

## High kinetic stability of HXeBr upon interaction with carbon dioxide: HXeBr...CO<sub>2</sub> complex in a xenon matrix and HXeBr in a carbon dioxide matrix.

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### Streszczenie

We investigate the conditions when noble-gas hydrides can be found in real environments and report on the preparation and identification of the HXeBr...CO(2) complex in a xenon matrix and HXeBr in a carbon dioxide matrix. The H-Xe stretching mode of the HXeBr...CO(2) complex in a xenon matrix is observed at 1557 cm<sup>-1</sup>, showing a spectral shift of +53 cm<sup>-1</sup> from the HXeBr monomer. The calculations at the CCSD(T)/aug-cc-pVTZ-PP(Xe,Br) level of theory give two stable structures for the HXeBr...CO(2) complex with frequency shifts of +55 and +103 cm<sup>-1</sup>, respectively. On the basis of the calculations, the experimentally observed band is assigned to the more stable structure with a "parallel" geometry. The HXeBr molecule was prepared in a carbon dioxide matrix and has the H-Xe stretching frequency of 1646 cm<sup>-1</sup>, meaning a strong matrix shift and stabilization of the H-Xe bond. The deuterated species DXeBr in a carbon dioxide matrix absorbs at 1200 cm<sup>-1</sup>. This is the first case where a noble-gas hydride is prepared in a molecular solid. The thermal stabilities of HXeBr and HXeBr...CO(2) complex in a xenon matrix and HXeBr in a carbon dioxide matrix were examined. We have found a high thermal stability of HXeBr in carbon dioxide ice (at least up to 100 K), i.e., under conditions that may occur in nature.

### Adres publiczny

<http://dx.doi.org/10.1021/jp301704n>

### Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>

