Supporting information for

Encapsulation of small organic molecules for affecting symmetry of supramolecular crystals

Pavel V. Nesterov [1], Vladimir V. Shilovskikh [1], Alexander D. Sokolov [1], Vladislav V. Gurzhiy [2],Alexander S. Novikov [1], Alexandra A. Timralieva [1], Elena V. Belogub [3], Nikolay D. Kondratyuk [4,5], Nikita D. Orekhov [4,5,6] and Ekaterina V. Skorb [1,*]

1. Infochemistry Scientific Center of ITMO University, Lomonosova str. 9, St. Petersburg 191002, Russian Federation

2. Crystallography Department, Institute of Earth Sciences, Saint-Petersburg State University, 199034, University emb. 7/9, Saint-Petersburg, Russian Federation

3. South Urals Federal Research Center of Mineralogy and Geoecology, Urals Branch of Russian Academy of Science, Miass, 456317, Russia

4. Joint Institute for High Temperatures of the Russian Academy of Sciences, 13 Izhorskaya Bd 2, Moscow, Russian Federation

5. Moscow Institute of Physics and Technology, 9 Institutskiy per., Dolgoprudny, Moscow Region, Russian Federation

6. Bauman Moscow State Technical University, 2nd Baumanskaya Str., 5, Moscow, Russia

*Correspondence: skorb@itmo.ru

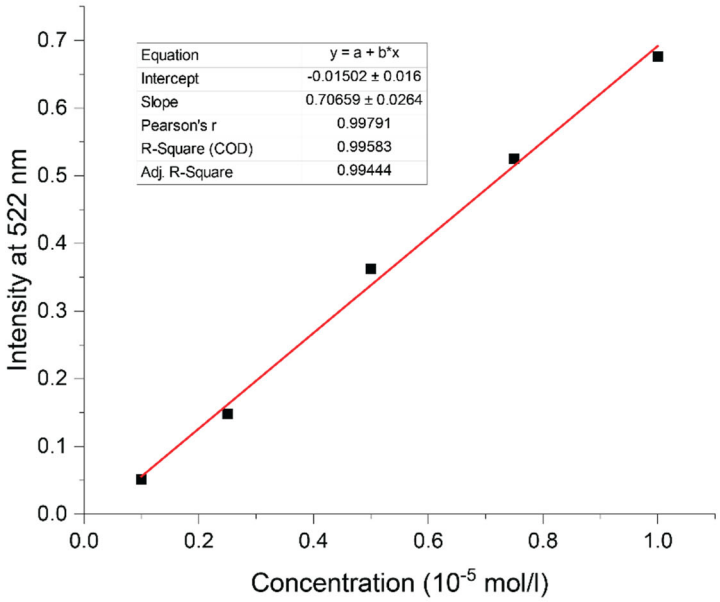

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Figure S1. Calibration curve for M-BA crystals dissolved in NaOH solution.

Figure S2. UV-vis spectra for solution obtained from dissolved M-BA crystals with (red curve) and without Rh6G inside the crystal. Prior to the dissolution the crystals were placed inside Rh6G solution with given concentrations: 10^{-7}, 10^{-6}, 10^{-5} (black, blue and red curves respectively) and after that washed in distilled water.

