0.3181	-0.3172	1.6641	0.2188	-0.7203
	MP2/aVDZ[g]	1.4062	0.2251	-0.1546			
	B3LYP/aVDZ[g]	1.4037	0.2277	-0.1499			
Ar	CCSD/aVTZ	1.7069	0.2450	-0.2392	1.9224	0.2327	-0.3375
	MP2/aVTZ	1.7090	0.2431	-0.2360	1.9346	0.2300	-0.3429
	B3LYP/aVTZ	1.6998	0.2453	-0.2300	1.9027	0.2337	-0.3173
	MP2/aVDZ	1.6653	0.2433	-0.2483	1.9754	0.2204	-0.2671
	B3LYP/aVDZ	1.6596	0.2458	-0.2453	1.9667	0.2228	-0.2637
Kr	CCSD/aVTZ	1.8812	0.2128	-0.20224	1.9926	0.2104	-0.2145
	MP2/aVTZ	1.8852	0.2111	-0.19945	2.0062	0.2084	-0.2144
	B3LYP/aVTZ	1.8778	0.2124	-0.19371	1.9821	0.2102	-0.2046
	MP2/aVDZ	1.7719	0.2124	-0.19422	2.0299	0.2044	-0.2286
	B3LYP/aVDZ	1.7752	0.2141	-0.19203	2.0242	0.2060	-0.2260
Xe	CCSD/aVTZ	1.9527	0.1731	-0.14544	2.0566	0.1720	-0.1471
	MP2/aVTZ	1.9659	0.1724	-0.14421	2.0763	0.1711	-0.1460
	B3LYP/aVTZ	1.9796	0.1722	-0.13833	2.0682	0.1713	-0.1396
	MP2/aVDZ	1.9229	0.1653	-0.12177	2.0070	0.1645	-0.1239
	B3LYP/aVDZ	1.9423	1.1670	-0.12107	2.0222	0.1662	-0.1233

[a] Distance (a_0) of the HCP from Ng. [b] Electron density ($e\ a_0^{-3}$) at the HCP. [c] Energy density (hartree a_0^{-3}) at the HCP. [d] Distance (a_0) of the BCP from Ng. [e] Electron density ($e\ a_0^{-3}$) at the BCP. [f] Energy density (hartree a_0^{-3}) at the BCP. [g] BCP not located at this computational level.

Table S15 Type of the Ng-X bonds of the Ng-Ar, Ng-HF, Ng-F^-, and Ng-Na^+, and average electron density ρ_s(ave) ($e\ a_0^{-3}$) over the volume enclosed by the $s(\boldsymbol{r}) = 0.4$ isosurface at around the BCP at the CCSD(T)/aVTZ geometries

		Ng-Ar	Ng-HF	Ng-F^-	Ng-Na^+
		type/ρ_s(ave)	type/ρ_s(ave)	type/ρ_s(ave)	type/ρ_s(ave)
He	CCSD/aVTZ	nCov(C)/0.0012	nCov(C)/0.0036	nCov(C)/0.0017	nCov(C)/0.0045
	MP2/aVTZ	nCov(C)/0.0012	nCov(C)/0.0036	nCov(C)/0.0017	nCov(C)/0.0044
	B3LYP/aVTZ	nCov(C)/0.0013	nCov(C)/0.0040	nCov(C)/0.0019	nCov(C)/0.0049
	MP2/aVDZ	nCov(C)/0.0014	nCov(C)/0.0037	nCov(C)/0.0017	nCov(C)/0.0047
	B3LYP/aVDZ	nCov(C)/0.0014	nCov(C)/0.0040	nCov(C)/0.0018	nCov(C)/0.0050
Ne	CCSD/aVTZ	nCov(C)/0.0021	nCov(C)/0.0065	nCov(C)/0.0032	nCov(C)/0.0059
