Structure Determination of Phosphoric Acid and Phosphate Ions in Aqueous Solution Using EXAFS Spectroscopy and Large Angle X-ray Scattering

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Supporting Material

Table 1a. Summary of reported crystal structures containing a phosphate ion, PO_4^{3-}, not bindning a metal ion except alkali metal ions.

Phosphate ion, PO_4^{3-}

CSD/ICSD code		
36045	1.548 Å	Larbot, A.; Durand, J. *Acta Crystallogr., Sect. C* **1983**, *39*, 12-15.
37021	1.539 Å	Averbuch-Pouchot, M. T.; Durif, A. *J. Solid State Chem.* **1983**, *46*, 193-196.
186466	1.541 Å	Vorob'eva, S. N.; Baidina, I. A.; Belyaev, A. V.; Alferova, N. I. *J. Struct. Chem. (USSR)* 2012, *53*, 125-131.
239004	1.545 Å	Leinemann, M.; Jess, I.; Boeckmann, J.; Naether, C. *Acta Crystallogr., Sect. E* 2015, *71*, i10-i11.
DUVLEM	1.538 Å	Jia, C.; Wu, B.; Li, S.; Yang, Z.; Zhao, Q.; Liang, J.; Li, Q.-S.; Yang, X.-J. *Chem. Commun.* **2010**, *46*, 5376.
HICWOH	1.511 Å	Zhang, Y.; Zhang, R.; Zhao, Y.; Ji, L.; Jia, C.; Wu, B., *New J. Chem.* **2013**, *37*, 2266.
IZOWAW	1.522 Å	Nohra, B.; Moll, H. E.; Albelo, L. M. R.; Mialane, P.; Marrot, J.; Mellot-Draznieks, C.; O'Keeffe, M.; Biboum, R. N.; Lemaire, J.; Keita, B.; Nadjo, L.; Dolbecq, A. *J. Am. Chem. Soc.* **2011**, *133*, 13363.
LIHZUZ	1.542 Å	Li, R.; Zhao, Y.; Li, S.; Yang, P.; Huang, X.; Yang, X.-J.; Wu, B. *Inorg. Chem.* **2013**, *52*, 5851.
LIJBAJ	1.535 Å	Li, R.; Zhao, Y.; Li, S.; Yang, P.; Huang, X.; Yang, X.-J.; Wu, B. *Inorg. Chem.* **2013**, *52*, 5851.
LINKOK	1.536 Å	Jana, D.; Mani, G.; Schulzke, C. *Inorg. Chem.* **2013**, *52*, 6427.
LUDZER	1.539 Å	Mezei, G. *Chem. Commun.* **2015**, *51*, 10341.
LUDZIV	1.545 Å	Mezei, G. *Chem. Commun.* **2015**, *51*, 10341.
NEZNUD	1.538 Å	Dey, S. K.; Das, G. *Dalton Trans.* **2012**, *41*, 8960.
NOWCOT	1.541 Å	Wu, B.; Li, S.; Lei, Y.; Hu, H.; Amadeu, N. de S.; Janiak, C.; Mathieson, J. S.; Long, D.-L.; Cronin, L.; Yang, X.-J. *Chem. Eur. J.* **2015**, *21*, 2588.

OCUXIV	1.540 Å	Day, S. K.; Das, G. *Dalton Trans.* **2011**, *40*, 12048.
OMIHUP	1.547 Å	Ji, L.; Yang, Z.; Zhao, Y.; Sun, M.; Cao, L.; Yang, X.-J.; Wang, Y.-Y.; Wu, B. *Chem. Commun.* **2016**, *52*, 7310.
OMIJAX	1.537 Å	Ji, L.; Yang, Z.; Zhao, Y.; Sun, M.; Cao, L.; Yang, X.-J.; Wang, Y.-Y.; Wu, B. *Chem. Commun.* **2016**, *52*, 7310.
PEPNIJ	1.532 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.; Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2013**, *52*, 5096.
VULYEI	1.537 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULYIM	1.541 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULYOS	1.537 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULYUY	1.534 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULZAF	1.547 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULZIN	1.537 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULZOT	1.532 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULZUZ	1.545 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VULBAI	1.538 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.

VUMLOG	1.541 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
VUMLUM	1.541 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
XAXJOX	1.525 Å	Zhang, Z.; Guo, J.; Fu, J.; Zheng, L.; Zhu, D.; Xu, Y.; Song, Y. *J. Cluster. Sci.* **2012**, *23*, 177.
OSUSAY	1.523Å	Turrina, A.; Garcia, R.; Cox, P. A.; Casci, J. L.; Wright, P. A. *Chem. Mater.* **2016**, *28*, 4998.
OSUSIG	1.518 Å	Turrina, A.; Garcia, R.; Cox, P. A.; Casci, J. L.; Wright, P. A. *Chem. Mater.* **2016**, *28*, 4998.
ZIDNAB	1.540 Å	Averbuch-Pouchot, M.-T.; Durif, A. *C. R. Seances Acad. Sci., Ser. II* **1993**, *317*, 1179.
Mean	**1.536 Å/28 structures**	

Table 1b. Summary of reported crystal structures containing a hydrogenphosphate ion, HPO_4^{2-}, not bindning a metal ion except alkali metal ions.

Hydrogenphosphate ion, HPO_4^{2-}

CSD/ISCD code		
1289	1.520 + 1.612 Å	Catti, M.; Ferraris, G.; Franchini-Angela, M. *Acta Crystallogr., Sect. B* **1977**, *33*, 3449-3452.
1433	1.515 + 1.593 Å	Catti, M.; Ferraris, G.; Ivaldi, G. *Acta Crystallogr., Sect. B* **1978**, *34*, 369-373.
14302	1.529 + 1.618 Å	Baur, W. H.; Khan, A. A. *Acta Crystallogr., Sect. B* **1970**, *26*, 1584-1596; *J. Chem. Phys.* **1990**, *94*, 7830-7834.
74543	1.510 + 1.607 Å	Lis, T. *Acta Crystallogr., Sect. C* **1994**, *50*, 484-487.
81304	1.530 + 1.618 Å	Baldus, M.; Meier, B. H.; Ernst, R. R.; Kentgens, A. P. M.; Meyer zu Altenschildesche, H.; Nesper, R. *J. Am. Chem. Soc.* **1995**, *117*, 5141-5147.
108837	1.520 + 1.602 Å	Templeton, D. H.; Ruben, H. W.; Zalkin, A. *J. Chem. Phys.* **1990**, *94*, 7830-7834.
108838	1.519 + 1.617 Å	Templeton, D. H.; Ruben, H. W.; Zalkin, A. *J. Chem. Phys.* **1990**, *94*, 7830-7834.
108839	1.515 + 1.601 Å	Templeton, D. H.; Ruben, H. W.; Zalkin, A. *J. Chem. Phys.* **1990**, *94*, 7830-7834.
108840	1.514 + 1.596 Å	Templeton, D. H.; Ruben, H. W.; Zalkin, A. *J. Chem. Phys.* **1990**, *94*, 7830-7834.
250548	1.523 + 1.606 Å	Stoeger, B.; Weil, M. *Acta Crystallogr., Sect. C* **2014**, *70*, 7-11.
250550	1.521 + 1.595 Å	Stoeger, B.; Weil, M. *Acta Crystallogr., Sect. C* **2014**, *70*, 7-11.
260729	1.526 + 1.589 Å	Kunz, P. C.; Wetzel, C.; Spingler, B. *Acta Crystallogr., Sect. E* **2010**, *66*, i26-i27.
AVOVOY	1.518 + 1.587 Å	Hoque, Md N.; Manna, U.; Das, G. *Polyhedron* **2016**, *119*, 307.
BIDMIK	1.519 + 1.587 Å	Baouab, L.; Jouini, A. *J. Solid State Chem.* **1998**, *141*, 343.
COMXAD06	1.515 + 1.584 Å	Jouffret, L.; Rivenet, M.; Abraham, F. *Inorg. Chem.* **2011**, *50*, 4619.

