Boron – Noble Gas Covalent Bond in Borenium and Boronium compounds

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SUPPORTING INFORMATION

Fig. S1. Structures for the D_{∞} Borenium (BH_2Ng^+) compounds and the first local minimum of Boronium cations ($BH_2Ng_2^+$). Ng = He – Rn at the PBE0-D3/def2-TZVP level. Pink spheres represent boron atoms, white hydrogen atoms and turquoise Ng atoms.

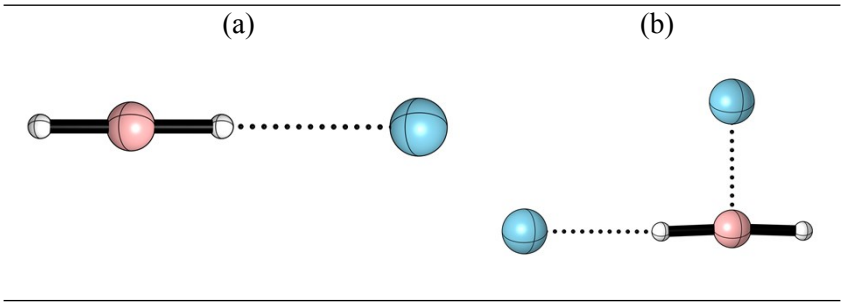

Table S1. Relative energies of BH_2Ng^+ and $BH_2Ng_2^+$ (Ng = He – Rn) with first local minima at corrected PBE0-D3/def2-TZVP, CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP and uncorrected CCSD(T)/def2-TZVP//PBE0/def2-TZVP levels.

System	$E_{relative,DFT}$	$E_{relative,CCSDT\ uncorrected}$	$E_{relative,CCSDT\ corrected}$
BH_2He^+	0.5	0.1	-0.4
BH_2Ne^+	1.7	0.8	0.1
BH_2Ar^+	14.3	12.0	10.5
BH_2Kr^+	20.0	17.8	16.0
BH_2Xe^+	28.1	25.8	24.5
BH_2Rn^+	50.7	30.9	29.1
$BH_2He_2^+$	0.2	0.1	0.6
$BH_2Ne_2^+$	1.5	1.0	0.4
$BH_2Ar_2^+$	7.2	12.8	11.5
$BH_2Kr_2^+$	9.2	7.9	6.7
$BH_2Xe_2^+$	12.0	10.5	9.4
$BH_2Rn_2^+$	13.5	13.1	12.1

Table S2. Geometrical parameters for BH_2^+, Ng-Borenium and Ng_2-Boronium cations at the PBE0-D3/ef2-TZVP level, and values for the T1 diagnostic for all the systems at the CCSD(T)/def2-TZVP//PBE0-D3/def2-TZVP level.

System	r_{B-H}	r_{B-Ng}	a_{H-B-H}	$a_{Ng-B-Ng}$	T1 diag
BH_2^+	1.18	-	180.00	-	0.0060
BH_2He^+	1.18	2.11	175.89	-	0.0057
BH_2Ne^+	1.18	2.12	172.10	-	0.0082
BH_2Ar^+	1.18	2.00	148.26	-	0.0071
BH_2Kr^+	1.18	2.11	144.81	-	0.0064
BH_2Xe^+	1.18	2.27	141.38	-	0.0074
BH_2Rn^+	1.18	2.35	140.55	-	0.0074
$BH_2He_2^+$	1.18	2.06	172.87	75.44	0.0057
$BH_2Ne_2^+$	1.18	2.16	169.56	83.68	0.0084
$BH_2Ar_2^+$	1.18	2.13	144.56	98.05	0.0071
$BH_2Kr_2^+$	1.18	2.25	140.80	101.49	0.0062
$BH_2Xe_2^+$	1.18	2.40	136.31	105.38	0.0070
$BH_2Rn_2^+$	1.18	2.49	135.61	106.64	0.0070

Table S3. van der Waals radii (R_{VdW}) and covalent radii (R_{Cov}) for B and Ng atoms (in Å) taken from references 81 and 82.

