

Supplementary Materials

Synthesis of α -Hydroxyethylphosphonates and α -Hydroxyethylphosphine oxides – Role of Solvents during Optical Resolution.

Zsuzsanna Szalai,¹ Anna Sára Kis,¹ József Schindler,^{1*} Konstantin Karaghiosoff² and György Keglevich^{1*}

¹*Department of Organic Chemistry and Technology, Faculty of Chemical Technology and Biotechnology, Budapest University of Technology and Economics, 1111 Budapest, Műegyetem rkp. 3., Hungary; szalai.zsuzsanna@edu.bme.hu; kisannasari@gmail.com; schindler.jozsef@vbk.bme.hu*

²*Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13, D-81377 München, Germany; klk@cup.uni-muenchen.de*

**Correspondence: keglevich.gyorgy@vbk.bme.hu; Tel.: +36-1-463-1111 (ext. 5883)*

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1. Geometrical data for (*S*)- α -hydroxyethyl-diphenylphosphine oxide ((*S*)-1c) obtained from the X-ray measurements

SI Table S1. Selected bond lengths (Å) of compound (*S*)-1c

P1 – O1	1.495(2)	C8 – C9	1.386(3)
P1 – C7	1.802(2)	C5 – C4	1.379(3)
P1 – C1	1.806(2)	C11 – C10	1.385(3)
P1 – C13	1.821(2)	C3 – C4	1.384(3)
O2 – C13	1.416(2)	C10 – C9	1.378(4)
C1 – C6	1.397(3)	C7 – C12	1.390(3)
C1 – C2	1.398(3)	C7 – C8	1.396(3)
C13 – C14	1.519(3)	C12 – C11	1.392(3)
C2 – C3	1.388(3)	C6 – C5	1.389(3)

SI Table S2. Selected bond angles (°) of compound (*S*)-1c

O1 – P1 – C7	110.1(1)	C9 – C8 – C7	120.2(2)
O1 – P1 – C1	112.3(1)	C4 – C5 – C6	120.3(2)
C7 – P1 – C1	107.0(1)	C10 – C11 – C12	119.8(2)
O1 – P1 – C13	111.5(1)	C4 – C3 – C2	120.0(2)
C7 – P1 – C13	107.4(1)	C5 – C4 – C3	120.2(2)
C1 – P1 – C13	108.4(1)	C9 – C10 – C11	120.6(2)
C6 – C1 – C2	119.1(2)	C10 – C9 – C8	119.9(2)
C6 – C1 – P1	124.0(2)	C12 – C7 – C8	119.6(2)
C2 – C1 – P1	116.9(2)	C12 – C7 – P1	122.5(2)
O2 – C13 – C14	110.8(2)	C8 – C7 – P1	117.9(2)
O2 – C13 – P1	108.6(1)	C7 – C12 – C11	119.9(2)
C14 – C13 – P1	110.6(2)	C5 – C6 – C1	120.1(2)
C3 – C2 – C1	120.3(2)		

