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Supporting information for article:

The typical crystal structures of a few representative α-aryl-α-hydroxy-phosphonates

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Table ST1. This shows unit cell dimensions in the $P2_1/n$ space group. The CCDC notes cell is included for comparison only. Similarities and differences are apparent.

Cell	KODYOS	KODYOS01	CCDC-Note Cell KODYOS01 ?	KODYOS02	**1a**
Formula	C_{11} H_{17} O_4 P	C_{11} H_{17} O_4 P	C_{11} H_{17} O_4 P	C_{11} H_{17} O_4 P	C_9 H_{13} O_4 P
T	296	273	*273*	293	173
S	9.2361	9.153	*9.128*	9.293	8.4039(5)
b	8.0719	8.017	*7.986*	8.103	7.7007(3)
c	17.4599	17.285	*17.238*	17.542	16.6012(7)
beta	95.096	95.035	*94.99*	95.329	99.149(4)
V	1296.5	1263.472	1251.82	1315.2	1060.69(9)
Dc	1.251	1.284	1.29	1.233	**1.354**

Remarks from the CSD

KODYOS

Disorder: *One ethyl group is disordered* with occupancies 0.273:0.727.

KODYOS01

CCDC Notes: Published unit-cell is *a 9.128, b 7.986, c 17.238 and beta 94.99*

Packing drawings for **1b**, **2a** and for **3a** (Supporting information Figures SF1, SF2 and SF3) show the basic primary propagation forms of O – H ··· O hydrogen bridges in the crystal packing for the chain, for the centrosymmetric dimer and for the pseudo-centrosymmetric types.

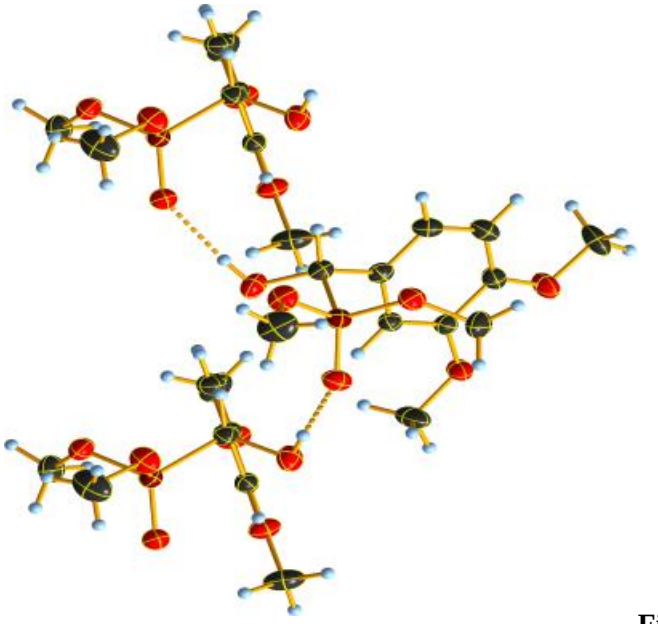


Figure 1 SF1. O···H–O H – bridges (dotted lines) in the **1b** crystal structure link molecules into 'infinite' chains

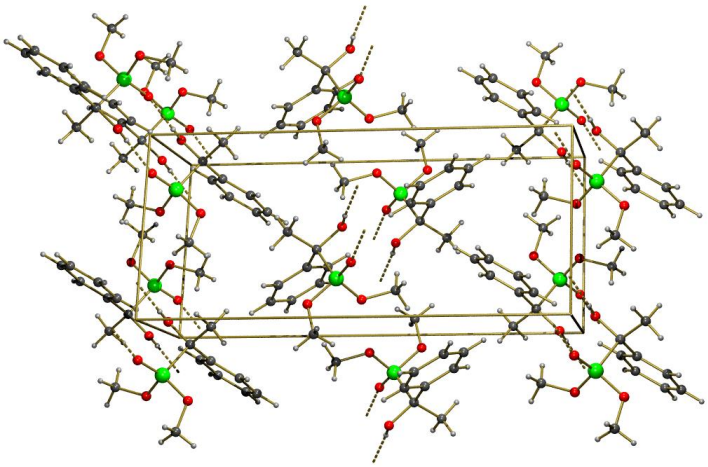


Figure 2

SF2. O···H–O H – bridges (dotted lines) in the **2a** crystal structure form dimers around symmetry centres of the lattice

