

Complex 1a

Table 1. Crystal data and structure refinement for 1a.

Identification code	sg411
Empirical formula	C20 H44 Cr
Formula weight	336.55
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pbc _a
Unit cell dimensions	a = 15.7617(18) Å alpha = 90 deg. b = 15.8066(18) Å beta = 90 deg. c = 17.8368(19) Å gamma = 90 deg.
Volume	4443.8(9) Å ³
Z, Calculated density	8, 1.006 Mg/m ³
Absorption coefficient	0.511 mm ⁻¹
F(000)	1504
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	2.15 to 28.76 deg.
Limiting indices	0 ≤ h ≤ 21, 0 ≤ k ≤ 21, 0 ≤ l ≤ 20
Reflections collected / unique	34844 / 4971 [R(int) = 0.0859]
Completeness to theta = 28.76	86.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928078 and 0.781909
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4971 / 0 / 238
Goodness-of-fit on F ²	1.085
Final R indices [I > 2σ(I)]	R1 = 0.0873, wR2 = 0.2965
R indices (all data)	R1 = 0.1461, wR2 = 0.3154
Largest diff. peak and hole	0.636 and -0.777 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cr	3731(1)	1261(1)	6288(1)	26(1)
C(1)	2738(8)	888(8)	5656(7)	31(2)
C(2)	2587(4)	184(4)	5144(4)	31(1)
C(3)	2606(9)	-669(9)	5588(8)	39(2)
C(4)	1754(9)	271(10)	4704(8)	48(3)
C(5)	3295(10)	152(10)	4532(9)	50(3)
C(1')	3314(8)	281(8)	5649(7)	31(2)
C(2')	2587(4)	184(4)	5144(4)	31(1)
C(3')	1735(8)	206(9)	5605(8)	39(2)
C(4')	2620(10)	-660(10)	4680(9)	48(3)
C(5')	2518(10)	946(10)	4589(9)	50(3)
C(6)	3345(8)	2270(9)	6867(8)	37(2)
C(7)	2635(4)	2412(4)	7404(4)	36(2)
C(8)	2506(10)	1618(11)	7958(9)	51(3)
C(9)	1722(9)	2416(9)	6938(8)	44(2)
C(10)	2691(12)	3196(11)	7851(10)	63(3)
C(6')	2746(9)	1651(8)	6879(8)	37(2)
C(7')	2635(4)	2412(4)	7404(4)	36(2)
C(8')	3512(10)	2550(10)	7850(9)	51(3)
C(9')	2590(9)	3235(9)	6924(8)	44(2)
C(10')	1939(11)	2347(11)	7955(10)	63(3)
C(11)	4733(8)	1642(8)	5686(8)	39(2)
C(12)	4863(4)	2398(4)	5189(4)	31(1)
C(13)	4040(10)	2542(9)	4690(8)	48(3)
C(14)	4907(10)	3197(9)	5682(9)	50(3)
C(15)	5678(9)	2303(9)	4697(9)	48(3)
C(11')	4132(8)	2245(9)	5721(8)	39(2)
C(12')	4863(4)	2398(4)	5189(4)	31(1)
C(13')	4934(10)	1663(9)	4613(8)	48(3)
C(14')	5731(9)	2397(10)	5648(9)	50(3)
C(15')	4766(10)	3235(9)	4759(9)	48(3)
C(16)	4109(8)	280(8)	6898(7)	31(2)
C(17)	4817(4)	142(4)	7436(3)	30(1)
C(18)	4911(9)	936(9)	7949(8)	43(2)
C(19)	5681(8)	113(9)	6976(8)	40(2)
C(20)	4737(10)	-639(10)	7890(10)	56(3)
C(16')	4698(8)	823(8)	6927(7)	31(2)
C(17')	4817(4)	142(4)	7436(3)	30(1)
C(18')	4055(9)	33(10)	7975(8)	43(2)
C(19')	4802(9)	-748(8)	6999(8)	40(2)
C(20')	5608(10)	187(11)	7927(9)	56(3)

Table 3. Bond lengths [Å] and angles [deg] for 1a.

Cr-C(11')	1.961(13)
Cr-C(6')	1.976(13)
Cr-C(16)	1.986(12)
Cr-C(6)	1.996(13)
Cr-C(11)	2.002(13)
Cr-C(1)	2.016(12)
Cr-C(16')	2.025(12)
Cr-C(1')	2.031(12)
C(1)-C(2)	1.459(13)
C(2)-C(4)	1.536(15)
C(2)-C(5)	1.562(16)
C(2)-C(3)	1.564(15)
C(6)-C(7)	1.489(14)
C(7)-C(10)	1.477(17)
C(7)-C(8)	1.611(17)
C(7)-C(9)	1.661(16)
C(11)-C(12)	1.503(14)
C(12)-C(14)	1.541(16)
C(12)-C(15)	1.563(15)
C(12)-C(13)	1.590(16)
C(16)-C(17)	1.488(13)
C(17)-C(20)	1.482(16)
C(17)-C(18)	1.561(15)
C(17)-C(19)	1.590(14)
C(11')-Cr-C(6')	106.3(6)
C(11')-Cr-C(16)	143.7(5)
C(6')-Cr-C(16)	100.7(6)
C(11')-Cr-C(6)	74.4(6)
C(6')-Cr-C(6)	40.0(5)
C(16)-Cr-C(6)	115.5(5)
C(11')-Cr-C(11)	39.7(5)
C(6')-Cr-C(11)	144.3(5)
C(16)-Cr-C(11)	107.0(5)
C(6)-Cr-C(11)	106.1(5)
C(11')-Cr-C(1)	101.2(5)
C(6')-Cr-C(1)	77.3(5)
C(16)-Cr-C(1)	108.1(5)
C(6)-Cr-C(1)	106.6(5)
C(11)-Cr-C(1)	113.6(5)
C(11')-Cr-C(16')	108.6(5)
C(6')-Cr-C(16')	113.4(5)
C(16)-Cr-C(16')	36.7(5)
C(6)-Cr-C(16')	102.2(5)
C(11)-Cr-C(16')	79.1(5)
C(1)-Cr-C(16')	143.0(5)
C(11')-Cr-C(1')	114.9(5)
C(6')-Cr-C(1')	106.4(5)
C(16)-Cr-C(1')	79.0(5)
C(6)-Cr-C(1')	143.2(5)
C(11)-Cr-C(1')	100.6(5)
C(1)-Cr-C(1')	38.1(5)
C(16')-Cr-C(1')	107.4(5)

