**Magic-angle spinning NMR spectroscopy provides insight into the impact of small molecule uptake by G-quartet hydrogels**

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Experimental NMR data for the NMR spectra presented in ***Materials Advances,*** 2020,

**Figure 1**  **1D MAS NMR spectra of alkali metal cations (7Li, 23Na, 39K and 133Cs)**

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| --- | --- |
| G4.M+ borate gels | High-resolution MAS NMR spectra |
| G4.Li+ borate gel | 7Li MAS NMR (20 T) |
| G4.K+ borate gel | 23Na MAS NMR (20 T) |
| G4.Na+ borate gel | 39K MAS NMR (20 T) |
| G4.Cs+ borate gel | 133Cs MAS NMR (20 T) |

**Figures 2 & S2: 11B MAS NMR spectra acquired at different magnetic fields**

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| --- | --- |
| G4.M+ borate gels | High-resolution MAS NMR spectra |
| G4.Li+ borate gel | 11B MAS NMR (11.7 T, 14.1 T, 20 T) |
| G4.K+ borate gel | 11B MAS NMR (11.7 T, 14.1 T, 20 T) |
| G4.Na+ borate gel | 11B MAS NMR (11.7 T, 14.1 T, 20 T) |
| G4.Cs+ borate gel | 11B MAS NMR (11.7 T, 14.1 T, 20 T) |

**Figure 3: Addition of methylene blue (MB) to G•K+ borate hydrogels**

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| --- | --- |
| G4.M+ borate gels | High-resolution MAS NMR spectra |
| G4.K+ borate gel | 11B MAS NMR (11.7 T, 20 T) |
| G4.K+ borate gel | 1H NMR |

**Figure 4: Addition of adenine to G•K+ borate hydrogels**

|  |  |
| --- | --- |
| G4.M+ borate gels | Solution-state NMR spectra |
| adenine added to G4.K+ borate gel | 1H NMR |

**Figures 5 & S5: Addition of adenine to G•Na+ borate hydrogels**

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| --- | --- |
| G4.M+ borate gels | High-resolution MAS NMR spectra |
| adenine loaded G4.Na+ borate gel | 1H NMR |
| 23Na MAS NMR (20 T) |
| 11B MAS NMR (20 T) |

**Figures 6 & S6: Addition of cytosine to G•Na+ borate hydrogels**

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| G4.M+ borate gels | High-resolution MAS NMR spectra |
| cytosine loaded G4.Na+ borate gel | 1H NMR |
| 23Na MAS NMR (20 T) |
| 11B MAS NMR (20 T) |

**Figure S3 and S4: DFT calculations of GB mono- and diesters**

|  |  |
| --- | --- |
| DFT calculation | Calculated chemical shifts |
| G4. borate monomer | 1H, 13C, 11B, 15N, 17O |
| G4. borate *cis* and *trans* dimers | 1H, 13C, 11B, 15N, 17O |

**Figure S7: Addition of 1-methylthymine to G•Na+ borate hydrogels**

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| --- | --- |
| G4.M+ borate gels | High-resolution MAS NMR spectra |
| 1-methylthymine added to G4.Na+ borate gel | 1H NMR |
| 23Na MAS NMR (20 T) |