

Publications

- (I) **Tunneling splittings. A classical trajectory approach**
K. Giese, H. Ushiyama, and O. Kühn
Chem. Phys. Lett. 371, pp. 681-687 (2003)
- (II) **Semiclassical tunneling splittings from short time dynamics: Herman-Kluk-propagation and harmonic inversion.**
K. Giese and O. Kühn
J. Chem. Phys. 120, pp. 4107-4118 (2004)
- (III) **On the Multidimensionality of Intramolecular Hydrogen Bond Dynamics: Hydrogen Transfer and IVR in 3,7-Dichlorotropolone**
K. Giese, D. Lahav, and O. Kühn
J. Theor. Comp. Chem. 3, pp. 567-597 (2004)
- (IV) **Dynamical hydrogen atom tunneling in dichlorotropolone: a combined quantum, semiclassical, and classical study.**
K. Giese, H. Ushiyama, K. Takatsuka, and O. Kühn
J. Chem. Phys. 122, 124307, pp. 1-14 (2005)
- (V) **The all-Cartesian reaction plane Hamiltonian: Formulation and application to the H-atom transfer in tropolone**
K. Giese and O. Kühn
J. Chem. Phys. 123, 54315, pp. 1-14 (2005)
- (VI) **Multidimensional Quantum Dynamics and Infrared Spectroscopy of Hydrogen Bonds**
O. Kühn and K. Giese
Phys. Rep. (invited review); in preparation