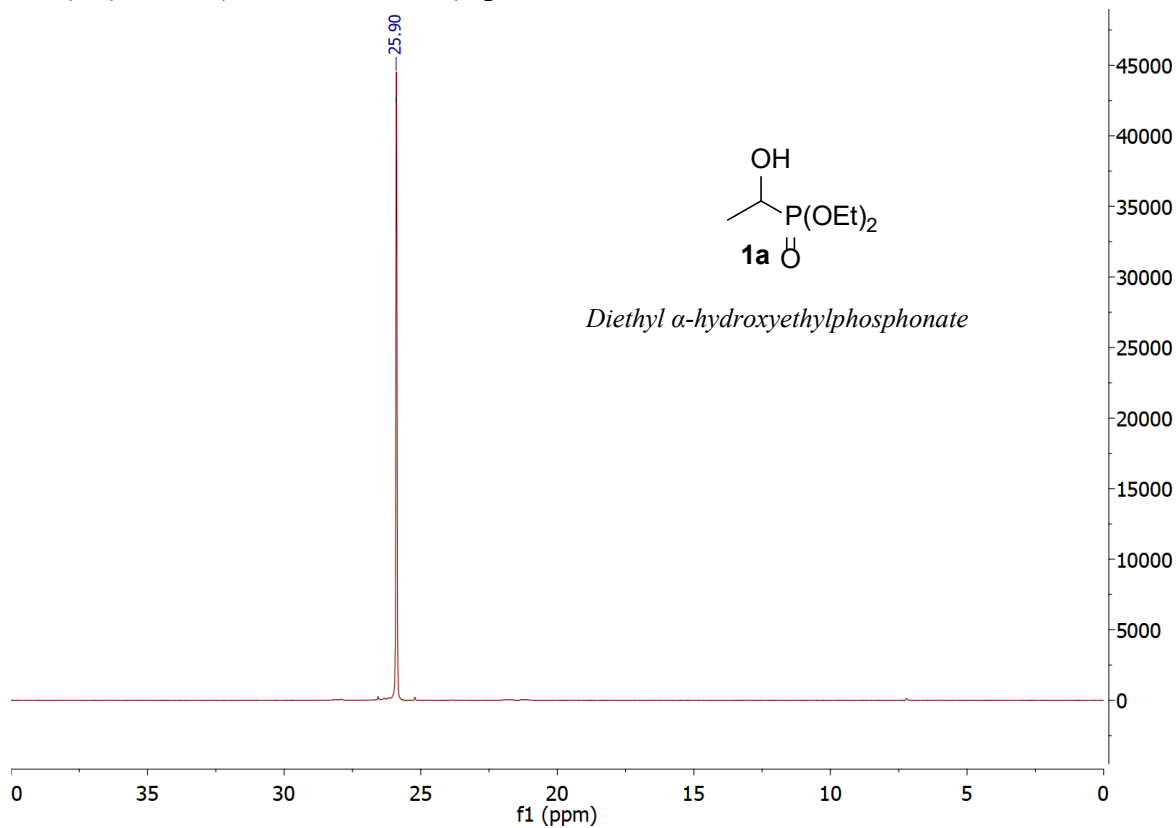
SI Table S3. Selected torsion angles (°) of compound (*S*)-1c

O1 – P1 – C1 – C6	122.9(2)	O1 – P1 – C7 – C8	-2.8(2)
C7 – P1 – C1 – C6	-116.2(2)	C1 – P1 – C7 – C8	-125.1(2)
C13 – P1 – C1 – C6	-0.7(2)	C13 – P1 – C7 – C8	118.8(2)
O1 – P1 – C1 – C2	-53.8(2)	C8 – C7 – C12 – C11	0.2(3)
C7 – P1 – C1 – C2	67.1(2)	P1 – C7 – C12 – C11	-179.2(2)
C13 – P1 – C1 – C2	-177.5(2)	C2 – C1 – C6 – C5	0.0(3)
O1 – P1 – C13 – O2	174.2(1)	P1 – C1 – C6 – C5	-176.7(2)
C7 – P1 – C13 – O2	53.5(2)	C12 – C7 – C8 – C9	-0.8(3)

