

Structure and Properties of 1,3-Phenylenediboronic Acid: Combined Experimental and Theoretical Investigations

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Single crystal XRD

Table S1. Selected geometrical parameters.

B(2)-O(21)	1.340(2)	C(1)-C(2)-B(2)	120.19(16)
B(2)-O(22)	1.379(2)	C(3)-C(2)-B(2)	122.06(14)
C(2)-B(2)	1.579(2)	C(2)#1-C(1)-C(2)	122.7(2)
O(21)-H(21)	0.81(3)	C(1)-C(2)-C(3)	117.75(15)
O(22)-H(22)	0.84(3)	C(4)-C(3)-C(2)	120.77(15)
C(2)-C(3)	1.399(2)	C(3)#1-C(4)-C(3)	120.2(2)
C(1)-C(2)#1	1.3985(19)		
C(1)-C(2)	1.3985(19)	C(1)-C(2)-B(2)-O(21)	-25.8(2)
C(3)-C(4)	1.390(2)	C(3)-C(2)-B(2)-O(21)	154.99(16)
C(4)-C(3)#1	1.390(2)	C(1)-C(2)-B(2)-O(22)	154.48(14)
		C(3)-C(2)-B(2)-O(22)	-24.7(2)
O(21)-B(2)-O(22)	118.35(16)	C(2)#1-C(1)-C(2)-C(3)	-1.09(11)
O(21)-B(2)-C(2)	119.67(15)	C(2)#1-C(1)-C(2)-B(2)	179.71(16)
O(22)-B(2)-C(2)	121.98(16)	B(2)-C(2)-C(3)-C(4)	-178.61(13)
B(2)-O(21)-H(21)	112.5(16)	C(1)-C(2)-C(3)-C(4)	2.2(2)
B(2)-O(22)-H(22)	115.5(17)	C(2)-C(3)-C(4)-C(3)#1	-1.14(11)

1. Spectrophotometric titration

Concentration of boronic acid: $c=2.7 \cdot 10^{-3}$ M

Concentration of NaOH: $c=0.04914$ M

Ionic strength: 0.1M KCl

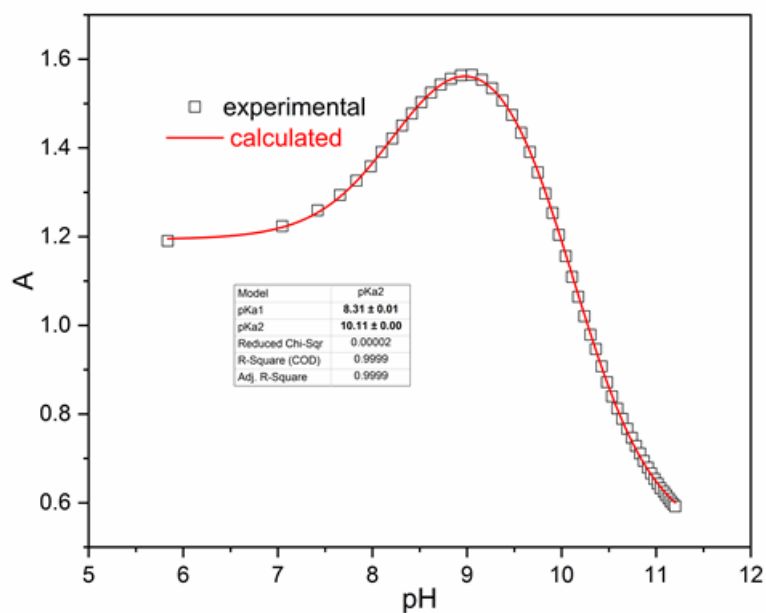


Figure S1. Analysis of spectroscopic data: absorbance change at 274 nm versus pH.

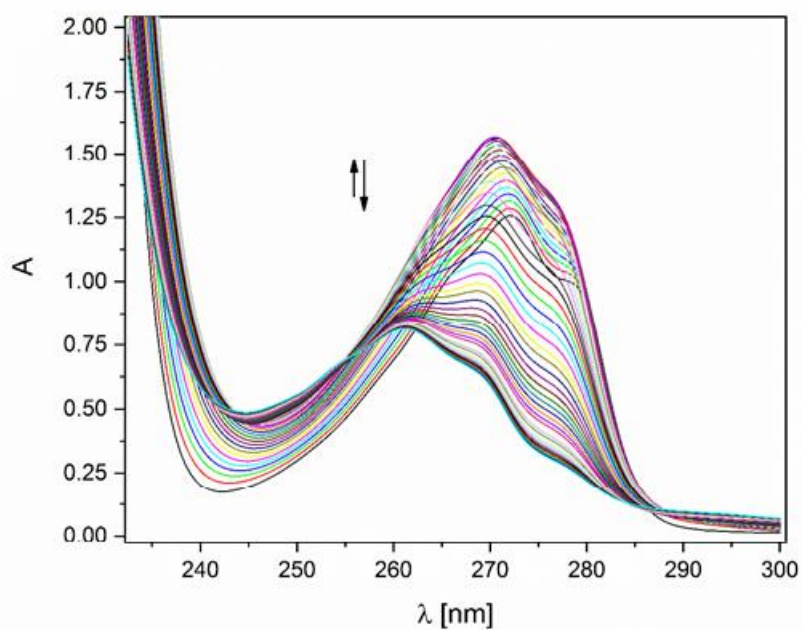


Figure S2. Spectrophotometric titration in pH range 5.5-11.5 in water (a correction to the dilution was taken into account). Arrows indicate changes in the absorbance with respect to the increase of pH.

