Syntheses and third-order NLO properties of η^6 complexes of *N*-ethylcarbazole with $Cr(CO)_3$ and $Cr(CO)_2PPh_3$ moieties

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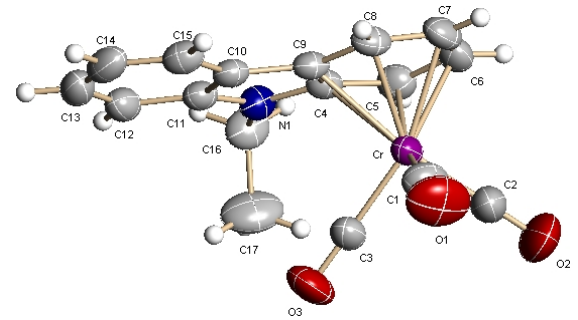
Crystallographic files for compound **2**



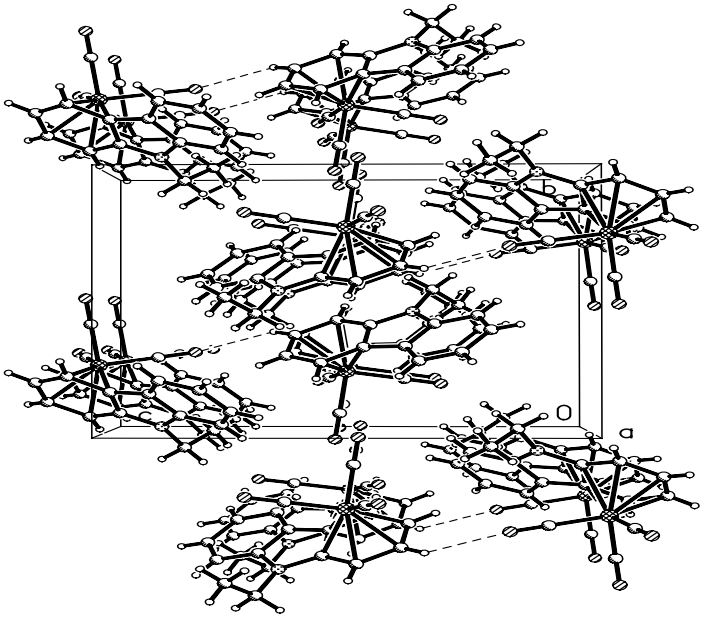


Table 1. Crystal data and structure refinement for compound **2**.

Identification code	cd25514
Empirical formula	C17 H13 Cr N O3
Formula weight	331.28
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.7347(7) A alpha = 90 deg.
	b = 11.5839(9) A beta = 90.8290(10) deg.
	c = 14.6847(11) A gamma = 90 deg.
Volume	1485.7(2) A^3
Z, Calculated density	4, 1.481 Mg/m^3
Absorption coefficient	0.781 mm^-1
F(000)	680

Crystal size	0.489 x 0.325 x 0.237 mm
Theta range for data collection	2.24 to 27.00 deg.
Limiting indices	-11<=h<=10, -14<=k<=14, -10<=l<=18
Reflections collected / unique	8541 / 3212 [R(int) = 0.0701]
Completeness to theta = 27.00	98.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.75333
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3212 / 0 / 217
Goodness-of-fit on F^2	1.021
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.1098
R indices (all data)	R1 = 0.0469, wR2 = 0.1141
Extinction coefficient	0.0087(15)
Largest diff. peak and hole	0.407 and -0.550 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr	7505(1)	2615(1)	10015(1)	39(1)
O(1)	8153(3)	5125(2)	10241(2)	99(1)
O(2)	4319(2)	3037(2)	10627(2)	114(1)
O(3)	6526(2)	3094(2)	8104(1)	79(1)
N(1)	8624(2)	370(1)	8690(1)	42(1)
C(1)	7925(3)	4161(2)	10151(2)	61(1)
C(2)	5551(3)	2887(2)	10388(2)	65(1)
C(3)	6895(2)	2908(2)	8843(1)	48(1)
C(4)	8496(2)	862(1)	9536(1)	39(1)
C(5)	7406(2)	683(2)	10203(2)	47(1)
C(6)	7632(3)	1245(2)	11052(1)	52(1)
C(7)	8850(3)	1998(2)	11202(1)	53(1)
C(8)	9870(2)	2251(2)	10503(1)	45(1)
C(9)	9716(2)	1674(1)	9664(1)	37(1)
C(10)	10613(2)	1632(1)	8848(1)	39(1)
C(11)	9913(2)	820(2)	8271(1)	40(1)
C(12)	10534(2)	522(2)	7436(1)	51(1)
C(13)	11905(3)	1034(2)	7210(2)	57(1)
C(14)	12621(2)	1825(2)	7779(2)	57(1)
C(15)	11992(2)	2141(2)	8595(2)	49(1)
C(16)	7564(2)	-456(2)	8279(2)	55(1)
C(17)	6309(3)	112(2)	7736(2)	86(1)

Table 3. Bond lengths [A] and angles [deg] for compound **2**.

Cr-C(3)	1.826(2)
Cr-C(2)	1.828(2)
Cr-C(1)	1.839(2)
Cr-C(6)	2.200(2)
Cr-C(7)	2.207(2)
Cr-C(8)	2.217(2)
Cr-C(5)	2.256(2)
Cr-C(9)	2.2834(17)
Cr-C(4)	2.3204(17)
O(1)-C(1)	1.142(3)
O(2)-C(2)	1.149(3)
O(3)-C(3)	1.149(2)
N(1)-C(4)	1.373(2)
N(1)-C(11)	1.392(2)
N(1)-C(16)	1.456(2)
C(4)-C(5)	1.392(3)
C(4)-C(9)	1.432(2)
C(5)-C(6)	1.417(3)
C(5)-H(5)	0.95(2)
C(6)-C(7)	1.391(3)
C(6)-H(6)	0.93(2)
C(7)-C(8)	1.400(3)
C(7)-H(7)	0.88(3)
C(8)-C(9)	1.406(3)
C(8)-H(8)	0.96(2)
C(9)-C(10)	1.442(3)
C(10)-C(15)	1.396(3)
C(10)-C(11)	1.400(2)
C(11)-C(12)	1.392(3)
C(12)-C(13)	1.381(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.383(3)
C(13)-H(13)	0.9300
C(14)-C(15)	1.375(3)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(17)	1.498(3)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600

C(3)-Cr-C(2)	89.39(10)
C(3)-Cr-C(1)	88.63(10)
C(2)-Cr-C(1)	89.16(12)
C(3)-Cr-C(6)	142.86(9)
C(2)-Cr-C(6)	87.42(10)
C(1)-Cr-C(6)	128.28(10)
C(3)-Cr-C(7)	161.70(9)
C(2)-Cr-C(7)	107.94(9)
C(1)-Cr-C(7)	97.26(10)
C(6)-Cr-C(7)	36.80(8)
C(3)-Cr-C(8)	126.70(9)
C(2)-Cr-C(8)	143.69(9)
C(1)-Cr-C(8)	88.07(9)
C(6)-Cr-C(8)	66.56(8)
C(7)-Cr-C(8)	36.90(8)
C(3)-Cr-C(5)	106.77(9)
C(2)-Cr-C(5)	95.55(10)
C(1)-Cr-C(5)	163.89(10)
C(6)-Cr-C(5)	37.05(8)
C(7)-Cr-C(5)	66.63(8)
C(8)-Cr-C(5)	79.01(7)
C(3)-Cr-C(9)	96.45(8)
C(2)-Cr-C(9)	161.24(10)
C(1)-Cr-C(9)	108.73(9)
C(6)-Cr-C(9)	77.15(7)
C(7)-Cr-C(9)	65.25(7)
C(8)-Cr-C(9)	36.37(6)
C(5)-Cr-C(9)	65.70(7)
C(3)-Cr-C(4)	88.97(8)
C(2)-Cr-C(4)	126.59(10)
C(1)-Cr-C(4)	144.13(9)
C(6)-Cr-C(4)	64.12(7)
C(7)-Cr-C(4)	76.09(7)
C(8)-Cr-C(4)	65.28(6)
C(5)-Cr-C(4)	35.37(7)
C(9)-Cr-C(4)	36.23(6)
C(4)-N(1)-C(11)	108.70(14)
C(4)-N(1)-C(16)	126.02(16)
C(11)-N(1)-C(16)	125.25(16)
O(1)-C(1)-Cr	178.5(2)
O(2)-C(2)-Cr	178.8(3)
O(3)-C(3)-Cr	179.3(2)
N(1)-C(4)-C(5)	129.84(17)
N(1)-C(4)-C(9)	108.77(15)

