

Supporting information for the manuscript

“Interaction of water with the model ionic liquid [bmim][BF₄]: molecular dynamics simulations and comparison with NMR data” by Moreno et al.

Table S1. Chemical shift data for [bmim][BF₄] at different water content.

RTIL conc. (mol/L)	5.354	5.302	5.251	5.171	5.077
RTIL conc. (mmol/L)	5353.509	5301.655	5251.49	5170.779	5077.163
Water conc. (mmol/L)	0	538.10	1058.69	1896.25	2867.75
Water molar fraction (χ_w)	0	0.09	0.17	0.27	0.36
Chemical shift (δ , ppm)					
H2	8.507	8.435	8.379	8.328	8.279
H4	7.050	7.022	6.999	6.977	6.956
H5	7.122	7.087	7.059	7.033	7.008
H6	3.619	3.611	3.604	3.597	3.590
H10	3.328	3.323	3.318	3.313	3.308
H7	1.168	1.167	1.165	1.164	1.164
H8	0.595	0.599	0.600	0.603	0.606
H9	0.158	0.161	0.163	0.165	0.169