Electronic Supplementary Material (ESI) for Dalton Transactions.

Structure and water exchange dynamics of hydrated oxo halo ions in aqueous solution using QMCF MD simulation, large angle X-ray scattering and EXAFS

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Electronic Supporting Information

Table S1. Summary of bond distances of oxo halo anions 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. 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.

Chlorite ion, ClO_2^-

ICSD code	***d*(Cl-O)**	**Reference**
1954	1.561 Å	Tarimci, C.; Schempp, E. *Acta Crystallogr., Sect. B* **1975**, *31*, 2146-2149. $NaClO_2 \cdot 3H_2O$
26511	1.562 Å	Gillespie, R. B.; Sparks, R. A.; Trueblood, K. N. *Acta Crystallogr.* **1959**, *12*, 867-872. NH_4ClO_2
22	1.564 Å	Tarimci, C.; Rosenstein, R. D.; Schempp, E. *Acta Crystallogr., Sect. B* **1976**, *32*, 610-612. $NaClO_2$
59935	1.565 Å	Smolentsev, A. I.; Naumov, D. Y. *Acta Crystallogr., Sect. E* **2005**, *61*, i17-i19. $KClO_2$
1858	1.566 Å	Tazzoli, V.; Riganti, V.; Giuseppetti, G.; Coda, A. *Acta Crystallogr., Sect. B* **1975**, *31*, 1032-1037. $NaClO_2 \cdot 3H_2O$
171021	1.570 Å	Smolentsev, A. I.; Naumov, D. Y. *Acta Crystallogr., Sect. E* **2005**, *61*, i249-i250. $Sr(ClO_2)$
170034	1.575 Å	Smolentsev, A. I.; Naumov, D. Y. *Acta Crystallogr., Sect. E* **2005**, *61*, i49-i50. $Ba(ClO_2) \cdot 3H_2O$
59921	1.576 Å	Smolentsev, A. I.; Naumov, D. Y. *Acta Crystallogr., Sect. E* **2005**, *61*, i38-i40. NH_4ClO_2
59936	1.578 Å	Smolentsev, A. I.; Naumov, D. Y. *Acta Crystallogr., Sect. E* **2005**, *61*, i17-i19. $LiClO_2$
162802	1.578 Å	Smolentsev, A. I.; Naumov, D.Y. *Zh. Strukt. Khim.* (Issue-No. from 1981) **2008**, *49*, 725-728. $RbClO_2$
69587	1.580 Å	Marsh, R. E. *Acta Crystallogr., Sect. C* **1991**, *47*, 1775-1775. $[Mg(H_2O)_6](ClO_2)_2$
68485	1.582 Å	Okuda, M.; Ishihara, M.; Yamanaka, M.; Ohba, S.; Saito, Y. *Acta Crystallogr., Sect. C* **1990**, *46*, 1755-1759. $[Mg(H_2O)_6](ClO_2)_2$
162803	1.582 Å	Smolentsev, A. I.; Naumov, D.Y. *Zh. Strukt. Khim.* (Issue-No. from 1981) **2008**, *49*, 725-728. $CsClO_2$
171020	1.585 Å	Smolentsev, A. I.; Naumov, D. Y. *Acta Crystallogr., Sect. E* **2005**, *61*, i246-i248. $Ca(ClO_2)$
Mean	**1.573 Å/14 structures**	

Chlorate ion, ClO_3^-

ICSD/CSD	*d*(Cl-O)	Reference
THURTL	1.451 Å	Mitchell, J..; Boeyens, J. C. A. *Acta Crystallogr., Sect. C* **1998**, *54*, 927. $[TlC_4H_{16}N_8S_4]_n(ClO_3)_n$
AYUXOH	1.455 Å	Chun-Xia Ren; Bao-Hui Ye; Feng He; Lin Cheng; Xiao-Ming Chen *CrystEngComm* **2000**, *6*, 200. $[Ag(C_{12}H_{14}N_4)_2](ClO_3)_2$
HUJVOX	1.457 Å	Gentile, P. S.; Ocampo, A. P. *Inorg. Chim. Acta* **1978**, *29*, 83. $Ca_2(C_4H_7NO_2)_4(ClO_3)_2 \cdot H_2O$
WONGUB	1.463 Å	Xiaopeng Hu; Jiwen Cai; Xiaoleng Feng; Liangnian Ji *J. Chem. Cryst.* **2000**, *30*, 27. $[Co(H_2N(C_2H_4N)_3H_2)(NO_2)_2]ClO_3$
NUMYID	1.467 Å	Todorov, T.; Petrova, R.; Kossev, K.; Macicek, J.; Angelova, O. *Acta Crystallogr., Sect. B* **1970**, *26*, 1121. $[Mg(OC(NH_2)_2)_6](ClO_3)_2$
59383	1.467 Å	Todorov, T.; Petrova, R.; Kossev, K.; Macicek, J.; Angelova, O. *Acta Crystallogr., Sect. C* **1998**, *54*, 927-929. $[Mg(OC(NH_2)_2)_6](ClO_3)_2$
NEWRAJ	1.468 Å	$[Co(H_2NC_2H_4NH_2)(NO_2)_2]ClO_3$
414606	1.472 Å	Sharma, R. P.; Bala, R.; Sharma, R.; Ferretti, V. *Inorg. Chim. Acta* **2005**, *358*, 3457-3464 $[Co(NH_3)_6]Br_2(ClO_3)$
VEQZEX	1.473 Å	Sharma, R. P.; Sharma, R.; Bala, R.; Venugopalan, P. *J. Mol. Struct.* **2006**, *789*, 133. $[Co(H_2NC_2H_4NH_2)Cl_2]ClO_3$
JAXGAR	1.474 Å	Petrosyan, A. M.; Karapetyan, H. A.; Sukiasyan, R. P.; Aghajanyan, A. E.; Morgunov, V. G.; Kravchenko, E. A.; Bush, A. A. *J. Mol. Struct.* **2005**, *752*, 144. $(C_6H_{15}N_4O_2)ClO_3$
1724	1.476 Å	Bats, J. W. *Acta Crystallogr., Sect. B* **1978**, *34*, 1679-1681. $KClO_3$
414607	1.476 Å	Sharma, R. P.; Bala, R.; Sharma, R.; Ferretti, V. *Inorg. Chim. Acta* **2005**, *358*, 3457-3464 $[Co(NH_3)_6]Cl_2(ClO_3)$
16714	1.477 Å	Ramachandran, G. N.; Chandrasekaran, K. S. *Acta Crystallogr.* **1957**, *10*, 671-675. $NaClO_3$
26684	1.477 Å	Zachariasen, W. H. *Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.* **1929**, *71*, 517-529. $NaClO_3$
40285	1.477 Å	Lutz, H. D.; Buchmeier, W.; Jung, M.; Kellersohn, T. *Z. Kristallogr.* **1989**, *189*, 131-139. $Ba(ClO_3)_2$
10283	1.478 Å	Brunton, G. *Mater. Res. Bull.* **1973**, *8*, 791-794. $RbClO_3$
26409	1.478 Å	Danielsen, J.; Hazell, A.; Larsen, F. K. *Acta Crystallogr., Sect. B* **1981**, *37*, 913-915. $KClO_3$
61157	1.478 Å	Lutz, H. D.; Buchmeier, W.; Alici, E.; Eckers, W. *Z. Anorg. Allg. Chem.* **1985**, *529*, 46-56. $Sr(ClO_3)_2$

80338	1.480 Å	Sowa, H. *J. Solid State Chem.* **1995**, *118*, 378-382. $NaClO_3$
80340	1.480 Å	Sowa, H. *J. Solid State Chem.* **1995**, *118*, 378-382. $NaClO_3$
80339	1.482 Å	Sowa, H. *J. Solid State Chem.* **1995**, *118*, 378-382. $NaClO_3$
31120	1.483 Å	Aravindakshan, C. *Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.* **1958**, *111*, 35-45. $KClO_3$
1301	1.485 Å	Abrahams, S. C.; Bernstein, J. L. *Acta Crystallogr., Sect. B* **1977**, *33*, 3601-3604. $NaClO_3$
63712	1.485 Å	Blackburn, A. C.; Gallucci, J. C.; Gerkin, R. E. *Acta Crystallogr., Sect. B* **1991**, *47*, 474-479. $[Cu(H_2O)_4](ClO_3)_2$
80341	1.485 Å	Sowa, H. *J. Solid State Chem.* **1995**, *118*, 378-382. $NaClO_3$
30452	1.486 Å	Sikka, S. K.; Momin, S. N.; Rajagopal, H.; Chidambaram, R. *J. Chem. Phys.* **1968**, *48*, 1883-1890. $Ba(ClO_3)_2 \cdot H_2O$
67106	1.487 Å	Gallucci, J. C.; Gerkin, R. E. *Acta Crystallogr., Sect. C* **1990**, *46*, 350-354. $[Ni(H_2O)_6](ClO_3)_2$
26408	1.488 Å	Danielsen, J.; Hazell, A.; Larsen, F. K. *Acta Crystallogr., Sect. B* **1981**, *37*, 913-915. $KClO_3$
1117	1.490 Å	Bruke-Laing, M. E.; Trueblood, K. N. *Acta Crystallogr., Sect. B* **1977**, *33*, 2698-2699. $NaClO_3$
23935	1.490 Å	Gillespie, R. B.; Gantzel, P. K.; Trueblood, K. N. *Acta Crystallogr.* **1962**, *15*, 1271-1272. NH_4ClO_3
63713	1.490 Å	Blackburn, A. C.; Gallucci, J. C.; Gerkin, R. E. *Acta Crystallogr., Sect. B* **1991**, *47*, 474-479. $[Cu(H_2O)_4](ClO_3)_2$
80337	1.490 Å	Sowa, H. *J. Solid State Chem.* **1995**, *118*, 378-382. $NaClO_3$
31121	1.491 Å	Aravindakshan, C. *Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.* **1959**, *111*, 241-248. $NaClO_3$
Mean	**1.477 Å/33 structures**	