C(2) - C(1) - Cr	134.4 (8)
C(1) - C(2) - C(4)	113.1 (9)
C(1) - C(2) - C(5)	110.2 (9)
C(4) - C(2) - C(5)	104.8 (9)
C(1) - C(2) - C(3)	109.7 (8)
C(4) - C(2) - C(3)	110.7 (9)
C(5) - C(2) - C(3)	108.2 (9)
C(7) - C(6) - Cr	133.1 (9)
C(10) - C(7) - C(6)	115.4 (10)
C(10) - C(7) - C(8)	109.3 (10)
C(6) - C(7) - C(8)	111.8 (9)
C(10) - C(7) - C(9)	108.7 (10)
C(6) - C(7) - C(9)	109.2 (8)
C(8) - C(7) - C(9)	101.6 (9)
C(12) - C(11) - Cr	131.6 (8)
C(11) - C(12) - C(14)	108.8 (9)
C(11) - C(12) - C(15)	111.5 (8)
C(14) - C(12) - C(15)	111.3 (9)
C(11) - C(12) - C(13)	109.5 (8)
C(14) - C(12) - C(13)	103.9 (9)
C(15) - C(12) - C(13)	111.7 (9)
C(17) - C(16) - Cr	133.9 (8)
C(20) - C(17) - C(16)	114.2 (9)
C(20) - C(17) - C(18)	111.0 (9)
C(16) - C(17) - C(18)	109.3 (8)
C(20) - C(17) - C(19)	109.3 (9)
C(16) - C(17) - C(19)	108.3 (8)
C(18) - C(17) - C(19)	104.1 (8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1a.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cr	27(1)	27(1)	25(1)	0(1)	-1(1)	0(1)
C(1)	32(4)	31(4)	29(5)	-1(4)	-1(4)	-6(4)
C(2)	34(3)	30(3)	29(3)	4(3)	-1(2)	0(2)
C(3)	36(5)	43(5)	39(5)	-1(4)	-1(4)	-2(4)
C(4)	45(6)	51(6)	47(6)	-7(5)	-7(5)	-3(5)
C(5)	50(6)	50(6)	50(7)	8(5)	-3(5)	-8(5)
C(1')	32(4)	31(4)	29(5)	-1(4)	-1(4)	-6(4)
C(2')	34(3)	30(3)	29(3)	4(3)	-1(2)	0(2)
C(3')	36(5)	43(5)	39(5)	-1(4)	-1(4)	-2(4)
C(4')	45(6)	51(6)	47(6)	-7(5)	-7(5)	-3(5)
C(5')	50(6)	50(6)	50(7)	8(5)	-3(5)	-8(5)
C(6)	34(5)	38(5)	41(5)	-2(4)	2(4)	-4(4)
C(7)	41(4)	34(4)	33(4)	-2(3)	7(3)	4(3)
C(8)	47(6)	57(7)	49(7)	-1(5)	1(5)	5(5)
C(9)	47(6)	43(5)	42(6)	-1(5)	4(5)	8(4)
C(10)	67(8)	58(7)	63(8)	-19(6)	13(7)	-3(6)
C(6')	34(5)	38(5)	41(5)	-2(4)	2(4)	-4(4)
C(7')	41(4)	34(4)	33(4)	-2(3)	7(3)	4(3)
C(8')	47(6)	57(7)	49(7)	-1(5)	1(5)	5(5)
C(9')	47(6)	43(5)	42(6)	-1(5)	4(5)	8(4)
C(10')	67(8)	58(7)	63(8)	-19(6)	13(7)	-3(6)
C(11)	37(5)	37(5)	42(5)	4(4)	3(4)	0(4)
C(12)	28(3)	34(3)	30(3)	2(3)	3(3)	1(2)
C(13)	52(6)	46(6)	45(6)	7(5)	-4(5)	3(5)
C(14)	44(6)	48(6)	58(7)	3(5)	7(5)	-4(5)
C(15)	48(6)	41(5)	56(7)	0(5)	13(5)	2(5)
C(11')	37(5)	37(5)	42(5)	4(4)	3(4)	0(4)
C(12')	28(3)	34(3)	30(3)	2(3)	3(3)	1(2)
C(13')	52(6)	46(6)	45(6)	7(5)	-4(5)	3(5)
C(14')	44(6)	48(6)	58(7)	3(5)	7(5)	-4(5)
C(15')	48(6)	41(5)	56(7)	0(5)	13(5)	2(5)
C(16)	32(4)	32(4)	30(5)	1(4)	-5(4)	-1(3)
C(17)	31(3)	33(3)	24(3)	2(2)	1(2)	4(3)
C(18)	42(5)	48(5)	41(6)	-5(5)	4(4)	5(4)
C(19)	40(5)	35(5)	46(6)	1(4)	2(4)	6(4)
C(20)	50(6)	55(7)	63(8)	14(6)	-5(6)	3(5)
C(16')	32(4)	32(4)	30(5)	1(4)	-5(4)	-1(3)
C(17')	31(3)	33(3)	24(3)	2(2)	1(2)	4(3)
C(18')	42(5)	48(5)	41(6)	-5(5)	4(4)	5(4)
C(19')	40(5)	35(5)	46(6)	1(4)	2(4)	6(4)
C(20')	50(6)	55(7)	63(8)	14(6)	-5(6)	3(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1a.