EBECOG	1.523 + 1.576 Å	Yoshii, Y.; Hoshino, N.; Takeda, T.; Akutagawa, T. *J. Phys. Chem. C* **2015**, *119*, 20845.
EBEDIB	1.521 + 1.589 Å	Yoshii, Y.; Hoshino, N.; Takeda, T.; Akutagawa, T. *J. Phys. Chem. C* **2015**, *119*, 20845.
EDUVUW	1.529 + 1.585 Å	Youcef, H. A.; Chafaa, S.; Doufnoune, R.; Douadi, T. *J. Mol. Struct.* **2016**, *1123*, 138.
FACWIR	1.521 + 1.595 Å	Dydio, P.; Zielinski, T.; Jurczak, J. *Org. Lett.* **2010**, *12*, 1076.
FETZEJ	1.516 + 1.608 Å	Jones, P. G. *Acta Crystallogr., Sect. C* **1987**, *43*, 367.
FIWTUA01	1.531 + 1.606 Å	You, X.; Zhu, L.- *Indian J. Chem., Sect. A* **2010**, *49*, 1478.
FUQXUM	1.519 + 1.600 Å	Matulkova, I.; Mathauserova, J.; Cisarova, I.; Nemec, I.; Fabry, J. *J. Mol. Struct.* **2016**, *1103*, 82.
FUYKOA	1.520 + 1.603 Å	Cihelka, J.; Havlicek, D.; Gyepes, R.; Nemec, I.; Koleva, Z. *J. Mol. Struct.* **2010**, *980*, 31.
GUANHP01	1.519 + 1.607 Å	Liu, X.; Wang, X.; Yin, X.; Liu, S.; He, W.; Zhu, L.; Zhang, G.; Xu, D. *CrystEngComm* **2014**, *16*, 930.
GURHUX	1.516 + 1.598 Å	Gale, P. A.; Hiscock, J. R.; Moore, S. J.; Caltagirone, C.; Hursthouse, M. B.; Light, M. E. *Chem. Asian J.* **2010**, *5*, 555.
HARMUK	1.521 + 1.598 Å	Clifford, S. E.; Runowski, M.; Parthasarathy, N.; Besnard, C.; Melich, X.; Williams, A. F. *New. J. Chem.* **2012,** *36*, 823.
HEGFIJ	1.535 + 1.576 Å	Fabry, J.; Krupkova, R.; Vanek, P.; Dusek, M. *Acta Crystallogr., Sect. C* **2006**, *62*, o73. $(CH_3NH_3)_3(HPO_4)(H_2PO_4)$
HUGQAC	1.524 + 1.578 Å	Li, X.-M.; Feng, S.-S.; Wang, F.; Ma, Q.; Zhu, M.-L. *Acta Crystallogr., Sect. E* **2010**, *66*, o239.
HUGQAC01	1.502 + 1.581 Å	Huang, S. T.; Wang, G. L.; Li, N. B.; Luo, H. Q. *RSC Advances* **2012**, *2*, 10948.
IJEVAW	1.515 + 1.588 Å	Zhao, J.; Yang, D.; Zhao, Y.; Cao, L.; Zhang, Z.; Yang, X.-J.; Wu, B. *Dalton Trans.* **2016**, *45*, 7360.
IZOWEA	1.514 + 1.574 Å	Nohra, B.; Moll, H. E.; Albelo, L. M. R.; Mialane, P.; Marrot, J.; Mellot-Draznieks, C.; O'Keeffe, M.; Biboum, R. N.; Lemaire, J.; Keita, B.; Nadjo, L.; Dolbecq, A. *J. Am. Chem. Soc.* **2011**, *133*, 13363.
KAWMOK	1.500 + 1.589 Å	Mukhopadhyay, B. P.; Dattagupta, J. K.; Simonetta, M. *Z. Kristallogr.* **1989**, *187*, 221.