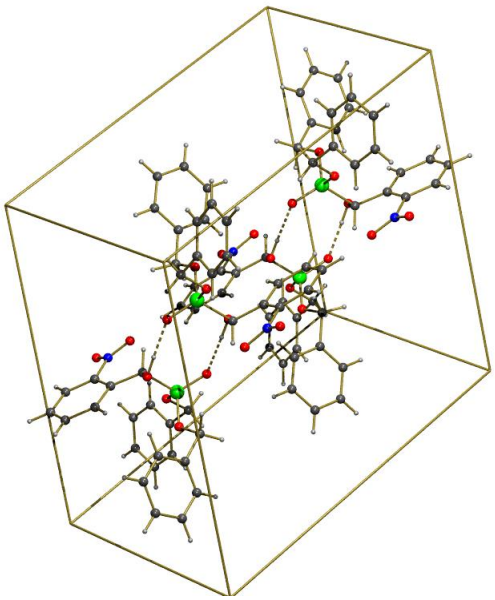


Figure 3 SF3. Two dimers with O···H–O H – bridges (dotted lines) in the **3a** crystal

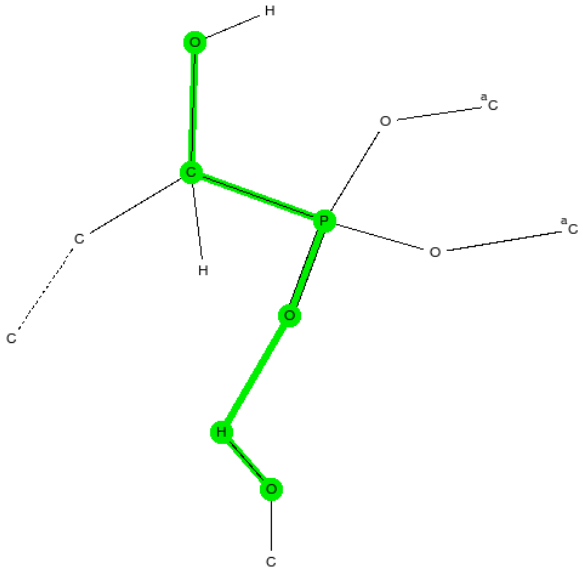


Figure 4 **SF4** Search fragment for the OPCO torsion angles with essential bonding such as acyclic ester feature. It shows the O–C–P=O part in heavy green lines as well as the intermolecular P=O···H–O contact that defines the O···H–O hydrogen bridge angle.

REFCODES and references for the CSD analysis of the OPCO torsion angles

REFCODE: AFININ

Authors/Journal

Authors: M.N.Tahir, N.Acar, H.Yilmaz, M.Danish, D.Ülkü

Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 63, o3817, 2007
Formula: C9 H12 Cl1 O4 P1
Name: (R)-Dimethyl ((2-chlorophenyl)hydroxymethyl)phosphonate

REFCODE: COLNOH
Authors/Journal
Authors: Hua Fang, Mei Juan Fang, Rui Zao Yi, Yu Fen Zhao
Journal: J.Chem.Cryst. , 38, 761, 2008
Formula: C14 H23 O5 P1
Name: di-isopropyl (hydroxy(4-methoxyphenyl)methyl)phosphonate

REFCODE: FALNOW
Authors/Journal
Authors: Anyu He, Bingli Yan, A.Thanavaro, C.D.Spilling, N.P.Rath
Journal: J.Org.Chem. , 69, 8643, 2004
Formula: C8 H18 O8 P2
Name: meso-Dimethyl 4-dimethoxyphosphoryl-1,4-dihydroxybut-2-enylphosphonate

REFCODE: FICVAO
Authors/Journal
Authors: A.T.Gubaidullin, I.A.Litvinov, V.M.Berestovitskaya, L.A.Dejiko, I.A.Bazhenova
Journal: Zh.Obshch.Khim.(Russ.)(Russ.J.Gen.Chem.) , 68, 1546, 1998
Formula: C6 H12 Cl2 N1 O6 P1
Name: bis(2-Chloroethyl) 1-hydroxy-2-nitroethylphosphonate