	x	y	z	U(eq)
H(1A)	2272	844	6017	37
H(1B)	2609	1388	5351	37
H(3A)	2167	-664	5969	59
H(3B)	3156	-737	5825	59
H(3C)	2508	-1136	5246	59
H(4A)	1280	284	5051	72
H(4B)	1691	-207	4368	72
H(4C)	1764	791	4415	72
H(5A)	3298	679	4254	75
H(5B)	3184	-314	4191	75
H(5C)	3842	69	4770	75
H(1'A)	3804	134	5337	37
H(1'B)	3253	-187	6006	37
H(3'A)	1737	-248	5971	59
H(3'B)	1259	133	5267	59
H(3'C)	1686	745	5861	59
H(4'A)	2642	-1138	5020	72
H(4'B)	3122	-661	4365	72
H(4'C)	2118	-702	4368	72
H(5'A)	3025	971	4282	75
H(5'B)	2461	1467	4871	75
H(5'C)	2025	871	4270	75
H(6A)	3850	2445	7146	45
H(6B)	3260	2706	6483	45
H(8A)	3010	1546	8264	77
H(8B)	2411	1110	7665	77
H(8C)	2020	1719	8279	77
H(9A)	1732	2862	6564	66
H(9B)	1259	2515	7285	66
H(9C)	1644	1874	6692	66
H(10A)	2770	3676	7519	94
H(10B)	3169	3158	8193	94
H(10C)	2172	3270	8136	94
H(6'A)	2289	1711	6510	45
H(6'B)	2590	1161	7187	45
H(8'A)	3618	2066	8172	77
H(8'B)	3473	3058	8154	77
H(8'C)	3974	2609	7494	77
H(9'A)	2088	3219	6609	66
H(9'B)	3092	3276	6611	66
H(9'C)	2561	3723	7252	66
H(10D)	1407	2257	7694	94
H(10E)	1907	2866	8244	94
H(10F)	2047	1875	8289	94
H(11A)	5196	1675	6051	46
H(11B)	4867	1157	5365	46
H(13A)	3962	2062	4358	71
H(13B)	4109	3052	4394	71

H(13C)	3548	2600	5012	71
H(14A)	5381	3150	6027	75
H(14B)	4384	3254	5964	75
H(14C)	4985	3691	5366	75
H(15A)	5631	1798	4391	72
H(15B)	6171	2258	5019	72
H(15C)	5736	2794	4375	72
H(11C)	3633	2420	5432	46
H(11D)	4206	2682	6105	46
H(13D)	4418	1633	4318	71
H(13E)	5017	1133	4877	71
H(13F)	5413	1764	4283	71
H(14D)	5713	2835	6029	75
H(14E)	6200	2504	5309	75
H(14F)	5808	1850	5886	75
H(15D)	4231	3233	4489	72
H(15E)	5230	3295	4406	72
H(15F)	4774	3703	5110	72
H(16A)	3602	126	7186	37
H(16B)	4182	-173	6529	37
H(18A)	4400	1007	8245	65
H(18B)	4999	1434	7641	65
H(18C)	5394	861	8280	65
H(19A)	5675	-368	6639	61
H(19B)	6154	60	7321	61
H(19C)	5742	630	6688	61
H(20A)	4681	-1123	7559	84
H(20B)	4239	-599	8207	84
H(20C)	5238	-707	8200	84
H(16C)	5158	744	6564	37
H(16D)	4862	1319	7222	37
H(18D)	3994	537	8280	65
H(18E)	4152	-452	8297	65
H(18F)	3541	-55	7686	65
H(19D)	5257	-761	6633	61
H(19E)	4261	-814	6746	61
H(19F)	4878	-1205	7355	61
H(20D)	5616	722	8194	84
H(20E)	6110	142	7615	84
H(20F)	5601	-275	8285	84

Complex **1b**

Table 6. Crystal data and structure refinement for 1b.

Identification code	sg412
Empirical formula	C16 H44 Cr Si4
Formula weight	400.87
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 18.7133(18) Å alpha = 90 deg. b = 8.3575(8) Å beta = 116.2890(10) deg. c = 18.7599(18) Å gamma = 90 deg.
Volume	2630.5(4) Å ³
Z, Calculated density	4, 1.012 Mg/m ³
Absorption coefficient	0.613 mm ⁻¹
F(000)	880
Crystal size	0.18 x 0.15 x 0.03 mm
Theta range for data collection	2.42 to 25.00 deg.
Limiting indices	-22<=h<=19, 0<=k<=9, 0<=l<=22
Reflections collected / unique	7547 / 2313 [R(int) = 0.0921]
Completeness to theta = 25.00	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928076 and 0.649701
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2313 / 0 / 168
Goodness-of-fit on F ²	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0904, wR2 = 0.2388
R indices (all data)	R1 = 0.0972, wR2 = 0.2420
Largest diff. peak and hole	0.388 and -0.412 e.Å ⁻³

Table 7. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1b**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cr	0	9857(2)	2500	33(1)
Si(1)	-565(1)	7675(3)	804(1)	52(1)
Si(2)	1697(1)	12076(3)	3041(1)	43(1)
C(1)	-439(9)	7974(17)	1830(8)	36(3)
C(2)	452(11)	7490(20)	809(11)	62(5)
C(3)	-1047(12)	9600(30)	197(11)	72(6)
C(4)	-1164(12)	5900(30)	248(13)	74(6)
C(5)	1050(8)	10350(17)	2545(8)	38(3)
C(6)	1749(10)	12370(20)	4053(10)	52(4)
C(7)	1255(10)	13980(20)	2488(10)	54(4)
C(8)	2695(12)	11940(20)	3137(13)	74(6)
C(1')	-82(10)	9380(20)	1444(10)	54(4)
C(2')	8(11)	5820(20)	1218(11)	65(5)
C(3')	-1563(10)	7360(20)	847(11)	54(4)
C(4')	-728(15)	7720(30)	-271(15)	98(8)
C(5')	670(8)	11798(16)	2897(8)	37(3)
C(6')	2351(10)	10400(20)	3619(11)	57(4)
C(7')	1755(11)	12040(20)	2056(11)	63(5)
C(8')	2153(12)	13950(30)	3589(12)	71(5)

Table 8. Bond lengths [Å] and angles [deg] for 1b.

