QM/MM calculation of formic acid in argon matrix

Teemu Järvinen\textsuperscript{a}, Przemysław Dopieralski\textsuperscript{b} and Jan Lundell\textsuperscript{a}

\textsuperscript{a}University of Jyväskylä, \textsuperscript{b}University of Wrocław

teemu.j.jarvinen@student.jyu.fi

We present results of QM/MM calculation of formic acid in argon matrix. Including site structure for both conformers, trans and cis, and present IR-spectrum and compare it to experimental spectrum \cite{1}. We also discuss how different argon-formic acid potentials affect the results and present a program that allows easy calculations of custom potentials.

\begin{center}
\textbf{Figure 1: Formic acid in argon matrix.}
\end{center}

\textbf{References}