Electronic Supplementary Information for Dalton Transactions

Supporting Information

for

Chromium(III) catalysed ethylene tetramerisation promoted by bis(phosphino)amines with an N-functionalised pendant

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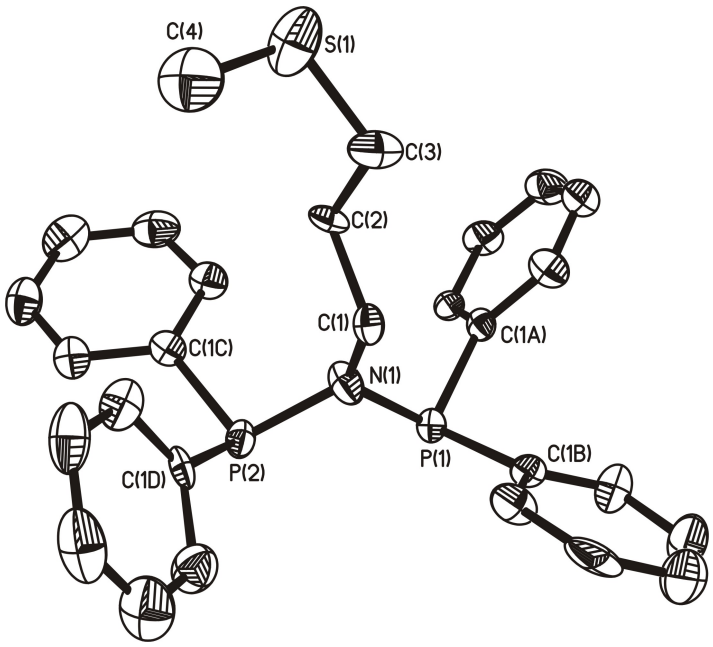
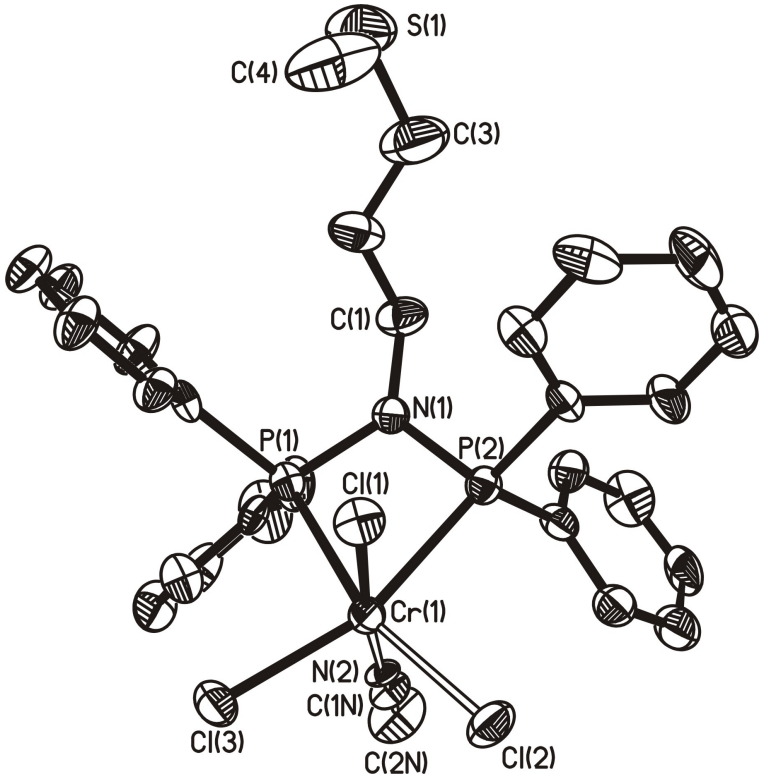
ORTEP diagrams and tables of crystallographic data for Compound **1d, 3a** and **3b**.



ORTEP diagram of compound **1d** (H atoms and the minor disorder components are omitted). Thermal ellipsoids are drawn at the 40% probability.

Table 1. Crystal data and structure refinement for 6192A (compound **1d**).

