

Are cyclopentadienylberyllium, magnesium and calcium hydrides carbon or metal acids in the gas phase?

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Supporting Information (total of 5 pages)

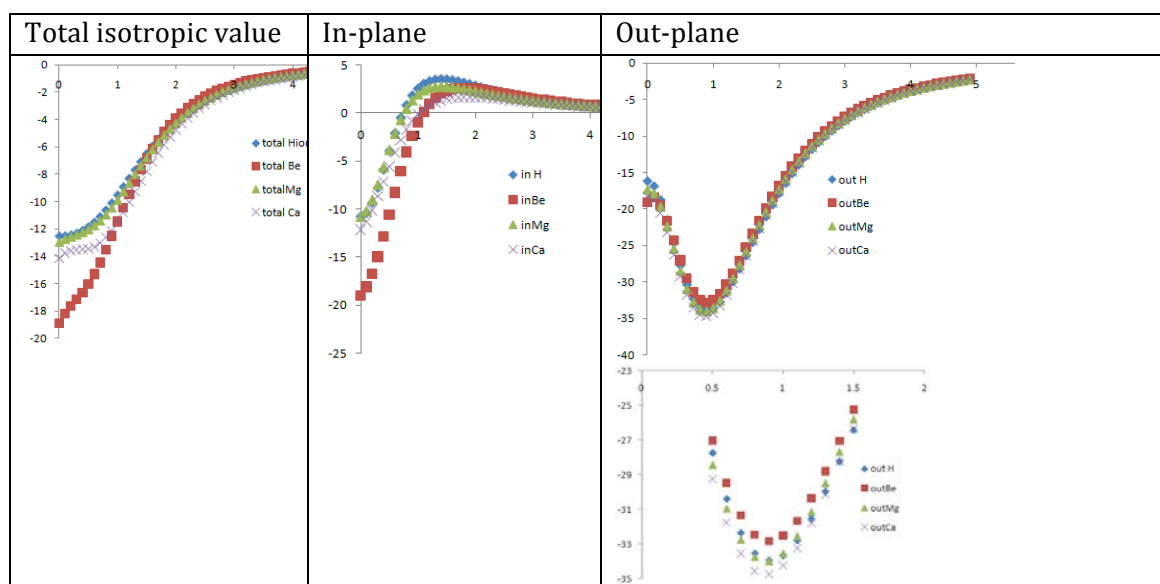
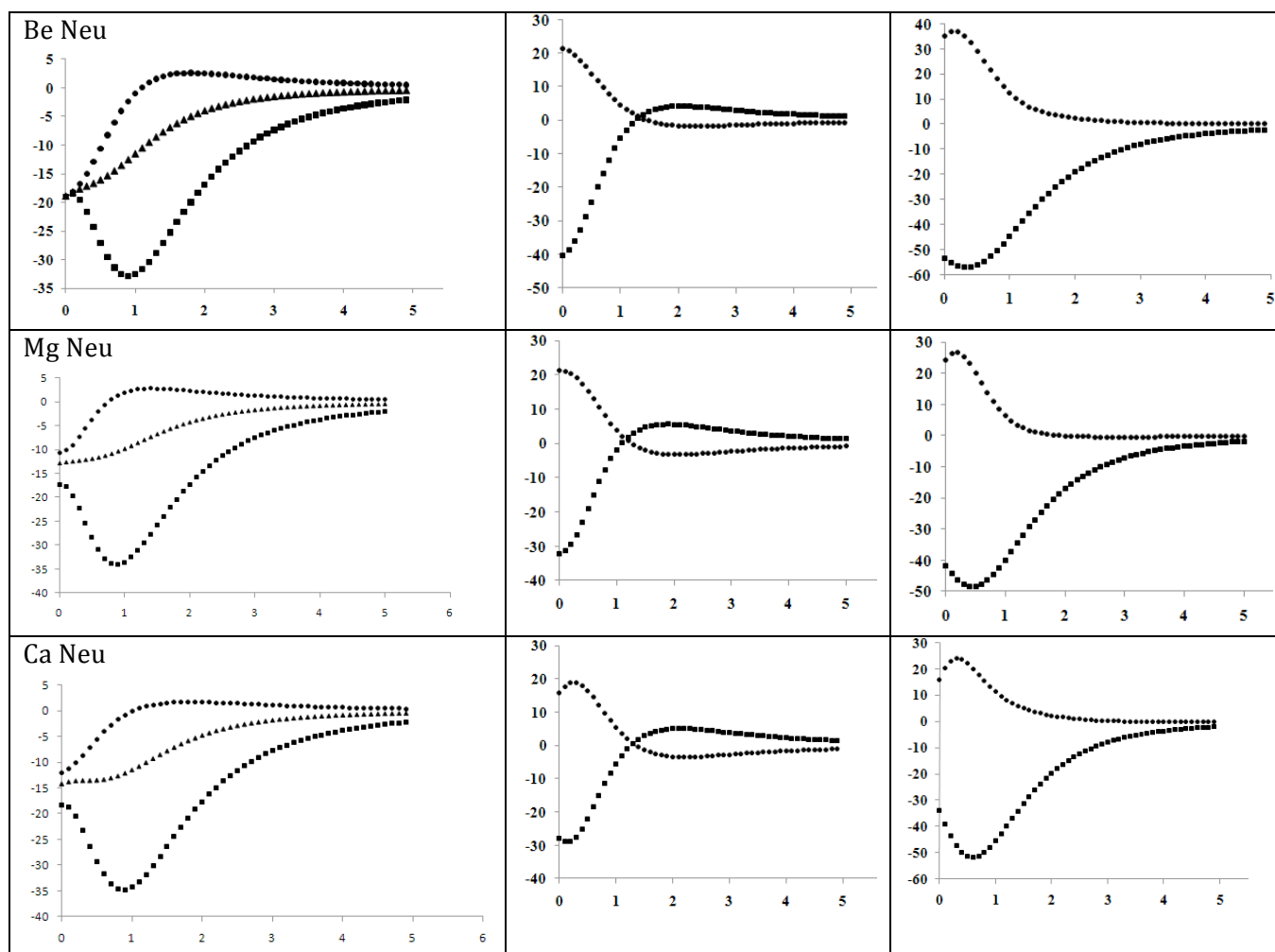
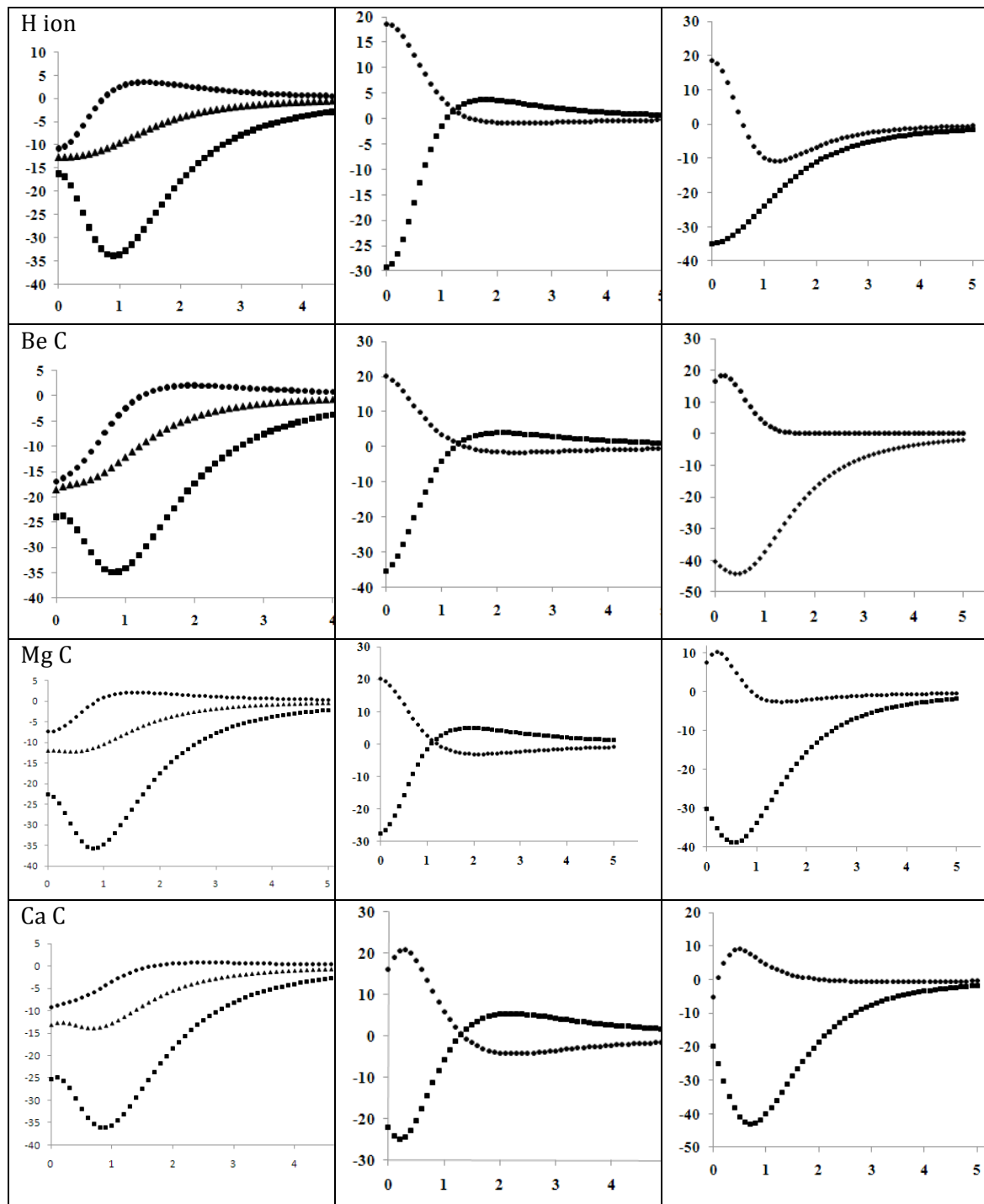


