Crystal structure of 1-(anilino)-1(-phenyl methylino)pentacarbonyl chromium, (C₁₉H₁₈N₂)(Cr(CO)₅)

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Fig. 1. ORTEP plot of the molecules.

Source of material: synthesized (see ref. 1).

The bond distances and angles do not show any large deviations. The ORTEP plot of the molecule is shown in Fig. 1. The packing of the molecules down *b* shown in Fig. 2.

C₂₄H₁₈CrN₂O₅, monoclinic, *P*12₁/c1 (No. 14), *a* = 14.60(2) Å, *b* = 6.38(2) Å, *c* = 24.58(2) Å, β = 97.24(7)°, *V* = 2271.3 Å³, *Z* = 4, *R*(*F*) = 0.040, *R*_w(*F*²) = 0.120.

Fig. 2. Packing of the molecules down *b*.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow, rectangular solid, size 0.20 x 0.25 x 0.35 mm
Wavelength:	Mo K α radiation (0.71069 Å)
μ :	5.41 cm ⁻¹
Diffractometer:	Rigaku AFC7S
Scan mode:	$\omega/2\theta$
<i>T</i> _{measurement} :	293 K
2 θ _{max} :	50°
<i>N</i> (<i>hkl</i>) _{unique} :	2254
Criterion for <i>I</i> _o :	<i>I</i> _o > 2 σ (<i>I</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	290
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	4e	0.1445(4)	0.521(1)	0.2918(2)	0.066(4)	0.055(4)	0.044(4)	0.008(3)	0.008(3)	0.004(3)
C(2)	4e	0.0918(4)	0.543(1)	0.2408(3)	0.069(4)	0.069(5)	0.050(4)	0.022(3)	0.005(3)	0.025(4)
C(3)	4e	0.0847(4)	0.383(1)	0.2040(3)	0.066(4)	0.097(6)	0.044(4)	0.009(4)	-0.010(3)	0.012(4)
C(4)	4e	0.1277(4)	0.197(1)	0.2166(3)	0.072(4)	0.082(5)	0.043(4)	0.002(4)	-0.009(3)	-0.010(4)
C(5)	4e	0.1794(4)	0.169(1)	0.2672(2)	0.053(3)	0.054(4)	0.048(4)	0.012(3)	0.000(3)	0.000(3)
C(6)	4e	0.1867(3)	0.3323(9)	0.3047(2)	0.039(2)	0.052(4)	0.033(3)	0.005(2)	0.004(2)	0.005(3)
N(7)	4e	0.2455(3)	0.2977(7)	0.3560(2)	0.038(2)	0.054(3)	0.029(2)	0.008(2)	0.001(2)	0.002(2)
C(8)	4e	0.2264(3)	0.3201(8)	0.4065(2)	0.040(3)	0.032(3)	0.035(3)	0.000(2)	0.001(2)	0.004(2)
C(9)	4e	0.1305(3)	0.3911(9)	0.4116(2)	0.048(3)	0.042(3)	0.026(3)	-0.001(2)	0.002(2)	0.002(2)
C(10)	4e	0.0584(4)	0.250(1)	0.3983(2)	0.047(3)	0.054(4)	0.046(4)	-0.001(3)	0.006(2)	0.000(3)
C(11)	4e	-0.0312(4)	0.309(1)	0.4050(3)	0.041(3)	0.084(5)	0.055(4)	-0.018(3)	0.006(3)	0.006(4)

Table 2. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(12)	4e	-0.0489(4)	0.506(1)	0.4237(2)	0.043(3)	0.090(5)	0.043(4)	0.016(3)	0.013(2)	0.006(4)
C(13)	4e	0.0218(4)	0.645(1)	0.4368(2)	0.059(3)	0.059(4)	0.045(4)	0.010(3)	0.011(3)	-0.005(3)
C(14)	4e	0.1110(3)	0.5859(9)	0.4309(2)	0.046(3)	0.048(4)	0.040(3)	0.002(3)	0.002(2)	-0.001(3)
C(15)	4e	0.4183(4)	0.3496(9)	0.4453(2)	0.049(3)	0.041(3)	0.044(4)	0.004(3)	0.002(2)	-0.005(3)
O(16)	4e	0.4792(3)	0.4231(8)	0.4282(2)	0.066(3)	0.083(4)	0.079(4)	-0.024(2)	0.025(2)	-0.008(3)
C(17)	4e	0.3293(4)	-0.027(1)	0.4382(2)	0.051(3)	0.047(4)	0.039(3)	0.005(3)	0.013(2)	0.008(3)
O(18)	4e	0.3348(3)	-0.1800(7)	0.4152(2)	0.106(4)	0.041(3)	0.075(4)	-0.001(3)	0.036(3)	-0.009(3)
C(19)	4e	0.3957(4)	0.134(1)	0.5366(2)	0.059(3)	0.048(4)	0.045(4)	0.009(3)	0.002(3)	0.001(3)
O(20)	4e	0.4434(3)	0.0758(8)	0.5740(2)	0.080(3)	0.096(4)	0.061(3)	0.008(3)	-0.026(2)	0.023(3)
C(21)	4e	0.2163(4)	0.1169(9)	0.5073(2)	0.050(3)	0.044(4)	0.054(4)	0.006(3)	0.010(3)	-0.001(3)
O(22)	4e	0.1576(3)	0.0475(7)	0.5279(2)	0.074(3)	0.066(3)	0.096(4)	0.002(2)	0.043(3)	0.017(3)
C(23)	4e	0.3002(4)	0.489(1)	0.5123(2)	0.055(3)	0.050(4)	0.035(3)	0.004(3)	0.001(2)	0.004(3)
O(24)	4e	0.2917(3)	0.6388(7)	0.5358(2)	0.102(3)	0.051(3)	0.048(3)	0.013(3)	0.002(2)	-0.011(2)
C(25)	4e	0.3994(4)	0.086(1)	0.2203(3)	0.064(4)	0.071(5)	0.064(5)	0.004(3)	0.017(3)	0.005(4)
C(26)	4e	0.3653(5)	-0.022(2)	0.1736(3)	0.090(5)	0.116(8)	0.052(5)	0.000(5)	0.021(4)	0.008(5)
C(27)	4e	0.3332(6)	-0.218(2)	0.1770(4)	0.089(5)	0.123(9)	0.075(6)	-0.011(5)	0.026(5)	-0.031(6)
C(28)	4e	0.3354(5)	-0.315(2)	0.2265(4)	0.086(5)	0.073(6)	0.111(8)	0.001(4)	0.043(5)	-0.014(6)
C(29)	4e	0.3699(5)	-0.207(1)	0.2739(3)	0.074(4)	0.087(6)	0.067(5)	0.016(4)	0.030(4)	0.019(5)
C(30)	4e	0.4022(4)	-0.005(1)	0.2713(3)	0.049(3)	0.072(5)	0.051(4)	0.008(3)	0.013(3)	0.000(4)
N(31)	4e	0.4303(4)	0.112(1)	0.3189(2)	0.070(3)	0.105(5)	0.054(4)	0.005(3)	0.005(3)	-0.008(4)
Cr	4e	0.31659(5)	0.2301(1)	0.47552(3)	0.0384(4)	0.0392(6)	0.0345(6)	0.0015(4)	0.0022(4)	0.0030(4)

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