C(5)-C(4)-C(9)	121.39(17)
N(1)-C(4)-Cr	132.34(12)
C(5)-C(4)-Cr	69.79(11)
C(9)-C(4)-Cr	70.48(9)
C(4)-C(5)-C(6)	117.55(19)
C(4)-C(5)-Cr	74.83(11)
C(6)-C(5)-Cr	69.33(12)
C(4)-C(5)-H(5)	116.9(12)
C(6)-C(5)-H(5)	125.5(12)
Cr-C(5)-H(5)	128.0(12)
C(7)-C(6)-C(5)	121.6(2)
C(7)-C(6)-Cr	71.84(12)
C(5)-C(6)-Cr	73.62(12)
C(7)-C(6)-H(6)	121.2(14)
C(5)-C(6)-H(6)	117.1(14)
Cr-C(6)-H(6)	124.1(13)
C(6)-C(7)-C(8)	120.55(19)
C(6)-C(7)-Cr	71.35(11)
C(8)-C(7)-Cr	71.97(11)
C(6)-C(7)-H(7)	120(2)
C(8)-C(7)-H(7)	119(2)
Cr-C(7)-H(7)	125.6(18)
C(7)-C(8)-C(9)	119.27(19)
C(7)-C(8)-Cr	71.13(12)
C(9)-C(8)-Cr	74.37(10)
C(7)-C(8)-H(8)	121.6(12)
C(9)-C(8)-H(8)	119.2(12)
Cr-C(8)-H(8)	126.0(12)
C(8)-C(9)-C(4)	119.28(17)
C(8)-C(9)-C(10)	134.26(17)
C(4)-C(9)-C(10)	106.30(15)
C(8)-C(9)-Cr	69.26(11)
C(4)-C(9)-Cr	73.29(10)
C(10)-C(9)-Cr	132.47(11)
C(15)-C(10)-C(11)	119.58(18)
C(15)-C(10)-C(9)	133.47(17)
C(11)-C(10)-C(9)	106.71(15)
N(1)-C(11)-C(12)	128.60(17)
N(1)-C(11)-C(10)	109.51(15)
C(12)-C(11)-C(10)	121.82(18)
C(13)-C(12)-C(11)	117.1(2)
C(13)-C(12)-H(12)	121.5
C(11)-C(12)-H(12)	121.5
C(12)-C(13)-C(14)	121.7(2)

C(12)-C(13)-H(13)	119.1
C(14)-C(13)-H(13)	119.1
C(15)-C(14)-C(13)	121.3(2)
C(15)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
C(14)-C(15)-C(10)	118.4(2)
C(14)-C(15)-H(15)	120.8
C(10)-C(15)-H(15)	120.8
N(1)-C(16)-C(17)	112.80(18)
N(1)-C(16)-H(16A)	109.0
C(17)-C(16)-H(16A)	109.0
N(1)-C(16)-H(16B)	109.0
C(17)-C(16)-H(16B)	109.0
H(16A)-C(16)-H(16B)	107.8
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for compound **2**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr	45(1)	39(1)	32(1)	2(1)	-1(1)	9(1)
O(1)	133(2)	43(1)	121(2)	-6(1)	-25(1)	6(1)
O(2)	77(1)	171(2)	97(2)	27(2)	36(1)	52(1)
O(3)	105(1)	88(1)	43(1)	14(1)	-13(1)	15(1)
N(1)	42(1)	38(1)	46(1)	-8(1)	-5(1)	0(1)
C(1)	73(1)	45(1)	64(1)	-4(1)	-12(1)	10(1)
C(2)	65(2)	81(2)	48(1)	11(1)	9(1)	25(1)
C(3)	57(1)	48(1)	41(1)	6(1)	2(1)	12(1)
C(4)	41(1)	33(1)	41(1)	2(1)	-6(1)	4(1)
C(5)	50(1)	40(1)	53(1)	8(1)	2(1)	-2(1)
C(6)	63(1)	53(1)	41(1)	13(1)	6(1)	11(1)
C(7)	71(1)	54(1)	34(1)	0(1)	-11(1)	14(1)
C(8)	50(1)	42(1)	43(1)	-2(1)	-14(1)	6(1)
C(9)	38(1)	33(1)	41(1)	1(1)	-9(1)	4(1)
C(10)	38(1)	35(1)	43(1)	2(1)	-6(1)	8(1)

C(11)	41(1)	38(1)	41(1)	1(1)	-5(1)	9(1)
C(12)	59(1)	52(1)	42(1)	-2(1)	-3(1)	16(1)
C(13)	62(1)	60(1)	49(1)	12(1)	13(1)	21(1)
C(14)	45(1)	55(1)	71(1)	20(1)	13(1)	10(1)
C(15)	42(1)	41(1)	62(1)	7(1)	-3(1)	2(1)
C(16)	56(1)	45(1)	65(1)	-14(1)	-10(1)	-7(1)
C(17)	68(2)	76(2)	112(2)	-12(2)	-43(2)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2x10^3) for compound **2**.

	x	y	z	U(eq)
H(12)	10047	0	7047	61
H(13)	12358	843	6661	68
H(14)	13547	2149	7606	68
H(15)	12474	2681	8969	58
H(16A)	7114	-919	8756	66
H(16B)	8128	-971	7885	66
H(17A)	5727	605	8127	118
H(17B)	5650	-469	7477	118
H(17C)	6746	563	7257	118
H(5)	6580(20)	174(18)	10054(14)	49(5)
H(6)	6890(20)	1126(18)	11493(15)	59(6)
H(7)	8950(30)	2360(20)	11730(20)	80(9)
H(8)	10670(20)	2809(17)	10583(14)	51(6)

Table 6. Torsion angles [deg] for compound **2**.

C(3)-Cr-C(1)-O(1)	89(9)
C(2)-Cr-C(1)-O(1)	0(9)
C(6)-Cr-C(1)-O(1)	-86(9)
C(7)-Cr-C(1)-O(1)	-108(9)
C(8)-Cr-C(1)-O(1)	-144(9)
C(5)-Cr-C(1)-O(1)	-108(9)
C(9)-Cr-C(1)-O(1)	-175(100)
C(4)-Cr-C(1)-O(1)	175(100)
C(3)-Cr-C(2)-O(2)	111(11)
C(1)-Cr-C(2)-O(2)	-161(11)
C(6)-Cr-C(2)-O(2)	-32(11)

C(7)-Cr-C(2)-O(2)	-63(11)
C(8)-Cr-C(2)-O(2)	-75(11)
C(5)-Cr-C(2)-O(2)	4(11)
C(9)-Cr-C(2)-O(2)	2(11)
C(4)-Cr-C(2)-O(2)	23(11)
C(2)-Cr-C(3)-O(3)	160(18)
C(1)-Cr-C(3)-O(3)	71(18)
C(6)-Cr-C(3)-O(3)	-115(18)
C(7)-Cr-C(3)-O(3)	-39(18)
C(8)-Cr-C(3)-O(3)	-16(18)
C(5)-Cr-C(3)-O(3)	-105(18)
C(9)-Cr-C(3)-O(3)	-38(18)
C(4)-Cr-C(3)-O(3)	-74(18)
C(11)-N(1)-C(4)-C(5)	-179.67(18)
C(16)-N(1)-C(4)-C(5)	2.3(3)
C(11)-N(1)-C(4)-C(9)	1.28(19)
C(16)-N(1)-C(4)-C(9)	-176.75(16)
C(11)-N(1)-C(4)-Cr	81.61(19)
C(16)-N(1)-C(4)-Cr	-96.4(2)
C(3)-Cr-C(4)-N(1)	4.43(17)
C(2)-Cr-C(4)-N(1)	92.90(18)
C(1)-Cr-C(4)-N(1)	-81.8(2)
C(6)-Cr-C(4)-N(1)	157.92(19)
C(7)-Cr-C(4)-N(1)	-164.90(18)
C(8)-Cr-C(4)-N(1)	-127.36(18)
C(5)-Cr-C(4)-N(1)	126.0(2)
C(9)-Cr-C(4)-N(1)	-97.98(19)
C(3)-Cr-C(4)-C(5)	-121.59(13)
C(2)-Cr-C(4)-C(5)	-33.12(15)
C(1)-Cr-C(4)-C(5)	152.18(17)
C(6)-Cr-C(4)-C(5)	31.90(12)
C(7)-Cr-C(4)-C(5)	69.08(13)
C(8)-Cr-C(4)-C(5)	106.62(13)
C(9)-Cr-C(4)-C(5)	136.00(16)
C(3)-Cr-C(4)-C(9)	102.40(12)
C(2)-Cr-C(4)-C(9)	-169.12(11)
C(1)-Cr-C(4)-C(9)	16.17(18)
C(6)-Cr-C(4)-C(9)	-104.11(12)
C(7)-Cr-C(4)-C(9)	-66.92(11)
C(8)-Cr-C(4)-C(9)	-29.38(10)
C(5)-Cr-C(4)-C(9)	-136.00(16)
N(1)-C(4)-C(5)-C(6)	174.76(18)
C(9)-C(4)-C(5)-C(6)	-6.3(3)
Cr-C(4)-C(5)-C(6)	-56.37(16)

