A Combined Experimental/Computational Study of Dicationic Ionic Liquids with Bromide and Tungstate Anions

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Supporting Information

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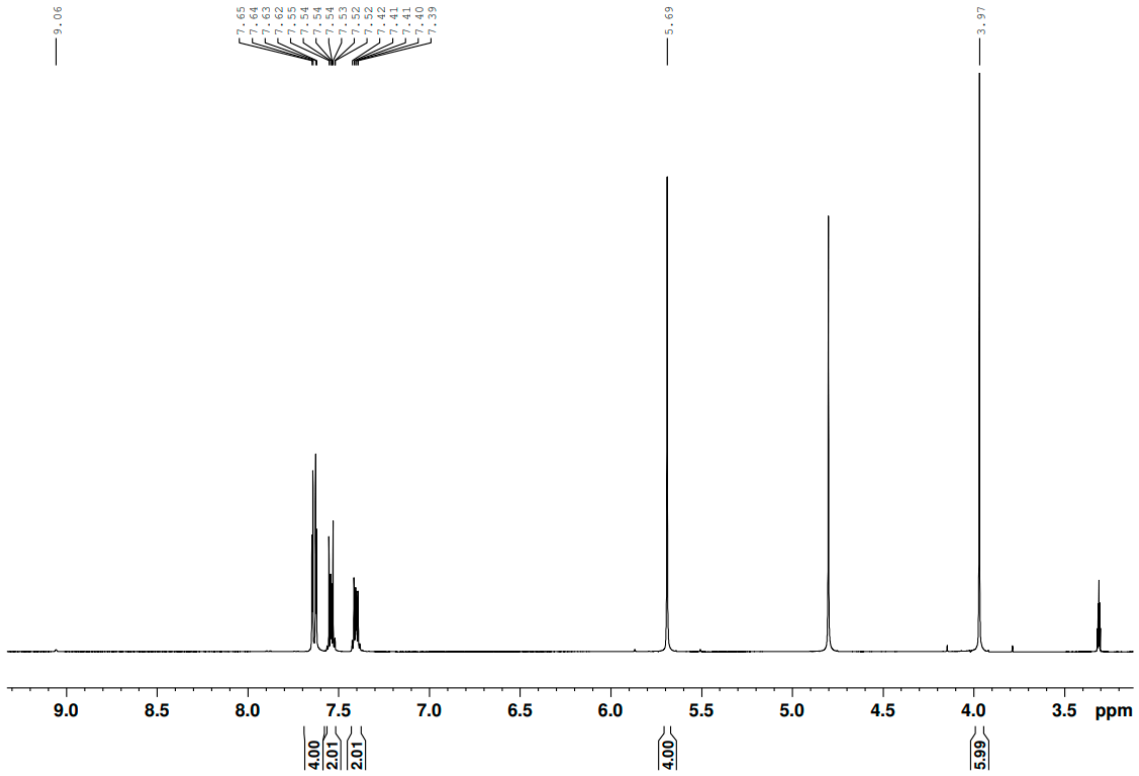

Figure S1. ^{1}H-NMR spectrum of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**1**).

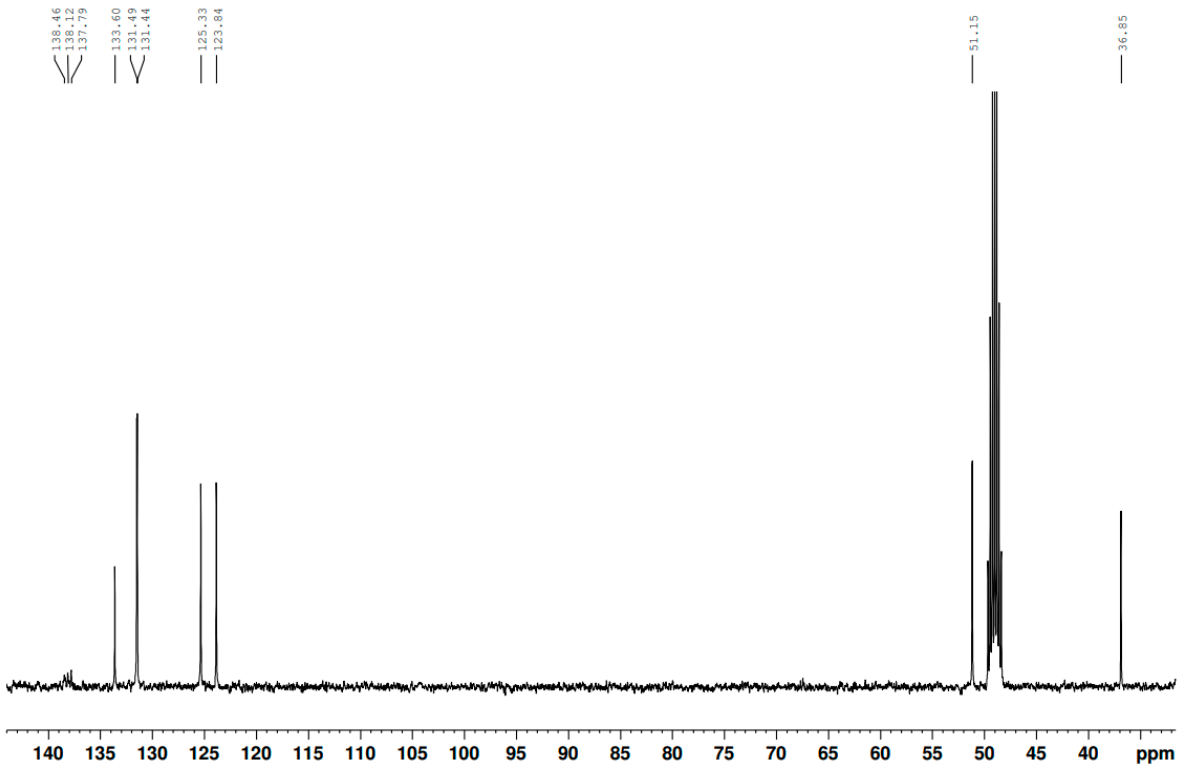

Figure S2. ^{13}C-NMR spectrum of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**1**).

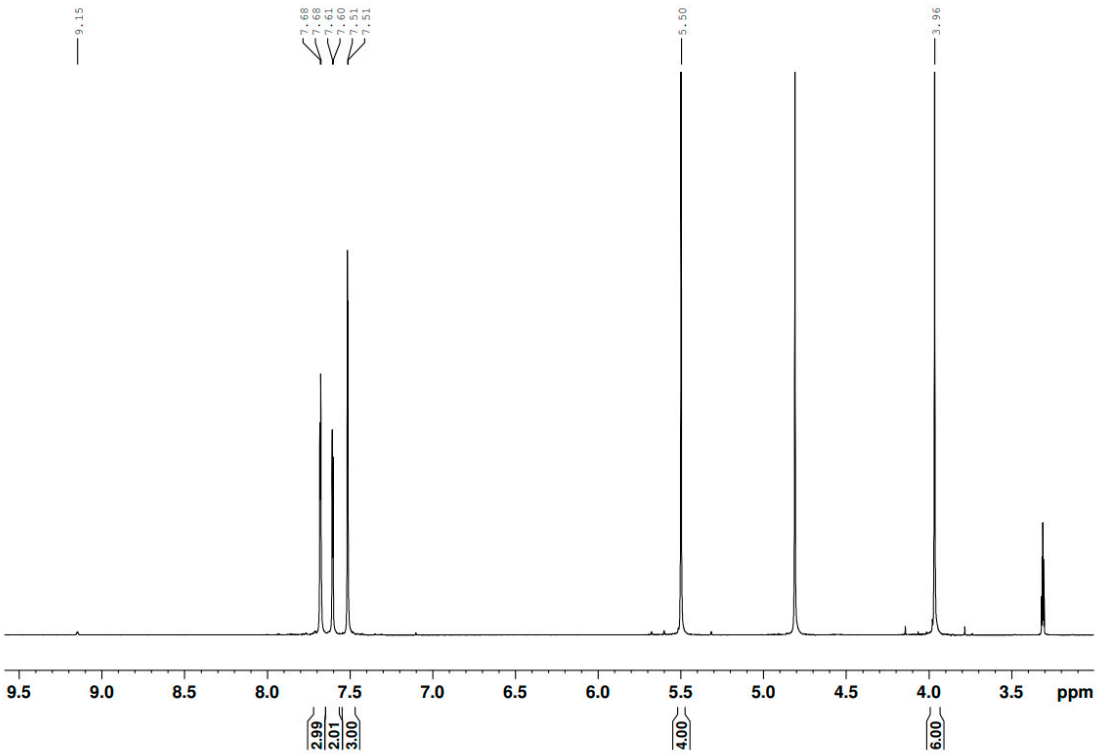

Figure S3. [1]H-NMR spectrum of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**2**).

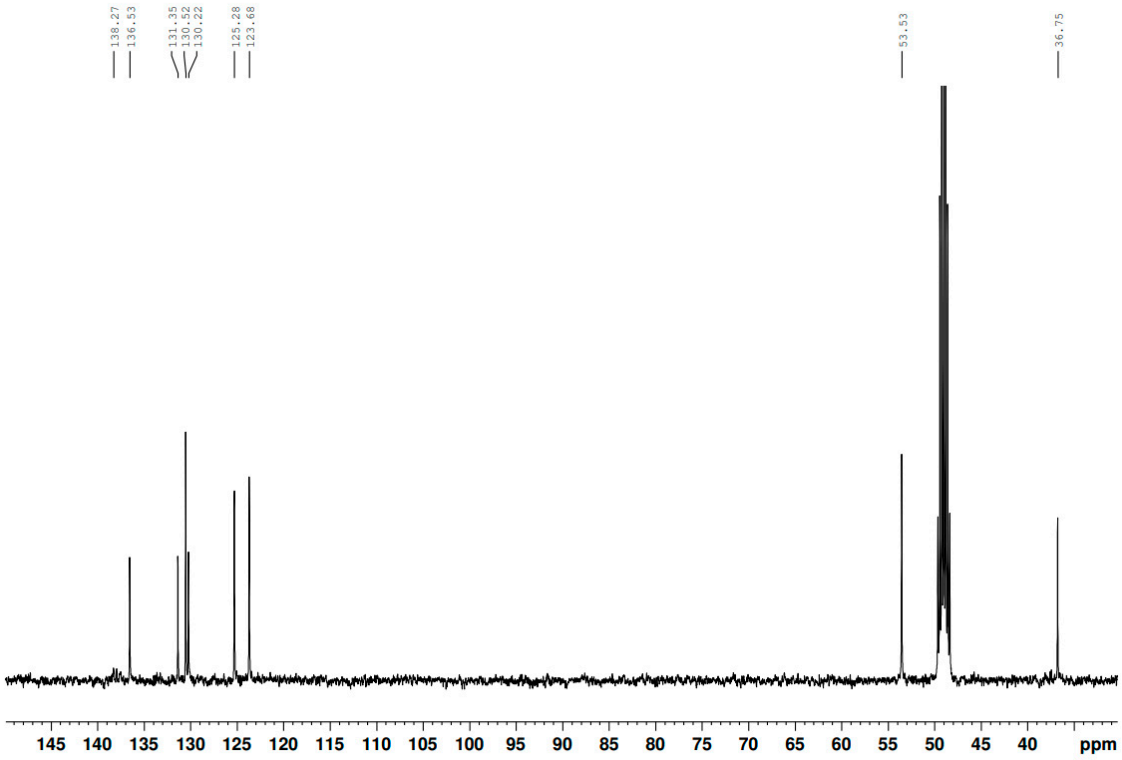

Figure S4. [13]C-NMR spectrum of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**2**).

