Computational Molecular Spectroscopy:
Fe-containing Molecules of Astrochemical Interest

Tsuneo Hirano,[1] Umpei Nagashima,[2] and Per Jensen[3]
[1)] Ochanomizu University, Japan.
[2)] Foundation for Computational Science (FOCUS), Japan.
[3)] Bergische Universität, Germany

The aim of Astrochemistry is to elucidate how molecules have evolved in space, *i.e.*, to determine which molecules are there and which reactions have formed them. More than 180 molecules have been detected already. Although Fe is known to have a large cosmic abundance comparable to those of Mg and Si, the only iron-containing molecules detected in the cosmic environment so far are FeH in sunspots [1], FeO toward Sgr B2 [2,3], and FeCN toward IRC +10216 [4]. In 1994, we made a preliminary *ab initio* calculation for FeCO as a candidate for observation in interstellar space, but attempts to detect it in space failed [5,6]. Then we started *ab initio* calculations on several Fe-containing molecules of astrochemical interest, including FeC [7], FeN [8], FeS, FeNC [9], FeCN [10], FeOH [11,12], and FeCO [13 (electronic properties)]. We will report here recent progress of computational molecular spectroscopy on Fe-containing molecules.

For FeCO, we have published a very accurate 3D potential energy surface [14], and reported many ro-vibrational properties. The calculated rotational constant B_0 deviates by only 0.03% from experimental value. For FeCN, observed by the Ziurys group toward IRC +10216 [4], the electronic ground state was erroneously claimed to be $^4\Delta_i$ [4] simply because rotational spectrum for the other electronic states was not observed in their laboratory. Our MR-SDCI+Q calculations show that the $^4\Delta_i$ state is higher in energy than the $^6\Delta_i$ state by *ca.* 4000 cm^{-1}.

FeOH is another possible interstellar molecule candidate, but neither laboratory experiments nor space observations have been reported. Stimulated by IR cold-chemistry experiments on FeO^+ reactions by the Dieter Gerlich group [15], we have calculated the equilibrium structures and energy levels of FeO, FeO^+, and $FeOH^+$. Presently, 3D PES calculations for $FeOH^+$ are in progress.

We hope these studies will be helpful for identification of more Fe-containing molecules in space.

References.

[1] P.K. Caroll, P. McCormack, and S. O'Connor, *Astrophys. J.*, **208**, 903 (1976). [2] C.M. Walmsley, R. Bachiller, G. Pineau des Forêts, and P. Schilke, *Astrophys. J.*, **566**, L109 (2002). [3] R.S. Furuya, C.M. Walmsley, K. Nakanishi, P. Schilke, and R. Bachiller, *A & A*, **409**, L21 (2003). [4] L.A.Zack, D.T. Halfen, L.M. Ziurys, ApJ,Lett.,733,L36 (2011). [5] Y. Kasai and K. Obi, Y. Ohshima, Y. Endo, and K. Kawaguchi, *J. Chem. Phys*.,**103**,90 (1995). [6] E. Kagi, Y. Kasai, H. Ungerechts, and K. Kawaguchi, *Astrophys. J.*, **488**, 766 (1997). [7] S. S. Itono, T. Taketsugu, T. Hirano, and U. Nagashima, *J. Chem. Phys.*, **115**, 11213 (2001). [8] P.M. Scheridan, L.M. Ziurys, and T. Hirano, *Astrophys. J.*, **593**, L141 (2003). [9] T. Hirano, R. Okuda, U. Nagashima, V. Špirko, and P. Jensen, *J. Mol. Spectrosc*., **236**, 234 (2006). [10] T. Hirano, M. Amano, Y. Mitsui, S. S. Itono, R. Okuda, U. Nagashima, and P. Jensen, *J. Mol. Spectrosc*., **243**, 267 (2007). [11] T. Hirano, P.R. Bunker, S. Patchkovskii, U. Nagashima, and P. Jensen, *J. Mol. Spectrosc.*, **256**, 45 (2009). [12] T. Hirano, U. Nagashima, G. Winnewisser, and P. Jensen, *J. Chem. Phys*., **132**, 094303 (2010). [13] Hirano, V. Derpmann, U. Nagashima, and P. Jensen, J. Mol. Spectrosc. 263, 150 (2010). [14] T. Hirano and U. Nagashima, J. Mol. Spectrosc. 314, 35 (2015). [15] D. Gerlich *et al*., private communication (2016).