N(1)-C(4)-C(5)-Cr	-128.87(19)
C(9)-C(4)-C(5)-Cr	50.08(15)
C(3)-Cr-C(5)-C(4)	62.81(13)
C(2)-Cr-C(5)-C(4)	153.85(13)
C(1)-Cr-C(5)-C(4)	-99.7(3)
C(6)-Cr-C(5)-C(4)	-127.91(17)
C(7)-Cr-C(5)-C(4)	-98.99(13)
C(8)-Cr-C(5)-C(4)	-62.46(11)
C(9)-Cr-C(5)-C(4)	-26.77(10)
C(3)-Cr-C(5)-C(6)	-169.28(13)
C(2)-Cr-C(5)-C(6)	-78.24(14)
C(1)-Cr-C(5)-C(6)	28.2(4)
C(7)-Cr-C(5)-C(6)	28.92(13)
C(8)-Cr-C(5)-C(6)	65.45(13)
C(9)-Cr-C(5)-C(6)	101.13(13)
C(4)-Cr-C(5)-C(6)	127.91(17)
C(4)-C(5)-C(6)-C(7)	3.4(3)
Cr-C(5)-C(6)-C(7)	-55.77(18)
C(4)-C(5)-C(6)-Cr	59.19(16)
C(3)-Cr-C(6)-C(7)	149.34(15)
C(2)-Cr-C(6)-C(7)	-125.08(15)
C(1)-Cr-C(6)-C(7)	-38.19(18)
C(8)-Cr-C(6)-C(7)	28.92(12)
C(5)-Cr-C(6)-C(7)	132.19(19)
C(9)-Cr-C(6)-C(7)	65.67(13)
C(4)-Cr-C(6)-C(7)	101.68(14)
C(3)-Cr-C(6)-C(5)	17.1(2)
C(2)-Cr-C(6)-C(5)	102.73(14)
C(1)-Cr-C(6)-C(5)	-170.37(13)
C(7)-Cr-C(6)-C(5)	-132.19(19)
C(8)-Cr-C(6)-C(5)	-103.27(13)
C(9)-Cr-C(6)-C(5)	-66.52(12)
C(4)-Cr-C(6)-C(5)	-30.51(11)
C(5)-C(6)-C(7)-C(8)	1.9(3)
Cr-C(6)-C(7)-C(8)	-54.66(17)
C(5)-C(6)-C(7)-Cr	56.60(18)
C(3)-Cr-C(7)-C(6)	-101.3(3)
C(2)-Cr-C(7)-C(6)	59.24(16)
C(1)-Cr-C(7)-C(6)	150.71(14)
C(8)-Cr-C(7)-C(6)	-132.37(19)
C(5)-Cr-C(7)-C(6)	-29.10(13)
C(9)-Cr-C(7)-C(6)	-101.97(14)
C(4)-Cr-C(7)-C(6)	-65.19(13)
C(3)-Cr-C(7)-C(8)	31.0(3)

C(2)-Cr-C(7)-C(8)	-168.39(14)
C(1)-Cr-C(7)-C(8)	-76.92(14)
C(6)-Cr-C(7)-C(8)	132.37(19)
C(5)-Cr-C(7)-C(8)	103.27(13)
C(9)-Cr-C(7)-C(8)	30.40(11)
C(4)-Cr-C(7)-C(8)	67.18(12)
C(6)-C(7)-C(8)-C(9)	-4.4(3)
Cr-C(7)-C(8)-C(9)	-58.80(16)
C(6)-C(7)-C(8)-Cr	54.37(17)
C(3)-Cr-C(8)-C(7)	-168.35(13)
C(2)-Cr-C(8)-C(7)	18.9(2)
C(1)-Cr-C(8)-C(7)	104.81(14)
C(6)-Cr-C(8)-C(7)	-28.84(13)
C(5)-Cr-C(8)-C(7)	-65.53(13)
C(9)-Cr-C(8)-C(7)	-129.21(18)
C(4)-Cr-C(8)-C(7)	-99.94(13)
C(3)-Cr-C(8)-C(9)	-39.13(15)
C(2)-Cr-C(8)-C(9)	148.07(17)
C(1)-Cr-C(8)-C(9)	-125.98(13)
C(6)-Cr-C(8)-C(9)	100.37(13)
C(7)-Cr-C(8)-C(9)	129.21(18)
C(5)-Cr-C(8)-C(9)	63.69(11)
C(4)-Cr-C(8)-C(9)	29.28(10)
C(7)-C(8)-C(9)-C(4)	1.6(3)
Cr-C(8)-C(9)-C(4)	-55.61(14)
C(7)-C(8)-C(9)-C(10)	-173.09(18)
Cr-C(8)-C(9)-C(10)	129.7(2)
C(7)-C(8)-C(9)-Cr	57.19(16)
N(1)-C(4)-C(9)-C(8)	-176.95(15)
C(5)-C(4)-C(9)-C(8)	3.9(3)
Cr-C(4)-C(9)-C(8)	53.69(14)
N(1)-C(4)-C(9)-C(10)	-0.93(18)
C(5)-C(4)-C(9)-C(10)	179.92(16)
Cr-C(4)-C(9)-C(10)	-130.29(12)
N(1)-C(4)-C(9)-Cr	129.36(13)
C(5)-C(4)-C(9)-Cr	-49.78(15)
C(3)-Cr-C(9)-C(8)	149.39(13)
C(2)-Cr-C(9)-C(8)	-103.2(3)
C(1)-Cr-C(9)-C(8)	58.65(14)
C(6)-Cr-C(9)-C(8)	-67.77(12)
C(7)-Cr-C(9)-C(8)	-30.82(12)
C(5)-Cr-C(9)-C(8)	-105.09(13)
C(4)-Cr-C(9)-C(8)	-131.28(16)
C(3)-Cr-C(9)-C(4)	-79.34(12)

C(2)-Cr-C(9)-C(4)	28.1(3)
C(1)-Cr-C(9)-C(4)	-170.08(11)
C(6)-Cr-C(9)-C(4)	63.51(11)
C(7)-Cr-C(9)-C(4)	100.46(12)
C(8)-Cr-C(9)-C(4)	131.28(16)
C(5)-Cr-C(9)-C(4)	26.18(10)
C(3)-Cr-C(9)-C(10)	17.70(18)
C(2)-Cr-C(9)-C(10)	125.1(3)
C(1)-Cr-C(9)-C(10)	-73.04(18)
C(6)-Cr-C(9)-C(10)	160.55(18)
C(7)-Cr-C(9)-C(10)	-162.50(19)
C(8)-Cr-C(9)-C(10)	-131.7(2)
C(5)-Cr-C(9)-C(10)	123.22(18)
C(4)-Cr-C(9)-C(10)	97.04(19)
C(8)-C(9)-C(10)-C(15)	1.3(3)
C(4)-C(9)-C(10)-C(15)	-173.90(18)
Cr-C(9)-C(10)-C(15)	104.1(2)
C(8)-C(9)-C(10)-C(11)	175.39(18)
C(4)-C(9)-C(10)-C(11)	0.23(17)
Cr-C(9)-C(10)-C(11)	-81.81(18)
C(4)-N(1)-C(11)-C(12)	175.88(17)
C(16)-N(1)-C(11)-C(12)	-6.1(3)
C(4)-N(1)-C(11)-C(10)	-1.14(19)
C(16)-N(1)-C(11)-C(10)	176.91(16)
C(15)-C(10)-C(11)-N(1)	175.64(15)
C(9)-C(10)-C(11)-N(1)	0.54(18)
C(15)-C(10)-C(11)-C(12)	-1.6(3)
C(9)-C(10)-C(11)-C(12)	-176.72(16)
N(1)-C(11)-C(12)-C(13)	-174.61(17)
C(10)-C(11)-C(12)-C(13)	2.1(3)
C(11)-C(12)-C(13)-C(14)	-1.1(3)
C(12)-C(13)-C(14)-C(15)	-0.4(3)
C(13)-C(14)-C(15)-C(10)	0.9(3)
C(11)-C(10)-C(15)-C(14)	0.1(3)
C(9)-C(10)-C(15)-C(14)	173.60(18)
C(4)-N(1)-C(16)-C(17)	90.2(3)
C(11)-N(1)-C(16)-C(17)	-87.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for compound **2**. [A and deg.].

D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)

Crystallographic files for compound **4**

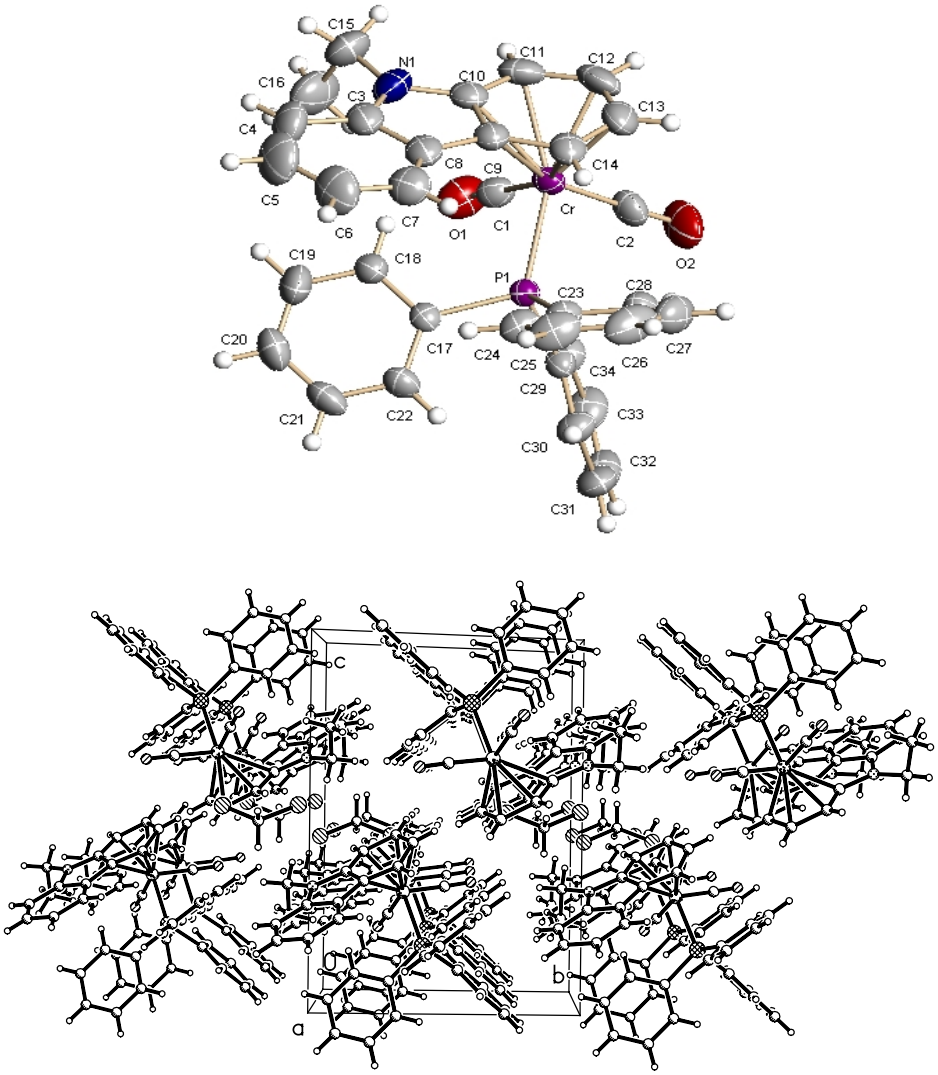


Table 1. Crystal data and structure refinement for compound **4.**

Identification code	cd25301
Empirical formula	C35 H30 Cl2 Cr N O2 P
Formula weight	650.47
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.0091(9) A alpha = 90.880(2) deg.
	b = 10.7369(10) A beta = 90.925(2) deg.
	c = 14.6282(14) A gamma = 101.742(2) deg.
Volume	1538.7(2) A^3
Z, Calculated density	2, 1.404 Mg/m^3