KIFZII	1.510 + 1.575 Å	Kamoun, S.; Jouini, A.; Daoud, A. *Acta Crystallogr., Sect. C* **1991**, *47*, 117.
KIFZII11	1.523 + 1.590 Å	Bartoszak-Adamska, E.; Figlerowicz, M.; Wiewiorowski, M.; Gustafsson, T.; Olovsson, I.; Jaskolski, M. *Pol. J. Chem.* **2000**, *74*, 393.
LUDYUG	1.538 + 1.574 Å	Mezei, G. *Chem. Commun.* **2015**, *51*, 10341.
MOPMOT	1.526 + 1.586 Å	Demir, S.; Yilmaz, V. T.; Andac, O.; Harrison, W. T. A. *Acta Crystallogr., Sect. C* **2002**, *58*, o407.
MUWQOL	1.504 + 1.627 Å	Gale, P. A.; Hiscock, J. R.; Jie, C. Z.; Hursthouse, M. B.; Light, M. E. *Chem. Sci.* **2010**, *1*, 215.
NOXBEJ	1.516 + 1.578 Å	Olivari, M.; Montis, R.; Karagiannidis, L. E.; Horton, P. N.; Mapp, L. K.; Coles, S. J.; Light, M. E.; Gale, P. A.; Caltagirone, C. *Dalton Trans.* **2015**, *44*, 2138.
OMIHOJ	1.518 + 1.591 Å	Ji, L.; Yang, Z.; Zhao, Y.; Sun, M.; Cao, L.; Yang, X.-J.; Wang, Y.-Y.; Wu, B. *Chem. Commun.* **2016**, *52*, 7310.
OZITUN	1.517 + 1.592 Å	Makuc, D.; Hiscock, J. R.; Light, M. E.; Gale, P. A.; Plavec, J. *Beilstein J. Org. Chem.* **2011**, *7*, 1205.
PEKZIQ	1.505 + 1.554 Å	Wei, M.; Wu, B.; Zhao, L.; Zhang, H.; Li, S.; Zhao, Y.; Yang, X.-J. *Org. Biomol. Chem.* **2012**, *10*, 8758.
SECLAP	1.503 + 1.586 Å	Mrad, M. L.; Ferretti, V.; Rzaigui, M.; Nasr, C. B. *Acta Crystallogr., Sect. E* **2012**, *68*, o3120.
TERLAE	1.523 + 1.586 Å	Hazell, A. *Acta Crystallogr., Sect. E* **2006**, *62*, o5941.
UJIDEY	1.520 + 1.586 Å	Ittyachan, R.; Ahigna, M. S.; Jagan, R. *Acta Crystallogr., Sect.E* **2016**, *72*, 530.
VEWFEK	1.501 + 1.561 Å	Mahroug, A.; Belhouchet, M.; Mhiri, T. *Phos.,Sulf.,Silic., Relat. Elem.* **2012**, *187*, 1482.
VIFYOA	1.526 + 1.592 Å	Akhuli, B.; Ravikumar, I.; Ghosh, P. *Chem. Sci.* **2012**, *3*, 1522.
VULYAE	1.509 + 1.632 Å	Wu, B.; Cui, F.; Lei, Y.; Li, S.: Amadeu, N. de S.; Janiak, C.; Lin, Y.-J.; Weng, L.-H.; Wang, Y.-Y.; Yang, X.-J. *Angew. Chem., Int. Ed.* **2015**, *54*, 8658.
WAKBAM	1.524 + 1.583 Å	Dakhlaoui, A.; Smiri, L. S.; Driss, A. *Acta Crystallogr., Sect. E* **2004**, *60*, o2241.
WUTGOH	1.525 + 1.594 Å	Craven, E.; Abu-Shandi, K.; Janiak, C. *Z. Anorg. Allg. Chem.* **2003**, *629*, 195.
WUTGUN	1.526 + 1.595 Å	Craven, E.; Abu-Shandi, K.; Janiak, C. *Z. Anorg. Allg. Chem.* **2003**, *629*, 195.

Mean **1.519 + 1.593 Å/50 (Mean 1.537 Å/50)**

Table 1c. Summary of reported crystal structures containing a dihydrogenphosphate ion, $H_2PO_4^-$, not bindning a metal ion except alkali metal ions.

Dihydrogenphosphate ion, $H_2PO_4^-$

Dihydrogenphosphate ions reported to have regular tetrahedral structure

1537, 16489, 16490, 20312, 24683, 30257, 33583, 54871, 54872, 65523, 65524, 65525, 65526, 65527, 65528, 65529, 65530, 65531, 65532, 65533, 66079, 76195, 86410, 87895, 151916, 159793, 173806, 173807, 192622, 192625, 200312, 200516, 200888, 200889, 201118, 201119, 201370, 201371, 201374, 201375, 202556

Mean 1.539 Å/41

Dihydrogenphosphate ions reported in the ICSD database

7, 65, 66, 2014, 24684, 29258, 31151, 34447, 36300, 37142, 47189, 52031, 54873, 56824, 61431, 68696, 79341, 79608, 79609, 100200, 166218, 167110, 167111,182308, 183037, 183038, 186817, 186818, 187005, 187006, 190487, 200318, 200885, 200890, 200895, 200896, 238714, 248318, 246948, 260211, 280455, 410084, 410085, 410086, 418249 **45 inorganic**

Dihydrogenphosphate ions reported in the CSD database

AJUKUL, ALURUQ, APAFAA, ASOWUC, AZIXEN, BIDPEJ, BOQJEW, CAFJAX, CAFJEB, DASNUH, DAVCEK, DAVVED, DAXYOR, DAYHOB, DAZJUL, DUSKAE, EBEBIZ, EBEBIZ01, EBECAS, EBECEW, EBECIA, EBEDEX, EBEFAV, EBEFUP, EDUVUW, EHUCAM, ELEVIC, ELEVOI, ELUQUT, EMOKIB, ERONEF, ESAJAL, ESAJEP, ESAJIT, ESAJOZ, ESAJUF, ESAKAM, ESALUH, ESAMAO, ESAMES, EVALAP, EXUQIY, EYICUM, EYUTEZ, FACWOX, FAGXUI, FASVAY, FUQMOT, FUQMUZ, FUQNAG, GEJYEA02, GEXXAI01, GEXXIA02, GICROB, GUNYET, GUNYIX, GUWNES, HAKDAA, HARMIY, MARMUK, HEDWUK, HEGDED, HEGFIJ, HICWOH, IKUSOY, ILEYUU, IMAROE, IPIPED, IQOKOQ, ISOLIM, IVUJOA, IWOQES, JIBDIH, JIZHEF, JOWQUJ, JUSMER, JUSMOB, JUSMUH, KAQSUS, KAWMOK, KICNUF, KIDTEY, KIDTEY01, KIVHOM, KUQRIY, KUQROE, KUQRIY01, KUQROE01,

KUQROE03, KUQROE04, KURCUW, KUZMIC, KUZMUO, KUZPAX, LACTEO, LEDBAZ, LEGJAK, LESCIX, LETCIW, LETLUT, LETMEE, LETMII, LIYWOH, LOFFIX, LUKMEL, LUKMIP, MECYUQ, MIFQEX, MINVIP01, MIFRIC, MOPHAC, MUGYUK, MUVDUE, MUVWIK, MUVXAD, NADGIL, NAHREV, NATNUU, NATWUC, NAVCOF, NELVUV, NINFEX, NIRFEB, NUPXAY, OCAWAS, OCIYOP, OLAWAH, OZEGIL, OZELIP, PAVTEN, PIFJAQ, PIYCOP, PUJTAQ, PUJTOE, QAJWAB, QAJWAB01, QALCAJ, QAYCAV, QEDHUE, QEDHUE01, QESNOS, QIFPIG, QIFPOM, QIFPUS, QITZOK, QULMOB, QUPSAW, QURPIC, RAFDUZ, RAHSEA, RAHSIF, REZNEP, RIBWAB, RONBOL, ROYWOT, SAJZUA, SECLAP, SEFDOW, SEFDUC, SENNUV, SODCUJ01, SOXFIV01, SUYKEQ, TANZOX, TEBMAQ, TECCOV, TIBQOM, TODNUV, TUPDEO, TUVDEU, TUVDIY, TUVDOE, UGISEI01, UNAXIS, UPALON, UPALON01, UPALON02, URAWUH, UZUHOO, VACSAW, VACSEA, VEGKIB, VEWFEK, VICZEN, VIDSOS, VIFMEE, VIXLUL, VOLWAW, VUNSAZ01, VUYMAD, WAKBAM, WAVHOQ, WAZWAX, WEBQEB, WEDZUC, WEFBIU, WETLOY, WIDXEO, WIGJEH, WIGYES, WINLAG, WUWMIL, WUWMIL01, WUXGAX, XAFBAK, XAQXAQ, XAZKAL, XEPREQ, XERBAX02, XIBVEK, XIWBEM, XOHLAJ, XOJKEO, XOZHEB, XOZJOM01, XULJEV, XULJIZ, YALWUE, YOWWEM, YUBKIR, YUPVOV, ZANFEC, ZAPGUU, ZASDIJ, ZASDOP, ZATNEP, ZISVAA

Mean **1.507+1.564 Å/227 (Mean 1.536 Å/227)**

Table 1d. Summary of reported crystal structures containing phosphoric acid, H_3PO_4, not bindning a metal ion.