Cr-C(1)	1.954 (14)
Cr-C(1)#1	1.954 (14)
Cr-C(1')	1.958 (16)
Cr-C(1')#1	1.958 (16)
Cr-C(5)#1	1.972 (14)
Cr-C(5)	1.972 (14)
Cr-C(5')	1.983 (14)
Cr-C(5')#1	1.983 (14)
Si(1)-C(1')	1.827 (18)
Si(1)-C(2')	1.85 (2)
Si(1)-C(1)	1.851 (13)
Si(1)-C(4)	1.88 (2)
Si(1)-C(4')	1.90 (3)
Si(1)-C(2)	1.905 (17)
Si(1)-C(3')	1.924 (17)
Si(1)-C(3)	1.95 (2)
Si(2)-C(8)	1.80 (2)
Si(2)-C(5')	1.834 (14)
Si(2)-C(5)	1.848 (14)
Si(2)-C(6')	1.860 (18)
Si(2)-C(8')	1.86 (2)
Si(2)-C(6)	1.874 (16)
Si(2)-C(7)	1.881 (17)
Si(2)-C(7')	1.898 (18)
C(1)-Cr-C(1)#1	72.7 (8)
C(1)-Cr-C(1')	50.6 (6)
C(1)#1-Cr-C(1')	108.1 (7)
C(1)-Cr-C(1')#1	108.1 (7)
C(1)#1-Cr-C(1')#1	50.6 (6)
C(1')-Cr-C(1')#1	156.7 (11)
C(1)-Cr-C(5)#1	90.8 (6)
C(1)#1-Cr-C(5)#1	108.9 (6)
C(1')-Cr-C(5)#1	111.6 (6)
C(1')#1-Cr-C(5)#1	73.5 (6)
C(1)-Cr-C(5)	108.9 (6)
C(1)#1-Cr-C(5)	90.8 (6)
C(1')-Cr-C(5)	73.5 (6)
C(1')#1-Cr-C(5)	111.6 (6)
C(5)#1-Cr-C(5)	155.9 (9)
C(1)-Cr-C(5')	156.5 (6)
C(1)#1-Cr-C(5')	113.7 (6)
C(1')-Cr-C(5')	107.4 (7)
C(1')#1-Cr-C(5')	91.8 (7)
C(5)#1-Cr-C(5')	107.3 (6)
C(5)-Cr-C(5')	50.3 (6)
C(1)-Cr-C(5')#1	113.7 (6)
C(1)#1-Cr-C(5')#1	156.5 (6)
C(1')-Cr-C(5')#1	91.8 (7)
C(1')#1-Cr-C(5')#1	107.4 (7)
C(5)#1-Cr-C(5')#1	50.3 (6)
C(5)-Cr-C(5')#1	107.3 (6)
C(5')-Cr-C(5')#1	70.2 (8)

C(1')-Si(1)-C(2')	110.7(8)
C(1')-Si(1)-C(1)	54.0(7)
C(2')-Si(1)-C(1)	83.8(7)
C(1')-Si(1)-C(4)	169.9(8)
C(2')-Si(1)-C(4)	70.3(9)
C(1)-Si(1)-C(4)	117.0(8)
C(1')-Si(1)-C(4')	118.9(9)
C(2')-Si(1)-C(4')	104.7(10)
C(1)-Si(1)-C(4')	171.0(9)
C(4)-Si(1)-C(4')	69.5(10)
C(1')-Si(1)-C(2)	81.8(8)
C(2')-Si(1)-C(2)	62.5(8)
C(1)-Si(1)-C(2)	109.8(7)
C(4)-Si(1)-C(2)	106.8(9)
C(4')-Si(1)-C(2)	72.5(10)
C(1')-Si(1)-C(3')	106.7(7)
C(2')-Si(1)-C(3')	105.0(8)
C(1)-Si(1)-C(3')	69.7(7)
C(4)-Si(1)-C(3')	63.9(8)
C(4')-Si(1)-C(3')	110.1(9)
C(2)-Si(1)-C(3')	167.2(8)
C(1')-Si(1)-C(3)	72.8(8)
C(2')-Si(1)-C(3)	166.3(8)
C(1)-Si(1)-C(3)	108.0(7)
C(4)-Si(1)-C(3)	108.8(9)
C(4')-Si(1)-C(3)	63.2(10)
C(2)-Si(1)-C(3)	105.9(8)
C(3')-Si(1)-C(3)	86.1(8)
C(8)-Si(2)-C(5')	168.9(8)
C(8)-Si(2)-C(5)	114.9(8)
C(5')-Si(2)-C(5)	54.3(6)
C(8)-Si(2)-C(6')	60.6(8)
C(5')-Si(2)-C(6')	111.5(7)
C(5)-Si(2)-C(6')	79.7(7)
C(8)-Si(2)-C(8')	78.2(9)
C(5')-Si(2)-C(8')	112.5(8)
C(5)-Si(2)-C(8')	166.7(8)
C(6')-Si(2)-C(8')	106.9(9)
C(8)-Si(2)-C(6)	108.8(9)
C(5')-Si(2)-C(6)	75.3(7)
C(5)-Si(2)-C(6)	109.8(7)
C(6')-Si(2)-C(6)	77.4(8)
C(8')-Si(2)-C(6)	61.7(8)
C(8)-Si(2)-C(7)	106.9(9)
C(5')-Si(2)-C(7)	81.4(7)
C(5)-Si(2)-C(7)	110.7(7)
C(6')-Si(2)-C(7)	167.0(7)
C(8')-Si(2)-C(7)	64.7(8)
C(6)-Si(2)-C(7)	105.1(8)
C(8)-Si(2)-C(7')	65.9(9)
C(5')-Si(2)-C(7')	111.3(7)
C(5)-Si(2)-C(7')	78.8(7)
C(6')-Si(2)-C(7')	104.4(8)
C(8')-Si(2)-C(7')	109.9(9)
C(6)-Si(2)-C(7')	171.4(8)
C(7)-Si(2)-C(7')	71.2(8)
Si(1)-C(1)-Cr	127.0(8)