Absorption coefficient	0.631 mm^-1
F(000)	672
Crystal size	0.486 x 0.432 x 0.120 mm
Theta range for data collection	1.39 to 27.00 deg.
Limiting indices	-12<=h<=12, -13<=k<=13, -13<=l<=18
Reflections collected / unique	9054 / 6528 [R(int) = 0.0520]
Completeness to theta = 27.00	97.1 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.76627
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6528 / 2 / 375
Goodness-of-fit on F^2	1.112
Final R indices [I>2sigma(I)]	R1 = 0.0699, wR2 = 0.2109
R indices (all data)	R1 = 0.0851, wR2 = 0.2249
Largest diff. peak and hole	1.948 and -1.079 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **4.** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cr	1534(1)	3442(1)	3261(1)	38(1)
P(1)	2622(1)	4171(1)	1925(1)	31(1)
Cl(1)	7004(2)	217(3)	4555(2)	149(1)
Cl(2)	7355(4)	2859(4)	4627(4)	169(3)
N(1)	1502(4)	219(3)	3351(2)	55(1)
O(1)	-1096(3)	2469(3)	2237(3)	73(1)
O(2)	577(4)	5870(3)	3512(2)	82(1)
C(1)	-46(4)	2855(4)	2617(3)	48(1)
C(2)	963(4)	4923(4)	3401(3)	52(1)
C(3)	2695(4)	100(4)	2920(3)	52(1)
C(4)	2987(6)	-956(4)	2429(3)	69(1)
C(5)	4259(7)	-816(5)	2082(4)	90(2)
C(6)	5270(6)	311(5)	2194(4)	82(2)
C(7)	4971(5)	1326(4)	2676(3)	60(1)
C(8)	3673(4)	1233(4)	3035(3)	49(1)
C(9)	3049(4)	2093(3)	3570(2)	43(1)
C(10)	1713(4)	1413(4)	3755(2)	47(1)
C(11)	808(5)	1983(4)	4269(3)	59(1)
C(12)	1336(5)	3161(5)	4718(3)	67(1)
C(13)	2695(5)	3796(4)	4562(3)	59(1)
C(14)	3516(4)	3308(4)	3962(2)	49(1)
C(15)	256(5)	-751(4)	3364(4)	72(1)

C(16)	-655(6)	-749(5)	2546(4)	90(2)
C(17)	2617(3)	2977(3)	1008(2)	33(1)
C(18)	1963(4)	1735(3)	1154(2)	44(1)
C(19)	1915(5)	806(4)	482(3)	65(1)
C(20)	2517(5)	1115(4)	-342(3)	62(1)
C(21)	3168(4)	2350(4)	-502(3)	54(1)
C(22)	3216(4)	3268(4)	165(2)	45(1)
C(23)	4436(3)	4879(3)	2124(2)	38(1)
C(24)	5498(3)	4314(4)	1816(3)	47(1)
C(25)	6829(4)	4813(5)	2124(3)	64(1)
C(26)	7119(5)	5828(5)	2712(4)	71(1)
C(27)	6087(5)	6401(4)	2996(3)	63(1)
C(28)	4756(4)	5927(4)	2710(3)	49(1)
C(29)	2039(3)	5427(3)	1279(2)	36(1)
C(30)	2919(4)	6263(3)	727(3)	49(1)
C(31)	2436(5)	7123(4)	186(3)	61(1)
C(32)	1059(5)	7167(4)	196(3)	67(1)
C(33)	195(5)	6364(4)	732(3)	62(1)
C(34)	670(4)	5495(4)	1275(3)	48(1)
C(35)	6336(14)	1540(11)	4964(10)	186(5)

Table 3. Bond lengths [A] and angles [deg] for compound **4.**

Cr-C(2)	1.806(4)
Cr-C(1)	1.820(4)
Cr-C(12)	2.164(4)
Cr-C(11)	2.190(4)
Cr-C(13)	2.200(4)
Cr-C(14)	2.250(4)
Cr-P(1)	2.3209(9)
Cr-C(9)	2.343(4)
Cr-C(10)	2.345(4)
P(1)-C(23)	1.837(3)
P(1)-C(17)	1.842(3)
P(1)-C(29)	1.842(3)
Cl(1)-C(35)	1.787(11)
Cl(2)-C(35)	1.655(11)
N(1)-C(10)	1.379(5)
N(1)-C(3)	1.387(5)
N(1)-C(15)	1.454(5)
O(1)-C(1)	1.176(5)
O(2)-C(2)	1.170(5)

C(3)-C(8)	1.404(6)
C(3)-C(4)	1.415(6)
C(4)-C(5)	1.359(7)
C(4)-H(4)	0.9300
C(5)-C(6)	1.416(8)
C(5)-H(5)	0.9300
C(6)-C(7)	1.375(6)
C(6)-H(6)	0.9300
C(7)-C(8)	1.394(6)
C(7)-H(7)	0.9300
C(8)-C(9)	1.444(5)
C(9)-C(14)	1.403(5)
C(9)-C(10)	1.419(5)
C(10)-C(11)	1.411(6)
C(11)-C(12)	1.415(7)
C(11)-H(11)	0.9300
C(12)-C(13)	1.416(7)
C(12)-H(12)	0.9300
C(13)-C(14)	1.381(6)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.494(8)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(18)	1.382(5)
C(17)-C(22)	1.392(5)
C(18)-C(19)	1.383(5)
C(18)-H(18)	0.9300
C(19)-C(20)	1.371(6)
C(19)-H(19)	0.9300
C(20)-C(21)	1.379(6)
C(20)-H(20)	0.9300
C(21)-C(22)	1.369(5)
C(21)-H(21)	0.9300
C(22)-H(22)	0.9300
C(23)-C(28)	1.385(5)
C(23)-C(24)	1.403(5)
C(24)-C(25)	1.395(5)
C(24)-H(24)	0.9300
C(25)-C(26)	1.358(7)
C(25)-H(25)	0.9300

C(26)-C(27)	1.372(7)
C(26)-H(26)	0.9300
C(27)-C(28)	1.382(6)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(29)-C(34)	1.388(5)
C(29)-C(30)	1.399(5)
C(30)-C(31)	1.380(6)
C(30)-H(30)	0.9300
C(31)-C(32)	1.389(7)
C(31)-H(31)	0.9300
C(32)-C(33)	1.358(7)
C(32)-H(32)	0.9300
C(33)-C(34)	1.385(6)
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(2)-Cr-C(1)	87.05(18)
C(2)-Cr-C(12)	89.03(17)
C(1)-Cr-C(12)	113.35(19)
C(2)-Cr-C(11)	116.07(17)
C(1)-Cr-C(11)	87.60(17)
C(12)-Cr-C(11)	37.93(17)
C(2)-Cr-C(13)	90.52(17)
C(1)-Cr-C(13)	151.17(17)
C(12)-Cr-C(13)	37.85(18)
C(11)-Cr-C(13)	67.78(17)
C(2)-Cr-C(14)	116.81(17)
C(1)-Cr-C(14)	155.97(16)
C(12)-Cr-C(14)	67.09(17)
C(11)-Cr-C(14)	79.51(16)
C(13)-Cr-C(14)	36.12(15)
C(2)-Cr-P(1)	90.15(13)
C(1)-Cr-P(1)	90.31(12)
C(12)-Cr-P(1)	156.25(15)
C(11)-Cr-P(1)	153.52(13)
C(13)-Cr-P(1)	118.44(13)
C(14)-Cr-P(1)	92.31(10)
C(2)-Cr-C(9)	152.19(16)
C(1)-Cr-C(9)	120.51(15)
C(12)-Cr-C(9)	77.09(15)
C(11)-Cr-C(9)	65.68(15)
C(13)-Cr-C(9)	63.75(15)

