Electronic Supplementary Information for

Noble gas hydrides: theoretical prediction of a first group of anionic species

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Table S1 CCSD(T)/aVTZ, MP2/aVTZ, and B3LYP/aVTZ optimized bond lengths (Å) of the linear $HNgBeO^-$ and NgBeO (Ng = Ar, Kr, Xe, Rn)

Species	Ng	Method	Ng-Be	Be-O	Ng-H
H-Ng-Be-O^-	Ar	CCSD(T)/aVTZ	2.0173	1.3528	2.5567
		MP2/aVTZ	2.0072	1.3623	2.5389
		B3LYP/aVTZ	2.0616	1.3388	2.5148
	Kr	CCSD(T)/aVTZ	2.1830	1.3553	2.5764
		MP2/aVTZ	2.1698	1.3648	2.5574
		B3LYP/aVTZ	2.2367	1.3415	2.5263
	Xe	CCSD(T)/aVTZ	2.4015	1.3595	2.5698
		MP2/aVTZ	2.3848	1.3689	2.5503
		B3LYP/aVTZ	2.4538	1.3453	2.5333
	Rn	CCSD(T)/aVTZ	2.5234	1.3622	2.5267
		MP2/aVTZ	2.5035	1.3716	2.5048
		B3LYP/aVTZ	2.5619	1.3472	2.5105
Ng-Be-O	Ar	CCSD(T)/aVTZ	2.0752	1.3413	
		MP2/aVTZ	2.0784	1.3513	
		B3LYP/aVTZ	2.0710	1.3240	
	Kr	CCSD(T)/aVTZ	2.2119	1.3424	
		MP2/aVTZ	2.2151	1.3523	
		B3LYP/aVTZ	2.2151	1.3252	
	Xe	CCSD(T)/aVTZ	2.3848	1.3440	
		MP2/aVTZ	2.3890	1.3537	
		B3LYP/aVTZ	2.3974	1.3268	
	Rn	CCSD(T)/aVTZ	2.4704	1.3449	
		MP2/aVTZ	2.4743	1.3546	
		B3LYP/aVTZ	2.4885	1.3276	

Table S2 CCSD(T)/aVTZ electron density ρ ($e\ a_0^{-3}$), Laplacian of the electron density $\nabla^2\rho$ ($e\ a_0^{-5}$), and energy density H (hartree a_0^{-3}) calculated at the BCP on the Ng-X bonds of the $HNgBeO^-$ and NgBeO

Species	Bond	ρ(BCP)	$\nabla^2\rho_{(BCP)}$	H(BCP)
$HArBeO^-$	Ar-H	0.0171	0.0400	0.00015
	Ar-Be	0.0444	0.241	-0.00387
ArBeO	Ar-Be	0.0325	0.223	0.00258
$HKrBeO^-$	Kr-H	0.0207	0.0382	-0.00107
	Kr-Be	0.0432	0.163	-0.00913
KrBeO	Kr-Be	0.0328	0.181	-0.00118
$HXeBeO^-$	Xe-H	0.0269	0.0374	-0.00275
	Xe-Be	0.0428	0.0864	-0.01479
XeBeO	Xe-Be	0.0333	0.136	-0.00524
$HRnBeO^-$	Rn-H	0.0308	0.0410	-0.00385
	Rn-Be	0.0410	0.0467	-0.01646
RnBeO	Rn-Be	0.0322	0.114	-0.00641

Table S3 Harmonic vibrational frequencies (cm^{-1}) of the linear $HNgBeO^-$ and NgBeO computed with the aVTZ basis set. IR intensities (km mol^{-1}) in parentheses

