Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

for

New azaheterocyclic aromatic diphosphonates for hybrid materials for fuel cell applications

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- ^{1}H and ^{13}C NMR spectra for 1-benzyl-4,7-dibromo-1*H*-benzimidazole **5** and 4,7-dibromo-1-(tetrahydro-2*H*-pyran-2-yl)-1*H*-benzimidazole **6**.

- ^{1}H, ^{13}C and ^{31}P NMR spectra for tetraethyl benzo[*c*][1,2,5]thiadiazole-4,7-diylbis(phosphonate) **10,** tetraethyl (2,3-diamino-1,4-phenylene)bis(phosphonate) **11,** tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9** and tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.

- ^{1}H and ^{31}P NMR spectra for tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9** in different solvents and concentrations.

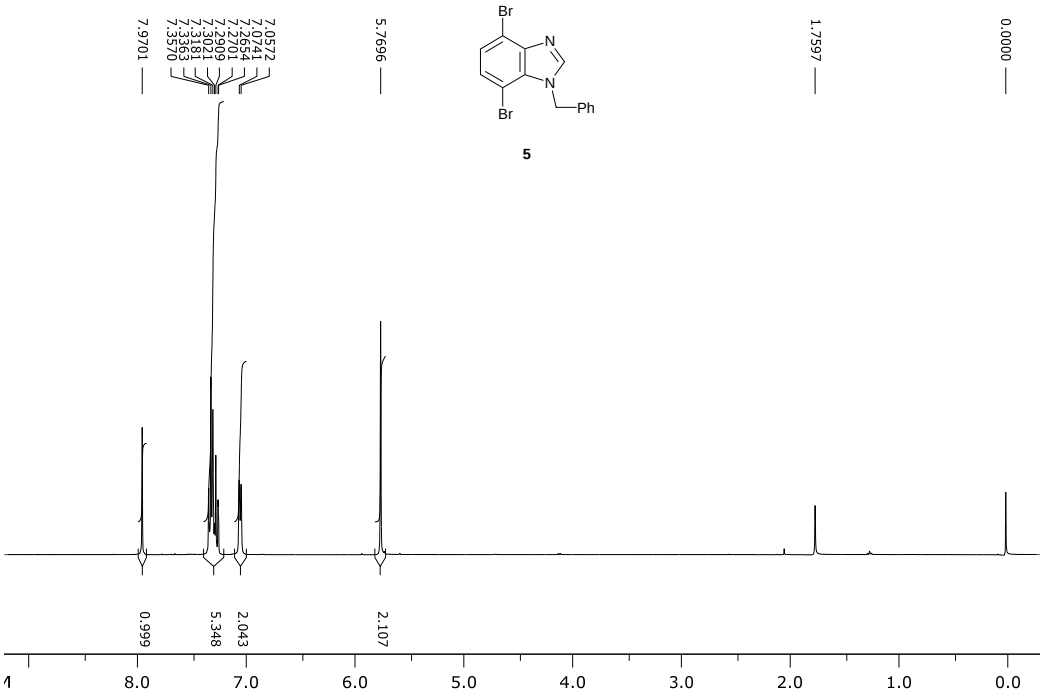

Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 1-benzyl-4,7-dibromo-1*H*-benzimidazole **5**.

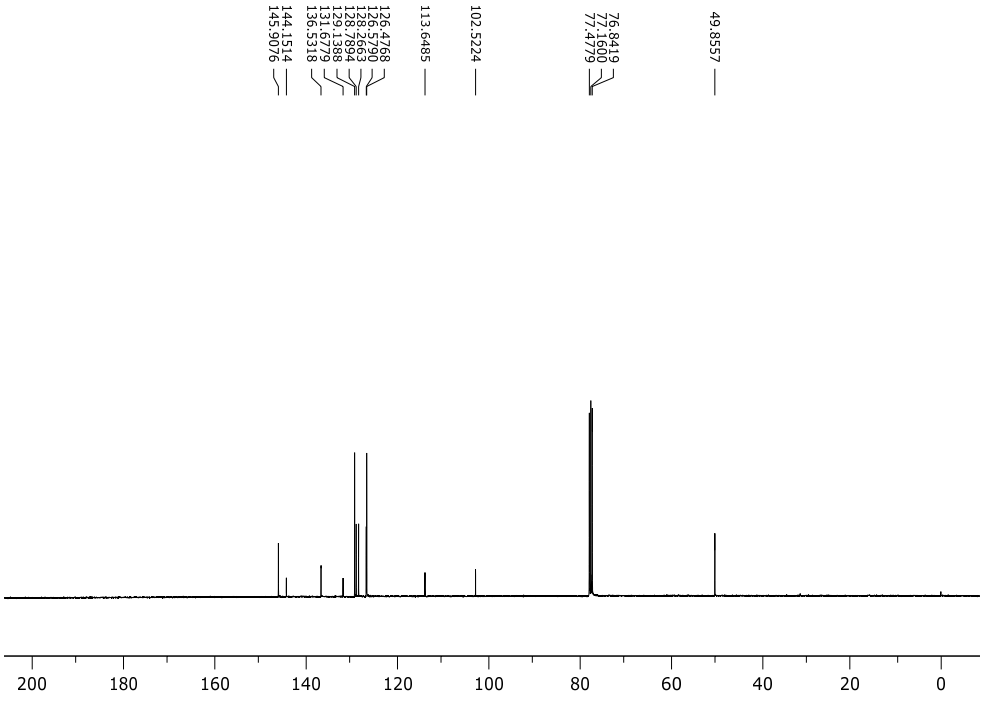

Figure S2. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 1-benzyl-4,7-dibromo-1*H*-benzimidazole **5**.

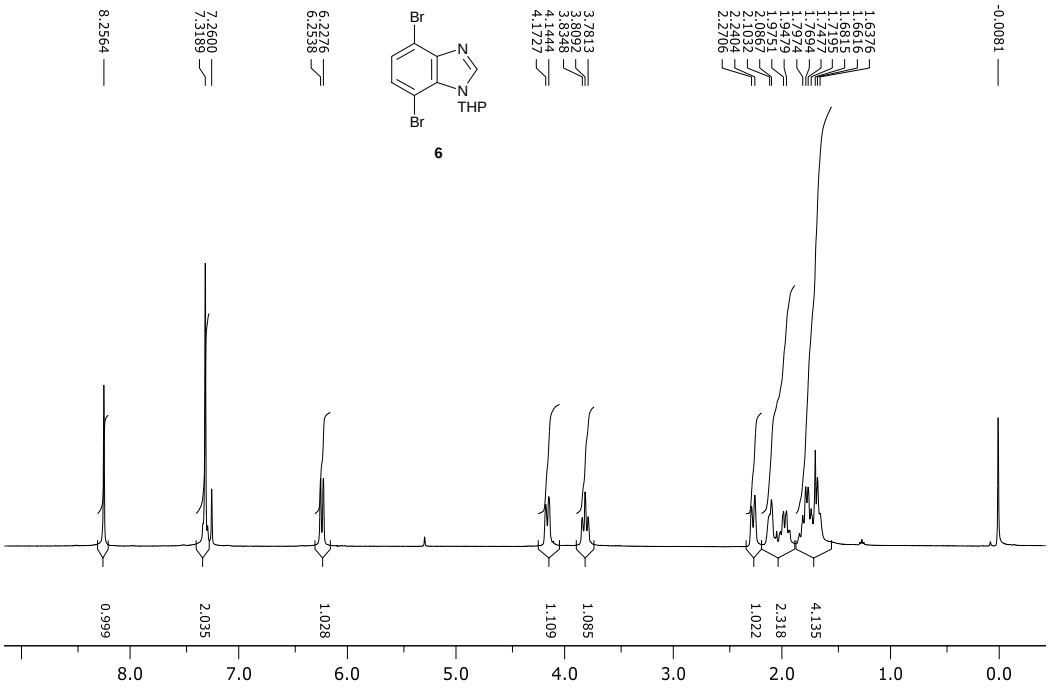

Figure S3. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of 4,7-dibromo-1-(tetrahydro-2*H*-pyran-2-yl)-1*H*-benzimidazole **6**.

