Electronic Supplementary Material (ESI) for Dalton Transactions.

Contrasting the Group 6 metal-metal bonding in sodium dichromate(II) and sodium dimolybdate(II) polymethyl complexes: Synthetic, X-ray Crystallographic and Theoretical Studies

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SUPPORTING INFORMATION

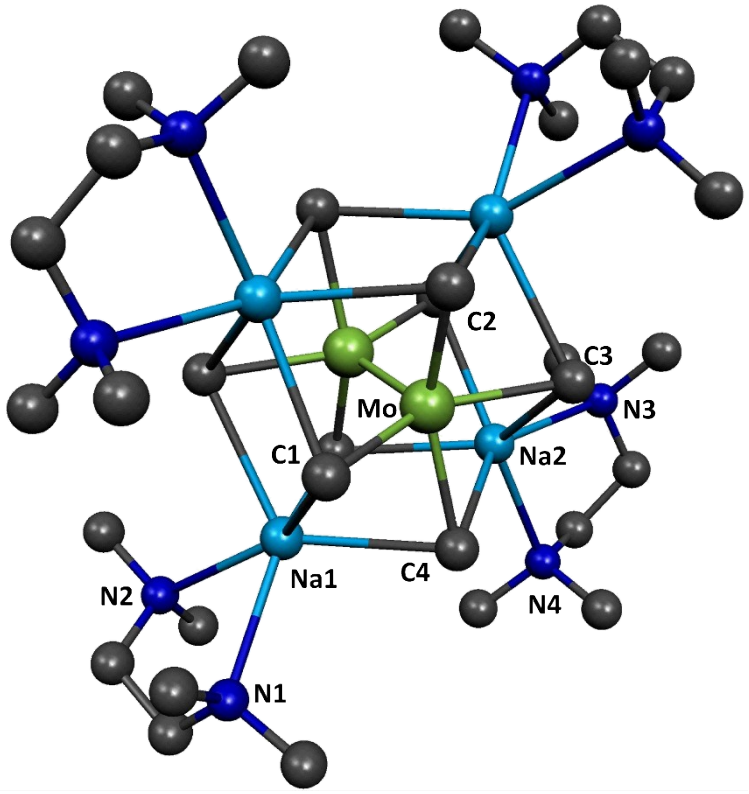

Figure S1. Geometry optimised structure of **5** (hydrogen atoms removed for clarity).

Table S1. Calculated and Experimental Bond Distances (Å) for **5**

	Exptl	Calcd
Mo(1)–Mo(1′)	2.1403(3)	2.137
Mo(1)–C(1)	2.318(2)	2.309
Mo(1)–C(2)	2.305(2)	2.306
Mo(1)–C(3)	2.318(2)	2.308
Mo(1)–C(4)	2.324(2)	2.316
C(1)–Na(1)	2.748(2)	2.740
C(2)–Na(1)	2.730(2)	2.668
C(3)–Na(1)	2.671(2)	2.675
C(4)–Na(1)	2.762(2)	2.734
C(1)–Na(2)	2.731(2)	2.640
C(2)–Na(2)	2.721(2)	2.688
C(3)–Na(2)	2.775(2)	2.751
C(4)–Na(2)	2.756(2)	2.823
Na(1)–N(1)	2.614(2)	2.553
Na(1)–N(2)	2.613(2)	2.564
Na(2)–N(3)	2.609(2)	2.582
Na(2)–N(4)	2.605(2)	2.573
Mo(1)···C_4[a]	0.69	0.70

[a] Distance Mo is displaced from C_4 plane.

