Electronic Supplementary Information

Anomaly in Stability of Hydroxides of Icosagens (B and Al) and Its Noble Gas (Xe and Rn) Derivatives: A Comparative Study

Ayan Ghosh#,‡, Atri Mallick†,§, and Tapan K. Ghanty†,‡,*

#Laser and Plasma Technology Division, Beam Technology Development Group, Bhabha Atomic Research Centre, Mumbai 400 085, INDIA.
†Theoretical Chemistry Section, Chemistry Group, Bhabha Atomic Research Centre, Mumbai 400 085, INDIA.
‡Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, INDIA.
§Present address: School of Materials Science and Nanotechnology, Jadavpur University, 188 Raja S. C. Mallick Road, Kolkata 700 032, INDIA.
List of Tables

Table S1. Optimized Structural Parameters (Bond Length R in Å, and Bond Angle \( \theta \) in Degree) for the Minima and Transition State (TS) Geometries of HNgBO and HNgOAI (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets.

Table S2. Optimized Structural Parameters (Bond Length R in Å, and Bond Angle \( \theta \) in Degree) for the Minima Structures of HNgOB and HNgAlO (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets and CCSD(T) Method with AVTZ Basis Set.

Table S3. Energies (in kJ mol\(^{-1}\)) of the Various Dissociated Species Relative to the HNgBO and HNgOAI (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets.

Table S4. Energies (in kJ mol\(^{-1}\)) of the Various Dissociated Species Relative to the HNgOB and HNgAlO (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets and CCSD(T) Method with AVTZ Basis Set.

Table S5. MP2 and B3LYP Calculated Values of the Partial Mulliken Charges in HNgBO and HNgOAI (Ng = Xe and Rn) Molecules using DEF2 and AVTZ Basis Set.

Table S6. Harmonic Vibrational Frequencies (in cm\(^{-1}\)) Calculated using MP2 [B3LYP] Methods with DEF2 and AVTZ Basis Sets for HNgBO and HNgAlO (Ng = Xe and Rn) Molecules for the Minima and the Transition States (TS). Corresponding IR Intensity Values Calculated using B3LYP and MP2 Methods are given within the Parentheses (in km mol\(^{-1}\)).

Table S7. MP2 [B3LYP] Calculated Values of the Harmonic Vibrational Frequencies (in cm\(^{-1}\)) and Intrinsic Force Constants in Parentheses (in N m\(^{-1}\)) Corresponding to Individual Internal Coordinates for the Minima Structure of HNgBO and HNgOAI (Ng = Xe and Rn) Molecules, Calculated using DEF2 and AVTZ Basis Sets.
Table S1. Optimized Structural Parameters (Bond Length $R$ in Å, and Bond Angle $\theta$ in Degree) for the Minima and Transition State (TS) Geometries of $\text{HN}_{\text{g}}\text{BO}$ and $\text{HN}_{\text{g}}\text{OAl}$ ($\text{Ng} = \text{Xe}$ and $\text{Rn}$) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets.