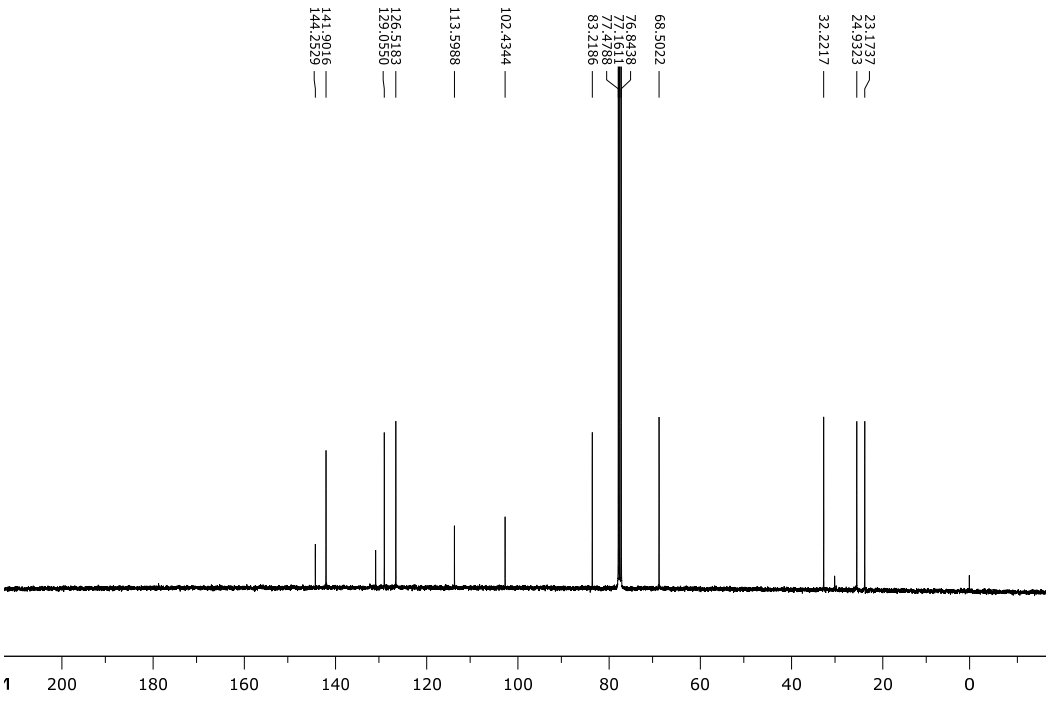

Figure S4. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of 4,7-dibromo-1-(tetrahydro-2*H*-pyran-2-yl)-1*H*-benzimidazole **6**.

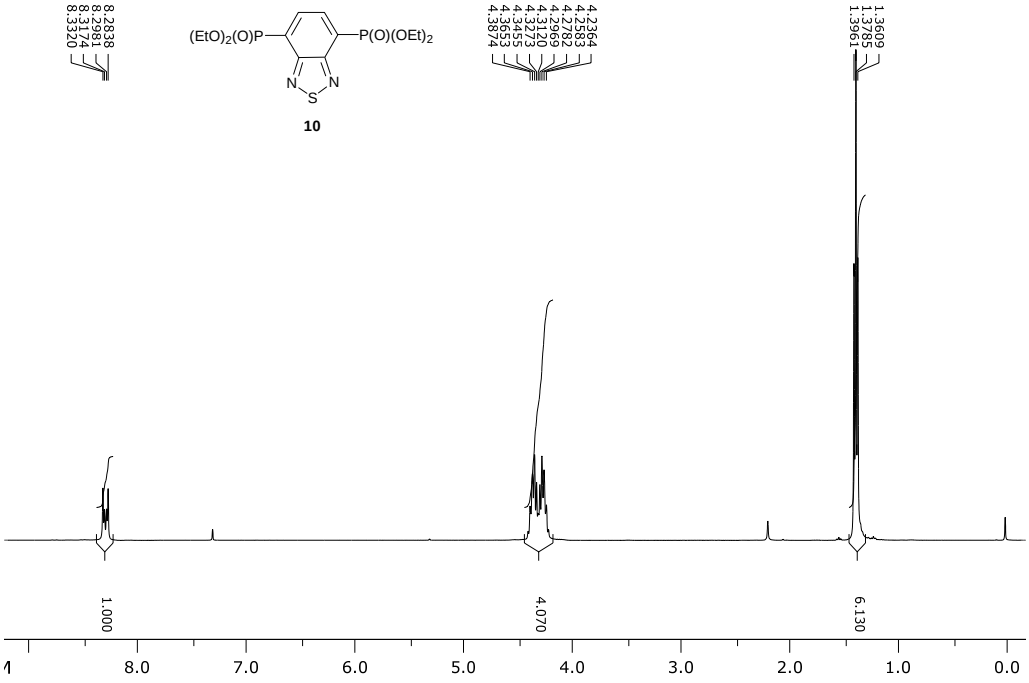

Figure S5. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of tetraethyl benzo[*c*][1,2,5]thiadiazole-4,7-diylbis(phosphonate) **10**.

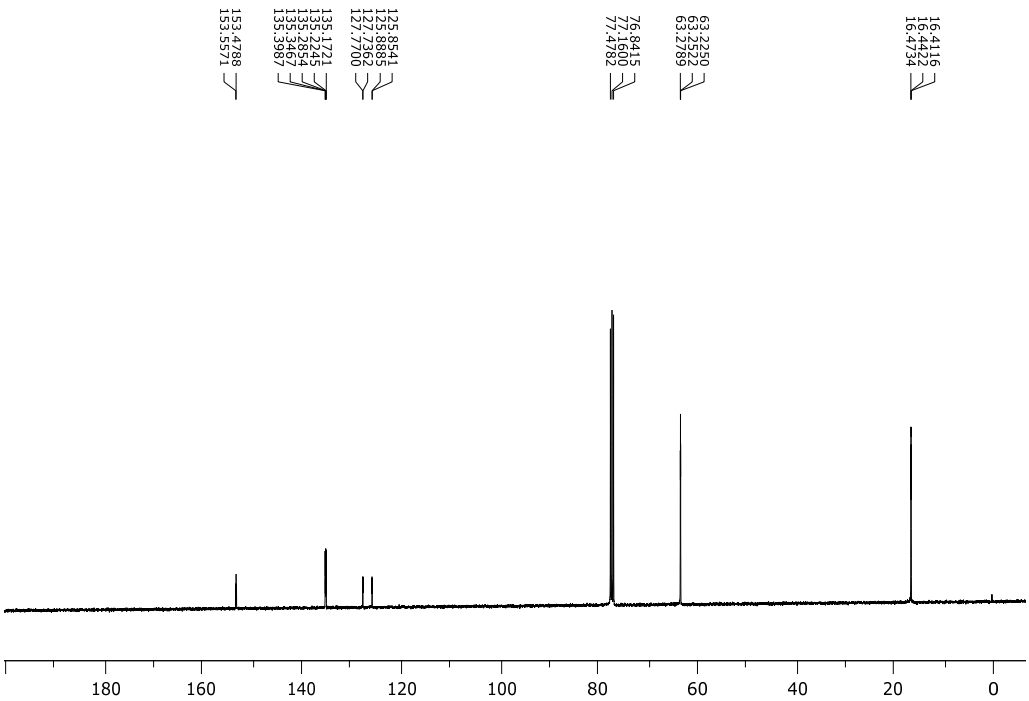

Figure S6. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of tetraethyl benzo[*c*][1,2,5]thiadiazole-4,7-diylbis(phosphonate) **10**.

