Supplementary Material for Organic & Biomolecular Chemistry


## Supplementary data

# Chelation-control in nucleophilic addition to $Cr(CO)_3$-complexed aryl aldehydes

Suresh Kumar Tipparaju[a], Vedavati G. Puranik[b] and Amitabha Sarkar[a,c]*

*Division of Organic Chemistry (Synthesis) and Physical Chemistry Division*

*National Chemical Laboratory*

*Pune – 411 008, India.*

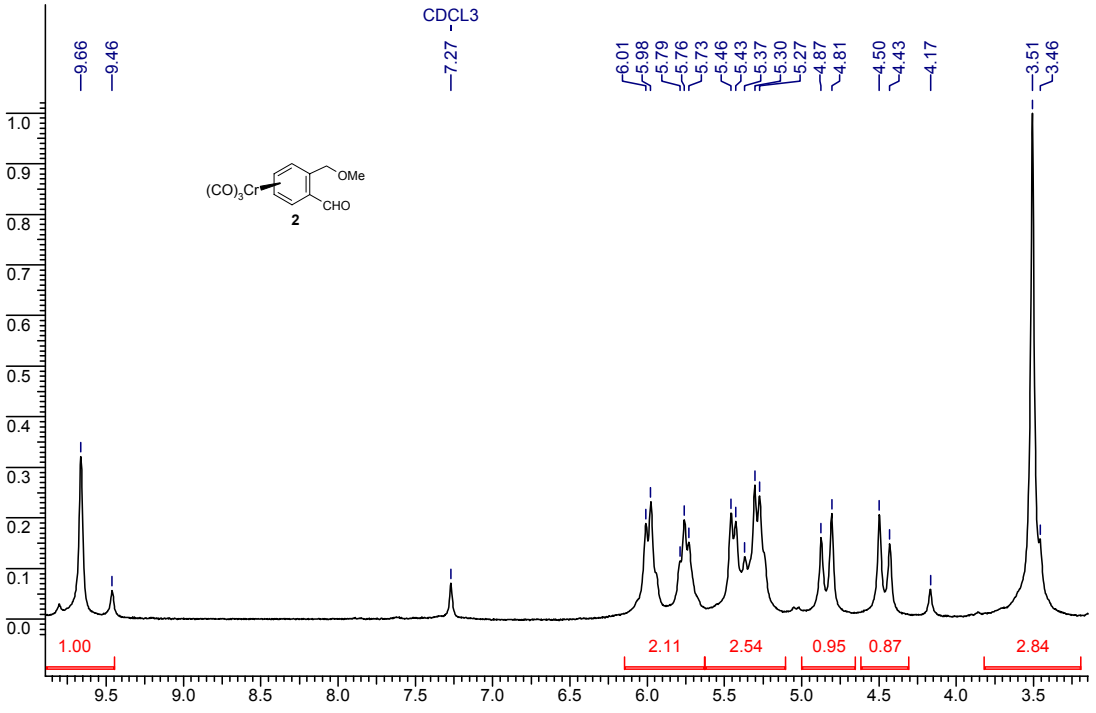
## Electronic Supplementary Information

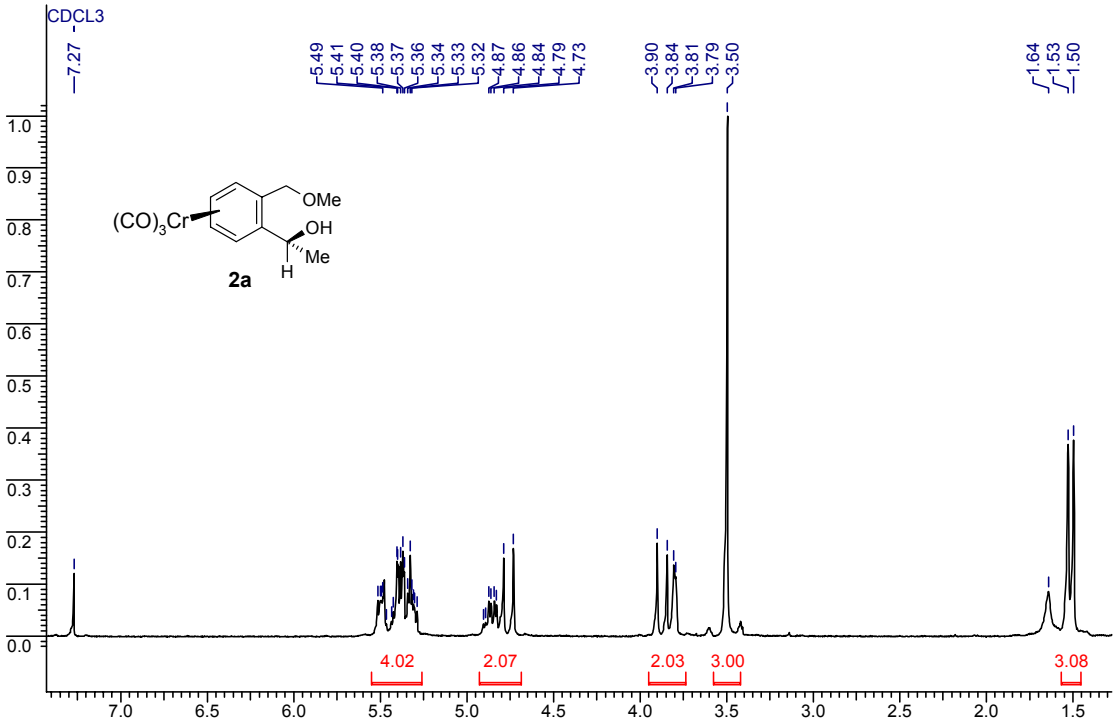
1) 200 and 300 MHz $H^1$ NMR Spectra of selected compounds

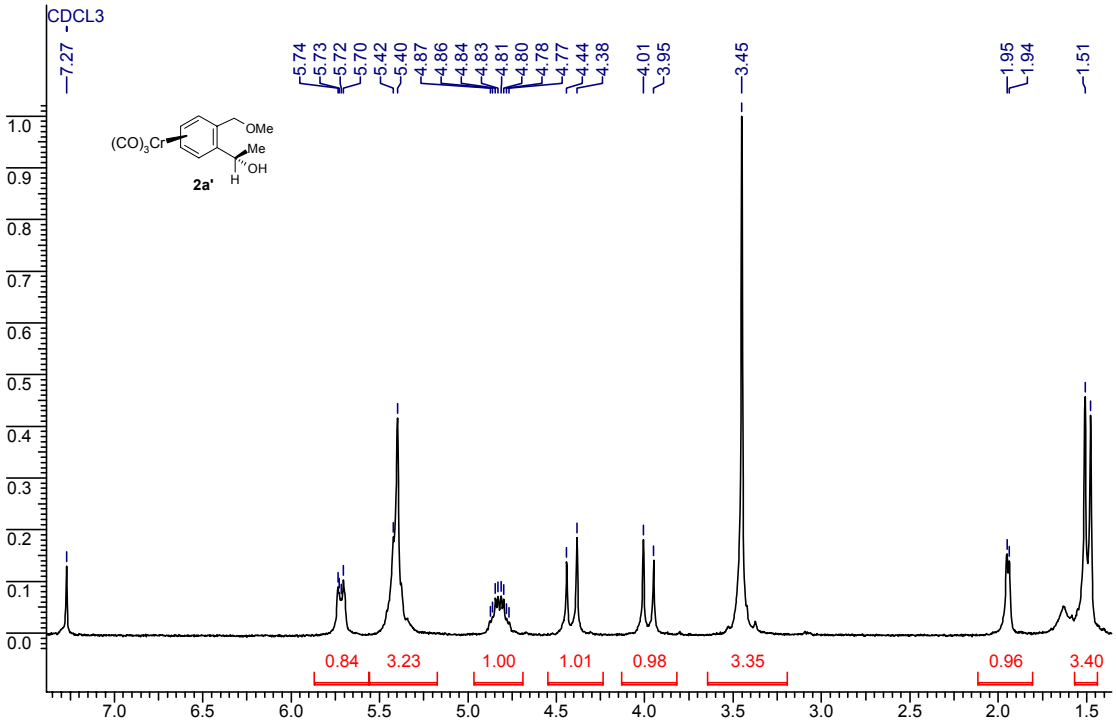
2) Crystallographic tables of bond angles, bond lengths, torsional angles etc for compounds **3a** and **3a'**

[a] Division of Organic Chemistry (Synthesis)
[b] Physical Chemistry Division
[c] Present address: Department of Organic Chemistry, Indian Association for the Cultivation of Science, Kolkata-700 064, India.