Bromite ion, BrO_2^-

ICSD/CSD	*d*(Br-O)	Reference
4323	1.825 Å	le Bihan, M. T.; Gurtner, B.; Kalt, A. *Bull. Soc. Franc. Mineral. Cristallogr.* **1975**, *98*, 223-226. $LiBrO_2 \cdot H_2O$
74654	1.716 Å	Levason, W.; Ogden, J. S.; Spicer, M. D.; Webster, M.; Young, N. A. *J. Am. Chem. Soc.* **1989**, *111*, 6210-6212. $NaBrO_2 \cdot 3H_2O$

Bromate ion, BrO_3^-

ICSD/CSD	*d*(Br-O)	Reference
28147	1.591 Å	Albertsson, J.; Elding, L. I. *Acta Crystallogr., Sect. B* **1977**, *33*, 1460-1469. $[Pr(H_2O)_9](BrO_3)_2$
28148	1.592 Å	Albertsson, J.; Elding, L. I. *Acta Crystallogr., Sect. B* **1977**, *33*, 1460-1469. $[Yb(H_2O)_9](BrO_3)_2$
23757	1.608 Å	Sikka, S. K. *Acta Crystallogr., Sect. A* **1969**, *25*, 621-626. $[Sm(H_2O)_9](BrO_3)_2$
AYUXIB	1.629 Å	Chun-Xia Ren, Bao-Hui Ye, Feng He, Lin Cheng, Xiao-Ming Chen *CrystEngComm* **2004**, *6*, 200. $[Ag_2C_{24}H_{28}N_8](BrO_3)_2$
BASLEM	1.634 Å	Paduan-Filho, A.; Sinn, E.; Chirico, R. D.; Carlin, R. L. *Inorg. Chem.* **1981**, *20*, 2688. $[Ni(ONC_5H_5)_6](BrO_3)_2$
415732	1.640 Å	Sharma, R. P.; Bala, R.; Sharma, R.; Perez, J.; Miguel, D. *J. Mol. Struct.* **2006**, *788*, 49-54. $[Co(NH_3)_6](BrO_3)_3 \cdot 0.5H_2O$
JAXFOE	1.641 Å	Petrosyan, A. M; Karapetyan, H. A.; Sukiasyan, R. P.; Aghajanyan, A. E.; Morgunov, V. G.; Kravchenko, E. A.; Bush, A. A. *J. Mol. Struct.* **2005**, *752*, 144. $(C_6H_{15}N_4O_2)BrO_3$
UKEHEX	1.641 Å	Cingolani, A.; Effendy; Hanna, J. V.; Pellei, M.; Pettinari, C.; Santini, C.; Skelton, B. W.; White, A. H. *Inorg. Chem.* **2003**, *42*, 4938. $[Ag(As(C_6H_5)_3)_4]BrO_3 \cdot CH_3OH$
VEQSAT	1.641 Å	Sharma, R. P.; Sharma, R.; Bala, R.; Venugopalan, P. *J. Mol. Struct.* **2006**, *789*, 133. $[Co(H_2N(CH_2)_2NH_2)_2]Cl_2](BrO_3)_2$
1302	1.648 Å	Abrahams, S. C.; Bernstein, J. L. *Acta Crystallogr., Sect. B* **1977**, *33*, 3601-3604. $NaBrO_3$
47173	1.648 Å	Templeton, D. H.; Templeton, L. K. *Acta Crystallogr., Sect A* **1985**, *41*, 133-142. $KBrO_3$
71863	1.649 Å	Blackburn, A. C.; Gallucci, J. H.; Gerkin, R. E. *Acta Crystallogr., Sect. C* **1992**, *48*, 1185-1188.

		$[Al(H_2O)_6](BrO_3)_2 \cdot 3H_2O$
404779	1.649 Å	Peter, S.; Suchanek, E.; Esser, D.; Lutz, H. D. *Z. Naturforsch., Teil B* **1996**, *51*, 1072-1072. $[Mg(H_2O)_6](BrO_3)_2$
71532	1.650 Å	Blackburn, A. C.; Gallucci, J. H.; Gerkin, R. E. *Acta Crystallogr., Sect. C* **1991**, *47*, 2019-2023. $[Cu(H_2O)_6](BrO_3)_2$
74767	1.651 Å	Szafranski, M.; Ståhl, K. *Z. Kristallogr.* **1994**, *209*, 491-494. $KBrO_3$
47174	1.653 Å	Templeton, D. H.; Templeton, L. K. *Acta Crystallogr., Sect A* **1985**, *41*, 133-142. $NaBrO_3$
68733	1.653 Å	Blackburn, A. C.; Gallucci, J. H.; Gerkin, R. E. *Acta Crystallogr., Sect. B* **1990**, *46*, 712-716. $[Co(H_2O)_6](BrO_3)_2$
74768	1.653 Å	Szafranski, M.; Ståhl, K. *Z. Kristallogr.* **1994**, *209*, 491-494. $RbBrO_3$
74769	1.654 Å	Szafranski, M.; Ståhl, K. *Z. Kristallogr.* **1994**, *209*, 491-494. $CsBrO_3$
69588	1.655 Å	Blackburn, A. C.; Gallucci, J. H.; Gerkin, R. E. *Acta Crystallogr., Sect. C* **1991**, *47*, 1786-1789. $[Ni(H_2O)_6](BrO_3)_2$
33663	1.682 Å	Zachariasen, W. H. *Norske Videnskaps-Akademi i Oslo 1*, **1928**, 1-165. $KBrO_3$
79821	1.683 Å	Lutoslawska-Rogoz, J.; Kapturkiewicz-Kowal, E.; Hodorowicz, S. A. *Cryst. Res. Technol.* **1995**, *30*, 255-262. $[Mg(H_2O)_6](BrO_3)_2$
UKEHAT	1.690 Å	Cingolani, A.; Effendy; Hanna, J. V.; Pellei, M.; Pettinari, C.; Santini, C.; Skelton, B. W.; White, A. H. *Inorg. Chem.* **2003**, *42*, 4938. $[Ag(As(C_6H_5)_3)_4]BrO_3 \cdot CH_3OH$
Mean	**1.646 Å/17 structures**	

Perbromate ion, BrO_4^-

ICSD/CSD	*d*(Br-O)	Reference
DEBSUY	1.580 Å	Beno, M. A.; Blackman, G. S.; Leung, P. C. W.; Carlson, K. D.; Copps, P. T.; Williams, J. M. *Mol. Cryst. Liq. Cryst.* **1985**, *119*, 409. $(C_{10}H_8S_8)_2(C_{10}H_8S_8)(BrO_4)_2$
CIYFOF	1.581 Å	Williams, J. M.; Beno, B. A.; Wang, H.-H.; Reed, P. E.; Azevedo, L. J.; Schirber, J. E. *Inorg. Chem.* **1984**, *23*, 1790. $(C_{10}H_8S_8)(C_{10}H_8S_8)BrO_4$
71538	1.601 Å	Blackburn, A. C.; Gallucci, J. C.; Gerkin, R. E.; Reppart, W. J. *Acta Crystallogr., Sect. C* **1992**, *48*, 419-424. $NaBrO_4 \cdot H_2O$
65047	1.603 Å	Gallucci, J. C.; Gerkin, R. E.; Reppart, W. J. *Acta Crystallogr., Sect. C* **1988**, *44*, 1345-1348. $[Ni(H_2O)_6]BrO_4$
73599	1.603 Å	Roegner, P.; Schiessl, U.; Range, K. J. *Z. Naturforsch., Teil B* **1993**, *48*, 235-236. $CsBrO_4$
68493	1.607 Å	Gallucci, J. C.; Gerkin, R. E.; Reppart, W. J. *Acta Crystallogr., Sect. C* **1990**, *46*, 1580-1584. $[Ni(H_2O)_6]BrO_4$
73397	1.608 Å	Blackburn, A. C.; Gerkin, R. E. *Acta Crystallogr., Sect. C* **1993**, *49*, 1271-1275. $[Co(H_2O)_6]BrO_4$
15222	1.609 Å	Siegel, S.; Tani, B. S.; Appelman, E. *Inorg. Chem.* **1969**, *8*, 1190-1191. $KBrO_4$
201158	1.610 Å	Gebert, E.; Peterson, S. W.; Reis, Jr., A. H..; Appelman, E. H. *J. Inorg. Nucl. Chem.* **1981**, *43*, 3085-3089. $CsBrO_4$
BUYRAO10	1.611 Å	Beno, M. A.; Blackman, G. S.; Leung, P. C. W.; Carlson, K. D.; Copps, P. T.; Williams, J. M. *Mol. Cryst. Liq. Cryst.* **1985**, *119*, 409. $(C_{10}H_8S_8)(C_{10}H_8S_8)BrO_4 \cdot 0.5C_2H_3Cl_3$
79714	1.611 Å	Blackburn, A. C.; Gerkin, R. E. *Acta Crystallogr., Sect. C* **1995**, *51*, 3-7. $LiBrO_4 \cdot H_2O$
CIYFOF01	1.614 Å	Williams, J. M.; Beno, B. A.; Wang, H.-H.; Reed, P. E.; Azevedo, L. J.; Schirber, J. E. *Inorg. Chem.* **1984**, *23*, 1790. $(C_{10}H_8S_8)(C_{10}H_8S_8)BrO_4$
165085	1.614 Å	Tutov, A. G.; Gavrilov, V. V.; Isupov, V. K.; Kolycheva, T. I.; Fundamenskii, V. S. *Zh. Neorg. Khim.* **1986**, *31*, 589-592. NH_4BrO_4
73706	1.623 Å	Blackburn, A. C.; Gallucci, J. C.; Gerkin, R. E.; Reppart, W. J. *Acta Crystallogr., Sect. C* **1993**, *49*, 1437-1439. $LiBrO_4 \cdot 3H_2O$
Mean	**1.605 Å/14 structures**	