Si(2)-C(5)-Cr	127.1(7)
Si(1)-C(1')-Cr	128.1(9)
Si(2)-C(5')-Cr	127.3(7)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 9. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for 1b.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cr	33(1)	33(1)	33(1)	0	15(1)	0
Si(1)	51(1)	57(2)	44(1)	-6(1)	18(1)	0(1)
Si(2)	39(1)	44(1)	42(1)	0(1)	16(1)	-1(1)
C(1)	44(8)	34(8)	33(7)	1(6)	19(6)	1(6)
C(2)	62(11)	69(12)	63(11)	1(9)	33(9)	9(9)
C(3)	71(12)	89(15)	62(11)	-16(11)	36(10)	-8(11)
C(4)	74(13)	70(14)	80(14)	-1(11)	36(11)	-3(11)
C(5)	44(8)	36(8)	36(7)	-4(6)	21(6)	2(6)
C(6)	59(10)	47(9)	55(10)	-1(8)	29(8)	0(8)
C(7)	51(9)	55(10)	53(10)	1(8)	22(8)	5(8)
C(8)	75(13)	56(12)	80(14)	3(11)	25(11)	2(10)
C(1')	50(9)	63(11)	50(9)	6(8)	21(8)	-2(8)
C(2')	58(11)	70(13)	67(12)	-11(10)	28(9)	-5(10)
C(3')	57(10)	44(9)	60(10)	1(8)	25(8)	6(8)
C(4')	101(18)	79(17)	103(19)	5(14)	35(15)	-19(14)
C(5')	38(7)	29(7)	38(7)	0(6)	13(6)	6(6)
C(6')	48(9)	59(11)	71(11)	3(9)	33(9)	-4(8)
C(7')	63(11)	66(12)	56(11)	-11(9)	23(9)	-13(10)
C(8')	68(12)	79(14)	68(12)	0(11)	31(10)	5(11)

Table 10. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1b**.

	x	y	z	U(eq)
H(1A)	-116	7070	2137	44
H(1B)	-970	7819	1802	44
H(2A)	727	6560	1117	93
H(2B)	764	8443	1045	93
H(2C)	384	7376	268	93
H(3A)	-1574	9745	166	108
H(3B)	-1089	9497	-335	108
H(3C)	-718	10519	458	108
H(4A)	-930	4931	546	111
H(4B)	-1166	5837	-269	111
H(4C)	-1707	6006	180	111
H(5A)	1378	9399	2776	45
H(5B)	962	10395	1991	45
H(6A)	1214	12499	4006	78
H(6B)	2061	13316	4297	78
H(6C)	1997	11442	4381	78
H(7A)	1219	13917	1957	81
H(7B)	1592	14878	2768	81
H(7C)	727	14134	2454	81
H(8A)	2675	11800	2615	111
H(8B)	2965	11035	3471	111
H(8C)	2983	12916	3376	111
H(1'A)	-332	10331	1122	65
H(1'B)	469	9373	1512	65
H(2'A)	526	5905	1221	97
H(2'B)	-278	4916	893	97
H(2'C)	76	5667	1757	97
H(3'A)	-1898	8290	633	81
H(3'B)	-1466	7196	1394	81
H(3'C)	-1828	6422	535	81
H(4'A)	-225	7924	-287	148
H(4'B)	-1104	8561	-555	148
H(4'C)	-939	6697	-519	148
H(5'A)	363	12665	2542	44
H(5'B)	682	12029	3415	44
H(6'A)	2339	10313	4128	85
H(6'B)	2893	10604	3703	85
H(6'C)	2163	9408	3326	85
H(7'A)	1423	12885	1716	95
H(7'B)	1568	11013	1800	95
H(7'C)	2302	12203	2149	95
H(8'A)	2110	13976	4085	107
H(8'B)	1877	14869	3268	107
H(8'C)	2711	13993	3700	107

Complex 2b

Table 15. Crystal data and structure refinement for 2b.

Identification code	sg415
Empirical formula	C ₃₂ H ₈₈ Cr ₄ Si ₈
Formula weight	905.74
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 17.0805(16) Å alpha = 90 deg. b = 13.4843(13) Å beta = 99.603(2) deg. c = 22.873(2) Å gamma = 90 deg.
Volume	5194.3(8) Å ³
Z, Calculated density	4, 1.158 Mg/m ³
Absorption coefficient	1.018 mm ⁻¹
F(000)	1952
Crystal size	0.10 x 0.10 x 0.02 mm
Theta range for data collection	1.38 to 26.37 deg.
Limiting indices	-21<=h<=21, 0<=k<=16, 0<=l<=28
Reflections collected / unique	46760 / 10605 [R(int) = 0.1157]
Completeness to theta = 26.37	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.928077 and 0.809644
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10605 / 0 / 397
Goodness-of-fit on F ²	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1153
R indices (all data)	R1 = 0.1292, wR2 = 0.1429
Largest diff. peak and hole	0.677 and -0.452 e.Å ⁻³

