THE ELECTRIC DIPOLE MOMENT OF IRIDIUM MONOSILICIDE, IrSi

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The optical spectrum of iridium monosilicide (IrSi) was recently observed using REMPI spectroscopy in the range 17200 to 23850 cm^{-1}[a]. The observation was supported by an *ab initio* calculation which predicted a $X^2\Delta_{5/2}$ state. Here, we report on the analysis of the optical Stark effect for the $X^2\Delta_{5/2}$ and [16.0]1.5 (v=6) states. The (6,0)[16.0]1.5 - $X^2\Delta_{5/2}$ and the (7,0)[16.0]3.5- $X^2\Delta_{5/2}$ bands of IrSi have been recorded using high-resolution laser-induced fluorescence spectroscopy. The observed optical Stark shifts for the ^{193}IrSi and ^{191}IrSi isotopologues were analyzed to produce the electric dipole moments of -0.4139(64)D and 0.7821(63)D for the $X^2\Delta_{5/2}$ and [16.0]1.5 (v=6) states, respectively. The negative sign of electric dipole moment of the $X^2\Delta_{5/2}$ state is supported by high-level quantum-chemical calculations employing all-electron scalar-relativistic CCSD(T) method augmented with spin-orbit corrections as well as corrections due to full triple excitations. In particular, electron-correlation effects have been shown to be essential in the prediction of the negative sign of the dipole moment. A comparison with other iridium containing molecules will be made.

[a]Maria A. Garcia, Carolin Vietz, Fernando Ruiprez, Michael D. Morse, and Ivan Infante, Kimika Fakultatea, Euskal Herriko. *J. Chem. Phys.*, (submitted)