# $H^1$ NMR Spectra of selected compounds:

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4.80
4.78
4.77
4.44
4.38
4.01
3.95
3.45
1.95
1.94
1.51
(CO)3Cr
OMe
Me
OH
H
2a'
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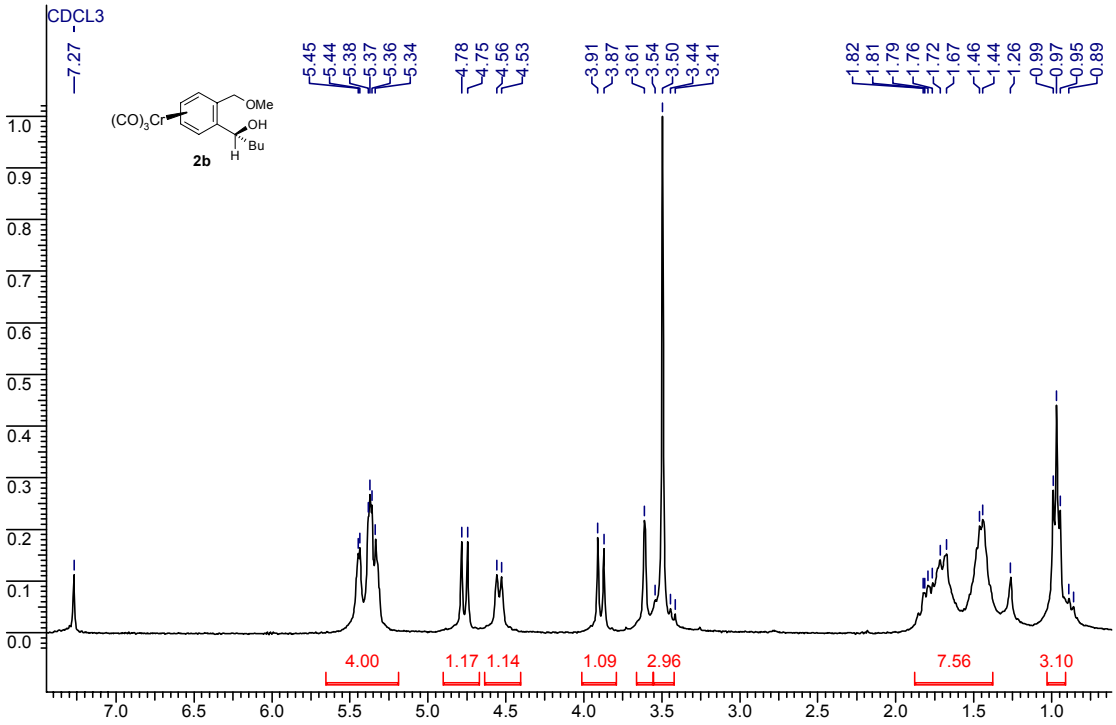
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3.61
3.54
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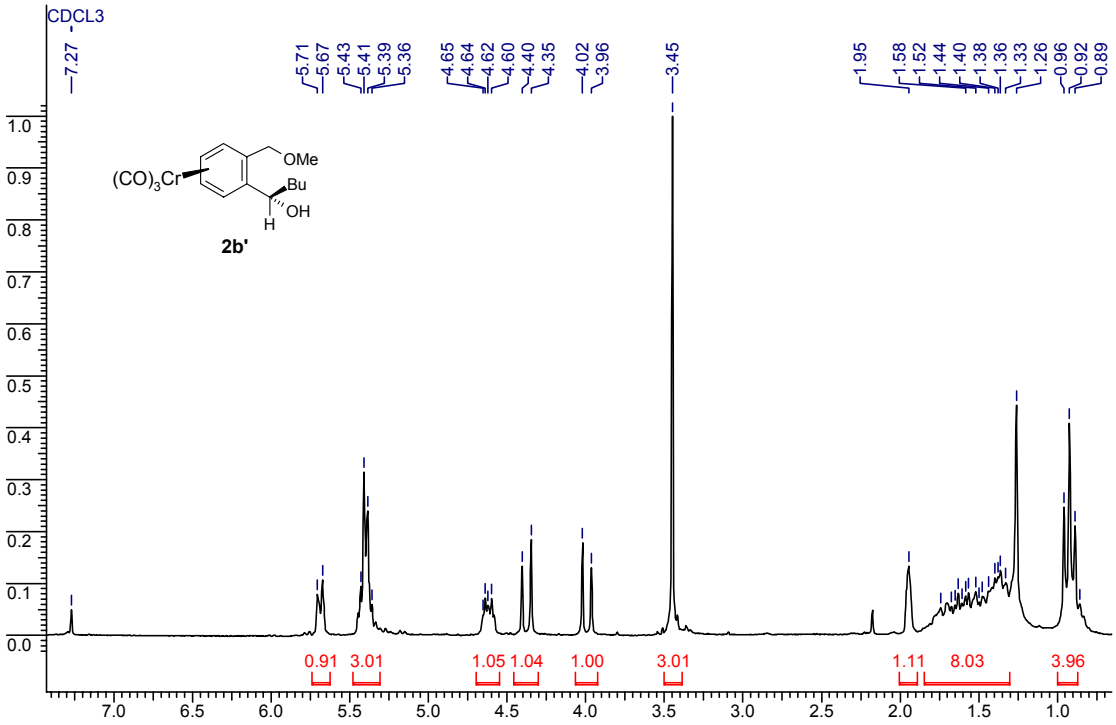
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1.52
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1.40
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1.36
1.33
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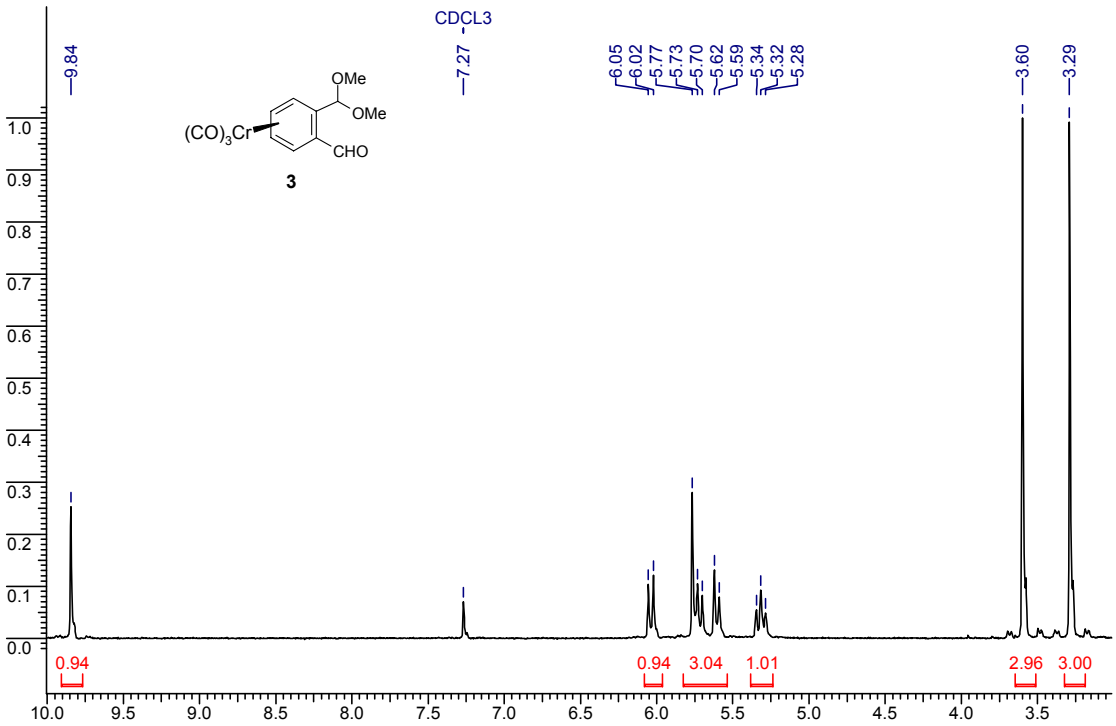
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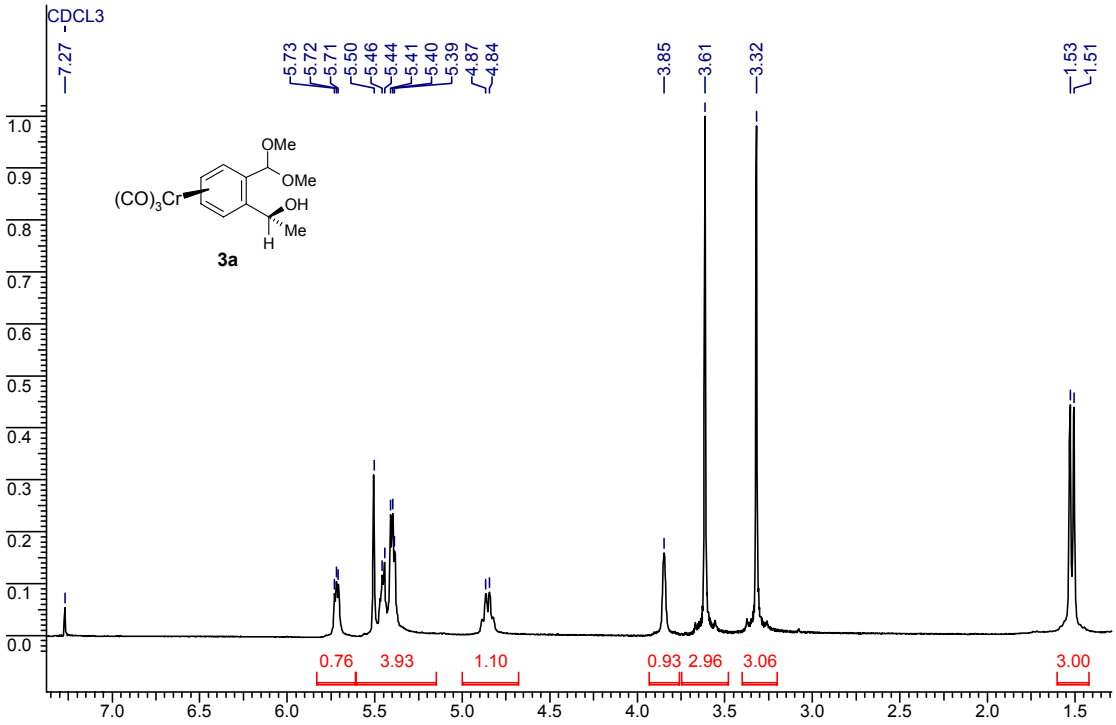
3.00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3.32
1.53
1.51
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3a
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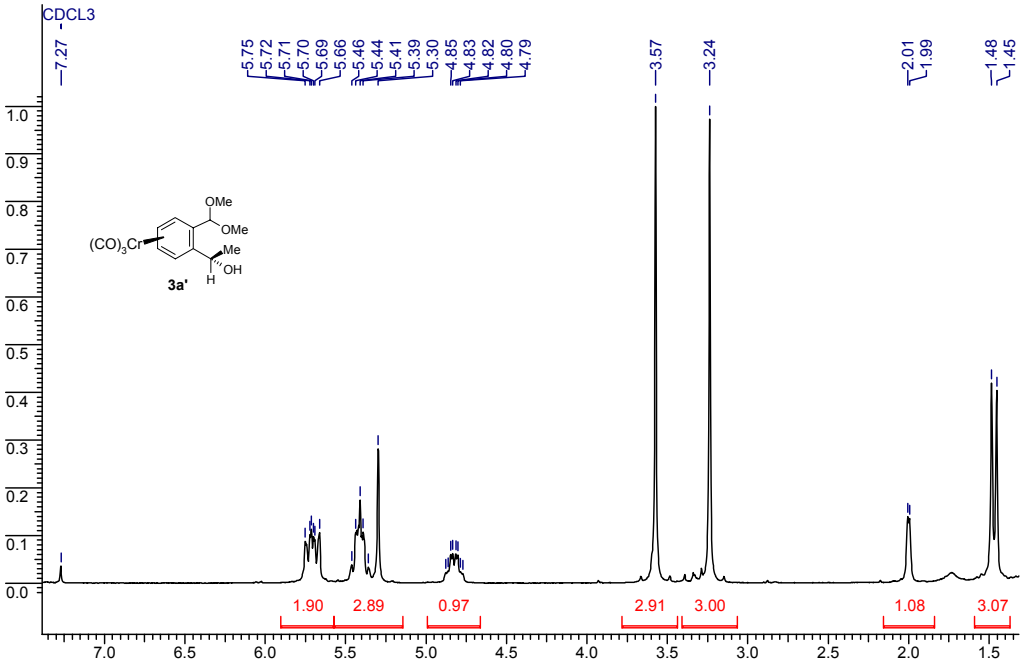