	MP2/aVTZ	nCov(C)/0.0022	nCov(C)/0.0066	nCov(C)/0.0034	nCov(C)/0.0060
	B3LYP/aVTZ	nCov(C)/0.0023	nCov(C)/0.0071	nCov(C)/0.0030	nCov(C)/0.0065
	MP2/aVDZ	nCov(C)/0.0021	nCov(C)/0.0065	nCov(C)/0.0030	nCov(C)/0.0059
	B3LYP/aVDZ	nCov(C)/0.0021	nCov(C)/0.0069	nCov(C)/0.0032	nCov(C)/0.0061
Ar	CCSD/aVTZ	nCov(C)/0.0026	nCov(C)/0.0084	nCov(C)/0.0089	nCov(C)/0.0072
	MP2/aVTZ	nCov(C)/0.0026	nCov(C)/0.0085	nCov(C)/0.0090	nCov(C)/ 0.0072
	B3LYP/aVTZ	nCov(C)/0.0027	nCov(C)/0.0089	nCov(C)/0.0090	nCov(C)/0.0078
	MP2/aVDZ	nCov(C)/0.0029	nCov(C)/0.0079	nCov(C)/0.0094	nCov(C)/0.0072
	B3LYP/aVDZ	nCov(C)/0.0029	nCov(C)/0.0083	nCov(C)/0.0093	nCov(C)/0.0074
Kr	CCSD/aVTZ	nCov(C)/0.0030	nCov(C)/0.0110	nCov(C)/0.0112	nCov(C)/0.0082
	MP2/aVTZ	nCov(C)/0.0030	nCov(C)/0.0111	nCov(C)/0.0114	nCov(C)/0.0082
	B3LYP/aVTZ	nCov(C)/0.0031	nCov(C)/0.0116	nCov(C)/0.0113	nCov(C)/0.0088
	MP2/aVDZ	nCov(C)/0.0034	nCov(C)/0.0100	nCov(C)/0.0117	nCov(C)/0.0080
	B3LYP/aVDZ	nCov(C)/0.0034	nCov(C)/0.0105	nCov(C)/0.0115	nCov(C)/0.0082
Xe	CCSD/aVTZ	nCov(C)/0.0029	nCov(C)/0.0116	nCov(C)/0.0160	nCov(C)/0.0089
	MP2/aVTZ	nCov(C)/0.0029	nCov(C)/0.0117	nCov(C)/0.0162	nCov(C)/0.0089
	B3LYP/aVTZ	nCov(C)/0.0030	nCov(C)/0.0122	nCov(C)/0.0161	nCov(C)/0.0095
	MP2/aVDZ	nCov(C)/0.0032	nCov(C)/0.0105	pCov(C/$H^{+/-}$)/0.0165	nCov(C)/0.0083
	B3LYP/aVDZ	nCov(C)/0.0031	nCov(C)/0.0110	nCov(C)/0.0163	nCov(C)/0.0085

Table S16 Type of the Ng-X bonds of the Ng-HOH_2^+, Ng-BeO, Ng-CuF, and F-NgO^- included in the NgBC47 reference set, and average electron density ρ_s(ave) ($e\ a_0^{-3}$) over the volume enclosed by the $s(\boldsymbol{r}) = 0.4$ isosurface at around the BCP at the CCSD(T)/aVTZ geometries

		Ng-HOH_2^+	Ng-BeO	Ng-CuF	F-NgO^-
		type/ρ_s(ave)	type/ρ_s(ave)	type/ρ_s(ave)	type/ρ_s(ave)
He	CCSD/aVTZ	nCov(C)/0.0118	nCov(C)/0.0281	pCov(A/H^-)/0.0579	pCov(A/$H^{-/+}$)/0.0700
	MP2/aVTZ	nCov(C)/0.0118	nCov(B)/0.0276	pCov(A/H^-)/0.0564	pCov(A/$H^{-/+}$)/0.0708
	B3LYP/aVTZ	nCov(C)/0.0127	nCov(C)/0.0296	pCov(A/H^-)/0.0583	pCov(A/$H^{-/+}$)/0.0720
	MP2/aVDZ	nCov(C)/0.0108	nCov(C)/0.0240	pCov(A/$H^{-/+}$)/0.0557	pCov(A/$H^{-/+}$)/0.0666