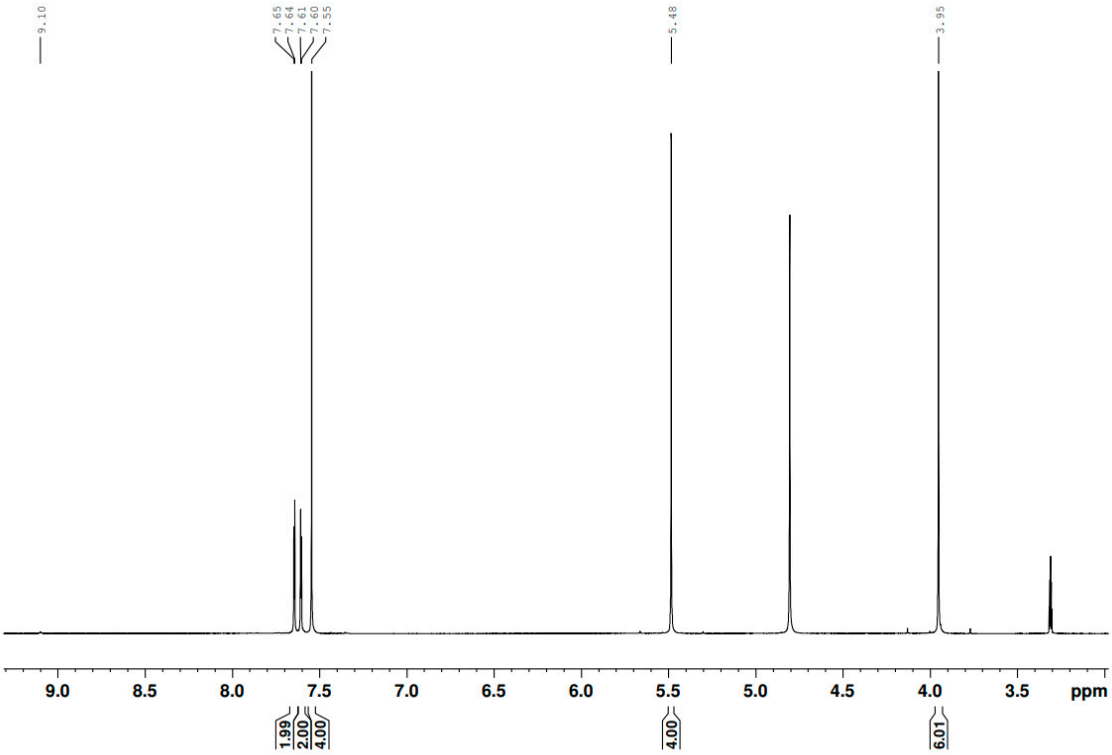

Figure S5. ^{1}H-NMR spectrum of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**3**).

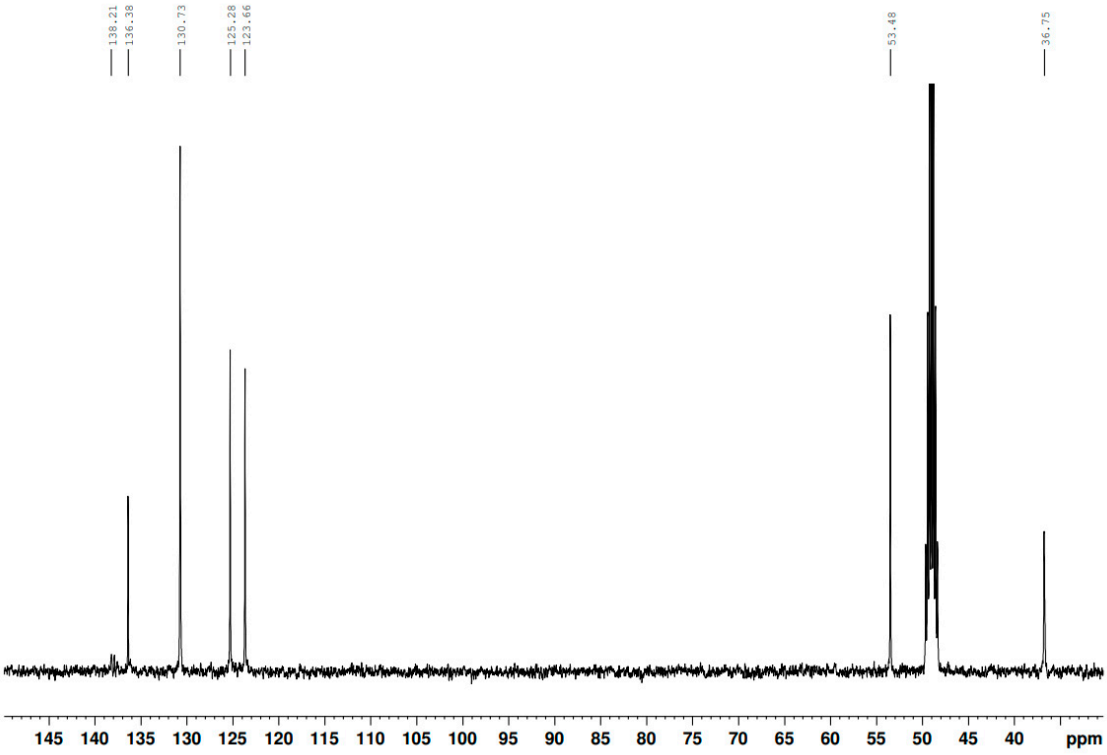

Figure S6. ^{13}C-NMR spectrum of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**3**).

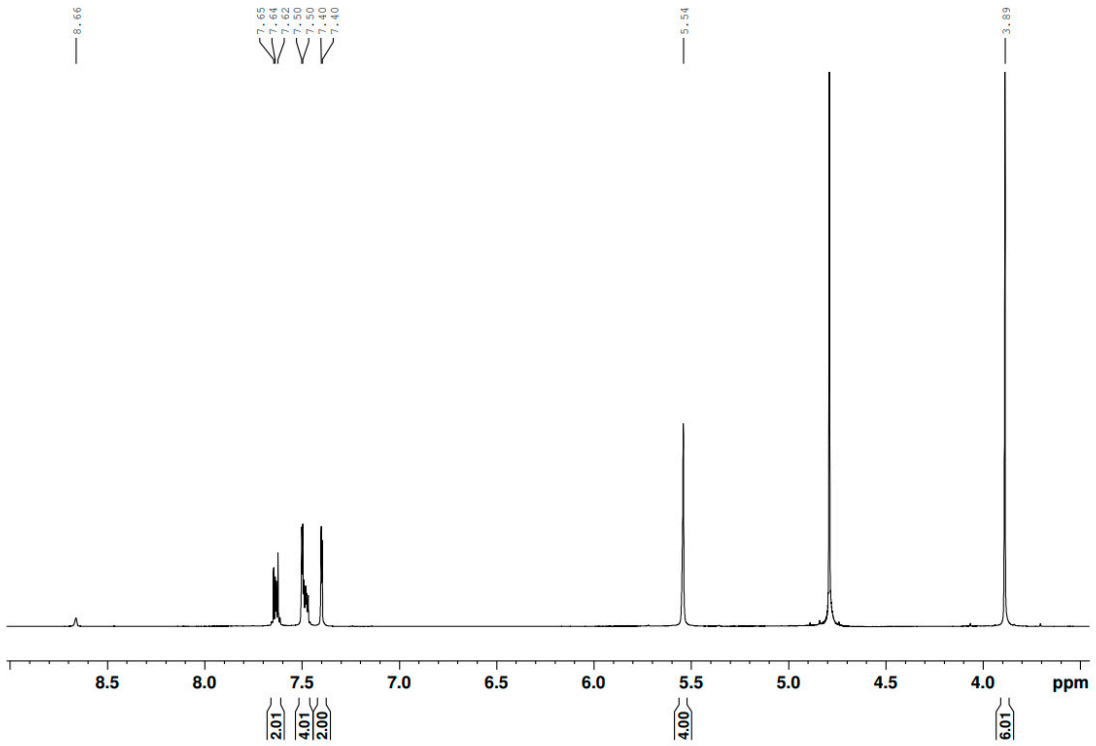

Figure S7. ^{1}H-NMR spectrum of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**4**).

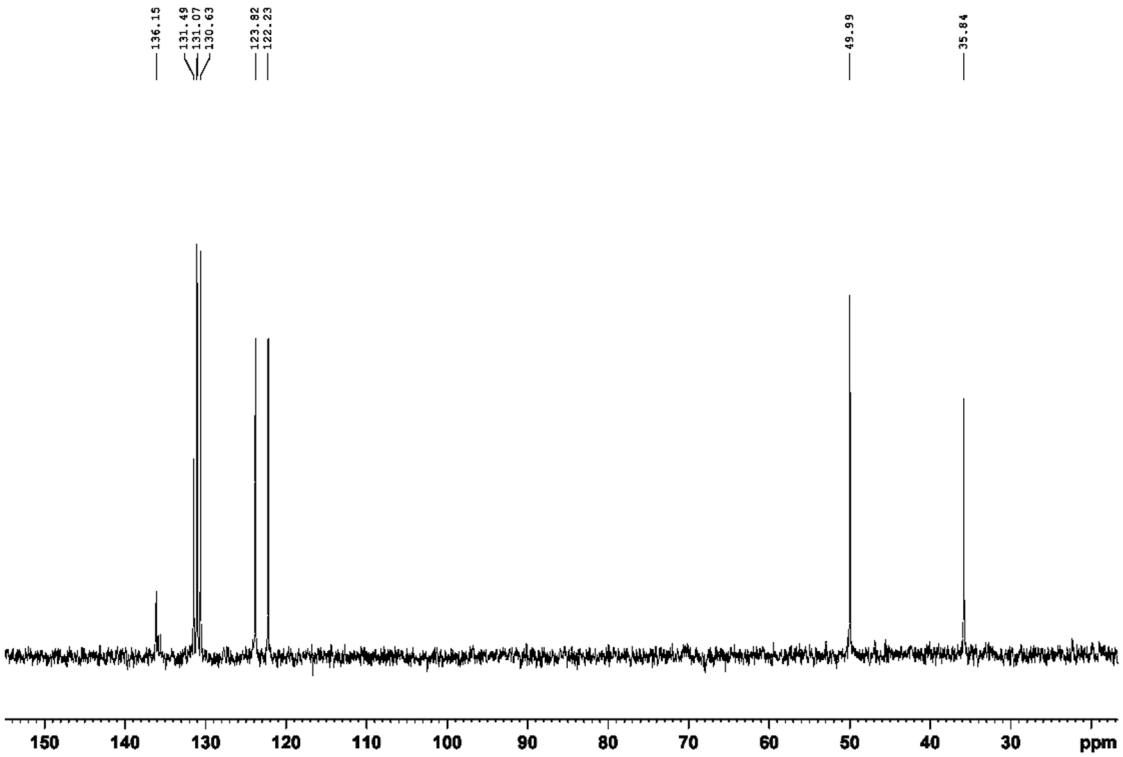

Figure S8. ^{13}C-NMR spectrum of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**4**).