<table>
<thead>
<tr>
<th>Geometrical Parameters</th>
<th>Methods</th>
<th>$\text{HXeBO}$</th>
<th>$\text{HRnBO}$</th>
<th>$\text{HXeOAl}$</th>
<th>$\text{HRnOAl}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Min</td>
<td>TS</td>
<td>Min</td>
<td>TS</td>
</tr>
<tr>
<td>$R(\text{H–Ng})$</td>
<td>MP2/DEF2</td>
<td>1.799</td>
<td>1.585</td>
<td>1.889</td>
<td>1.673</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>1.805</td>
<td>1.589</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>1.824</td>
<td>1.826</td>
<td>1.913</td>
<td>1.872</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>1.826</td>
<td>1.831</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$R(\text{Ng–B})/R(\text{Ng–O})$</td>
<td>MP2/DEF2</td>
<td>2.487</td>
<td>3.207</td>
<td>2.549</td>
<td>3.249</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>2.490</td>
<td>3.203</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>2.526</td>
<td>3.617</td>
<td>2.584</td>
<td>3.583</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>2.527</td>
<td>3.620</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$R(\text{B–O})/R(\text{O–Al})$</td>
<td>MP2/DEF2</td>
<td>1.223</td>
<td>1.236</td>
<td>1.223</td>
<td>1.236</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>1.224</td>
<td>1.238</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>1.208</td>
<td>1.214</td>
<td>1.208</td>
<td>1.215</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>1.209</td>
<td>1.215</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$\theta(\text{H–Ng–B})/\theta(\text{H–Ng–O})$</td>
<td>MP2/DEF2</td>
<td>180</td>
<td>98.7</td>
<td>180</td>
<td>92.3</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>180</td>
<td>98.7</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>180</td>
<td>86.2</td>
<td>180</td>
<td>82.5</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>180</td>
<td>86.4</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$\theta(\text{Ng–B–O})/\theta(\text{Ng–O–Al})$</td>
<td>MP2/DEF2</td>
<td>180</td>
<td>177.9</td>
<td>180</td>
<td>178.8</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>180</td>
<td>177.6</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>180</td>
<td>173.6</td>
<td>180</td>
<td>173.7</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>180</td>
<td>172.8</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

$^a$It is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.
Table S2. Optimized Structural Parameters (Bond Length R in Å, and Bond Angle θ in Degree) for the Minima Structures of HNgOB and HNgAlO (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets and CCSD(T) Method with AVTZ Basis Set.

<table>
<thead>
<tr>
<th>Geometrical Parameters</th>
<th>Methods</th>
<th>HXeOB</th>
<th>HRnOB</th>
<th>HXeAlO</th>
<th>HRnAlO</th>
</tr>
</thead>
<tbody>
<tr>
<td>R(H–Ng)</td>
<td>MP2/DEF2</td>
<td>1.637</td>
<td>1.738</td>
<td>1.917</td>
<td>1.969</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>1.642</td>
<td>...a</td>
<td>1.924</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>1.682</td>
<td>1.779</td>
<td>1.911</td>
<td>1.980</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>1.685</td>
<td>...a</td>
<td>1.913</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>1.656</td>
<td>1.758</td>
<td>...b</td>
<td>2.044</td>
</tr>
<tr>
<td>R(Ng–O)/R(Ng–Al)</td>
<td>MP2/DEF2</td>
<td>2.340</td>
<td>2.411</td>
<td>2.945</td>
<td>2.990</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>2.331</td>
<td>...a</td>
<td>2.951</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>2.354</td>
<td>2.407</td>
<td>2.998</td>
<td>3.041</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>2.349</td>
<td>...a</td>
<td>2.997</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>2.324</td>
<td>2.394</td>
<td>...b</td>
<td>3.066</td>
</tr>
<tr>
<td>R(O–B)/R(Al–O)</td>
<td>MP2/DEF2</td>
<td>1.273</td>
<td>1.272</td>
<td>1.633</td>
<td>1.632</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>1.276</td>
<td>...a</td>
<td>1.642</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>1.260</td>
<td>1.259</td>
<td>1.610</td>
<td>1.610</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>1.261</td>
<td>...a</td>
<td>1.618</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>1.275</td>
<td>1.273</td>
<td>...b</td>
<td>1.630</td>
</tr>
<tr>
<td>θ(H–Ng–O)/θ(H–Ng–Al)</td>
<td>MP2/DEF2</td>
<td>176.6</td>
<td>175.3</td>
<td>180.0</td>
<td>180.0</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>176.5</td>
<td>...a</td>
<td>180.0</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>177.3</td>
<td>176.7</td>
<td>180.0</td>
<td>180.0</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>177.3</td>
<td>...a</td>
<td>180.0</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>176.9</td>
<td>176.0</td>
<td>...b</td>
<td>180.0</td>
</tr>
<tr>
<td>θ(Ng–O–B)/θ(Ng–Al–O)</td>
<td>MP2/DEF2</td>
<td>121.3</td>
<td>114.2</td>
<td>180.0</td>
<td>180.0</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>121.1</td>
<td>...a</td>
<td>180.0</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>130.9</td>
<td>127.2</td>
<td>180.0</td>
<td>180.0</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>131.4</td>
<td>...a</td>
<td>180.0</td>
<td>...a</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>123.8</td>
<td>118.4</td>
<td>...b</td>
<td>180.0</td>
</tr>
</tbody>
</table>

