Structure and water exchange of the hydrated thiosulfate ion in aqueous solution using QMCF MD simulation and large angle X-ray scattering

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Electronic supplementary information

Table S1. Comparison of structural parameters obtained for minimum structures of $[S_2O_3.H_2O]^{2-}$ at HF, MP2 and CCSD level (see also figure S1, left structure). S-O distance r_{SO} of the coordinated oxygen and the two non-coordinated oxygen atoms (average value), S-S distance r_{SS} and acceptor-hydrogen distance of the H-Bond r_{O-H} in Å. Hydrogen bond angle α_{O-HO} in degree.

	r_{SO}	r_{SS}	r_{O-H}	α_{O-HO}
HF	1.473/1.463	2.017	1.830	176.90
CCSD	1.508/1.492	2.023	1.733	176.98
MP2	1.514/1.495	2.019	1.702	176.68

Table S2. Summary of S-O and S_C-S_T bond distances in solid state structures containing individual thiosulfate ions where the counter ion is monovalent, has a complete hydration shell or is an organic cation not forming specific interactions with the thiosulfate ion. The ICSD and CSD codes refer to the Inorganic Crystal Structure Database and Cambridge Structure Database, respectively.

Compounds with a fully hydrated metal ion

ICSD/ CSD code	***d*(S-O)+*d*(S_C-S_T)**	**Reference and formula of compound**
2428	1.458 + 2.016 Å	Elerman, Y.; Uraz, A. A.; Armagan, N. *Acta Crystallogr., Sect. B* **1978**, *34*, 3330-3332. $[Ni(H_2O)_6]S_2O_3$.
24841	1.465 + 2.011 Å	Elerman, Y.; Fuess, H.; Joswig, W. *Acta Crystallogr., Sect. B* **1982**, *38*, 1799-1801. $[Mg(H_2O)_6]S_2O_3$.
24842	1.466 + 2.047 Å	Elerman, Y.; Fuess, H.; Joswig, W. *Acta Crystallogr., Sect. B* **1982**, *38*, 1799-1801. $[Mg(H_2O)_6]S_2O_3$.
59268	1.467 + 1.982 Å	Sobolev, A. N.; Figgis, B. N. *Acta Crystallogr., Sect. C* **1997**, *53*, 661-663. $[Co(NH_3)_6](S_2O_3)Cl{\cdot}H_2O$.
35664	1.470 + 2.019 Å	Elerman, Y.; Bats, J. W.; Fuess, H. *Acta Crystallogr., Sect. B* **1983**, *39*, 515-518. $[Mg(H_2O)_6]S_2O_3$.
8126	1.471 + 1.979 Å	Teng, S. T.; Fuess, H.; Bats, J. W. *Acta Crystallogr., Sect. B* **1979**, *35*, 1682-1684. $(NH_4)_2S_2O_3$.
16035	1.471 + 2.012 Å	Baggio, S.; Amzel, L.; Becka, L. N. *Acta Crystallogr., Sect. B* **1969**, *25*, 1650-1653. $[Mg(H_2O)_6]S_2O_3$.
34705		
DMSOST	1.475 + 2.001 Å	Jansen, M.; Wiench, D. M. *Cryst. Struct. Commun.* **1978**, *7*, 423. $Na_2S_2O_3{\cdot}(CH_3)_2SO$.
35665	1.476 + 2.018 Å	Elerman, Y.; Bats, J. W.; Fuess, H. *Acta Crystallogr., Sect. B* **1983**, *39*, 515-518. $[Mg(H_2O)_6]S_2O_3$.
23881	1.482 + 2.020 Å	Nardelli, M.; Fava, G.; Giraldi, G. *Acta Crystallogr.* **1962**, *15*, 227-231. $[Mg(H_2O)_6]S_2O_3$.

Mean 1.470 + 2.011 Å/10 structures

Compounds with monovalent metal ion not forming specific interactions with thiosulfate

9054 1.456 + 1.941 Å Padmanabhan, V. M.; Yadava, V. S.; Navarro, Q. O.; Garcia, A.; Karsono, L.; Suh, I.-H.; Chien, L. S. *Acta Crystallogr., Sect. B* **1971**, *27*, 253-257. $Na_2S_2O_3 \cdot 5H_2O$.

4436 1.456 + 1.996 Å Csordas, L. *Acta Chim. Acad. Sci. Hung.* **1969**, *62*, 371-393. $K_2S_2O_3 \cdot 0.33H_2O$.

37093 1.466 + 2.001 Å von Benda, H.; von Benda, K. *Z. Naturforsch., Teil B* **1979**, *34*, 957-968. $Na_2S_2O_3$.

2226 1.466 + 2.025 Å Lisensky, G. C.; Levy, H. A. *Acta Crystallogr., Sect. B* **1978**, *34*, 1975-1977. $Na_2S_2O_3 \cdot 5H_2O$.

279595 1.466 + 2.016 Å Prasad, S. M.; Rani, A. *Acta Crystallogr., Sect. E* **2001**, *57*, 67-69. $Na_2S_2O_3 \cdot 5H_2O$.

15476 1.467 + 2.018 Å Sandor, E.; Csordas, L. *Acta Crystallogr.* **1961**, *14*, 237-243. $Na_2S_2O_3$.

936 1.468 + 2.016 Å Uraz, A. A.; Armagan, N. *Acta Crystallogr., Sect. B* **1977**, *33*, 1396-1399. $Na_2S_2O_3 \cdot 5H_2O$.

59815 1.468 + 2.008 Å Held, P.; Bohaty, L. *Acta Crystallogr., Sect. C* **2004**, *60*, i97-i100. $CaS_2O_3 \cdot 6H_2O$.

37094 1.472 + 1.999 Å von Benda, H.; von Benda, K. *Z. Naturforsch., Teil B* **1979**, *34*, 957-968. $Na_2S_2O_3$.

72924 1.472 + 1.996 Å Hesse, W.; Leutner, B.; Boehn, K. H.; Walker, N. P. C. *Acta Crystallogr., Sect. C* **1993**, *49*, 363-365. $Na_2S_2O_3 \cdot 0.667H_2O$.

60026 1.475 + 2.005 Å Teng, S. T.; Fuess, H.; Bats, J.W. *Acta Crystallogr., Sect. C* **1984**, *40*, 1785-1787. $Na_2S_2O_3$.

60022 1.476 + 2.006 Å Teng, S. T.; Fuess, H.; Bats, J.W. *Acta Crystallogr., Sect. C* **1984**, *40*, 1785-1787. $Na_2S_2O_3$.

Mean 1.467 + 2.002 Å/12 structures

Compounds with solvated metal ions

KOLXOY 1.446 + 1.969 Å Freire, E.; Baggio, S.; Mombru, A.; Baggio, R. *Acta Crystallogr., Sect. C* **2000**, *56*, 541. $[Ni(C_{10}H_8N_2)_3](S_2O_3) \cdot 7H_2O$.