	B3LYP/aVDZ	nCov(C)/0.0116	nCov(C)/0.0260	pCov(A/H^-)/0.0577	pCov(C/$H^{+/-}$)/0.0676
Ne	CCSD/aVTZ	pCov(C/$H^{+/-}$)/0.0169	nCov(C)/0.0223	nCov(C)/0.0233	
	MP2/aVTZ	pCov(C/$H^{+/-}$)/0.0172	nCov(C)/0.0222	pCov(C/$H^{+/-}$)/0.0228	
	B3LYP/aVTZ	pCov(C/$H^{+/-}$)/0.0181	nCov(C)/0.0238	pCov(C/$H^{+/-}$)/0.0235	
	MP2/aVDZ	nCov(C)/0.0170	nCov(C)/0.0220	nCov(C)/0.0239	
	B3LYP/aVDZ	nCov(C)/0.0179	nCov(C)/0.0234	nCov(C)/0.0244	
Ar	CCSD/aVTZ	pCov(A/H^-)/0.0269	pCov(B/$H^{+/-}$)/0.0306	pCov(A/H^-)/0.0490	
	MP2/aVTZ	pCov(A/H^-)/0.0271	pCov(B/$H^{+/-}$)/0.0301	pCov(A/H^-)/0.0491	
	B3LYP/aVTZ	pCov(A/H^-)/0.0282	pCov(B/$H^{-/+}$)/0.0318	pCov(A/H^-)/0.0499	
	MP2/aVDZ	nCov(C)/0.0246	pCov(B/$H^{+/-}$)/0.0273	pCov(A/H^-)/0.0484	
	B3LYP/aVDZ	nCov(C)/0.0258	pCov(B/$H^{+/-}$)/0.0288	pCov(A/H^-)/0.0492	
Kr	CCSD/aVTZ	pCov(A/H^-)/0.0283	pCov(B/$H^{-/+}$)/0.0310	pCov(A/H^-)/0.0526	pCov(A/$H^{-/+}$)/0.0505
	MP2/aVTZ	pCov(A/H^-)/0.0283	pCov(B/$H^{-/+}$)/0.0304	pCov(A/H^-)/0.0525	pCov(A/$H^{-/+}$)/0.0517
	B3LYP/aVTZ	pCov(A/H^-)/0.0294	pCov(B/$H^{-/+}$)/0.0322	pCov(A/H^-)/0.0529	pCov(A/$H^{-/+}$)/0.0516
	MP2/aVDZ	pCov(C/$H^{+/-}$)/0.0256	pCov(B/$H^{-/+}$)/0.0278	pCov(A/H^-)/0.0524	pCov(A/$H^{-/+}$)/0.0507
	B3LYP/aVDZ	pCov(C/$H^{+/-}$)/0.0268	pCov(B/$H^{-/+}$)/0.0294	pCov(A/H^-)/0.0526	pCov(C/$H^{-/+}$)/0.0507
Xe	CCSD/aVTZ	pCov(A/H^-)/0.0296	pCov(B/$H^{-/+}$)/0.0314	pCov(A/H^-)/0.0538	pCov(A/H^-)/0.0523
	MP2/aVTZ	pCov(A/H^-)/0.0297	pCov(B/$H^{-/+}$)/0.0307	pCov(A/H^-)/0.0549	pCov(A/H^-)/0.0538
	B3LYP/aVTZ	pCov(A/H^-)/0.0305	pCov(B/$H^{-/+}$)/0.0325	pCov(A/H^-)/0.0540	pCov(A/H^-)/0.0536
	MP2/aVDZ	pCov(A/H^-)/0.0273	pCov(B/$H^{-/+}$)/0.0287	pCov(A/H^-)/0.0564	pCov(A/H^-)/0.0526
	B3LYP/aVDZ	pCov(A/H^-)/0.0283	pCov(B/$H^{-/+}$)/0.0304	pCov(A/H^-)/0.0545	pCov(C/H^-)/0.0527

Table S17 Volume Ω_s (a_0^3) enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP, and total electronic charge (me) over Ω_s, $N(\Omega_s)$, of the Ng-X interactions included in the NgBC47 reference set at the CCSD(T)/aVTZ geometries