Table 12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2b**.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cr(1)	5638(1)	6401(1)	2432(1)	25(1)
Cr(2)	5357(1)	7121(1)	3300(1)	25(1)
Cr(3)	4407(1)	8195(1)	2722(1)	26(1)
Cr(4)	4681(1)	7465(1)	1850(1)	27(1)
Si(1)	4066(1)	5568(1)	1001(1)	44(1)
C(1)	4605(3)	5837(3)	1758(2)	31(1)
C(2)	4229(4)	4242(5)	799(3)	69(2)
C(3)	4378(4)	6403(5)	427(2)	66(2)
C(4)	2967(3)	5702(6)	963(3)	70(2)
Si(2)	6755(1)	6612(1)	1396(1)	42(1)
C(5)	5970(3)	7295(3)	1715(2)	33(1)
C(6)	7707(3)	6485(4)	1940(2)	48(1)
C(7)	6449(4)	5335(4)	1141(3)	67(2)
C(8)	6970(4)	7309(5)	730(3)	66(2)
Si(3)	7267(1)	7044(1)	3872(1)	45(1)
C(9)	6582(3)	7077(3)	3143(2)	31(1)
C(10)	7171(3)	8168(4)	4331(3)	63(2)
C(11)	7102(4)	5940(5)	4330(2)	68(2)
C(12)	8320(3)	7001(6)	3730(3)	79(2)
Si(4)	5844(1)	4256(1)	3068(1)	36(1)
C(13)	5332(3)	5462(3)	3140(2)	30(1)
C(14)	5869(3)	3526(4)	3768(2)	46(1)
C(15)	6884(3)	4386(4)	2919(3)	59(2)
C(16)	5293(3)	3503(4)	2447(2)	52(2)
Si(5)	4140(1)	6826(1)	4239(1)	40(1)
C(17)	4115(3)	7185(3)	3448(2)	31(1)
C(18)	4129(4)	5444(4)	4316(2)	61(2)
C(19)	5034(4)	7305(5)	4739(2)	60(2)
C(20)	3244(4)	7301(5)	4506(3)	64(2)
Si(6)	5032(1)	10001(1)	3659(1)	39(1)
C(21)	5371(3)	8795(3)	3379(2)	30(1)
C(22)	5818(4)	10465(4)	4272(2)	61(2)
C(23)	4096(4)	9865(4)	3970(3)	67(2)
C(24)	4882(3)	10974(4)	3070(2)	51(2)
Si(7)	4594(1)	9708(1)	1227(1)	44(1)
C(25)	4775(3)	9083(3)	1967(2)	32(1)
C(26)	4491(4)	11074(4)	1324(3)	66(2)
C(27)	3655(4)	9286(5)	741(3)	80(2)
C(28)	5440(4)	9479(5)	822(3)	66(2)
Si(8)	2514(1)	8288(1)	2153(1)	46(1)
C(29)	3438(3)	7613(4)	2062(2)	35(1)
C(30)	1721(3)	8032(5)	1500(3)	65(2)
C(31)	2648(4)	9673(4)	2218(3)	75(2)
C(32)	2117(3)	7833(6)	2823(3)	79(2)

Table 13. Bond lengths [Å] and angles [deg] for 2b.

Cr(1)-C(5)	2.184(4)
Cr(1)-C(13)	2.188(4)
Cr(1)-Cr(2)	2.3310(10)
Cr(1)-Cr(4)	2.4026(10)
Cr(2)-C(9)	2.183(4)
Cr(2)-C(17)	2.205(4)
Cr(2)-Cr(3)	2.4004(10)
Cr(3)-C(29)	2.192(5)
Cr(3)-C(21)	2.191(4)
Cr(3)-Cr(4)	2.3396(10)
Cr(4)-C(25)	2.200(5)
Cr(4)-C(1)	2.207(5)
Si(1)-C(1)	1.856(5)
Si(1)-C(4)	1.872(6)
Si(1)-C(3)	1.873(6)
Si(1)-C(2)	1.880(6)
Si(2)-C(7)	1.865(6)
Si(2)-C(8)	1.878(6)
Si(2)-C(5)	1.871(5)
Si(2)-C(6)	1.884(5)
Si(3)-C(10)	1.867(6)
Si(3)-C(11)	1.869(6)
Si(3)-C(12)	1.880(6)
Si(3)-C(9)	1.870(5)
Si(4)-C(14)	1.872(5)
Si(4)-C(15)	1.871(6)
Si(4)-C(16)	1.868(5)
Si(4)-C(13)	1.868(5)
Si(5)-C(20)	1.854(6)
Si(5)-C(19)	1.863(6)
Si(5)-C(18)	1.872(5)
Si(5)-C(17)	1.867(5)
Si(6)-C(23)	1.863(6)
Si(6)-C(24)	1.868(5)
Si(6)-C(22)	1.879(6)
Si(6)-C(21)	1.875(4)
Si(7)-C(28)	1.868(6)
Si(7)-C(26)	1.867(6)
Si(7)-C(27)	1.881(6)
Si(7)-C(25)	1.871(4)
Si(8)-C(30)	1.874(6)
Si(8)-C(32)	1.878(6)
Si(8)-C(29)	1.863(5)
Si(8)-C(31)	1.885(6)
C(5)-Cr(1)-C(13)	177.91(17)
C(5)-Cr(1)-Cr(2)	121.74(13)
C(13)-Cr(1)-Cr(2)	60.09(12)
C(5)-Cr(1)-Cr(4)	59.51(13)
C(13)-Cr(1)-Cr(4)	122.08(13)
Cr(2)-Cr(1)-Cr(4)	90.30(3)
C(9)-Cr(2)-C(17)	179.08(18)
C(9)-Cr(2)-Cr(1)	60.59(12)

