Supporting Information

Infrared Identification of Proton-bound Rare-gas Dimers $(XeHXe)^+$, $(KrHKr)^+$, $(KrHXe)^+$, and Their Deuterated Species in Solid Hydrogen

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Table S1. Harmonic and anharmonic vibrational wavenumbers (cm^{-1}) of $(XeHXe)^+$, $(KrHKr)^+$, $(KrHXe)^+$, and their deuterated species (given in brackets) calculated with various methods.[a,b]

method		$(XeHXe)^+$			$(KrHKr)^+$			$(KrHXe)^+$		
		ν_1	ν_2	ν_3	ν_1	ν_2	ν_3	ν_1	ν_2	ν_3
R-CCSD(T)(full)	harm.	151 [151]	624 [442]	800 [567]	210 [210]	734 [521]	985 [699]	120 [119]	570 [405]	1384 [985]
	anharm.	132 [149]	615 [441]	726 [551]	203 [197]	737 [511]	919 [676]	122 [116]	574 [405]	1279 [916]
CCSD(T)(full)	harm.	151 [151]	622 [441]	822 [582]	210 [210]	733 [520]	999 [708]	122 [122]	572 [405]	1371 [975]
	anharm.	130 [149]	627 [439]	799 [568]	201 [199]	737 [515]	944 [687]	127 [122]	581 [405]	1259 [921]
MP2(full)	harm.	152 [152]	577 [409]	944 [669]	208 [208]	633 [499]	1010 [716]	129 [128]	536 [380]	1318 [937]
	anharm.	131 [145]	556 [401]	879 [644]	199 [201]	628 [445]	970 [696]	139 [125]	531 [376]	1155 [821]
B3LYP	harm.	140 [140]	542 [384]	976 [692]	194 [194]	601 [427]	1079 [765]	138 [137]	530 [376]	1217 [864]
	anharm.	120 [135]	540 [383]	934 [669]	188 [184]	598 [425]	1027 [742]	140 [125]	533 [378]	1130 [802]

[a]The ν_1, ν_2, and ν_3 modes correspond to the Rg–H–Rg' symmetric stretching, doubly-degenerated Rg–H–Rg' bending, and Rg–H–Rg' antisymmetric stretch modes, respectively. [b]with aug-cc-pVTZ-PP basis set.

Table S2. Binding energies and shifts in harmonic vibrational wavenumbers ($\Delta\nu$ in cm^{-1}) of linear and T-shaped $(RgHRg')^+$–Rg/Rg' complexes calculated with the CCSD(T)(full)/aug-cc-pVTZ-PP method.

	$\Delta\nu_1$	$\Delta\nu_2$[a]	$\Delta\nu_3$	binding energy[b]
	$(XeHXe)^+$–Xe complex			
Linear	−20.0	+11.4	+113.8	−12.5
T-shaped	−0.1	−19.8, +6.0	−11.6	−14.9
	$(KrHKr)^+$–Kr complex			
Linear	−6.6	+14.0	+29.6	−10.9
T-shaped	−0.3	−24.6, −1.1	−14.3	−13.3
	$(KrHXe)^+$–Xe complex			
Linear $(KrHXe)^+$–Xe	−20.0	−16.1	+241.2	−16.7
Linear Xe–$(KrHXe)^+$	+21.6	+47.9	−169.8	−10.1
T-shaped	−1.8	−30.2, −0.3	+21.8	−15.4
	$(KrHXe)^+$–Kr complex			
Linear $(KrHXe)^+$–Kr	−15.0	−12.3	+184.7	−12.9
Linear Kr–$(KrHXe)^+$	+16.8	+37.3	−123.5	−8.5
T-shaped	−1.6	−26.1, −0.6	+16.2	−13.0

[a]The degenerated ν_2 mode (bending) is split into two vibrations in the case of T-shaped complexes because of symmetry.

[b]Binding energies in kJ mol^{-1} are corrected for zero-point vibrational energy.

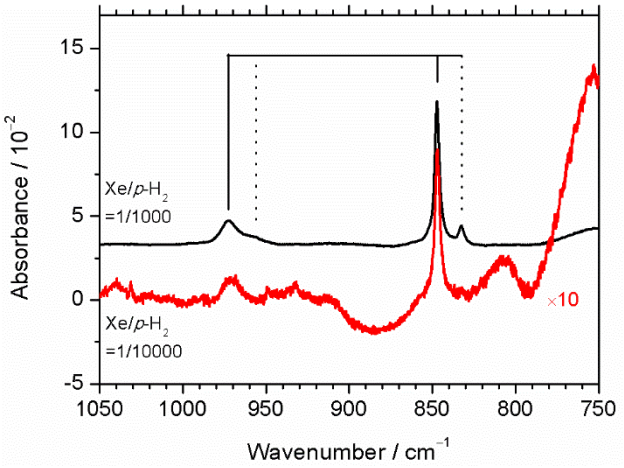

Figure S1. Partial IR spectra of electron-bombarded matrices with Xe/p-H_2 = 1/1000 (upper trace, black) and 1/10000 (lower trace, red). Spectra were measured right after deposition. Lines due to $(XeHXe)^+$ and $(XeHXe)^+$–Xe are indicated with solid and dotted lines, respectively.