Supporting Information for:

Polyvinyl alcohol-boronate gel for sodium hydroxide extraction

Gretchen Marie Peters, Xiaodong Chi, Chandler Brockman, Jonathan L. Sessler Department of Chemistry, the University of Texas at Austin, 105 E. 24th Street, Stop A5300, Austin, TX 78712

Table of Contents	
General Experimental	S 2
Procedure for Gel Preparation	S2
Procedure for NaOH Absorption	S 2
Rheology Studies	S 2
Figure S1. Frequency sweeps and strain sweep of 10 mM BdBA: 5% PVA gel	S 3
Figure S2. Frequency sweeps and strain sweep of 50 mM BdBA: 5% PVA gel	S4
Figure S3. Visual and spectroscopic change in phph as a function of [NaOH]	S5
Figure S4. UV-visible spectra of NaOH aliquots with phph	S6
Figure S5. NaOH absorption by the BdBA-PVA gel after 24 h	S 7
Figure S6. Percent of NaOH absorbed as a function of the amount of BdBA- PVA gel	S 8

General Experimental: Chemicals and solvents were purchased from Aldrich, Alfa Aeser, Fisher, and Acros. UV-visible spectroscopy measurements were made on a Cary 5000 spectrometer. All rheological data was collected using an AR2000 stress-controlled rheometer from TA instruments.

Procedure for Gel Preparation: Stock solutions of **BdBA** and **PVA** (98-99% hydrolyzed, average MW = 11,000-31,000 g/mol) were prepared in DMSO at 100 mM and 10%, respectively. The **PVA** stock solution was heated and stirred until the **PVA** solid was fully dissolved. Gels were prepared by combining the appropriate amounts of these stock solutions at room temperature. A spatula was used to stir the material and ensure proper combination. Gels formed within minutes.

Procedure for NaOH Absorption: A **BdBA-PVA** gel (50 mM **BdBA**, 5% **PVA** in DMSO) was prepared in a vial according to the general preparation procedure given above. The gels were then placed in a drawer and allowed to set at room temperature overnight. A spatula was used to scrape the gel from the edges of the vial and form a ball to maximize the surface area of the material. The gel ball was then washed three times with H₂O (3 mL) to ensure that any free **BdBA** and DMSO was removed. At this point, 1 mL of 25 mM aqueous NaOH was added. Aliquots of the solution surrounding the gel ball (50 µL) were removed at various time points and combined with 50 µL of a 10 mM solution of **phph** in MeOH. The concentration of NaOH was evaluated by UV-visible spectroscopy by recording the intensity of the **phph** λ_{max} at 555 nm. Spectra were obtained using a quartz Starna 16.10-Q-10 sub-micro cell with 10 mm path length. The pH was also confirmed using litmus paper and a pH probe. These experiments were done in triplicate.

Rheology Studies: Gels were prepared by following the general gel-forming procedure presented above. They were then allowed to set at room temperature overnight. Rheological experiments were performed at 20 °C using the parallel plate geometry (25 mm diameter). The gel samples were allowed to equilibrate on the plate for 10 min. Frequency sweeps were performed at 1% strain from 0.1 to 100 rad/s. Strain sweeps were performed at 10 rad/sec by varying the strain from 0.1 to 100%



Figure S1. (A) Dynamic frequency sweep and (B) strain sweep of a BdBA-PVA gel (10 mM BdBA, 5% PVA).



Figure S2. (A) Dynamic frequency sweep and (B) strain sweep of a BdBA-PVA gel (50 mM BdBA, 5% PVA).



Figure S3. Visible color change seen upon treating **phph** with increasing [NaOH] (top) and changes in the UV-visible absorbance intensity at 555 nm as a function of [NaOH] (bottom) (5 mM in 50:50 H₂O:MeOH).



Figure S4. UV-visible spectra of mixtures of 50 μ L **phph** (10 mM in MeOH) and 50 μ L aliquots of the bulk aqueous NaOH solution after exposure to the **BdBA-PVA** gel (50 mM and 5%, respectively) for the indicated times. The gel was prepared to a volume of 0.3 mL and combined with 1 mL of NaOH (25 mM in H₂O).



Figure S5. Decrease in [NaOH] as a function of time in the presence of the **BdBA-PVA** gel. The changes were monitored for up to 24 h. This figure provides the results from a longer time period than the corresponding figure in the main text.



Figure S6. Plot of the % NaOH absorbed from the bulk aqueous solution after 5 h of contact with the **BdBA-PVA** gel (50 mM, 5%). Gels were prepared in vials to final volumes of 0.2, 0.3, 0.4, 0.5 and 0.6 mL using the appropriate amounts of the **BdBA** and **PVA** stock solutions. The gels were also weighed to confirm that the mass of the gel employed matched what would be expected based on the indicated volumes. To each vial, 1 mL of NaOH (25 mM in H₂O) was added and allowed to soak. After 5 h, 50 µL of the bulk NaOH solution was removed from each system and added to 50 µL of **phph** (10 mM in MeOH). UV-visible spectra were then recorded, and the concentration of NaOH absorbed was calculated using the value of the **phph** absorbance intensity at 555 nm.