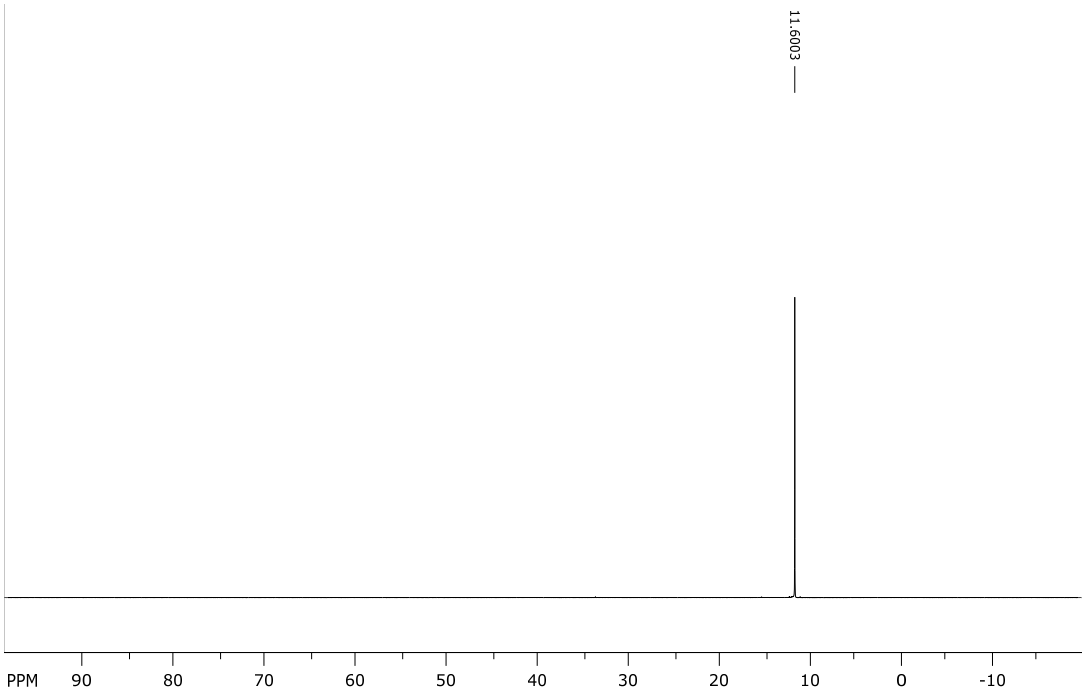

Figure S7. ^{31}P NMR spectrum (162 MHz, $H_3PO_4/CDCl_3$) tetraethyl benzo[*c*][1,2,5]thiadiazole-4,7-diylbis(phosphonate) **10**.

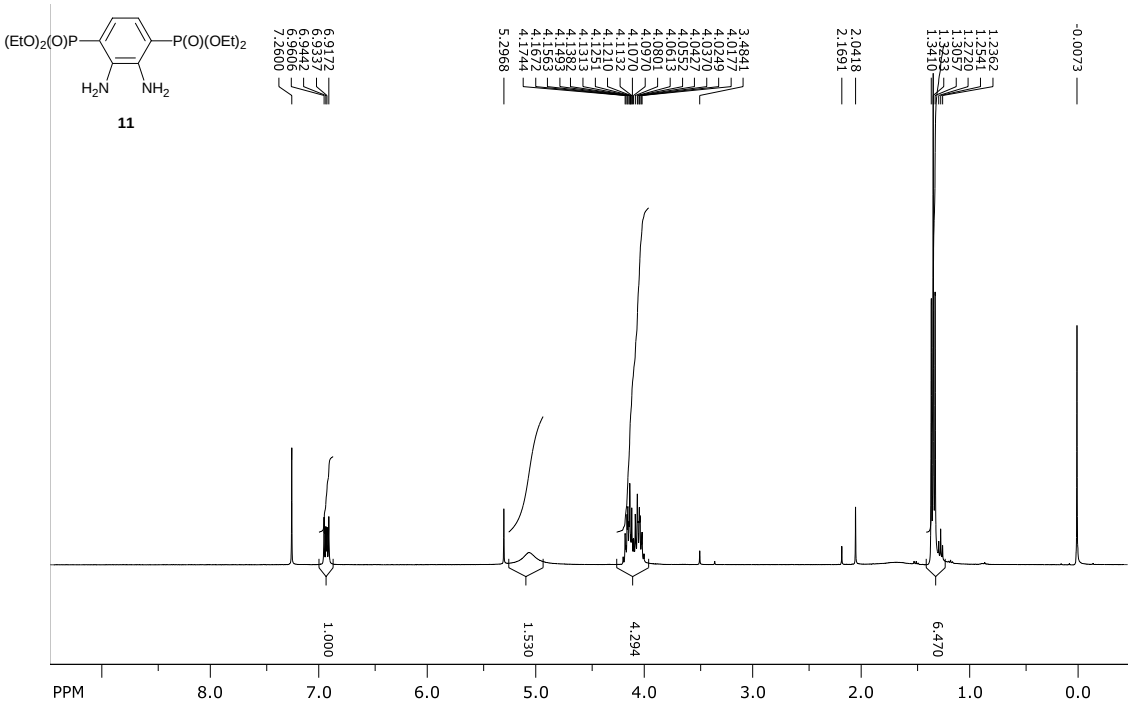

Figure S8. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of tetraethyl (2,3-diamino-1,4-phenylene)bis(phosphonate) **11**.

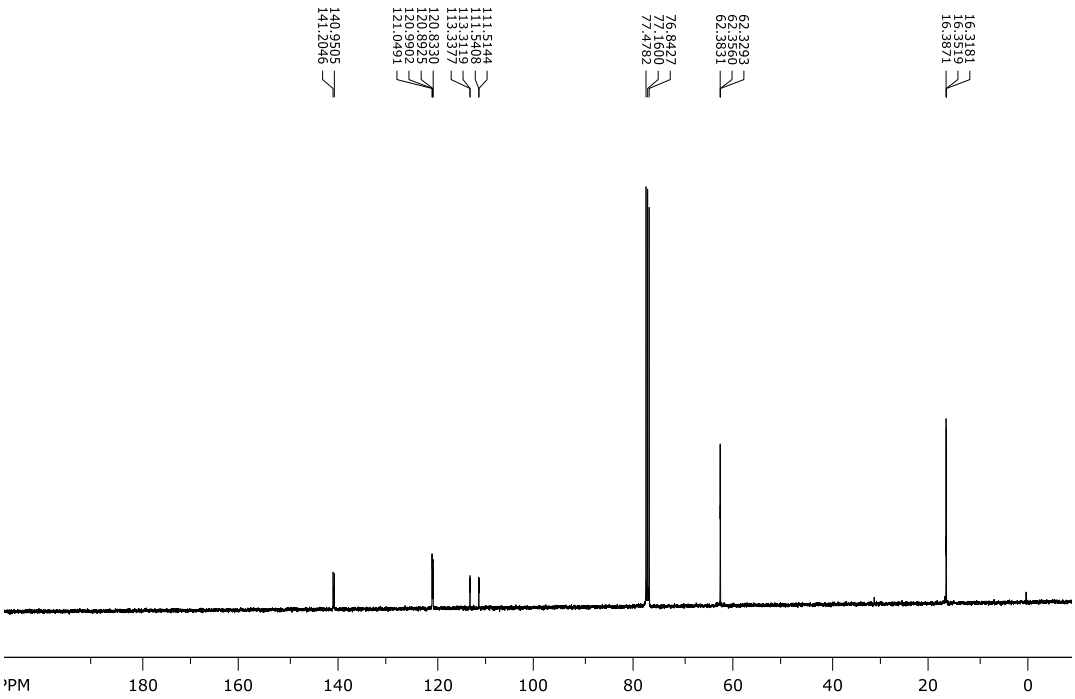

Figure S9. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of tetraethyl (2,3-diamino-1,4-phenylene)bis(phosphonate) **11**.

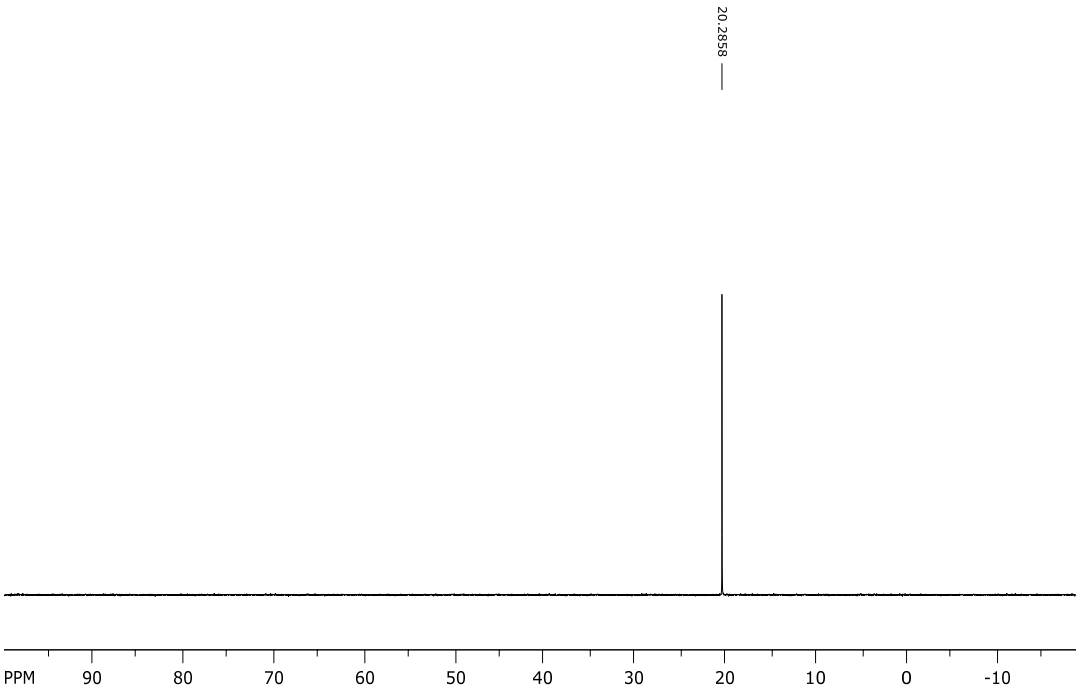

Figure S10. ^{31}P NMR spectrum (162 MHz, $H_3PO_4/CDCl_3$) of tetraethyl (2,3-diamino-1,4-phenylene)bis(phosphonate) **11**.