2. Potentiometric titration

Concentration of boronic acid: $c=2.7 \cdot 10^{-3}$ M

Concentration of NaOH: $c=0.04914$ M

Ionic strength: 0.1M KCl

(the same conditions as in spectrophotometric experiment).

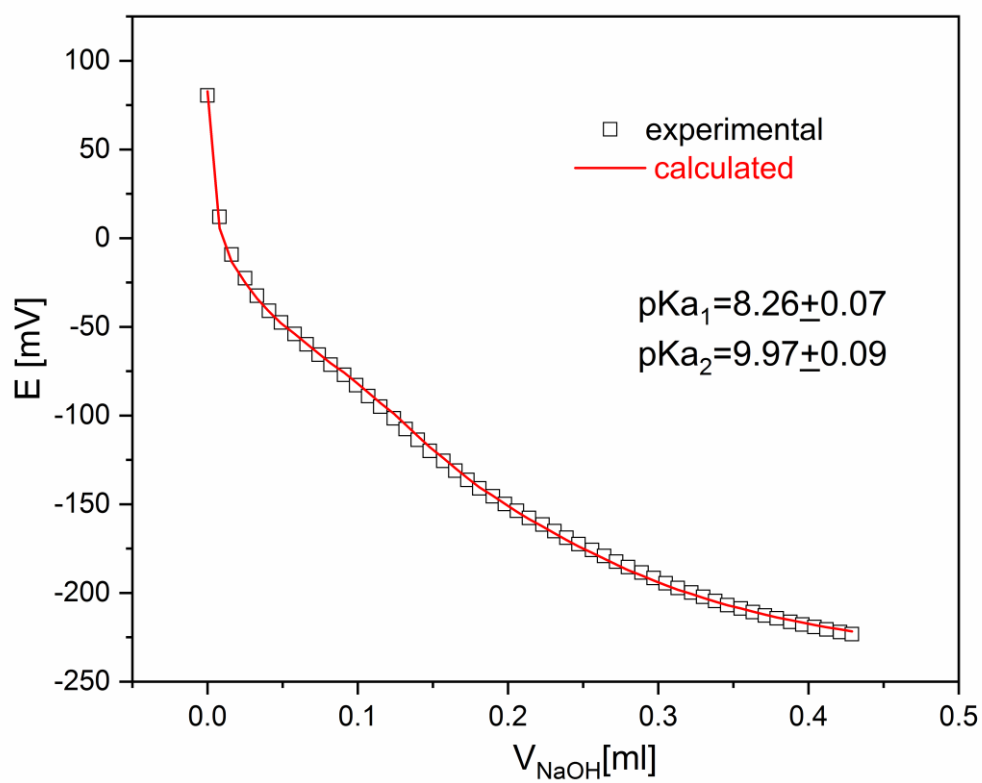
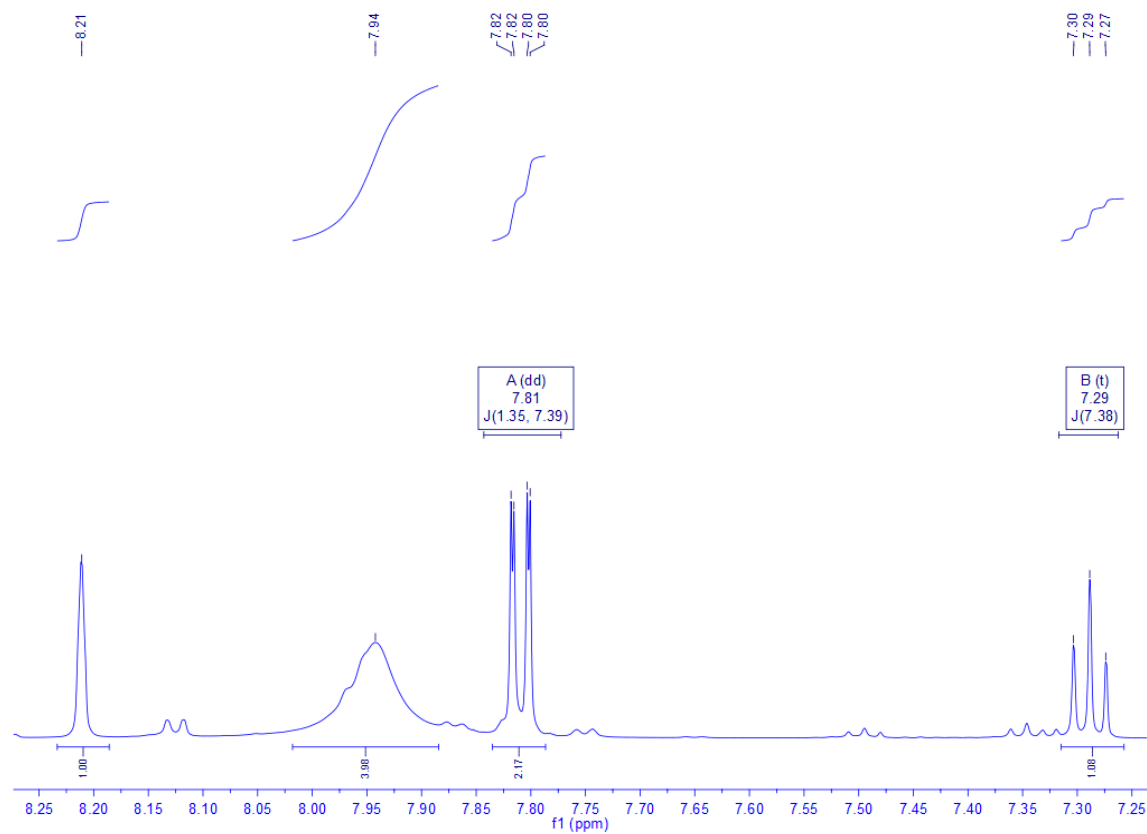