Phosphoric acid, H_3PO_4

CSD/ICSD code		
2096	1.492+1.551 Å	Dickens, B.; Prince, E.; Schroeder, L.W.; Jordan, T. H. *Acta Crystallogr., Sect. B* **1974**, *30*, 1470-1473.
15103	1.483+1.547 Å	Mootz, D.; Goldmann, J. *Z. Anorg. Allg. Chem.* **1969**, *368*, 231-242.
15887	1.517+1.571 Å	Furberg, S. *Acta Chem. Scand.* **1955**, *9*, 1557-1566.
23193	1.490+1.552 Å	Mighell, A. D.; Smith, J. P.; Brown, W. E. *Acta Crystallogr., Sect. B* **1969**, *25*, 776-780.
36149	1.515+1.573 Å	Smith, J. P.; Brown, W. E.; Lehr, J. R. *J. Am. Chem. Soc.* **1955**, *77*, 2728-2730.
63660	1.494+1.548 Å	Blessing, R.H. *Acta Crystallogr., Sect. B* **1988**, *44*, 334-340.
79784	1.493+1.549 Å	Souhassou, M.; Espinosa, E.; Lecomte, C.; Blessing, R.H. *Acta Crystallogr., Sect. B* **1995**, *51*, 661-668.
80137	1.496+1.547 Å	Moss, G. R.; Souhassou, M.; Blessing, R. H.; Espinosa, E.; Lecomte, C. *Acta Crystallogr., Sect. B* **1995**, *51*, 650-660.
80138	1.496+1.547 Å	Moss, G. R.; Souhassou, M.; Blessing, R. H.; Espinosa, E.; Lecomte, C. *Acta Crystallogr., Sect. B* **1995**, *51*, 650-660.
ACETPA	1.487+1.536 Å	Jonsson, P.-G. *Acta Chem. Scand.* **1972**, *26*, 1599.
ACETPA01	1.489+1.541 Å	Jonsson, P.-G. *Acta Chem. Scand.* **1972**, *26*, 1599.
APAFAA	1.493+1.547 Å	Phukan, N.; Baruah, J. B. *New. J. Chem.* **2016**, *40*, 6899.
CRBAMP19	1.509+1.544 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.

CRBAMP20	1.504+1.545 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP21	1.507+1.538 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP22	1.504+1.537 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP23	1.502+1.535 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP24	1.501+1.536 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP25	1.495+1.535 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP29	1.508+1.544 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
CRBAMP30	1.504+1.542 Å	Wolfram, W.; Arutyunyan, E. G.; Antsyshkina, A. S.; Porai-Koshits, M. A. *Bull. Acad. Pol. Sci., Ser. Sci. Chim.* **1967**, *15*, 83.
DUJPED	1.479+1.537 Å	Nordlander, E. H.; Burns, J. H. *Inorg. Chim. Acta* **1986**, *115*, 31.
ECEDEW	1.490+1.544 Å	Oueslati, J.; Oueslati, A.; Nasr, C. B.; Lefebvre, F. *Solid State Sci.* **2006**, *8*, 1067.
ELEVOI	1.492+1,537 Å	Freire, E.; Polla, G.; Baggio, R. *J. Mol. Struct.* **2014**, *1068*, 43.
ESAMAO	1.496+1.528 Å	Huang, J.; Liu, T.-P.; Huo, L-H.; Deng, Z.-P.; Gao, S. *J. Mol. Struct.* **2017**, *1127*, 361.
GUNYET	1.498+1.540 Å	Grepioni, F.; Rossini, M.; Braga, D. *Cryst. Eng. Comm.* **2001**, *3*, 36.
HAHGED	1.470+1.541 Å	Braga, D.; Curzi, M.; Maini, L.; Polito, M.; Grepioni, F. *Dalton Trans.* **2004**, 2432.
HAHGIH	1.472+1.541 Å	Braga, D.; Curzi, M.; Maini, L.; Polito, M.; Grepioni, F. *Dalton Trans.* **2004**, 2432.

HAHGON	1.492+1.536 Å	Braga, D.; Curzi, M.; Maini, L.; Polito, M.; Grepioni, F. *Dalton Trans.* **2004**, 2432.
HAKDED	1.502+1.544 Å	Warden, A. C.; Warren, M.; Hearn, M. T. W.; Spiccia, L. *Inorg. Chem.* **2004**, *43*, 6936.
HEGDED	1.487+1.548 Å	Bourne, S. A.; De Villiers, K.; Egan, T. J. *Acta Crystallogr., Sect. C* **2006**, *62*, o53.
HISTPA10	1.489+1.548 Å	Blessing, R. H. *Acta Crystallogr., Sect. B* **1986**, *42*, 613.
HISTPA12	1.490+1.549 Å	Mata, I.; Espinosa, E.; Molins, E.; Veintemillas, S.; Maniukiewicz, W.; Lecomte, C.; Cousson, A.; Paulus, W. *Acta Crystallogr., Sect. A* **2006**, *62*, 365.
HISTPA13	1.487+1.550 Å	Mata, I.; Espinosa, E.; Molins, E.; Veintemillas, S.; Maniukiewicz, W.; Lecomte, C.; Cousson, A.; Paulus, W. *Acta Crystallogr., Sect. A* **2006**, *62*, 365.
HISTPA14	1.486+1.548 Å	Mata, I.; Espinosa, E.; Molins, E.; Veintemillas, S.; Maniukiewicz, W.; Lecomte, C.; Cousson, A.; Paulus, W. *Acta Crystallogr., Sect. A* **2006**, *62*, 365.
HISTPA15	1.493+1.555 Å	Mata, I.; Espinosa, E.; Molins, E.; Veintemillas, S.; Maniukiewicz, W.; Lecomte, C.; Cousson, A.; Paulus, W. *Acta Crystallogr., Sect. A* **2006**, *62*, 365.
IBATIP	1.496+1.533 Å	Al'bov, D. V.; Mazina, O. S.; Rybakov, V. B.; Babaev, E. V.; Chernyshev, V. V.; Aslanov, L. A. *Kristallografiya* **2004**, *49*, 208.
IPIPED	1.486+1.539 Å	Fu, X.-Q.; Hang, T.; Ye, Q.; Xiong, R.-G. *Inorg. Chem. Commun.* **2011**, *14*, 281.
JAYQIJ	1.473+1.555 Å	Berry, R. E.; Armstrong, E. M.; Beddoes, R. L.; Collison, D.; Ertok, S. N.; Helliwell, M.; Garner, C. D. *Angew. Chem., Int. Ed.* **1999**, *38*, 795.
JAYXUD	1.489+1.543 Å	Matulkova, I.; Teubner, K.; Nemec, I.; Rohovec, J.; Micka, Z. *Acta Crystallogr., Sect. E* **2005**, *61*, o3941.
LUKMEL	1.493+1.534 Å	Chutia, R.; Dey, S. K.; Das, G. *Cryst. Growth Des.* **2015**, *15*, 4993.
LUKMIP	1.500+1.543 Å	Chutia, R.; Dey, S. K.; Das, G. *Cryst. Growth Des.* **2015**, *15*, 4993.
MAYGAV	1.500+1.549 Å	Sattler, A.; Seyfarth, L.; Senker, J.; Schnick, W. *Z. Anorg. Allg. Chem.* **2005**, *631*, 2545.
MAGYUK	1.512+1.545 Å	Andrepont, C.; Pakhomova, S.; Marzilli, P. A.; Marzilli, L. G. *Inorg. Chem.* **2015**, *54*, 4895.

