Title:	Does borazine–water behave like benzene-water? A matrix isolation infrared and ab initio study
Authors:	Mishra, Piyush (/jspui/browse?type=author&value=Mishra%2C+Piyush) Verma, Kanupriya (/jspui/browse?type=author&value=Verma%2C+Kanupriya) Bawari, D. (/jspui/browse?type=author&value=Bawari%2C+D.) Viswanathan, K.S. (/jspui/browse?type=author&value=Viswanathan%2C+K.S.)
Keywords:	Inorganic Benzene Isoelectronic
Issue Date:	2016
Publisher:	American Institute of Physics
Citation:	Journal of Chemical Physics,144(23).
Abstract:	Borazine is isoelectronic with benzene and is popularly referred to as inorganic benzene. The study of non-covalent interactions with borazine and comparison with its organic counterpart promises to show interesting similarities and differences. The motivation of the present study of the borazine-water interaction, for the first time, stems from such interesting possibilities. Hydrogen-bonded complexes of borazine and water were studied using matrix isolation infrared spectroscopy and quantum chemical calculations. Computations were performed at M06-2X and MP2 levels of theory using 6-311++G(d,p) and aug-cc-pVDZ basis sets. At both the levels of theory, the complex involving an N–H···O interaction, where the N–H of borazine serves as the proton donor to the oxygen of water was found to be the global minimum, in contrast to the benzene-water system, which showed an H–π interaction. The experimentally observed infrared spectra of the complexes corroborated well with our computations for the complex corresponding to the global minimum. In addition to the global minimum, our computations also located two local minima on the borazine-water potential energy surface. Of the two local minima, one corresponded to a structure where the water was the proton donor to the nitrogen of borazine, approaching the borazine ring from above the plane of the ring; a structure that resembled the global minimum in the benzene-water H–π complex. The second local minimum corresponded to an interaction of the oxygen of water with the boron of borazine, which can be termed as the boron bond. Clearly the borazine-water system presents a richer landscape than the benzene-water system.
URI:	https://aip.scitation.org/doi/10.1063/1.4953793 (https://aip.scitation.org/doi/10.1063/1.4953793) http://hdl.handle.net/123456789/2561 (http://hdl.handle.net/123456789/2561)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/2561/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/12345

Show full item record (/jspui/handle/123456789/2561?mode=full)

(/jspui/handle/123456789/2561/statistics)