Species	Method	ν(Ng-Be)	ν(Be-O)	ν(Ng-H)	δ(Ng-Be-O)[a]	δ(H-Ng-Be)[a]
$HArBeO^-$	CCSD(T)	318	1508	569	233	134
	MP2	330 (0.4)	1472 (124)	585 (1284)	241 (15)	138 (713)
	B3LYP	267 (38)	1534 (120)	578 (1190)	234 (3)	141 (577)
ArBeO	CCSD(T)	272	1536		155	
	MP2	268 (2)	1490 (72)		160 (64)	
	B3LYP	270 (1)	1590 (146)		160 (73)	
$HKrBeO^-$	CCSD(T)	267	1495	591	250	153
	MP2	281 (19)	1460 (117)	605 (1635)	256 (8)	158 (638)
	B3LYP	229 (65)	1522 (130)	607 (1440)	259 (44)	150 (459)
KrBeO	CCSD(T)	246	1533		155	
	MP2	243 (1)	1488 (77)		158 (59)	
	B3LYP	240 (0.7)	1585 (154)		157 (68)	
$HXeBeO^-$	CCSD(T)	267	1495	591	250	153
	MP2	248 (69)	1442 (107)	654 (2273)	292 (84)	167 (420)
	B3LYP	214 (78)	1506 (145)	648 (1838)	296 (86)	155 (312)
XeBeO	CCSD(T)	237	1527		150	
	MP2	233 (0.6)	1483 (78)		151 (50)	
	B3LYP	225 (0.2)	1577 (159)		149 (59)	
$HRnBeO^-$	CCSD(T)	234	1476	641	286	161
	MP2	225 (94)	1429 (101)	728 (2548)	305 (90)	164 (300)
	B3LYP	205 (72)	1497 (158)	720 (1930)	302 (79)	158 (243)
RnBeO	CCSD(T)	224	1522		145	
	MP2	221 (0.5)	1478 (81)		147 (46)	
	B3LYP	214 (0.2)	1572 (165)		145 (55)	

[a]Doubly-degenerate bending.

Table S4 CCSD(T)/aVTZ dissociation energies (kcal mol^{-1}) of the $HNgBeO^-$ (reference species)

Species		H^- + NgBeO	H^- + Ng + BeO	H + Ng + BeO^-	Ng + $HBeO^-$	$E^{\#a}$
$HArBeO^-$	ΔE_{el}	28.1	40.0	7.1	-83.1	2.9
	ΔE (0 K)	26.7	37.6	4.5	-81.4	2.5
	ΔE (298.15 K)	26.8	37.6	4.5	-82.1	2.0
	ΔH (298.15 K)	27.4	38.7	5.7	-81.5	2.0
	ΔG (298.15 K)	21.0	25.8	-7.7	-87.3	1.7
$HKrBeO^-$	ΔE_{el}	30.3	44.5	11.5	-78.7	6.1
	ΔE (0 K)	28.8	42.0	8.9	-76.9	5.5
	ΔE (298.15 K)	29.0	42.0	8.9	-77.6	5.0
	ΔH (298.15 K)	29.5	43.2	10.1	-77.1	5.0
	ΔG (298.15 K)	23.0	30.0	-3.5	-83.0	4.5
$HXeBeO^-$	ΔE_{el}	34.3	51.3	18.3	-71.8	11.0
	ΔE (0 K)	32.6	48.7	15.7	-70.2	10.2
	ΔE (298.15 K)	32.9	48.8	15.7	-70.9	9.9
	ΔH (298.15 K)	33.5	50.0	16.9	-70.3	9.9
	ΔG (298.15 K)	26.7	36.7	3.2	-76.4	9.1
$HRnBeO^-$	ΔE_{el}	39.0	56.9	24.0	-66.2	14.3
	ΔE (0 K)	37.2	54.3	21.2	-64.7	13.5
	ΔE (298.15 K)	37.5	54.4	21.3	-65.3	13.2
	ΔH (298.15 K)	38.1	55.5	22.4	-64.7	13.2
	ΔG (298.15 K)	31.3	42.3	8.8	-70.8	12.3

[a]Energy barrier for the reaction $HNgBeO^- \rightarrow Ng + HBeO^-$

Table S5 MP2/aVTZ dissociation energies (kcal mol^{-1}) of the $HNgBeO^-$ (reference species)

Species		H^- + NgBeO	H^- + Ng + BeO	H + Ng + BeO^-	Ng + $HBeO^-$	$E^{\#a}$
$HArBeO^-$	ΔE_{el}	28.6	40.3	2.8	-84.9	3.1
	ΔE (0 K)	27.0	37.8	0.3	-83.1	2.6
	ΔE (298.15 K)	27.2	37.8	0.3	-83.8	2.1
	ΔH (298.15 K)	27.8	38.9	1.4	-83.2	2.1
	ΔG (298.15 K)	21.3	25.9	-12.5	-89.1	1.9
$HKrBeO^-$	ΔE_{el}	30.8	44.7	7.2	-80.5	6.3
	ΔE (0 K)	29.2	42.1	4.6	-78.8	5.6
	ΔE (298.15 K)	29.4	42.1	4.6	-79.4	5.2
	ΔH (298.15 K)	30.0	43.3	5.8	-78.9	5.2
	ΔG (298.15 K)	23.3	30.1	-8.3	-84.9	4.6
$HXeBeO^-$	ΔE_{el}	34.8	51.4	13.9	-73.8	11.1
	ΔE (0 K)	33.0	48.7	11.2	-72.2	10.3
	ΔE (298.15 K)	33.4	48.8	11.3	-72.8	10.0
	ΔH (298.15 K)	33.9	49.9	12.4	-72.2	10.0
	ΔG (298.15 K)	27.1	36.6	-1.8	-78.4	9.1
$HRnBeO^-$	ΔE_{el}	39.4	56.8	19.3	-68.4	14.6
	ΔE (0 K)	37.5	54.0	16.5	-66.9	13.7
	ΔE (298.15 K)	37.8	54.1	16.6	-67.5	13.4
	ΔH (298.15 K)	38.4	55.3	17.8	-66.9	13.4
	ΔG (298.15 K)	31.5	41.9	3.6	-73.1	14.6