C(14)-Cr-C(9)	35.49(13)
P(1)-Cr-C(9)	93.12(9)
C(2)-Cr-C(10)	151.87(16)
C(1)-Cr-C(10)	93.69(15)
C(12)-Cr-C(10)	64.87(15)
C(11)-Cr-C(10)	36.06(14)
C(13)-Cr-C(10)	75.46(15)
C(14)-Cr-C(10)	64.12(14)
P(1)-Cr-C(10)	117.94(10)
C(9)-Cr-C(10)	35.24(13)
C(23)-P(1)-C(17)	104.32(15)
C(23)-P(1)-C(29)	101.62(15)
C(17)-P(1)-C(29)	100.39(14)
C(23)-P(1)-Cr	112.33(11)
C(17)-P(1)-Cr	116.38(11)
C(29)-P(1)-Cr	119.63(11)
C(10)-N(1)-C(3)	107.9(3)
C(10)-N(1)-C(15)	126.7(4)
C(3)-N(1)-C(15)	125.5(4)
O(1)-C(1)-Cr	177.1(3)
O(2)-C(2)-Cr	178.2(4)
N(1)-C(3)-C(8)	109.7(3)
N(1)-C(3)-C(4)	129.0(4)
C(8)-C(3)-C(4)	121.3(4)
C(5)-C(4)-C(3)	116.6(4)
C(5)-C(4)-H(4)	121.7
C(3)-C(4)-H(4)	121.7
C(4)-C(5)-C(6)	123.3(5)
C(4)-C(5)-H(5)	118.3
C(6)-C(5)-H(5)	118.3
C(7)-C(6)-C(5)	119.3(5)
C(7)-C(6)-H(6)	120.3
C(5)-C(6)-H(6)	120.3
C(6)-C(7)-C(8)	119.4(5)
C(6)-C(7)-H(7)	120.3
C(8)-C(7)-H(7)	120.3
C(7)-C(8)-C(3)	120.0(4)
C(7)-C(8)-C(9)	133.2(4)
C(3)-C(8)-C(9)	106.8(3)
C(14)-C(9)-C(10)	119.7(3)
C(14)-C(9)-C(8)	134.3(4)
C(10)-C(9)-C(8)	105.8(3)
C(14)-C(9)-Cr	68.6(2)
C(10)-C(9)-Cr	72.5(2)

C(8)-C(9)-Cr	135.3(3)
N(1)-C(10)-C(11)	129.3(4)
N(1)-C(10)-C(9)	109.9(3)
C(11)-C(10)-C(9)	120.8(4)
N(1)-C(10)-Cr	134.8(3)
C(11)-C(10)-Cr	66.0(2)
C(9)-C(10)-Cr	72.3(2)
C(10)-C(11)-C(12)	118.0(4)
C(10)-C(11)-Cr	78.0(2)
C(12)-C(11)-Cr	70.0(2)
C(10)-C(11)-H(11)	121.0
C(12)-C(11)-H(11)	121.0
Cr-C(11)-H(11)	122.3
C(11)-C(12)-C(13)	119.7(4)
C(11)-C(12)-Cr	72.0(2)
C(13)-C(12)-Cr	72.5(2)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
Cr-C(12)-H(12)	127.4
C(14)-C(13)-C(12)	121.5(4)
C(14)-C(13)-Cr	73.9(2)
C(12)-C(13)-Cr	69.7(2)
C(14)-C(13)-H(13)	119.2
C(12)-C(13)-H(13)	119.2
Cr-C(13)-H(13)	129.7
C(13)-C(14)-C(9)	119.3(4)
C(13)-C(14)-Cr	70.0(2)
C(9)-C(14)-Cr	75.9(2)
C(13)-C(14)-H(14)	120.3
C(9)-C(14)-H(14)	120.3
Cr-C(14)-H(14)	125.5
N(1)-C(15)-C(16)	113.8(4)
N(1)-C(15)-H(15A)	108.8
C(16)-C(15)-H(15A)	108.8
N(1)-C(15)-H(15B)	108.8
C(16)-C(15)-H(15B)	108.8
H(15A)-C(15)-H(15B)	107.7
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(22)	118.3(3)

C(18)-C(17)-P(1)	118.5(2)
C(22)-C(17)-P(1)	123.2(3)
C(17)-C(18)-C(19)	120.8(4)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.6
C(20)-C(19)-C(18)	119.9(4)
C(20)-C(19)-H(19)	120.1
C(18)-C(19)-H(19)	120.1
C(19)-C(20)-C(21)	120.1(4)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(22)-C(21)-C(20)	119.9(4)
C(22)-C(21)-H(21)	120.1
C(20)-C(21)-H(21)	120.1
C(21)-C(22)-C(17)	121.1(4)
C(21)-C(22)-H(22)	119.5
C(17)-C(22)-H(22)	119.5
C(28)-C(23)-C(24)	118.5(3)
C(28)-C(23)-P(1)	117.6(3)
C(24)-C(23)-P(1)	123.3(3)
C(25)-C(24)-C(23)	118.9(4)
C(25)-C(24)-H(24)	120.6
C(23)-C(24)-H(24)	120.6
C(26)-C(25)-C(24)	121.7(4)
C(26)-C(25)-H(25)	119.1
C(24)-C(25)-H(25)	119.1
C(25)-C(26)-C(27)	119.5(4)
C(25)-C(26)-H(26)	120.3
C(27)-C(26)-H(26)	120.3
C(26)-C(27)-C(28)	120.4(4)
C(26)-C(27)-H(27)	119.8
C(28)-C(27)-H(27)	119.8
C(27)-C(28)-C(23)	121.0(4)
C(27)-C(28)-H(28)	119.5
C(23)-C(28)-H(28)	119.5
C(34)-C(29)-C(30)	118.1(3)
C(34)-C(29)-P(1)	119.8(3)
C(30)-C(29)-P(1)	121.9(3)
C(31)-C(30)-C(29)	121.0(4)
C(31)-C(30)-H(30)	119.5
C(29)-C(30)-H(30)	119.5
C(30)-C(31)-C(32)	119.5(4)
C(30)-C(31)-H(31)	120.2
C(32)-C(31)-H(31)	120.2

C(33)-C(32)-C(31)	120.1(4)
C(33)-C(32)-H(32)	119.9
C(31)-C(32)-H(32)	119.9
C(32)-C(33)-C(34)	120.8(4)
C(32)-C(33)-H(33)	119.6
C(34)-C(33)-H(33)	119.6
C(33)-C(34)-C(29)	120.5(4)
C(33)-C(34)-H(34)	119.7
C(29)-C(34)-H(34)	119.7
Cl(2)-C(35)-Cl(1)	108.0(7)
Cl(2)-C(35)-H(35A)	110.1
Cl(1)-C(35)-H(35A)	110.1
Cl(2)-C(35)-H(35B)	110.1
Cl(1)-C(35)-H(35B)	110.1
H(35A)-C(35)-H(35B)	108.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for compound **4.** The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cr	45(1)	40(1)	31(1)	2(1)	8(1)	14(1)
P(1)	30(1)	32(1)	32(1)	1(1)	3(1)	10(1)
Cl(1)	142(2)	171(2)	144(2)	51(2)	-9(1)	53(2)
Cl(2)	175(3)	240(4)	542(8)	-239(5)	-108(4)	72(3)
N(1)	62(2)	39(2)	62(2)	9(2)	-1(2)	7(2)
O(1)	51(2)	72(2)	92(2)	12(2)	-7(2)	4(2)
O(2)	114(3)	74(2)	76(2)	-15(2)	8(2)	59(2)
C(1)	48(2)	46(2)	51(2)	9(2)	11(2)	13(2)
C(2)	60(2)	58(2)	42(2)	-7(2)	9(2)	23(2)
C(3)	70(3)	45(2)	46(2)	6(2)	-3(2)	22(2)
C(4)	89(4)	41(2)	80(3)	-9(2)	-4(3)	24(2)
C(5)	111(5)	66(3)	107(4)	-16(3)	4(4)	50(3)
C(6)	87(4)	80(4)	90(4)	-10(3)	10(3)	48(3)
C(7)	61(3)	60(3)	66(3)	5(2)	2(2)	27(2)
C(8)	62(2)	44(2)	44(2)	7(2)	-4(2)	22(2)
C(9)	55(2)	40(2)	36(2)	7(1)	0(2)	14(2)
C(10)	61(2)	49(2)	34(2)	10(2)	1(2)	17(2)
C(11)	68(3)	70(3)	41(2)	20(2)	15(2)	15(2)
C(12)	101(4)	81(3)	30(2)	7(2)	17(2)	42(3)
C(13)	84(3)	57(2)	37(2)	-4(2)	-8(2)	16(2)

C(14)	62(2)	48(2)	39(2)	3(2)	-9(2)	19(2)
C(15)	85(3)	47(2)	79(3)	15(2)	11(3)	-1(2)
C(16)	89(4)	68(3)	99(4)	8(3)	-12(3)	-21(3)
C(17)	33(2)	36(2)	33(2)	0(1)	-2(1)	14(1)
C(18)	54(2)	38(2)	40(2)	2(1)	4(2)	14(2)
C(19)	90(3)	38(2)	65(3)	-9(2)	0(2)	13(2)
C(20)	72(3)	62(3)	54(3)	-21(2)	1(2)	21(2)
C(21)	63(3)	72(3)	33(2)	-2(2)	8(2)	26(2)
C(22)	45(2)	52(2)	38(2)	1(2)	9(2)	13(2)
C(23)	34(2)	41(2)	38(2)	8(1)	0(1)	6(1)
C(24)	35(2)	48(2)	58(2)	9(2)	2(2)	11(2)
C(25)	37(2)	71(3)	88(3)	21(2)	1(2)	20(2)
C(26)	46(2)	71(3)	88(3)	22(3)	-20(2)	-5(2)
C(27)	64(3)	53(2)	64(3)	1(2)	-11(2)	-10(2)
C(28)	49(2)	50(2)	47(2)	-3(2)	2(2)	5(2)
C(29)	43(2)	34(2)	35(2)	-1(1)	-1(1)	14(1)
C(30)	50(2)	41(2)	57(2)	10(2)	5(2)	12(2)
C(31)	88(3)	41(2)	57(2)	14(2)	7(2)	17(2)
C(32)	96(4)	48(2)	65(3)	-5(2)	-34(3)	34(2)
C(33)	63(3)	56(2)	72(3)	-3(2)	-20(2)	28(2)
C(34)	44(2)	48(2)	56(2)	-2(2)	-7(2)	17(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **4.**

	x	y	z	U(eq)
H(4)	2341	-1707	2347	82
H(5)	4477	-1495	1755	108
H(6)	6128	363	1945	98
H(7)	5628	2069	2761	72
H(11)	-108	1595	4311	71
H(12)	793	3516	5115	80
H(13)	3042	4560	4870	71
H(14)	4371	3779	3819	58
H(15A)	-243	-624	3909	87
H(15B)	498	-1579	3403	87
H(16A)	-704	112	2405	115
H(16B)	-1552	-1222	2673	115
H(16C)	-295	-1134	2034	115
H(18)	1549	1522	1711	52
H(19)	1475	-28	589	77

