

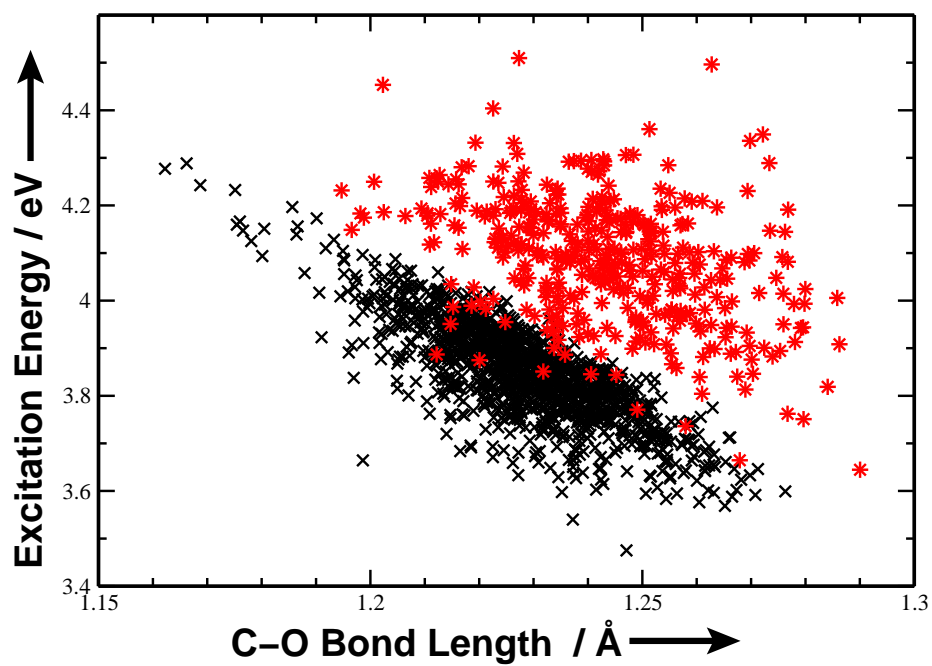
© 2003 WILEY-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim (Germany)

Supporting Information for *ChemPhysChem* F650

QM/MM Car-Parrinello Molecular Dynamics Study of the Solvent Effects on
the Ground State and on the First Excited Singlet State of Acetone in Water

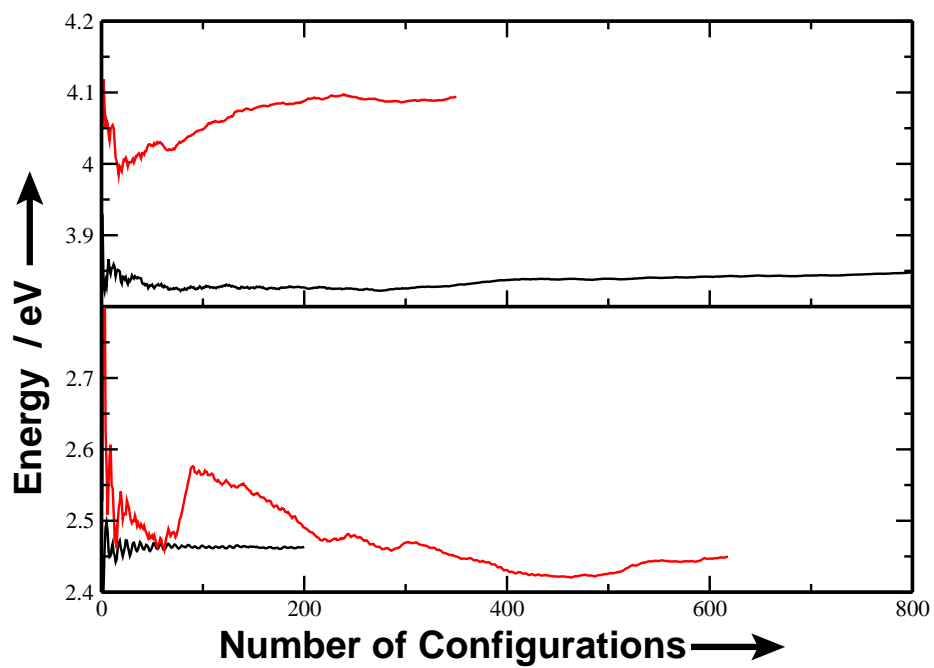
Ute F. Röhrig, Irmgard Frank, Jürg Hutter, Alessandro Laio, Joost VandeVondele, and Ursula
Röthlisberger

Supporting Information



Correlation between the C-O bond length and the ROKS excitation energy in the gas phase (crosses) and in solution (stars).

Supporting Information



Running averages. Upper panel: ROKS excitation energy in gas phase (red) and in water (black). Lower panel: ROKS fluorescence energy in gas phase (black) and in water (red).