Iodate ion, IO_3^-

ICSD/CSD	*d*(I-O)	Reference
LOFKOG	1.785 Å	Terzyan, S. S.; Petrosyan, A. M. *Kristallografiya* **1999**, *44*, 846. $N(CH_3)_4IO_4 \cdot 2H_2O$
20198	1.787 Å	Kalinin, V. P.; Ilyukhin, V. V.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1978**, *239*, 590-593. KIO_3
97995	1.790 Å	Kasatani, H.; Aoyagi, S.; Kuroiwa, Y.; Yagi, K.; Katayama, R.; Terauchi, H. *Nucl. Instr. Methods Phys. Res. B* **2003**, *199*, 49-53. KIO_3
86285	1.792 Å	Chen, Y.; Zhang, P.-L.; Yan, Q.-W.; Cheng, Y.-F.; Cheng, Z.-X. *Wu Li Hsueh Pao* **1986**, *35*, 1102-1107. $K_2(IO_3)Cl \cdot HIO_3$
201816	1.792 Å	Crettez, J. M.; Coquet, E.; Pannetier, J.; Bouillot, J.; Durand-Le Floch, M. *J. Solid State Chem.* **1985**, *56*, 133-147. $Li(IO_3)$
2642	1.794 Å	Schulz, H. *Acta Crystallogr., Sect B* **1973**, *29*, 2285-2289. $LiIO_3$
23772	1.794 Å	Chan, L. Y. Y.; Einstein, F. W. B. *Can. J. Chem.* **1971**, *49*, 468-476. $KIO_3 \cdot HIO_3$
9508	1.796 Å	Emiraliev, A.; Kocharov, A. G.; Yamzin, I. I.; Lyubimtsev, V. A. *Kristallografiya* **1973**, *18*, 1177-1181 $LiIO_3$
35474	1.800 Å	Coquet, E.; Crettez, J. M.; Pannetier, J.; Bouillot, J.; Damien, J. C. *Acta Crystallogr., Sect. B* **1983**, *39*, 408-413. $LiIO_3$
35646	1.801 Å	Averbuch-Pouchot, M. T. *J. Solid State Chem.* **1983**, *49*, 368-378. $NH_4IO_3 \cdot Te(OH)_6 \cdot H_2O$
156001	1.801 Å	Chen Xue An; Zhang Li; Chang Xi Nan; Xue Hai Ping; Zang Hegui; Xiao Wei Qiang; Song Xuemei; Yan Hui *J. Alloys Compd.* **2007**, *428*, 54-58. $KIO_3 \cdot MoO_3$
200669	1.801 Å	Kalinin, V.R.; Ilyukhin, V. V.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1978**, *241*, 583-585. $RbLi_2(IO_3)_3$
200793	1.801 Å	Soldatov, E. A.; Ilyukhin, V. V.; Kuz'min, E. A.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1980**, *252*, 108-110. $NH_4(IO_3) \cdot 2HIO_3$
40361	1.803 Å	Svensson, C.; Albertsson, J.; Liminga, R.; Kvick, Å.; Abrahams, S. C. *J. Chem. Phys.* **1983**, *78*, 7343-7352. $LiIO_3$
20858	1.804 Å	Sorokina, N. I.; Murodyan, L. A.; Loshmanov, A. A.; Fykin, L. E.; Rider, E. E.; Dobrzhanskii, G. F.; Simonov, V. I. *Kristallografiya* **1984**, *29*, 220-227. $NH_4(IO_3) \cdot 2HIO_3$

23695	1.804 Å	Keve, E. T.; Abrahams, S. C.; Bernstein, J. L. *J. Chem. Phys.* **1971**, *54*, 2556-2563. NH_4IO_3
200239	1.805 Å	Sorokina, N. I.; Ilyukhin, V. V.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1977**, *236*, 1361-1363. $(C(NH_2)_3)IO_3$
414608	1.805 Å	Sharma, R. P.; Bala, R.; Sharma, R.; Ferretti, V. *Inorg. Chim. Acta* **2005**, *358*, 3457-3464. $[Co(NH_3)_6]Cl_2(IO_3)\cdot H_2O$
420353	1.805 Å	Gautier Luneau, I.; Suffren, Y.; Jamet, H.; Pilme, J. *Z. Anorg. Allgem. Chem.* **2010**, *636*, 1368-1379. $Cs_2(IO_3)(I_3O_8)$
35645	1.806 Å	Averbuch-Pouchot, M. T. *J. Solid State Chem.* **1983**, *49*, 368-378. $KIO_3\cdot Te(OH)_6$
35647	1.806 Å	Averbuch-Pouchot, M. T. *J. Solid State Chem.* **1983**, *49*, 368-378. $(KIO_3)_2\cdot Te(OH)_6$
14045	1.807 Å	Kalinin, V. P.; Karataeva, I. M.; Vinogradov, E. E.; Vavilin, V. I.; Plyukhin, V. V.; Pakhomov, V. I. *Koord. Khim.* **1978**, *4*, 444-447. $RbLi_2(IO_3)_3$
62499	1.807 Å	Sorokina, N. I.; Loshmanov, A. A.; Fykin, L. E.; Rider, E. E. *Kristallografiya* **1985**, *30*, 895-898. $KIO_3\cdot HIO_3$
80025	1.807 Å	Cheng, Y.-F.; Yang, Z.; Cheng, Z.-X.; Guo, L.-P. *Jiegon Huaxue* **1995**, *14*, 11-14. $LiIO_3$
80026	1.807 Å	Cheng, Y.-F.; Yang, Z.; Cheng, Z.-X.; Guo, L.-P. *Jiegon Huaxue* **1995**, *14*, 11-14. $LiIO_3$
405832	1.807 Å	Suchanek, E.; Peter, S.; Lutz, H. D. *J. Mol. Struct.* **1997**, *416*, 249-260. $[Ca(H_2O)_6](IO_3)_2$
ICAYEQ	1.807 Å	Petrosyan, A. M.; Burbelo, V. M.; Tamazyan, R. A.; Karapetyan, H. A.; Sukiasyan, R. P. *Z. Naturforsch., Teil B* **2000**, *55*, 119. $(H_3NCH_3CHCOOH)IO_3\cdot H_2O$
2825	1.808 Å	Alcock, N. W. *Acta Crystallogr., Sect B* **1972**, *28*, 2783-2788. $RbIO_3$
20168	1.808 Å	Sorokina, N. I.; Ilyukhin, V. V.; Pakhomov, V. I.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1979**, *249*, 613-616. $NaIO_3$
47138	1.808 Å	Podlahova, J.; Loub, J.; Pechar, F.; Petricek, V. *Acta Crystallogr., Sect. C* **1984**, *40*, 1999-2001. $KIO_3\cdot Te(OH)_6$
200804	1.808 Å	Soldatov, E. A.; Ilyukhin, V. V.; Kuz'min, E. A.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1980**, *252*, 615-618. $Rb(IO_3)\cdot 2HIO_3$
202679	1.808 Å	Svensson, C.; Ståhl, K. *J. Solid State Chem.* **1988**, *77*, 112-116. $NaIO_3$
ICAYAM	1.808 Å	Petrosyan, A. M.; Burbelo, V. M.; Tamazyan, R. A.; Karapetyan, H. A.; Sukiasyan, R. P. *Z. Naturforsch., Teil B* **2000**, *55*, 119. $(H_3N(CH_2)_2COOH)IO_3\cdot H_2O$
14344	1.809 Å	de Boer, J. L.; van Bolhuis, F.; Olthof-Hazekamp, R.; Vos, A. *Acta Crystallogr.* **1966**, *21*, 841-843. $LiIO_3$
420354	1.809 Å	Gautier Luneau, I.; Suffren, Y.; Jamet, H.; Pilme, J. *Z. Anorg. Allgem. Chem.* **2010**, *636*, 1368-1379.