H(20)	2487	491	-793	74
H(21)	3574	2560	-1061	65
H(22)	3657	4100	53	53
H(24)	5318	3619	1414	56
H(25)	7535	4441	1922	76
H(26)	8011	6132	2920	85
H(27)	6285	7112	3383	76
H(28)	4065	6318	2914	59
H(30)	3842	6239	725	58
H(31)	3029	7670	-182	74
H(32)	727	7746	-165	81
H(33)	-726	6398	735	74
H(34)	66	4953	1639	58
H(35A)	5420	1492	4719	210
H(35B)	6297	1534	5626	210

Table 6. Torsion angles [deg] for compound **4**.

C(2)-Cr-P(1)-C(23)	95.20(18)
C(1)-Cr-P(1)-C(23)	-177.75(16)
C(12)-Cr-P(1)-C(23)	7.3(3)
C(11)-Cr-P(1)-C(23)	-92.5(3)
C(13)-Cr-P(1)-C(23)	4.53(18)
C(14)-Cr-P(1)-C(23)	-21.64(15)
C(9)-Cr-P(1)-C(23)	-57.17(15)
C(10)-Cr-P(1)-C(23)	-83.41(17)
C(2)-Cr-P(1)-C(17)	-144.65(17)
C(1)-Cr-P(1)-C(17)	-57.60(16)
C(12)-Cr-P(1)-C(17)	127.4(3)
C(11)-Cr-P(1)-C(17)	27.6(3)
C(13)-Cr-P(1)-C(17)	124.68(17)
C(14)-Cr-P(1)-C(17)	98.51(15)
C(9)-Cr-P(1)-C(17)	62.98(14)
C(10)-Cr-P(1)-C(17)	36.74(16)
C(2)-Cr-P(1)-C(29)	-23.75(19)
C(1)-Cr-P(1)-C(29)	63.30(17)
C(12)-Cr-P(1)-C(29)	-111.7(3)
C(11)-Cr-P(1)-C(29)	148.5(3)
C(13)-Cr-P(1)-C(29)	-114.42(18)
C(14)-Cr-P(1)-C(29)	-140.59(16)
C(9)-Cr-P(1)-C(29)	-176.12(15)
C(10)-Cr-P(1)-C(29)	157.64(17)

C(2)-Cr-C(1)-O(1)	-78(7)
C(12)-Cr-C(1)-O(1)	10(7)
C(11)-Cr-C(1)-O(1)	39(7)
C(13)-Cr-C(1)-O(1)	8(7)
C(14)-Cr-C(1)-O(1)	96(7)
P(1)-Cr-C(1)-O(1)	-168(7)
C(9)-Cr-C(1)-O(1)	98(7)
C(10)-Cr-C(1)-O(1)	74(7)
C(1)-Cr-C(2)-O(2)	89(14)
C(12)-Cr-C(2)-O(2)	-24(14)
C(11)-Cr-C(2)-O(2)	3(14)
C(13)-Cr-C(2)-O(2)	-62(14)
C(14)-Cr-C(2)-O(2)	-88(14)
P(1)-Cr-C(2)-O(2)	180(100)
C(9)-Cr-C(2)-O(2)	-83(14)
C(10)-Cr-C(2)-O(2)	-3(14)
C(10)-N(1)-C(3)-C(8)	-1.0(4)
C(15)-N(1)-C(3)-C(8)	178.8(4)
C(10)-N(1)-C(3)-C(4)	178.7(4)
C(15)-N(1)-C(3)-C(4)	-1.5(7)
N(1)-C(3)-C(4)-C(5)	-179.3(5)
C(8)-C(3)-C(4)-C(5)	0.4(7)
C(3)-C(4)-C(5)-C(6)	0.2(9)
C(4)-C(5)-C(6)-C(7)	0.0(9)
C(5)-C(6)-C(7)-C(8)	-0.7(8)
C(6)-C(7)-C(8)-C(3)	1.3(6)
C(6)-C(7)-C(8)-C(9)	179.0(4)
N(1)-C(3)-C(8)-C(7)	178.6(3)
C(4)-C(3)-C(8)-C(7)	-1.2(6)
N(1)-C(3)-C(8)-C(9)	0.3(4)
C(4)-C(3)-C(8)-C(9)	-179.4(4)
C(7)-C(8)-C(9)-C(14)	-3.4(7)
C(3)-C(8)-C(9)-C(14)	174.5(4)
C(7)-C(8)-C(9)-C(10)	-177.5(4)
C(3)-C(8)-C(9)-C(10)	0.4(4)
C(7)-C(8)-C(9)-Cr	101.7(5)
C(3)-C(8)-C(9)-Cr	-80.3(4)
C(2)-Cr-C(9)-C(14)	-6.7(4)
C(1)-Cr-C(9)-C(14)	-178.2(2)
C(12)-Cr-C(9)-C(14)	-68.5(3)
C(11)-Cr-C(9)-C(14)	-106.8(3)
C(13)-Cr-C(9)-C(14)	-30.7(2)
P(1)-Cr-C(9)-C(14)	89.6(2)
C(10)-Cr-C(9)-C(14)	-133.0(3)

C(2)-Cr-C(9)-C(10)	126.3(3)
C(1)-Cr-C(9)-C(10)	-45.2(3)
C(12)-Cr-C(9)-C(10)	64.5(2)
C(11)-Cr-C(9)-C(10)	26.2(2)
C(13)-Cr-C(9)-C(10)	102.3(2)
C(14)-Cr-C(9)-C(10)	133.0(3)
P(1)-Cr-C(9)-C(10)	-137.4(2)
C(2)-Cr-C(9)-C(8)	-138.7(4)
C(1)-Cr-C(9)-C(8)	49.7(4)
C(12)-Cr-C(9)-C(8)	159.4(4)
C(11)-Cr-C(9)-C(8)	121.1(4)
C(13)-Cr-C(9)-C(8)	-162.8(4)
C(14)-Cr-C(9)-C(8)	-132.1(5)
P(1)-Cr-C(9)-C(8)	-42.5(4)
C(10)-Cr-C(9)-C(8)	94.9(4)
C(3)-N(1)-C(10)-C(11)	179.8(4)
C(15)-N(1)-C(10)-C(11)	0.1(7)
C(3)-N(1)-C(10)-C(9)	1.3(4)
C(15)-N(1)-C(10)-C(9)	-178.5(4)
C(3)-N(1)-C(10)-Cr	85.7(4)
C(15)-N(1)-C(10)-Cr	-94.0(5)
C(14)-C(9)-C(10)-N(1)	-176.2(3)
C(8)-C(9)-C(10)-N(1)	-1.0(4)
Cr-C(9)-C(10)-N(1)	132.2(3)
C(14)-C(9)-C(10)-C(11)	5.1(5)
C(8)-C(9)-C(10)-C(11)	-179.8(3)
Cr-C(9)-C(10)-C(11)	-46.5(3)
C(14)-C(9)-C(10)-Cr	51.6(3)
C(8)-C(9)-C(10)-Cr	-133.2(3)
C(2)-Cr-C(10)-N(1)	132.2(4)
C(1)-Cr-C(10)-N(1)	41.5(4)
C(12)-Cr-C(10)-N(1)	155.7(5)
C(11)-Cr-C(10)-N(1)	122.3(5)
C(13)-Cr-C(10)-N(1)	-165.6(4)
C(14)-Cr-C(10)-N(1)	-128.8(4)
P(1)-Cr-C(10)-N(1)	-50.8(4)
C(9)-Cr-C(10)-N(1)	-100.7(4)
C(2)-Cr-C(10)-C(11)	9.8(5)
C(1)-Cr-C(10)-C(11)	-80.8(3)
C(12)-Cr-C(10)-C(11)	33.3(3)
C(13)-Cr-C(10)-C(11)	72.1(3)
C(14)-Cr-C(10)-C(11)	108.8(3)
P(1)-Cr-C(10)-C(11)	-173.1(2)
C(9)-Cr-C(10)-C(11)	137.0(4)