LICCIK 1.460 + 1.982 Å de Vivar, M. E. D.; Baggio, S.; Garland, M. T.; Baggio, R. *Acta Crystallogr., Sect. C* **2007**, *63*, m153. $[Ni(C_{10}H_8N_2)(H_2O)_4]_n(S_2O_3)_n \cdot 7H_2O$.

ROKHII 1.460 + 1.982 Å Baggio, S.; Pardo, M. I.; Baggio, R.; Garland, M. T. *Acta Crystallogr., Sect. C* **1997**, *53*, 1570. $[Zn(C_{10}H_8N_2)(H_2O)_4]_n(S_2O_3)_n \cdot 7H_2O$.

GINDUC 1.461 + 2.008 Å Leyten, W.; Rettig, S. J.; Trotter, J. *Acta Crystallogr., Sect. C* **1988**, *44*, 1749. $(C_2H_5)_4N)_2(S_2O_3) \cdot 2H_2O$.

PUMTUM 1.465 + 1.987 Å Tong Jiang; Lough, A.; Ozin, G. A.; Bedard, R. L. *J. Mater. Chem.* **1998,** *8*, 733. $(C_{10}H_{18}N)_2S_2O_3$.

PADBEC 1.475 + 2.004 Å Nelson, J.; Nieuwenhuyzen, M.; Pal, I.; Town, R. M. *Dalton Trans.* **2004**, 2003. $(C_{30}H_{54}N_8O_3)(S_2O_3)(ClO_4)_4 \cdot 8H_2O$.

QIXPIW 1.476 + 1.994 Å Maubert, B. M.; Nelson, J.; McKee, V.; Town, R. T.; Pal, I. *J. Chem. Soc., Dalton Trans.* **2001**, 1395. $(C_{36}H_{60}N_8O_3)(S_2O_3)(ClO_4)_4 \cdot 11H_2O$.

IZAVAG 1.480 + 1.989 Å Diaz de Vivar, M. E.; Baggio, S.; Ibanez, A.; Baggio, R. *Acta Crystallogr., Sect. C* **2004**, *60*, m451. $[ZnC_8H_{24}N_2(H_2O)_4]S_2O_3$.

Mean 1.465 + 1.989 Å/8 structures

Total mean 1.467 + 2.002 Å/30 structures

Table S3. Summary of bond distances of the oxo sulfur anions dithionite, $S_2O_4^{2-}$, disulfite, $S_2O_5^{2-}$, dithionate, $S_2O_6^{2-}$, disulfate, $S_2O_7^{2-}$, and peroxodisulfate, $S_2O_8^{2-}$, in the solid state where the anion is not bound to any counter ion with the charge of +2 or higher or to silver(I) or thallium(I) ions; for the dithionite ion are all structures included due to limited reported structures . The list is based on the data collected from the Inorganic Crystal Structure Database (ICSD) and the Cambridge Structural Database (CSD); references marked in red text are omitted from the mean bond distance and angle.

Dithionite ion, $S_2O_4^{2-}$

ICSD/CSD	***d*(S-O) + *d*(S-S)**	**Reference**
SESBEY	1.458 + 2.297 Å	Nakai, H.; Miyano, Y.; Hayashi, Y.; Isobe, K. *Mol. Cryst. Liq. Cryst. Sci. Technol., Sect. A* **2006**, *456*, 63. $[Rh_2(S_2O_4)(C_{16}H_{19})_2]\cdot 0.5CH_2Cl_2\cdot C_7H_8$.
SESBEY01	1.461 + 2.297 Å	Nakai, H.; Miyano, Y.; Hayashi, Y.; Isobe, K. *J. Organometal. Chem.* **2007**, *692*, 122. $[Rh_2(S_2O_4)(C_{16}H_{19})_2]\cdot 0.5CH_2Cl_2\cdot C_7H_8$.
16646	1.507 + 2.387 Å	Dunitz, J. D. *Acta Crystallogr.* **1956**, *9*, 579. $Na_2S_2O_4$.
PYZNDT	1.514 + 2.386 Å	Kiers, C. T.; Vos, A. *Acta Crystallogr., Sect. B* **1978**, *34*, 1499. $Zn(S_2O_4)(NC_5H_5)$
32684	1.515 + 2.349 Å	Magnusson, A.; Johansson, L. G. *Acta Chem. Scand., Ser. A* **1982**, *36*, 429. $Sn_2(S_2O_4)_2$
Mean	**1.491 + 2.343 Å/5**	

Disulfite ion, $S_2O_5^{2-}$

ICSD/CSD	***d*(S-O, S-O) + *d*(S-S)**	**Reference**
JAFKUW	1.402, 1.491 + 2.198 Å	Reynolds, M. S.; Holm, R. H. *Inorg. Chim. Acta* **1989**, *155*, 113.
31817	1.426, 1.464 + 2.212 Å	Zachariasen, W. H. *Phys. Rev.* **1932**, *40*, 923-935. $K_2S_2O_5$.
9074	1.456, 1.497 + 2.171 Å	Baggio, S. *Acta Crystallogr., Sect. B* **1971**, *27*, 517-522. $(NH_4)_2S_2O_5$.
16701	1.459, 1.498 + 2.208 Å	Lindqvist, I.; Moertsell, M. *Acta Crystallogr.* **1957**, *10*, 406-409. $K_2S_2O_5$.
37172	1.462, 1.489 + 2.226 Å	Magnusson, A.; Johansson, L. G.; Lindqvist, O. *Acta Crystallogr., Sect. C* **1983**, *39*, 819-822. $K_5(HSO_3)(S_2O_5)$
60025	1.487 + 2.220 Å	Chen, I. C.; Wang, Y. *Acta Crystallogr., Sect. C* **1984**, *40*, 1780-1781. $K_2S_2O_5$.
Mean	**1.477 + 2.206 Å/6**	

