Supplementary Material (ESI) for Chemical Communications

Supplementary Material

Title: Gallium(I)-Alkaline Earth Metal Donor-Acceptor bonds.

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Table 1. Computed selected structural constants of [(η^5-C_5Me_5)Ga] (**1a**), [(η^5-C_5Me_5)$_2$Ca] (**1b**), and [(η^5-C_5Me_5)$_2$Ca-Ga(η^5-C_5Me_5)] (**1**). Structure optimizations have been performed at MP2 and density functional theory (DFT) level with the functional BP86. The basis set is def2-TZVP (triple zeta valence augmented by polarization functions, e. g. 2d1f for C) and def2-QZVP for Ca. Lengths in Å, angles in degrees, ED = electron diffraction experiment, Cg = centroid of the C_5Me_5 ring.

		BP86	**MP2**	**XRD**	**ED**
1a	Cg-Ga	2.096	2.025	208.1[(a)]	208.1(5)[(b)]
1b	Cg-Ca	2.632	2.278	233-236[(c)]	2.312(6)[(d)]
	Cg_1-Ca-Cg_2	180	157.6	146-148[(c)]	154(3)[(d)]
1	Ga-Ca	3.423	3.068	3.183(2) [(e)]	
	Cg_{Ga}-Ga	2.047	1.964	1.99(2)	
	Cg_1-Ca	2.367	2.307	2.347(5)	
	Cg_1-Ca-Cg_2	148.74	149.32	147.44(1)	

[(a)] D. Loos, E. Baum, A. Ecker, H. Schnöckel, A. J. Downs, *Angew. Chem.* **1997**, *109*, 894-895; *Angew. Chem., Int. Ed. Engl.* **1997**, *36*, 860-862.
[(b)] A. Haaland, K.-G. Martinsen, H. V. Volden, D. Loos, H. Schnöckel, *Acta Chem. Scand.* **1994**, 48, 172-174.
[(c)] R. A. Williams, T. P. Hanusa, and J. C. Huffman, *Organometallics* **1990**, 9, 1128-1134.
[(d)] R. A. Andersen, R. Blom, J. M. Boncella, C. J. Burns, H. V. Volden, *Acta Chem. Scand. A* **1987**, 41, 24-35.
[(e)] This work.