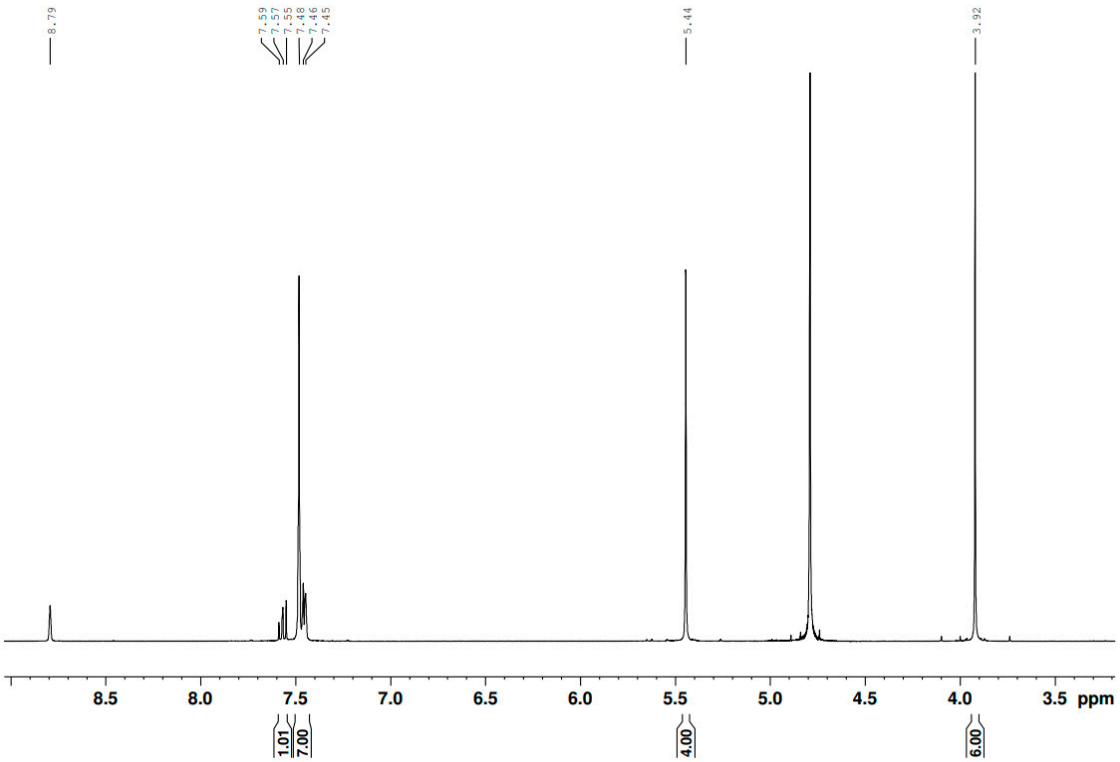

Figure S9. ^{1}H-NMR spectrum of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**5**).

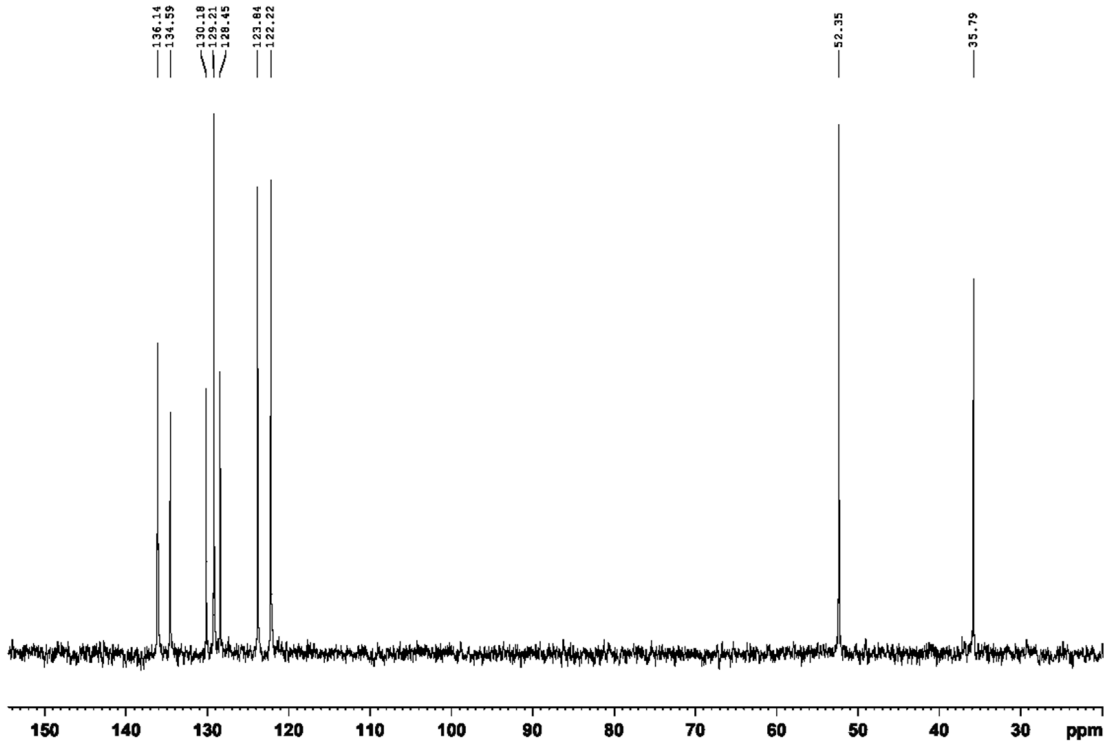

Figure S10. ^{13}C-NMR spectrum of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**5**).

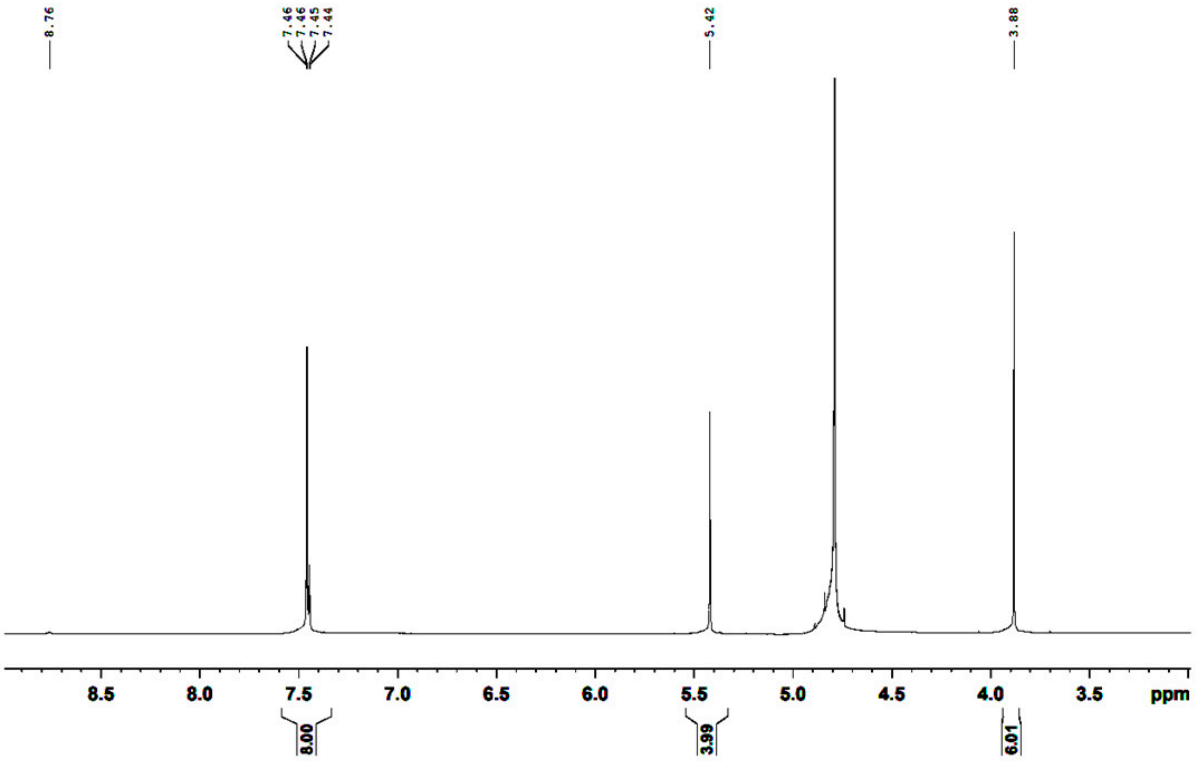

Figure S11. [1]H-NMR spectrum of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**6**).

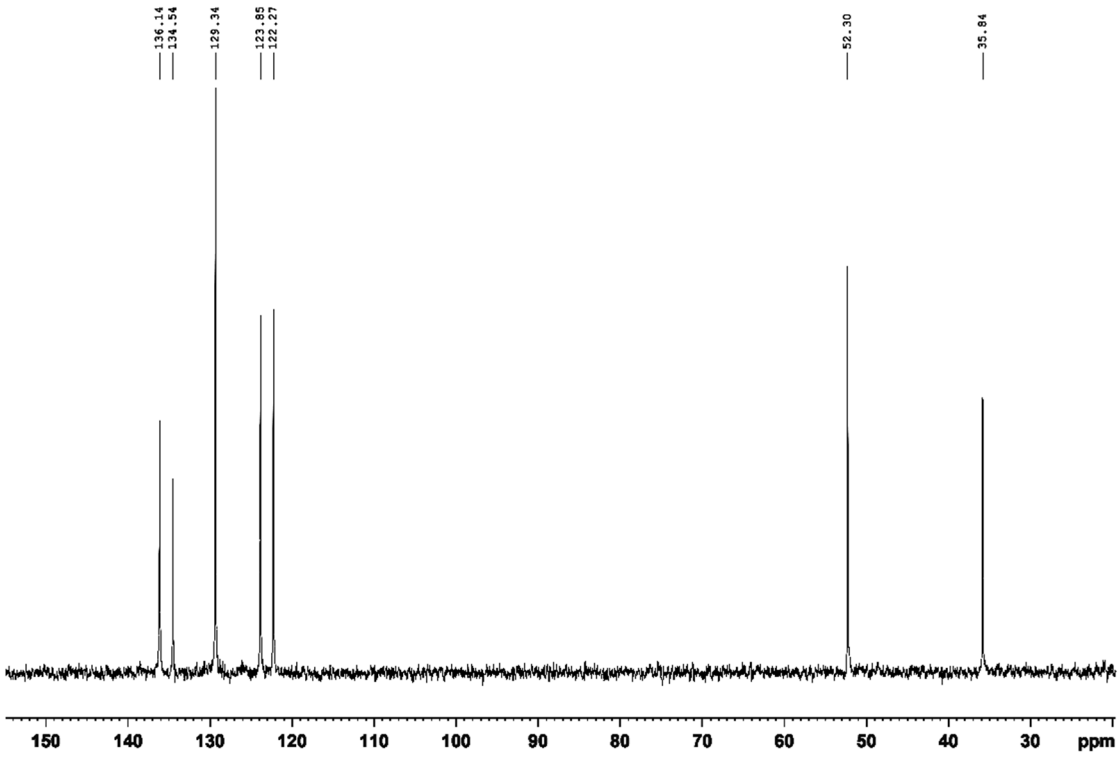

Figure S12. [13]C-NMR spectrum of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**6**).