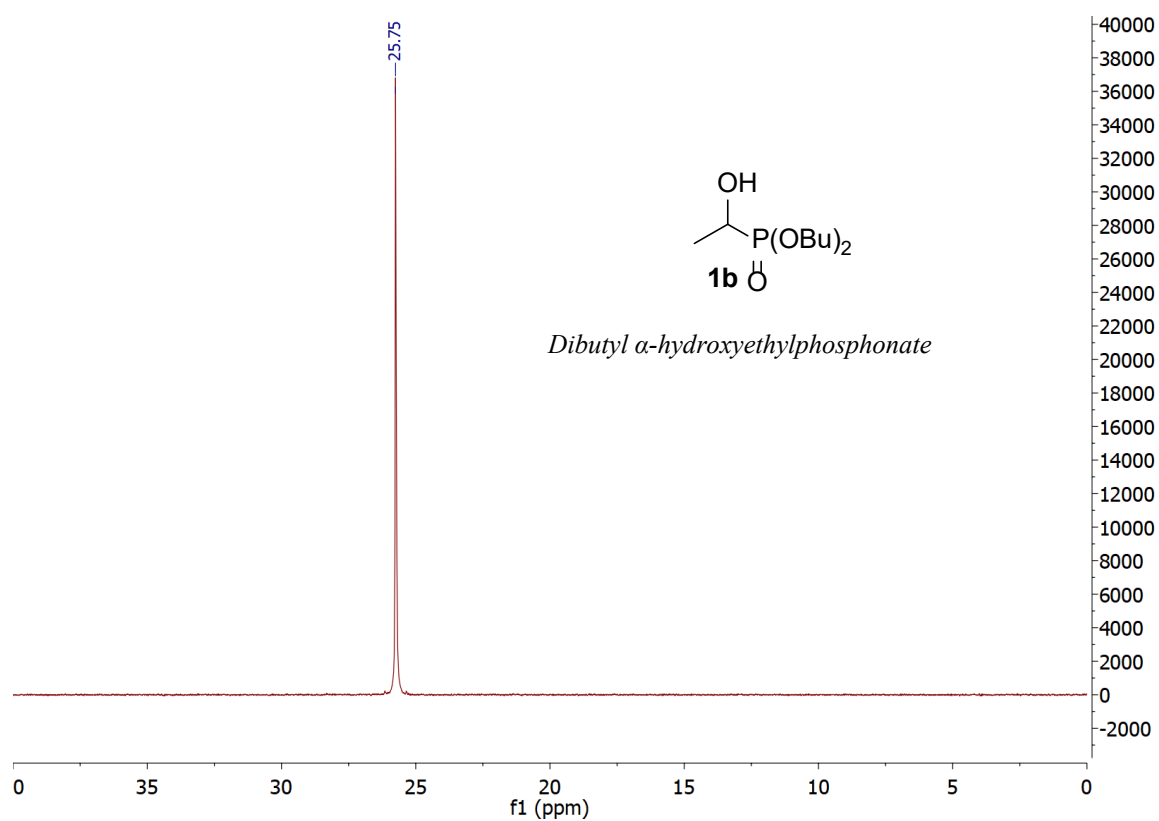
C1 – P1 – C13 – O2	-61.7(2)	P1 – C7 – C8 – C9	178.6(2)
O1 – P1 – C13 – C14	52.3(2)	C1 – C6 – C5 – C4	0.1(3)
C7 – P1 – C13 – C14	-68.4(2)	C7 – C12 – C11 – C10	0.6(3)
C1 – P1 – C13 – C14	176.4(2)	C1 – C2 – C3 – C4	0.4(3)
C6 – C1 – C2 – C3	-0.2(3)	C6 – C5 – C4 – C3	0.1(3)
P1 – C1 – C2 – C3	176.7(2)	C2 – C3 – C4 – C5	-0.4(4)
O1 – P1 – C7 – C12	176.6(2)	C12 – C11 – C10 – C9	-0.7(4)
C1 – P1 – C7 – C12	54.3(2)	C11 – C10 – C9 – C8	0.1(4)
C13 – P1 – C7 – C12	-61.8(2)	C7 – C8 – C9 – C10	0.6(3)