1.10
0.93
2.96
3.06
3.00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4.85
4.83
4.82
4.80
4.79
3.57
3.24
2.01
1.99
1.48
1.45
OMe
OMe
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OH
H
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0.97
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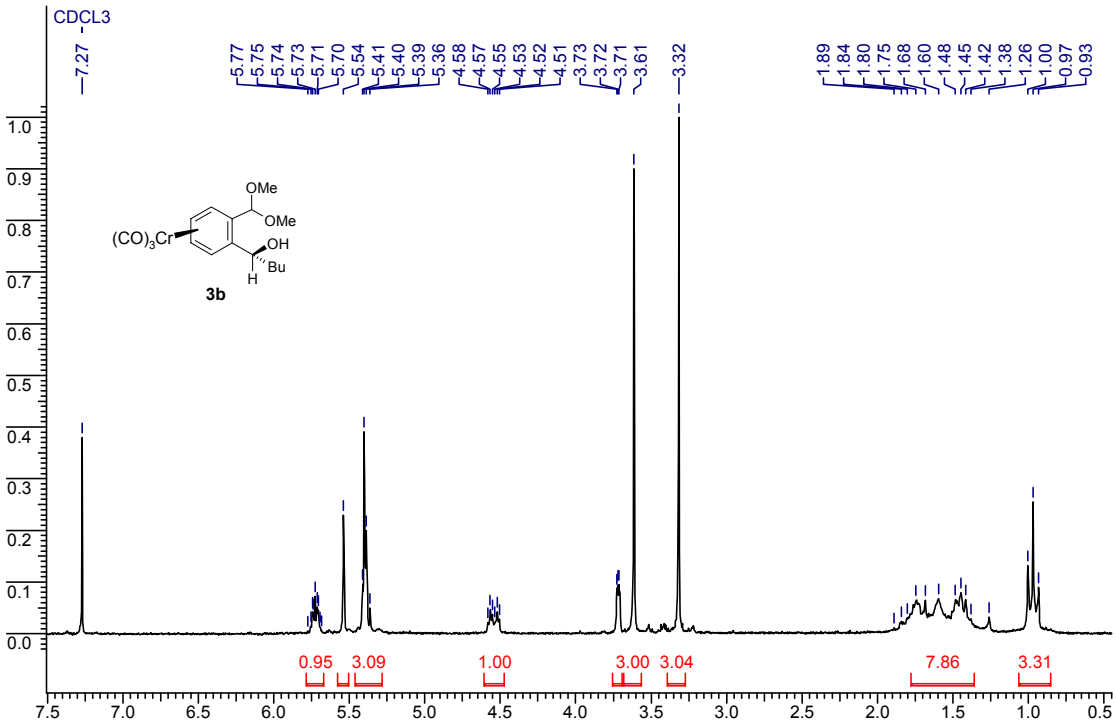
3.00
1.08
3.07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4.55
4.53
4.52
4.51
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3.72
3.71
3.61
3.32
1.89
1.84
1.80
1.75
1.68
1.60
1.48
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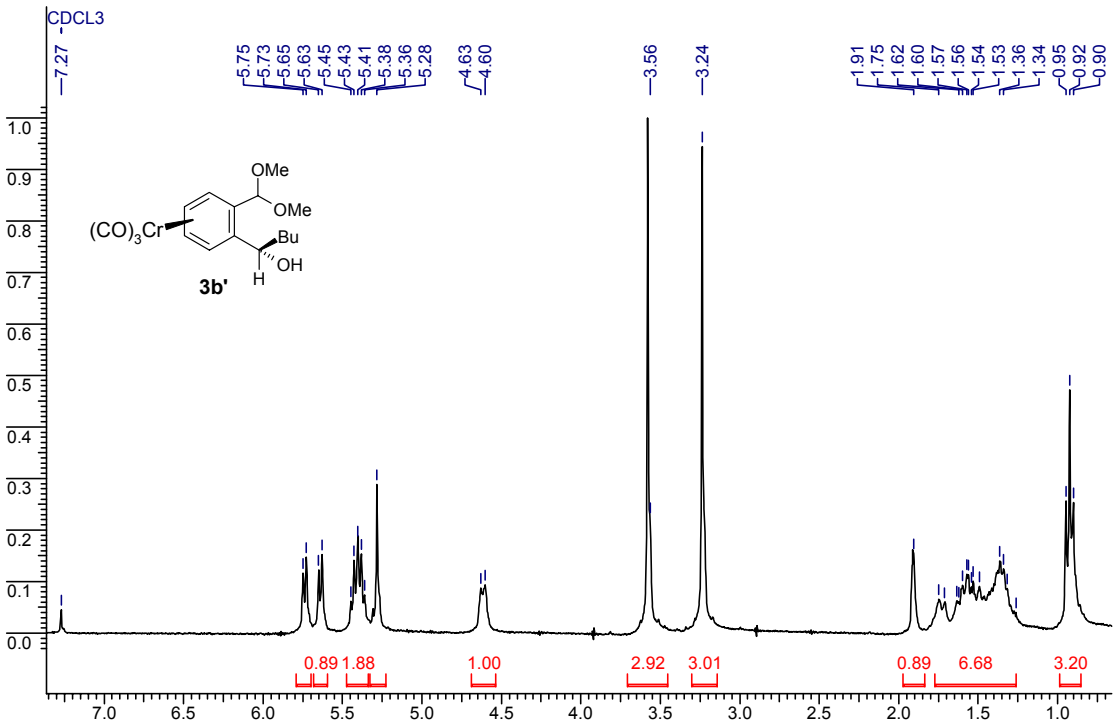
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4.60
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1.91
1.75
1.62
1.60
1.57
1.56
1.54
1.53
1.36
1.34
0.95
0.92
0.90
OMe
OMe
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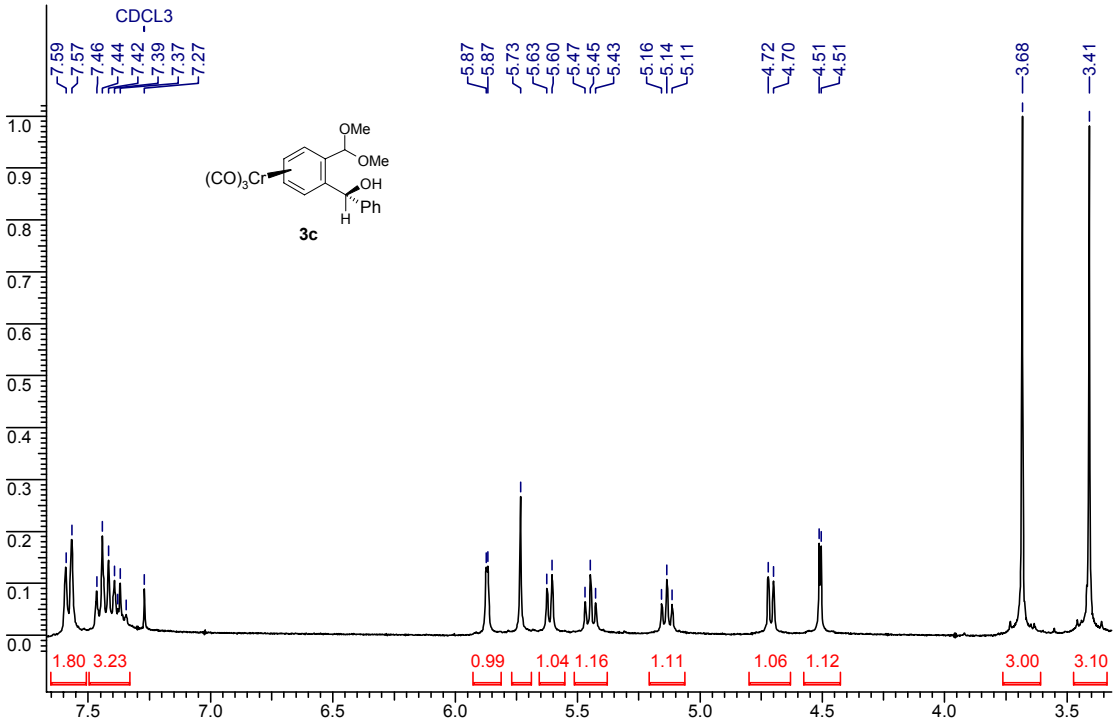