Dithionate ion, $S_2O_6^{2-}$

ICSD/CSD	*d*(S-O) + *d*(S-S)	Reference
2933	1.401 + 2.138 Å	Hargreaves, R. N.; Stanley, E. *Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem.* **1972**, *135*, 399.
PIVJAF	1.411 + 2.063 Å	Rominger, F.; Muller, A.; Thewalt, U. *Chem. Ber.* **1994**, *127*, 797.
ARUFTH	1.418 + 2.099 Å	Lehmann, H.; Schenk, K. J.; Chapuis, G.; Ludi, A. *J. Am. Chem. Soc.* **1979**, *101*, 6197.
GEPSUP	1.419 + 2.128 Å	Towle, D. K.; Botsford, C. A.; Hodgson, D. J. *Inorg. Chim. Acta* **1988**, *141*, 167.
JATKEU	1.421 + 2.163 Å	Corbin, K. M.; Hodgson, D. J.; Lynn, M. H.; Michelsen, K.; Nielsen, K. M.; Pedersen, E. *Inorg. Chim. Acta* **1989**, *129*, 159.
JATKEU10	1.421 + 2.163 Å	Corbin, K. M.; Glerup, J.; Hodgson, D. J.; Lynn, M. H.; Michelsen, K.; Nielsen, K. M. *Inorg. Chem.* **1993**, *32*, 18.
FATZUV	1.422 + 2.122 Å	Hodgson, D. J.; Pedersen, E.; Toftlund, H.; Weiss, C. *Inorg. Chim. Acta* **1986**, *120*, 177.
OZBPIT	1.422 + 2.071 Å	Mikami, M.; Konno, M.; Saito, Y. *Acta Crystallogr., Sect. B* **1979**, *35*, 3096.
DOFVEZ	1.423 + 2.218 Å	Elschenbroich, C.; Gondrum, R.; Massa, W. *Angew. Chem., Int. Ed.* **1985**, *24*, 967.
AMCOTN	1.425 + 2.131 Å	Hambley, T. W.; Hawkins, C. J.; Palmer, J. A.; Snow, M. R. *Aust. J. Chem.* **1981**, *34*, 45.
XSENCR	1.425 + 2.138 Å	Kaas, K. *Acta Crystallogr., Sect. B* **1979**, *35*, 596.
XAZDUX	1.430 + 2.131 Å	Ming-Liang Tong; Shao-Liang Zheng; Xiao-Ming Chen
YOPBUA	1.430 + 2.132 Å	Harrowfield, J. M.; Mocerino, M.; Skelton, B. W.; Wenyan Wei; White, A. H. *J. Chem. Soc., Dalton Trans.* **1995**, 783.
ENCOXT	1.431 + 2.134 Å	Thewalt, U.; Struckmeier, G. *Z. Anorg. Allg. Chem.* **1976**, *419*, 163.
FIHKUC	1.431 + 2.125 Å	Ardon, M.; Bino, A.; Michelsen, K. *J. Am. Chem. Soc.* **1987**, *109*, 1986.
CIGLUZ	1.432 + 2.137 Å	Bang, E.; Monsted, O. *Acta. Chem. Scand., Ser. A* **1984**, *38*, 281.
KEZLAC	1.433 + 2.120 Å	Goodson, P. A.; Hodgson, D. J.; Michelsen, K. *Inorg. Chim. Acta* **1990**, *172*, 49.
CIXWUB	1.434 + 2.137 Å	xxxx
COPWOT	1.434 + 2.117 Å	Curtis, N. J.; Hagen, K. S.; Sargeson, A. M. *Chem. Commun.* **1984**, 1571.
JATJUJ	1.435 + 2.130 Å	Corbin, K. M.; Hodgson, D. J.; Lynn, M. H.; Michelsen, K.; Nielsen, K. M.; Pedersen, E. *Inorg. Chim. Acta* **1989**, *129*, 159.
JATJUJ10	1.435 + 2.130 Å	Corbin, K. M.; Glerup, J.; Hodgson, D. J.; Lynn, M. H.; Michelsen, K.; Nielsen, K. M. *Inorg. Chem.* **1993**, *32*, 18.
JUNCOK	1.435 + 2.138 Å	Bernhardt, P. V.; Comba, P.; Mahu-Rickenbach, A.; Stebler, S.; Steiner, S.; Varnagy, K.; Zehnder, M. *Inorg. Chem.* **1992**, *31*, 4194.
COHJEO	1.436 + 2.137 Å	Larsen, S.; Nielsen, K. B.; Trabjerg, I. *Acta. Chem. Scand., Ser. A* **1983**, *37*, 833.

TADCOT10	1.436 + 2.117 Å	Bourshteyn, I. F.; Mazus, M. D.; Byushkin, V. N.; Popa, E. V.; Ablov, A. V.; Malinovskii, T. I.; Rannev, N. V.; Shchedrin, B. M. *Koord. Khim.* **1978**, *4*, 282.
ACAVEG	1.437 + 2.127 Å	Alzoubi, B. M.; Liehr, G.; van Eldik, R. *Inorg. Chem.* **2004**, *63*, 6093.
JULTEP	1.437 + 2.119 Å	Atkinson, I. M.; Keene, F. R.; Gulbis, J. M.; Searle, G. H.; Tiekink, E. R. T. *J. Mol. Struct.* **1992**, *265*, 189.
16466	1.438 + 2.119 Å	Hodgson, D. J.; Pedersen, E. *Inorg. Chem.* **1980**, *19*, 3116.
EAMOCO10	1.438 + 2.117 Å	Thewalt, U. *Chem. Ber.* **1971**, *104*, 2657.
PADNEO	1.438 + 2.119 Å	Sisley, M. J.; McDonald, R.; Jordan, R. B. *Inorg. Chem.* **2004**, *43*, 5339.
60785	1.439 + 2.127 Å	Andersen, P.; Bang, E. *Acta Chem. Scand., Ser. A* **1986**, *40*, 476.
ACHYZN	1.439 + 2.124 Å	Krol, L. A.; Agre, V. M.; Kvernadze, M. S.; Pirtskhalava, N. I.; Nyudochkin, A. G. *Koord. Khim.* **1981**, *7*, 800.
BAZDOX	1.439 + 2.135 Å	Chang-Jin Qin; James, L.; Chartres, J. D.; Alcock, L. J.; Davis, K. J.; Willis, A. C.; Sargeson, A. M.; Bernhardt, P. V.; Ralph, S. F. *Inorg. Chem.* **2011**, *50*, 9131.
GADSOT	1.439 + 2.129 Å	Gaus, P. L.; Benefield, R. M.; Hicsasmaz, H.; Perry, B.; Villanueva, J.; Flack, C. E.; Pett, V. B.; Demoulini, S. A.; Faulhaber, J. C.; Lynch, D. E.; Bacon J. W. *Inorg. Chim. Acta* **1988**, *141*, 61.
PATACO10	1.439 + 2.112 Å	Robertson, G. B.; Whimp, P. O. *Aust. J. Chem.* **1975**, *28*, 729.
RUZEF	1.439 + 2.132 Å	Fairlie, D. P.; Wickramasinghe, W. A.; Byriel, K.A.; Taube, H. *Inorg. Chem.* **1997**, *36*, 2242.
SUWTOT	1.439 + 2.125 Å	Burnet, S.; Min-Ho Choi; Donnelly, P. S.; Harrowfield, J. M.; Ivanova, I.; Seong-Hoon Jeong; Yang Kim; Mocerino, M.; Skelton, B. W.; White, A. H.; Williams, C. C.; Zhi-Ling Zeng *Eur. J. Inorg. Chem.* **2001**, 1869.
TOENCO	1.439 + 2.119 Å	Lydon, J. D.; Mulligan, K. J.; Elder, R. C.; Deutsch, E. *Inorg. Chem.* **1980**, *19*, 2083.
TUQNEY	1.439 + 2.123 Å	Russell, V. A.; Evans, C. C.; Wenjie Li; Ward, M. D. *Science* **1997**, *276*, 575.
DORTIN	1.440 + 2.132 Å	Wieghardt, K.; Walz, W.; Nuber, B.; Weiss, J.; Ozarowski, A.; Stratemeier, H.; Reinen, D. *Inorg. Chem.* **1986**, *25*, 1650.
FUPFEB	1.440 + 2.115 Å	Roecker, L.; Sargeson, A. M.; Willis, A. C. *Chem. Commun.* **1988**, 119.
KEXZIW	1.440 + 2.123 Å	Donlevy, T. M.; Gahan, L. R.; Hambley, T. W.; Hanson, G. R.; Markiewicz, A.; Murray, K. S.; Swann, I. L.; Pickering, S. R. *Aust.J. Chem.* **1990**, *43*, 1407.
BULLEZ	1.441 + 2.119 Å	Searle, G. H.; Hambley, T. W. *Aust. J. Chem.* **1982**, *35*, 2399.
PATZUF	1.441 + 2.123 Å	Corbin, K. M.; Glerup, J.; Hodgson, D. J.; Lynn, M. H.; Michelsen, K.; Nielsen, K. M. *Inorg. Chem.* **1993**, *32*, 18.
RIPDID	1.441 + 2.124 Å	Fairlie, D. P.; Jackson, W. G.; Skelton, B. W.; Huo Wen; White, A. H.; Wickramasinghe, W. A.; Tai Chin Woon; Taube, H. *Inorg. Chem.* **1997**, *36*, 1020.
68293	1.442 + 2.126 Å	Frank, W.; Stetzer, T.; Heck, L. *Z. Naturforsch., Teil B* **1988**, *43*, 189.