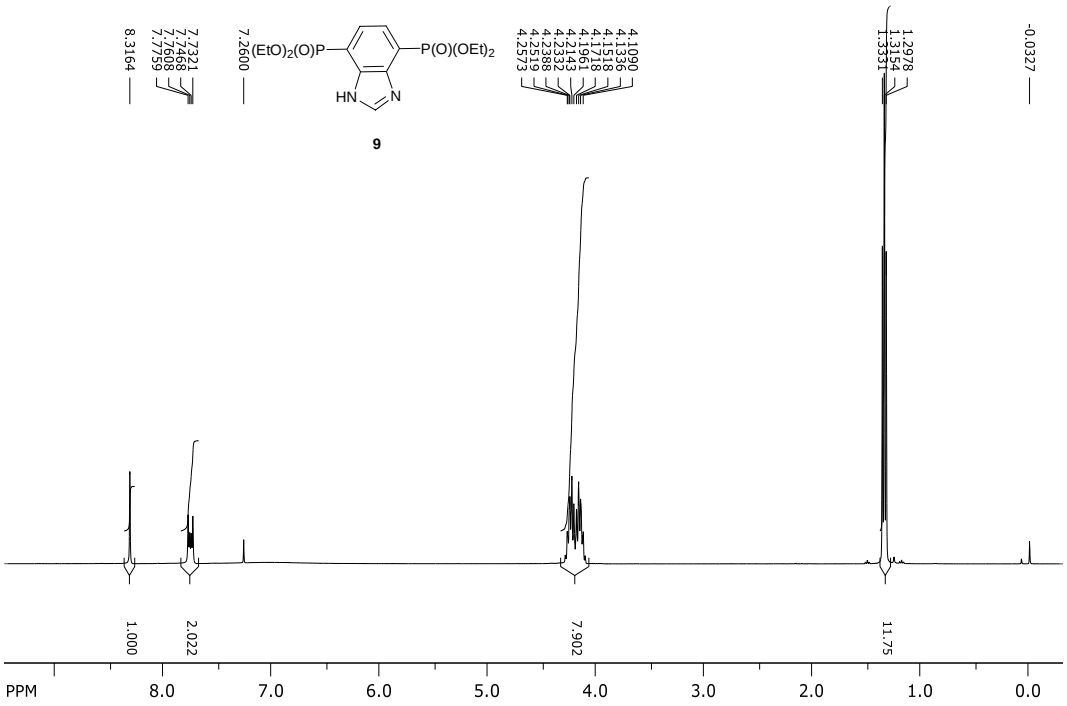

Figure S11. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9**.

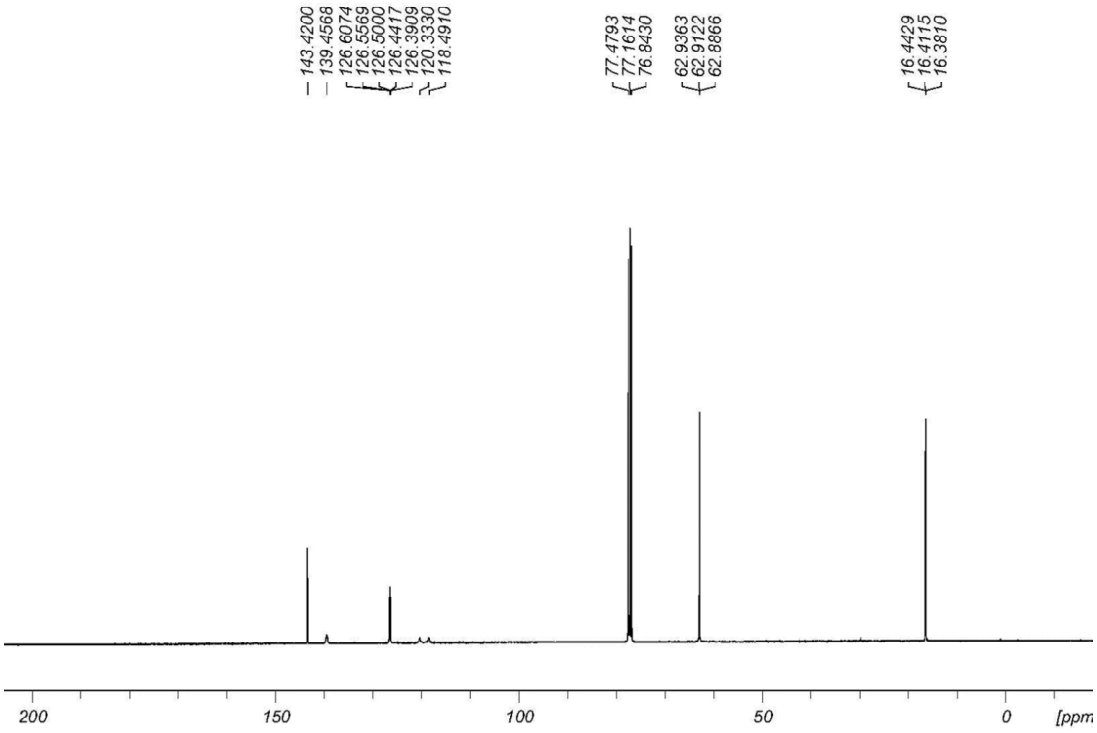

Figure S12. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9**.

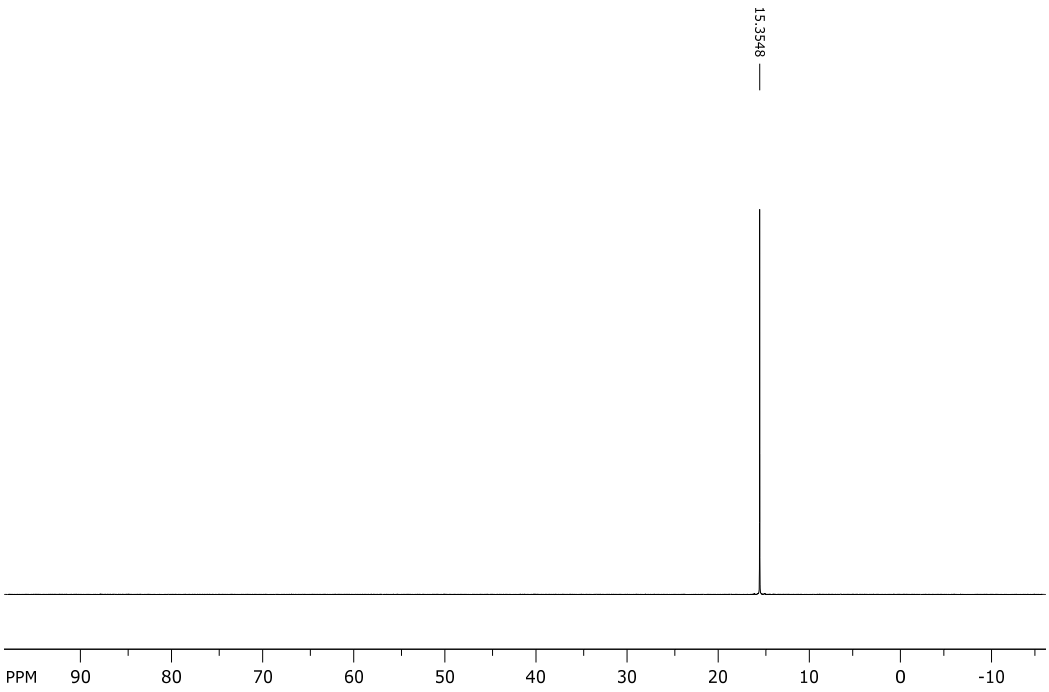

Figure S13. ^{31}P NMR spectrum (162 MHz, H_3PO_4/$CDCl_3$) of tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9**.