		$Rb_2(IO_3)(I_3O_8)\cdot 2HIO_3\cdot H_2O$
TULRIB	1.809 Å	Haussuhl, S.; Schreuer, J. *Z. Kristallogr.* **1996**, *211*, 903. $(C_5H_{12}NO_2)HI_2O_6\cdot HIO_3$
10306	1.810 Å	Kemper, G.; Vos, A.; Rietveld, H. M. *Can. J. Chem.* **1972**, *50*, 1134-1143. $KIO_3\cdot HIO_3$
200717	1.811 Å	Kalinin, V. R.; Ilyukhin, V. V.; Pakhomov, V. I.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1978**, *239*, 318-321. $KIO_3\cdot HIO_3$
20209	1.812 Å	Kalinin, V.R.; Ilyukhin, V. V.; Belov, N. V. *Dokl. Akad. Nauk SSSR* **1978**, *239*, 1340-1342. $K_2(IO_3)(NO_3)\cdot 2HIO_3$
202145	1.812 Å	Bordet, P.; Boucherle, J. X.; Santoro, A.; Marezio, M. *Solid State Ionics* **1986**, *21*, 243-254. $NH_4(IO_3)\cdot 2HIO_3$
423584	1.812 Å	Belokoneva, E. L.; Stefanovich, S. Y.; Dimitrova, O. V. J. Solid State Chem. 2012, 195, 79-85. KIO_3
61009	1.813 Å	Wang, C.-G. *Hua Hsueh Hsueh Pao* **1985**, *43*, 271-274. $CsIO_3$
202144	1.814 Å	Bordet, P.; Boucherle, J. X.; Santoro, A.; Marezio, M. *Solid State Ionics* **1986**, *21*, 243-254. $NH_4(IO_3)\cdot 2HIO_3$
280857	1.814 Å	Sykora, R.E.; Ok, K. M.; Halasyamani, P. S.; Albrecht Schmitt, T. E. *J. Am. Chem. Soc.* **2002**, *124*, 1951-1957. $KIO_3\cdot MoO_3$
280859	1.814 Å	Sykora, R.E.; Ok, K. M.; Halasyamani, P. S.; Albrecht Schmitt, T. E. *J. Am. Chem. Soc.* **2002**, *124*, 1951-1957. $CsIO_3\cdot MoO_3$
410914	1.814 Å	Engelen, B.; Gavrilko, T.; Panthoefer, M.; Puchkovskaya, G.; Sekirin, I. *J. Mol. Struct.* **2000**, *523*, 163-173. $KIO_3\cdot HIO_3$
416527	1.814 Å	Gerken, M.; Hazendonk, P.; Iuga, A.; Mack, J. P.; Mercier, H. P. A.; Schrobilgen, G. J. D. *J. Fluor. Chem.* **2006**, *127*, 1328-1338. $(CH_3)_4N(IO_3)$
HIRMOK	1.814 Å	Petrosyan, A. M.; Sukiasyan, R. P.; Terzyan, S. S.; Burbelo, V. M. *Acta Crystallogr., Sect. B* **1999**, *55*, 221. $(C_6H_{16}NO_2)(HI_2O_6)IO_3$
REWRUH	1.814 Å	Gerken, M.; Hazendonk, P.; Iuga, A.; Mack, J. P.; Mercier, H. P.A.; Schrobilgen, G. J. *J. Fluorine Chem.* **2006**, *127*, 1328. $N(CH_3)_4IO_4$
14377	1.817 Å	Rosenzweig, A.; Morosin, B. *Acta Crystallogr.* **1966**, *21*, 758-761. $LiIO_3$
15564	1.818 Å	MacGillavry, C. H.; Panthaleon van Eck, C. L. Rec. Trav. Chim. Pays-Bas Belg. 1943, 62, 729-736. $NaIO_3$
423864	1.819 Å	Bayarjargal, L.; Wiehl, L.; Friedrich, A.; Winkler, B.; Juarez-Arellano, E. A.; Morgenroth, W.; Haussuehl, E. *J.*

		Physics: Condensed Matter **2012**, *24*, 325401-11. KIO_3
280858	1.820 Å	Sykora, R.E.; Ok, K. M.; Halasyamani, P. S.; Albrecht Schmitt, T. E. *J. Am. Chem. Soc.* **2002**, *124*, 1951-1957. $RbIO_3 \cdot MoO_3$
ICAYIU	1.823 Å	Petrosyan, A. M.; Burbelo, V. M.; Tamazyan, R. A.; Karapetyan, H. A.; Sukiasyan, R. P. *Z. Naturforsch., Teil B* **2000**, *55*, 119. $(H_3N(CH_2)_4CH(NH_3)COOH)(IO_3)_2 \cdot 4HIO_3$
247719	1.832 Å	Bayarjargal, L.; Wiehl, L.; Friedrich, A.; Winkler, B.; Juarez-Arellano, E. A.; Morgenroth, W.; Haussuehl, E. *J. Physics: Condensed Matter* **2012**, *24*, 325401-11. KIO_3
Mean	**1.807 Å/55 structures**	

Metaperiodate ion, IO_4^-

ICSD/CSD	*d*(I-O)	Reference
BUAMPI	1.672 Å	Carpy, A.; Goursolle, M.; Leger, J. M..; Nivaud, E. *KC. R. Acad. Sci., Ser.C (Chim)* **1977**, *285*, 311. $N(C_4H_9)_4IO_4$
ROQLIS	1.668 Å	Belaj, F.; Trnoska, A.; Nachbaur, E. *Z. Kristallogr.* **1997**, *212*, 355. $[NaO_6C_{18}H_{36}N_2])IO_4$
VAVTAO	1.693 Å	Campos-Fernandez, C. S.; Schottel, B. L.; Chifotides, H. T.; Bera, J. K.;Bacsa, J.; Koomen, J. M.; Russell, D. H.; Dunbar, K. R. *J. Am. Chem. Soc.* **2005**, *127*, 12909. $[Ni_4C_{56}H_{52}N_{28}O_{48}]ClO_4(IO_4)_7 \cdot 3CH_3CN$
HOHMOG01	1.735 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2001**, *13*, 11053. $(C_5H_6N)IO_4$
HOHMOG02	1.737 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2001**, *13*, 11053. $(C_5H_6N)IO_4$
ZZZUYA02	1.738 Å	Wagner, R. I.; Bau, R.; Gnann, R. Z.; Jones, P. F.; Christe, K. O. *Inorg. Chem.* **1997**, *36*, 2564. $N(CH_3)_4IO_4$
HOHMOG04	1.745 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2003**, *15*, 5663. $(C_5H_6N)IO_4$
83375	1.747 Å	de Waal, D.; Zabel, M.; Range, K. J. *Naturforschung, Teil B* **1996**, *51*, 441-443. $CsIO_4$
89509	1.748 Å	Hoppe, R.; Fischer, D.; Schneider, J. *Z. Anorg. Allgem. Chem.* **1999**, *625*, 1135-1142. $CsIO_4$
HOHMOG03	1.750 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2001**, *13*, 11053. $(C_5H_6N)IO_4$
HOHMOG07	1.751 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2003**, *15*, 5663. $(C_5H_6N)IO_4$
HOHMOG06	1.752 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2003**, *15*, 5663. $(C_5H_6N)IO_4$
HOHMOG	1.752 Å	Dutkiewicz, G.; Pajak, Z. *Z. Naturforsch., Teil B* **1998**, *53*, 1323. $(C_5H_6N)IO_4$
83365	1.759 Å	de Waal, D.; Range, K. J. *Z. Naturforschung, Teil B* **1996**, *51*, 1365-1367. $RbIO_4$
83377	1.761 Å	de Waal, D.; Range, K. J. *Naturforschung, Teil B* **1996**, *51*, 444-446. KIO_4
400552	1.761 Å	Kraft, T.; Jansen, M. *Z. Anorg. Allgem. Chem.* **1995**, *621*, 484-487. $LiIO_4$

83376	1.762 Å	de Waal, D.; Range, K. J. *Naturforschung, Teil B* **1996**, *51*, 444-446. KIO_4
89510	1.765 Å	Hoppe, R.; Fischer, D.; Schneider, J. *Z. Anorg. Allgem. Chem.* **1999**, *625*, 1135-1142. $RbIO_4$
83365	1.766 Å	de Waal, D.; Range, K. J. *Z. Naturforschung, Teil B* **1996**, *51*, 1365-1367. $RbIO_4$
WEMSUD	1.767 Å	Sharma, R. P.; Sharma, R.; Bala, R.; Burrows, A. D.; Mahon, M. F.; Cassar, K. *J. Mol. Struct.* **2006**, *794*, 173. $[Co(H_2N(CH_2)_2NH_2)_2Cl_2]IO_4$
14287	1.769 Å	Kalman, A.; Cruickshank, D. W. J. *Acta Crystallogr., Sect. B* **1970**, *26*, 1782-1785. $NaIO_4$
HOHMOG05	1.772 Å	Maluszynska, H.; Czarnecki, P.; Lewicki, S.; Wasicki, J.; Gdaniec, M. *J. Phys.: Condens. Matter* **2003**, *15*, 5663. $(C_5H_6N)IO_4$
LANNEU	1.772 Å	Sharma, R. P.; Sharma, R.; Bala, R.; Bond, A. D. *Acta Crystallogr., Sect. E* **2005**, *61*, m997. $[Co(H_2N(CH_2)_2NH_2)_2(NO_2)_2]IO_4$
280083	1.773 Å	Levason, W.; Webster, M. *Acta Crystallogr., Sect. C* **1999**, *55*, 1-1. NH_4IO_4
Mean	**1.756 Å/21 structures**	

Orthoperiodate ion, $H_6IO_6^+$, H_5IO_6, $H_4IO_6^-$, $H_3IO_6^{2-}$, $H_2IO_6^{3-}$, HIO_6^{4-}, HIO_6^{5-}