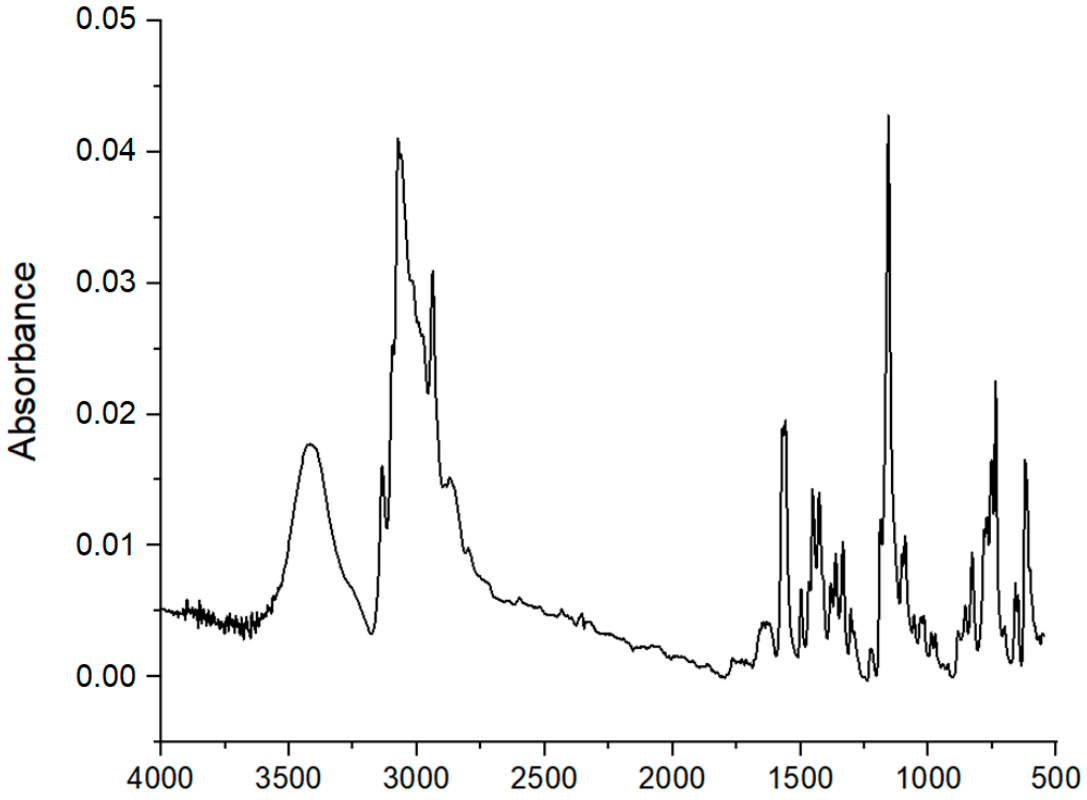

Figure S13. ATR-FTIR spectrum of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**1**).

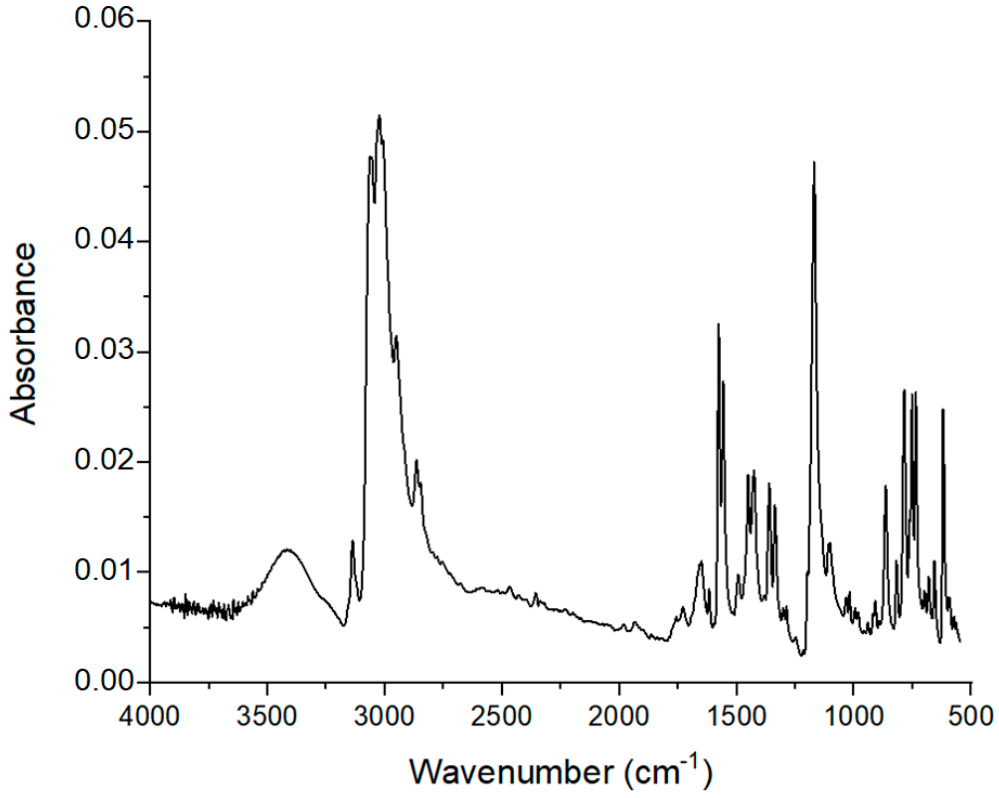

Figure S14. ATR-FTIR spectrum of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**2**).

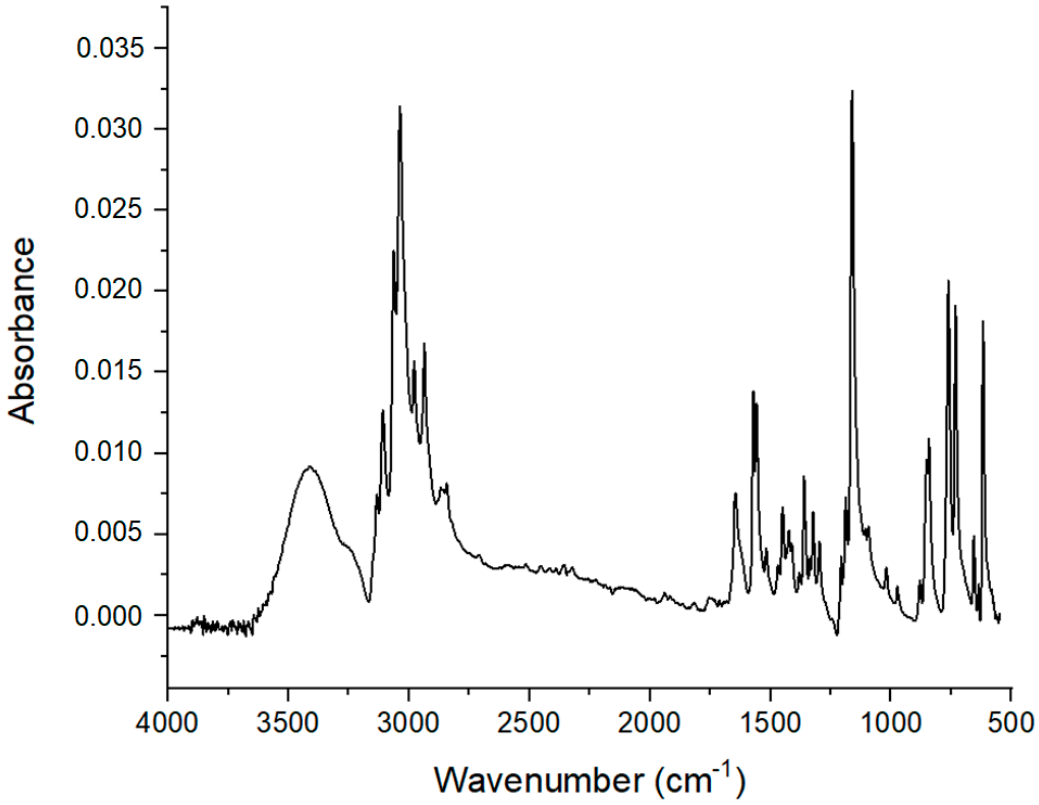

Figure S15. ATR-FTIR spectrum of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**3**).

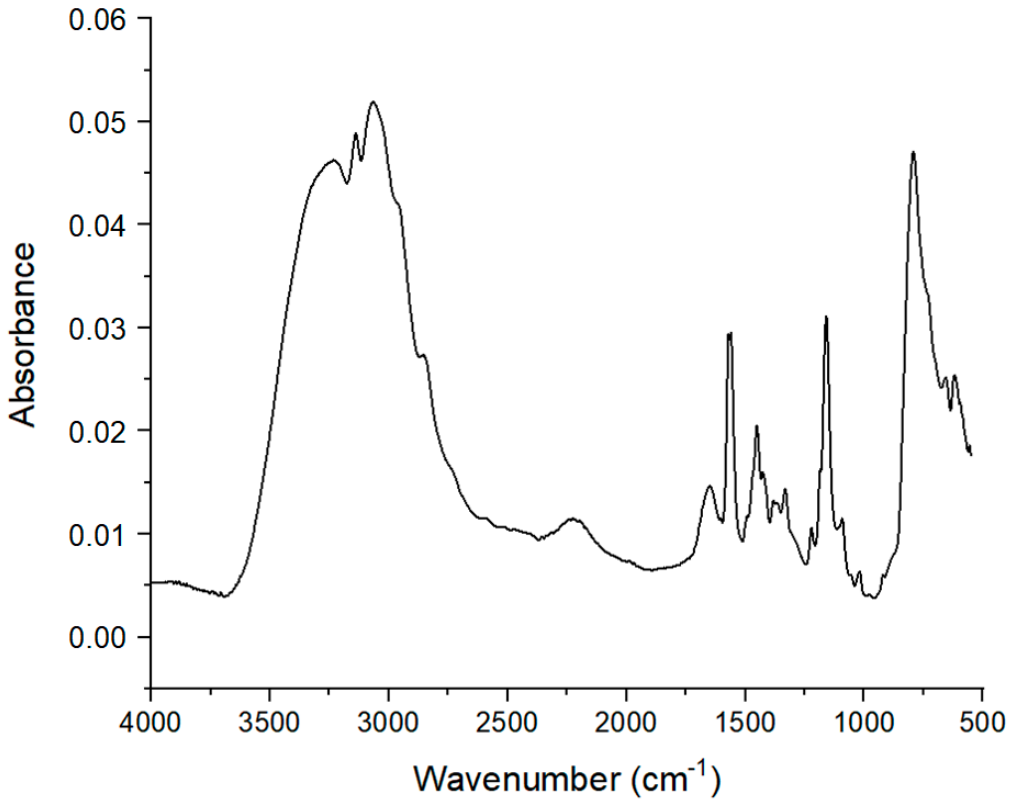

Figure S16. ATR-FTIR spectrum of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**4**).