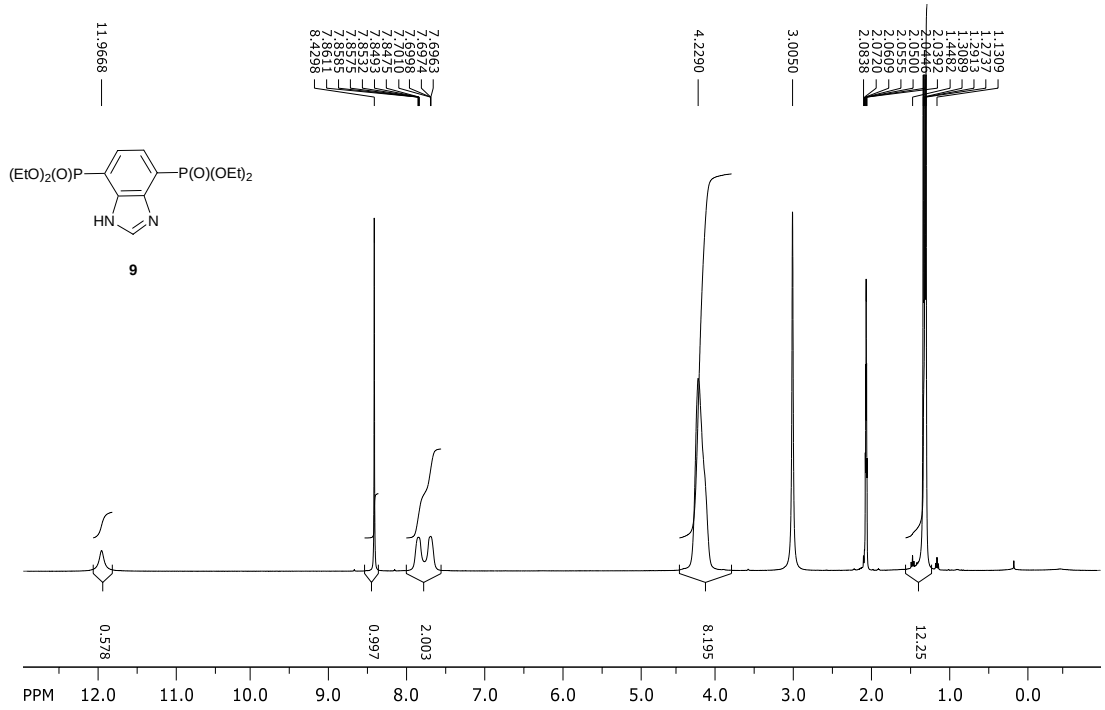

Figure S14. ^{1}H NMR spectrum (400 MHz, acetone-d_6) of tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9**.

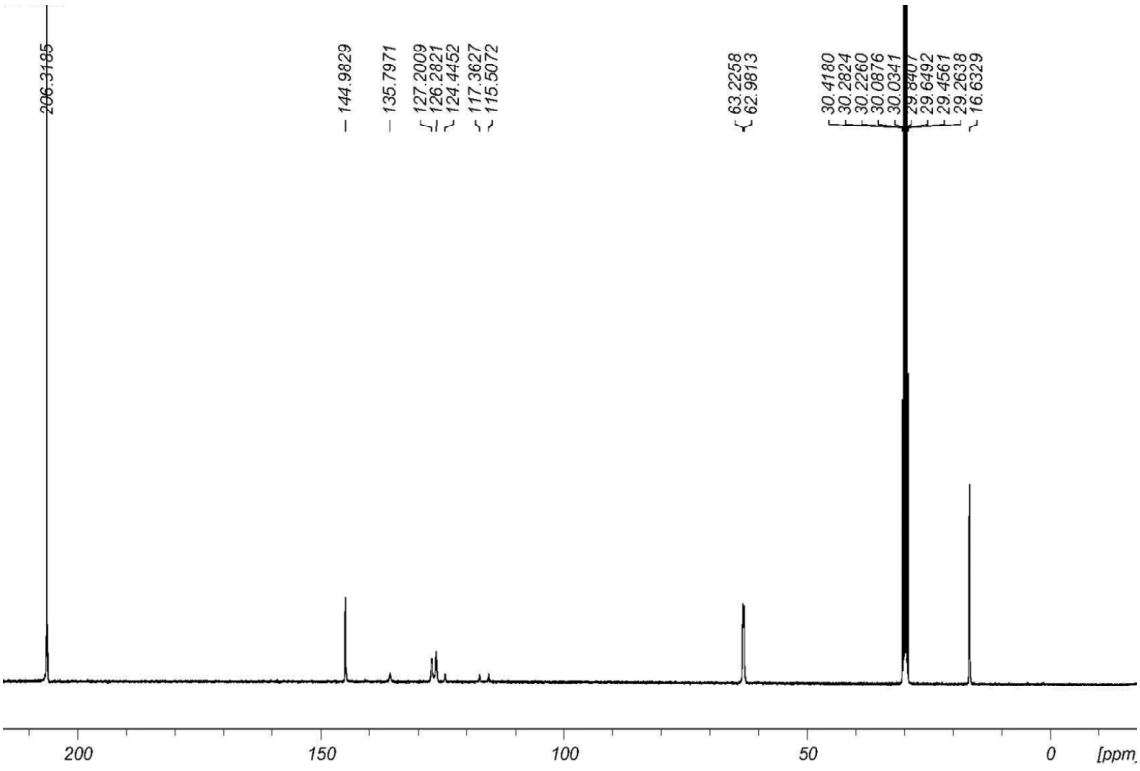

Figure S15. ^{13}C NMR spectrum (100 MHz, acetone-d_6) of tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9**.

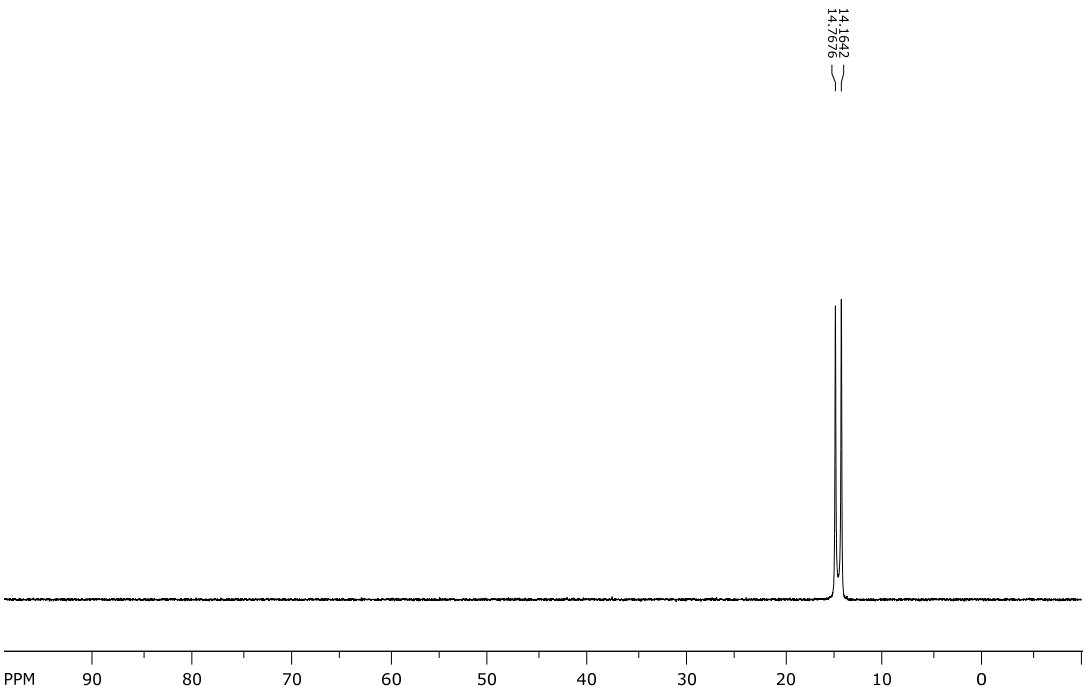

Figure S16. ^{31}P NMR spectrum (162 MHz, H_3PO_4/ acetone-d_6) of tetraethyl 1*H*-benzo[*d*]imidazole-4,7-diylbis(phosphonate) **9**.