ICSD/CSD	***d*(I-O)**	**Reference**
15398	1.848 Å	Feikema, Y. D. *Acta Crystallogr.* **1961**, *14*, 315-316. H_5IO_6
25791	1.851 Å	Feikema, Y. D. *Acta Crystallogr.* **1966**, *20*, 765-769. H_5IO_6
380001	1.869 Å	Kraft, T.; Jansen, M. *Chem. Ber.* **1993**, *126*, 2415-2419. $(H_6IO_6)(HSO_4)$
380002	1.869 Å	Kraft, T.; Jansen, M. *Chem. Ber.* **1993**, *126*, 2415-2419. $(H_6IO_6)(HSO_4)$
25790	1.871 Å	Feikema, Y. D. *Acta Crystallogr.* **1966**, *20*, 765-769. H_5IO_6
16447	1.878 Å	Tichy, K.; Rueegg, A.; Benes, J. *Acta Crystallogr., Sect B* **1980**, *36*, 1028-1032. $(ND_4)D_3IO_6$
16446	1.879 Å	Tichy, K.; Rueegg, A.; Benes, J. *Acta Crystallogr., Sect B* **1980**, *36*, 1028-1032. $(NH_4)H_3IO_6$
400439	1.879 Å	Kraft, T.; Jansen, M. *Anorg. Allgem. Chem.* **1994**, *620*, 805-808. $Li(H_4IO_6)\cdot H_2O$
BOVMEE	1.879 Å	Fabry, F.; Podlahova, J.; Loub, J.; Langer, V. *Acta Crystallogr., Sect. B* **1982**, *38*, 1048. $(NH_2)_2CO\cdot OI(OH)_5$
400104	1.880 Å	Jansen, M.; Kraft, T. *Z. Anorg. Allgem. Chem.* **1994**, *620*, 53-57. $Li_2(H_3IO_6)$
200568	1.882 Å	Abrahams, S. C.; Bernstein, J. L. *J. Chem. Phys.* **1978**, *69*, 4234-4237. $Na(H_3O)H_3IO_6$
69554	1.887 Å	Kellersohn, T. *Acta Crystallogr., Sect. C* **1991**, *47*, 1133-1136. $K_2Na(H_2IO_6)\cdot 4H_2O$
202560	1.890 Å	Hoppe, R.; Schneider, J. *J. Less-Common Met.* **1988**, *137*, 85-103. $K_4Li(IO_6)$
62102	1.899 Å	Untenecker, H.; Hoppe, R. *Z. Anorg. Allgem. Chem.* **1987**, *549*, 129-138. $K_9Li_3(IO_6)_2O$
65443	1.905 Å	Schneider, J.; Hoppe, R. *Z. Anorg. Allgem. Chem.* **1989**, *574*, 54-164. $K_9Na(IO_6)[Au_2O]$
66248	1.912 Å	Jansen, M.; Rehr, A. *Z. Anorg. Allgem. Chem.* **1988**, *567*, 95-100. $Na_2H_3IO_6$
77725	1.912 Å	Kraft, T.; Jansen, M. *Angew. Chem., German Ed.* **1997**, *109*, 1842-1843. HIO_4
16007	1.917 Å	Bigoli, F.; Manotti Lanfredi, A. M.; Tiripicchio, A.; Tiripicchio Camellini, M. *Acta Crystallogr.* **1970**, *26*, 1075-1079. $[Mg(H_2O)_6]H_3IO_6$
77726	1.932 Å	Kraft, T.; Jansen, M. *Angew. Chem., German Ed.* **1997**, *109*, 1842-1843. HIO_4
Mean	**1.886 Å/19 structures**	

Pentaoxoiodate, IO_5^{3-}

ICSD/CSD	***d*(I-O)**	**Reference**
4325, 10102	1.786 Å	Trömel, M.; Dölling, H. *Z. Anorg. Allgem. Chem.* **1975**, *411*, 41-48. KIO_5
4326	1.803 Å	Trömel, M.; Dölling, H. *Z. Anorg. Allgem. Chem.* **1975**, *411*, 49-53. $RbIO_5$
23624	1.773 Å	Dölling, H.; Trömel, M. *Naturwissenschaften* **1973**, *60*, 153-154. KIO_5
Mean	**1.787 Å/3 structures**	

Legends to Figures

Figure S1. LAXS, chlorite ion. Top: the individual peak shapes for all contributing species in the 1.5006 mol·dm^{-3} aqueous solution of sodium chlorite, the hydrated chlorite 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, $si_{exp}(s)$ (thin black line); model $si_{calc}(s)$ (red line).

Figure S2. LAXS, perchlorate ion. Top: the individual peak shapes for all contributing species in the 1.5006 mol·dm^{-3} aqueous solution of perchloric acid, the hydrated perchlorate ion (orange line), hydrated oxonium 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, $si_{exp}(s)$ (thin black line); model $si_{calc}(s)$ (red line).

Figure S3. Simulation data $D(r)/4pr^2\rho_o$ of the Cl---O distances of chlorite (top), chlorate (middle) and perchlorate (bottom), with full range displayed on the left side and focused on the features in the area between 3 and 5 Å for each ion.

Figure S4. LAXS, hypochlorite ion. Top: the individual peak shapes for all contributing species in the 1.5006 mol·dm^{-3} aqueous solution of sodium hypochlorite, the hydrated hypochlorite 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, $si_{exp}(s)$ (thin black line); model $si_{calc}(s)$ (red line).

Figure S5. LAXS, bromate ion. Top: the individual peak shapes for all contributing species in the 1.5006 mol·dm^{-3} aqueous solution of sodium bromate, the hydrated bromate 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 S6. LAXS, iodate ion. Top: the individual peak shapes for all contributing species in the 1.5006 mol·dm^{-3} aqueous solution of sodium iodate, the hydrated iodate 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 S7. LAXS, metaperiodate ion. Top: the individual peak shapes for all contributing species in the 1.5006 mol·dm^{-3} aqueous solution of sodium metaperiodate, the hydrated metaperiodate 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 S8. Upper: k^3 weighted EXAFS of (a) solid sodium orthoperiodate, offset: 16, (b) aqueous solution of sodium orthoperiodate, offset: 18, (c) solid sodium metaperiodate, offset: 4, (d) aqueous solution of solid sodium metaperiodate, no offset; experiment (thin black line); model (red line).

Figure S9. Upper: Fourier transform of the k^3 weighted EXAFS function of solid sodium orthoperiodate, offset: 1.5, (b) aqueous solution of sodium orthoperiodate, offset: 1.0, (c) solid sodium metaperiodate, offset: 0.5,(d) aqueous solution of solid sodium metaperiodate, no offset; experiment (thin black line); model (red line).

Figure S10. Angular radial distribution functions for the hydrated perchlorate (left panel) and sulfate (right panels) ions; enlarged part of Figure 7. Notice the more well-defined positions of the hydrating water molecules around the sulfate ion in comparison to the perchlorate ion.

