Electronic Supplementary Material (ESI) for Dalton Transactions

On the Structure and Dynamics of the Asymmetrically Hydrated Sulfite Ion in Aqueous Solution – An ab initio QMCF MD Simulation and Large Angle X-ray Scattering Study

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Supporting Material

Complete reference 16

(16) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 03, Revision E.01*.

Table S1. Summary of solid state structures containing individual sulfite ions where the counter ion is monovalent or has a complete hydration shell.

ICSD code	*d*(S-O)	Reference
4432	1.505 Å	Larsson, L. O.; Kierkegaard, P. *Acta Chem. Scand.* **1969**, *23*, 2253-2260; *Powder Diffraction* **1986**, *1*, 265-275. Na_2SO_3.
1626	1.508 Å	Oddon, Y.; Pepe, G.; Tranquard, A. *J. Chem. Res. S* **1977**, *1977*, 138-139. $NaTl_3(SO_3)_2$.
60762	1.515 Å	Andersen, L.;Strömberg, D. *Acta Chem. Scand., Ser. A* **1986**, *40*, 479-480. K_2SO_3
23824	1.524 Å	Battelle, L. F.; Trueblood, K. N. *Acta Crystallogr.* **1965**, *19*, 531-535. $(NH_4)_2SO_3 \cdot H_2O$

Mean 1.513 Å/4

ICSD code	*d*(S-O)	*d*(S···H)	Reference
48112	1.528 Å	2.800 Å	Andersen, L.; Lindqvist, O. *Acta Crystallogr., Sect. B* **1984**, *40*, 584-586. $[Mg(H_2O)_6]SO_3$.
26149	1.532 Å	2.789 Å	Baggio, S.; Becka, L. N. *Acta Crystallogr., Sect. B* **1969**, *25*, 1150-1155. . $[Ni(H_2O)_6]SO_3$.
62636	1.533 Å	2.782 Å	Bats, J. W.; Fuess, H.; Elerman, Y. *Acta Crystallogr., Sect. B* **1986**, *42*, 552-557. $[Mg(H_2O)_6]SO_3$.
2524	1.536 Å		Flack, H. D. *Acta Crystallogr., Sect. B* **1973**, *29*, 656-658. $[Mg(H_2O)_6]SO_3$.
62637	1.536 Å		Bats, J. W.; Fuess, H.; Elerman, Y. *Acta Crystallogr., Sect. B* **1986**, *42*, 552-557. $[Mg(H_2O)_6]SO_3$.
62638	1.536 Å		Bats, J. W.; Fuess, H.; Elerman, Y. *Acta Crystallogr., Sect. B* **1986**, *42*, 552-557. $[Mg(H_2O)_6]SO_3$.

Mean 1.534 Å/6

Table S2. Numeric values of the peaks in Figure 2.

Figure 2a

Center	**FWHM**
1.0	0.058
1.5	0.074
1.9	0.427
2.8	0.324
3.1	0.346
3.7	0.823
4.3	2.011

Figure 2b

Center	**FWHM**
2.792	0.372
2.994	0.620
4.196	1.435

Figure 2c

Center	**FWHM**
0.975	0.058
1.921	0.418

Figure 2d

Center	**FWHM**
1.526	0.075
3.725	0.530
4.114	0.370

Figure 2e

Center	**FWHM**
2.827	0.330
4.368	2.047