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5.60
5.47
5.45
5.43
5.16
5.14
5.11
4.72
4.70
4.51
4.51
3.68
3.41
OMe
OMe
(CO)3Cr
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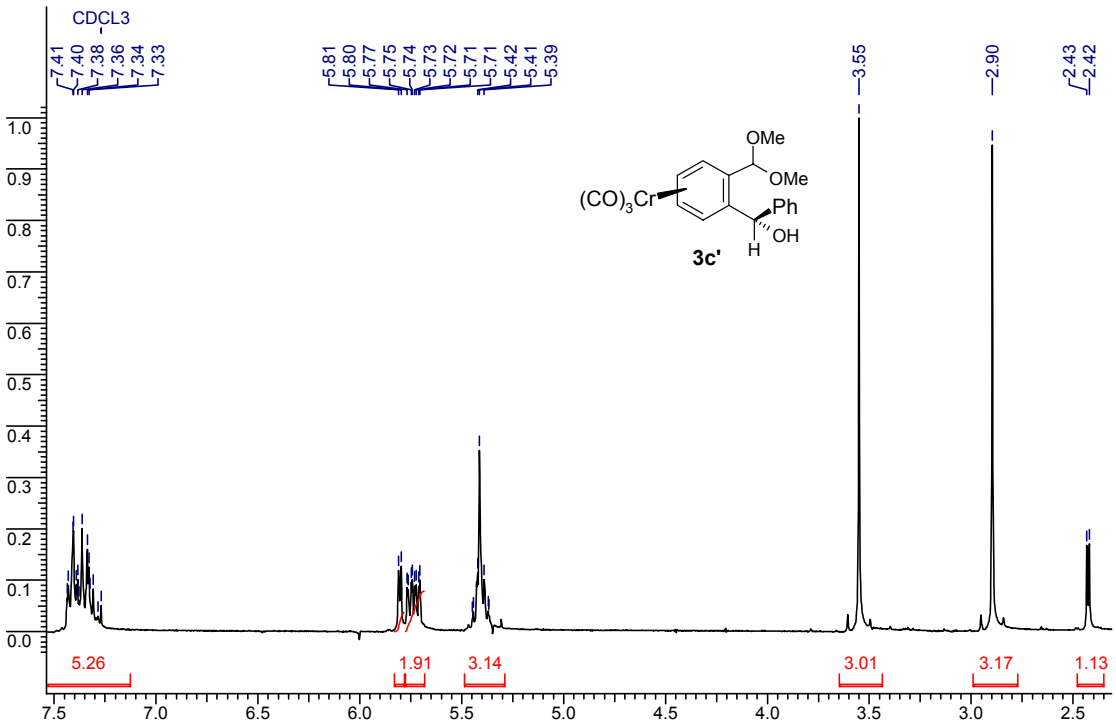
1.12
3.00
3.10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5.72
5.71
5.71
5.42
5.41
5.39
3.55
2.90
2.43
2.42
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Ph
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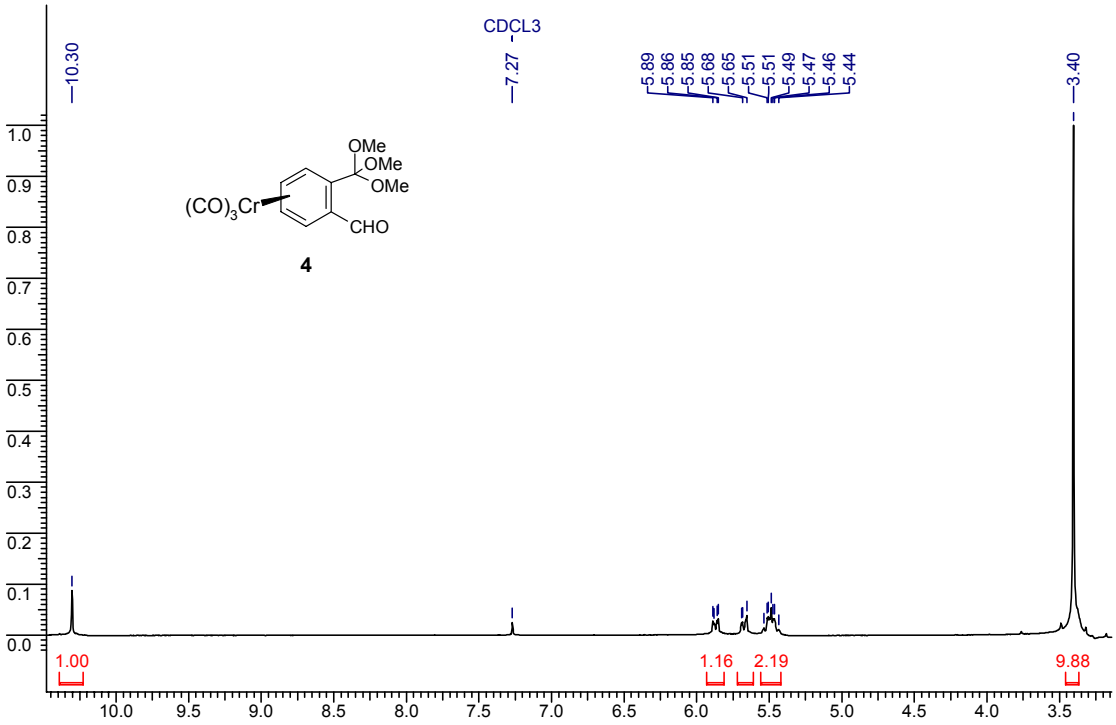
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CHO
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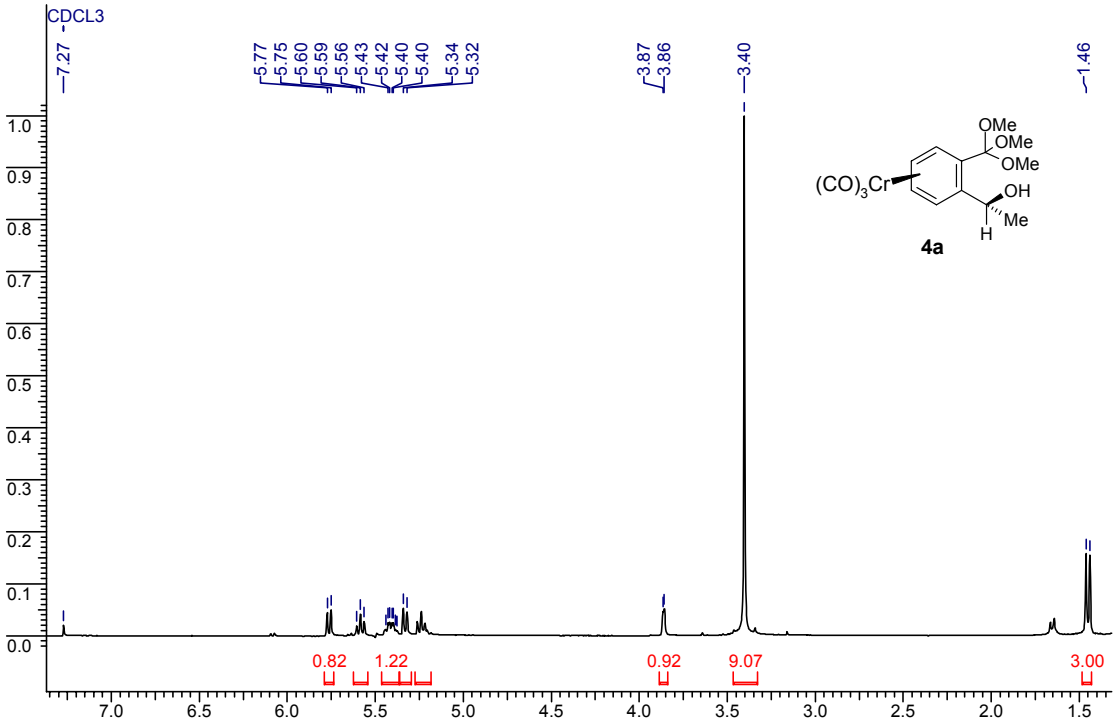
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3.87
3.86
3.40
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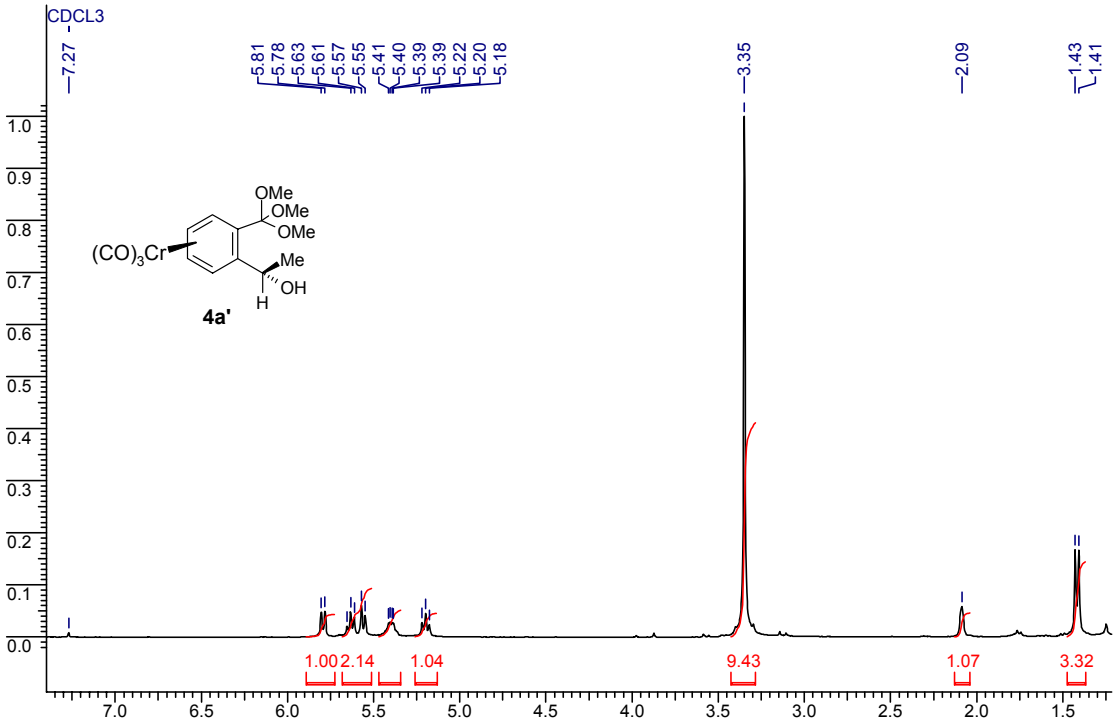
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5.40
5.39
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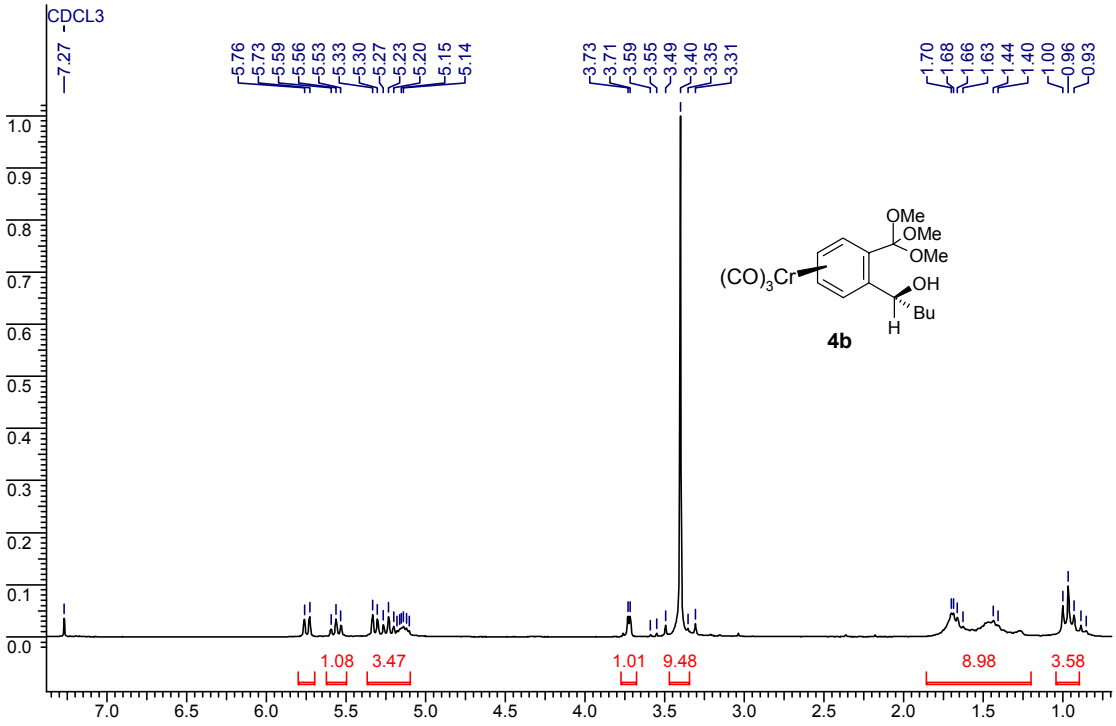
5.22
5.20
5.18
3.35
2.09