Atom	R_{VdW}	R_{Cov}
B	2.05	0.84
He	1.43	0.28
Ne	1.58	0.58
Ar	1.94	1.06
Kr	2.07	1.16
Xe	2.28	1.40
Rn	2.40	1.50

Table S4. QTAIM parameters (in a.u.) at B-Ng bond critical points (BCP) at PBE0-D3/def2-TZVP level.

System	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$
BH_2He^+	0.0164	0.0522	0.0118	-0.0105	0.0013
BH_2Ne^+	0.0259	0.0675	0.0190	-0.0211	-0.0021
$BH_2He_2^+$	0.0178	0.0545	0.0128	-0.0119	0.0009
$BH_2Ne_2^+$	0.0234	0.0659	0.0175	-0.0186	-0.0010

Fig. S2. Contour plots of Laplacian of electron density ($\nabla^2\rho(r_c)$) for Borenium BH_2Ng^+ cations (Ng = He and Ne) at the PBE0-D3/def2-TZVP level. Blue solid lines represent positive values (Charge depletion), whereas red dashed lines represent negative values (Charge concentration).

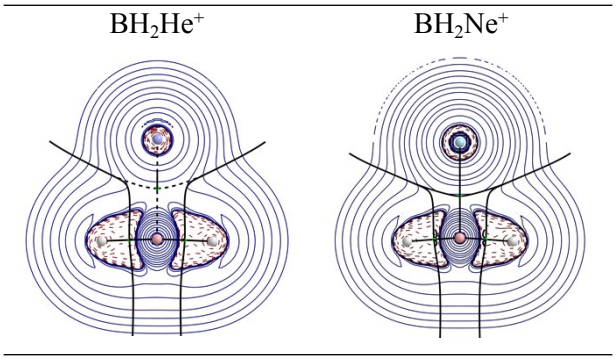

Table S5. NPA Charges (q) for the B and Ng centers (a.u), Wiberg bond indices for B-Ng (Ng = He and Ne) at the PBE0-D3/def2-TZVP level.

System	Wiberg	q_B	q_{Ng}
BH_2He^+	0.06	1.09	0.03
BH_2Ne^+	0.10	1.04	0.05
$BH_2He_2^+$	0.08	1.04	0.04
$BH_2Ne_2^+$	0.09	0.98	0.05

Fig. S3. NBO plots of B-Ng (He and Ne) for Borenium ($BH_2N_2^+$) and Boronium cations ($BH_2Ng_2^+$). At the PBE0-D3/def2-TZVP level.

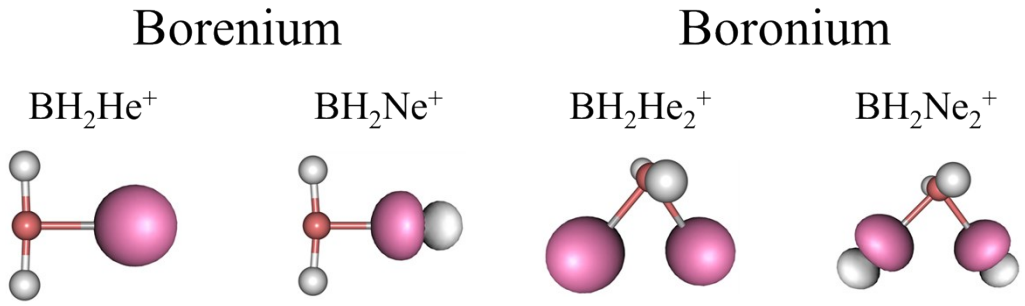

Table S6. EDA results for Borenium, BH_2Ng^+ and Boronium, $BH_2Ng_2^+$ (Ng = He an Ne) at the PBE-D3/TZ2P//PBE0-D3/def2-TZVP level.

System	ΔE_{int}	ΔE_{Pauli}	ΔV_{elstat}	ΔE_{orb}	ΔE_{disp}	$\%\Delta E_{cov}$	$\%\Delta E_{non\text{-}cov}$
BH_2He^+	-2.12	4.05	-0.90	-5.07	-0.20	82.17	17.83
BH_2Ne^+	-4.78	9.29	-2.85	-10.92	-0.30	77.61	22.39
$BH_2He_2^+$	-4.36	9.36	-2.03	-11.30	-0.39	82.36	17.64
$BH_2Ne_2^+$	-8.76	15.92	-4.80	-19.30	-0.59	78.17	21.83