

## Supplementary Information (ESI)

for

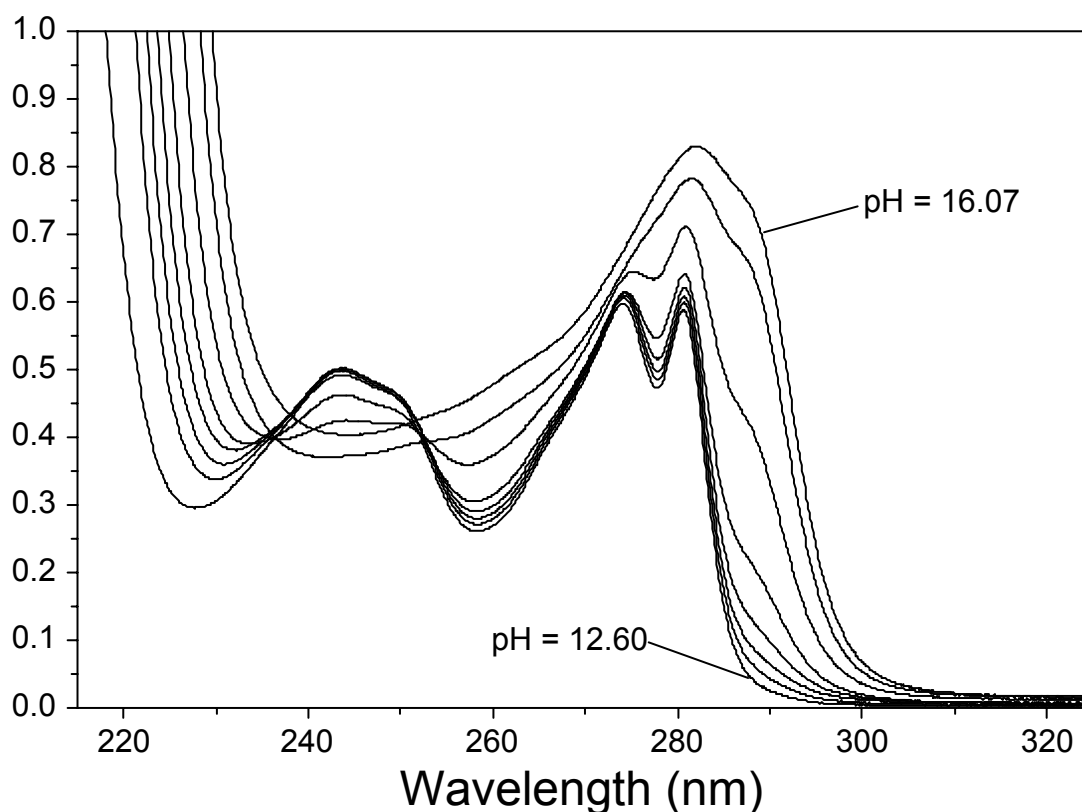
**Synthesis and acid-base properties of (1*H*-benzimidazol-2-yl-methyl)phosphonate (Bimp<sup>2-</sup>).**

**Evidence for intramolecular hydrogen-bond formation in aqueous solution between (N-1)H and the phosphonate group<sup>†</sup>**

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**Fig. S1** UV absorption spectra measured in 1-cm quartz cells of (1*H*-benzimidazole-2-ylmethyl)phosphonate ([Bimp] = 0.08 mM; aqueous solution; 25 °C) in dependence on pH; i.e., the pH values varied from 12.60, 13.31, 13.63 ([KOH] = 0.455 M), 13.92 ([KOH] = 0.727 M), 14.33 ([KOH] = 1.364 M), 14.62 ([KOH] = 2.273 M), 15.31 ([KOH] = 4.546 M) to 16.07 ([KOH] = 7.273 M). The pH values below 13.60 were measured with a pH meter equipped with a glass electrode and where necessary they were corrected for the "alkali error" (see Section 4.4). The pH values above 13.60 were calculated from the KOH concentration employed by using the  $H_+$  scale provided by Yagil<sup>31</sup> (see also Section 2.4 and 4.4). In the solutions with [KOH] < 0.1 M the ionic strength *I* was adjusted with KCl to 0.1 M. The sample beam contained Bimp and KOH, and the reference beam only water since KOH and KCl begin to absorb only below about 240 nm (cf. also ref. 31). The absorption spectrum for the solution with pH =  $H_+$  = 16.07 ([KOH] = 7.273 M), does not fit well anymore to the isosbestic points at 236 and 252 nm; this might be due to some carbonate absorption by the solution. However, this deviation had no effect on the evaluations at and above 260 nm. For the evaluation of the spectra see Fig. 2 of the publication.