*aIt is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.

*bIt is not possible to optimize the HXeAlO molecule using CCSD(T)/AVTZ level of theory.
Table S3. Energies (in kJ mol\(^{-1}\)) of the Various Dissociated Species Relative to the HNgBO and HNgOAl (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets.

<table>
<thead>
<tr>
<th>Molecular Species</th>
<th>Methods</th>
<th>HXeBO</th>
<th>HRnBO</th>
<th>HXeOAl</th>
<th>HRnOAl</th>
</tr>
</thead>
<tbody>
<tr>
<td>HNgBO/HNgOAl</td>
<td>All</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Ng + HBO/HOAl</td>
<td>MP2/DEF2</td>
<td>−457.5</td>
<td>−417.7</td>
<td>−411.7</td>
<td>−378.9</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−453.9</td>
<td>...(^{a})</td>
<td>−403.6</td>
<td>...(^{a})</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>−437.9</td>
<td>−401.1</td>
<td>−411.4</td>
<td>−378.9</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−437.4</td>
<td>...(^{a})</td>
<td>−408.4</td>
<td>...(^{a})</td>
</tr>
<tr>
<td>HNg + BO/OAl</td>
<td>MP2/DEF2</td>
<td>16.7</td>
<td>56.6</td>
<td>140.9</td>
<td>173.8</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>20.5</td>
<td>...(^{a})</td>
<td>151.9</td>
<td>...(^{a})</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>51.0</td>
<td>87.7</td>
<td>77.7</td>
<td>110.3</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>51.0</td>
<td>...(^{a})</td>
<td>76.3</td>
<td>...(^{a})</td>
</tr>
<tr>
<td>HNg(^{+}) + BO(^{-})/OAl(^{-})</td>
<td>MP2/DEF2</td>
<td>594.6</td>
<td>609.4</td>
<td>615.1</td>
<td>622.9</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>597.8</td>
<td>...(^{a})</td>
<td>624.8</td>
<td>...(^{a})</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>610.9</td>
<td>621.5</td>
<td>637.5</td>
<td>643.9</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>611.4</td>
<td>...(^{a})</td>
<td>641.7</td>
<td>...(^{a})</td>
</tr>
<tr>
<td>H + Ng + BO/OAl</td>
<td>MP2/DEF2</td>
<td>17.0</td>
<td>56.8</td>
<td>141.3</td>
<td>174.0</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>20.8</td>
<td>...(^{a})</td>
<td>152.2</td>
<td>...(^{a})</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>51.0</td>
<td>87.8</td>
<td>77.7</td>
<td>110.3</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>51.0</td>
<td>...(^{a})</td>
<td>76.2</td>
<td>...(^{a})</td>
</tr>
<tr>
<td>H(^{+}) + Ng + BO(^{-})/OAl(^{-})</td>
<td>MP2/DEF2</td>
<td>1102.1</td>
<td>1141.9</td>
<td>1122.6</td>
<td>1155.4</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>1102.5</td>
<td>...(^{a})</td>
<td>1129.5</td>
<td>...(^{a})</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>1120.6</td>
<td>1157.4</td>
<td>1147.2</td>
<td>1179.8</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>1120.0</td>
<td>...(^{a})</td>
<td>1150.2</td>
<td>...(^{a})</td>
</tr>
<tr>
<td><strong>Barrier Height(^{b})</strong></td>
<td>MP2/DEF2</td>
<td>208.1</td>
<td>222.5</td>
<td>164.0</td>
<td>174.0</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>209.0</td>
<td>...(^{a})</td>
<td>168.1</td>
<td>...(^{a})</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>200.6</td>
<td>211.9</td>
<td>172.9</td>
<td>182.8</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>200.6</td>
<td>...(^{a})</td>
<td>175.8</td>
<td>...(^{a})</td>
</tr>
</tbody>
</table>