REFCODE: FUNYEU
Authors/Journal
Authors: J.Guin, Qinggang Wang, M.van Gemmeren, B.List
Journal: Angew.Chem.,Int.Ed. , 54, 355, 2015
Formula: C17 H22 Br1 O4 P1
Name: Di-isopropyl ((6-bromo-2-naphthyl)(hydroxy)methyl)phosphonate

REFCODE: GIRTIL
Authors/Journal
Authors: Cai-bao Chen, Wei-wei Jin, Xin-yong Li
Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 64, o144, 2008
Formula: C11 H16 N1 O6 P1
Name: Diethyl (hydroxy(2-nitrophenyl)methyl)phosphonate

REFCODE: GITQUW

Authors/Journal

Authors: J.Hajduch, Ghilsoo Nam, Eun Ju Kim, R.Frohlich, J.A.Hanover, K.L.Kirk

Journal: Carbohydr.Res. , 343, 189, 2008

Formula: C19 H32 N1 O12 P1

Name: Diethyl (2-(acetylamino)-3,4,6-tri-O-acetyl-2-deoxy-alpha-D-glucopyranosyl)-1-hydroxymethylphosphonate

REFCODE: JAHBUQ

Authors/Journal

Authors: M.Malecka, K.Th.Wanner, E.Budzisz

Journal: Acta Crystallogr.,Sect.C:Cryst.Struct.Commun. , 59, o317, 2003

Formula: C15 H26 N1 O7 P1

Name: Dimethyl (1S,1'R,3'S,6'S)-(6'-t-butyl-5'-methoxy-6'-methyl-7'-oxa-8'-oxo-4'-azaspiro(2.5)oct-4'-en-1'-yl)hydroxymethylphosphonate

REFCODE: JEMPIA

Authors/Journal

Authors: A.I.Yanovsky, Yu.T.Struchkov, L.A.Uzlova, G.K.Kist'yan, Yu.A.Zhdanov

Journal: Zh.Strukt.Khim.(Russ.)(J.Struct.Chem.) , 30, 158-1, 1989

Formula: C13 H25 O8 P1

Name: Diethyl 1,2-O-isopropylidene-3-O-methyl-alpha-D-xylopentadialdo-1,4-furanose-5-phosphate

REFCODE: JOGBUD

Authors/Journal

Authors: J.P.Abell, H.Yamamoto

Journal: J.Am.Chem.Soc. , 130, 10521, 2008

Formula: C11 H10 Br1 F6 O4 P1

Name: 1-(4-bromophenyl)-1-(bis(2,2,2-trifluoroethoxy)phosphite)methanol

REFCODE: KODYOS

Authors/Journal

Authors: Li-Tao An, Gui-Xia Gong, Xing Liu, Min Xia, Jian-Feng Zhou

Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 64, o1320, 2008

Formula: C11 H17 O4 P1

Name: Diethyl (hydroxy(phenyl)methyl)phosphonate

REFCODE: KODYOS01

Authors/Journal

Authors: Hua Fang, Weizhu Chen, Bihong Hong, Yufen Zhao, Meijuan Fang

Journal: Phosphorus,Sulfur,Silicon,Relat.Elem. , 185, 2182, 2010

Formula: C11 H17 O4 P1
Name: Diethyl hydroxy(phenyl)methylphosphonate

REFCODE: KODYOS02
Authors/Journal
Authors: L.Ouksel, S.Chafaa, R.Bourzami, N.Hamdouni, M.Sebais, Nadjib Chafai
Journal: J.Mol.Struct. , 1144, 389, 2017
Formula: C11 H17 O4 P1

REFCODE: KORLUY
Authors/Journal
Authors: Z.Galdecki, B.Luciak, M.Hoffmann
Journal: Cryst.Res.Technol. , 26, K174, 1991
Formula: C18 H23 O4 P1
Name: (-)-Dibenzyl-(1-hydroxy-2-methylpropyl)phosphonate