PYETCR	1.442 + 2.103 Å	Larsen, S.; Hansen, B. *Acta Chem. Scand., Ser. A* **1981**, *35*, 105.
SUWTIN	1.442 + 2.105 Å	Burnet, S.; Min-Ho Choi; Donnelly, P. S.; Harrowfield, J. M.; Ivanova, I.; Seong-Hoon Jeong; Yang Kim; Mocerino, M.; Skelton, B. W.; White, A. H.; Williams, C. C.; Zhi-Ling Zeng *Eur. J. Inorg. Chem. 2001*, 1869.
BEFHID	1.443 + 2.121 Å	Kiyoda, S.; Akashi, H.; Ohtani, T.; Shibahara, T. *Chem. Lett.* **1999**, 41.
BEFHID01	1.443 + 2.121 Å	Kiyoda, S.; Akashi, H.; Ichimura, A.; Shibahara, T. *Bull. Chem. Soc. Jpn.* **2003**, *76*, 1155.
CEKLEJ	1.443 + 2.144 Å	Hambley, T. W.; Searle, G. H. *Acta Crystallogr., Sect. C* **1984**, *40*, 383.
GUCFAM	1.443 + 2.113 Å	Boldog, I.; Daran, J.-C.; Chernega, A. N.; Rusanov, E. B.; Krautscheid, H.; Domasevitch, K. V. *Cryst. Growth Des.* **2009**, *9*, 2895.
KENPIC	1.443 + 2.116 Å	Alcock, N. W.; Creaser, I. I.; Curtis, N. J.; Roecker, L.; Sargeson, A. M.; Willis, A. C. *Aust. J. Chem.* **1990**, *43*, 643.
KIBZAW01	1.443 + 2.109 Å	Marsh, R. E. *Acta Crystallogr., Sect. B* **1997**, *53*, 317.
NEFYIG	1.443 + 2.135 Å	Shin, Y. K.; Szalda, D. J.; Brunschwig, B.S.; Creutz, C.; Sutin, N. *Inorg. Chem.* **1997**, *36*, 3190.
OAZCOS	1.443 + 2.118 Å	Zehnder, M.; Thewalt, U. *Z. Anorg. Allg. Chem.* **1980**, *461*, 53.
VIDXUB	1.443 + 2.124 Å	Donnelly, P. S.; Harrowfield, J. M.; Skelton, B. W.; White, A. H. *Inorg. Chem.* **2000**, *39*, 5817.
YOPBEK	1.443 + 2.133 Å	Harrowfield, J. M.; Mocerino, M.; Skelton, B. W.; Wenyan Wei; White, A. H. *J. Chem. Soc., Dalton Trans.* **1995**, 783.
YOPBIO	1.443 + 2.128 Å	Harrowfield, J. M.; Mocerino, M.; Skelton, B. W.; Wenyan Wei; White, A. H. *J. Chem. Soc., Dalton Trans.* **1995**, 783.
BOPVIL	1.444 + 2.132 Å	Creaser, I. I.; Geue, R. J..; Harrowfield, J. M.; Herit, A. J.; Sargeson, A. M.; Snow, M. R.; Springborg, J. *J. Am. Chem. Soc.* **1982**, *104*, 6016.
CEGBUL	1.445 + 2.145 Å	Keene, F. R.; Ridd, M. J.; Snow, M. R. *J. Am. Chem. Soc.* **1983**, *105*, 7075.
CULQOP	1.445 + 2.115 Å	Hyungphil Chun; Jackson, W. G.; McKeon, J. A.; Somoza Jr., F. B.; Bernal, I. *Eur. J. Inorg. Chem.* **2000**, 189.
24676	1.446 + 2.081 Å	Stanley, E. *Acta Crystallogr.* **1953**, *6*, 187.
CULQIJ	1.446 + 2.136 Å	Hyungphil Chun; Jackson, W. G.; McKeon, J. A.; Somoza Jr., F. B.; Bernal, I. *Eur. J. Inorg. Chem.* **2000**, 189.
DOGRIA	1.446 + 2.128 Å	Galsbol, F.; Larsen, S.; Rasmussen, B.; Springborg, J. *Inorg. Chem.* **1986**, *25*, 290.
DUCMET	1.446 + 2.114 Å	Szalda, D. J.; Keene, F. R. *Inorg. Chem.* **1986**, *25*, 2795.
FIGFEH	1.446 + 2.126 Å	Harrowfield, J. M.; Ogden, M. I.; Skelton, B. W.; White, A. H. *Compt. Rendus Chim.* **2005**, *8*, 121.
JAMWUP	1.446 + 2.126 Å	Krogh-Jespersen, K.; Xiaohua Zhang; Westbrook, J. D.; Fikar, R.; Nayak, K.; Whei-Lu Kwik; Potenza, J. A; Schugar, H. J. *J. Am. Chem. Soc.* **1989**, *111*, 4082.

