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Ab initio investigations of the binary complexes Rg-IBr (Rg=He, Ne, Ar, Kr, Xe)

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Highlights

- *ab initio* intermolecular PESs of Rg-IBr are constructed.
- Characteristics of the PESs are identified.
- Intermolecular vibrational states are assigned.
- The occurred quantum tunneling effects are discussed.
- Transition frequencies and spectroscopic constants are predicted.

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