



Library Indian Institute of Science Education and Research Mohali



DSpace@IISERMohali (/jspui/)

/ Publications of IISER Mohali (/jspui/handle/123456789/4)

/ Research Articles (/jspui/handle/123456789/9)

Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/2946>

Title: An ab initio quantum chemical investigation of the structure and stability of ozone-water complexes

Authors: Kumar, Pradeep (/jspui/browse?type=author&value=Kumar%2C+Pradeep)
Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)

Keywords: Ozone-water
Vertical excitation
MRCI
Atoms-in-molecules

Issue Date: 2013

Publisher: Elsevier

Citation: Chemical Physics, 415, pp.214-221.

Abstract: Ab initio quantum chemical calculations have been carried out to investigate the structure and stability of 1:1 and 1:2 ozone-water complexes. All the geometries have been optimized at the CCSD level of theory using aug-cc-pVDZ and aug-cc-pVTZ basis sets. The importance of correlation-consistent basis sets in deciding the nature of critical points on these complexes is emphasized. An analysis based on the dipole moment of the complexes and the charge distribution on atoms follows. The effect of ozone molecule on the structure and properties of water dimer is also investigated. Values of the vertical electronic excitation energy and the corresponding transition dipole moment have been calculated for the ozone-water complexes using the multi-reference-configuration-interaction method and the aug-cc-pVTZ basis set. The calculated shift in vibrational frequencies due to complex formation is compared with the earlier reported experimental and theoretical values.

URI: <https://www.sciencedirect.com/science/article/pii/S0301010413000293>
(<https://www.sciencedirect.com/science/article/pii/S0301010413000293>)
<http://hdl.handle.net/123456789/2946> (<http://hdl.handle.net/123456789/2946>)

Appears in Research Articles (/jspui/handle/123456789/9)
Collections:

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/2946/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/123456789/2946/1/Need%20to%20add%20pdf.odt)

Show full item record (/jspui/handle/123456789/2946?mode=full)

(/jspui/handle/123456789/2946/statistics)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.