REFCODE: LAKQEV
Authors/Journal
Authors: J.-C.Monbaliu, B.Tinant, J.Marchand-Brynaert
Journal: J.Org.Chem. , 75, 5478, 2010
Formula: C15 H24 N1 O4 P1
Name: (Z)-Diethyl (1-hydroxy-4-((2-methylphenyl)amino)but-2-en-1-yl)phosphonate

REFCODE: LAKQOF
Authors/Journal
Authors: J.-C.Monbaliu, B.Tinant, J.Marchand-Brynaert
Journal: J.Org.Chem. , 75, 5478, 2010
Formula: C22 H42 N1 O8 P1 S1 Si1
Name: 1-(Diethoxyphosphonyl) 4-(o-tolylamino)-1-hydroxy-2-methanesulfonatobutan- -3-yl-t-butyl(dimethyl)silane

REFCODE: MEHBOR
Authors/Journal
Authors: Hua Fang, Mei-Juan Fang, Zhi-Ping Zeng, Zan-Bin Wei, Yu-Fen Zhao
Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 62, o1378, 2006
Formula: C9 H13 O4 P1
Name: Dimethyl (hydroxy(phenyl)methyl)phosphonate

REFCODE: MELROL
Authors/Journal

Authors: D.Plazuk, J.Zakrzewski, A.J.Rybarczyk-Pirek
Journal: Tetrahedron:Asymm. , 17, 1975, 2006
Formula: C13 H17 Fe1 O4 P1
Name: (R)-Dimethyl-(hydroxy(ferrocenyl)methyl)phosphonate

REFCODE: MHCEPO
Authors/Journal
Authors: E.Hohne, K.Lohs
Journal: Z.Naturforsch.,B:Chem.Sci. , 24, 1071, 1969
Formula: C4 H8 Cl3 O4 P1
Name: O,O-Dimethyl-(1-hydroxy-2,2,2-trichloroethyl)-phosphonate
Synonym: Trichlorofon

REFCODE: MITLEG
Authors/Journal
Authors: H.Sun, G.B.Reddy, C.George, E.J.Meuillet, M.Berggren, G.Powis, A.P.Kozikowski
Journal: Tetrahedron Lett. , 43, 2835, 2002
Formula: C34 H41 O9 P1
Name: 1,2:4,5-bis(O,O'-Isopropylidene)-6-O-benzyl-3-deoxy-3-(dibenzyl phosphono(hydroxy)methyl)inositol

REFCODE: NOLDAU
Authors/Journal
Authors: Fei Wang, Yadan Wang, Lingchao Cai, Zhiwei Miao, Ruyu Chen
Journal: Adv.Synth.Catal. , 350, 2733, 2008
Formula: C17 H17 O4 P1
Name: dimethyl (hydroxy(2-(phenylethynyl)phenyl)methyl)phosphonate

REFCODE: NUXXEJ
Authors/Journal
Authors: T.Yokomatsu, T.Yamagishi, T.Sada, K.Suemune, S.Shibuya
Journal: Tetrahedron , 54, 781, 1998
Formula: C16 H25 O6 P1
Name: (4S,5R,1'R)-4-(1'-(Diethylphosphono)hydroxymethyl)-5-phenyl-2,2-dimethyl-1,3-dioxolane

REFCODE: OSIXOF

Authors/Journal
Authors: V.B.Vangala, H.N.Pati
Journal: Synth.Commun. , 46, 374, 2016

Formula: C21 H26 N1 O6 P1
Name: diethyl (hydroxy(1-(4-methoxyphenyl)-4-oxo-3-phenylazetidin-2-yl)methyl)phosphonate

REFCODE: OTELEF
Authors/Journal
Authors: M.Petrova, M.Budesinsky, B.Klepetarova, I.Rosenberg
Journal: Tetrahedron , 67, 4227, 2011
Formula: C13 H19 N2 O8 P1
Name: Diethyl (5'R)-3'-deoxy-3',4'-didehydrouridine-5'-C-phosphonate
Synonym: Diethyl ((5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-4-hydroxy-4,5-dihydrofuran-2-yl)(hydroxy)methyl)phosphonate

