

Abstract Submitted  
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**Investigation of Bonding in the  $\text{BF}_3\text{-H}_2\text{O}$  Complex** ARCHANA DUBEY, H.P. SAHA, LEE CHOW, UCF Orlando, R.H. PINK, DIP N. MAHATO, M.B. HUANG, T.P. DAS<sup>1</sup>, SUNY Albany, R.H. SCHEICHER, MTU Houghton, MAHENDRA K. MAHANTI, NEHU, Shillong, India — The catalytic properties of  $\text{BF}_3$  involving its complexes with different classes of molecules is of great current interest. As a typical system of complexes involving the B-O bond we have studied the  $\text{BF}_3\text{-H}_2\text{O}$  system using first-principle Hartree-Fock-Roothaan procedure combined with many-body perturbation theory to include Van der Waals (VDW) interaction between  $\text{BF}_3$  and  $\text{H}_2\text{O}$  molecules. From our results, the VDW contribution to the binding energy of the  $\text{BF}_3\text{-H}_2\text{O}$  complex comes out as 34.5% of the covalency, close to the 36.4% result from our earlier investigations on  $\text{BF}_3\text{-NH}_3$ . The absolute values for the covalency and VDW contributions are both about 35% of the  $\text{BF}_3\text{-NH}_3$  result. Physical implications of these results will be discussed.

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