

QM/MM calculation of formic acid in argon matrix

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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 [1]. We also discuss how different argon-formic acid potentials affect the results and present a program that allows easy calculations of custom potentials.

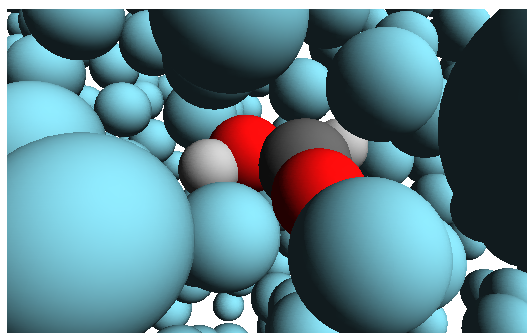


Figure 1: Formic acid in argon matrix.

References

1. M. Pettersson and J.Lundell, L. Khriachtchev, M. Räsänen, *J. Am. Chem. Soc.* **119** (1997), 11715.