Understanding and modulating high-energy property of noble-gas hydrides from their long-bonding: an NBO/NRT investigation on HNgCO⁺/CS⁺/OSi⁺ and HNgCN/NC (Ng = He, Ar, Kr, Xe, Rn) molecules

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### Table S1  CCSD(T) calculated values of the harmonic vibrational frequencies (in cm$^{-1}$) of HNgAB Molecules

<table>
<thead>
<tr>
<th>Molecules</th>
<th>H-Ng stretch</th>
<th>Ng-A stretch</th>
<th>A-B stretch</th>
<th>H-Ng-A bend</th>
<th>Ng-A-B bend</th>
</tr>
</thead>
<tbody>
<tr>
<td>HHeCO$^+$</td>
<td>336.5(3004.6)$^b$</td>
<td>318.2(423.4)$^b$</td>
<td>2216.1(2285.4)$^b$</td>
<td>357.3(439.7)$^b$</td>
<td>222.3(203.5)$^b$</td>
</tr>
<tr>
<td>HaCO$^+$</td>
<td>237.9(2535.5)$^b$</td>
<td>129.0(196.3)$^b$</td>
<td>2198.9(2267.4)$^b$</td>
<td>272.3(311.7)$^b$</td>
<td>140.1(138.7)$^b$</td>
</tr>
<tr>
<td>HkCO$^+$</td>
<td>2534.6(2400.5)$^b$</td>
<td>124.7(112.7)$^b$</td>
<td>2202.7(2268.8)$^b$</td>
<td>307.9(314.0)$^b$</td>
<td>143.8(130.3)$^b$</td>
</tr>
<tr>
<td>HxeCO$^+$</td>
<td>2314.2(2213.6)$^b$</td>
<td>120.1(172.4)$^b$</td>
<td>2202.9(2267.5)$^b$</td>
<td>306.4(294.1)$^b$</td>
<td>139.0(126.4)$^b$</td>
</tr>
<tr>
<td>Hrnc$^+$</td>
<td>2185.6</td>
<td>126.7</td>
<td>2207.4</td>
<td>320.3</td>
<td>143.9</td>
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<tr>
<td>HHeCl$^+$</td>
<td>3272.4(3398.9)$^b$</td>
<td>411.9(485.2)$^b$</td>
<td>1376.9(1336.0)$^b$</td>
<td>550.8(556.0)$^b$</td>
<td>178.4(190.8)$^b$</td>
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<tr>
<td>HaCl$^+$</td>
<td>2661.6(2638.5)$^b$</td>
<td>152.0(241.6)$^b$</td>
<td>1348.6(1323.4)$^b$</td>
<td>392.3(416.0)$^b$</td>
<td>123.1(139.6)$^b$</td>
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<td>HkCl$^+$</td>
<td>2459.6(2521.1)$^b$</td>
<td>141.6(239.8)$^b$</td>
<td>1357.0(1325.5)$^b$</td>
<td>439.6(432.9)$^b$</td>
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<tr>
<td>HxeCl$^+$</td>
<td>2239.7(2278.3)$^b$</td>
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<td>555.1</td>
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$^a$ From ref. 10. $^b$ From ref. 11. $^c$ From ref. 12.

### Table S2  Covalent limits $R_{coy}$ and vdW limits $R_{vdw}$ for H–Ng, Ng–A and H–A bonds of HNgAB Molecules

<table>
<thead>
<tr>
<th>Molecules</th>
<th>$R_{coy}$, H–Ng (Å)</th>
<th>$R_{coy}$, Ng–A (Å)</th>
<th>$R_{vdw}$, H–Ng (Å)</th>
<th>$R_{vdw}$, Ng–A (Å)</th>
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<td>0.78</td>
<td>1.21</td>
<td>1.07</td>
<td>2.88</td>
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<td>HaCO$^+$</td>
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Figure S1. Correlation plot for long-bond orders ($b_{H-A}$) – dissociation energies ($\Delta E_2$) of HNgNC species.

Figure S2. Correlation plot for long-bond orders ($b_{H-A}$) – dissociation energies ($\Delta E_2$) of HArAB species.
Figure S3. Correlation plot for long-bond orders ($b_{H-A}$) – dissociation energies ($\Delta E_2$) of HKrAB species.

Figure S4. Correlation plot for long-bond orders ($b_{H-A}$) – dissociation energies ($\Delta E_2$) of HXeAB species.
Figure S5. Correlation plot for long-bond orders ($b_{\text{H-A}}$) – dissociation energies ($\Delta E_2$) of HRnAB species.