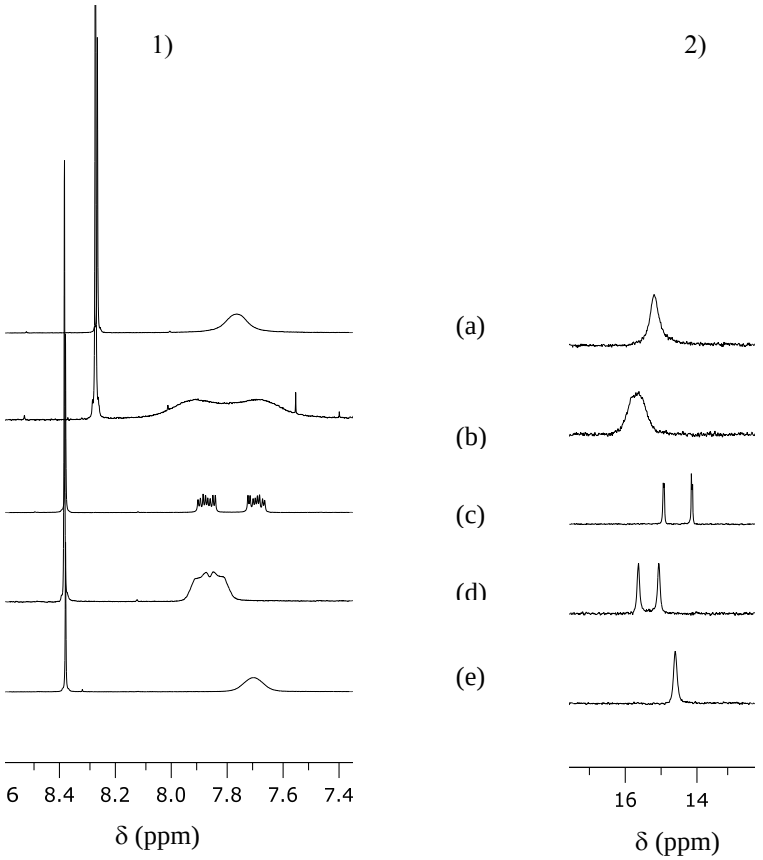

Figure S17. The 1) ^{1}H NMR and 2) ^{31}P NMR spectra of compound **9** in different solvents in 0.01M solutions: (a) CD_2Cl_2, (b) $CDCl_3$, (c) acetone-d_6, (d) MeOD, (e) DMSO-d_6.

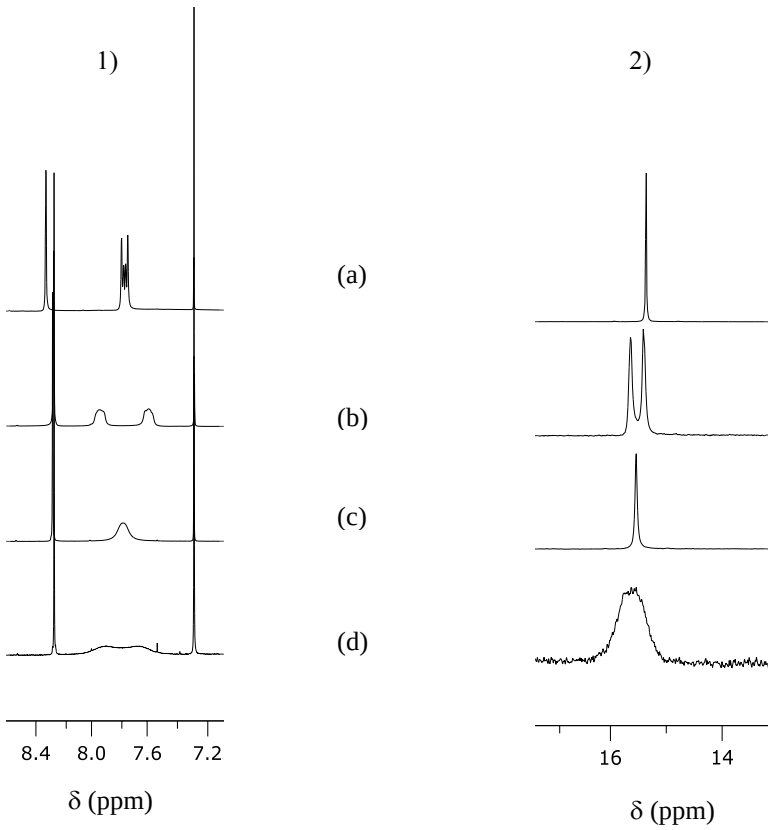

Figure S18. The 1) ^{1}H NMR and 2) ^{31}P NMR spectra of compound **9** in $CDCl_3$ for different concentrations: (a) 0.1 M (after redissolution of the sample), (b) 0.1 M, (c) 0.05 M, (d) 0.01 M.

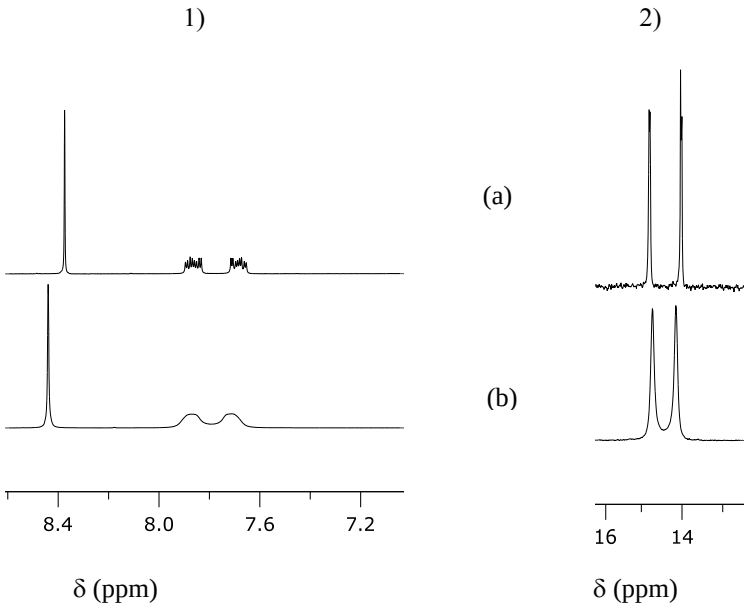

Figure S19. The 1) ^{1}H NMR and 2) ^{31}P NMR spectra of compound **9** in acetone-d_6 in different concentrations: (a) 0.01M, (b) 0.1 M.

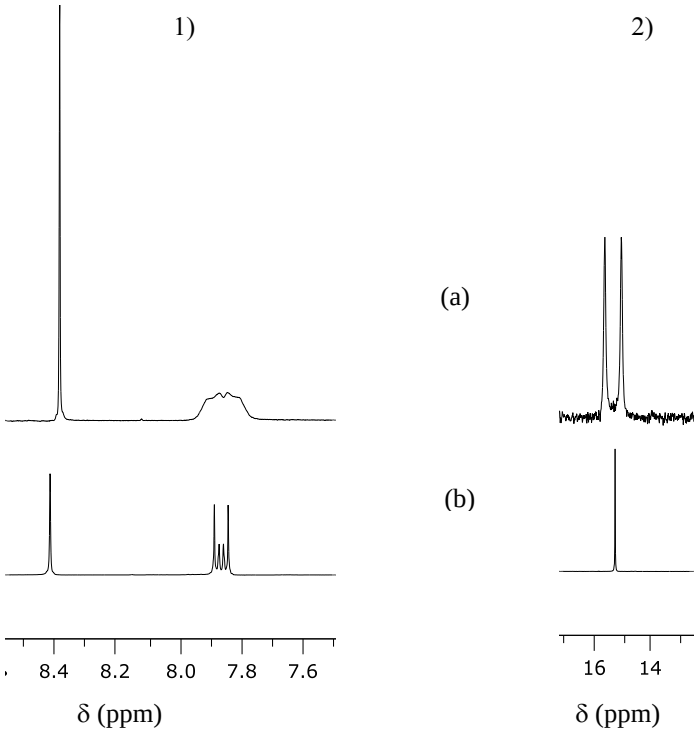

Figure S20. The 1) ^{1}H NMR and 2) ^{31}P NMR spectra of compound **9** in MeOD in different concentrations: (a) 0.01M, (b) 0.1 M.