		Ng-Ar	Ng-HF	Ng-F^-	Ng-Na^+	Ng-HOH_2^+	Ng-BeO	Ng-CuF	F-NgO^-
		$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$	$\Omega_s/N(\Omega_s)$
He	CCSD/aVTZ	0.0222/0.027	0.0192/0.069	0.0306/0.052	0.0107/0.048	0.0330/0.39	0.0219/0.62	0.1385/8.02	0.1224/8.57
	MP2/aVTZ	0.0225/0.027	0.0196/0.071	0.0322/0.055	0.0110/0.048	0.0331/0.39	0.0222/0.61	0.1496/8.44	0.1273/9.01
	B3LYP/aVTZ	0.0259/0.034	0.0233/0.093	0.0423/0.080	0.0158/0.077	0.0380/0.48	0.0289/0.86	0.1593/9.29	0.1320/9.50
	MP2/aVDZ	0.0201/0.028	0.0335/0.12	0.0339/0.058	0.0163/0.077	0.0496/0.54	0.0213/0.51	0.1329/7.40	0.1395/9.29
	B3LYP/aVDZ	0.0252/0.035	0.0389/0.16	0.0414/0.075	0.0196/0.098	0.0553/0.64	0.0277/0.72	0.1333/7.69	0.1322/8.94
Ne	CCSD/aVTZ	0.0357/0.075	0.0336/0.22	0.0554/0.18	0.0199/0.12	0.0528/0.89	0.0278/0.62	0.1393/3.25	
	MP2/aVTZ	0.0370/0.081	0.0365/0.24	0.0659/0.22	0.0210/0.13	0.0564/0.97	0.0301/0.67	0.1598/3.64	
	B3LYP/aVTZ	0.0411/0.095	0.0411/0.29	0.0754/0.26	0.0265/0.17	0.0616/1.11	0.0386/0.92	0.1717/4.03	
	MP2/aVDZ	0.0260/0.055	0.0414/0.27	0.0365/0.11	0.0160/0.094	0.0609/1.04	0.0258/0.57	0.1744/4.17	
	B3LYP/aVDZ	0.0295/0.062	0.0477/0.33	0.0460/0.15	0.0188/0.11	0.0700/1.25	0.0362/0.85	0.1885/4.60	
Ar	CCSD/aVTZ	0.0877/0.23	0.0763/0.64	0.1818/1.62	0.0488/0.35	0.1540/4.14	0.0856/2.62	0.4607/22.6	
	MP2/aVTZ	0.0906/0.24	0.0768/0.65	0.1978/1.78	0.0492/0.35	0.1592/4.31	0.0905/2.72	0.5151/25.3	
	B3LYP/aVTZ	0.1026/0.28	0.0843/0.75	0.2091/1.88	0.0633/0.49	0.1705/4.81	0.1186/3.77	0.5278/26.3	
	MP2/aVDZ	0.1036/0.30	0.1264/1.00	0.1926/1.81	0.0594/0.43	0.1676/4.12	0.1201/3.28	0.4891/23.7	
	B3LYP/aVDZ	0.1097/0.32	0.1351/1.12	0.1977/1.84	0.0671/0.50	0.1769/4.56	0.1439/4.14	0.4777/23.5	
Kr	CCSD/aVTZ	0.1138/0.34	0.1112/1.22	0.2530/2.83	0.0676/0.55	0.2346/6.64	0.1407/4.36	0.7368/38.8	0.4996/25.2
	MP2/aVTZ	0.1156/0.35	0.1155/1.28	0.2693/3.07	0.0683/0.56	0.2404/6.80	0.1522/4.63	0.8258/43.4	0.5381/27.8
	B3LYP/aVTZ	0.1305/0.40	0.1246/1.45	0.2833/3.20	0.0904/0.80	0.2590/7.61	0.1990/6.41	0.8306/43.9	0.5016/25.9
	MP2/aVDZ	0.1448/0.49	0.1828/1.83	0.2749/3.22	0.0857/0.69	0.2516/6.44	0.2266/6.30	0.7647/40.1	0.6206/31.5