1.43
1.41
OMe
OMe
OMe
(CO)3Cr
Me
OH
H
4a'
1.00
2.14
1.04
9.43
1.07
3.32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3.59
3.55
3.49
3.40
3.35
3.31
1.70
1.68
1.66
1.63
1.44
1.40
1.00
0.96
0.93
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OMe
OMe
(CO)3Cr
OH
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H
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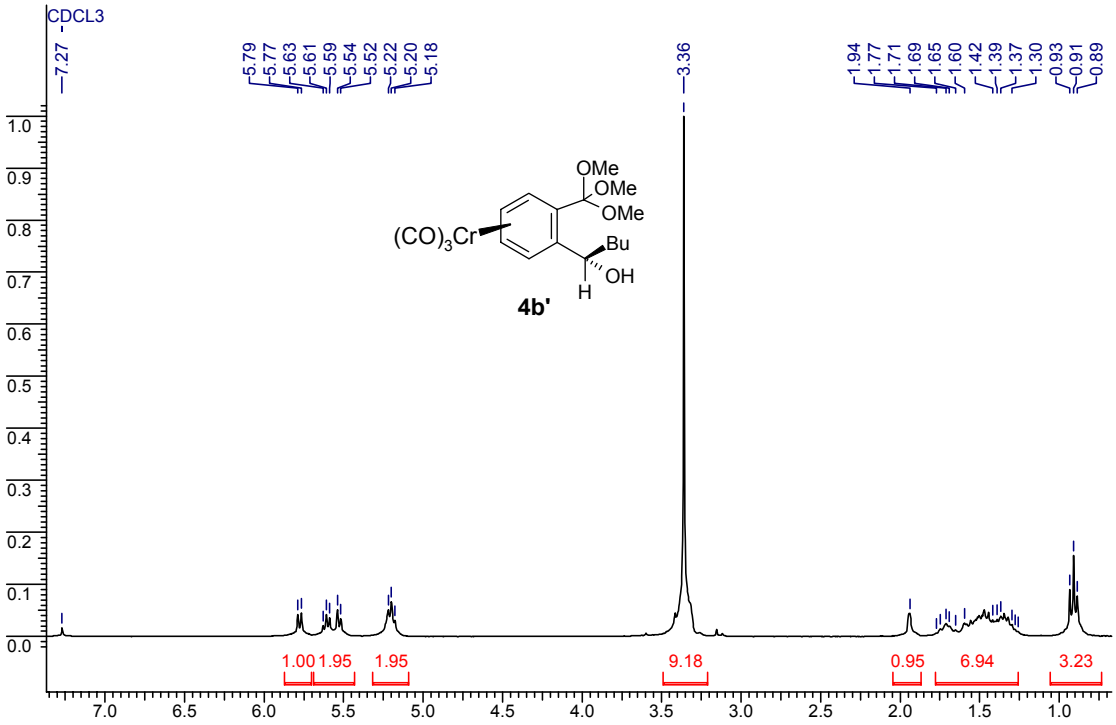
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1.94
1.77
1.71
1.69
1.65
1.60
1.42
1.39
1.37
1.30
0.93
0.91
0.89
OMe
OMe
OMe
(CO)3Cr
Bu
OH
H
4b'
1.00
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1.95
9.18
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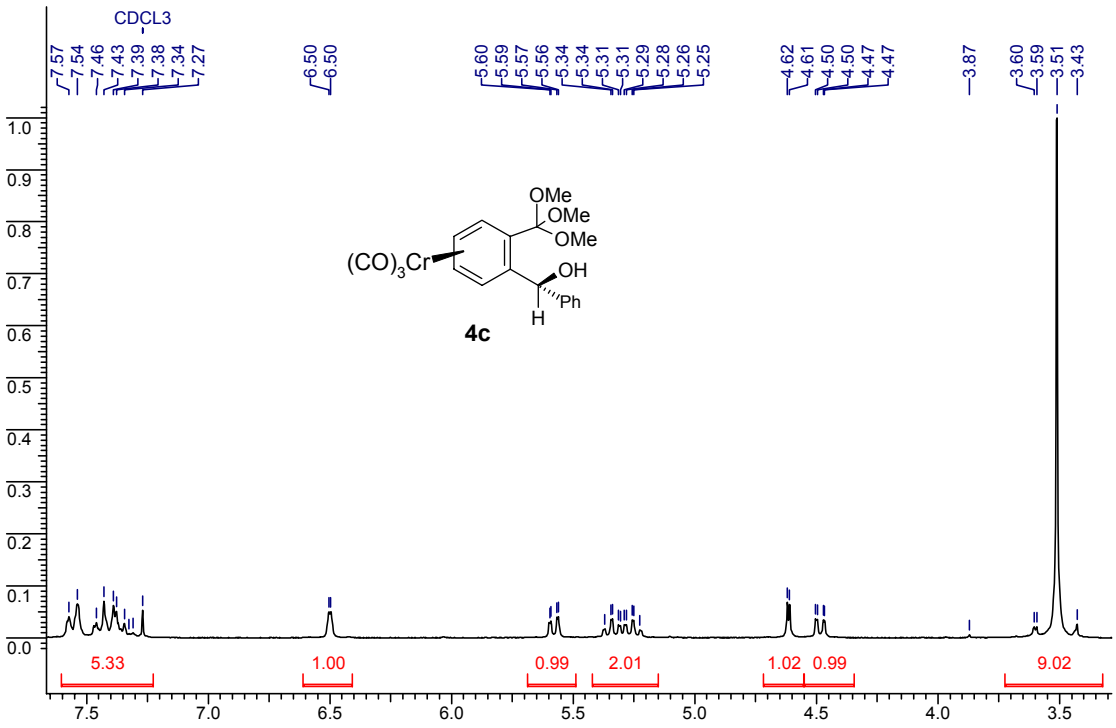
6.94
3.23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5.31
5.29
5.28
5.26
5.25
4.62
4.61
4.50
4.50
4.47
4.47
3.87
3.60
3.59
3.51
3.43
OMe
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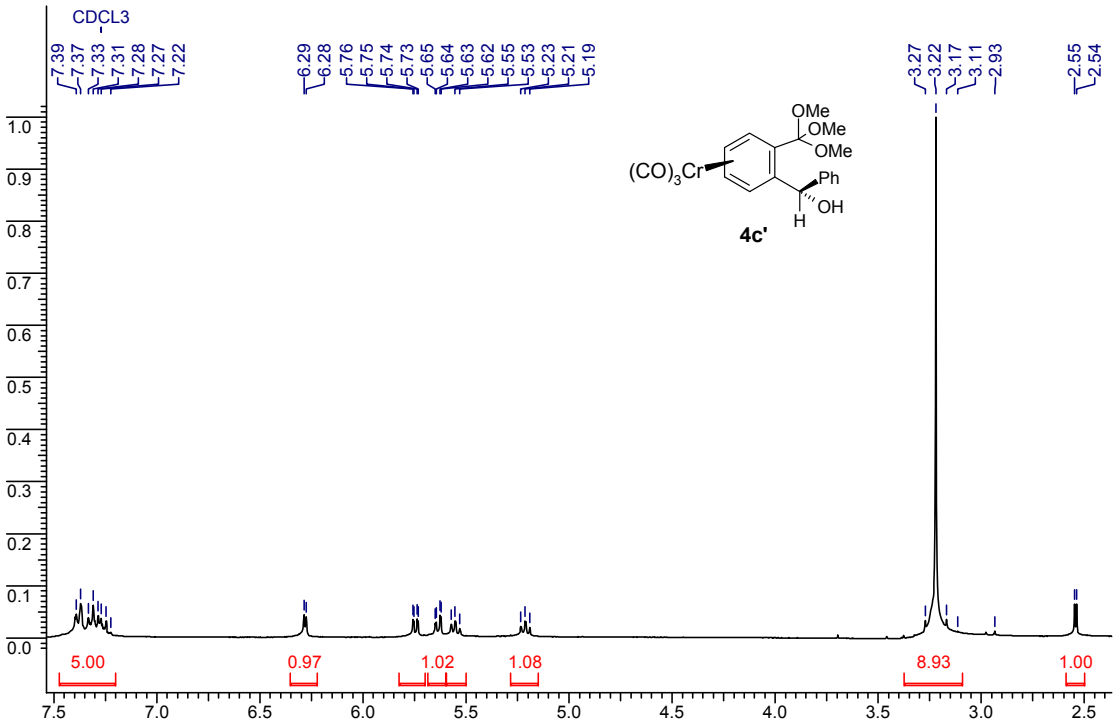