\(^{a}\)It is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.

\(^{b}\)Barrier Height corresponding to TS (Transition State), (HNgBO → HBO + Ng; HNgOAl → HOAl + Ng).
Table S4. Energies (in kJ mol\(^{-1}\)) of the Various Dissociated Species Relative to the HNgOB and HNgAlO (Ng = Xe and Rn) Molecules, Calculated using MP2 and B3LYP Methods with DEF2 and AVTZ Basis Sets and CCSD(T) Method with AVTZ Basis Set.

<table>
<thead>
<tr>
<th>Molecular Species</th>
<th>Methods</th>
<th>HXeOB</th>
<th>HRnOB</th>
<th>HXeAlO</th>
<th>HRnAlO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>All</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>HNgOB/HNgAlO</td>
<td>MP2/DEF2</td>
<td>−337.3</td>
<td>−301.1</td>
<td>−369.2</td>
<td>−331.6</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−332.7</td>
<td>...(^a)</td>
<td>−364.2</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>−333.4</td>
<td>−298.2</td>
<td>−342.0</td>
<td>−307.5</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−332.1</td>
<td>...(^a)</td>
<td>−342.3</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>−339.3</td>
<td>−301.8</td>
<td>...(^b)</td>
<td>−308.4</td>
</tr>
<tr>
<td>Ng + HOB/HAIO</td>
<td>MP2/DEF2</td>
<td>−73.5</td>
<td>−37.2</td>
<td>35.2</td>
<td>72.8</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−66.9</td>
<td>...(^a)</td>
<td>42.0</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>−41.4</td>
<td>−6.2</td>
<td>−26.9</td>
<td>7.5</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−40.0</td>
<td>...(^a)</td>
<td>−32.0</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>−41.6</td>
<td>−4.2</td>
<td>...(^b)</td>
<td>11.0</td>
</tr>
<tr>
<td>HNg + OB/AlO</td>
<td>MP2/DEF2</td>
<td>504.5</td>
<td>515.7</td>
<td>509.3</td>
<td>522.0</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>510.4</td>
<td>...(^a)</td>
<td>514.9</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>518.5</td>
<td>527.5</td>
<td>532.8</td>
<td>541.2</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>520.4</td>
<td>...(^a)</td>
<td>533.5</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>515.5</td>
<td>526.6</td>
<td>...(^b)</td>
<td>531.2</td>
</tr>
<tr>
<td>H(^+) + Ng + OB/AlO(^-)</td>
<td>MP2/DEF2</td>
<td>−73.2</td>
<td>−36.9</td>
<td>35.5</td>
<td>73.1</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−66.6</td>
<td>...(^a)</td>
<td>42.3</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>−41.4</td>
<td>−6.2</td>
<td>−26.9</td>
<td>7.6</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−40.0</td>
<td>...(^a)</td>
<td>−32.0</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>−41.0</td>
<td>−3.6</td>
<td>...(^b)</td>
<td>11.6</td>
</tr>
<tr>
<td>H(^+) + Ng + OB(^-)/AlO(^-)</td>
<td>MP2/DEF2</td>
<td>1012.0</td>
<td>1048.2</td>
<td>1016.8</td>
<td>1054.5</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>1015.1</td>
<td>...(^a)</td>
<td>1019.6</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>1028.2</td>
<td>1063.4</td>
<td>1042.5</td>
<td>1077.1</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>1028.9</td>
<td>...(^a)</td>
<td>1042.0</td>
<td>...(^a)</td>
</tr>
<tr>
<td></td>
<td>CCSD(T)/AVTZ</td>
<td>1031.5</td>
<td>1068.9</td>
<td>...(^b)</td>
<td>1073.4</td>
</tr>
</tbody>
</table>

\(^a\)It is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.

