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

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