Figure S1

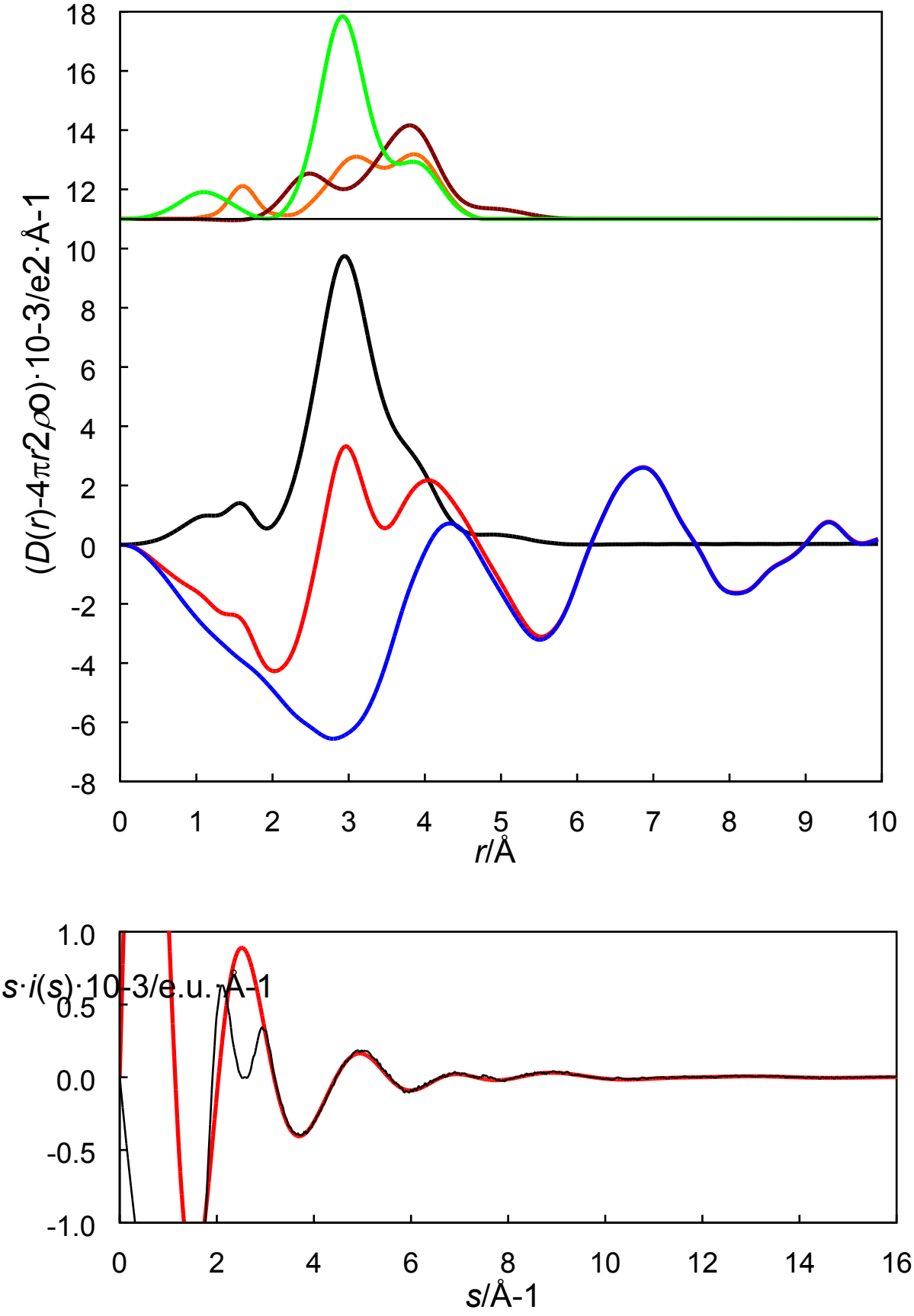


Figure S2

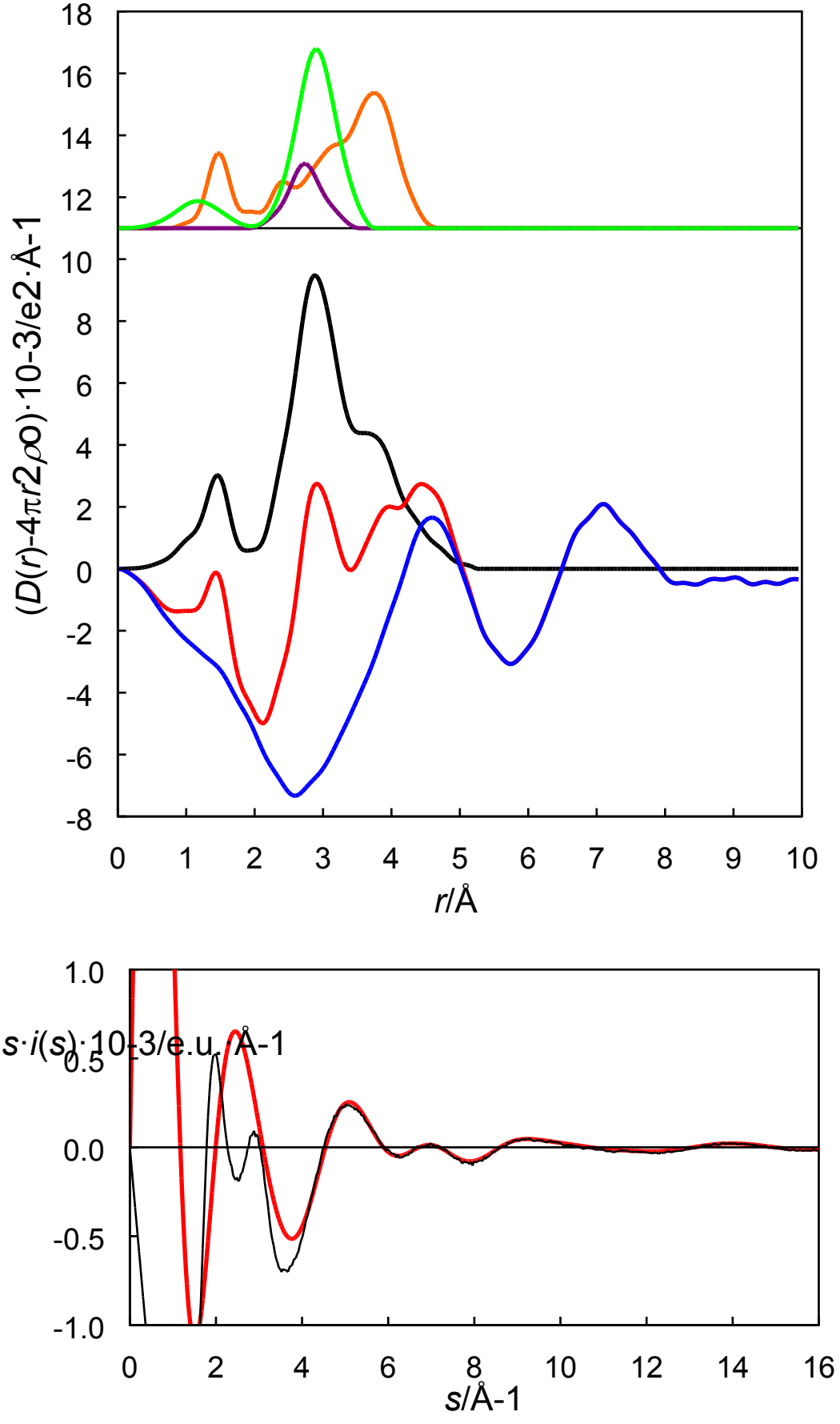
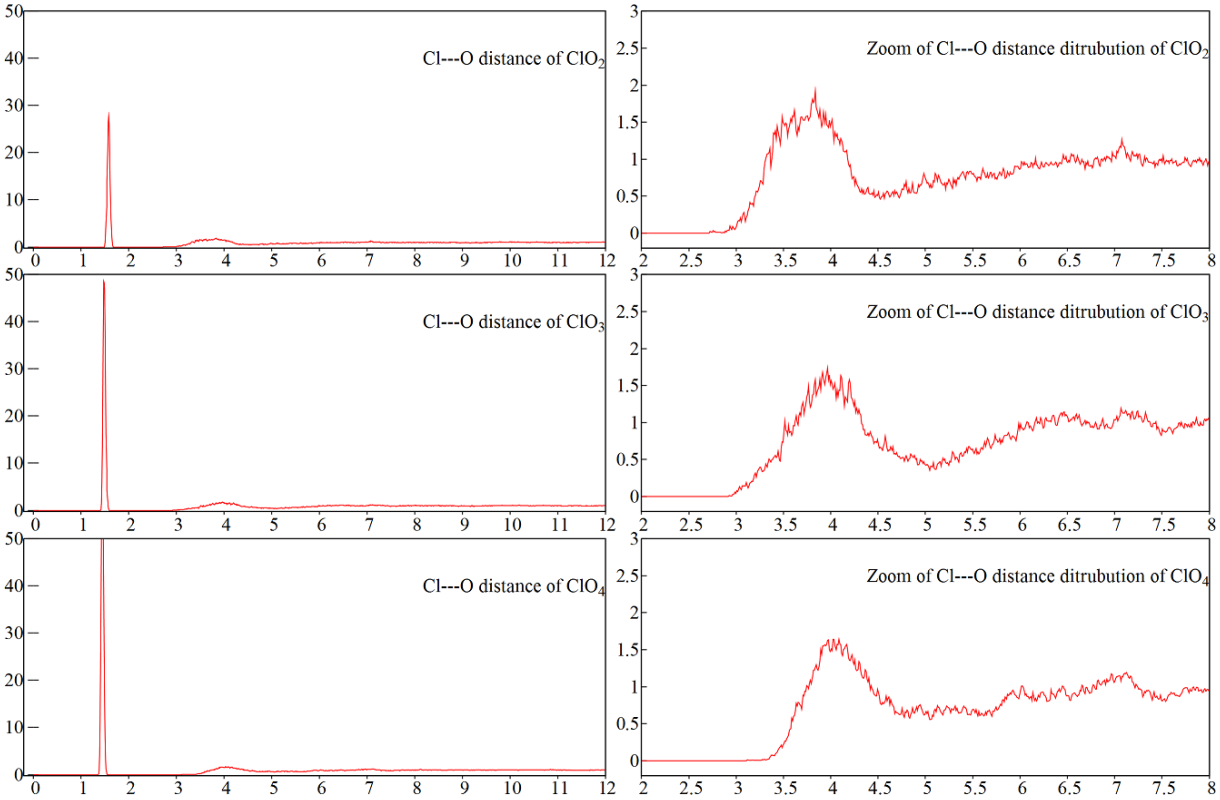


Figure S3


Cl---O distance of ClO2
Zoom of Cl---O distance ditrubution of ClO2
Cl---O distance of ClO3
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Cl---O distance of ClO4
Zoom of Cl---O distance ditrubution of ClO4