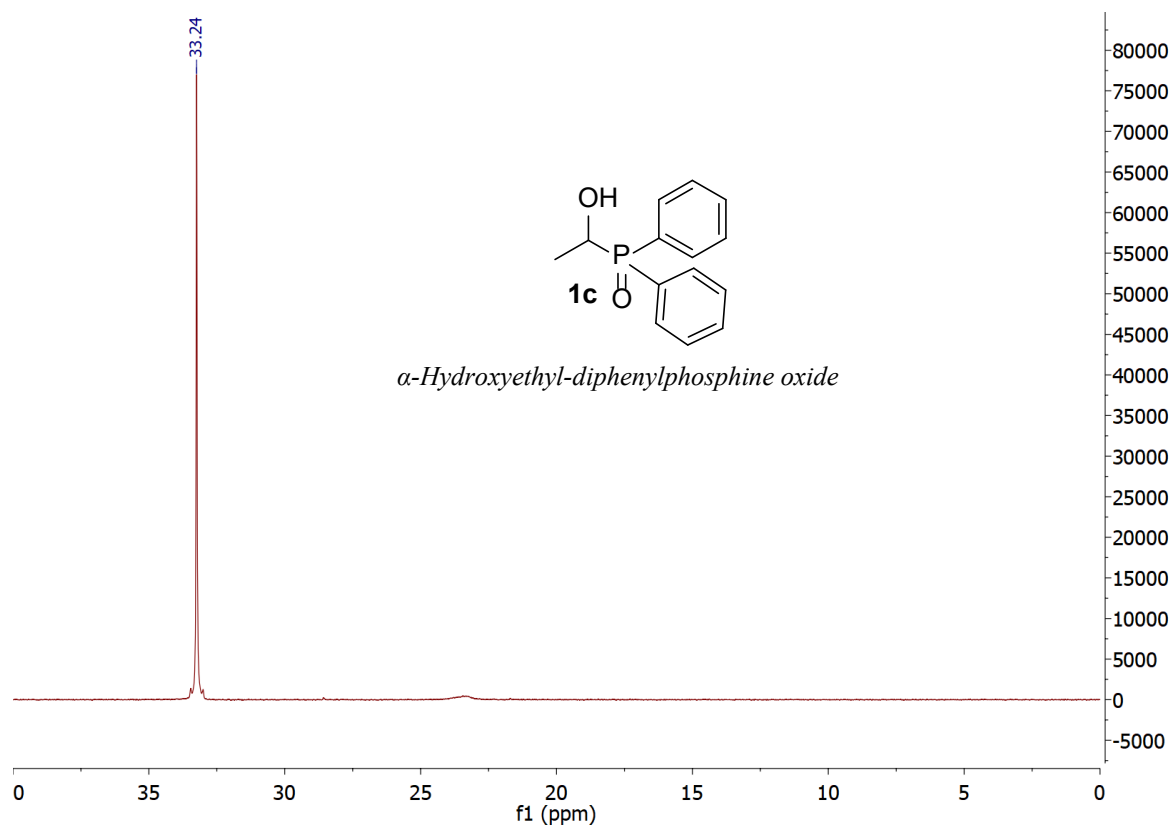
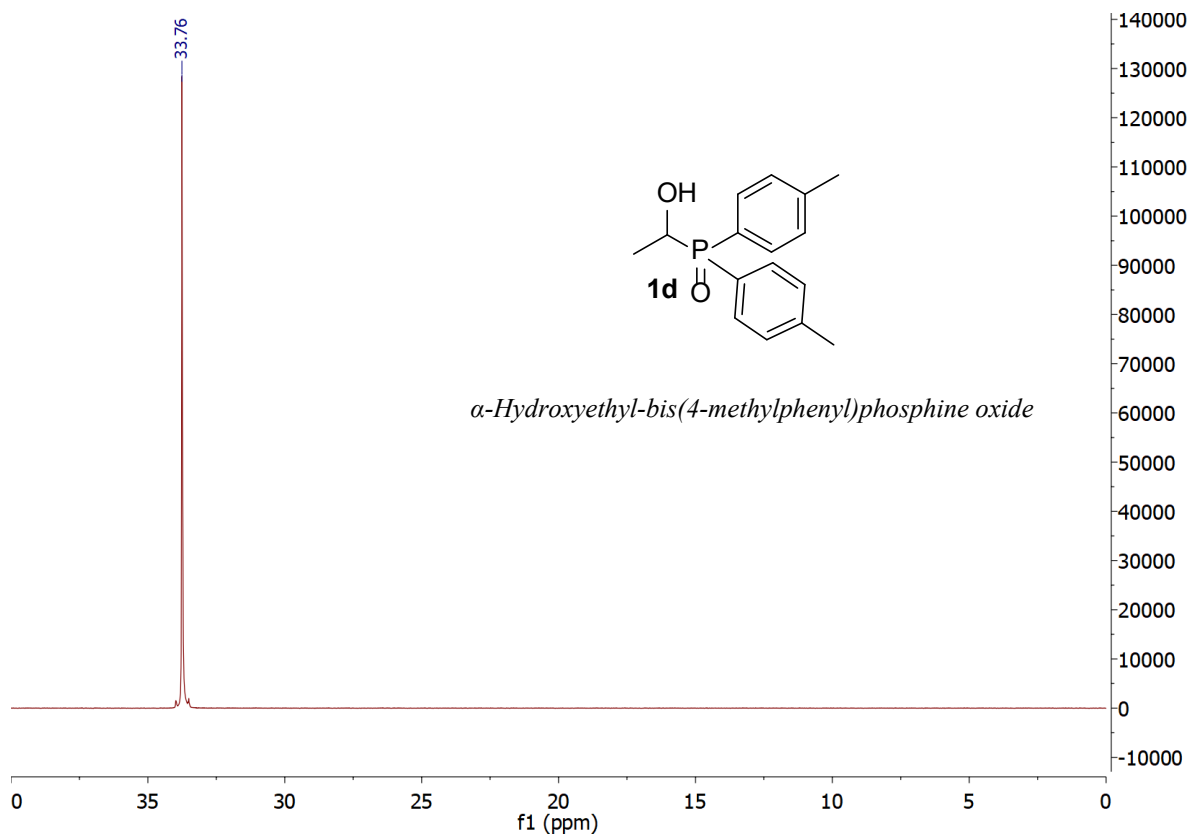
2. ^{31}P , ^{13}C , ^1H NMR spectra for the hydroxyphosphonate derivatives 1a-e synthesized