REFCODE: OTELIJ
Authors/Journal
Authors: M.Petrova, M.Budesinsky, B.Klepetarova, I.Rosenberg
Journal: Tetrahedron , 67, 4227, 2011
Formula: C13 H19 N2 O8 P1
Name: Diethyl (5'S)-3'-deoxy-3',4'-didehydrouridine-5'-C-phosphonate
Synonym: Diethyl ((5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-4-hydroxy-4,5-dihydrofuran-2-yl)(hydroxy)methyl)phosphonate

REFCODE: PUQBAG
Authors/Journal
Authors: T.Cytlak, M.Saweliew, M.Kubicki, H.Koroniak
Journal: Org.Biomol.Chem. , 13, 10050, 2015
Formula: C21 H27 F3 N1 O4 P1 S1
Name: diethyl (3-(benzylamino)-4,4,4-trifluoro-1-hydroxy-2-(phenylsulfanyl)butyl)phosphonate

REFCODE: PUQBEK
Authors/Journal
Authors: T.Cytlak, M.Saweliew, M.Kubicki, H.Koroniak
Journal: Org.Biomol.Chem. , 13, 10050, 2015
Formula: C21 H26 F4 N1 O4 P1 S1
Name: diethyl (3-(benzylamino)-4,4,4-trifluoro-2-((4-fluorophenyl)sulfanyl)-1-hydroxybutyl)phosphonate

REFCODE: PUQBIO
Authors/Journal
Authors: T.Cytlak, M.Saweliew, M.Kubicki, H.Koroniak
Journal: Org.Biomol.Chem. , 13, 10050, 2015

Formula: C15 H21 F3 N1 O4 P1
Name: (1S*2R*,3S*)-diethyl ((1-benzyl-3-(trifluoromethyl)aziridin-2-yl)(hydroxy)methyl)phosphonate

REFCODE: PUQBOU
Authors/Journal
Authors: T.Cytlak, M.Saweliew, M.Kubicki, H.Koroniak
Journal: Org.Biomol.Chem. , 13, 10050, 2015
Formula: C15 H21 F3 N1 O4 P1
Name: (1R*,2R*,3S*)-diethyl ((1-benzyl-3-(trifluoromethyl)aziridin-2-yl)(hydroxy)methyl)phosphonate

REFCODE: ROPRAP
Authors/Journal
Authors: V.J.Blazis, K.J.Koeller, N.P.Rath, C.D.Spilling
Journal: Acta Crystallogr.,Sect.B:Struct.Sci. , 53, 838, 1997
Formula: C11 H15 O4 P1
Name: rac-(1-Hydroxy-3-phenyl-2-propenyl) dimethylphosphonate

REFCODE: ROPRET
Authors/Journal
Authors: V.J.Blazis, K.J.Koeller, N.P.Rath, C.D.Spilling
Journal: Acta Crystallogr.,Sect.B:Struct.Sci. , 53, 838, 1997
Formula: C11 H15 O4 P1
Name: (S)-(1-Hydroxy-3-phenyl-2-propenyl) dimethylphosphonate

REFCODE: SILQEK
Authors/Journal
Authors: Hua Fang, Mei-Juan Fang, Yu-Fen Zhao
Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 63, o4002, 2007
Formula: C12 H19 O5 P1
Name: Diethyl hydroxy(4-methoxyphenyl)methylphosphonate

REFCODE: SOMBOM
Authors/Journal
Authors: M.N.Tahir, N.Acar, H.Yilmaz, M.I.Tariq, D.Ulku
Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 65, o562, 2009
Formula: C9 H12 N1 O6 P1
Name: Dimethyl ((S)-hydroxy(2-nitrophenyl)methyl)phosphonate

