CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Synthesis and Relaxometric Studies of a Dendrimer-based pH responsive MRI Contrast Agent

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Electronic Supplementary Information S1

Table S1. Crystallographic data for 5

Identification code	jf1426ffmi
Empirical formula	$C_{18}H_{30}N_2O_8P_2$
Formula weight	464.38
Temperature	90(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P\,n\,a\,2_1$
Unit cell dimensions	a = 19.2299(12) Å $\quad\alpha = 90°$.
	b = 15.1795(9) Å $\quad\beta = 90°$.
	c = 15.6480(10) Å $\quad\gamma = 90°$.
Volume	4567.7(5) $Å^3$
Z	8
Density (calculated)	1.351 Mg/m^3
Absorption coefficient	0.236 mm^{-1}
F(000)	1968
Crystal size	0.46 x 0.41 x 0.25 mm^3
Crystal color and habit	Colorless Irregular Block
Diffractometer	Bruker SMART1000
Theta range for data collection	1.71 to 30.00°.
Index ranges	-27 = h = 27, -21 = k = 21, -22 = l = 22
Reflections collected	51060
Independent reflections	13322 [R(int) = 0.0393]
Observed reflections (I > 2sigma(I))	11744
Completeness to theta = 30.00°	100.0 %
Absorption correction	SADABS, Analytical
Max. and min. transmission	0.9430 and 0.8994
Solution method	SHELXS-97 (Sheldrick, 1990)
Refinement method	SHELXL-97 (Sheldrick, 1997) Full-matrix least-squares on F^2
Data / restraints / parameters	13322 / 27 / 645
Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0572, wR2 = 0.1202
R indices (all data)	R1 = 0.0655, wR2 = 0.1239
Absolute structure parameter	0.38(9)
Largest diff. peak and hole	0.450 and -0.458 $e.Å^{-3}$

Electronic Supplementary Information S2
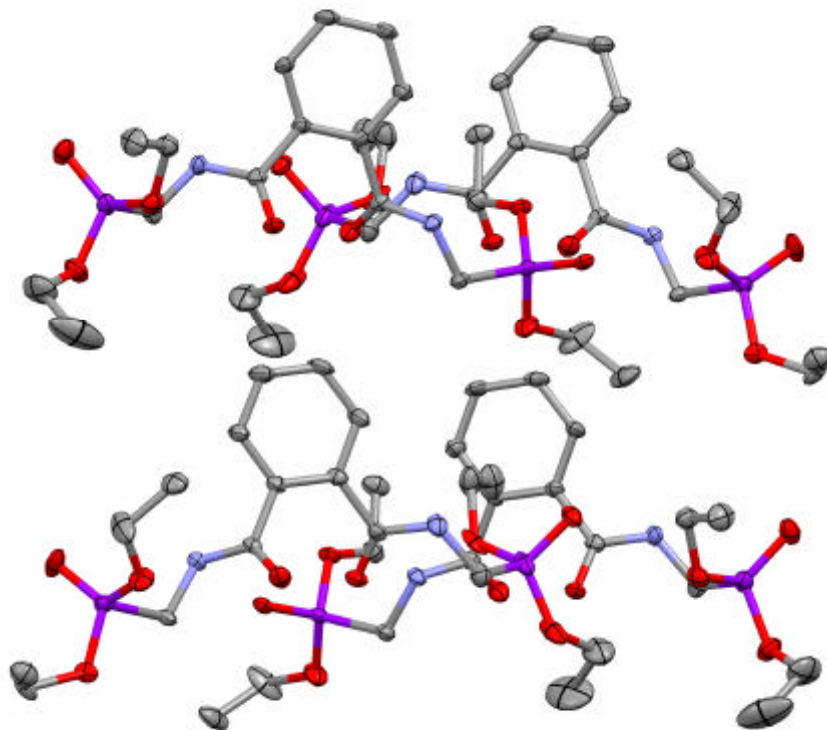
Figure S1. Packing diagram of the crystal structure of **5** view down the c-axis
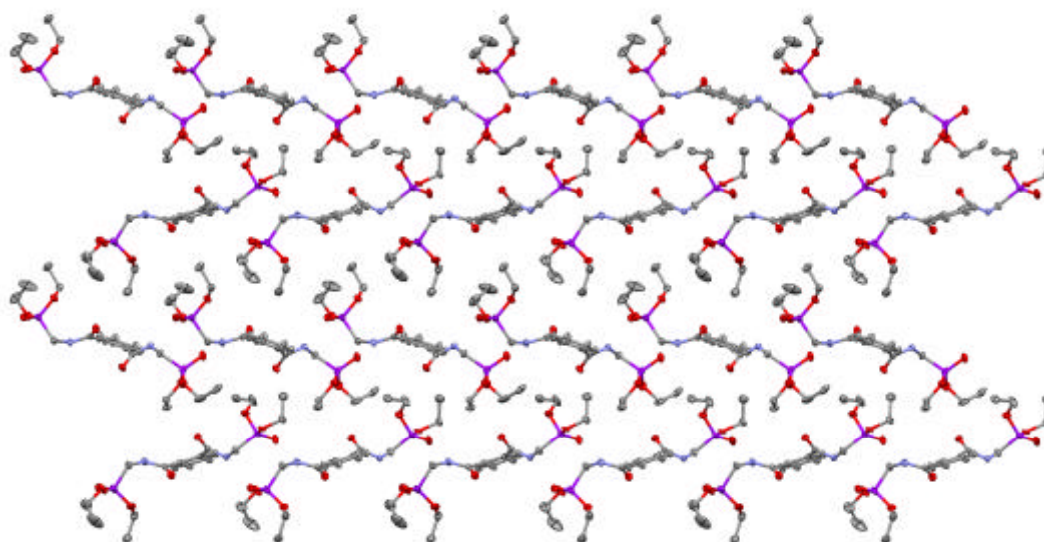
Figure S2. Packing diagram of the crystal structure of **5** view down the b-axis