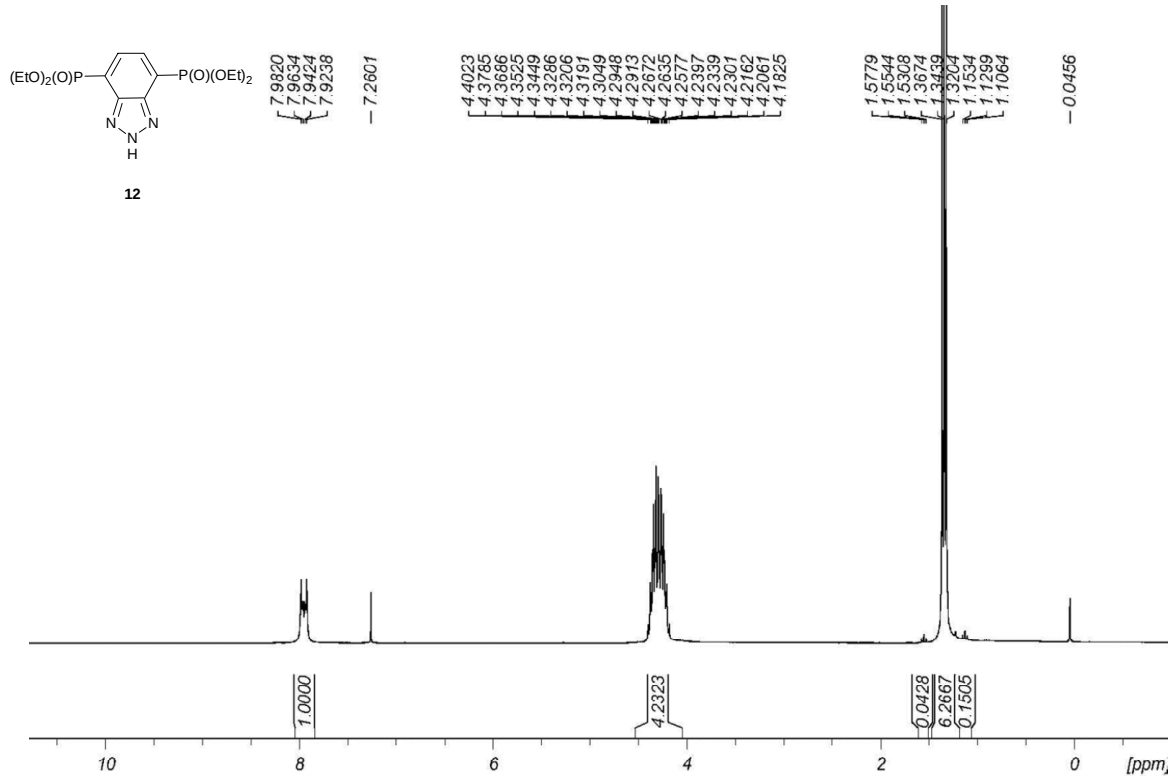

Figure S21. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.

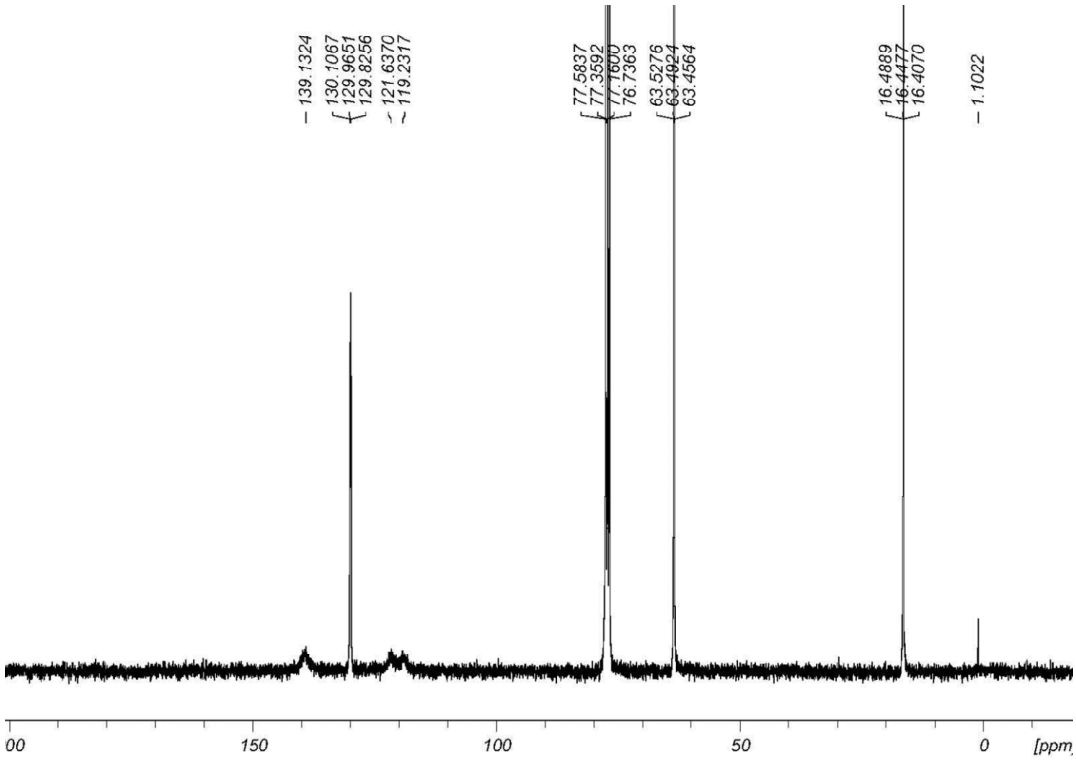

Figure S22. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.

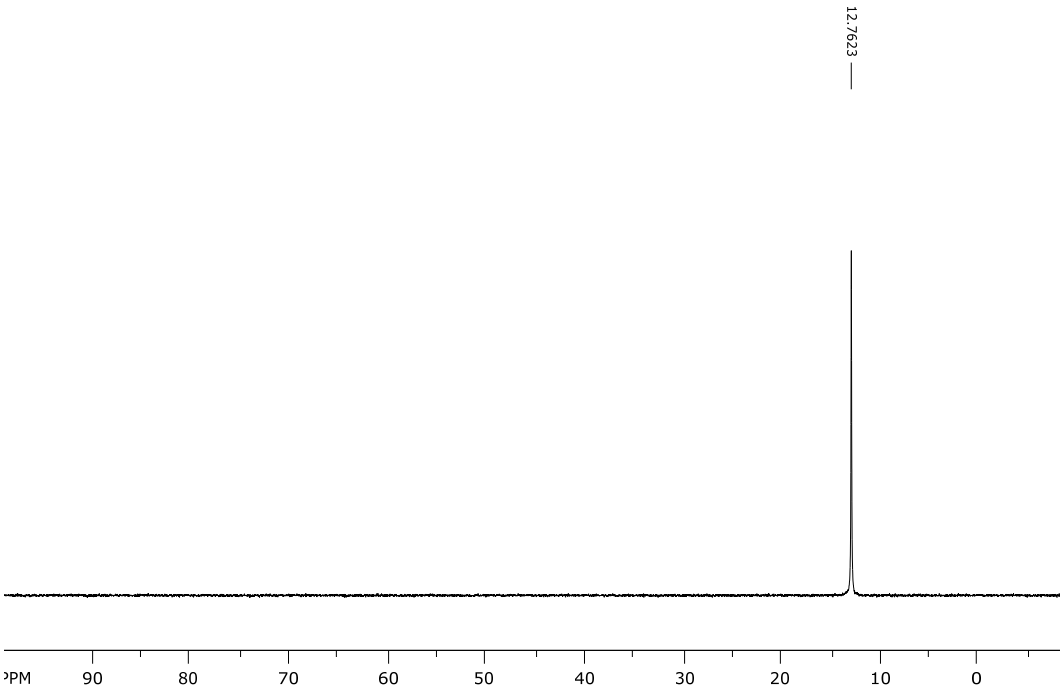

Figure S23. ^{31}P NMR spectrum (162 MHz, H_3PO_4/ $CDCl_3$) of tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.