REFCODE: TAQPOT

Authors/Journal

Authors: K.Pallitsch, A.Schweifer, A.Roller, F.Hammerschmidt

Journal: Org.Biomol.Chem. , 15, 3276, 2017

Formula: C7 H14 F3 O5 P1

Name: (rac)-(1R,2S)-diethyl (3,3,3-trifluoro-1,2-dihydroxypropyl)phosphonate

REFCODE: TIVREX

Authors/Journal

Authors: M.T.Corbett, J.S.Johnson

Journal: J.Am.Chem.Soc. , 135, 594, 2013

Formula: C12 H19 O4 P1

Name: Dimethyl (1-hydroxy-2-(4-methylphenyl)propyl)phosphonate

REFCODE: TIVRUN

Authors/Journal

Authors: M.T.Corbett, J.S.Johnson

Journal: J.Am.Chem.Soc. , 135, 594, 2013

Formula: C13 H19 O4 P1

Name: Dimethyl (hydroxy(1,2,3,4-tetrahydronaphthalen-1-yl)methyl)phosphonate

REFCODE: TOSDOU

Authors/Journal

Authors: T.Yokomatsu, T.Yamagishi, K.Matsumoto, S.Shibuya

Journal: Tetrahedron , 52, 11725, 1996

Formula: C23 H30 N1 O8 P1

Name: Methyl 4-(diethylphosphinyl(hydroxy)methyl)-N-benzyloxycarbonyl-L-phenylalaninate

REFCODE: VEMVOZ

Authors/Journal

Authors: D.Plazuk, J.Zakrzewski, A.Rybarczyk-Pirek

Journal: J.Organomet.Chem. , 691, 3098, 2006

Formula: C15 H23 Fe1 O4 P3

Name: 2-(Dimethylphosphito(hydroxy)methyl)-3,3',4,4'-tetramethyl-1,1'-diphosphaferrocene

REFCODE: XUWLOS

Authors/Journal

Authors: Angelique Ferry, X.Guinchard, P.Retailleau, D.Crich

Journal: J.Am.Chem.Soc. , 134, 12289, 2012

Formula: C29 H35 O9 P1

Name: (1R)-2,3,5-Tri-O-benzyl-4-O-formyl-D-arabinose 1-(dimethyl phosphonate)