C(17)-Cr(2)-Cr(1)	119.19(13)
C(9)-Cr(2)-Cr(3)	120.26(12)
C(17)-Cr(2)-Cr(3)	58.82(12)
Cr(1)-Cr(2)-Cr(3)	89.90(3)
C(29)-Cr(3)-C(21)	179.34(18)
C(29)-Cr(3)-Cr(4)	59.87(12)
C(21)-Cr(3)-Cr(4)	120.41(13)
C(29)-Cr(3)-Cr(2)	121.78(13)
C(21)-Cr(3)-Cr(2)	58.88(11)
Cr(4)-Cr(3)-Cr(2)	90.15(3)
C(25)-Cr(4)-C(1)	178.40(17)
C(25)-Cr(4)-Cr(3)	59.99(12)
C(1)-Cr(4)-Cr(3)	118.86(12)
C(25)-Cr(4)-Cr(1)	119.70(12)
C(1)-Cr(4)-Cr(1)	58.86(12)
Cr(3)-Cr(4)-Cr(1)	89.65(3)
C(1)-Si(1)-C(4)	111.2(2)
C(1)-Si(1)-C(3)	112.4(2)
C(4)-Si(1)-C(3)	108.1(3)
C(1)-Si(1)-C(2)	110.2(3)
C(4)-Si(1)-C(2)	105.6(3)
C(3)-Si(1)-C(2)	109.1(3)
Si(1)-C(1)-Cr(4)	107.2(2)
C(7)-Si(2)-C(8)	106.9(3)
C(7)-Si(2)-C(5)	113.3(2)
C(8)-Si(2)-C(5)	108.7(3)
C(7)-Si(2)-C(6)	106.7(3)
C(8)-Si(2)-C(6)	108.4(3)
C(5)-Si(2)-C(6)	112.6(2)
Si(2)-C(5)-Cr(1)	108.3(2)
C(10)-Si(3)-C(11)	107.2(3)
C(10)-Si(3)-C(12)	107.4(3)
C(11)-Si(3)-C(12)	108.0(3)
C(10)-Si(3)-C(9)	112.4(2)
C(11)-Si(3)-C(9)	112.9(2)
C(12)-Si(3)-C(9)	108.7(3)
Si(3)-C(9)-Cr(2)	109.1(2)
C(14)-Si(4)-C(15)	108.6(3)
C(14)-Si(4)-C(16)	107.5(2)
C(15)-Si(4)-C(16)	106.6(3)
C(14)-Si(4)-C(13)	109.1(2)
C(15)-Si(4)-C(13)	114.0(2)
C(16)-Si(4)-C(13)	110.8(2)
Si(4)-C(13)-Cr(1)	105.4(2)
C(20)-Si(5)-C(19)	108.4(3)
C(20)-Si(5)-C(18)	107.0(3)
C(19)-Si(5)-C(18)	107.9(3)
C(20)-Si(5)-C(17)	110.0(2)
C(19)-Si(5)-C(17)	112.8(2)
C(18)-Si(5)-C(17)	110.5(2)
Si(5)-C(17)-Cr(2)	105.8(2)
C(23)-Si(6)-C(24)	108.8(3)
C(23)-Si(6)-C(22)	107.5(3)
C(24)-Si(6)-C(22)	107.4(3)
C(23)-Si(6)-C(21)	112.2(2)
C(24)-Si(6)-C(21)	112.1(2)
C(22)-Si(6)-C(21)	108.7(2)

Si (6) -C (21) -Cr (3)	108.4 (2)
C (28) -Si (7) -C (26)	108.6 (3)
C (28) -Si (7) -C (27)	108.1 (3)
C (26) -Si (7) -C (27)	106.3 (3)
C (28) -Si (7) -C (25)	110.5 (2)
C (26) -Si (7) -C (25)	110.0 (2)
C (27) -Si (7) -C (25)	113.2 (3)
Si (7) -C (25) -Cr (4)	109.8 (2)
C (30) -Si (8) -C (32)	106.3 (3)
C (30) -Si (8) -C (29)	109.5 (3)
C (32) -Si (8) -C (29)	111.1 (3)
C (30) -Si (8) -C (31)	107.9 (3)
C (32) -Si (8) -C (31)	108.4 (3)
C (29) -Si (8) -C (31)	113.5 (3)
Si (8) -C (29) -Cr (3)	107.7 (2)