## X-ray Crystal Structure Analysis For 3a' and 3a:

Data for both the compounds were collected on *MACH-3* diffractometer using Mo $K_\alpha$ radiation with fine focus tube. All the data were corrected for Lorentzian, polarisation and absorption effects. SHELX-97 (SHELXTL)[ref] was used for structure solution and full matrix least squares refinement on $F^2$. Data collection and refinement parameters are listed in table 1 and 2 respectively.

**Crystal Data for 3a':** Rectangular pale yellow single crystals were grown by slow evaporation of solvent from a mixture of dichloromethane and petroleum ether. $C_{14}H_{22}CrO_6$, $M$ = 332.27. Crystals belong to monoclinic, space group P21/n$^o$, $a$ = 13.639(1), $b$ = 8.994(1), $c$ = 13.74(1) Å, β = 113.594 (7) °, $V$ = 1544.6 (3) Å$^3$, $Z$ = 4, $D_c$ = 1.429 mg m$^{-3}$, $\mu$ (Mo–$K_\alpha$) = 0.763 mm$^{-1}$, $T$ = 293(2) K, 2710 unique [I>2σ(I)], $R_1$ = 0.0289, $wR_2$ = 0.0838.

**Crystal Data for 3a:** Cubic yellow single crystals were grown by slow evaporation of solvent from a mixture of dichloromethane and petroleum ether. $C_{14}H_{22}CrO_6$, $M$ =

332.27. Crystals belong to monoclinic, space group P21/c$^{o}$, $a$ = 8.099(1), $b$ = 8.084(6), $c$ = 23.252(2) Å, β = 99.51(1) °, $V$ = 1501.4(3) Å$^3$, $Z$ = 4, $D_c$ = 1.47 mg m$^{-3}$, $\mu$ (Mo–K$_\alpha$) = 0.785 mm$^{-1}$, $T$ = 293(2) K, 2649unique [I>2σ(I)], $R_1$ = 0.0350, w$R_2$ = 0.0889.

Reference

G. M. Sheldrick, SHELX-97 program for crystal structure solution and refinement, University of Gottingen, Germany, 1997

## Table 1. Crystal data and structure refinement for 3a

| | |
|---|---|
| Empirical formula | C14 H16 Cr O6 |
| Formula weight | 332.27 |
| Temperature | 293(2) K |
| Wavelength | 0.70930 Å |
| Crystal system, space group | Monoclinic, P21/c$^{o}$ |
| Unit cell dimensions | a = 8.099(1) Å<br>b = 8.084(6)Å β = 99.51(1) °<br>c = 23.252(2) Å |
| Volume | 1501.4(3) Å$^3$ |
| Z, Calculated density | 4, 1.470 Mg/m$^3$ |
| Absorption coefficient | 0.785 mm$^{-1}$ |
| F(000) | 688 |
| Crystal size | 0.25 x 0.20 x 0.20 mm |
| Theta range for data collection | 1.77 to 24.91°. |
| Limiting indices | -9<=h<=9, 0<=k<=9, 0<=l<=27 |
| Reflections collected / unique | 2649 / 2649 [R(int)= 0.0000] |
| Completeness to theta = 24.91 | 100.0 % |
| Refinement method | Full-matrix least-squares on F$^2$ |
| Data / restraints / parameters | 2649 / 0 / 254 |
| Goodness-of-fit on F$^2$ | 1.022 |
| Final R indices [I>2sigma(I)] | R1 = 0.0350, wR2 = 0.0889 |
| R indices (all data) | R1 = 0.0527, wR2 = 0.0949 |