REFCODE: YEDVOT

Authors/Journal

Authors: Hua Fang, Mei-Juan Fang, Shu-Na Luo, Rong-Bin Huang, Yu-Fen Zhao

Journal: Acta Crystallogr.,Sect.E:Struct.Rep.Online , 62, o637, 2006

Formula: C13 H21 O4 P1

Name: Diisopropyl (hydroxyphenylmethyl)phosphonate

REFCODE: ZOBWIX

Authors/Journal

Authors: C.Meier, W.H.G.Laux, J.W.Bats

Journal: Liebigs Ann. , , 1963, 1995

Formula: C13 H20 Cl1 O4 P1

Name: (S)-Di-isopropyl (2-chlorophenyl)hydroxymethyl-phosphonate

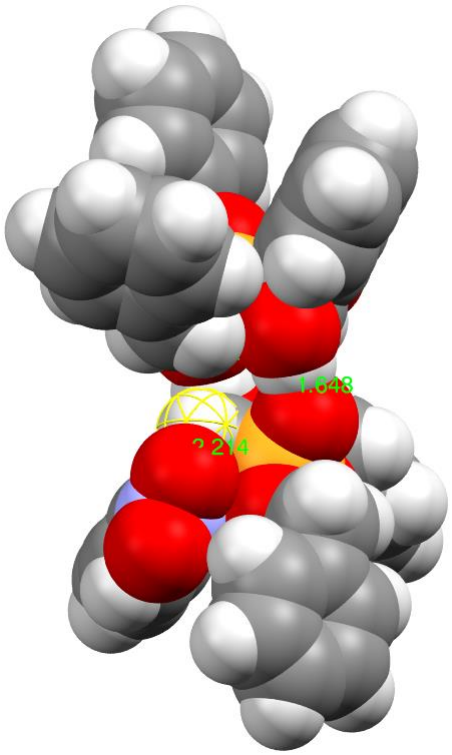


Figure 1

Figure 2

Figure 3

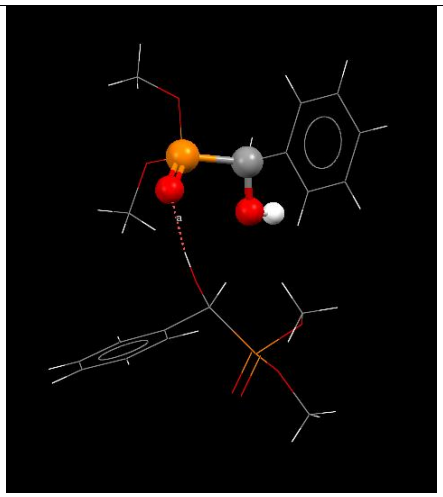
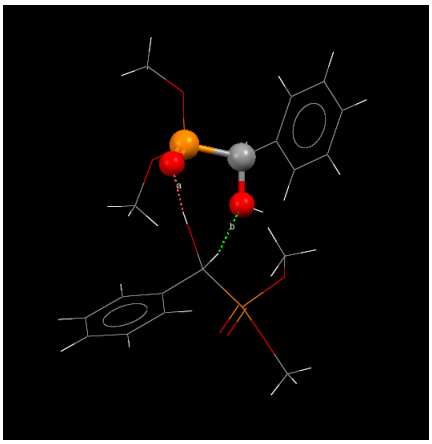
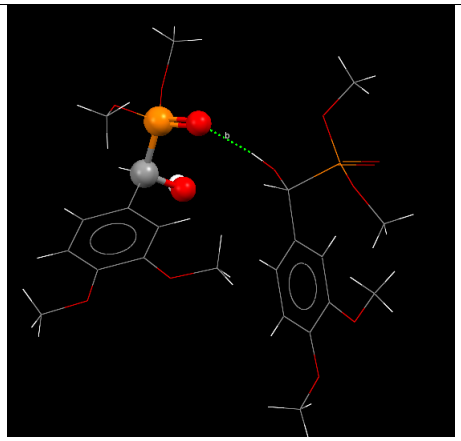
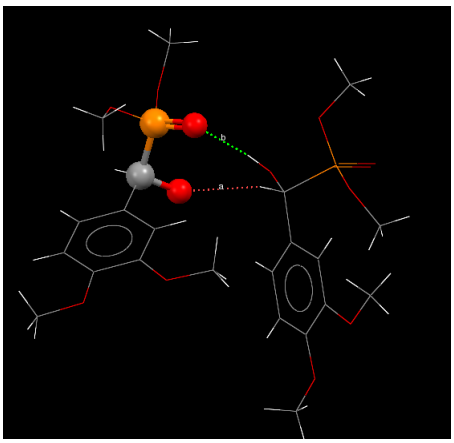
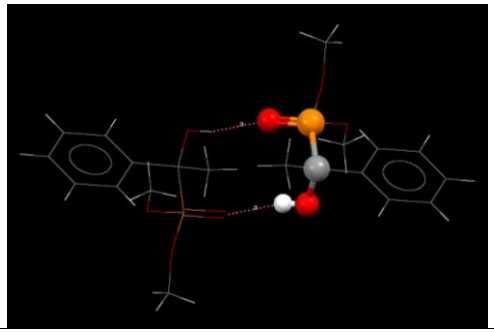
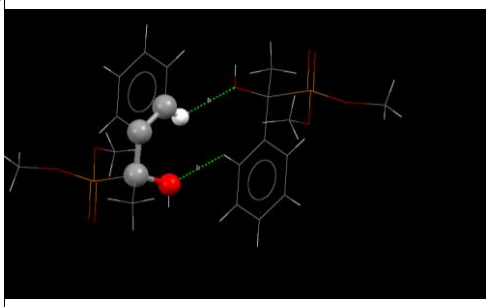
Figure 4