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2b.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cr(1)	23(1)	27(1)	27(1)	-1(1)	6(1)	-1(1)
Cr(2)	25(1)	26(1)	24(1)	1(1)	4(1)	1(1)
Cr(3)	24(1)	28(1)	26(1)	3(1)	6(1)	1(1)
Cr(4)	24(1)	32(1)	24(1)	2(1)	4(1)	-3(1)
Si(1)	40(1)	58(1)	33(1)	-8(1)	4(1)	-12(1)
C(1)	27(3)	36(3)	32(3)	-4(2)	10(2)	-1(2)
C(2)	71(5)	75(5)	59(4)	-35(4)	10(3)	-19(4)
C(3)	60(4)	104(5)	31(3)	-2(3)	3(3)	-17(4)
C(4)	40(4)	119(6)	48(4)	-16(4)	-2(3)	-21(4)
Si(2)	37(1)	50(1)	45(1)	-3(1)	20(1)	-2(1)
C(5)	29(3)	35(3)	36(3)	-3(2)	10(2)	-10(2)
C(6)	35(3)	51(3)	63(4)	0(3)	21(3)	1(3)
C(7)	57(4)	65(4)	81(5)	-30(4)	21(4)	7(3)
C(8)	60(4)	92(5)	54(4)	6(4)	39(3)	-1(4)
Si(3)	33(1)	52(1)	45(1)	-4(1)	-7(1)	0(1)
C(9)	28(3)	27(3)	36(3)	-1(2)	2(2)	-2(2)
C(10)	49(4)	71(4)	62(4)	-21(3)	-14(3)	-17(3)
C(11)	74(5)	71(4)	47(4)	10(3)	-23(3)	-2(4)
C(12)	36(4)	105(6)	88(5)	-3(4)	-14(3)	2(4)
Si(4)	42(1)	26(1)	42(1)	4(1)	12(1)	1(1)
C(13)	33(3)	32(3)	25(3)	-4(2)	4(2)	-2(2)
C(14)	58(4)	33(3)	50(3)	10(2)	13(3)	6(3)
C(15)	59(4)	33(3)	89(5)	2(3)	25(3)	6(3)
C(16)	69(4)	29(3)	62(4)	-2(3)	18(3)	-5(3)
Si(5)	45(1)	43(1)	35(1)	4(1)	17(1)	0(1)
C(17)	30(3)	29(3)	34(3)	4(2)	8(2)	2(2)
C(18)	91(5)	50(4)	49(4)	9(3)	26(3)	-10(3)
C(19)	74(4)	72(4)	33(3)	2(3)	8(3)	-6(3)
C(20)	61(4)	88(5)	48(4)	12(3)	30(3)	8(4)
Si(6)	46(1)	30(1)	42(1)	-3(1)	13(1)	3(1)
C(21)	40(3)	21(2)	31(3)	2(2)	5(2)	0(2)
C(22)	88(5)	46(4)	47(4)	-20(3)	5(3)	1(3)
C(23)	68(4)	51(4)	91(5)	-5(3)	43(4)	14(3)
C(24)	67(4)	26(3)	62(4)	1(3)	12(3)	1(3)
Si(7)	49(1)	47(1)	36(1)	13(1)	4(1)	-4(1)
C(25)	35(3)	35(3)	27(3)	5(2)	6(2)	-9(2)
C(26)	81(5)	52(4)	67(4)	28(3)	18(4)	11(3)
C(27)	77(5)	101(6)	52(4)	20(4)	-21(4)	-17(4)
C(28)	81(5)	72(4)	49(4)	25(3)	27(3)	4(4)
Si(8)	27(1)	54(1)	59(1)	7(1)	7(1)	3(1)
C(29)	29(3)	43(3)	32(3)	3(2)	5(2)	-3(2)
C(30)	33(3)	71(4)	83(5)	17(4)	-7(3)	2(3)
C(31)	56(4)	65(4)	104(6)	-8(4)	12(4)	18(3)
C(32)	35(4)	124(6)	86(5)	34(5)	30(3)	21(4)

Table 15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2b**.

	x	y	z	U(eq)
H(1A)	5138	5547	1813	37
H(1B)	4318	5556	2057	37
H(2A)	4792	4128	808	103
H(2B)	3943	4109	403	103
H(2C)	4037	3805	1080	103
H(3A)	4290	7088	527	99
H(3B)	4070	6250	42	99
H(3C)	4938	6302	415	99
H(4A)	2844	6378	1060	105
H(4B)	2788	5251	1244	105
H(4C)	2700	5545	566	105
H(5A)	5505	7406	1407	40
H(5B)	6172	7941	1868	40
H(6A)	8093	6124	1755	72
H(6B)	7606	6127	2287	72
H(6C)	7914	7139	2057	72
H(7A)	5958	5366	859	100
H(7B)	6371	4934	1478	100
H(7C)	6861	5039	952	100
H(8A)	6484	7384	446	98
H(8B)	7357	6945	549	98
H(8C)	7181	7959	852	98
H(9A)	6664	6487	2910	37
H(9B)	6693	7665	2918	37
H(10A)	7251	8758	4105	95
H(10B)	7567	8145	4688	95
H(10C)	6645	8186	4438	95
H(11A)	6559	5942	4403	102
H(11B)	7463	5967	4705	102
H(11C)	7198	5339	4120	102
H(12A)	8419	7568	3492	119
H(12B)	8402	6395	3520	119
H(12C)	8681	7016	4105	119
H(13A)	5518	5761	3529	36
H(13B)	4756	5367	3092	36
H(14A)	6155	3898	4099	70
H(14B)	6135	2898	3733	70
H(14C)	5331	3404	3833	70
H(15A)	6879	4757	2555	89
H(15B)	7108	3733	2879	89
H(15C)	7203	4735	3246	89
H(16A)	5277	3859	2076	78
H(16B)	4755	3388	2516	78
H(16C)	5560	2872	2425	78
H(17A)	3901	7856	3376	37
H(17B)	3783	6723	3183	37
H(18A)	3668	5176	4059	92
H(18B)	4106	5270	4724	92

H(18C)	4608	5169	4204	92
H(19A)	5056	8021	4704	89
H(19B)	5508	7016	4627	89
H(19C)	5005	7127	5145	89
H(20A)	2772	7058	4251	95
H(20B)	3247	8021	4499	95
H(20C)	3244	7074	4909	95
H(21A)	5505	8327	3709	36
H(21B)	5845	8901	3198	36
H(22A)	5648	11088	4422	92
H(22B)	6309	10566	4120	92
H(22C)	5903	9981	4590	92
H(23A)	3676	9627	3663	100
H(23B)	3946	10503	4113	100
H(23C)	4178	9395	4295	100
H(24A)	4474	10760	2748	77
H(24B)	5375	11079	2921	77
H(24C)	4719	11589	3234	77
H(25A)	4384	9311	2206	38
H(25B)	5305	9255	2178	38
H(26A)	4402	11393	939	100
H(26B)	4972	11333	1559	100
H(26C)	4044	11204	1525	100
H(27A)	3596	9628	364	120
H(27B)	3204	9434	934	120
H(27C)	3681	8576	676	120
H(28A)	5337	9807	439	98
H(28B)	5497	8772	764	98
H(28C)	5925	9740	1051	98
H(29A)	3555	7716	1661	42
H(29B)	3372	6900	2122	42
H(30A)	1898	8254	1140	97
H(30B)	1240	8383	1547	97
H(30D)	1615	7325	1473	97
H(31A)	2858	9919	1877	113
H(31D)	3014	9828	2577	113
H(31B)	2139	9984	2232	113
H(32D)	2047	7120	2798	119
H(32A)	1611	8148	2839	119
H(32B)	2490	7998	3178	119