NIRFEB	1.486+1.541 Å	Wu, B.; Li, S.; Lei, Y.; Hu, H.; Amadeu, N. de S.; Janiak, C.; Mathieson, J. S.; Long, D.-L.; Cronin, L. Yang, X.-J. *Chem. Eur. J.* **2015**, *21*, 2588.
PAVTEN	1.481+1.556 Å	Wang, Y.-C. *Acta Crystallogr. Sect. E* **2012**, *68*, o1693.
PAZVAO	1.493+1.543 Å	Mrad, M. L.; Nasr, C. B.; Rzaigui, M.; Lefebvre, F. *Phos., Sulf., Silic., Relat.Elem.* **2006**, *181*, 39.
PETTIS	1.475+1.515 Å	Chen, A. M.; Ellison, M. E.; Peresypkin, A.; Wenslow, R. M.; Variankaval, N.; Savarin, C. G.; Natishan, T. K.; Mathre, D. J.; Dormer, P. G.; Euler, D. H.; Ball, R. G.; Zhixiong Ye; Yaling Wang; Santos, I. *Chem. Commun.* **2007**, 419.
PUJTAQ	1.479+1.546 Å	Xia, D.-C.; Yao, J.-H. *Acta Crystallogr. Sect. E* **2010**, *66*, o609.
QALCAJ	1.494+1.539 Å	Khemiri, H.; Akriche, S. T.; Al-Deyab, S. S.; Rzaigui, M. *Acta Crystallogr. Sect. E* **2011**, *67*, o101.
QAYCAV	1.489+1.539 Å	Belam, W.; Khedhiri, L.; Daoud, A. *Z. Kristallogr.-New Cryst. Struct.* **2005**, *220*, 147.
RAFDUZ	1.505+1.550 Å	Mahroug, A.; Belhouchet, M.; Hemon-Ribaud, A.; Mhiri, T. *Phosphorus, Sulfur, Silicon, Relat. Elem.* **2011**, *186*, 2332.
RONBOL	1.491+1.545 Å	Ainscough, E. W.; Brodie, A. M.; Ranford, J. D.; Waters, J. M. *J. Chem. Soc., Dalton Trans.* **1997**, 1251.
SANDUH	1.479+1.544 Å	Chekhlov, A. N. *Zh. Neorg. Khim.* **2004**, *49*, 1101.
SECFIQ	1.503+1.527 Å	Chekhlov, A. N. *Zh. Neorg. Khim.* **2005**, *50*, 1096.
SOXFIV01	1.500+1.548 Å	Anderson, K. M.; Goeta, A. E.; Martin, J. E.; Mason, S. A.; McIntyre, G. J.; Sansam, B. C. R.; Wilkinson, C.; Steed, J. W. *Cryst Growth Des.* **2011**, *11*, 4904.
TEBMAQ	1,481+1.531 Å	Wang, W.-X; Zhu, R.-Q.; Fu, X.-Q.; Zhang, W. *Z. Anorg. Allg. Chem.* **2012**, *638*, 1123.
TODNUV	1.502+1.549 Å	Zaccaro, J.; Bagieu-Beucher, M.; Ibanez, A.; Masse, R. *J. Solid State Chem.* **2006**, *124*, 8.
TUPDEO	1.468+1.548 Å	Xiao, J.-M. *Acta Crystallogr. Sect. E* **2010**, *66*, o1339.
VEGKIB	1.487+1.547 Å	Masse, R.; Tordjman, I. *Acta Crystallogr., Sect. C* **1990**, *46*, 606.

WAVHOQ	1.487+1.544 Å	Gerasimchuk, O. A.; Mason, S.; Llinares, J. M.; Maoping Song; Alcock, N. W. ; Bowman-James, K. *Inorg. Chem.* **2000**, *39*, 1371.
WETDIJ	1.486+1.552 Å	Rashdan, S.; Light, M. E.; Kilburn, J. D. *Chem. Commun.* **2006**, 4578.
WEVXAX	1.485+1.538 Å	Halasz, I.; Lukic, K.; Vancik, H. *Acta Crystallogr., Sect. C* **2007**, *63*, o61.
WOJKIP	1.485+1.529 Å	Ming-Liang Tong; Xiao-Ming Chen; Seik Weng Ng Inorg. *Chem. Commun.* **2000**, *3*, 436.
WUWZOD	1.504+1.525 Å	Wikstad, E.; Kritikos, M. *Acta Crystallogr., Sect. C* **2003**, *59*, m87.
XAZGEK	1.493+1.533 Å	Ming-Liang Tong; Shao-Liang Zheng; Xiao-Ming Chen *Chem. Eur. J.* **2000**, *6*, 3729.
XAZKAL	1.497+1.536 Å	Chen Chen; Zavalij, P. Y.; Whittingham, M. S. *Acta Crystallogr., Sect. E* **2006**, *62*, o258.
YEMJIJ	1.468+1.512 Å	Wallet, J. C.; Cody, V.; Wojtczak, A.; Blessing, R. H. *Anti-Cancer Drug Des.* **1993**, *8*, 325.
XULJIZ	1.485+1.540 Å	Jagan, R.; Sathya, D.; Sivakumar, K. *Acta Crystallogr., Sect. C* **2015**, *71*, 374.
ZANFEC	1.487+1.535 Å	Butler, C. R.; Ogilvie, K.; Martinez-Alsina, L.; Barreiro, G.; Beck, E. M.; Nolan, C. E.; Atchison, K.; Benvenuti, E.; Buzon, L.; Doran, S.; Gonzales, C.; Helal, C. J.; Hou, X.; Hsu, M.-H.; Johnson, E. F.; Lapham, K.; Lanyon, L.; Parris, K.; ONeill, B. T.; Riddell, D.; Robshaw, A.; Vajdos, F.; Brodney, M. A. *J. Med. Chem.* **2017**, *60*, 386.
ZOXVAJ	1.492+1.550 Å	Kral, V.; Furuta, H.; Shreder, K.; Lynch, V.; Sessler, J. L. *J. Am. Chem. Soc.* **1996**, *118*, 1595.
Mean	**1.493+1.542 Å/72 (Mean 1.530 Å/72)**	