\(^b\)It has not been possible to optimize the geometry of HXeAlO by employing CCSD(T) method with AVTZ basis set.
Table S5. MP2 and B3LYP Calculated Values of the Partial Mulliken Charges in HNgBO and HNgOAl (Ng = Xe and Rn) Molecules using DEF2 and AVTZ Basis Set.

<table>
<thead>
<tr>
<th>Charges</th>
<th>Methods</th>
<th>HXeBO</th>
<th>HRnBO</th>
<th>HXeOAl</th>
<th>HRnOAl</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Min</td>
<td>TS&lt;sup&gt;a&lt;/sup&gt;</td>
<td>Min</td>
<td>TS&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>q(H)</td>
<td>MP2/DEF2</td>
<td>−0.159</td>
<td>0.179</td>
<td>−0.206</td>
<td>0.138</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−0.223</td>
<td>0.008</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>−0.123</td>
<td>0.070</td>
<td>−0.177</td>
<td>0.036</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−0.179</td>
<td>−0.073</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>q(Ng)</td>
<td>MP2/DEF2</td>
<td>0.506</td>
<td>0.720</td>
<td>0.538</td>
<td>0.761</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>0.663</td>
<td>0.886</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>0.428</td>
<td>0.443</td>
<td>0.478</td>
<td>0.508</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>0.613</td>
<td>0.554</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>q(O)</td>
<td>MP2/DEF2</td>
<td>−0.345</td>
<td>−0.434</td>
<td>−0.399</td>
<td>−0.384</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−0.308</td>
<td>−0.423</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>−0.310</td>
<td>−0.315</td>
<td>−0.369</td>
<td>−0.300</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−0.420</td>
<td>−0.398</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>q(B)/q(Al)</td>
<td>MP2/DEF2</td>
<td>−0.002</td>
<td>−0.465</td>
<td>0.067</td>
<td>−0.515</td>
</tr>
<tr>
<td></td>
<td>MP2/AVTZ</td>
<td>−0.132</td>
<td>−0.471</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td></td>
<td>B3LYP/DEF2</td>
<td>0.005</td>
<td>−0.197</td>
<td>0.068</td>
<td>−0.244</td>
</tr>
<tr>
<td></td>
<td>B3LYP/AVTZ</td>
<td>−0.014</td>
<td>−0.084</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
<td>...&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup>Transition state

<sup>b</sup>It is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.
Table S6. Harmonic Vibrational Frequencies (in cm$^{-1}$) Calculated using MP2 [B3LYP] Methods with DEF2 and AVTZ Basis Sets for HNgBO and HNgOAl (Ng = Xe and Rn) Molecules for the Minima and the Transition States (TS). Corresponding IR Intensity Values Calculated using B3LYP and MP2 Methods are given within the Parentheses (in km mol$^{-1}$).

