





www.HidenAnalytical.com



Mass Spectrometers for
Real time Gas Analysis



■ Knowledge,
■ Experience,
■ Expertise

[Click Here](#)



[Home](#) > [The Journal of Chemical Physics](#) > [Volume 138, Issue 6](#) > [10.1063/1.4775589](https://doi.org/10.1063/1.4775589)



< PREV

NEXT >

 No Access

Submitted: 25 February 2012

Accepted: 23 December 2012

Published Online: 11 February 2013

Different structures give similar vibrational spectra: The case of OH⁻ in aqueous solution

J. Chem. Phys. **138**, 064503 (2013); <https://doi.org/10.1063/1.4775589>

Pavlin D. Mitev^{1,2}, Philippe A. Bopp³, Jasmina Petreska⁴, Kaline Coutinho⁵, Hans Ågren², Ljupco Pejov^{4, a)}, and Kersti Hermansson^{1,2, a)}

[View Affiliations](#)[View Contributors](#) PDF

We have calculated the anharmonic OH⁻(aq) vibrational spectrum in aqueous solution with a “classical Monte Carlo simulation + QM/MM + vibrational” sequential approach. A new interaction model was used in the Monte Carlo simulations: a modified version of the charged-ring hydroxide-water model from the literature. This spectrum is compared with experiment and with a spectrum based on CPMD-generated structures, and the hydration structures and H-bonding for the two models are compared. We find that: (i) the solvent-induced frequency shift as well as the absolute OH⁻ frequency are in good agreement with experiment using the two models; (ii) the Raman and IR bands are very similar, in agreement with experiment; (iii) the hydration structure and H-bonding around the ion are very different with the two ion-water interaction models (charged-ring and CPMD); (iv) a cancellation effect between different regions of the hydration shell makes the total spectra similar for the two interaction models, although their hydration structures are different; (v) the net OH⁻ frequency shift is a blueshift of about +80 cm⁻¹ with respect to frequency of the gas-phase ion.

ACKNOWLEDGMENTS

The authors acknowledge the support of The Swedish Research Council (VR). Lj.P. acknowledges the financial support of the Swedish Institute (post-doctoral research grant). P.A.B. thanks the Wenner-Gren foundation (Sweden) for a grant and the Ångström Laboratory for its hospitality. Computer time was provided by the Uppsala Multidisciplinary Center for Advanced Computational Science (UPPMAX) at Uppsala University and the Swedish National Infrastructure for Computing (SNIC). This work was performed within the framework of the MATTER Consortium (supported



programme (a strategic research program in e-science supported by the Swedish Government).

SELECT YOUR ACCESS

INDIVIDUAL ACCESS

If you have an individual subscription, a subscription provided by one of AIP's Member Societies, have claimed access to a Conference Proceeding, or have made an individual purchase, sign in below.

Username:

Password

Remember me

LOG IN

[Forgot password?](#)

INSTITUTIONAL ACCESS



Access through
USP - Universidade de Sao Paulo

Access via the **USP - Universidade de Sao Paulo** is not supported.
Please [choose one of the other](#) institutional login options

PURCHASE

Standard PPV for \$35.00

ADD TO CART



PDF

Pdf document note icon in... Download	File upload line... Download	Set of isolate... Down
---	--	----------------------------------

Resources

AUTHOR

LIBRARIAN

ADVERTISER

General Information

ABOUT

CONTACT

HELP

PRIVACY POLICY

TERMS OF USE

FOLLOW AIP PUBLISHING:



specified within the article.