C(2)-Cr-C(10)-C(9)	-127.1(4)
C(1)-Cr-C(10)-C(9)	142.2(2)
C(12)-Cr-C(10)-C(9)	-103.7(3)
C(11)-Cr-C(10)-C(9)	-137.0(4)
C(13)-Cr-C(10)-C(9)	-64.9(2)
C(14)-Cr-C(10)-C(9)	-28.2(2)
P(1)-Cr-C(10)-C(9)	49.9(2)
N(1)-C(10)-C(11)-C(12)	171.3(4)
C(9)-C(10)-C(11)-C(12)	-10.2(6)
Cr-C(10)-C(11)-C(12)	-59.4(3)
N(1)-C(10)-C(11)-Cr	-129.2(4)
C(9)-C(10)-C(11)-Cr	49.2(3)
C(2)-Cr-C(11)-C(10)	-174.9(3)
C(1)-Cr-C(11)-C(10)	99.6(3)
C(12)-Cr-C(11)-C(10)	-126.0(4)
C(13)-Cr-C(11)-C(10)	-95.8(3)
C(14)-Cr-C(11)-C(10)	-60.0(2)
P(1)-Cr-C(11)-C(10)	13.7(5)
C(9)-Cr-C(11)-C(10)	-25.6(2)
C(2)-Cr-C(11)-C(12)	-48.8(3)
C(1)-Cr-C(11)-C(12)	-134.4(3)
C(13)-Cr-C(11)-C(12)	30.3(3)
C(14)-Cr-C(11)-C(12)	66.0(3)
P(1)-Cr-C(11)-C(12)	139.8(3)
C(9)-Cr-C(11)-C(12)	100.4(3)
C(10)-Cr-C(11)-C(12)	126.0(4)
C(10)-C(11)-C(12)-C(13)	7.0(6)
Cr-C(11)-C(12)-C(13)	-56.7(4)
C(10)-C(11)-C(12)-Cr	63.6(3)
C(2)-Cr-C(12)-C(11)	137.5(3)
C(1)-Cr-C(12)-C(11)	51.1(3)
C(13)-Cr-C(12)-C(11)	-130.5(4)
C(14)-Cr-C(12)-C(11)	-102.8(3)
P(1)-Cr-C(12)-C(11)	-134.4(3)
C(9)-Cr-C(12)-C(11)	-66.8(3)
C(10)-Cr-C(12)-C(11)	-31.7(3)
C(2)-Cr-C(12)-C(13)	-92.1(3)
C(1)-Cr-C(12)-C(13)	-178.5(3)
C(11)-Cr-C(12)-C(13)	130.5(4)
C(14)-Cr-C(12)-C(13)	27.7(2)
P(1)-Cr-C(12)-C(13)	-3.9(5)
C(9)-Cr-C(12)-C(13)	63.6(3)
C(10)-Cr-C(12)-C(13)	98.7(3)
C(11)-C(12)-C(13)-C(14)	1.5(6)

Cr-C(12)-C(13)-C(14)	-55.0(4)
C(11)-C(12)-C(13)-Cr	56.4(4)
C(2)-Cr-C(13)-C(14)	-138.8(3)
C(1)-Cr-C(13)-C(14)	136.4(3)
C(12)-Cr-C(13)-C(14)	133.4(4)
C(11)-Cr-C(13)-C(14)	103.1(3)
P(1)-Cr-C(13)-C(14)	-48.4(3)
C(9)-Cr-C(13)-C(14)	30.2(2)
C(10)-Cr-C(13)-C(14)	65.8(2)
C(2)-Cr-C(13)-C(12)	87.8(3)
C(1)-Cr-C(13)-C(12)	2.9(5)
C(11)-Cr-C(13)-C(12)	-30.3(3)
C(14)-Cr-C(13)-C(12)	-133.4(4)
P(1)-Cr-C(13)-C(12)	178.2(2)
C(9)-Cr-C(13)-C(12)	-103.2(3)
C(10)-Cr-C(13)-C(12)	-67.6(3)
C(12)-C(13)-C(14)-C(9)	-6.8(6)
Cr-C(13)-C(14)-C(9)	-59.8(3)
C(12)-C(13)-C(14)-Cr	53.1(4)
C(10)-C(9)-C(14)-C(13)	3.5(5)
C(8)-C(9)-C(14)-C(13)	-170.0(4)
Cr-C(9)-C(14)-C(13)	56.9(3)
C(10)-C(9)-C(14)-Cr	-53.4(3)
C(8)-C(9)-C(14)-Cr	133.2(4)
C(2)-Cr-C(14)-C(13)	47.5(3)
C(1)-Cr-C(14)-C(13)	-125.2(4)
C(12)-Cr-C(14)-C(13)	-28.9(3)
C(11)-Cr-C(14)-C(13)	-66.5(3)
P(1)-Cr-C(14)-C(13)	138.9(2)
C(9)-Cr-C(14)-C(13)	-129.0(4)
C(10)-Cr-C(14)-C(13)	-101.0(3)
C(2)-Cr-C(14)-C(9)	176.5(2)
C(1)-Cr-C(14)-C(9)	3.8(5)
C(12)-Cr-C(14)-C(9)	100.1(3)
C(11)-Cr-C(14)-C(9)	62.5(2)
C(13)-Cr-C(14)-C(9)	129.0(4)
P(1)-Cr-C(14)-C(9)	-92.1(2)
C(10)-Cr-C(14)-C(9)	28.0(2)
C(10)-N(1)-C(15)-C(16)	94.8(6)
C(3)-N(1)-C(15)-C(16)	-84.9(6)
C(23)-P(1)-C(17)-C(18)	125.2(3)
C(29)-P(1)-C(17)-C(18)	-129.8(3)
Cr-P(1)-C(17)-C(18)	0.8(3)
C(23)-P(1)-C(17)-C(22)	-56.2(3)

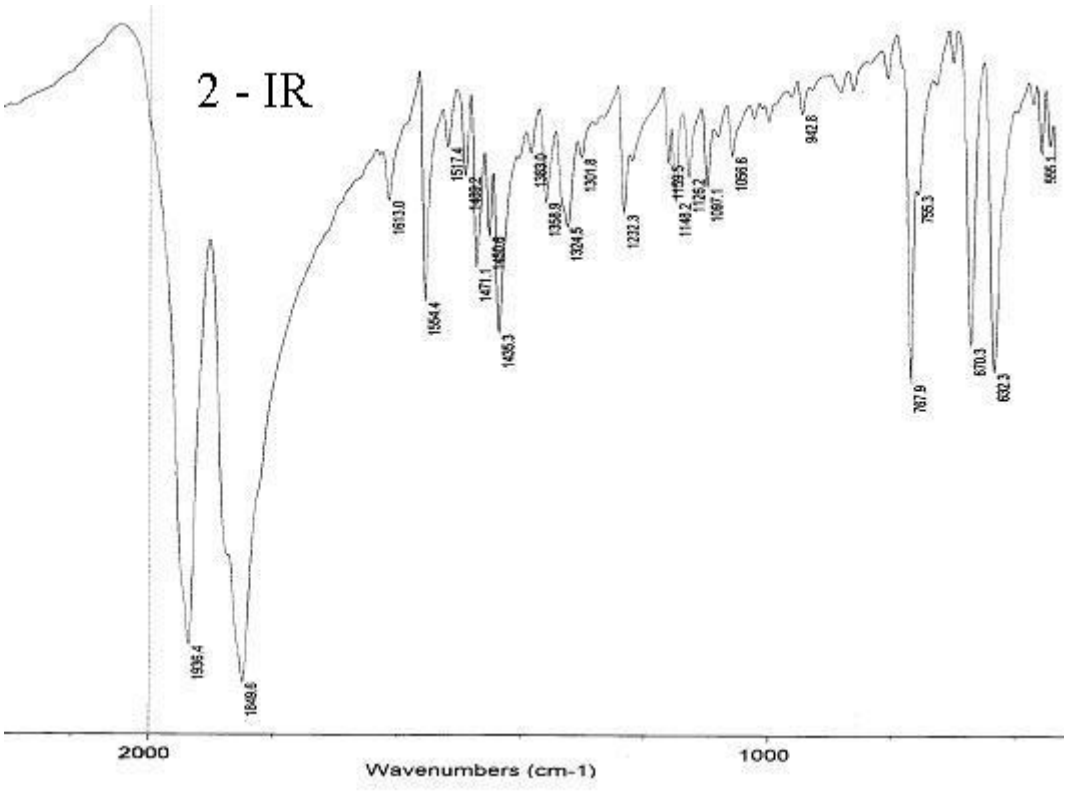
C(29)-P(1)-C(17)-C(22)	48.8(3)
Cr-P(1)-C(17)-C(22)	179.5(2)
C(22)-C(17)-C(18)-C(19)	0.5(5)
P(1)-C(17)-C(18)-C(19)	179.2(3)
C(17)-C(18)-C(19)-C(20)	-0.3(7)
C(18)-C(19)-C(20)-C(21)	-0.1(7)
C(19)-C(20)-C(21)-C(22)	0.2(7)
C(20)-C(21)-C(22)-C(17)	0.0(6)
C(18)-C(17)-C(22)-C(21)	-0.3(5)
P(1)-C(17)-C(22)-C(21)	-179.0(3)
C(17)-P(1)-C(23)-C(28)	172.4(3)
C(29)-P(1)-C(23)-C(28)	68.4(3)
Cr-P(1)-C(23)-C(28)	-60.7(3)
C(17)-P(1)-C(23)-C(24)	-16.6(3)
C(29)-P(1)-C(23)-C(24)	-120.6(3)
Cr-P(1)-C(23)-C(24)	110.3(3)
C(28)-C(23)-C(24)-C(25)	1.2(5)
P(1)-C(23)-C(24)-C(25)	-169.7(3)
C(23)-C(24)-C(25)-C(26)	0.0(6)
C(24)-C(25)-C(26)-C(27)	-1.5(7)
C(25)-C(26)-C(27)-C(28)	2.0(7)
C(26)-C(27)-C(28)-C(23)	-0.8(7)
C(24)-C(23)-C(28)-C(27)	-0.8(6)
P(1)-C(23)-C(28)-C(27)	170.7(3)
C(23)-P(1)-C(29)-C(34)	-156.7(3)
C(17)-P(1)-C(29)-C(34)	96.2(3)
Cr-P(1)-C(29)-C(34)	-32.4(3)
C(23)-P(1)-C(29)-C(30)	28.5(3)
C(17)-P(1)-C(29)-C(30)	-78.6(3)
Cr-P(1)-C(29)-C(30)	152.8(3)
C(34)-C(29)-C(30)-C(31)	-0.7(6)
P(1)-C(29)-C(30)-C(31)	174.2(3)
C(29)-C(30)-C(31)-C(32)	0.6(6)
C(30)-C(31)-C(32)-C(33)	-0.2(7)
C(31)-C(32)-C(33)-C(34)	0.0(7)
C(32)-C(33)-C(34)-C(29)	-0.1(6)
C(30)-C(29)-C(34)-C(33)	0.4(6)
P(1)-C(29)-C(34)-C(33)	-174.5(3)