Table S2. Mean P-O and P-O(-H) bond distances in phosphoric and arsenic acid and the $H_2PO_4^-$, HPO_4^{2-}, PO_4^{3-}, $H_2AsO_4^-$, $HAsO_4^{2-}$, and AsO_4^{3-} ions in solid compounds where the acids and the ions not bind to metal ions except alkali metal ions. These structures are summarized in Table S2 for phosphoric acid and the phosphate ions, and in Tables S1-S4 in Mähler, J, Persson, I. *Dalton Trans.* 2013, **42**, 1364-1377.

	d(P-O)	*d*(P-O(-H))	Mean *d*(P-O)	*d*(P-O)-*d*(P-O(-H))
H_3PO_4	1.493	1.542	1.530	0.049
$H_2PO_4^-$	1.507	1.564	1.536	0.057
HPO_4^{2-}	1.519	1.593	1.537	0.074
PO_4^{3-}	1.536		1.536	
	d(As-O)	*d*(As-O(-H))	Mean *d*(As-O)	*d*(As-O)-*d*(As-O(-H))
H_3AsO_4	1.641	1.686	1.674	0.045
$H_2AsO_4^-$	1.655	1.708	1.681	0.053
$HAs_2O_4^-$	1.670	1.736	1.687	0.066
AsO_4^{3-}	1.674		1.674	

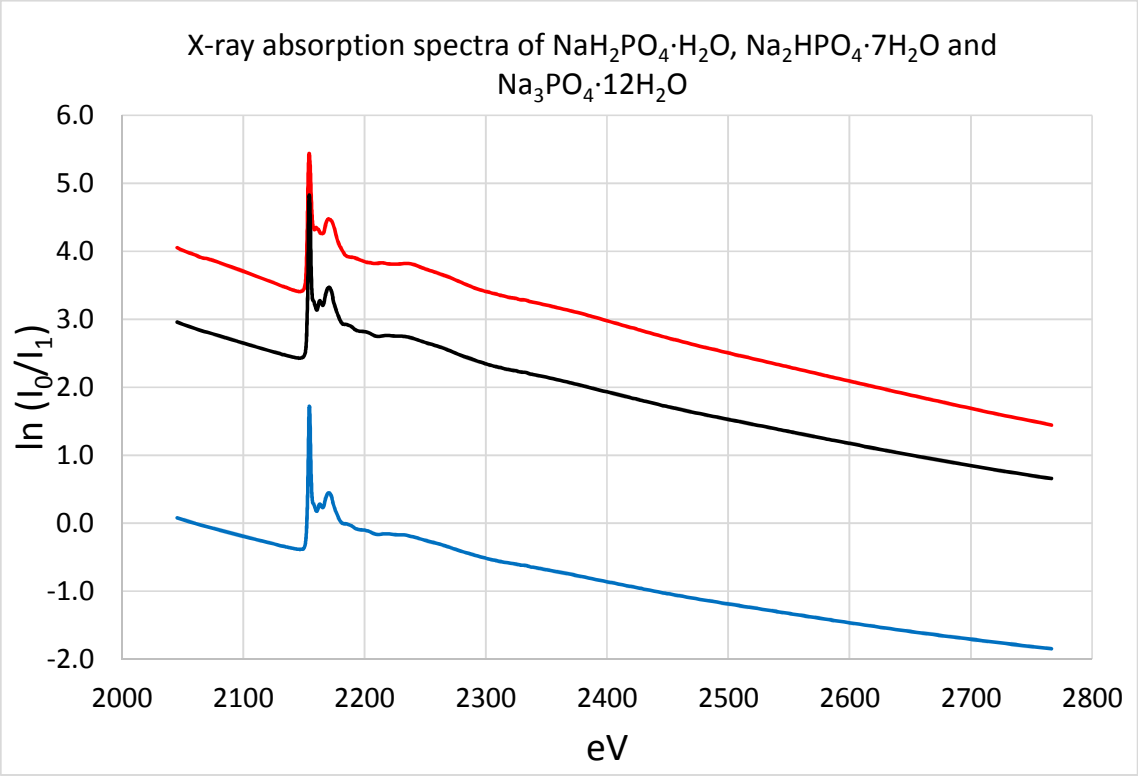

Figure S1. X-ray absorption spectra at the P K edge of $NaH_2PO_4 \cdot H_2O$ (blue line), $Na_2HPO_4 \cdot 7H_2O$ (red line) and $Na_3PO_4 \cdot 12H_2O$ (black line).