	B3LYP/aVDZ	0.1551/0.53	0.1993/2.09	0.2805/3.23	0.1012/0.83	0.2676/7.17	0.2633/7.74	0.7218/38.0	0.5521/28.0
Xe	CCSD/aVTZ	0.1427/0.41	0.1665/1.93	0.4049/6.48	0.1165/1.04	0.3938/11.7	0.2811/8.83	1.2657/68.1	0.7305/38.2
	MP2/aVTZ	0.1452/0.42	0.1734/2.03	0.4288/6.95	0.1174/1.04	0.4000/11.9	0.3067/9.42	1.4893/81.8	0.7911/42.6
	B3LYP/aVTZ	0.1600/0.48	0.1889/2.30	0.4322/6.96	0.1506/1.43	0.4238/12.9	0.4211/13.7	1.3737/74.2	0.7136/38.2
	MP2/aVDZ	0.1914/0.61	0.2515/2.64	0.4092/6.75	0.1284/1.07	0.4148/11.3	0.4627/13.3	1.4965/84.4	0.9793/51.5
	B3LYP/aVDZ	0.2005/0.62	0.2636/2.90	0.4071/6.64	0.1538/1.31	0.4248/12.0	0.5226/15.9	1.2807/69.8	0.8572/45.2

Table S18 Average, maximum and minimum value (ave/max/min) of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over the volume enclosed by the $s(\boldsymbol{r})$ = 0.4 isosurface at around the BCP of the Ng-X interactions (X = Ar, HF, F^-, Na^+) at the CCSD(T)/aVTZ geometries

		Ng-Ar	Ng-HF	Ng-F^-	Ng-Na^+
		ave/max/min	ave/max/min	ave/max/min	ave/max/min
He	CCSD/aVTZ	0.0004/0.0005/0.0004	0.0015/0.0015/0.0014	0.0006/0.0006/0.0005	0.0029/0.0031/0.0028
	MP2/aVTZ	0.0004/0.0005/0.0004	0.0014/0.0015/0.0014	0.0006/0.0006/0.0005	0.0029/0.0031/0.0028
	B3LYP/aVTZ	0.0004/0.0005/0.0004	0.0014/0.0015/0.0014	0.0005/0.0006/0.0005	0.0029/0.0031/0.0027
	MP2/aVDZ	0.0004/0.0004/0.0004	0.0007/0.0007/0.0006	0.0006/0.0006/0.0005	0.0020/0.0022/0.0019
	B3LYP/aVDZ	0.0004/0.0004/0.0004	0.0006/0.0007/0.0006	0.0005/0.0005/0.0005	0.0020/0.0022/0.0018
Ne	CCSD/aVTZ	0.0006/0.0007/0.0006	0.0015/0.0015/0.0014	0.0005/0.0006/0.0005	0.0029/0.0033/0.0026
	MP2/aVTZ	0.0006/0.0007/0.0006	0.0014/0.0015/0.0013	0.0005/0.0006/0.0005	0.0029/0.0033/0.0026
	B3LYP/aVTZ	0.0006/0.0006/0.0006	0.0014/0.0015/0.0013	0.0005/0.0005/0.0004	0.0028/0.0033/0.0024
	MP2/aVDZ	0.0009/0.0009/0.0008	0.0019/0.0022/0.0017	0.0012/0.0012/0.0012	0.0033/0.0036/0.0030
	B3LYP/aVDZ	0.0008/0.0008/0.0008	0.0017/0.0021/0.0015	0.0011/0.0012/0.0011	0.0032/0.0036/0.0029
Ar	CCSD/aVTZ	0.0007/0.0007/0.0006	0.0015/0.0016/0.0014	0.0015/0.0018/0.0013	0.0031/0.0036/0.0027