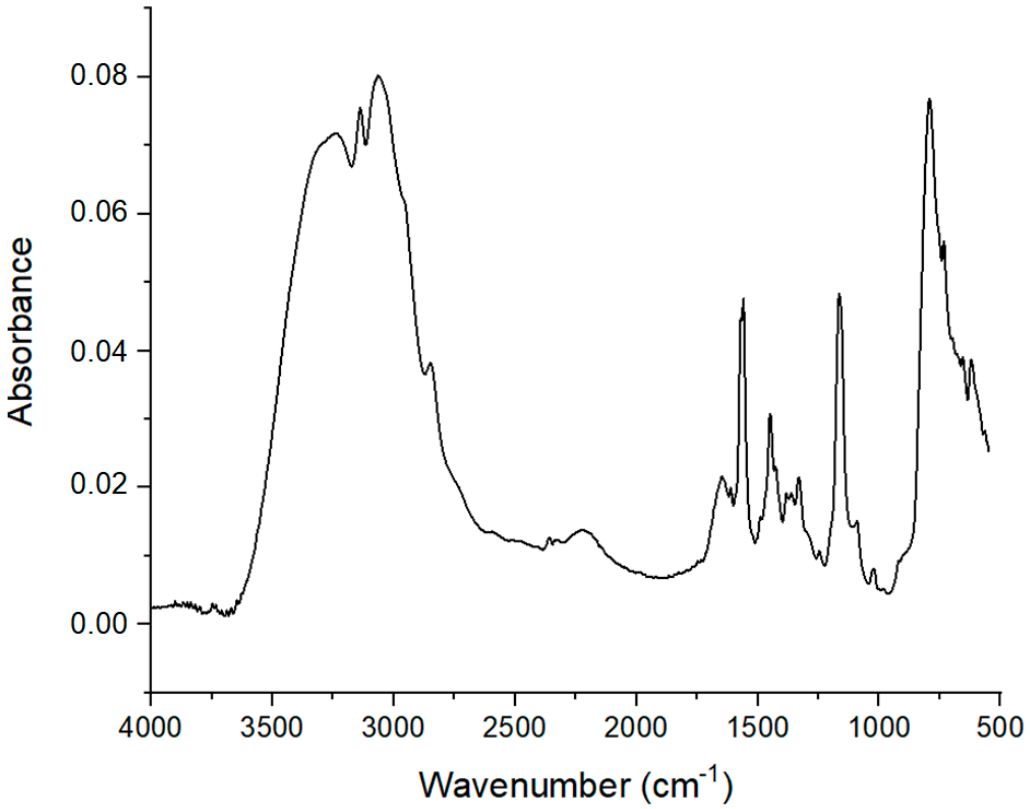

Figure S17. ATR-FTIR spectrum of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**5**).

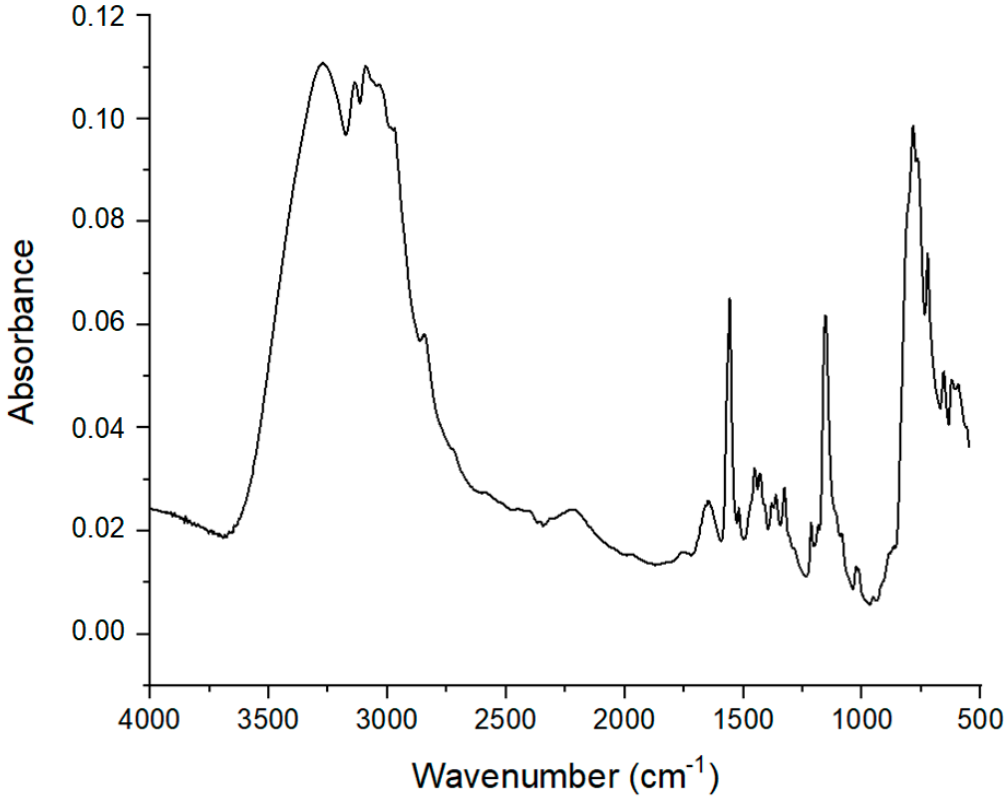

Figure S18. ATR-FTIR spectrum of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**6**).

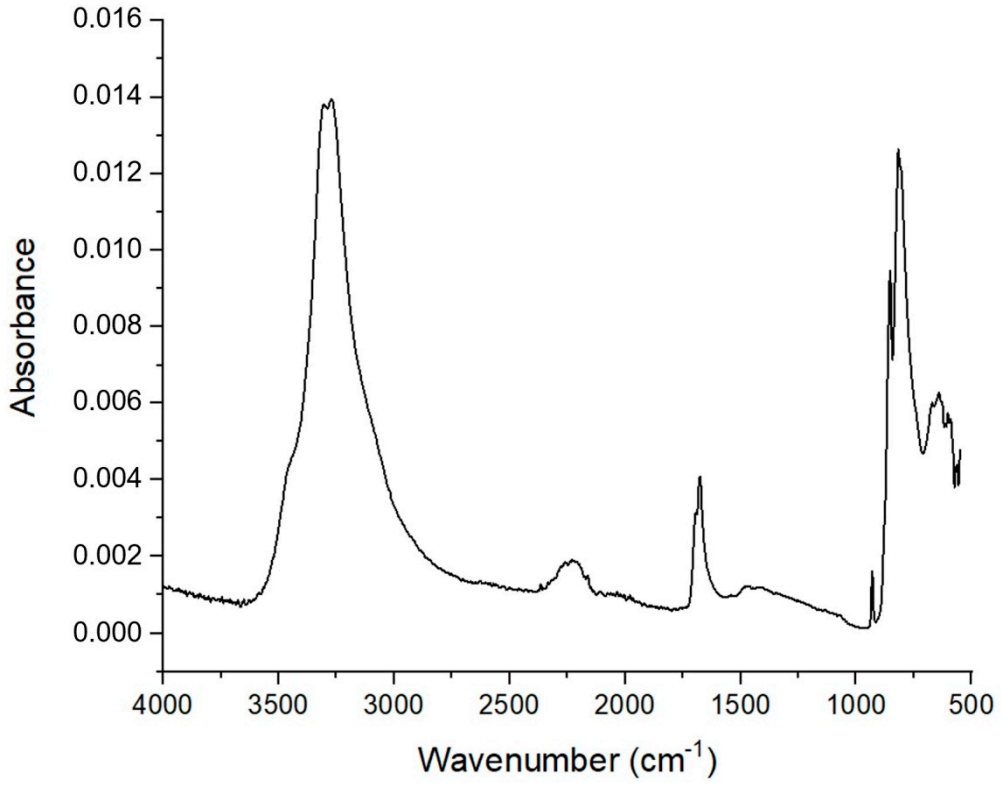

Figure S19. ATR-FTIR spectrum of sodium tungstate.

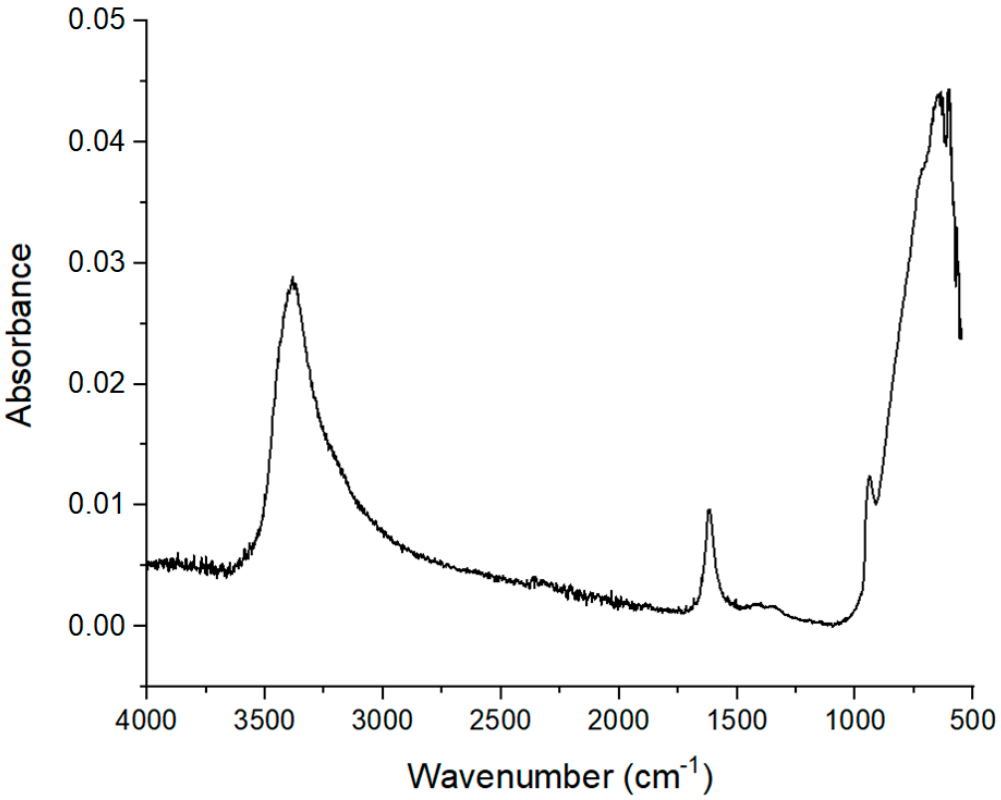

Figure S20. ATR-FTIR spectrum of tungstic acid.

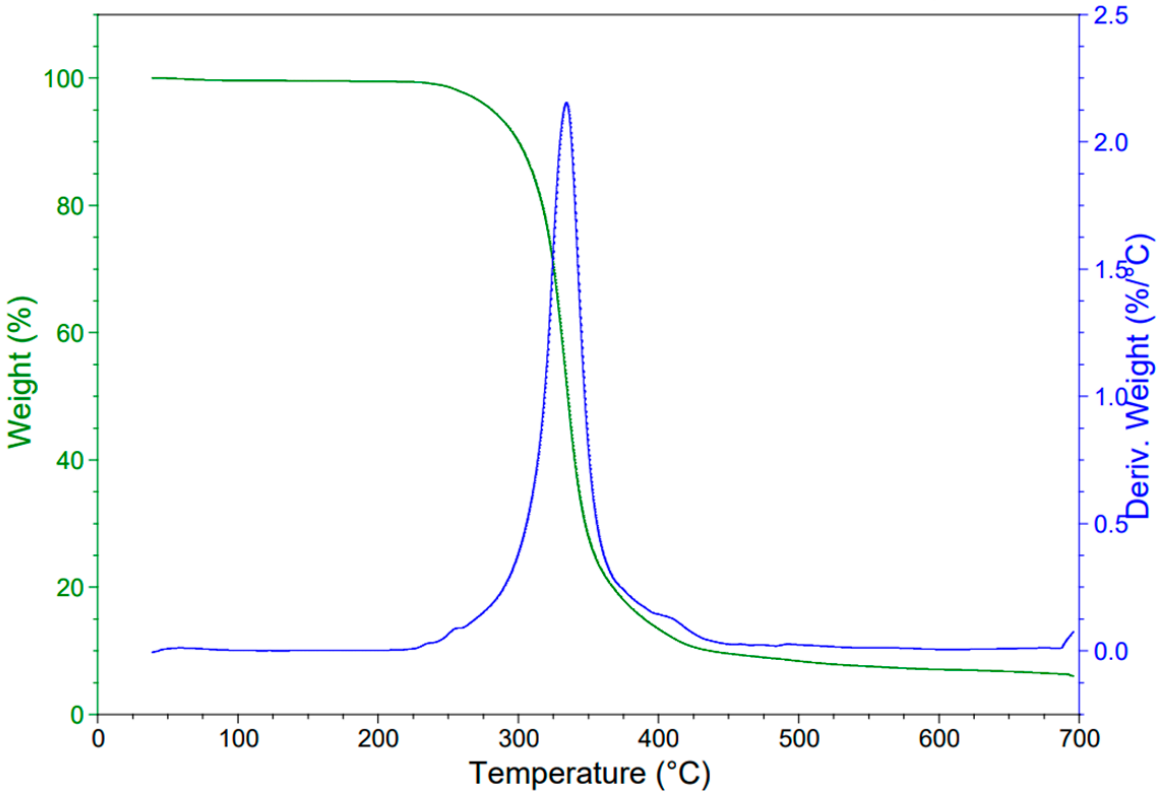

Figure S21. Thermal gravimetric analysis and derivative of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**1**)