[a]Energy barrier for the reaction $HNgBeO^- \rightarrow Ng + HBeO^-$

Table S6 B3LYP/aVTZ dissociation energies (kcal mol^{-1}) of the $HNgBeO^-$ (reference species)

Species		H^- + NgBeO	H^- + Ng + BeO	H + Ng + BeO^-	Ng + $HBeO^-$	$E^{\#a}$
$HArBeO^-$	ΔE_{el}	29.9	41.7	10.4	-82.0	4.0
	ΔE (0 K)	28.5	39.4	7.9	-80.1	3.5
	ΔE (298.15 K)	28.6	39.3	7.8	-80.9	3.1
	ΔH (298.15 K)	29.2	40.5	9.0	-80.3	3.1
	ΔG (298.15 K)	22.9	27.6	-4.8	-86.0	2.7
$HKrBeO^-$	ΔE_{el}	32.3	45.9	14.6	-77.8	7.6
	ΔE (0 K)	30.8	43.6	12.1	-76.0	6.9
	ΔE (298.15 K)	31.0	43.6	12.0	-76.7	6.5
	ΔH (298.15 K)	31.6	44.7	13.2	-76.1	6.5
	ΔG (298.15 K)	25.0	31.7	-0.7	-82.0	5.9
$HXeBeO^-$	ΔE_{el}	36.1	52.0	20.7	-71.7	12.8
	ΔE (0 K)	34.4	49.6	18.1	-70.0	11.9
	ΔE (298.15 K)	34.7	49.6	18.1	-70.7	11.6
	ΔH (298.15 K)	35.3	50.8	19.3	-70.1	11.6
	ΔG (298.15 K)	28.5	37.6	5.2	-76.1	10.7
$HRnBeO^-$	ΔE_{el}	40.5	57.1	25.8	-66.6	15.6
	ΔE (0 K)	38.7	54.5	23.0	-65.1	14.6
	ΔE (298.15 K)	39.0	54.6	23.1	-65.7	14.3
	ΔH (298.15 K)	39.6	55.7	24.2	-65.1	14.3
	ΔG (298.15 K)	32.7	42.5	10.2	-71.1	13.3

[a]Energy barrier for the reaction $HNgBeO^- \rightarrow Ng + HBeO^-$

Table S7 CCSD(T)/aVTZ, MP2/aVTZ, and B3LYP/aVTZ optimized bond lengths (Å) and bond angles (°) of the $HNgBeO^-$ TS

Ng	Method	Ng-Be	Be-O	Ng-H	H-Ng-Be	Ng-Be-O
Ar	CCSD(T)/aVTZ	2.0269	1.3519	2.6842	114.4	163.5
	MP2/aVTZ	2.0191	1.3611	2.6673	113.1	163.6
	B3LYP/aVTZ	2.0527	1.3368	2.7050	111.8	162.6
Kr	CCSD(T)/aVTZ	2.1815	1.3527	2.8188	103.7	161.8
	MP2/aVTZ	2.1743	1.3618	2.7968	102.8	161.9
	B3LYP/aVTZ	2.2103	1.3373	2.8417	102.5	161.3
Xe	CCSD(T)/aVTZ	2.3689	1.3537	2.9587	94.5	160.8
	MP2/aVTZ	2.3649	1.3627	2.9289	93.9	160.9
	B3LYP/aVTZ	2.3997	1.3379	2.9851	94.2	160.7
Rn	CCSD(T)/aVTZ	2.4681	1.3548	2.9486	91.6	161.2
	MP2/aVTZ	2.4603	1.3638	2.9228	89.9	161.1
	B3LYP/aVTZ	2.5061	1.3390	2.9774	90.1	161.1