	MP2/aVTZ	0.0007/0.0007/0.0006	0.0015/0.0016/0.0014	0.0014/0.0017/0.0012	0.0031/0.0036/0.0027
	B3LYP/aVTZ	0.0007/0.0007/0.0006	0.0015/0.0016/0.0013	0.0015/0.0018/0.0013	0.0029/0.0035/0.0025
	MP2/aVDZ	0.0005/0.0005/0.0004	0.0014/0.0020/0.0011	0.0014/0.0019/0.0009	0.0024/0.0030/0.0021
	B3LYP/aVDZ	0.0005/0.0005/0.0004	0.0013/0.0019/0.0010	0.0014/0.0020/0.0009	0.0024/0.0030/0.0020
Kr	CCSD/aVTZ	0.0008/0.0008/0.0007	0.0010/0.0011/0.0007	0.00134/0.00153/0.00119	0.0028/0.0034/0.0023
	MP2/aVTZ	0.0008/0.0008/0.0007	0.0009/0.0011/0.0006	0.00126/0.00150/0.00111	0.0028/0.0034/0.0023
	B3LYP/aVTZ	0.0008/0.0008/0.0007	0.0009/0.0011/0.0005	0.00134/0.00166/0.00116	0.0026/0.0033/0.0020
	MP2/aVDZ	0.0005/0.0005/0.0004	0.0015/0.0024/0.0010	0.00117/0.00183/0.00058	0.0023/0.0030/0.0018
	B3LYP/aVDZ	0.0005/0.0005/0.0004	0.0013/0.0023/0.0009	0.00125/0.00195/0.00068	0.0022/0.0030/0.0017
Xe	CCSD/aVTZ	0.0006/0.0007/0.0006	0.0005/0.0007/0.0002	0.00132/0.00198/0.00104	0.0023/0.0032/0.0015
	MP2/aVTZ	0.0006/0.0007/0.0006	0.0004/0.0006/0.0001	0.00120/0.00186/0.00087	0.0023/0.0032/0.0015
	B3LYP/aVTZ	0.0006/0.0007/0.0006	0.0005/0.0007/0.0001	0.00144/0.00218/0.00114	0.0020/0.0031/0.0012
	MP2/aVDZ	0.0004/0.0004/0.0004	0.0012/0.0024/0.0082	0.00061/0.00107/-0.00017	0.0020/0.0029/0.0015
	B3LYP/aVDZ	0.0004/0.0004/0.0004	0.0011/0.0020/0.0008	0.00080/0.00124/0.00016	0.0020/0.0029/0.0015

Table S19 Average, maximum and minimum value (ave/max/min) of the $H(\boldsymbol{r})$ (hartree a_0^{-3}) over the volume enclosed by the $s(\boldsymbol{r}) = 0.4$ isosurface at around the BCP of the Ng-X interactions (X = HOH_2^+, BeO, CuF), and the Ng-F bond of F-NgO^- at the CCSD(T)/aVTZ geometries

		Ng-HOH_2^+	Ng-BeO	Ng-CuF	F-NgO^-
		ave/max/min	ave/max/min	ave/max/min	ave/max/min
He	CCSD/aVTZ	0.0019/0.0022/0.0014	0.0111/0.0168/0.0070	-0.0060/-0.0044/-0.0097	-0.00003/0.0039/-0.0085
	MP2/aVTZ	0.0019/0.0023/0.0014	0.0117/0.0173/0.0075	-0.0062/-0.0048/-0.0089	-0.0007/0.0033/-0.0091
	B3LYP/aVTZ	0.0017/0.0021/0.0009	0.0091/0.0154/0.0047	-0.0059/-0.0042/-0.0100	0.0011/0.0050/-0.0082
