

A density functional theory study of the formation and spectroscopy of the formate (HCOO^-) and ammonium (NH_4^+) ions in interstellar ices

David E. Woon and Jin-Young Park

Molecular Research Institute, 2495 Old Middlefield Way, Mountain View, CA 94043, USA
email: woon@purisima.molres.org

Abstract. Following our recent success confirming the identification of OCN^- as the carrier for the XCN feature (Park & Woon 2004a, 2004b), we have explored the formation of the formate ion from formic acid (HCOOH) in an ice matrix using quantum chemical density functional theory (DFT) cluster calculations at the B3LYP/6-31+G** level. The formate ion is thought to account for interstellar infrared features at 1381 and 1349 cm^{-1} (Schutte et al. 1999). Both are broad features, indicating that they most likely arise from a species embedded in a condensed phase medium. We performed cluster calculations where up to 15 explicit water molecules were included. As in OCN^- , we considered both ammonia and water as potential proton acceptors for charge transfer. The vibrational mode coupling is very different in HCOOH , where there is a single CO carbonyl stretch, and HCOO^- , where there are two CO stretches that can couple symmetrically and asymmetrically. Our DFT calculations for this band are 1338 and 1343 cm^{-1} , respectively, for the cases where NH_4^+ and H_3O^+ are the counterion. The latter is quite close to the band at 1349 cm^{-1} that is observed both in the protostellar W33 source and in experiments. Other formate ion features and the bands of NH_4^+ will also be described.

The support of the NASA Exobiology program (NAG5-13482) is gratefully acknowledged.

Keywords. astrochemistry, molecular processes, ISM: molecules, ISM: lines and bands

References

- Schutte, W. A.; Boogert, A. C. A.; Tielens, A. G. G. M.; Whittet, D. C. B.; Gerakines, P. A.; Chiar, J. E.; Ehrenfreund, P.; Greenberg, J. M.; van Dishoeck, E. F. & de Graauw, T. 1999, *Astron. Astrophys.* 343, 966
Park, J.-Y. & Woon, D. E. 2004a, *Astrophys. J.* 601, L63
Park, J.-Y. & Woon, D. E. 2004b, *J. Phys. Chem. A* 108, 6589