KAJFIK	1.446 + 2.123 Å	Begley, M. J.; Hubberstey, P.; Walton, P. H. *Chem. Commun.* **1989**, 502.
KAJFIK10	1.446 + 2.123 Å	Begley, M. J.; Hubberstey, P.; Walton, P. H. *J. Chem. Soc., Dalton Trans.* **1995**, 957.
4313	1.447 + 2.126 Å	Thewalt, U. *Z. Anorg. Allg. Chem.* **1975**, *412*, 29.
BPACUT	1.447 + 2.146 Å	Harrison, W. D.; Hathaway, B. J. *Acta Crystallogr., Sect. B* **1979**, *35*, 2910.
HCRENT	1.447 + 2.127 Å	Cline, S. J.; Scaringe, R. P.; Hatfield, W. E.; Hodgson, D. J. *J. Chem. Soc., Dalton Trans.* **1977**, 1662.
WIZMUN	1.447 + 2.108 Å	Schmidt, S.; Heinemann, F. W.; Grohmann, A. *Eur. J. Inorg. Chem.* **2000**, 1657.
XODKEG	1.447 + 2.141 Å	Harrowfield, J. M.; Seong-Hoon Jeong; Man-Kil Lee; Yang Kim; Rukmini, E.; Skelton, B. W.; White, A. H. *Aust. J. Chem.* **2001**, *54*, 63.
1834	1.448 + 2.123 Å	Black, W. H.; Griffith, E. A. H.; Robertson, B. E. *Acta Crystallogr., Sect. B* **1975**, *31*, 615.
CUGKOE	1.448 + 2.134 Å	Comba, P.; Engelhardt, L. M.; Harrowfield, J. M..; Lawrance, G. A.; Martin, I. L.; Sargeson, A. M.; White, A. H. *Chem. Commun.* **1985**, 174.
GOKBIR	1.448 + 2.128 Å	Diamantis, A. A.; Moritz, P. S.; Snow, M. R.; Tiekink, E. R. T. *Aust. J. Chem.* **1988**, *41*, 1251.
1835	1.449 + 2.124 Å	Black, W. H.; Griffith, E. A. H.; Robertson, B. E. *Acta Crystallogr., Sect. B* **1975**, *31*, 615.
FECQIN	1.449 + 2.130 Å	Grohmann, A.; Heinemann, F. W.; Kofod, P. *Inorg. Chim. Acta* **1999**, *286*, 98.
POKWIW	1.449 + 2.145 Å	Turba, S.; Walter, O.; Schindler, S.; Nielsen, L. P.; Hazell, A.; McKenzie, C. J.; Lloret, F.; Cano, J.; Julve, M. *Inorg. Chem.* **2008**, *47*, 9612.
XATLAH	1.449 + 2.133 Å	Wang, R.; Sherburn, M. S.; Willis, A. C., CDS no. XATLAH
8172	1.450 + 2.154 Å	Zwoll, K. *Ber. Kernforschungsanlage Juelich* **1974**, *1057*, 95-116.
8173	1.450 + 2.154 Å	Zwoll, K. *Ber. Kernforschungsanlage Juelich* **1974**, *1057*, 95.
8209	1.450 + 2.080 Å	Solans, X.; Miravitlles, C.; Germain, G.; Declercq, J. P. *Acta Crystallogr., Sect. B* **1979**, *35*, 2181.
BIKJAG	1.450 + 2.060 Å	Gahan, L. R.; Hambley, T. W.; Sargeson, A. M.; Snow, M. R. *Inorg. Chem.* **1982**, *21*, 2699.
FISQUT	1.450 + 2.162 Å	Krebs, F. C.; Laursen, B. W.; Johannsen, I.; Faldi, A.; Bechgaard, K.; Jacobsen, C. S.; Thorup, N.; Boubekeur, K. *Acta Crystallogr., Sect. B* **1999**, *55*, 410.
GEMWOK	1.450 + 2.138 Å	Keene, F. R.; Snow, M. R.; Stephenson, P. J.; Tiekink, E. R. T. *Inorg. Chem.* **1988**, *27*, 2040.
LEJWIG	1.450 + 2.152 Å	Kofod, P.; Larsen, E.; Springborg, J.; Larsen, S.; Larsen, T. A.; Geue, R. J.; Searle, G. H. *Aust. J. Chem.* **1994**, *47*, 111.
MULCAY	1.450 + 2.128 Å	Clegg, J. K.; Lindoy, L. F.; Thuery, P.; Young Hoon Lee; Kusumohastuti, D. K. A.; Mora, C.; Hyang Hoo Kim; Jeong Hwan Cho; Yang Kim *J. Inclusion Phenom. Macrocyclic Chem.* **2009**, *65*, 49.
WIZNAU	1.450 + 2.144 Å	Schmidt, S.; Heinemann, F. W.; Grohmann, A. *Eur. J. Inorg. Chem.* **2000**, 1657.

1836	1.451 +2.127 Å	Black, W. H.; Griffith, E. A. H.; Robertson, B. E. *Acta Crystallogr., Sect. B* **1975**, *31*, 615.
26326	1.451 + 2.140 Å	Kirfel, A.; Will, G.; Weiss, A. *Acta Crystallogr., Sect. B* **1980**, *36*, 223.
31858	1.451 + 2.140 Å	Berthold, I.; Weiss, A. *Z. Naturforsch., Teil A* **1967**, *22*, 1440-1451; *Ber. Kernforschungsanlage Jülich* **1974**, *1057*, 1.
41148	1.451 +2.131 Å	de Matos Gomes, E. *Acta Crystallogr., Sect. B* **1991**, *47*, 7.
82843	1.451 + 2.142 Å	de Matos Gomes, E.; Ortega, J.; Extebarria, J.; Zuniga, F. J.; Breczewski, T. *J. Phys.: Condensed Matter* **1996**, *8*, 2063.
NESXAM	1.451 + 2.132 Å	Clegg, J. K.; Harrowfield, J. M.; Yang Kim; Young Hoon Lee; Madalan, A.; Thuery, P.; Arim Woo *Aust. J. Chem.* **2012**, *65*, 734.
PIVJEJ	1.451 + 2.129 Å	Rominger, F.; Muller, A.; Thewalt, U. *Chem. Ber.* **1994**, *127*, 797.
1525	1.452 + 2.141 Å	Kiers, C. T.; Piepenbroek, A.; Vos, A. *Acta Crystallogr., Sect. B* **1978**, *34*, 888.
60032	1.452 + 2.142 Å	Kirfel, A.; Will, G. *Acta Crystallogr., Sect. B* **1980**, *36*, 512.
HIFYOL	1.452 + 2.129 Å	Domasevitch, K. V.; Gural'skiy, I. A.; Solntsev, P. V.; Rusanov, E. B.; Krautscheid, H.; Howard, J. A. K.; Chernega, A. N. *Dalton Trans.* **2007**, 3140.
MULBIF	1.452 + 2.147 Å	Clegg, J. K.; Lindoy, L. F.; Thuery, P.; Young Hoon Lee; Kusumohastuti, D. K. A.; Mora, C.; Hyang Hoo Kim; Jeong Hwan Cho; Yang Kim *J. Inclusion Phenom. Macrocyclic Chem.* **2009**, *65*, 49.
NATNUR	1.452 + 2.115 Å	Ama, T., Okamoto, K.-I.; Yonemura, T.; Kawaguchi, H.; Ogasawara, Y.; Yasui, T. *Chem. Lett.* **1996**, 29.
WEHPEF	1.452 + 2.142 Å	Mantero, D. G.; Neels, A.; Stoeckli-Evans, H. *Inorg. Chem.* **2006**, *45*, 3287.
WEHPIJ	1.452 + 2.096 Å	Mantero, D. G.; Neels, A.; Stoeckli-Evans, H. *Inorg. Chem.* **2006**, *45*, 3287.
200867	1.453 + 2.107 Å	Liminga, R.; Abrahams, S. C.; Bernstein, J. L. *J. Chem. Phys.* **1980**, **73**, 1432.
XODKIK	1.453 + 2.132 Å	Harrowfield, J. M.; Seong-Hoon Jeong; Man-Kil Lee; Yang Kim; Rukmini, E.; Skelton, B. W.; White, A. H. *Aust. J. Chem.* **2001**, *54*, 63.
AGUTIG	1.453 + 2.124 Å	Govor, E. V.; Lysenko, A. B.; Rusanov, E. B.; Chernega, A. N.; Krautscheid, H.; Domasevitch, K. V. *Z. Anorg. Allg. Chem.* **2010**, *636*, 209.
16622	1.454 + 2.157 Å	Martinez, S.; Garcia Blanco, S.; Rivoir, L. *Acta Crystallogr.* **1956**, *9*, 145-150; *Acta Crystallogr., Sect. B* **1968**, *24*, 1131-1133; *Z. Phys. Chem.* **1963**, *38*, 140.
DODVOH	1.454 + 2.138 Å	Larsen, S.; Michelsen, K.; Pedersen, E. *Acta. Chem. Scand., Ser. A* **1986**, *40*, 63.
RATDOF	1.454 + 2.138 Å	Kofod, P.; Harris, P.; Larsen, S. *Inorg. Chem.* **1997**, *36*, 2258.
XOTQUS	1.454 + 2.129 Å	Bendahl, L.; Hammershoi, A.; Jensen, D. K.; Larsen, S.; Riisager, A.; Sargeson, A.M.; Sorensen. H. O. *J. Chem.*