<table>
<thead>
<tr>
<th>Normal Modes</th>
<th>Basis Set</th>
<th>HXeBO</th>
<th>HRnBO</th>
<th>HXeOAl</th>
<th>HRnOAl</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Min</td>
<td>TS</td>
<td>Min</td>
<td>TS</td>
</tr>
<tr>
<td>H–Ng Stretch</td>
<td>DEF2</td>
<td>1510.3</td>
<td>1757.1</td>
<td>1536.2</td>
<td>1759.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1615.5)</td>
<td>(46.9)</td>
<td>(1393.9)</td>
<td>(57.2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[1468.4]</td>
<td>[1050.0]</td>
<td>[1478.4]</td>
<td>[1162.5]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3933.8)</td>
<td>(1153.7)</td>
<td>(3575.8)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>1496.3</td>
<td>1755.3</td>
<td>1510.3</td>
<td>1759.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1585.7)</td>
<td>(47.5)</td>
<td>(1393.9)</td>
<td>(57.2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[1470.5]</td>
<td>[1040.7]</td>
<td>[1478.4]</td>
<td>[1162.5]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(1291.7)</td>
<td>(4012.4)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ng–B/ Ng–O Stretch</td>
<td>DEF2</td>
<td>253.3</td>
<td>167.7</td>
<td>253.3</td>
<td>161.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(89.3)</td>
<td>(52.9)</td>
<td>(80.8)</td>
<td>(52.7)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[234.1]</td>
<td>[95.2]</td>
<td>[235.9]</td>
<td>[99.5]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(77.8)</td>
<td>(1.0)</td>
<td>(69.0)</td>
<td>(1.8)</td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>252.0</td>
<td>168.7</td>
<td>252.0</td>
<td>161.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(87.8)</td>
<td>(52.5)</td>
<td>(94.2)</td>
<td>(52.5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[234.6]</td>
<td>[94.2]</td>
<td>[94.2]</td>
<td>(1.5)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(77.8)</td>
<td>(1.5)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B–O/ O–Al Stretch</td>
<td>DEF2</td>
<td>1846.9</td>
<td>2390.5</td>
<td>1849.1</td>
<td>2247.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(22.7)</td>
<td>(151.1)</td>
<td>(30.5)</td>
<td>(131.7)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>[1912.6]</td>
<td>[1843.3]</td>
<td>[1914.6]</td>
<td>[1843.0]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(71.0)</td>
<td>(180.0)</td>
<td>(81.1)</td>
<td>(174.1)</td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>1843.6</td>
<td>2379.2</td>
<td>1843.6</td>
<td>2247.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(23.4)</td>
<td>(139.5)</td>
<td>(183.2)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>[1913.0]</td>
<td>[1843.4]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(70.4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>DEF2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---------------------------</td>
<td>-------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>H–Ng–B/</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H–Ng–O</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bend(^a)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>634.1 (0.6)</td>
<td></td>
<td>649.8 (6.6)</td>
<td></td>
<td>569.4 (2.2)</td>
</tr>
<tr>
<td></td>
<td>[598.6 (0.3)]</td>
<td></td>
<td>[504.0 (1.7)]</td>
<td></td>
<td>[536.2 (1.5)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>627.7 (35.1)</td>
<td></td>
<td>651.9 (14.0)</td>
<td></td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>[599.7 (34.6)]</td>
<td></td>
<td>[500.8 (25.0)]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>152.9 (5.8)</td>
<td></td>
<td>89.4 (9.5)</td>
<td></td>
<td>162.3 (7.1)</td>
</tr>
<tr>
<td></td>
<td>[154.0 (7.8)]</td>
<td></td>
<td>[64.1 (0.6)]</td>
<td></td>
<td>[161.1 (9.4)]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>148.6 (10.3)</td>
<td></td>
<td>88.9 (8.8)</td>
<td></td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>[152.9 (12.0)]</td>
<td></td>
<td>[58.4 (1.3)]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>84.2 (13.5)</td>
<td></td>
<td>83.7 (9.5)</td>
<td></td>
<td>...</td>
</tr>
<tr>
<td></td>
<td>[51.4 (0.0)]</td>
<td></td>
<td>[57.3 (0.003)]</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>81.6 (22.3)</td>
<td></td>
<td>...</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>[50.9 (0.01)]</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^a\)The modes are doubly degenerate for minima.

\(^b\)It is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.