Figure S4

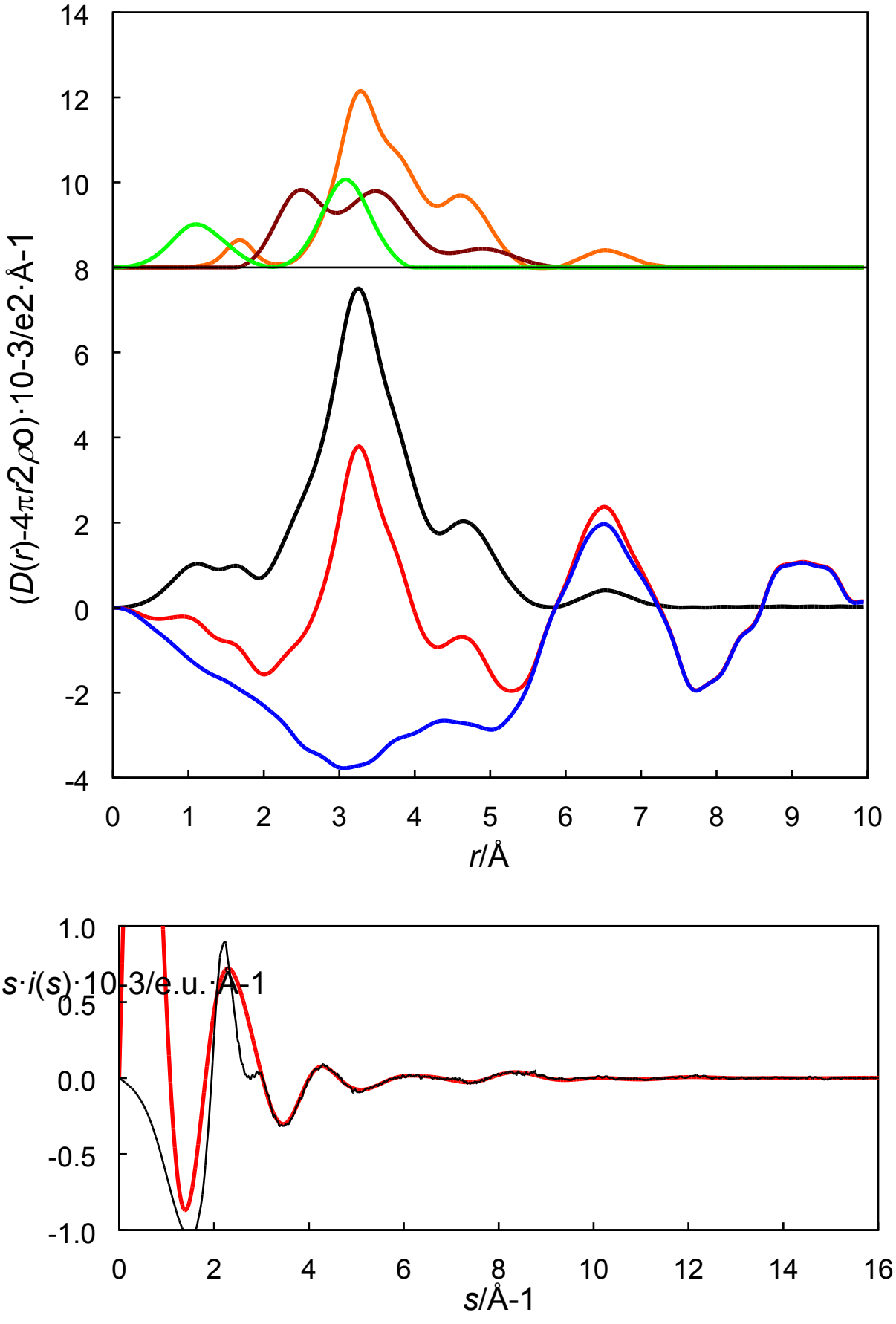
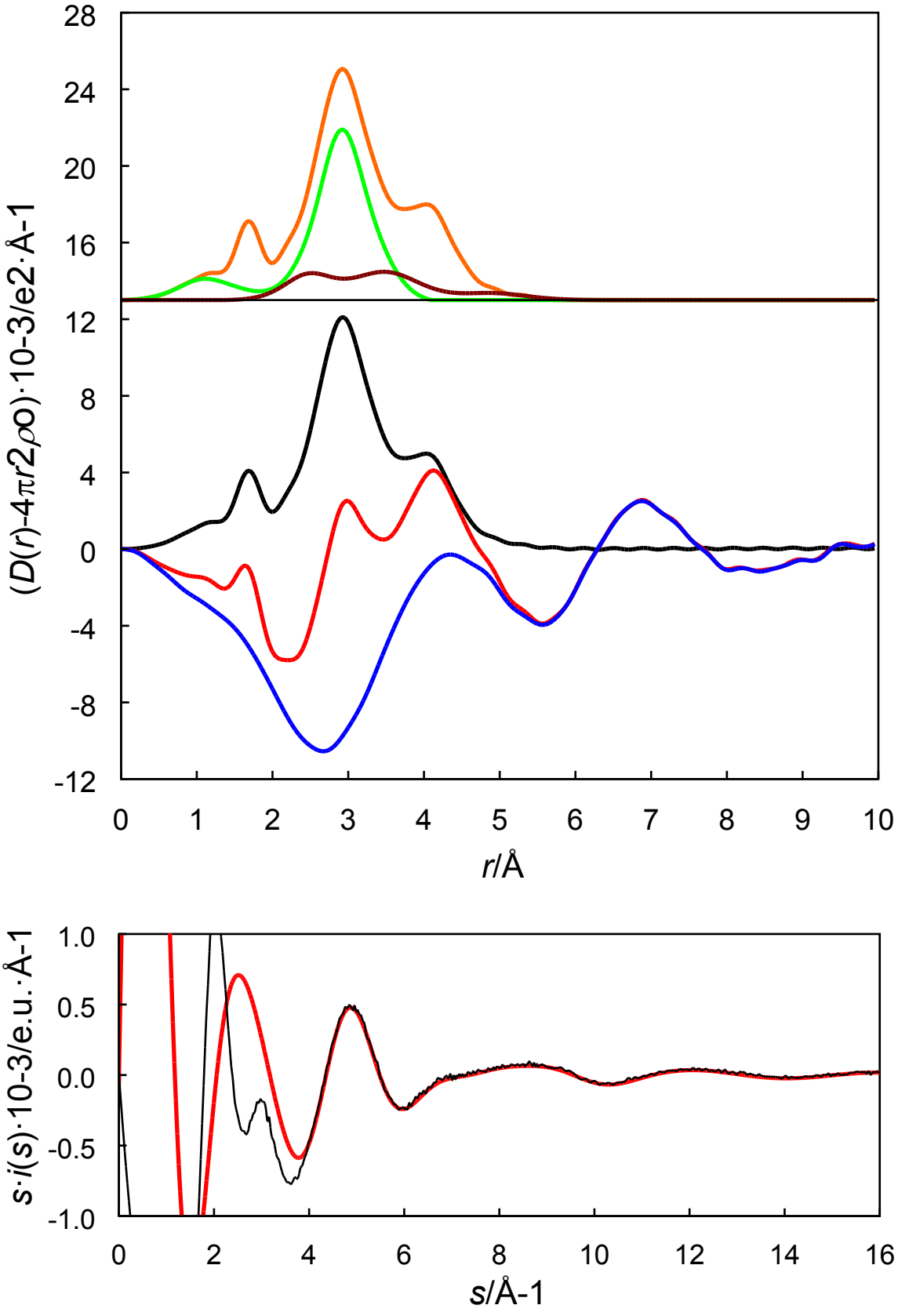


Figure S5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3
4
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6
7
8
9
10
r/Å
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0.5
0.0
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s·i(s)·10-3/e.u.·Å-1
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2
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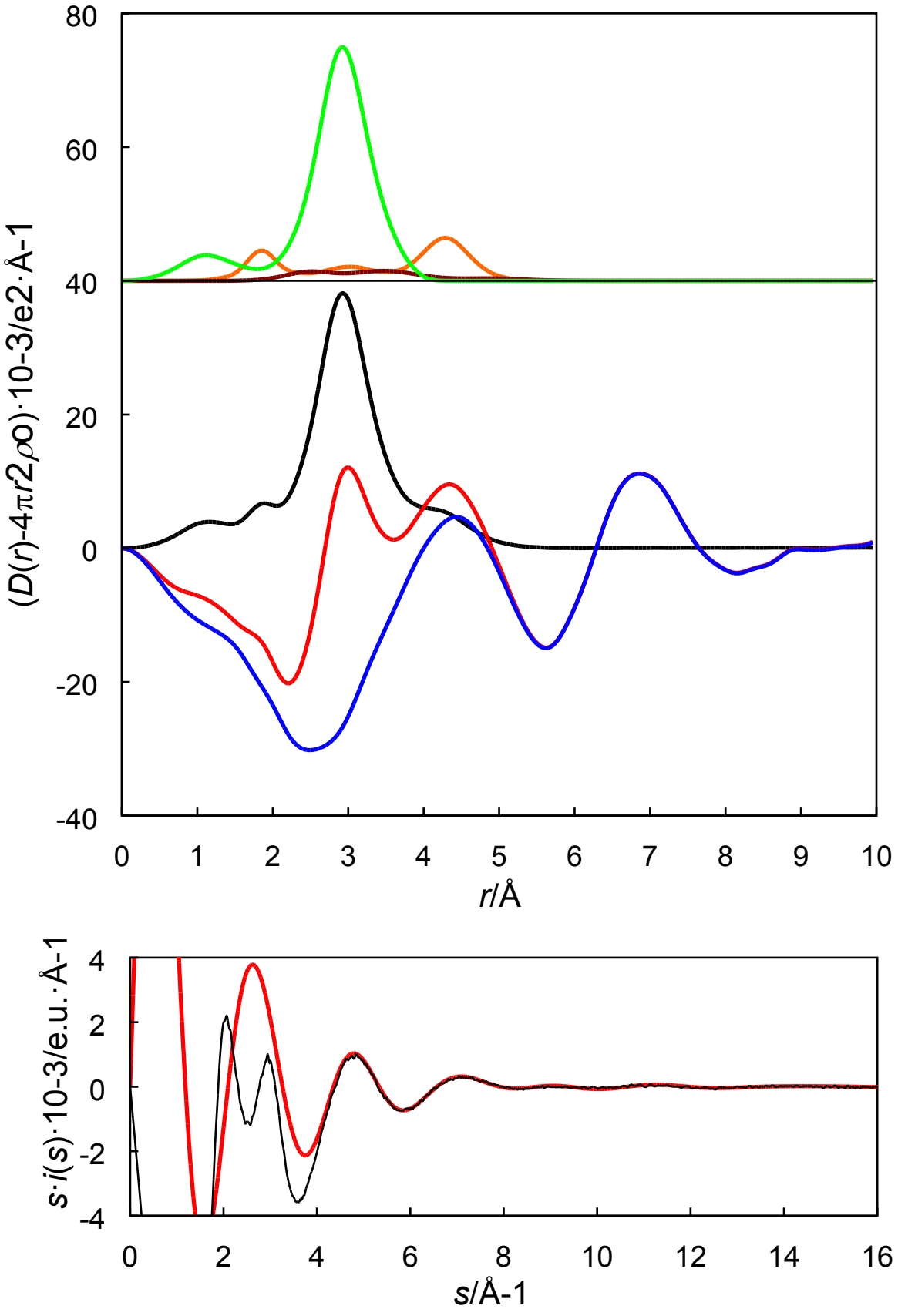
8
10
12
14
16
s/Å-1