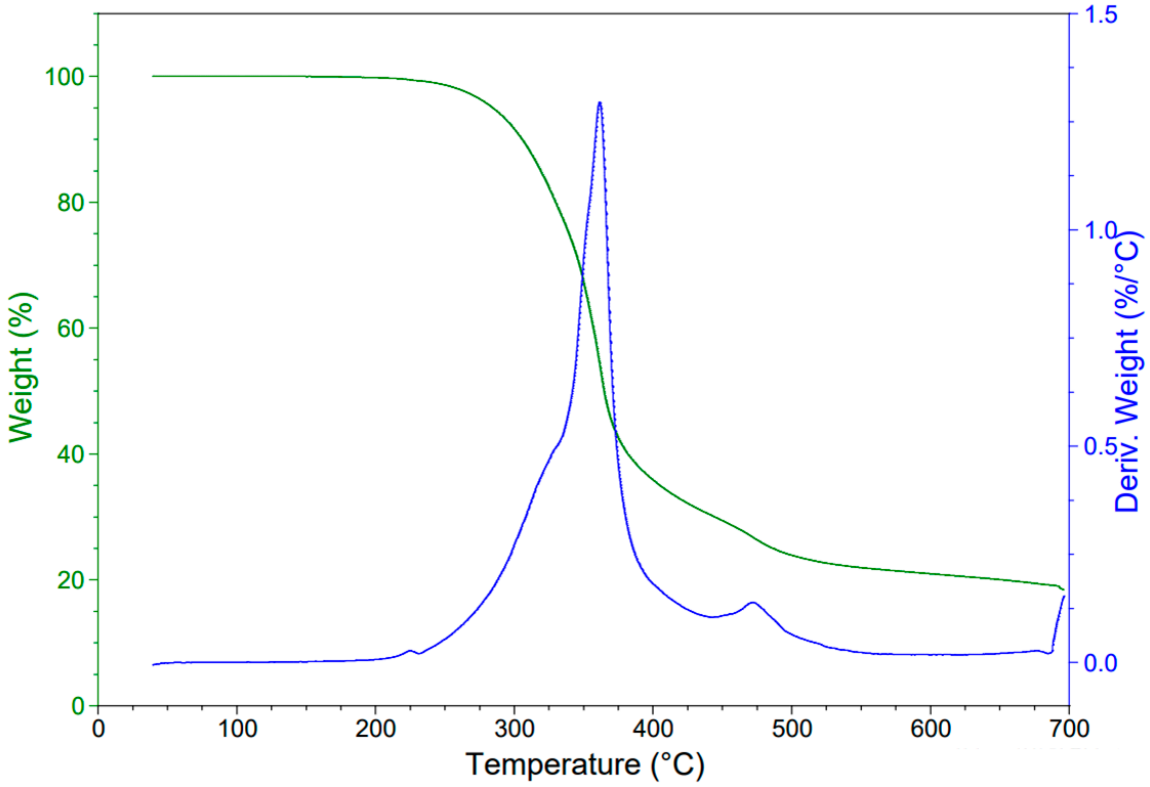

Figure S22. Thermal gravimetric analysis and derivative of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**2**)

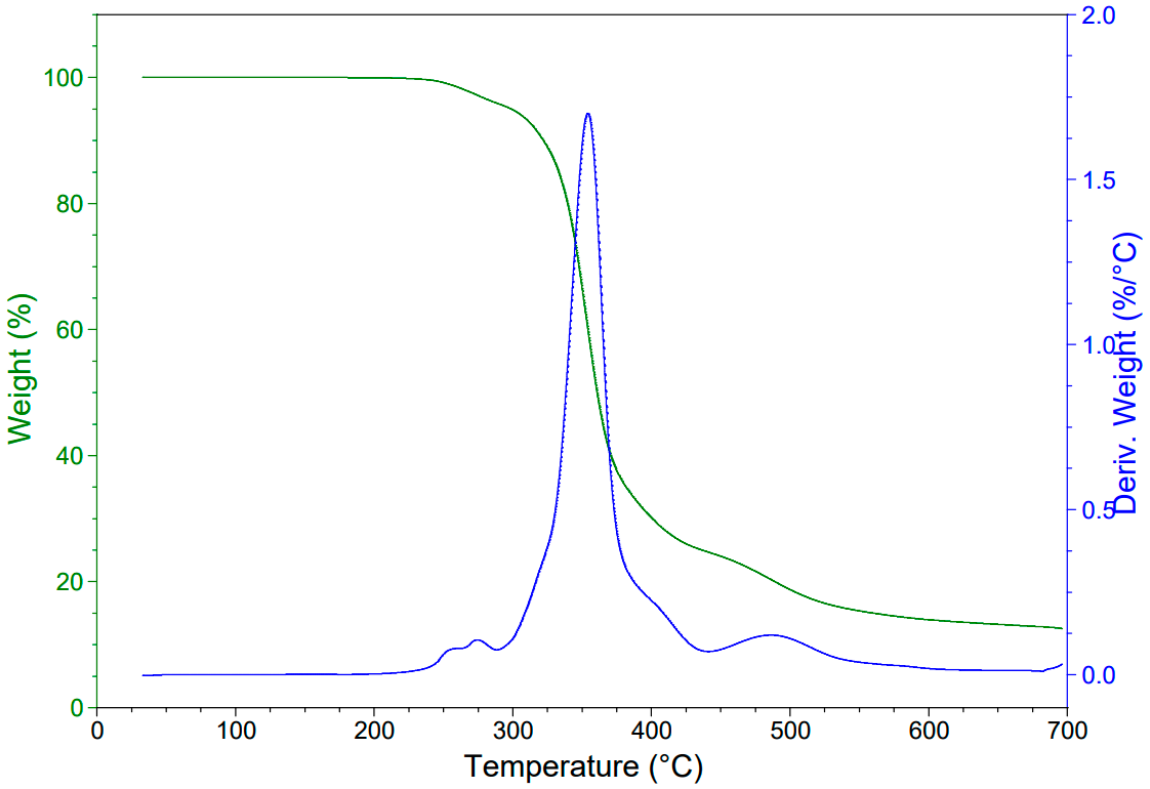

Figure S23. Thermal gravimetric analysis and derivative of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) bromide (**3**)

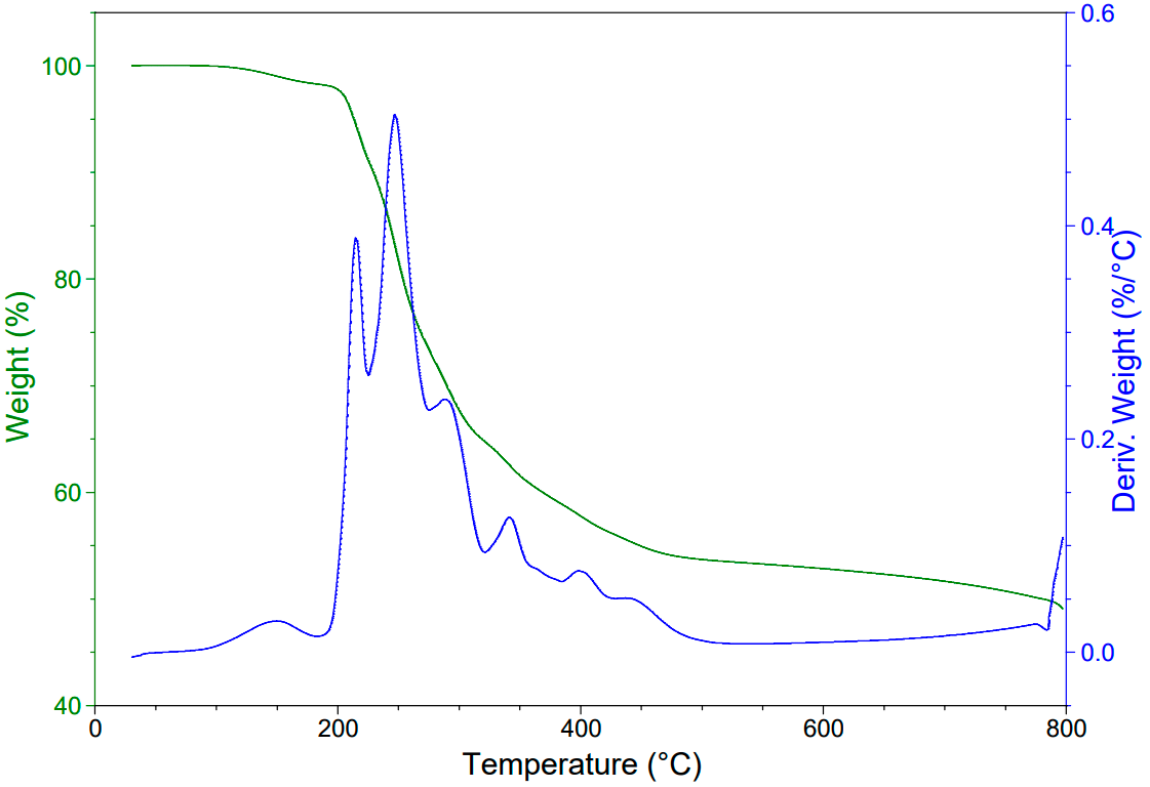

Figure S24. Thermal gravimetric analysis and derivative of 1,1'-(1,2-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**4**).

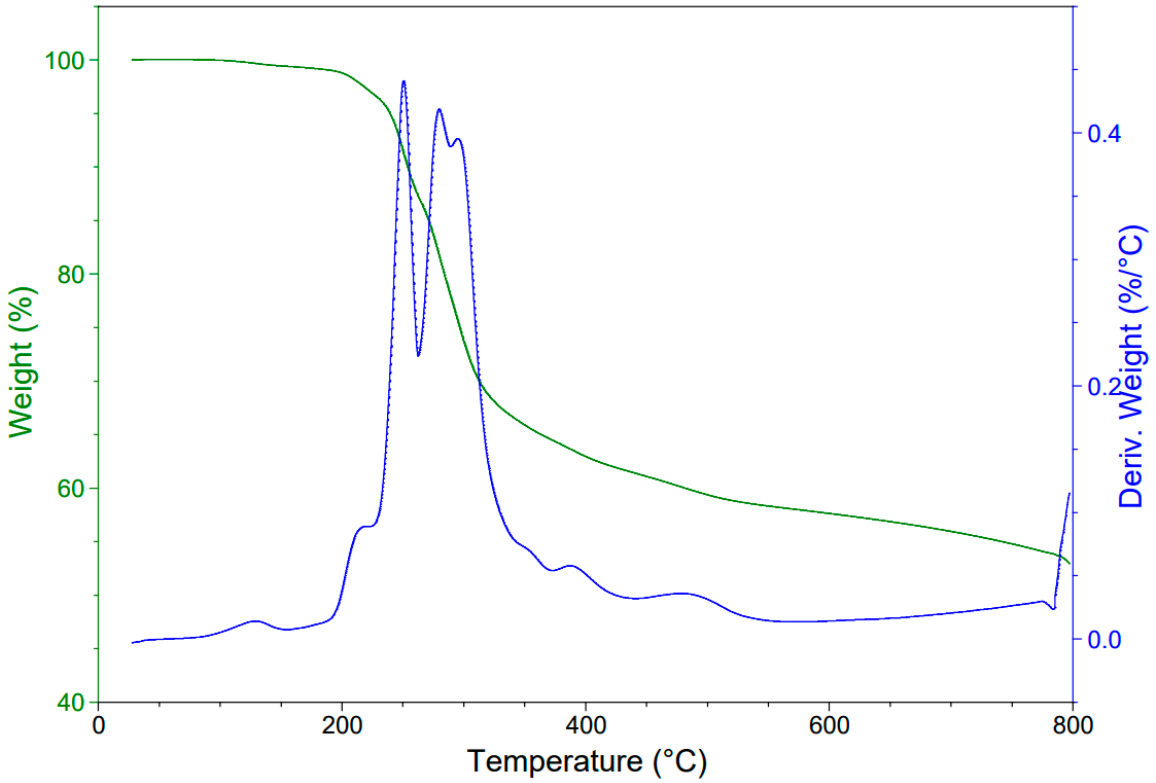

Figure S25. Thermal gravimetric analysis and derivative of 1,1'-(1,3-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**5**).

