

**High-resolution FTIR spectroscopy of trisulfane HSSH: a candidate for detecting parity violation in chiral molecules**I. Bolotova<sup>1</sup>, S. Albert<sup>1</sup>, Z. Chen<sup>2</sup>, C. Fabri<sup>2</sup>, M. Quack<sup>2\*</sup>, G. Seyfang<sup>2</sup>, D. Zindel<sup>2</sup><sup>1</sup>ETH Zurich, <sup>2</sup>Physical Chemistry, ETH Zurich, Vladimir-Prelog-weg 2, 8093 Zurich, Switzerland

According to traditional quantum chemistry involving only the electromagnetic force the ground state energies of the enantiomers of chiral molecules as well as the energies of equivalent excited quantum states are exactly identical by symmetry. When the parity violating weak "nuclear" force causing beta-decay is included in the "electroweak quantum chemistry", one predicts an energy difference  $\Delta_{\text{pv}}E_0$  between the ground states of enantiomers and a corresponding reaction enthalpy  $\Delta_{\text{pv}}H_0^\ominus$  for the stereomutation reaction converting *P* and *M* enantiomers in the case of axially chiral molecules, [1, 2]:

$$P = M \quad \Delta_{\text{pv}}H_0^\ominus = E_0(M) - E_0(P) = N_A \Delta_{\text{pv}}E_0 \quad (1)$$

We report the first successful high-resolution analyses of the Fourier transform infrared (FTIR) spectrum of trisulfane. A band centered at 861.0292 cm<sup>-1</sup> can be assigned unambiguously to the chiral *trans* conformer by means of ground state combination differences in comparison with known rotational spectra. A second band near 864.698 cm<sup>-1</sup> is tentatively assigned to the *cis* conformer by comparison with theory. The results are discussed in relation to their importance for experimental attempts to measure the parity violating energy difference  $\Delta_{\text{pv}}E$  between the ground states of enantiomers of chiral molecules, [3, 4].

[1] M. Quack *Fundamental Symmetries and Symmetry Violations from High-Resolution Spectroscopy*, Vol. 1, pp. 659-722 in *Handbook of High Resolution Spectroscopy*, M. Quack and F. Merkt eds., Wiley Chichester **2011**.

[2] C. Fabri, L. Horny, M. Quack, *ChemPhysChem*, **2015**, 16, 3584.

[3] P. Dietiker, E. Miloglyadov, M. Quack, A. Schneider, and G. Seyfang, *Journal of Chemical Physics* **2015** 143, 244305.

[4] S. Albert, I. Bolotova, Z. Chen, C. Fabri, M. Quack, G. Seyfang, D. Zindel, *Physical Chemistry Chemical Physics* **2017**, 19, 11738.