Figure S6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10
r/Å
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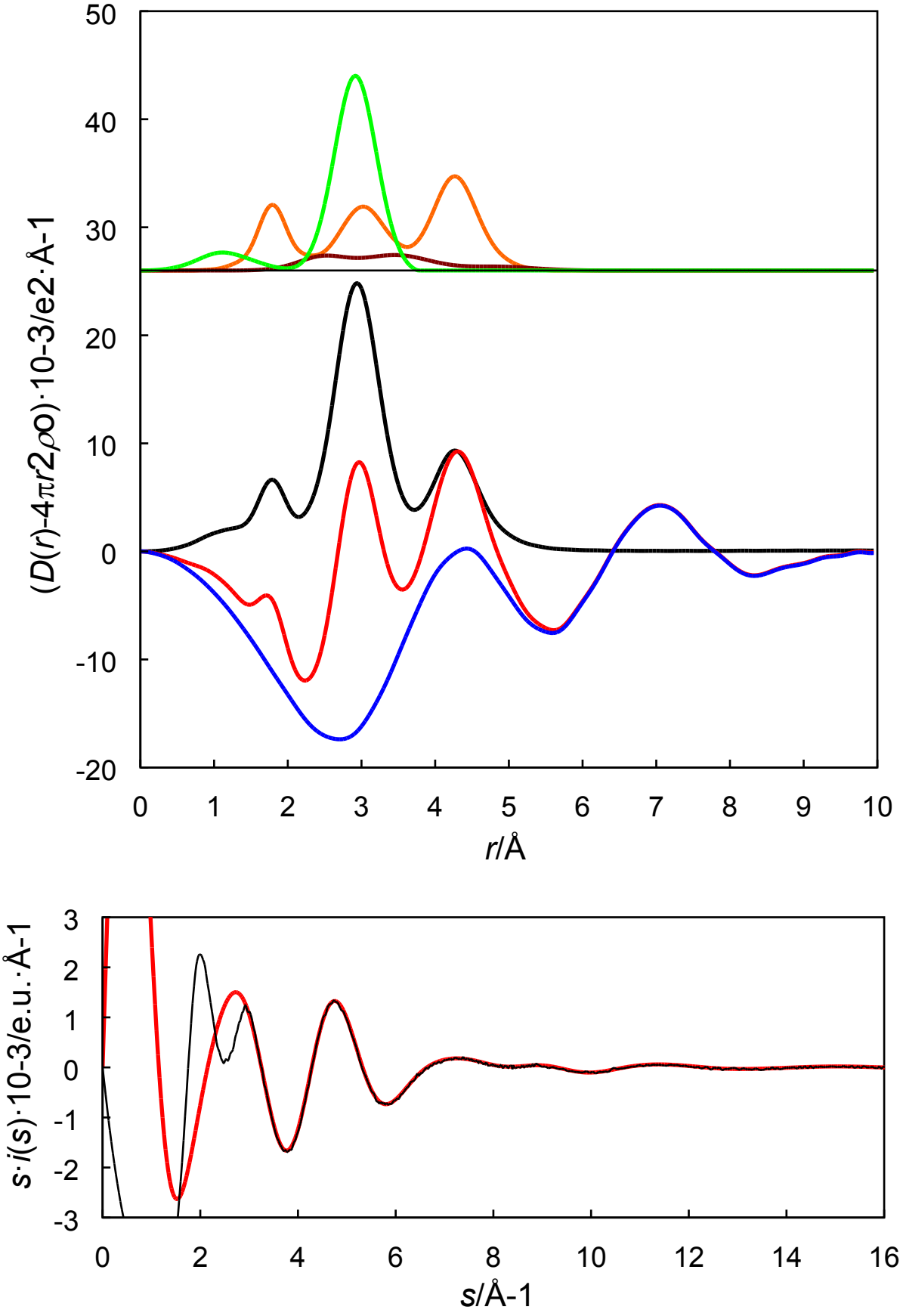
16
s/Å-1

Figure S7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r/Å
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10
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14
16
s/Å-1

Figure S8

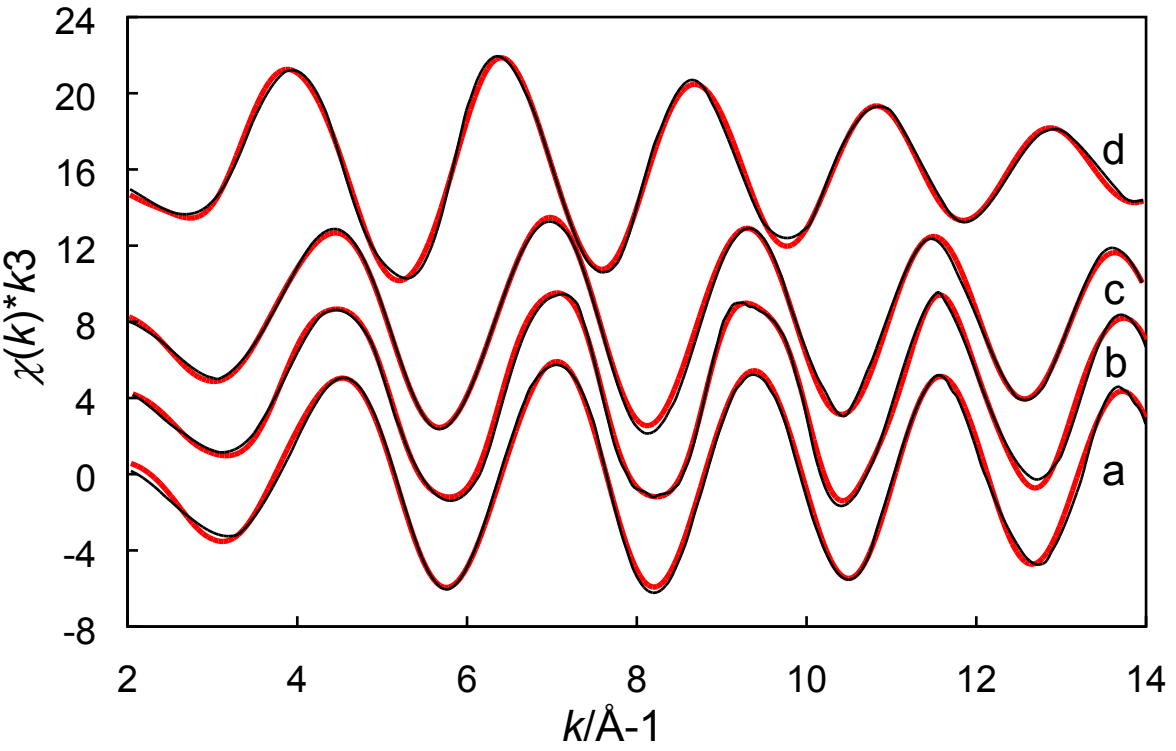

Figure S9

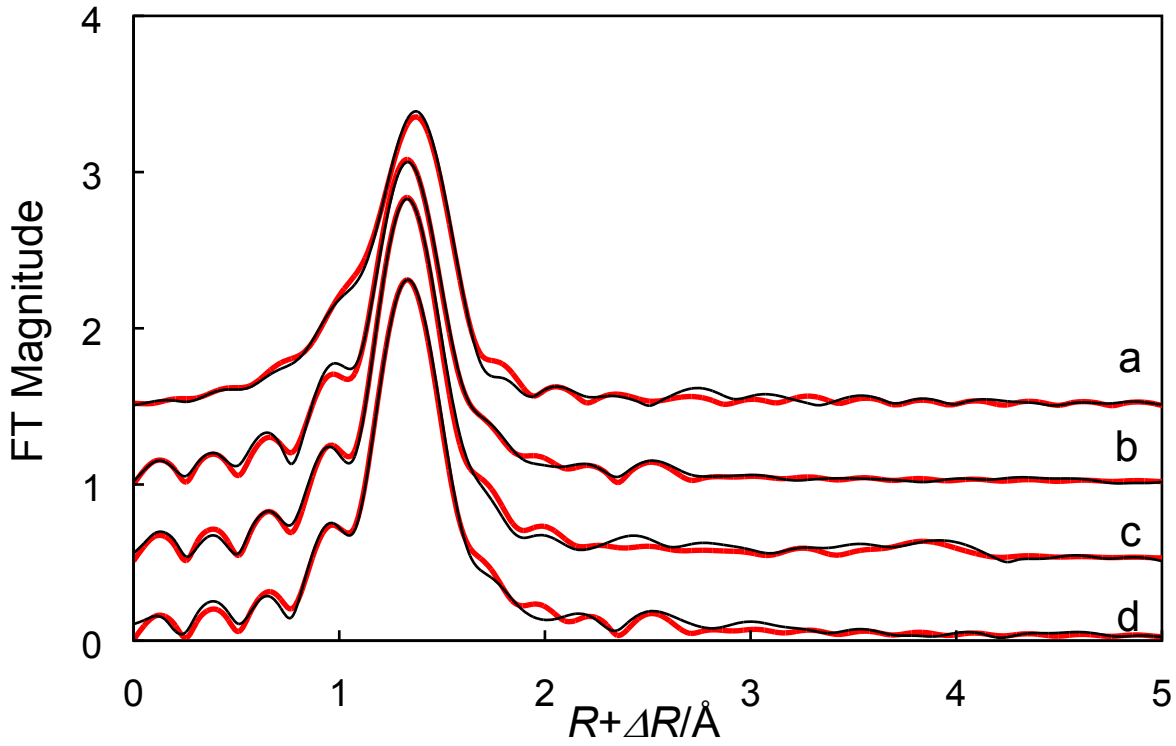

Figure S10