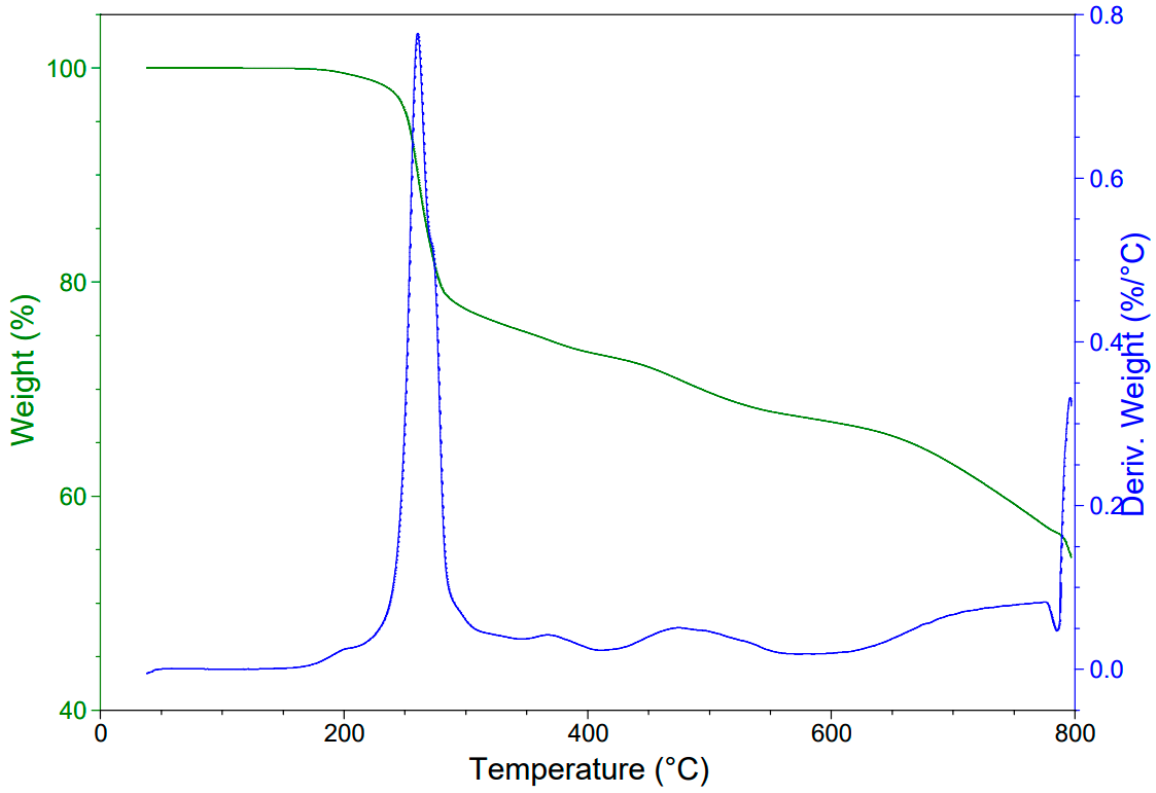

Figure S26. Thermal gravimetric analysis and derivative of 1,1'-(1,4-phenylenebis(methylene))bis(3-methylimidazolium) tungstate (**6**).

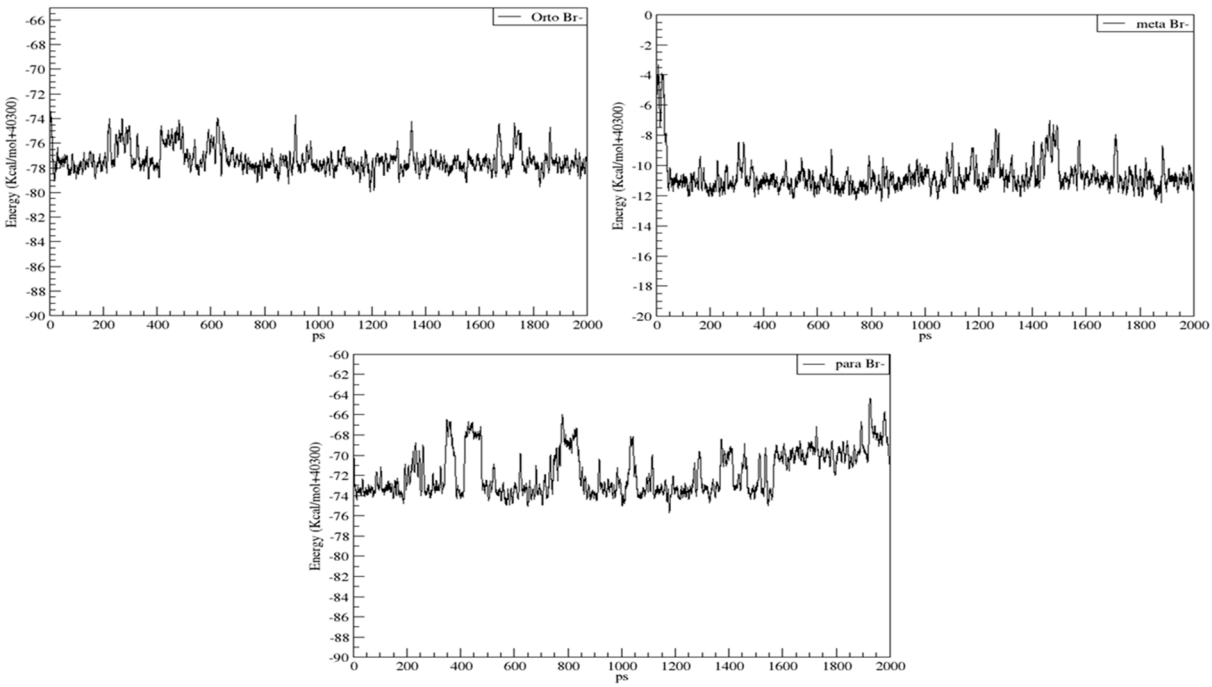

Figure S27: Energy variation along the simulation time to the IL using the Bromide anion (Conformations Ortho, Meta and Para).

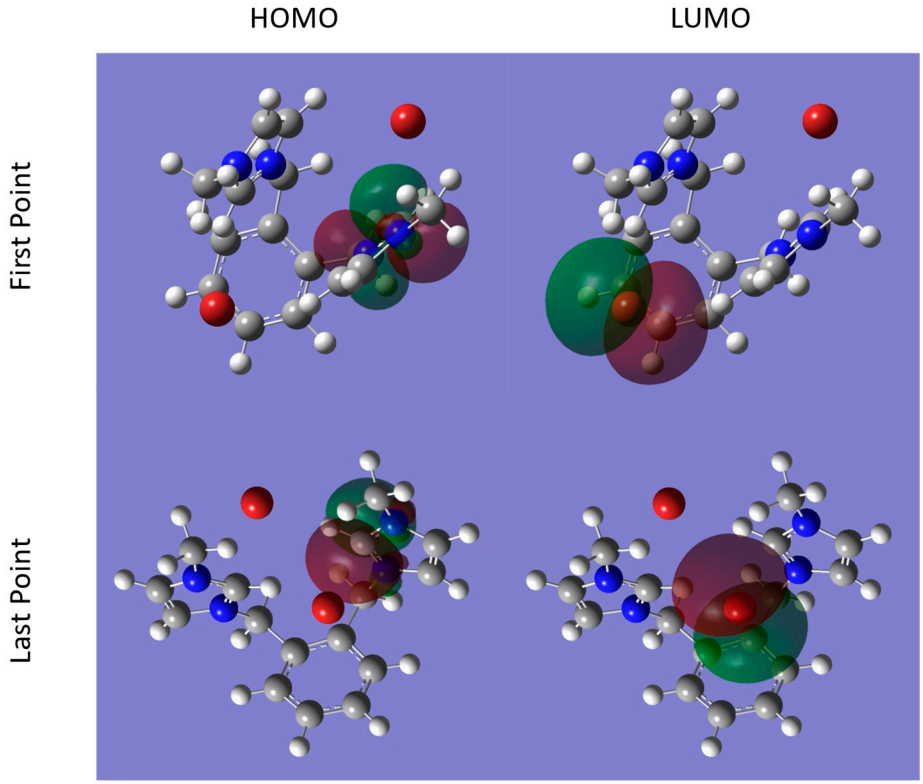

Figure S28: HOMO-LUMO analyses for the IL with bromide anion in the configuration ortho.