	MP2/aVDZ	0.0034/0.0041/0.0029	0.0159/0.0204/0.0130	-0.0011/0.0008/-0.0037	0.0047/0.0096/-0.0059
	B3LYP/aVDZ	0.0032/0.0038/0.0027	0.0139/0.0189/0.0110	-0.0010/0.0014/-0.0045	0.0087/0.0145/-0.0019
Ne	CCSD/aVTZ	0.0014/0.0027/-0.0002	0.0106/0.0150/0.0080	0.0014/0.0031/0.0002	
	MP2/aVTZ	0.0012/0.0026/-0.0006	0.0106/0.0150/0.0079	0.0007/0.0027/-0.0005	
	B3LYP/aVTZ	0.0011/0.0028/-0.0010	0.0091/0.0064/0.01395	0.0012/0.0032/-0.00004	
	MP2/aVDZ	0.0031/0.0045/0.0018	0.00841/0.0131/0.0049	-0.0029/-0.0026/-0.0031	
	B3LYP/aVDZ	0.0026/0.0040/0.0012	0.0062/0.0117/0.0027	-0.0025/-0.0023/0.0027	
Ar	CCSD/aVTZ	-0.0034/-0.0017/-0.0065	0.0015/0.0098/-0.0044	-0.0095/-0.0061/-0.0148	
	MP2/aVTZ	-0.0035/-0.0018/-0.0067	0.0016/0.0101/-0.0042	-0.0101/-0.0065/-0.0151	
	B3LYP/aVTZ	-0.0033/-0.0014/-0.0070	-0.0004/0.0082/-0.0060	-0.0092/-0.0058/-0.0136	
	MP2/aVDZ	0.0024/0.0026/0.0018	0.0028/0.0118/-0.0012	-0.0082/-0.0048/-0.0125	
	B3LYP/aVDZ	0.0023/0.0025/0.0019	0.0010/0.0090/-0.0028	-0.0070/-0.0038/-0.0114	
Kr	CCSD/aVTZ	-0.0047/-0.0027/-0.0083	-0.0026/0.0053/-0.0094	-0.0123/-0.0078/-0.0198	-0.0019/0.0011/-0.0095
	MP2/aVTZ	-0.0047/-0.0027/-0.0084	-0.0023/0.0056/-0.0082	-0.0131/-0.0083/-0.0210	-0.0028/0.0010/-0.0119
	B3LYP/aVTZ	-0.0044/-0.0024/-0.0088	-0.0046/0.0038/-0.0104	-0.0117/-0.0073/-0.0187	-0.0004/0.0024/-0.0079
	MP2/aVDZ	0.0007/0.0011/-0.0003	-0.0018/0.0085/-0.0064	-0.0123/-0.0070/-0.0209	-0.0046/0.0005/-0.0161
	B3LYP/aVDZ	0.0006/0.0010/-0.0002	-0.0034/0.0072/-0.0074	-0.0106/-0.0056/-0.0180	-0.0017/0.0045/-0.0136
Xe	CCSD/aVTZ	-0.0047/-0.0027/-0.0083	-0.0068/0.0031/-0.0143	-0.0150/-0.0083/-0.0325	-0.0062/-0.0007/-0.0201
	MP2/aVTZ	-0.0056/-0.0033/-0.0103	-0.0064/0.0035/-0.0134	-0.0161/-0.0088/-0.0401	-0.0072/-0.0011/-0.0235
	B3LYP/aVTZ	-0.0050/-0.0028/-0.0106	-0.0082/0.0013/-0.0146	-0.0140/-0.0076/-0.0316	-0.0048/0.0005/-0.0197
	MP2/aVDZ	-0.0015/-0.0005/-0.0037	-0.0064/0.0055/-0.0120	-0.0179/-0.0088/-0.0538	-0.0099/-0.0038/-0.0267
	B3LYP/aVDZ	0.0006/0.0010/-0.0002	-0.0076/0.0042/-0.0124	-0.0148/-0.0074/-0.0356	-0.0074/-0.0002/-0.0237