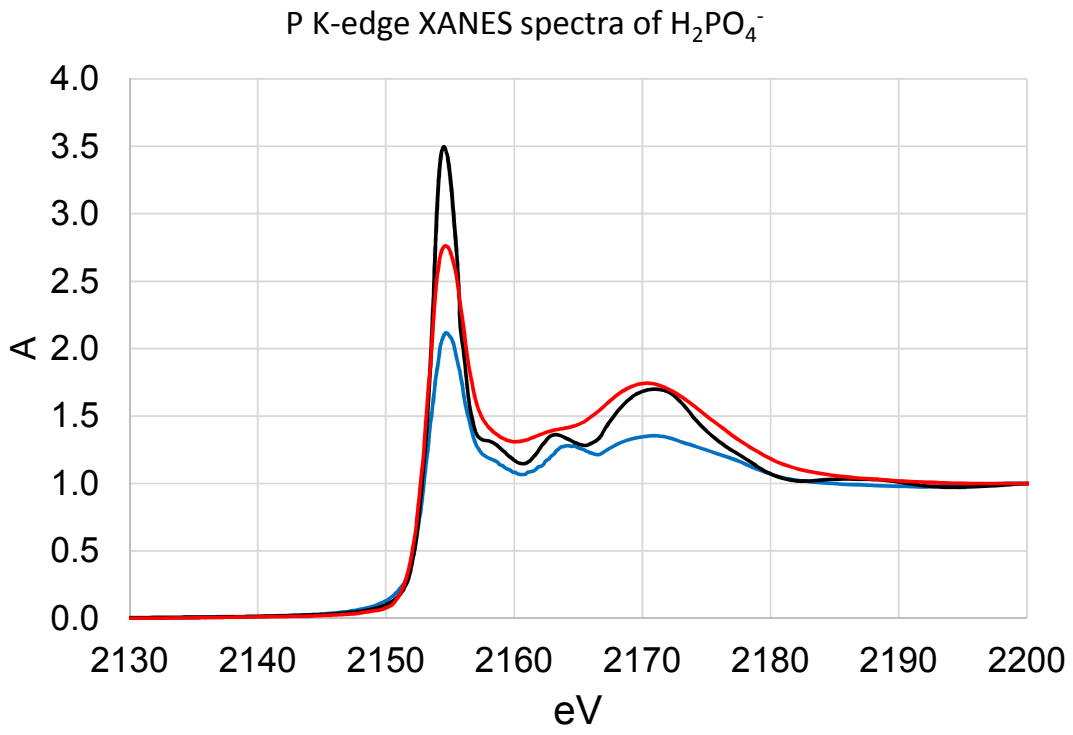

Figure S2. P K-edge XANES spectra of solid $NaH_2PO_4 \cdot H_2O$ collected in transmission mode (black line) and in fluorescence mode (blue line), and an 1.0 $mol \cdot dm^{-3}$ aqueous solution of NaH_2PO_4 collected in transmission mode (red line). All spectra are normalized to an absorption at 2200 eV to unity.

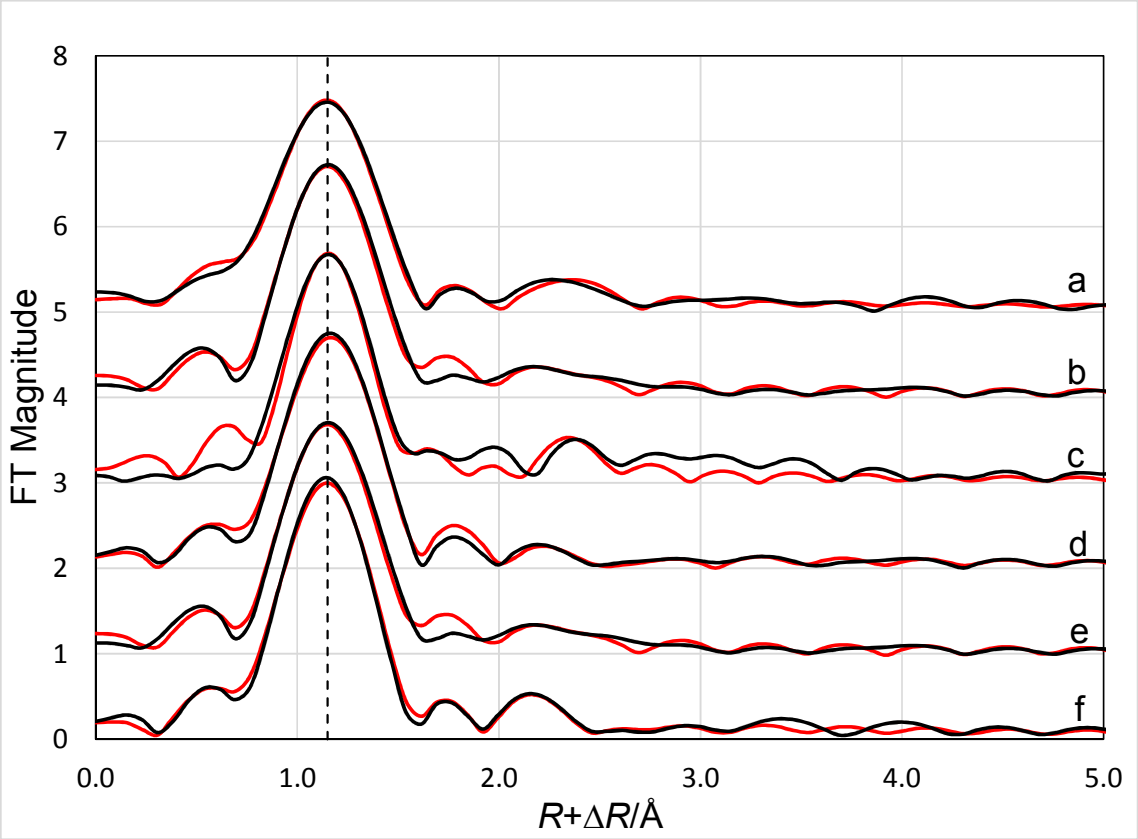

Figure S3. Fitting of Fourier transforms of k^3-weighted EXAFS raw data of a/ solid $NaH_2PO_4 \cdot H_2O$, b/ 1.0 $mol \cdot dm^{-3}$ aqueous solution of sodium dihydrogenphosphate, c/ solid $NaH_2PO_4 \cdot H_2O$ data collected fluorescence mode, d/ solid $Na_2HPO_4 \cdot 7H_2O$, e/ 1.0 $mol \cdot dm^{-3}$ aqueous solution of sodium hydrogenphosphate and f/ solid $Na_3PO_4 \cdot 12H_2O$; experimental data – black line, model – red line.