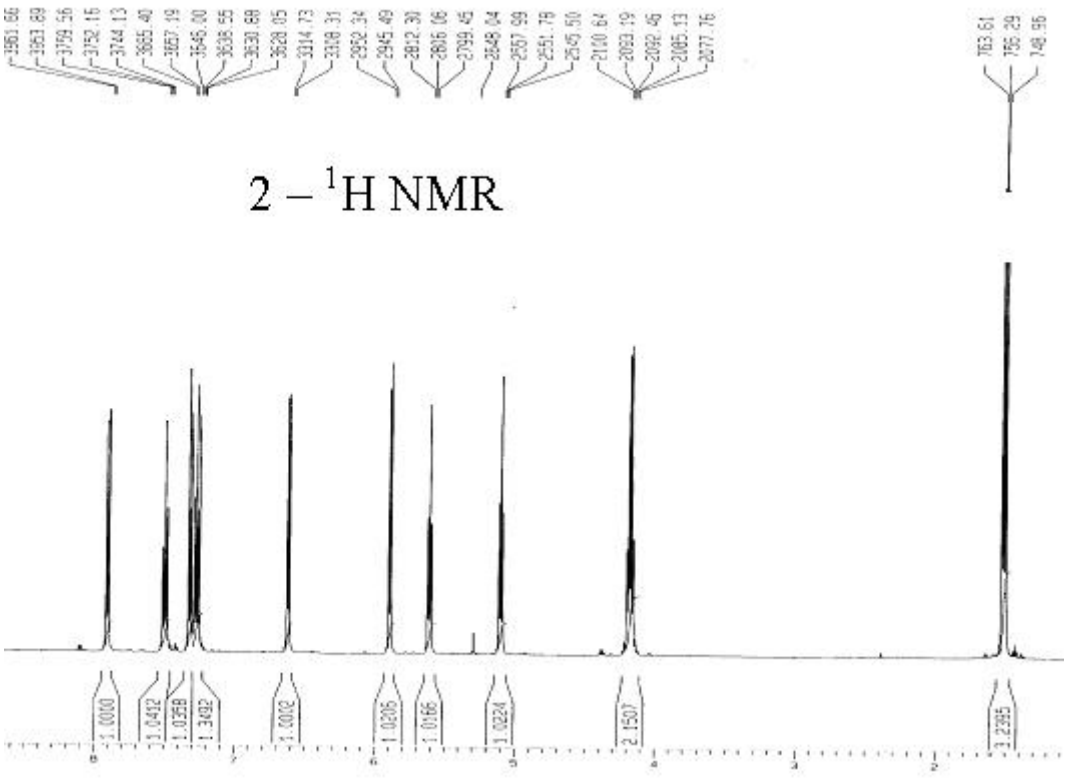
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for compound **4.** [A and deg.].

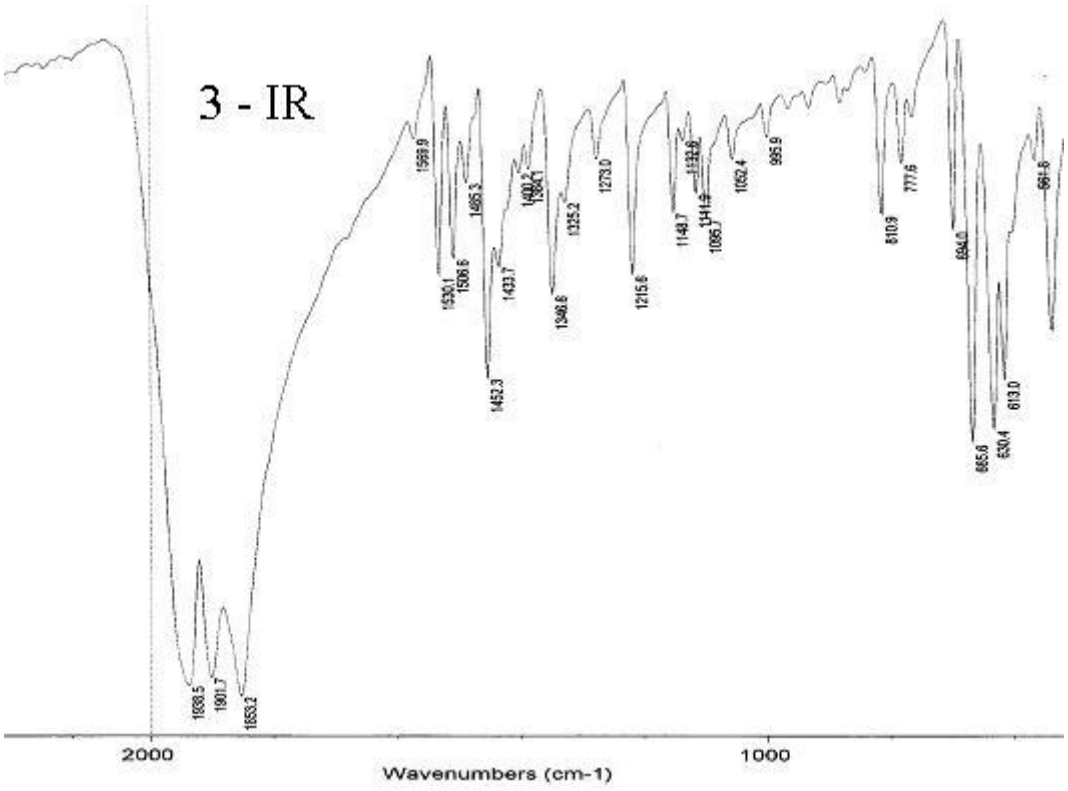
D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

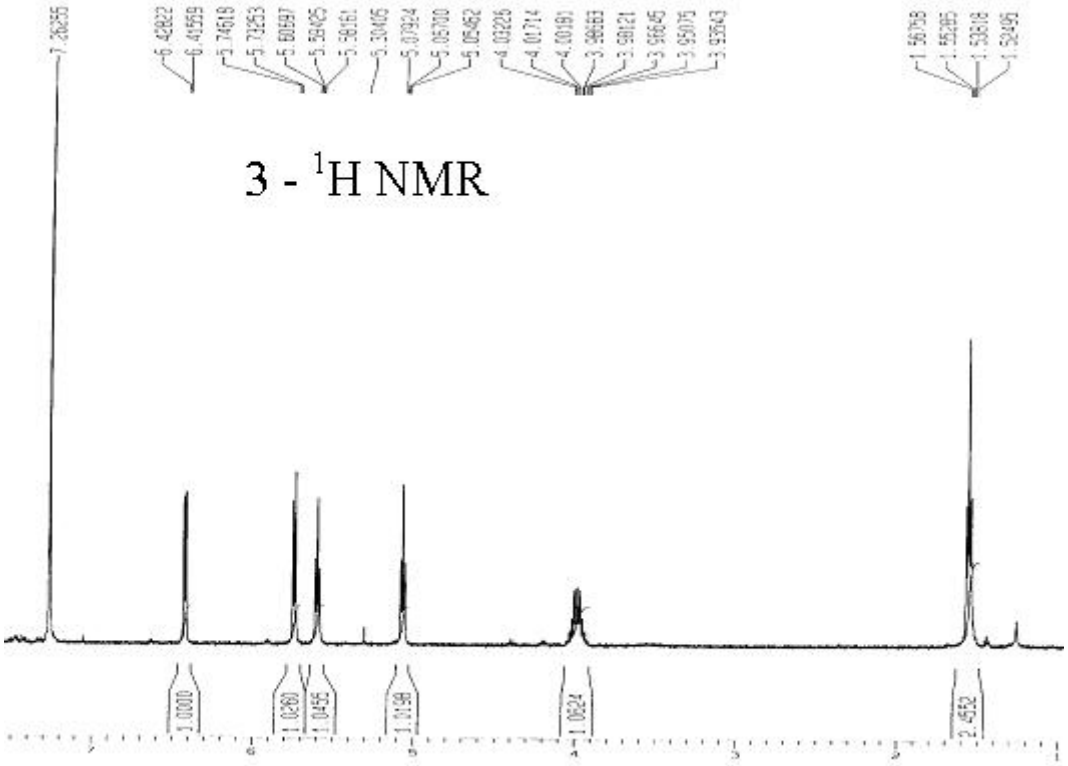
IR and ^{1}H NMR spectra for compound 2





IR and ^{1}H NMR spectra for compound 3





IR and ^{1}H NMR spectra for compound 4