Largest diff. peak and hole 0.365 and -0.269 e. $Å^{-3}$

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cr | 9874(1) | 7413(1) | 3652(1) | 37(1) |
| O(1) | 13190(2) | 9011(3) | 3605(1) | 82(1) |
| O(2) | 9168(4) | 7445(3) | 2348(1) | 104(1) |
| O(3) | 8593(3) | 10865(3) | 3657(1) | 91(1) |
| O(6) | 5904(3) | 6639(3) | 4826(1) | 58(1) |
| O(4) | 5958(2) | 5062(2) | 2920(1) | 54(1) |
| O(5) | 4921(2) | 4833(2) | 3797(1) | 45(1) |
| C(1) | 11919(3) | 8372(4) | 3624(1) | 55(1) |
| C(2) | 9446(4) | 7435(4) | 2850(1) | 62(1) |
| C(3) | 9063(3) | 9528(4) | 3651(1) | 54(1) |
| C(4) | 8229(3) | 6750(3) | 4296(1) | 37(1) |
| C(5) | 9916(3) | 6732(4) | 4581(1) | 46(1) |
| C(6) | 11139(3) | 5808(4) | 4357(1) | 54(1) |
| C(7) | 10683(3) | 4832(3) | 3864(1) | 52(1) |
| C(8) | 9034(3) | 4816(3) | 3581(1) | 44(1) |
| C(9) | 7781(3) | 5767(3) | 3789(1) | 36(1) |
| C(10) | 6896(3) | 7742(3) | 4545(1) | 45(1) |
| C(11) | 5980(3) | 5731(3) | 3472(1) | 40(1) |
| C(12) | 4389(5) | 5307(6) | 2541(2) | 76(1) |
| C(13) | 5287(5) | 3119(4) | 3869(2) | 65(1) |
| C(14) | 7563(5) | 9019(5) | 4990(2) | 68(1) |

Table 3. Bond lengths [Å] and angles [°] for **3a**.

| | |
|---|---|
| Cr-C(3) | 1.832(3) |
| Cr-C(2) | 1.839(3) |
| Cr-C(1) | 1.840(3) |
| Cr-C(8) | 2.204(3) |
| Cr-C(6) | 2.205(3) |
| Cr-C(7) | 2.217(3) |
| Cr-C(9) | 2.218(2) |
| Cr-C(5) | 2.222(3) |
| Cr-C(4) | 2.228(2) |
| O(1)-C(1) | 1.159(3) |
| O(2)-C(2) | 1.153(4) |
| O(3)-C(3) | 1.147(3) |
| O(6)-C(10) | 1.428(3) |
| O(6)-H(6O) | 0.71(3) |

| | |
|---|---|
| O(4)-C(11) | 1.391(3) |
| O(4)-C(12) | 1.435(4) |
| O(5)-C(13) | 1.420(4) |
| O(5)-C(11) | 1.432(3) |
| C(4)-C(5) | 1.416(3) |
| C(4)-C(9) | 1.420(3) |
| C(4)-C(10) | 1.533(3) |
| C(5)-C(6) | 1.407(4) |
| C(5)-H(5) | 0.91(3) |
| C(6)-C(7) | 1.390(4) |
| C(6)-H(6) | 0.92(3) |
| C(7)-C(8) | 1.387(4) |
| C(7)-H(7) | 0.84(3) |
| C(8)-C(9) | 1.419(3) |
| C(8)-H(8) | 0.95(2) |
| C(9)-C(11) | 1.522(3) |
| C(10)-C(14) | 1.498(4) |
| C(10)-H(10) | 0.90(2) |
| C(11)-H(11A) | 0.96(2) |
| C(12)-H(12A) | 1.00(5) |
| C(12)-H(12B) | 1.03(4) |
| C(12)-H(12C) | 0.97(4) |
| C(13)-H(13A) | 0.87(4) |
| C(13)-H(13B) | 0.95(4) |
| C(13)-H(13C) | 1.02(5) |
| C(14)-H(14A) | 0.90(3) |
| C(14)-H(14B) | 0.94(4) |
| C(14)-H(14C) | 0.95(3) |
| C(3)-Cr-C(2) | 88.93(13) |
| C(3)-Cr-C(1) | 86.04(12) |
| C(2)-Cr-C(1) | 88.82(13) |
| C(3)-Cr-C(8) | 141.54(11) |
| C(2)-Cr-C(8) | 85.95(12) |
| C(1)-Cr-C(8) | 131.84(11) |
| C(3)-Cr-C(6) | 132.33(13) |
| C(2)-Cr-C(6) | 138.19(13) |
| C(1)-Cr-C(6) | 87.93(11) |
| C(8)-Cr-C(6) | 66.11(11) |
| C(3)-Cr-C(7) | 166.29(12) |
| C(2)-Cr-C(7) | 103.50(13) |
| C(1)-Cr-C(7) | 99.77(11) |
| C(8)-Cr-C(7) | 36.57(10) |
| C(6)-Cr-C(7) | 36.63(11) |
| C(3)-Cr-C(9) | 106.15(10) |
| C(2)-Cr-C(9) | 97.50(11) |
| C(1)-Cr-C(9) | 166.29(10) |
| C(8)-Cr-C(9) | 37.45(9) |
| C(6)-Cr-C(9) | 79.24(9) |
| C(7)-Cr-C(9) | 66.97(9) |
| C(3)-Cr-C(5) | 100.44(12) |
| C(2)-Cr-C(5) | 163.17(13) |
| C(1)-Cr-C(5) | 105.63(11) |
| C(8)-Cr-C(5) | 78.00(11) |
| C(6)-Cr-C(5) | 37.06(10) |
| C(7)-Cr-C(5) | 66.10(11) |
| C(9)-Cr-C(5) | 66.57(9) |
| C(3)-Cr-C(4) | 88.40(10) |

| | |
|---|---|
| C(2)-Cr-C(4) | 130.58(11) |
| C(1)-Cr-C(4) | 140.09(11) |
| C(8)-Cr-C(4) | 67.05(9) |
| C(6)-Cr-C(4) | 67.37(9) |
| C(7)-Cr-C(4) | 79.16(9) |
| C(9)-Cr-C(4) | 37.24(8) |
| C(5)-Cr-C(4) | 37.11(8) |
| C(10)-O(6)-H(6O) | 110(2) |
| C(11)-O(4)-C(12) | 112.8(2) |
| C(13)-O(5)-C(11) | 115.1(2) |
| O(1)-C(1)-Cr | 178.5(3) |
| O(2)-C(2)-Cr | 179.5(3) |
| O(3)-C(3)-Cr | 178.3(3) |
| C(5)-C(4)-C(9) | 118.5(2) |
| C(5)-C(4)-C(10) | 120.9(2) |
| C(9)-C(4)-C(10) | 120.5(2) |
| C(5)-C(4)-Cr | 71.23(14) |
| C(9)-C(4)-Cr | 70.99(12) |
| C(10)-C(4)-Cr | 131.64(17) |
| C(6)-C(5)-C(4) | 121.1(3) |
| C(6)-C(5)-Cr | 70.79(16) |
| C(4)-C(5)-Cr | 71.65(14) |
| C(6)-C(5)-H(5) | 119.8(18) |
| C(4)-C(5)-H(5) | 118.7(18) |
| Cr-C(5)-H(5) | 124.7(16) |
| C(7)-C(6)-C(5) | 119.9(3) |
| C(7)-C(6)-Cr | 72.19(16) |
| C(5)-C(6)-Cr | 72.15(15) |
| C(7)-C(6)-H(6) | 123.3(18) |
| C(5)-C(6)-H(6) | 116.8(18) |
| Cr-C(6)-H(6) | 128.3(18) |
| C(8)-C(7)-C(6) | 120.0(3) |
| C(8)-C(7)-Cr | 71.20(15) |
| C(6)-C(7)-Cr | 71.18(16) |
| C(8)-C(7)-H(7) | 123.4(19) |
| C(6)-C(7)-H(7) | 116.5(19) |
| Cr-C(7)-H(7) | 128.2(18) |
| C(7)-C(8)-C(9) | 121.3(3) |
| C(7)-C(8)-Cr | 72.23(16) |
| C(9)-C(8)-Cr | 71.79(14) |
| C(7)-C(8)-H(8) | 118.4(15) |
| C(9)-C(8)-H(8) | 120.3(15) |
| Cr-C(8)-H(8) | 128.0(15) |
| C(8)-C(9)-C(4) | 119.1(2) |
| C(8)-C(9)-C(11) | 120.5(2) |
| C(4)-C(9)-C(11) | 120.38(19) |
| C(8)-C(9)-Cr | 70.76(14) |
| C(4)-C(9)-Cr | 71.76(13) |
| C(11)-C(9)-Cr | 129.55(16) |
| O(6)-C(10)-C(14) | 106.3(2) |
| O(6)-C(10)-C(4) | 109.3(2) |
| C(14)-C(10)-C(4) | 115.2(2) |
| O(6)-C(10)-H(10) | 110.2(15) |
| C(14)-C(10)-H(10) | 109.7(15) |
| C(4)-C(10)-H(10) | 106.2(15) |
| O(4)-C(11)-O(5) | 111.91(19) |
| O(4)-C(11)-C(9) | 108.60(19) |

| | |
|---|---|
| O(5)-C(11)-C(9) | 111.39(19) |
| O(4)-C(11)-H(11A) | 109.6(12) |
| O(5)-C(11)-H(11A) | 104.1(13) |
| C(9)-C(11)-H(11A) | 111.1(13) |
| O(4)-C(12)-H(12A) | 111(2) |
| O(4)-C(12)-H(12B) | 111(2) |
| H(12A)-C(12)-H(12B) | 101(3) |
| O(4)-C(12)-H(12C) | 110(2) |
| H(12A)-C(12)-H(12C) | 107(3) |
| H(12B)-C(12)-H(12C) | 117(3) |
| O(5)-C(13)-H(13A) | 108(3) |
| O(5)-C(13)-H(13B) | 111(2) |
| H(13A)-C(13)-H(13B) | 119(3) |
| O(5)-C(13)-H(13C) | 110(3) |
| H(13A)-C(13)-H(13C) | 112(4) |
| H(13B)-C(13)-H(13C) | 96(3) |
| C(10)-C(14)-H(14A) | 109(2) |
| C(10)-C(14)-H(14B) | 110(2) |
| H(14A)-C(14)-H(14B) | 101(3) |
| C(10)-C(14)-H(14C) | 110(2) |
| H(14A)-C(14)-H(14C) | 112(3) |
| H(14B)-C(14)-H(14C) | 115(3) |