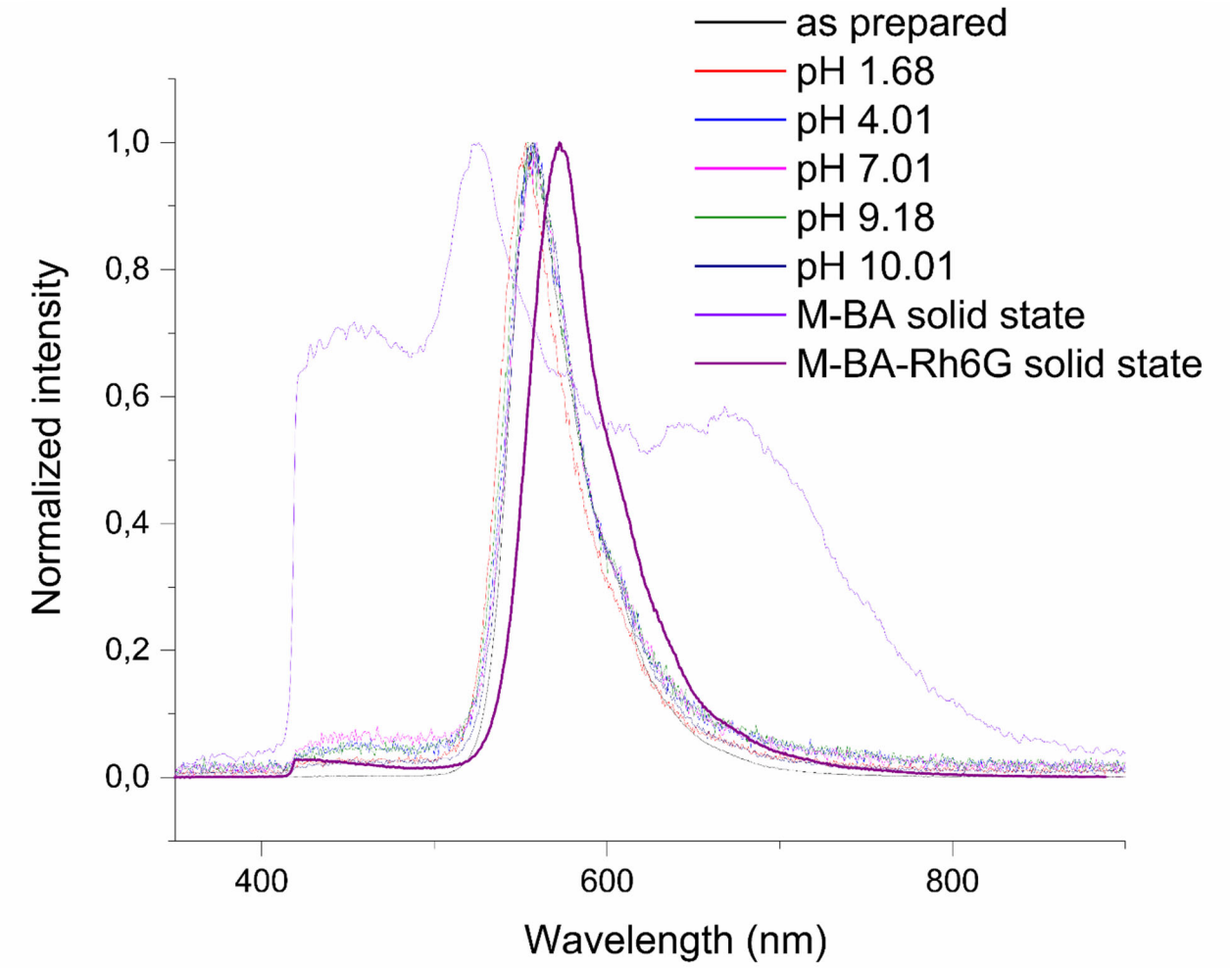

Figure S3. Luminescence spectra of Rh6G solutions at different pH and luminescence spectra of solid state M-BA and M-BA-Rh6G

Table S1. Crystallinity data for M-BA and M-BA-Rh6G crystals

Rh6G Concentration, mol/l	Crystallinity	Crystal I_{cr}	Amorphous
0	89.87	16.11	1.82
10^{-7}	82.91	13.53	2.79
10^{-6}	89.09	15.79	1.93
10^{-5}	84.35	15.78	2.93
10^{-4}	85.88	16.95	2.79

Table S2. Crystallographic data for M-Ba.

Crystal System	Orthorhombic
Space group	*Ccc*2
a (Å)	5.0575(4)
b (Å)	12.1663(9)
c (Å)	15.7377(11)
V (Å^3)	968.36(12)
Molecular weight	254.23
μ (mm^{-1})	1.211
Temperature (K)	100(2)
Z	4
D_{calc} (g/cm^3)	1.744
Crystal size (mm^3)	0.05 × 0.03 × 0.01
Radiation	Cu*K*α
Total reflections	2461
Unique reflections	843
Angle range 2θ (°)	11.24–140.00
Reflections with $\|F_o\| \geq 4\sigma_F$	801
R_{int}	0.0259
R_σ	0.0259
R_1 ($\|F_o\| \geq 4\sigma_F$)	0.0303
wR_2 ($\|F_o\| \geq 4\sigma_F$)	0.0788
R_1 (all data)	0.0327
wR_2 (all data)	0.0834
S	1.104
ρ_{min}, ρ_{max}, *e*/Å^3	−0.192, 0.191
CSD	2087674

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$; $s = \{\Sigma[w(F_o^2 - F_c^2)]/(n - p)\}^{1/2}$ where n is the number of reflections and p is the number of refinement parameters.