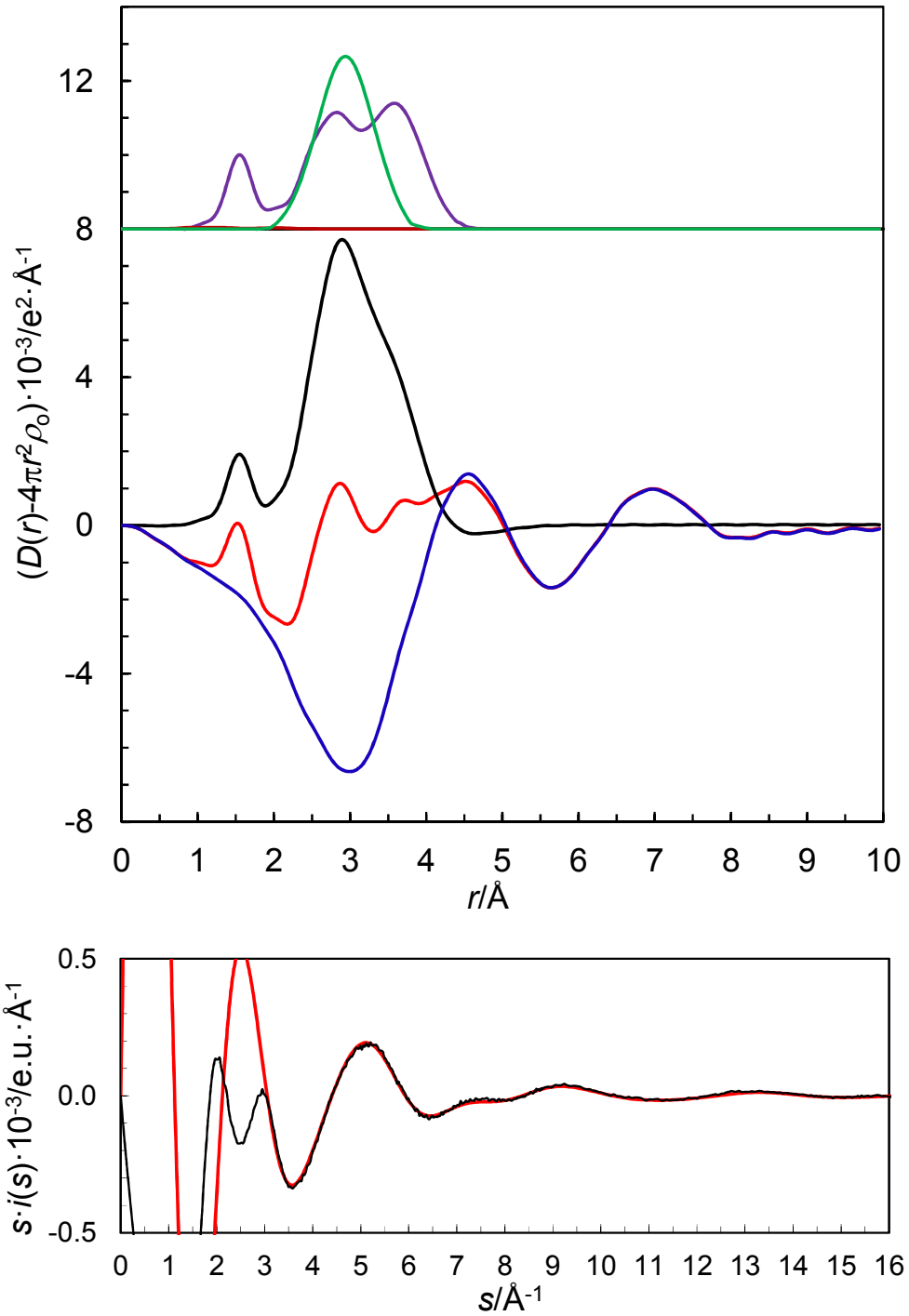

Figure S4. (Top) LAXS radial distribution curves for a 3.02 mol·dm^{-3} phosphoric acidic aqueous solution at pH=0.6 (acidified by nitric acid). Upper part: Separate model contributions (offset: 8) of hydrated phosphoric acid (purple line), nitrate ion (brown line) and aqueous bulk (green line). (Middle) Experimental RDF: $D(r)$-$4\pi r^2\rho_o$ (red line); sum of model contributions (black line); difference (blue line). (Bottom) Reduced LAXS intensity functions $s\cdot i(s)$ (black line); model $s\cdot i_{calc}(s)$ (red line).

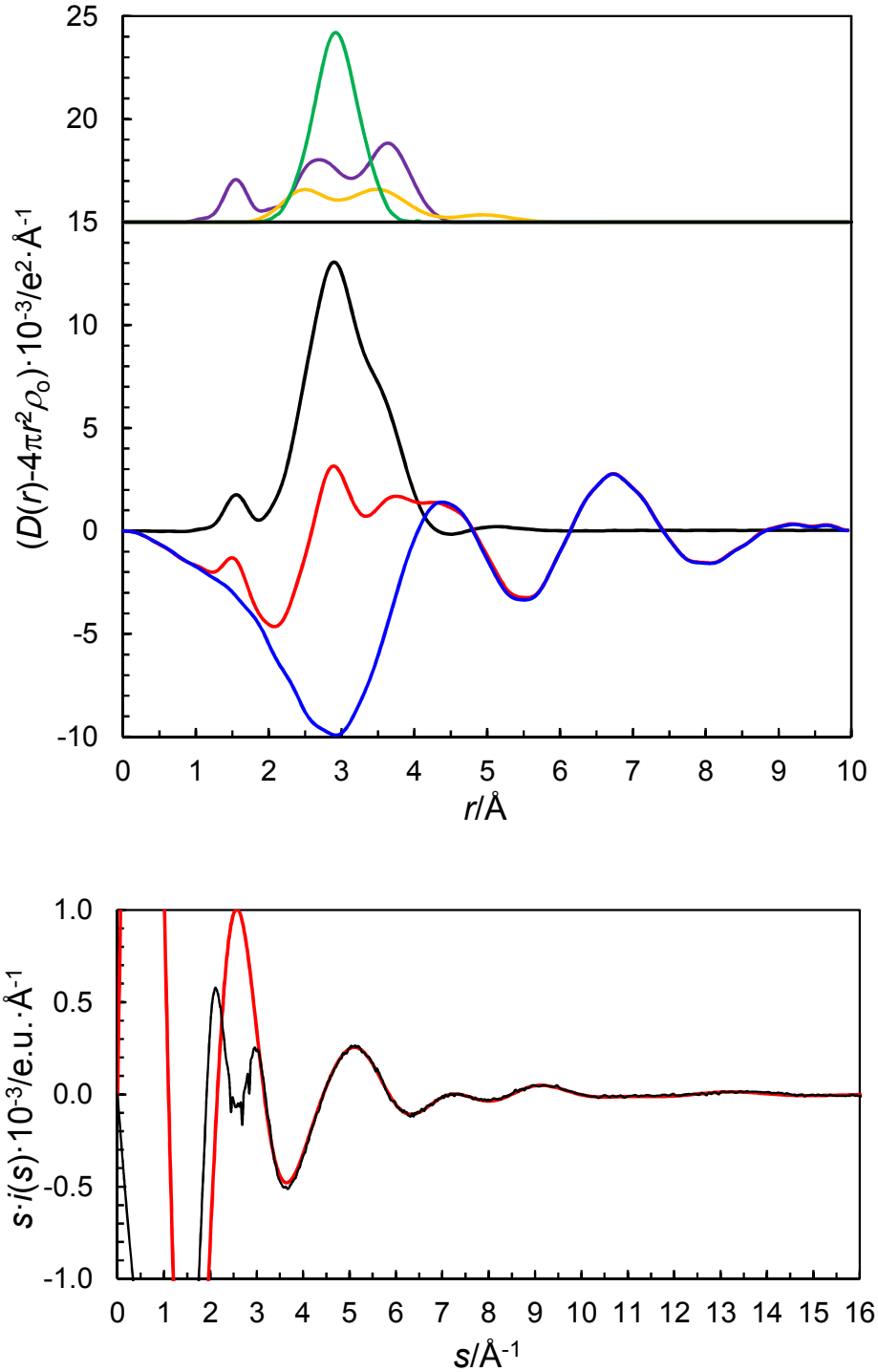

Figure S5. (Top) LAXS radial distribution curves for a 2.00 mol·dm^{-3} aqueous solution of sodium dihydrogenphosphate. Upper part: Separate model contributions (offset: 12) of the hydrated dihydrogenphosphate ion (purple line), the hydrated sodium ion (yellow line) and aqueous bulk (green line). (Middle) Experimental RDF: $D(r)$-4pr^2□ $_o$ (red line); sum of model contributions (black line); difference (blue line).

(Bottom) Reduced LAXS intensity functions $s \cdot i(s)$ (black line); model $s \cdot i_{calc}(s)$ (red line).