Electronic Supplementary Material (ESI) for Dalton Transactions

The Kubas Interaction in M(II) (M = Ti, V, Cr) Hydrazide-Based Hydrogen Storage Materials: a DFT Study

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Supplementary Information

		Method of partial charge calculation				
Ancillary ligand	Number of H_2 bound	Mulliken	Voronoi	Hirshfeld	Gaussian Mulliken	AIM
(Trimethylsilyl)methyl	0	0.668	0.352	0.404	0.704	1.151
	1	0.598	0.319	0.400	-0.202	1.137
Hydride	0	0.658	0.351	0.317	0.387	1.099
	1	0.616	0.327	0.338	-0.046	1.102
2 Hydride	0	0.572	0.370	0.294	0.124	1.027
	1	0.559	0.345	0.282	0.013	1.032
Hydrazine based	0	0.689	0.332	0.384	0.444	1.140
	1	0.663	0.324	0.391	-0.329	1.173

Table S1: Partial charge on the Cr atom for the BSR with various different ancillary ligands, number of H_2 molecules bound and methods of calculating the partial charge. The values highlighted in green and red show the partial charge decreasing and increasing respectively as more H_2 molecules are bound.

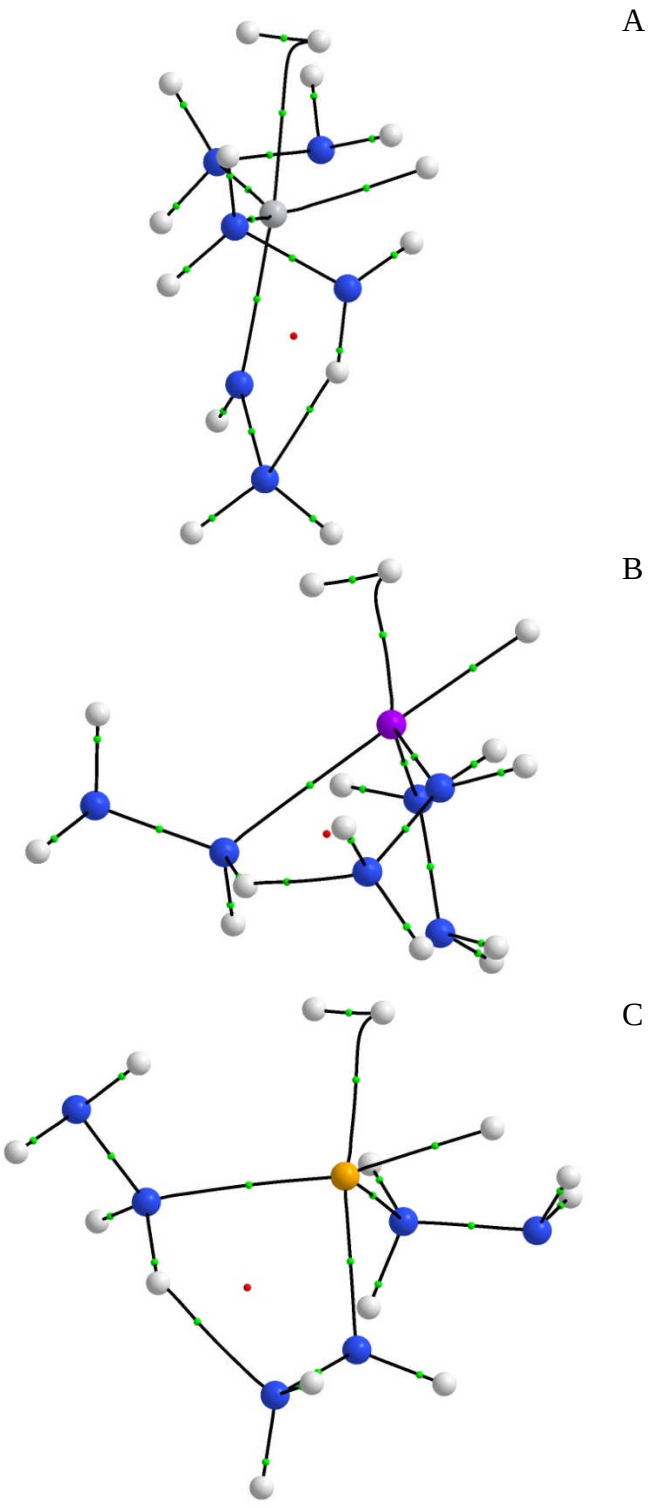

Figure S2: Molecular graphs showing the bond paths (black lines) and bond and ring critical points (green and red circles respectively) for the 4 coordinate BSRs with ancillary hydride ligand and one bound H_2; A Ti, B V and C Cr.