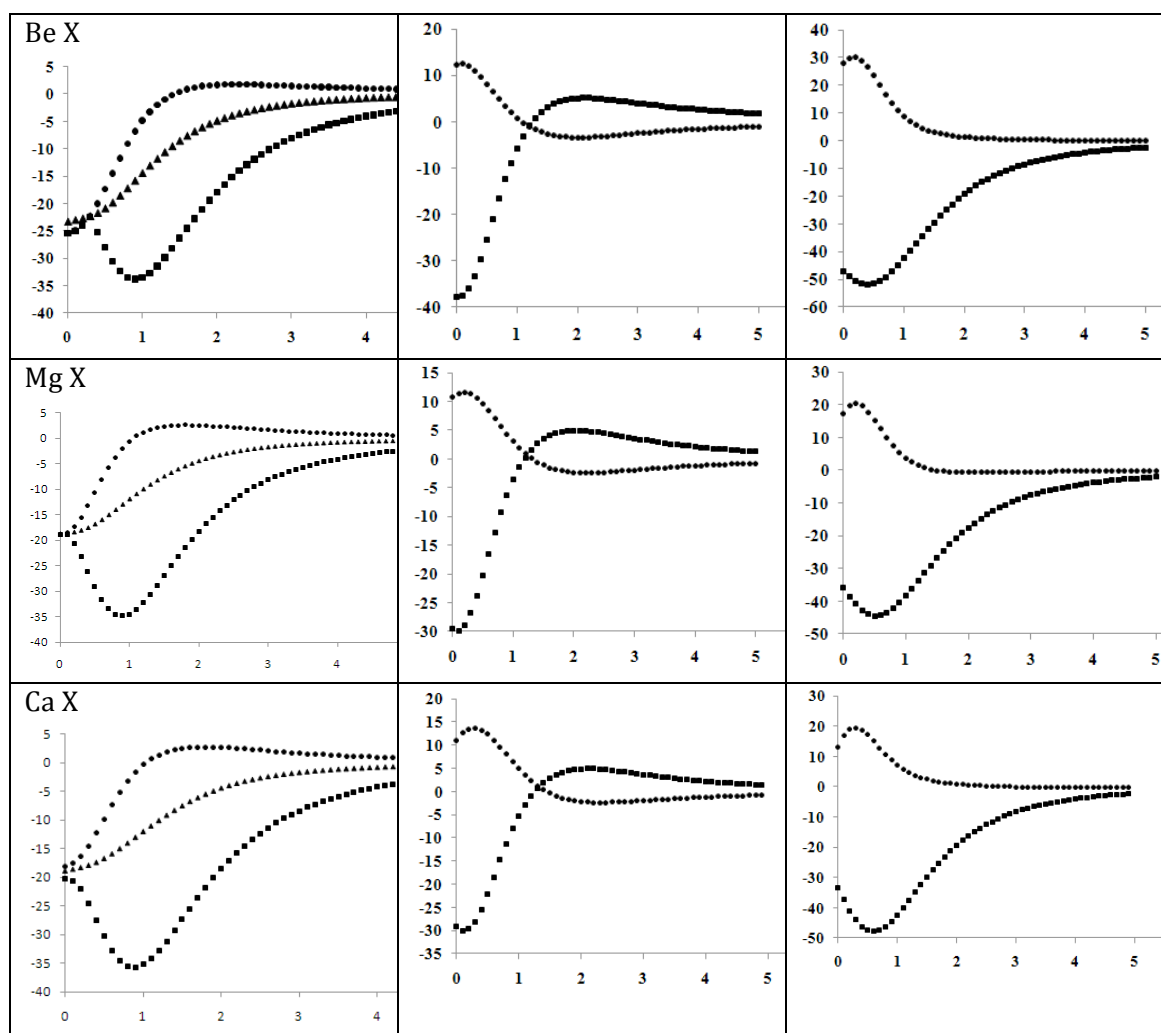
Figure S1. Total isotropic chemical shift and its in-plane and out-of-plane components for cyclopentadienyl anion and CpXH (X = Be, Mg, Ca) neutral compounds. Values in ppm.



(a)



(b)



(c)

Figure S2. NICS scans for: (a) CPXH (X = Be, Mg, Ca) neutral compounds, (b) cyclopentadienyl anion and the CH deprotonated species of CPXH (X = Be, Mg, Ca) derivatives, (c) XH deprotonated species of CPXH (X = Be, Mg, Ca) derivatives. First column shows NICS values (▲) and the out-of-plane (■) and in-plane (●) components, as a function of the distance to the Cp ring. Second column shows the diamagnetic (●) and paramagnetic (■) contributions to the in-plane component, and the third column gives the same information for the out-of-plane component. All values in ppm.