Computational Molecular Spectroscopy:
Fe-containing Molecules of Astrochemical Interest

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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.