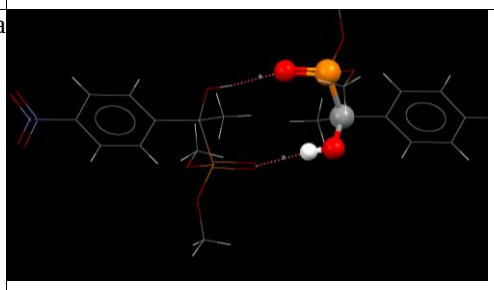
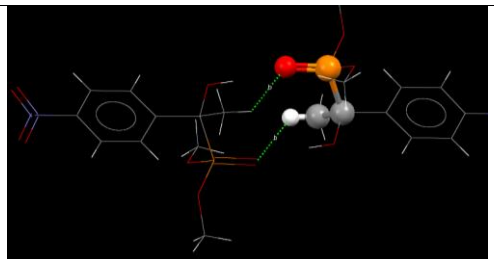
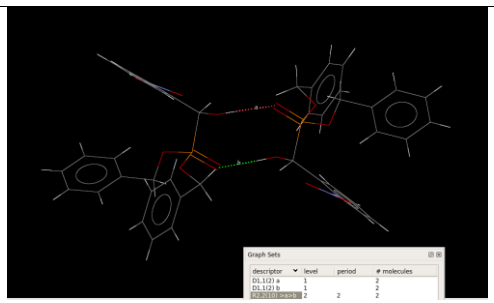
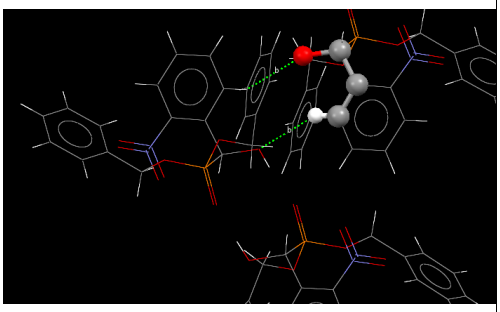
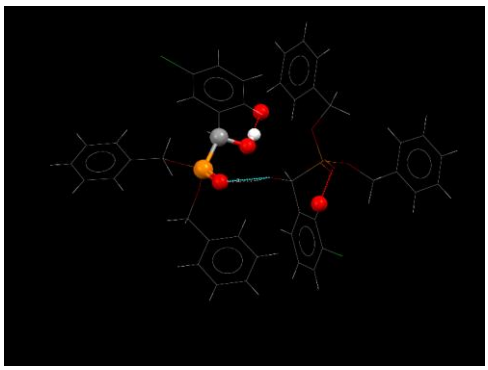
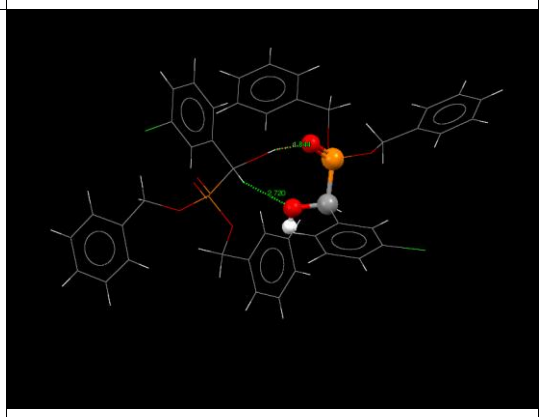
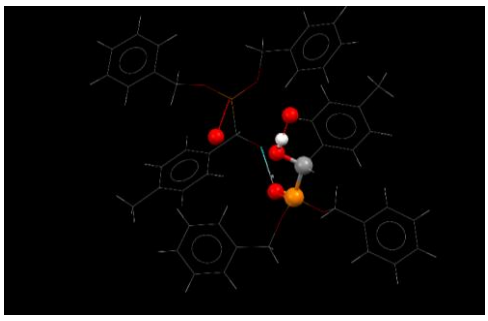
Figure 5

Figure 6

Figure 5 SF5. Space filling drawing of the **3a** molecules showing the a – H atom in a hatched sphere. The a – H atom – NO_2 group and one of the OH ··· O bridges O ··· H distances are also shown

Table ST2. Graph set analyses of compounds **1a** – **3c** for deposition. Sets are tabulated as text / drawings description of the primary graph set, then secondary set output from Mercury (Macrae *et al*., 2009)

	Primary GS	Primary GS	Secondary GS	Secondary GS
1a	C1,1(5)		R2,2(8)	
1b	C1,1(5)		R2,2(8)	
2a	R2,2(10)a,a		R2,2(10)b,b	

	Primary GS	Primary GS	Secondary GS	Secondary GS
2b	R2,2(10)a,a		R2,2(10)b,b	
3a	R2,2(10) >a>b		R2,2(10) >b>b; & S1,1(6) & S1,1(5)	
3b	C1,1(5) a		$R_2^2(8)$	
3c	C1,1(5) a		*S1,1(7) b* C1,1(8) c