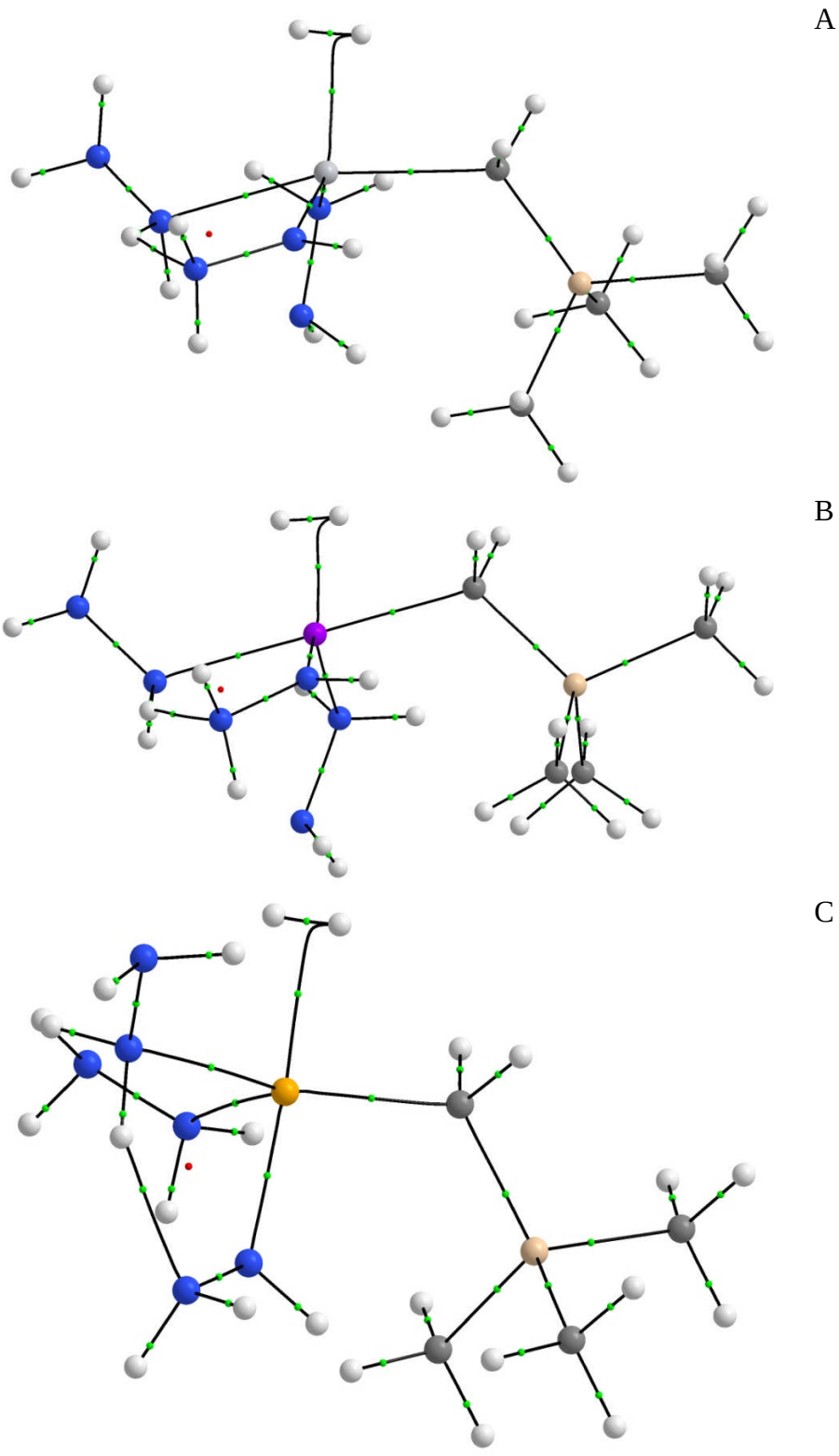

Figure S3: Molecular graphs showing the bond paths (black lines) and bond and ring critical points (green and red circles respectively) for the 4 coordinate BSRs with ancillary bis[(trimethylsilyl) methyl] ligand and one bound H_2; A Ti, B V and C Cr.