Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Detection of Hydrogen Peroxide using Dioxazaborocanes: Elucidation of the Sensing Mechanism at the Molecular Level by NMR and XPS Measurements

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Supporting information:

Figure S1. ^{11}B NMR spectra of Dioxazaborocane 2 in $CDCl_3$ before and after 48 h of exposure to HP.

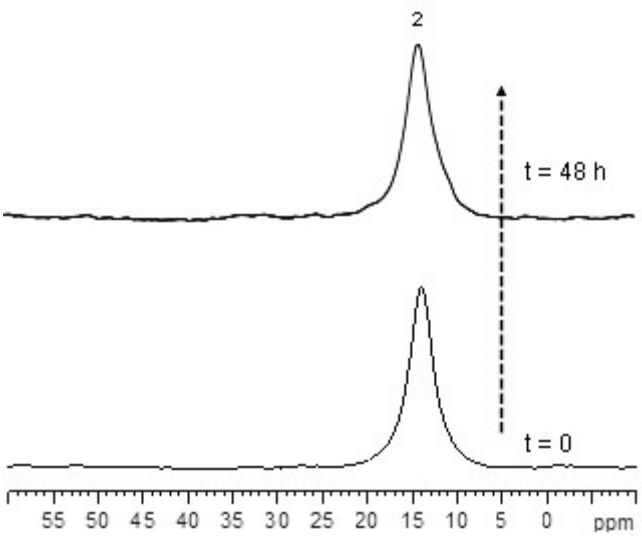

Table S1. Dioxazaborocane **2** characterization

M.p	257°C
^{1}H NMR (400 MHz, $CDCl_3$)	δ = 8.50 (s, 1 H, CH), 8.03 (m, 6 H, CH), 7.50 (m, 7 H, CH), 4.61 (s, 2 H, CH_2), 4.21 (t, 4 H, CH_2), 2.96 (s, 4 H, CH_2) ppm
^{13}C NMR (100 MHz, $CDCl_3$)	δ=133.7, 132.13, 131.6, 130.1, 129.8, 128.3, 128.0, 127.2, 125.4, 124.6, 123.9, 63.0, 56.4, 51.8 ppm
IR (ATR):	ν~=3049, 2982, 2938, 2889, 2855, 2835, 1622, 1590, 1522, 1493, 1446, 1433, 1357, 1211, 1155, 1084, 1067, 1010, 953, 895, 830, 795, 727, 705 cm^{-1}
HRMS (M^{+*})	*m/z* found 381.1860 u., calculated for $^{12}C_{25}{}^{1}H_{24}{}^{10}B^{14}N^{16}O_2$ 381.1905u

Table S2. Crystallographic characteristics and X-Ray data collection and refinement statistics for Dioxazaborocane **2**.

Parameter	Compound **2**
Molecular formula	C50H48B2N2O4 (2 molecules)
Temperature (K)	293
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	10.0855(6)
b (Å)	22.4497(14)
c (Å)	17.1902(11)
a (°)	90
b (°)	90.037(6)
g (°)	90
V ($Å^3$)	3892.1(4)
Z	4
Crystal size (mm)	0.3
r (gcm^{-3})	1.301
Radiation	Mo K\ a
λ (Å)	0.71073
Exp. resolution (Å)	16.0143
N_{reftot}	13291
N_{refls}	8083
N_{par}	523
R_1	0.1977
wR_2	0.0654
GOF	1.0757

Comment S1. Evaluation of the limit of detection of the device

Based on a previous article dedicated to the detection of TNT vapors using the same laboratory prototype [Talanta Volume 81, Issues 1–2, 15 April 2010, Pages 543-548], the limit of detection Ld for hydrogen peroxide can be calculated.
We postulate a linear relationship between the response of the sensor and the hydrogen peroxide concentration. When exposed to 50 ppmv of HP, the response is 64 %.

$$Ld = \frac{3 \times noise}{\frac{response}{Concentration}}$$

Ld is thus given according to , with noise = 1.5 %.
It leads to Ld = 4 ppmv.