**University of
Zurich**^{UZH}

**Zurich Open Repository and
Archive**

University of Zurich
University Library
Strickhofstrasse 39
CH-8057 Zurich
www.zora.uzh.ch

Year: 2012

Erratum: “Azide–water intermolecular coupling measured by two-color two-dimensional infrared spectroscopy” [J. Chem. Phys. 136, 224503 (2012)]

Borek, Joanna ; Perakis, Fivos ; Kläsi, Felix ; Garrett-Roe, Sean ; Hamm, Peter

DOI: <https://doi.org/10.1063/1.4739535>

Posted at the Zurich Open Repository and Archive, University of Zurich

ZORA URL: <https://doi.org/10.5167/uzh-73360>

Journal Article

Accepted Version

Originally published at:

Borek, Joanna; Perakis, Fivos; Kläsi, Felix; Garrett-Roe, Sean; Hamm, Peter (2012). Erratum: “Azide–water intermolecular coupling measured by two-color two-dimensional infrared spectroscopy” [J. Chem. Phys. 136, 224503 (2012)]. Journal of Chemical Physics, 137(6):069902.

DOI: <https://doi.org/10.1063/1.4739535>

Erratum: Azide–water intermolecular coupling measured by two–color two-dimensional infrared spectroscopy

Joanna Borek¹, Fivos Perakis¹, Felix Kläsi¹, Sean Garrett-Roe², Peter Hamm¹

¹*Physikalisch-Chemisches Institut, Universität Zürich,
Winterthurerstrasse 190, CH-8057 Zürich, Switzerland and*

²*Department of Chemistry, University of Pittsburgh,
Chevron Science Center, 219 Parkman Avenue, Pittsburgh, PA 15260**

(Dated: July 20, 2012)

*Electronic address: phamm@pci.uzh.ch

After publication of Ref. [1], it has been brought to our attention that Hochstrasser and coworkers have studied essentially the same molecular system (i.e., N_3^- in H_2O instead of D_2O) by two-color 2D IR spectroscopy before us [2]. A cross peak is also observed, which less likely is due to population transfer because of the even larger energy gap from the N_3^- asymmetric stretch vibration to the H_2O band. We had based our conclusion, that population transfer is the dominant coupling mechanism, mostly on the large frequency separation of the 0-1 and the 1-2 transition in the 2D IR spectra, which reflects the large anharmonicity of the OD vibrator itself [1]. The 1-2 transition is not shown in Ref. [2], so we cannot decide whether an alternative coupling mechanism might be responsible for the cross-peak between N_3^- in H_2O . Nonetheless, Ref. [2] found a tilt in the cross-peak, evidencing a correlation in the vibrational frequencies the of N_3^- and the H_2O vibrations, which is another consequence of the coupling to azide-bound water.

-
- [1] J. Borek, F. Perakis, F. Kläsi, S. Garrett-Roe, and P. Hamm, J. Chem. Phys. **136**, 224503 (2012).
- [2] C.-H. Kuo, D. Y. Vorobyev, J. Chen, and R. M. Hochstrasser, J. Phys. Chem. B **111**, 14028 (2007).