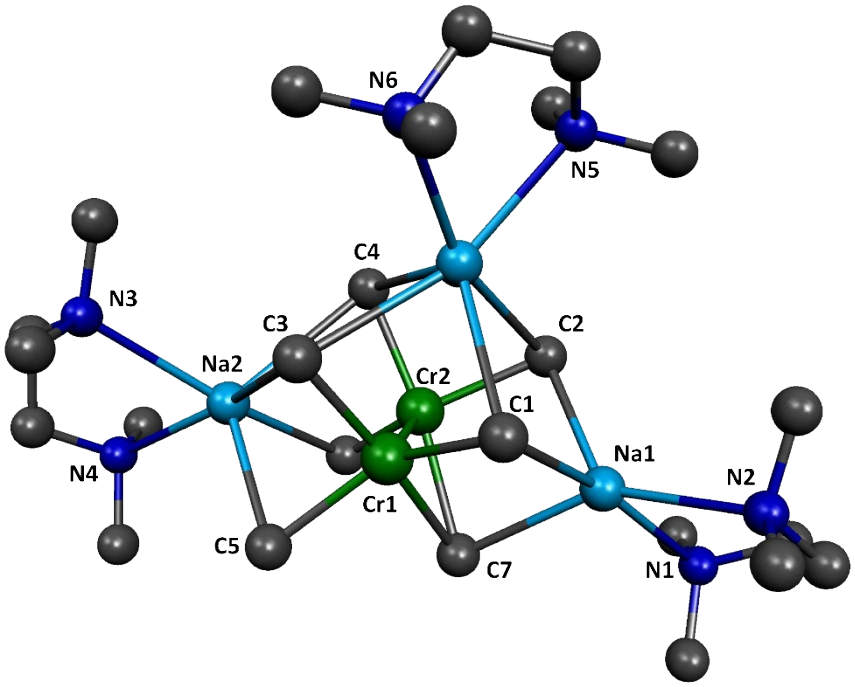

Figure S2. Geometry optimised structure of **6** (hydrogen atoms removed for clarity).

Table S2. Calculated and Experimental Bond Distances (Å) and Angles for **6**

	Exptl[a]	Calcd
Cr(1)–Cr(2)	1.9136(4)	1.858
Cr(1)–C(1)	2.205(2)	2.205
Cr(1)–C(3)	2.160(2)	2.161
Cr(1)–C(5)	2.160(2)	2.140
Cr(1)–C(7)	2.302(2)	2.279
Cr(2)–C(2)	2.174(2)	2.188
Cr(2)–C(4)	2.185(2)	2.160
Cr(2)–C(6)	2.142(2)	2.117
Cr(2)–C(7)	2.286(2)	2.398
C(1)–Na(1)	2.544(2)	2.509
C(2)–Na(1)	2.634(2)	2.492
C(7)–Na(1)	2.625(2)	2.483
C(3)–Na(2)	2.814(2)	2.841
C(4)–Na(2)	2.993(2)	2.946
C(5)–Na(2)	2.631(3)	2.520
C(6)–Na(2)	2.786(3)	2.588
C(1)–Na(3)	2.851(3)	2.735
C(2)–Na(3)	2.899(2)	2.818
C(3)–Na(3)	2.759(2)	2.711
C(4)–Na(3)	2.769(2)	2.705
Na(1)–N(1)	2.512(2)	2.490
Na(1)–N(2)	2.544(2)	2.531
Na(2)–N(3)	2.558(2)	2.534
Na(2)–N(4)	2.663(2)	2.541
Na(3)–N(5)	2.609(2)	2.632
Na(3)–N(6)	2.607(2)	2.561
Cr(1)–C(7)–Cr(2)	49.30(5)°	46.72°

[a] Calculated data are compared with the more highly resolved structure **7**.

Table S3. Crystallographic data and refinement details for complexes **5**, **6** and **7**.

	5	**6**	**7**
Empirical formula	$C_{32}H_{88}Mo_2N_8Na_4$	$C_{25}H_{69}Cr_2N_6Na_3$	$C_{37}H_{87}Cr_2N_6Na_3$
Mol. Mass	868.94	626.83	789.10
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	P 2_1/n	P 2_1 2_1 2_1	P 2_1
a/ Å	11.3776(2)	13.5520(7)	12.0585(3)
b/ Å	17.0310(4)	14.8524(6)	15.7116(5)
c/ Å	12.7810(3)	18.5398(8)	12.5776(4)
α	90	90	90
β	105.031(2)	90	103.980(3)
γ	90	90	90
V/ Å^3	2391.86(9)	3731.7(3)	2312.35(12)
Z	2	4	2
λ/ Å	0.71073	0.71073	0.71073
Measured reflections	15939	22619	14038
Unique reflections	5647	9490	8711
R_{int}	0.0358	0.0504	0.0201
Observed rflns [I>2σ(I)]	4010	6618	8281
GooF	0.851	1.037	1.020
R [on F, obs rflns only]	0.0275	0.0551	0.0282
ωR [on F^2, all data]	0.0461	0.0942	0.0667
Largest diff. Peak/hole. e/ Å^{-3}	0.42/-0.27	0.34/-0.26	0.39/-0.19
Flack parameter	-	-0.009(12)	-0.013(10)