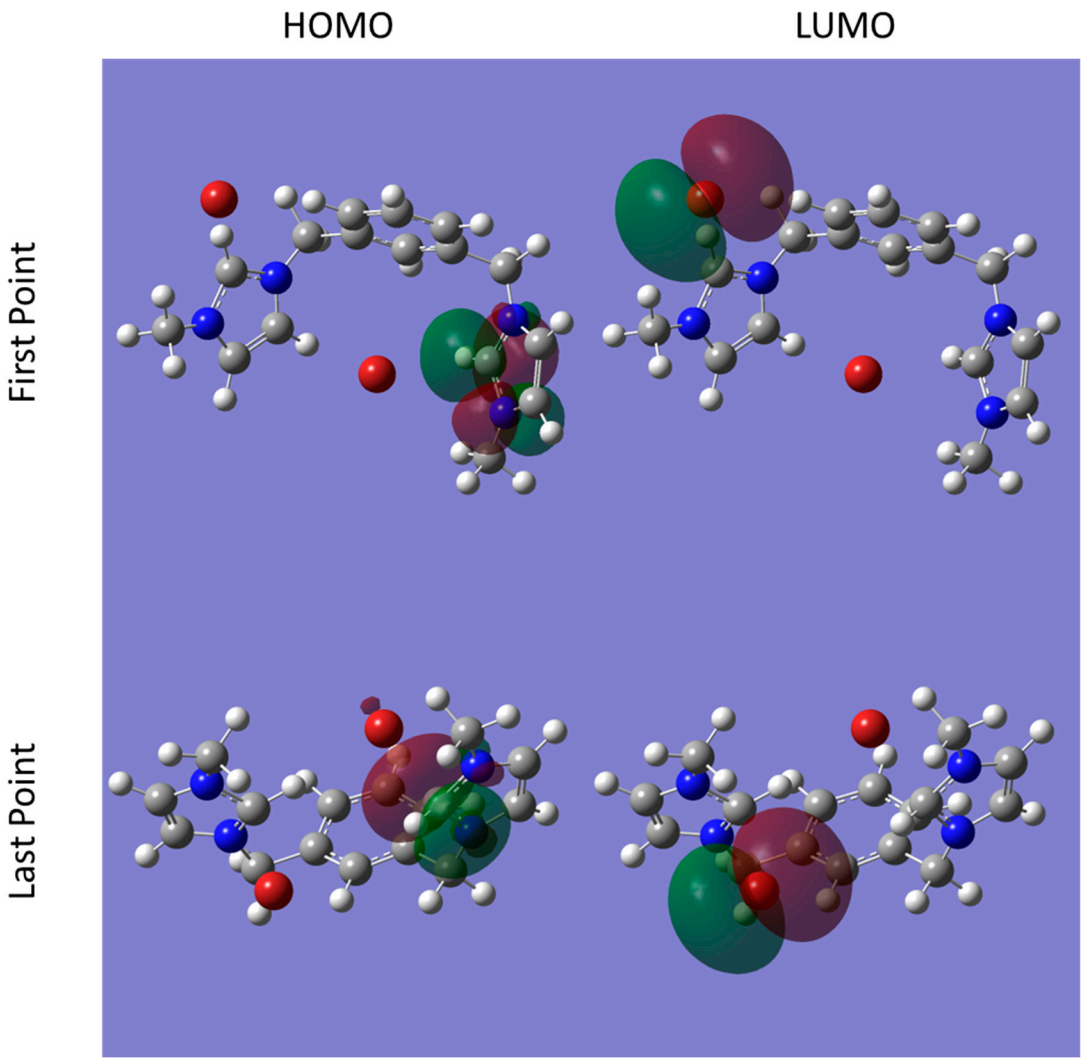

Figure S29: HOMO-LUMO analyses for the IL with bromide anion in the configuration meta.

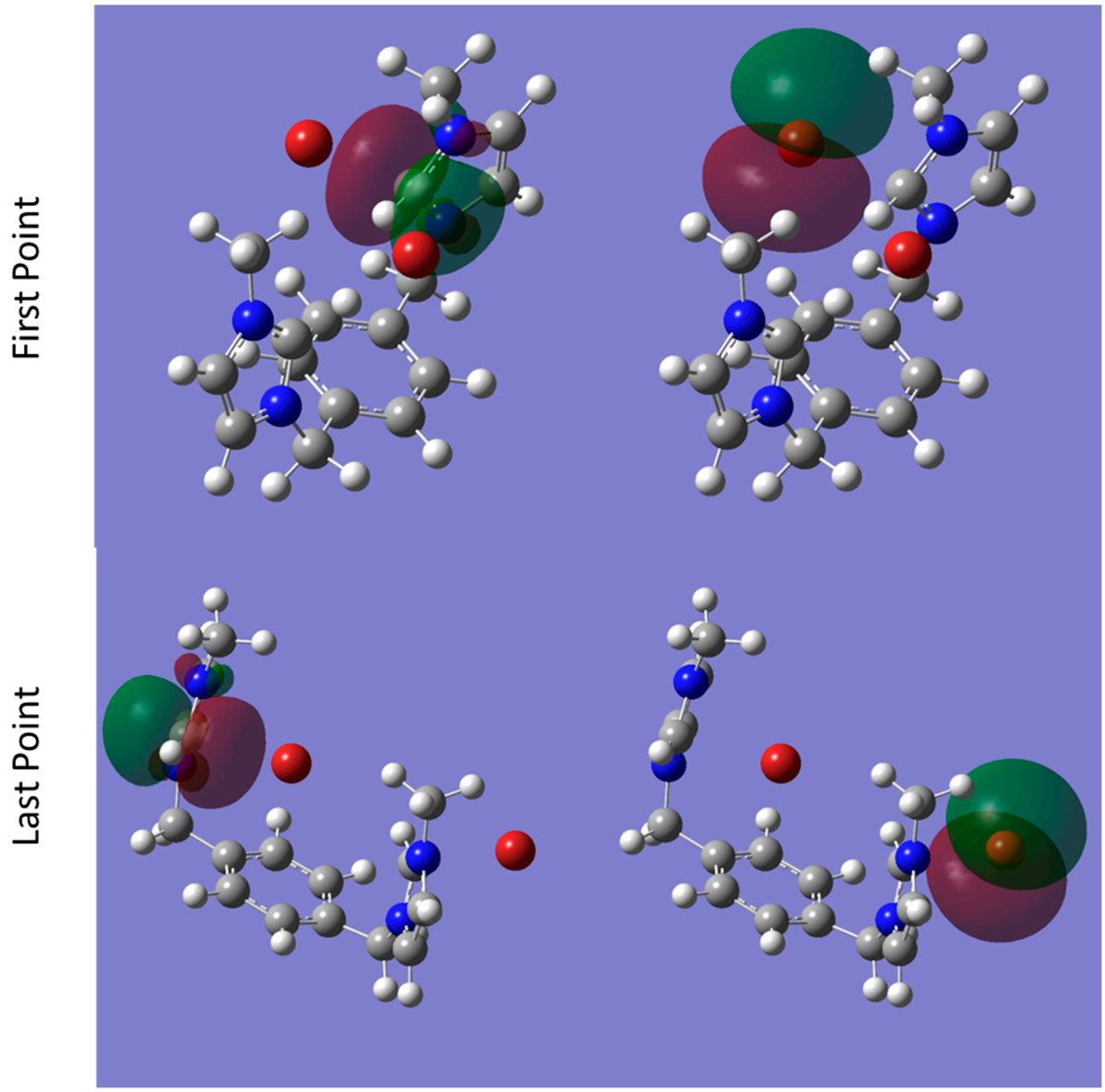

Figure S30: HOMO-LUMO analyses for the IL with bromide anion in the configuration para.

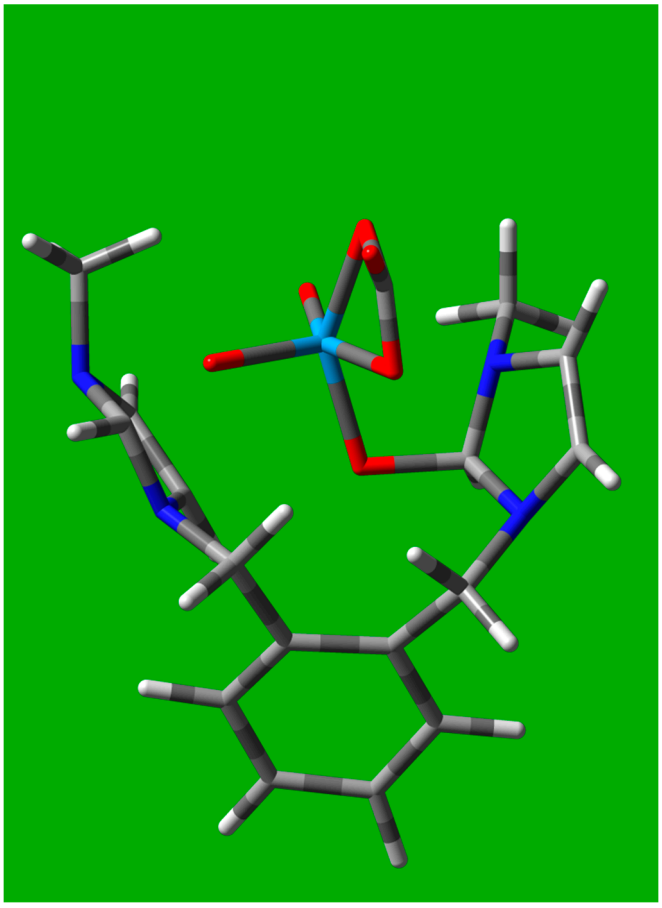

Figure S31. Structure of cluster with CO_2. Ortho configuration.

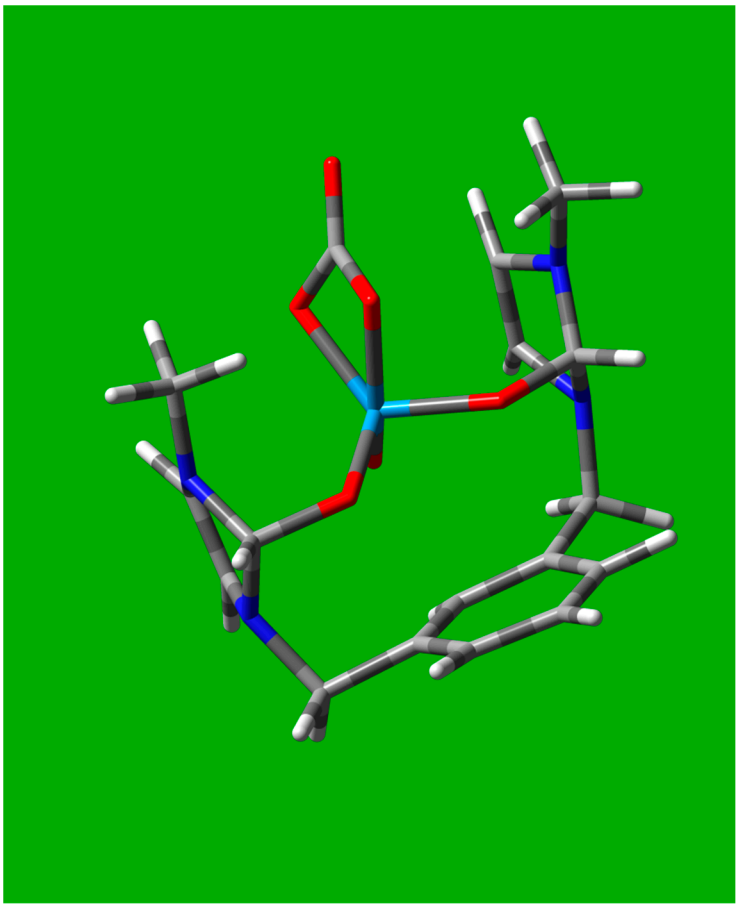

Figure S32. Structure of cluster with CO_2. Meta configuration.

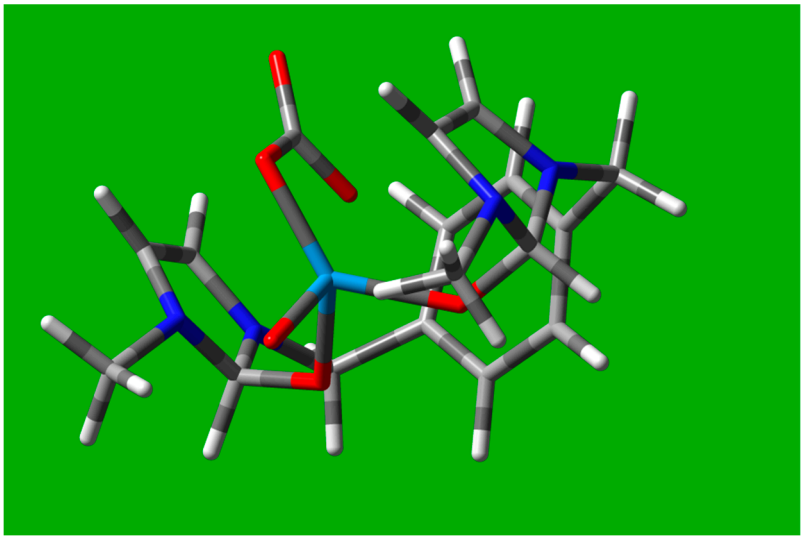

Figure S33. Structure of cluster with CO_2. Para configuration.