1,3-Diketone Fluids and their Complexes with Iron

Michael Walter$^{1,2,*}$, Tobias Amann$^2$, Ke Li$^3$, Andreas Kailer$^2$, Jürgen Rühe$^3$, and Michael Moseler$^2$

$^1$Freiburg Materials Research Center, University of Freiburg, Stefan-Meier-Straße 21, 79104 Freiburg, Germany.
$^2$IWM - Fraunhofer Institute for Mechanics of Materials, Woehlerstr. 11, 79108 Freiburg, Germany.
$^3$Department of Microsystems Engineering, University of Freiburg, Georges-Köhler-Allee 103, D-79110 Freiburg, Germany.

*Corresponding author Michael.Walter@fmf.uni-freiburg.de

Tribological experiments with 1,3-diketone fluids in contact with iron surfaces show ultralow friction[1], which was suggested to be connected to the formation of iron complexes. In order to support this assumption, we calculate infrared and optical spectra of various substituted 1,3-diketones and their iron complexes using gradient corrected density functional theory (DFT). The description of the complexes requires the application of the DFT+U scheme for a correct prediction of the high spin state on the central iron atom. With this approach we obtain excellent agreement between experiment and simulation in infrared and optical spectra (see fig. 1), allowing for the determination of 1,3-diketone tautomeric forms [2]. The match in the spectra of the complex strongly supports the assumption of iron complex formation by these lubricants.

Fig. 1 Comparison of simulated and experimental UV-Vis spectra.

References