Figure S3. Potentiometric titration with fitting of calculated data.

¹H NMR



¹³C NMR

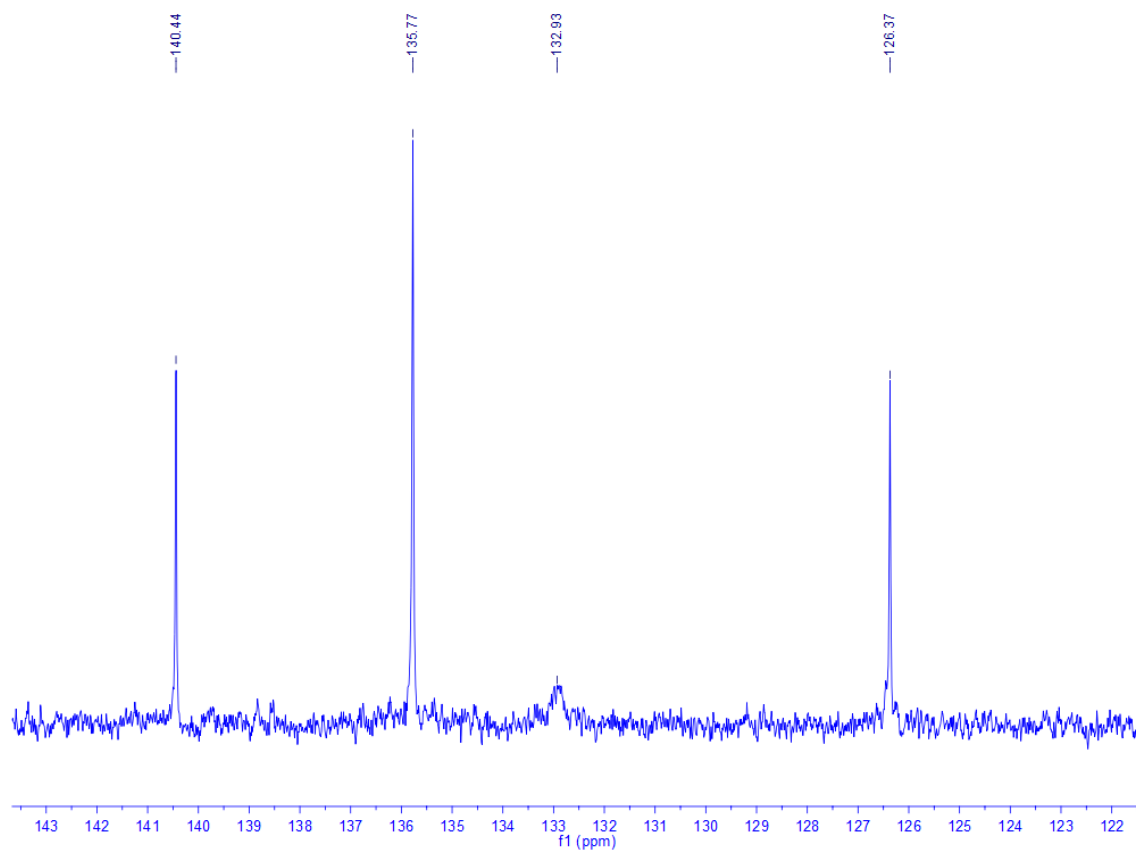


Figure S4. One-dimensional NMR spectra of the title compound in DMSO-d₆.