Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Planar Tetracoordinate Beryllium compounds with a partially covalent Be–Ng bond

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SUPPORTING INFORMATION

Table S1. Vibrational modes (in cm^{-1}) computed at the CCSD(T)/def2-TZVP level.

ν	BeH_3He^+	BeH_3Ne^+	BeH_3Ar^+	BeH_3Kr^+	BeH_3Xe^+	BeH_3Rn^+
1	178.9689	167.1509	288.5872	298.9603	317.2628	315.2484
2	277.3450	226.5630	330.6105	321.8707	334.7953	352.5582
3	358.8748	291.4269	387.5636	376.5439	369.4408	369.1903
4	387.0698	389.4762	461.0397	469.8148	488.3960	503.2793
5	461.4693	441.7424	548.5065	561.2152	578.1852	588.4945
6	927.4407	912.9368	835.2901	814.3065	788.1754	768.8169
7	1087.1397	1076.3623	1096.2433	1099.9413	1109.7799	1112.7938
8	2294.5637	2290.9223	2275.8393	2266.2788	2253.9624	2246.0672
9	4060.8522	4072.4054	4091.0738	4093.6972	4085.8644	4083.1592

Table S2. Moment of Inertia (*I*, in amu.$Å^2$) computed at the CCSD(T)/def2-TZVP level.

I	BeH_3He^+	BeH_3Ne^+	BeH_3Ar^+	BeH_3Kr^+	BeH_3Xe^+	BeH_3Rn^+
XX	70.5396	41.0450	24.6912	18.9425	15.1813	13.4955
YY	30.1441	13.3204	9.4698	7.5556	6.3051	5.7944
ZZ	52.6384	19.7172	15.3612	12.5689	10.7838	10.1540

Table S3. Rotational constants (*B*, in GHz) computed at the CCSD(T)/def2-TZVP level.

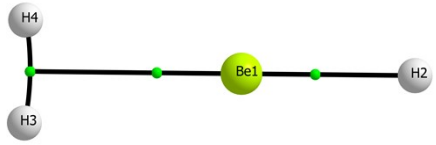
B	BeH_3He^+	BeH_3Ne^+	BeH_3Ar^+	BeH_3Kr^+	BeH_3Xe^+	BeH_3Rn^+
XX	82.2934	82.4607	15.3612	91.1154	92.7804	93.5009
YY	30.1441	13.3197	9.4698	7.5556	6.3051	5.7944
ZZ	30.1441	13.3197	10.5871	8.2388	6.7648	6.1772

Table S4. Natural atomic charges and Wiberg bond index for all bonds in BeH_3Ng^+. Calculations were performed at the CCSD/def2–TZVP level.

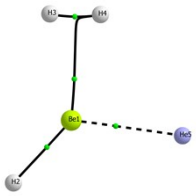
Compound	Q_{Be}	Q_H	Q_{Ha}	Q_{Hb}	Q_{Ng}	$WBI_{Be–Ng}$	$WBI_{Be–H}$	$WBI_{Be–Ha}$	$WBI_{Be–Hb}$
BeH_3^+	1.32	–0.44	0.06	0.06	——	——	0.71	0.10	0.10
BeH_3He^+	1.34	–0.49	0.09	0.02	0.04	0.06	0.66	0.10	0.09
BeH_3Ne^+	1.35	–0.49	0.09	0.01	0.04	0.05	0.65	0.10	0.08
BeH_3Ar^+	1.31	–0.52	0.08	0.00	0.13	0.42	0.61	0.09	0.07
BeH_3Kr^+	1.28	–0.52	0.08	0.00	0.16	0.23	0.60	0.09	0.07
BeH_3Xe^+	1.24	–0.53	0.08	–0.01	0.22	0.30	0.59	0.08	0.07
BeH_3Rn^+	1.22	–0.53	0.07	–0.01	0.25	0.57	0.58	0.08	0.07

Figure S1. Bond paths for all systems studied in this work. Computed at the CCSD/def2-TZVP level.

BeH_3^+

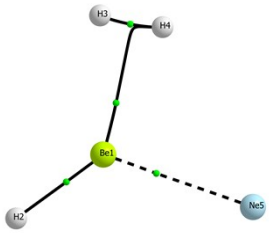


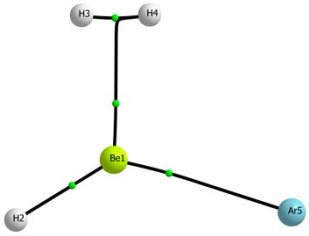
BeH_3He^+



BeH_3Ne^+

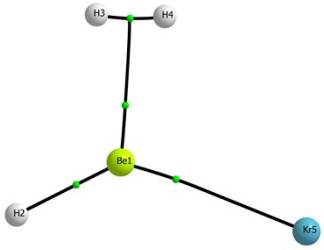
BeH_3Ar^+

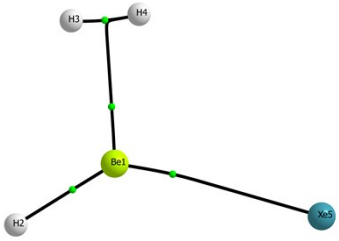




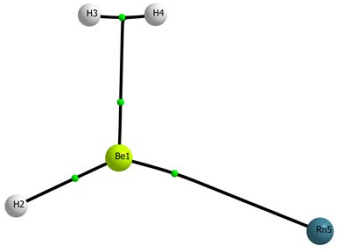
BeH_3Kr^+

BeH_3Xe^+





BeH_3Rn^+



Cartesian Coordinates

BeH_3^+			
Be	0.000000000	0.000000000	0.279852315
H	0.000000000	0.000000000	1.591869381
H	0.000000000	0.387784045	-1.355639318
H	0.000000000	-0.387784045	-1.355639318

BeH_3He^+			
Be	0.000000000	0.356822026	0.000000000
H	-0.285066020	1.631370119	0.000000000
H	1.528920112	-0.312431023	0.000000000
H	1.079698079	-0.940810070	0.000000000
He	-1.161776085	-0.902708065	0.000000000

BeH_3Ne^+			
Be	0.128230009	1.063157078	0.000000000
H	1.201846084	1.807948131	0.000000000
H	-1.440355103	1.650723120	0.000000000
H	-1.556714110	0.888054062	0.000000000
Ne	0.128230009	-0.859935059	0.000000000

BeH_3Ar^+			
Be	0.088397000	1.435405000	0.000000000
H	1.064141000	2.308093000	0.000000000
H	-1.391060000	2.233129000	0.000000000
H	-1.617820000	1.498050000	0.000000000
Ar	0.088397000	-0.654494000	0.000000000

BeH_3Kr^+			
Be	0.051398004	1.823579133	0.000000000
H	1.010406070	2.716907198	0.000000000
H	-1.408759104	2.652590190	0.000000000
H	-1.657573119	1.925272141	0.000000000
Kr	0.051398004	-0.405252029	0.000000000

BeH_3Xe^+			
Be	0.036089003	2.102272152	0.000000000
H	0.981399071	3.013210219	0.000000000
H	-1.407351101	2.974445213	0.000000000
H	-1.667221120	2.250863160	0.000000000
Xe	0.036089003	-0.308289022	0.000000000

BeH_3Rn^+			
Be	0.023769000	2.272835000	0.000000000
H	0.955877000	3.199249000	0.000000000
H	-1.413411000	3.161464000	0.000000000
H	-1.681712000	2.441038000	0.000000000
Rn	0.023769000	-0.208059000	0.000000000