\(^c\)There is no torsional modes of vibration for the minima structures.
Table S7. MP2 [B3LYP] Calculated Values of the Harmonic Vibrational Frequencies (in cm\(^{-1}\)) and Intrinsic Force Constants in Parentheses (in N m\(^{-1}\)) Corresponding to Individual Internal Coordinates for the Minima Structure of HNgBO and HNgOAl (Ng = Xe and Rn) Molecules, Calculated using DEF2 and AVTZ Basis Sets.

<table>
<thead>
<tr>
<th>Normal Modes</th>
<th>Basis Set</th>
<th>HXeBO</th>
<th>HRnBO</th>
<th>HXeOAl</th>
<th>HRnOAl</th>
</tr>
</thead>
<tbody>
<tr>
<td>H–Ng Stretch</td>
<td>DEF2</td>
<td>1510.5 (134.5)</td>
<td>1536.1 (139.5)</td>
<td>1940.5 (221.9)</td>
<td>1849.5 (202.2)</td>
</tr>
<tr>
<td></td>
<td>[1468.4] (127.0)</td>
<td>[1478.1] (129.1)</td>
<td>[1756.5] (181.8)</td>
<td>[1690.1] (168.8)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>1496.4 (131.9)</td>
<td>…</td>
<td>1922.0 (217.7)</td>
<td>…</td>
</tr>
<tr>
<td></td>
<td>[1470.5] (127.4)</td>
<td>...</td>
<td>[1753.2] (181.1)</td>
<td>...</td>
<td></td>
</tr>
<tr>
<td>Ng–B/Ng–O Stretch</td>
<td>DEF2</td>
<td>396.4 (94.0)</td>
<td>405.1 (101.4)</td>
<td>422.4 (149.9)</td>
<td>423.9 (158.0)</td>
</tr>
<tr>
<td></td>
<td>[371.3] (82.5)</td>
<td>[380.5] (89.5)</td>
<td>[384.8] (124.5)</td>
<td>[389.4] (133.3)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>393.6 (92.7)</td>
<td>…</td>
<td>438.0 (161.3)</td>
<td>…</td>
</tr>
<tr>
<td></td>
<td>[372.3] (83.0)</td>
<td>...</td>
<td>[396.0] (131.8)</td>
<td>...</td>
<td></td>
</tr>
<tr>
<td>B–O/O–Al Stretch</td>
<td>DEF2</td>
<td>1821.5 (1274.6)</td>
<td>1821.9 (1275.3)</td>
<td>836.7 (414.2)</td>
<td>842.0 (419.4)</td>
</tr>
<tr>
<td></td>
<td>[1890.8] (1373.5)</td>
<td>[1891.3] (1374.4)</td>
<td>[844.0] (421.5)</td>
<td>[850.0] (427.5)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>1818.5 (1270.6)</td>
<td>…</td>
<td>828.4 (406.0)</td>
<td>…</td>
</tr>
<tr>
<td></td>
<td>[1891.0] (1373.8)</td>
<td>...</td>
<td>[837.0] (414.5)</td>
<td>...</td>
<td></td>
</tr>
<tr>
<td>H–Ng–B/H–Ng–O Bend</td>
<td>DEF2</td>
<td>620.8 [585.2]</td>
<td>555.9 [522.6]</td>
<td>639.1 [602.1]</td>
<td>560.7 [526.0]</td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>614.1 [586.4]</td>
<td>…</td>
<td>634.2 [605.5]</td>
<td>…</td>
</tr>
<tr>
<td>Ng–B–O/Ng–O–Al Bend</td>
<td>DEF2</td>
<td>200.3 [198.8]</td>
<td>203.7 [201.0]</td>
<td>49.9 [74.5]</td>
<td>48.7 [75.6]</td>
</tr>
<tr>
<td></td>
<td>AVTZ</td>
<td>197.3 [197.9]</td>
<td>…</td>
<td>66.0 [62.3]</td>
<td>…</td>
</tr>
</tbody>
</table>

*a*It is not possible to optimize the Rn containing molecules through GAMESS software due to the presence of h function in the AVTZ basis set.