		Soc., Dalton Trans. **2002**, 3054.
200865	1.455 + 2.112 Å	Liminga, R.; Abrahams, S. C.; Bernstein, J. L. *J. Chem. Phys.* **1980**, **73**, 1432.
AGACEQ	1.455 + 2.145 Å	Brooker, S.; de Geest, D. J.; Kelly, R. J.; Plieger, P. G.; Moubaraki, B.; Murray, K. S.; Jameson, G. B. *J. Chem. Soc., Dalton Trans.* **2002**, 2080.
EMIDUZ	1.455 + 2.134 Å	Yang Kim; Skelton, B. W.; White, A. H. *Acta Crystallogr., Sect. C* **2003**, *59*, m546.
FAZCUF	1.455 + 2.125 Å	Warden, A. C.; Warren, M.; Hearn, M. T. W.; Spiccia, L. *New. J. Chem.* **2004**, *28*, 1301.
GUCDOY	1.455 + 2.134 Å	Boldog, I.; Daran, J.-C.; Chernega, A. N.; Rusanov, E. B.; Krautscheid, H.; Domasevitch, K. V. *Cryst. Growth Des.* **2009**, *9*, 2895.
MEJGOX	1.455 + 2.130 Å	Sanzenbacher, R.; Sotofte, I.; Springborg, J. *Acta Chem. Scand.* **1999**, *53*, 457.
MUFKED	1.455 + 2.123 Å	Harris, P.; Kofod, P. *Acta Crystallogr., Sect. E* **2002**, *58*, m460.
NIGVII	1.455 + 2.135 Å	Buchen, T.; Hazell, A.; Jessen, L.; McKenzie, C. J.; Nielsen, L. P.; Pedersen, J. Z.; Schollmeyer, D. *J. Chem. Soc., Dalton Trans.* **1997**, 2697.
QAXHIG	1.455 + 2.147 Å	Kalsbeek, N.; Larsen, S. *Acta Chem. Scand.* **1999**, *53*, 149.
RATDIZ	1.455 + 2.130 Å	Kofod, P.; Harris, P.; Larsen, S. *Inorg. Chem.* **1997**, *36*, 2258.
VABKUE	1.455 + 2.134 Å	Bjerrum, M. J.; Gejhede, M.; Larsen, E.; Springborg, J. *Inorg. Chem.* **1988**, *27*, 3960.
31857	1.456 + 2.153 Å	Berthold, I.; Weiss, A. *Z. Naturforsch., Teil A* **1967**, *22*, 1440-1451; *Ber. Kernforschungsanlage Jülich* **1974**, *1057*, 1.
DIBRAI	1.456 + 2.133 Å	Schiessl, W.; Puchta, R.; Bugarcic, Z. D.; Heinemann, F. W.; van Eldik, R. *Eur. J. Inorg. Chem.* **2007**, 1390.
WURROQ	1.456 + 2.139 Å	Harris, P.; Kofod, P.; Yong Sheng Song; Larsen, E. *Eur. J. Inorg. Chem.* **2000**, 1657.
37067	1.457 + 2.138 Å	Cline, S. J.; Hodgson, D. J.; Kallesoe, S.; Larsen, S.; Pedersen, E. *Inorg. Chem.* **1983**, *22*, 637.
KIBZAW	1.457 + 2.108 Å	Schreiber, P.; Wieghardt, K.; Nuber, B.; Weiss, J. *Z. Anorg. Allg. Chem.* **1990**, *587*, 174.
10065	1.464 + 2.138 Å	Leskelae, M.; Valkonen, J.; Hoppe, R. *Acta Chem. Scand., Ser. A* **1978**, *32*, 805.
14329	1.464 + 2.151 Å	Rausell-Colom, J. A.; Garcia-Blanco, S. *Acta Crystallogr.* **1966**, *21*, 672.
200866	1.464 + 2.112 Å	Liminga, R.; Abrahams, S. C.; Bernstein, J. L. *J. Chem. Phys.* **1980**, **73**, 1432.
DURWOC	1.470 + 2.119 Å	Hawkins, C. J.; Horn, E.; Martin, J.; Palmer, J. A. L.; Snow, M. R. *Aust. J. Chem.* **1986**, *39*, 1213.
DORYOY	1.471 + 2.111 Å	Wieghardt, K.; Kleine-Boymann, M.; Nuber, B.; Weiss, J. *Inorg. Chem.* **1986**, *25*, 1654.
14258	1.478 + 2.158 Å	Chan, J.; Stanley, E. *Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem.* **1970**, *132*, 404.
GEMRAR	1.480 + 2.125 Å	Schreiber, P.; Wieghardt, K.; Florke, U.; Haupt, H.-J. *Inorg. Chem.* **1988**, *27*, 2111.
24677	1.481 + 2.080 Å	Stanley, E. *Acta Crystallogr.* **1953**, *6*, 187.