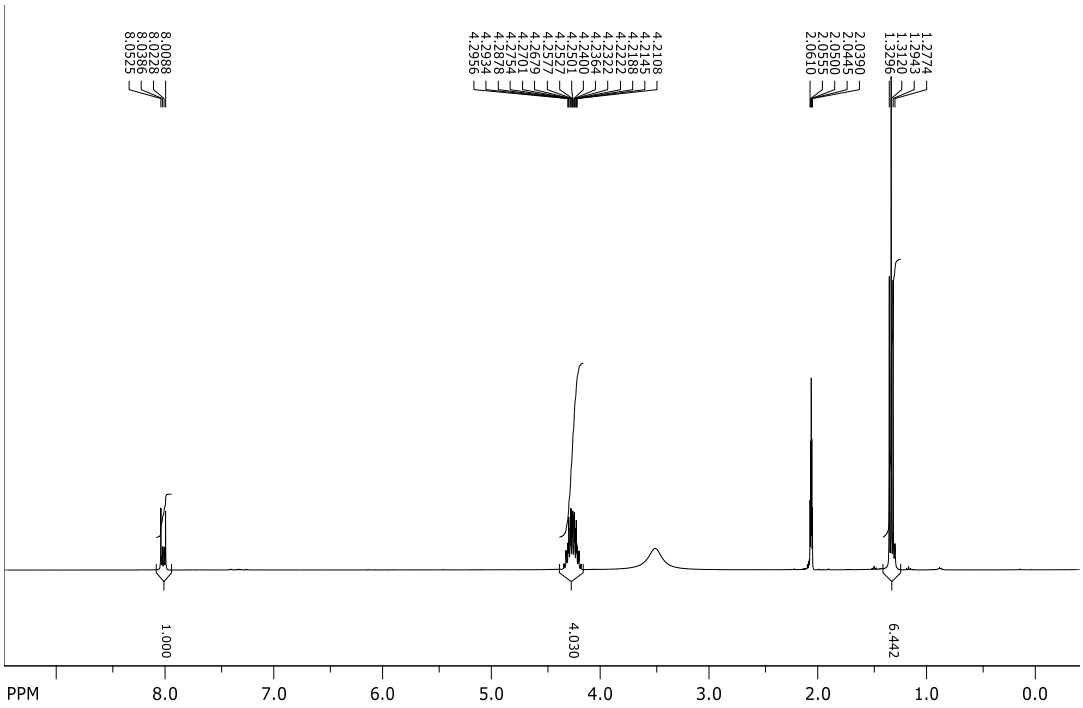

Figure S24. ^{1}H NMR spectrum (400 MHz, acetone-d_6) of tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.

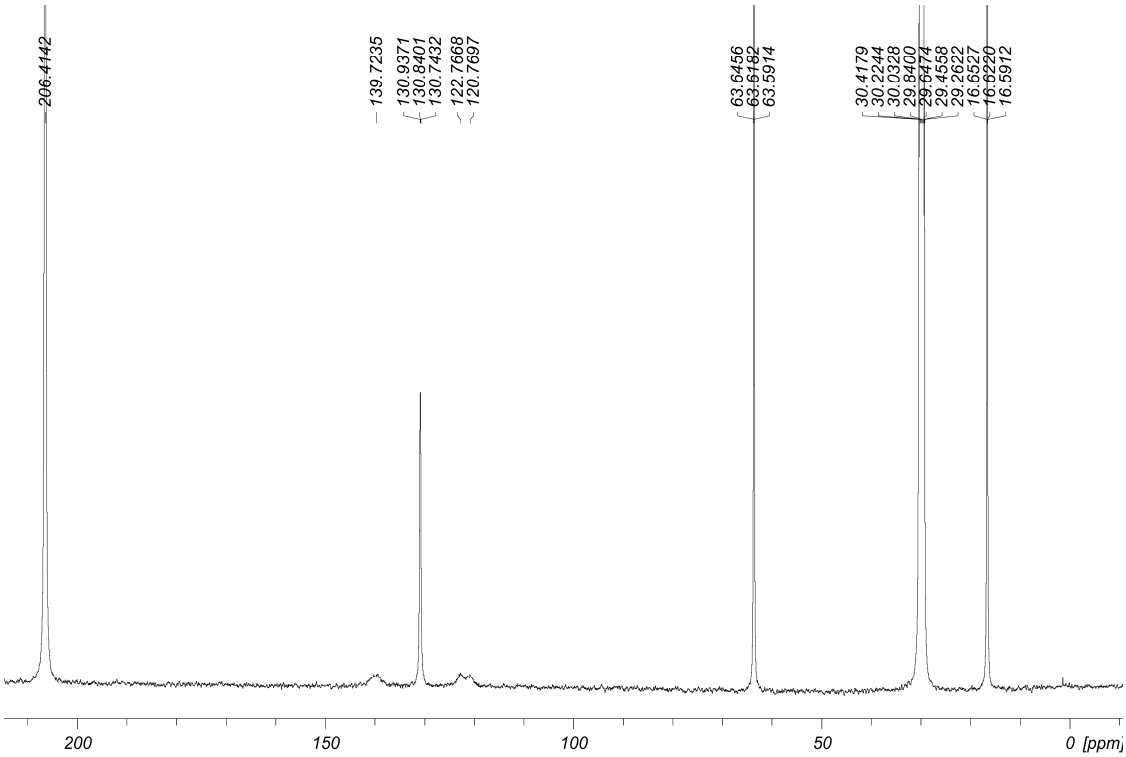

Figure S25. ^{13}C NMR spectrum (100 MHz, acetone-d_6) of tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.

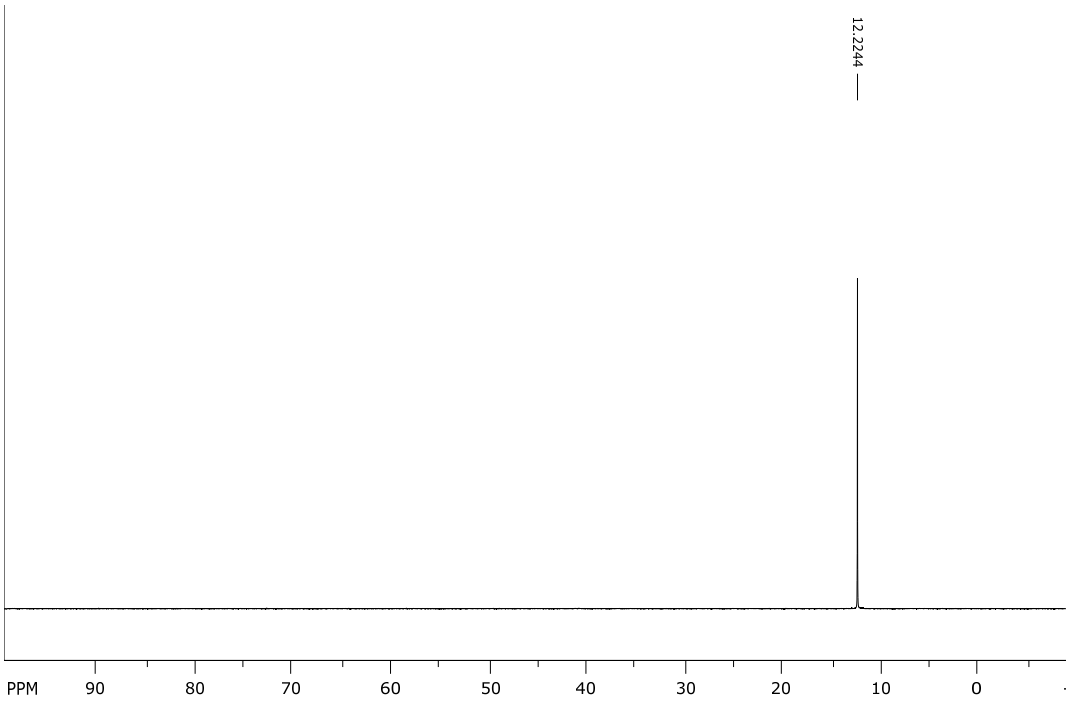

Figure S26. ^{31}P NMR spectrum (162 MHz, H_3PO_4/ acetone-d_6) of tetraethyl 1*H*-benzo[*d*][1,2,3]triazole-4,7-diylbis(phosphonate) **12**.