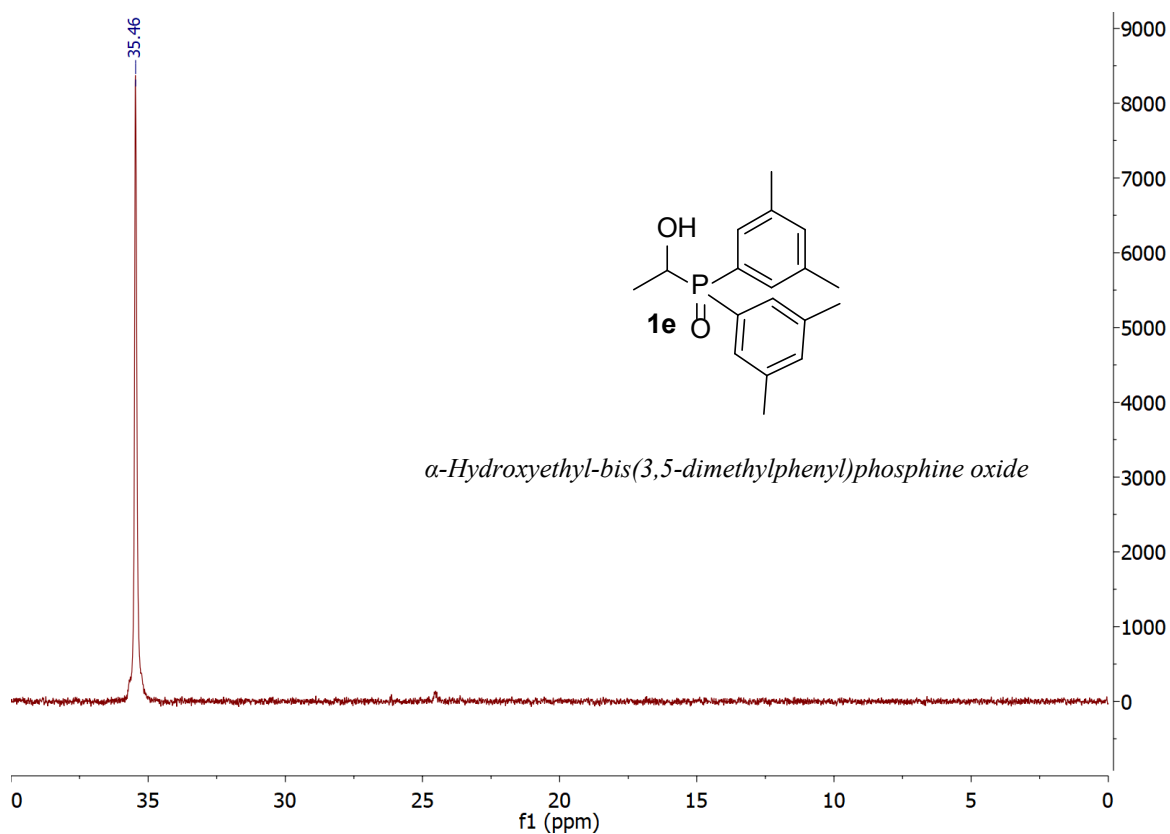
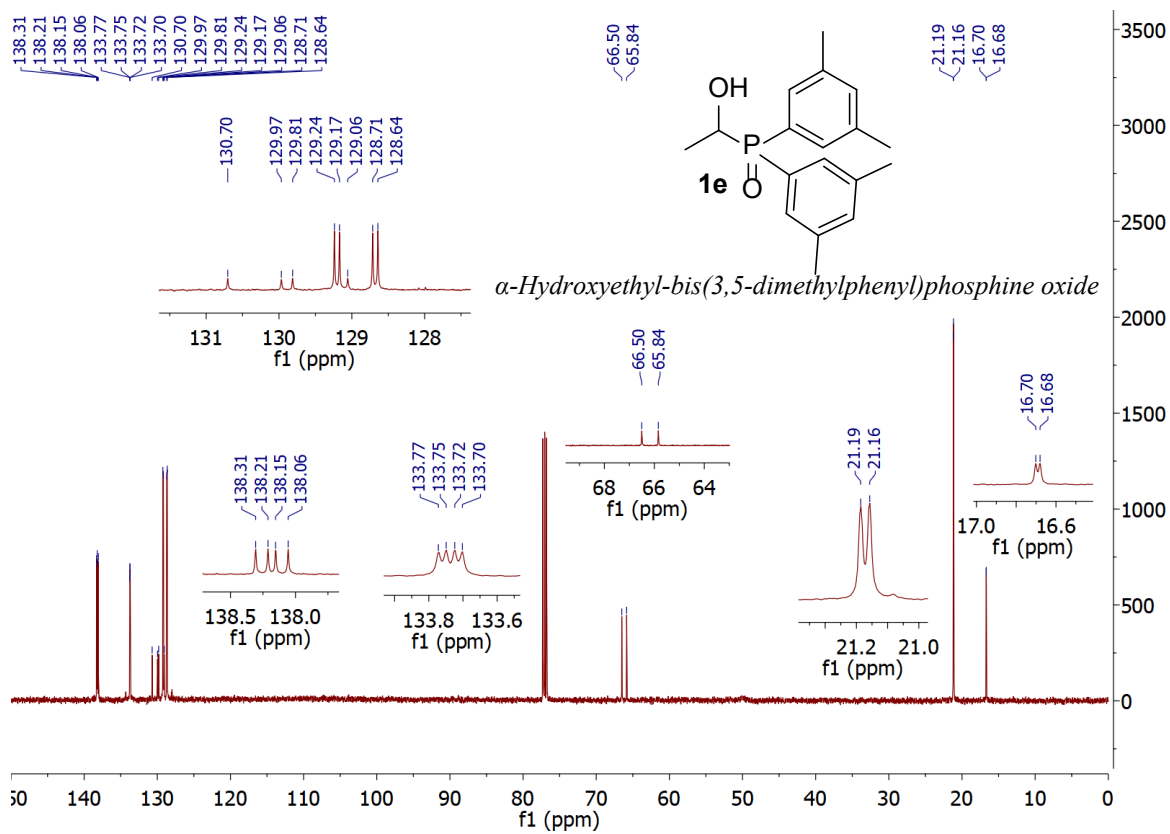
^{31}P $\{^1\text{H}\}$ NMR (122 MHz, CDCl_3) spectra for 1a



^{31}P $\{^1\text{H}\}$ NMR (202 MHz, CDCl_3) spectra for 1b



^{31}P { ^1H } NMR (202 MHz, CDCl_3) spectra for 1c **^{31}P { ^1H } NMR (202 MHz, CDCl_3) spectra for 1d**

^{31}P $\{^1\text{H}\}$ NMR (202 MHz, CDCl_3) spectra for 1d **^{13}C $\{^1\text{H}\}$ NMR (126 MHz, CDCl_3) spectra for 1e**

¹H NMR (500 MHz, CDCl₃) spectra for 1e