27580	1.489 + 2.012 Å	Huggins, M. L.; Frank, G. O. *Amer. Mineral.* **1931**, *16*, 580.
15966	1.490 + 2.095 Å	Barnes, W. H.; Wendling, A. V. *Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem.* **1938**, *99*, 153.
27581	1.520 + 2.016 Å	Huggins, M. L.; Frank, G. O. *Amer. Mineral.* **1931**, *16*, 580.
36154	1.578 + 2.035 Å	Helwig, G. V. *Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem.* **1932**, *83*, 485.
Mean	**1.446 Å + 2.127 Å/135**	

Disulfate ion, $S_2O_7^{2-}$

ICSD/CSD	*d*(S-O) + *d*(S-O)	Reference
413050	1.405 + 1.578 Å	Ståhl, K.; Balic-Zunic, T.; da Silva, F.; Eriksen, K. M.; Berg, R. W.; Fehrmann, R. *J. Solid State Chem.* **2005**, *178*, 1697.
16392	1.417 + 1.632 Å	Einstein, F. W. B.; Wilis, A. C. *Acta Crystallogr., Sect. B* **1981**, *37*, 218.
172461	1.421 + 1.619 Å	Kornath, A.; Blecher, O. *Z. Anorg. Allg. Chem.* **2002**, *628*, 625.
249741	1.426 + 1.632 Å	Swain, D.; Guru Row, T. N. *Inorg. Chem.* **2008**, *47*, 8613.
4435	1.427 + 1.644 Å	Sivertsen, B.K.;Sorum, H. *Z. Kristallograph., Kristallgeom., Kristallphys., Kristallchem.* **1969**, *130*, 449.
249740	1.427 + 1.639 Å	Swain, D.; Guru Row, T. N. *Inorg. Chem.* **2008**, *47*, 8613.
418072	1.427 + 1.629 Å	Ståhl, K.; Berg, R. W.; Eriksen, K. M.; Fehrmann, R. *Acta Crystallogr., Sect. B* **2009**, *65*, 5.
FAGYAO	1.431 + 1.629 Å	Kornath, A.; Blecher, O. *Z. Anorg. Allg. Chem.* **2002**, *628*, 622.
34169	1.432 + 1.642 Å	Lynton, H.; Truter, M. R. *J. Chem. Soc.* **1960**, 5112.
8033	1.435 + 1.623 Å	Douglade, J.; Mercier, R. *Acta Crystallogr., Sect. B* **1979**, *35*, 1062.
414672	1.437 + 1.660 Å	Stahl, K.; Balic-Zunic, T.; da Silva, F.; Eriksen, K. M.; Berg, R. W.; Fehrmann, R. *J. Solid State Chem.* **2005**, *178*, 1697.
ZOWVAI	1.438 + 1.632 Å	Kuhn, N.; Bohnen, H.; Henkel, G. *Z. Kristallogr.* **1996,** *211*, 57.
411052	1.438 + 1.630 Å	Wickleder, M. S. *Z. Anorg. Allg. Chem.* **2000**, *626*, 621.
413049	1.439 + 1.629 Å	Stahl, K.; Balic-Zunic, T.; da Silva, F.; Eriksen, K. M.; Berg, R. W.; Fehrmann, R. *J. Solid State Chem.* **2005**, *178*, 1697.
418071	1.439 + 1.641 Å	Ståhl, K.; Berg, R. W.; Eriksen, K. M.; Fehrmann, R. *Acta Crystallogr., Sect. B* **2009**, *65*, 551.
DIXTIN	1.438 + 1.651 Å	Hvoslef, J.; Tracy, M. L.; Nash, C. P. *Acta Crystallogr., Sect. C* **1986**, *42*, 353.
63067	1.442 + 1.625 Å	Simonov, M. A.; Shkovrov, S. V.; Troyanov, S. I. *Kristallografiya* **1988**, *33*, 502.
188009	1.442 + 1.667 Å	Logemann, C.; Witt, J.; Wickleder, M. S. Z. Kristallogr. - New Cryst. Struct. 2013, 228, 159.
LEFMEP	1.444 + 1.631 Å	Richtera, L.; Taraba, J.; Touzin, J. *Collect. Czech. Chem. Commun.* **2006**, *71*, 155.
405696	1.448 + 1.628 Å	Jansen, M.; Müller, R. *Z. Anorg. Allg. Chem.* **1997**, *623*, 1055.
Mean	**1.434 + 1.636 Å/19**	

Peoxodisulfate ion, $S_2O_8^{2-}$

ICSD/CSD	d(S-O) + d(S-O_{peroxo})	Reference
XAMFEX	1.390 + 1.602 Å	Harvey, M. A.; Baggio, S.; Garland, M. T.; Baggio, R. *J. Coord. Chem.* **2005**, *58*, 243.
EYIMOO	1.391 + 1.557 Å	Harvey, M. A.; Baggio, S.; Ibanez, A.; Baggio, R. *Acta Crystallogr., Sect. C* **2004**, *60*, m375.
CITLEX	1.391 + 1.661 Å	Youngme, S.; Phatchimkun, J.; Wannarit, N.; Chaichit, N.; Meejoo, S.; van Albada, G. A.; Reedijk, J. *Polyhedron* **2008**, *27*, 304.
ROZWUZ	1.393 + 1.679 Å	Singh, A.; Sharma, R. P.; Ferretti, V.; Rossetti, S.; Venugopalan, P. *J. Mol. Struct.* **2009**, *927*, 111.
NEPSAE	1.408 + 1.615 Å	Harvey, M. A.; Suarez, S.; Doctorovich, F.; Baggio, R. *Acta Crystallogr., Sect. E* **2013**, *69*, m63.
EYIMUU	1.413 + 1.611 Å	Harvey, M. A.; Baggio, S.; Ibanez, A.; Baggio, R. *Acta Crystallogr., Sect. C* **2004**, *60*, m375.
IMAZUS	1.414 + 1.615 Å	Skogareva, L. S.; Minacheva, L. K.; Sergienko, V. S. *Kristallografiya* **2009**, *54*, 46.
EYINAB	1.418 + 1.647 Å	Harvey, M. A.; Baggio, S.; Ibanez, A.; Baggio, R. *Acta Crystallogr., Sect. C* **2004**, *60*, m375.
FEDZIY	1.423 + 1.653 Å	Skogareva, L. S.; Minacheva, L. K.; Sergienko, V. S.; Minaeva, N. A.; Filippova, T. V. *Zh. Neorg. Khim.* **2004**, *49*, 938.
54024	1.425 + 1.645 Å	Naumov, D. Y.; Virovets, A. V.; Podberezskaya, N. V.; Novikov, P. B.; Politov, A. A. *J. Struc. Chem. (USSR)***1997** *38*, 772.
4435	1.427 + 1.644 Å	Sivertsen, B. K.; Sorum, H. *Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.* **1969**, *130*, 449.
165104	1.427 + 1.674 Å	Skogareva, L. S.; Minaeva, N. A.; Filippova, T. V. *Russ. J. Inorg. Chem.* **2009**, *54*, 1341.
BULYIR	1.429 + 1.643 Å	Baffert, C.; Orio, M.; Pantazis, D. A.; Duboc, C.; Blackman, A. G.; Blondin, G.; Neese, F., Deronzier, A.; Collomb, M.-N. *Inorg. Chem.* **2009**, *48*, 10281.
HOFVEE	1.431 + 1.650 Å	Harvey, M. A.; Baggio, S.; Garland, M. T.; Baggio, R. *Acta Crystallogr., Sect. C* **2008**, *64*, o489.
171374	1.438 + 1.639 Å	Allan, D. R. *Acta Crystallogr., Sect. E* **2006**, *62*, i44.
281002	1.439 + 1.652 Å	Schmidt, T.; Schmitt, H.; Zimmermann, H.; Haeberlen, U.; Lalowicz, Z. T.; Olejniczak, Z.; Oeser, T. *Acta Crystallogr., Sect. B* **2002**, *58*, 760.
Mean	**1.424 + 1.641 Å/12**	