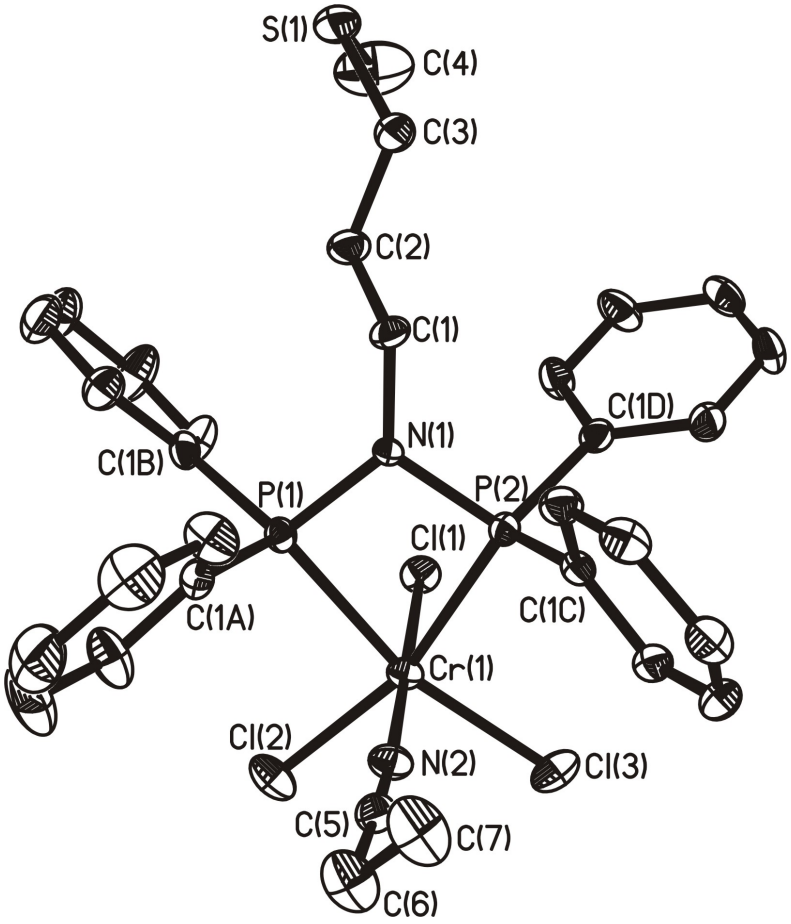
Identification code	6192a	
Empirical formula	C28 H29 N P2 S	
Formula weight	473.52	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.2813(10) Å	α= 90°.
	b = 9.8308(8) Å	β= 90°.
	c = 27.659(3) Å	γ = 90°.
Volume	2523.6(4) $Å^3$	
Z	4	
Density (calculated)	1.246 Mg/m^3	
Absorption coefficient	0.271 mm^{-1}	
F(000)	1000	
Crystal size	0.26 x 0.10 x 0.06 mm^3	
Theta range for data collection	1.47 to 25.00°.	
Index ranges	-10<=h<=11, -10<=k<=9, -32<=l<=8	
Reflections collected	6731	
Independent reflections	3723 [R(int) = 0.0731]	
Completeness to theta = 25.00°	94.9 %	
Absorption correction	Sadabs, (Sheldrick 2001)	
Max. and min. transmission	0.9839 and 0.9328	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3723 / 6 / 298	
Goodness-of-fit on F^2	1.077	
Final R indices [I>2sigma(I)]	R1 = 0.0838, wR2 = 0.1564	
R indices (all data)	R1 = 0.1113, wR2 = 0.1758	
Absolute structure parameter	0.0(2)	
Largest diff. peak and hole	0.447 and -0.382 $e.Å^{-3}$	



ORTEP diagram of compound **3a** (H atoms and the minor disorder components are omitted). Thermal ellipsoids are drawn at the 40% probability.

Table 1. Crystal data and structure refinement for 6150 (compound **3a**).

Identification code	6150	
Empirical formula	C30 H32 Cl3 Cr N2 P2 S	
Formula weight	672.93	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.3331(13) Å	= 90°.
	b = 16.3009(19) Å	= 99.248(4)°.
	c = 17.286(2) Å	= 90°.
Volume	3151.8(6) $Å^3$	
Z	4	
Density (calculated)	1.418 Mg/m^3	
Absorption coefficient	0.808 mm^{-1}	
F(000)	1388	
Crystal size	0.10 x 0.08 x 0.02 mm^3	
Theta range for data collection	1.73 to 25.00°.	
Index ranges	-12<=h<=13, -19<=k<=17, -20<=l<=20	
Reflections collected	18076	
Independent reflections	5559 [R(int) = 0.1524]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	None	
Max. and min. transmission	0.9840 and 0.9235	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5559 / 22 / 373	
Goodness-of-fit on F^2	1.094	
Final R indices [I>2sigma(I)]	R1 = 0.1172, wR2 = 0.1964	
R indices (all data)	R1 = 0.1918, wR2 = 0.2264	
Largest diff. peak and hole	0.610 and -0.498 $e.Å^{-3}$	



ORTEP diagram of compound **3b**(Thermal ellipsoids are drawn at the 40% probability)

Table 1. Crystal data and structure refinement for 6246 (compound **3b**).

Identification code	6246	
Empirical formula	C31 H34 Cl3 Cr N2 P2 S	
Formula weight	686.95	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 11.213(2) Å	= 90°.
	b = 16.453(3) Å	= 90°.
	c = 34.766(7) Å	= 90°.
Volume	6414(2) $Å^3$	
Z	8	
Density (calculated)	1.423 Mg/m^3	
Absorption coefficient	0.796 mm^{-1}	
F(000)	2840	
Crystal size	0.18 x 0.06 x 0.02 mm^3	
Theta range for data collection	2.16 to 25.00°.	
Index ranges	-13<=h<=13, -19<=k<=15, -41<=l<=41	
Reflections collected	35350	
Independent reflections	5646 [R(int) = 0.1304]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Sadabs, (sheldrick 2001)	
Max. and min. transmission	0.9843 and 0.8700	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5646 / 0 / 363	
Goodness-of-fit on F^2	1.112	
Final R indices [I>2sigma(I)]	R1 = 0.0713, wR2 = 0.1314	
R indices (all data)	R1 = 0.1024, wR2 = 0.1432	
Largest diff. peak and hole	0.401 and -0.445 $e.Å^{-3}$	