Legends to Figures

Figure S1: Minimum structures obtained via energy minimization at MP2 level in implicit solvent. Energy minimization made via HF and CCSD yield similar topologies (see Table S1). Although a solution-like coordination is observed for the oxygen-coordinated H-bond (left), a bi-coordinated complex results in case a sulfur-coordinated H-bond is present in the starting structure (right). Since the latter is not relevant in the context of aqueous solution, a comparison of the structural properties is not meaningful.

Figure S2: Radial Distribution Function from simulation, pair wise depicted left showing the entire distribution and right details of smaller peaks. The graphs are from bottom to top, central sulfur S_C to oxygen distances, terminal sulfur S_T to oxygen, thiosulfate oxygen O_{S2O3} to oxygen (both on ion and water), oxygen to hydrogen distances and finally the top shows s summation over all previous graphs.

Figure S3. LAXS, peroxodisulfate ion. Top: the individual peak shapes for all contributing species in the 1.5000 mol·dm^{-3} aqueous solution of sodium peroxodisulfate, the hydrated peroxodisulfate ion (orange line), hydrated sodium ion (brown line) and the aqueous bulk (green line). (b) Experimental $D(r) - 4\pi r^2\rho_o$ (red line); model (black line), the modelled distances are given in Table 2; difference (blue line). Bottom: reduced LAXS intensity function, $si(s)$ (thin black line); model $si_{calc}(s)$ (red line).

Figure S1

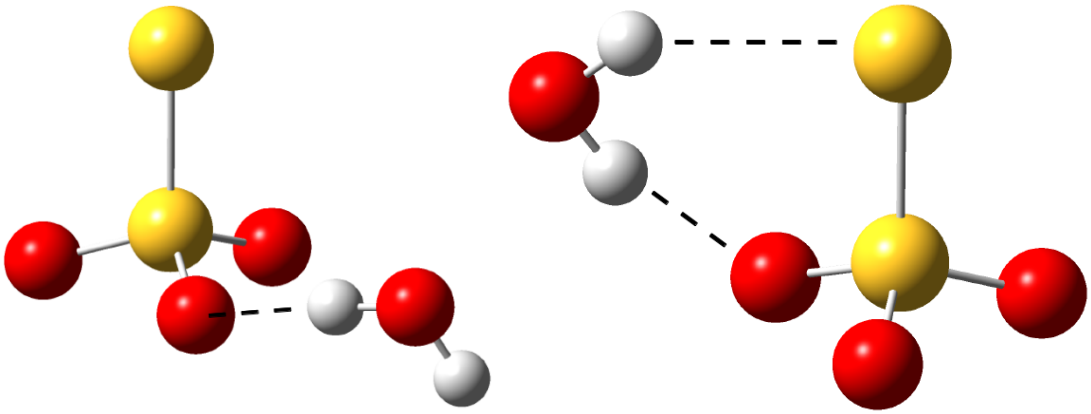

Figure S2

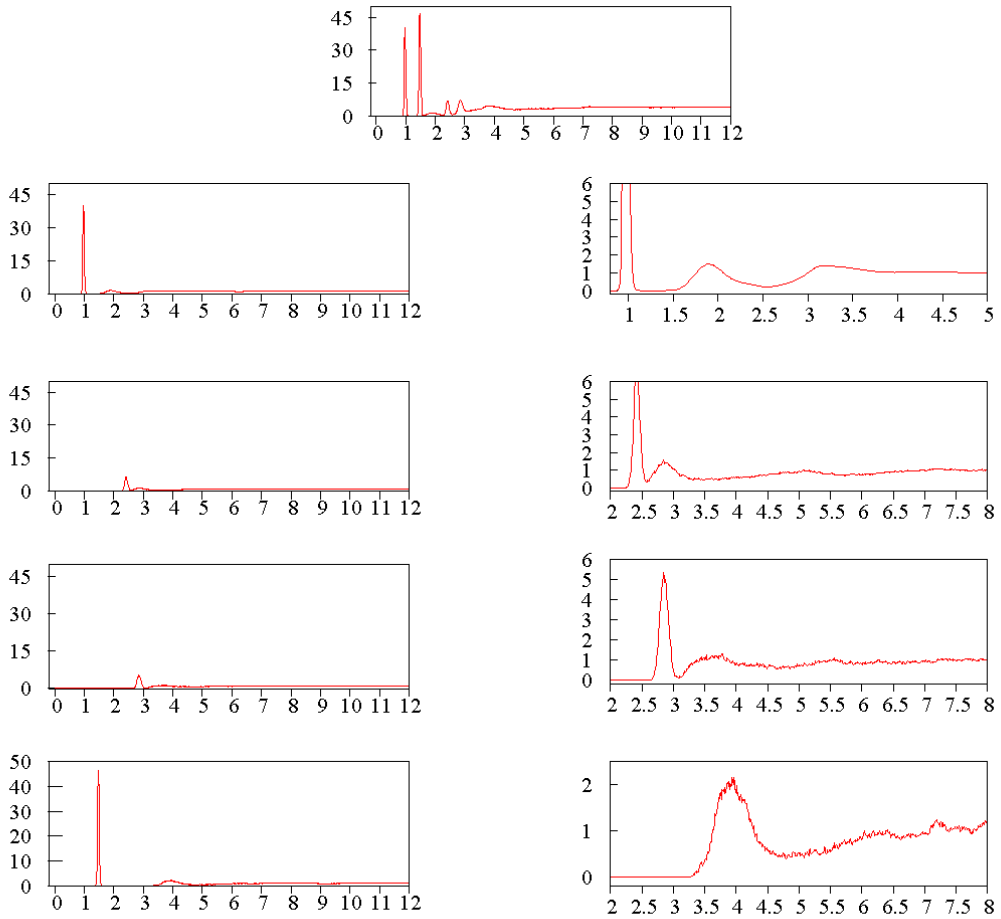
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Figure S3