Table 4. Anisotropic displacement parameters ($A^2$ x $10^3$) for **3a**. 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 | 25(1) | 42(1) | 47(1) | 8(1) | 11(1) | 3(1) |
| O(1) | 36(1) | 85(2) | 128(2) | 24(1) | 25(1) | -7(1) |
| O(2) | 138(3) | 125(2) | 51(1) | 13(1) | 19(2) | -13(2) |
| O(3) | 86(2) | 49(1) | 144(2) | 18(1) | 40(2) | 22(1) |
| O(6) | 44(1) | 82(2) | 54(1) | -15(1) | 24(1) | -13(1) |
| O(4) | 47(1) | 73(1) | 44(1) | -8(1) | 8(1) | -5(1) |
| O(5) | 30(1) | 56(1) | 53(1) | -6(1) | 15(1) | -6(1) |
| C(1) | 36(1) | 58(2) | 72(2) | 12(1) | 14(1) | 5(1) |
| C(2) | 65(2) | 67(2) | 57(2) | 11(2) | 20(2) | -6(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(3) | 40(1) | 54(2) | 72(2) | 14(1) | 19(1) | 3(1) |
| C(4) | 26(1) | 46(1) | 40(1) | 6(1) | 12(1) | 1(1) |
| C(5) | 30(1) | 64(2) | 44(1) | 9(1) | 3(1) | -3(1) |
| C(6) | 26(1) | 70(2) | 64(2) | 27(2) | 6(1) | 8(1) |
| C(7) | 36(1) | 47(2) | 77(2) | 15(1) | 25(1) | 15(1) |
| C(8) | 41(1) | 38(1) | 59(2) | 2(1) | 23(1) | 4(1) |
| C(9) | 28(1) | 39(1) | 45(1) | 4(1) | 12(1) | 0(1) |
| C(10) | 35(1) | 56(2) | 45(1) | -3(1) | 11(1) | 2(1) |
| C(11) | 29(1) | 47(1) | 44(1) | -5(1) | 10(1) | -3(1) |
| C(12) | 62(2) | 108(3) | 52(2) | -6(2) | -8(2) | -10(2) |
| C(13) | 73(2) | 55(2) | 77(2) | -3(2) | 38(2) | -9(2) |
| C(14) | 59(2) | 78(2) | 70(2) | -25(2) | 19(2) | -3(2) |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(5) | 10230(30) | 7420(30) | 4887(12) | 46(8) |
| H(6) | 12210(40) | 5880(30) | 4553(12) | 62(8) |
| H(7) | 11460(40) | 4300(30) | 3747(12) | 52(8) |
| H(8) | 8760(30) | 4170(30) | 3239(11) | 41(7) |
| H(10) | 6260(30) | 8230(30) | 4241(10) | 29(6) |
| H(11A) | 5510(30) | 6820(30) | 3437(8) | 23(5) |
| H(12A) | 3470(60) | 4710(60) | 2688(19) | 129(16) |
| H(12B) | 3990(50) | 6510(50) | 2559(16) | 99(13) |
| H(12C) | 4460(50) | 4860(40) | 2157(17) | 96(12) |
| H(13A) | 5160(50) | 2680(50) | 3524(18) | 98(14) |
| H(13B) | 4720(50) | 2660(40) | 4156(16) | 88(12) |
| H(13C) | 6470(70) | 2960(50) | 4094(19) | 135(18) |
| H(14A) | 6700(40) | 9630(40) | 5074(13) | 70(10) |
| H(14B) | 8170(40) | 9830(40) | 4825(14) | 77(11) |
| H(14C) | 8160(40) | 8490(40) | 5329(15) | 79(11) |
| H(6O) | 5520(40) | 6040(40) | 4622(12) | 50(10) |

Table 6. Torsion angles [°] for **3a**.

| | |
|---|---|
| C(3)-Cr-C(1)-O(1) | -6(10) |
| C(2)-Cr-C(1)-O(1) | 83(10) |
| C(8)-Cr-C(1)-O(1) | 166(100) |
| C(6)-Cr-C(1)-O(1) | -139(10) |
| C(7)-Cr-C(1)-O(1) | -174(100) |
| C(9)-Cr-C(1)-O(1) | -159(10) |
| C(5)-Cr-C(1)-O(1) | -106(10) |
| C(4)-Cr-C(1)-O(1) | -89(10) |
| C(3)-Cr-C(2)-O(2) | -94(43) |
| C(1)-Cr-C(2)-O(2) | 180(100) |
| C(8)-Cr-C(2)-O(2) | 48(43) |
| C(6)-Cr-C(2)-O(2) | 94(43) |
| C(7)-Cr-C(2)-O(2) | 80(43) |
| C(9)-Cr-C(2)-O(2) | 12(43) |
| C(5)-Cr-C(2)-O(2) | 30(43) |
| C(4)-Cr-C(2)-O(2) | -7(43) |
| C(2)-Cr-C(3)-O(3) | -121(9) |
| C(1)-Cr-C(3)-O(3) | -32(9) |
| C(8)-Cr-C(3)-O(3) | 157(9) |
| C(6)-Cr-C(3)-O(3) | 51(9) |
| C(7)-Cr-C(3)-O(3) | 83(9) |
| C(9)-Cr-C(3)-O(3) | 141(9) |
| C(5)-Cr-C(3)-O(3) | 73(9) |
| C(4)-Cr-C(3)-O(3) | 108(9) |
| C(3)-Cr-C(4)-C(5) | -109.72(19) |
| C(2)-Cr-C(4)-C(5) | 163.06(19) |
| C(1)-Cr-C(4)-C(5) | -27.8(2) |
| C(8)-Cr-C(4)-C(5) | 100.69(18) |
| C(6)-Cr-C(4)-C(5) | 28.14(17) |
| C(7)-Cr-C(4)-C(5) | 64.49(18) |
| C(9)-Cr-C(4)-C(5) | 130.5(2) |
| C(3)-Cr-C(4)-C(9) | 119.77(15) |
| C(2)-Cr-C(4)-C(9) | 32.6(2) |
| C(1)-Cr-C(4)-C(9) | -158.34(17) |
| C(8)-Cr-C(4)-C(9) | -29.82(14) |
| C(6)-Cr-C(4)-C(9) | -102.36(16) |
| C(7)-Cr-C(4)-C(9) | -66.02(15) |
| C(5)-Cr-C(4)-C(9) | -130.5(2) |
| C(3)-Cr-C(4)-C(10) | 5.4(2) |
| C(2)-Cr-C(4)-C(10) | -81.8(3) |
| C(1)-Cr-C(4)-C(10) | 87.3(3) |
| C(8)-Cr-C(4)-C(10) | -144.2(2) |
| C(6)-Cr-C(4)-C(10) | 143.3(2) |

| | | |
|---|---|---|
| | C(7)-Cr-C(4)-C(10) | 179.6(2) |
| | C(9)-Cr-C(4)-C(10) | -114.4(3) |
| | C(5)-Cr-C(4)-C(10) | 115.1(3) |
| | C(9)-C(4)-C(5)-C(6) | 2.1(4) |
| | C(10)-C(4)-C(5)-C(6) | 179.3(2) |
| | Cr-C(4)-C(5)-C(6) | -52.8(2) |
| | C(9)-C(4)-C(5)-Cr | |
| 54.86(19) | | |
| | C(10)-C(4)-C(5)-Cr | -127.9(2) |
| | C(3)-Cr-C(5)-C(6) | - |
| 153.14(18) | | |
| | C(2)-Cr-C(5)-C(6) | 83.9(4) |
| | C(1)-Cr-C(5)-C(6) | -64.4(2) |
| | C(8)-Cr-C(5)-C(6) | |
| 66.07(18) | | |
| | C(7)-Cr-C(5)-C(6) | |
| 29.58(17) | | |
| | C(9)-Cr-C(5)-C(6) | |
| 103.65(19) | | |
| | C(4)-Cr-C(5)-C(6) | 133.8(3) |
| | C(3)-Cr-C(5)-C(4) | |
| 73.10(18) | | |
| | C(2)-Cr-C(5)-C(4) | -49.8(5) |
| | C(1)-Cr-C(5)-C(4) | |
| 161.87(16) | | |
| | C(8)-Cr-C(5)-C(4) | - |
| 67.68(16) | | |
| | C(6)-Cr-C(5)-C(4) | -133.8(3) |
| | C(7)-Cr-C(5)-C(4) | - |
| 104.18(18) | | |
| | C(9)-Cr-C(5)-C(4) | - |
| 30.10(14) | | |
| | C(4)-C(5)-C(6)-C(7) | -3.0(4) |
| | Cr-C(5)-C(6)-C(7) | -56.2(2) |
| | C(4)-C(5)-C(6)-Cr | 53.2(2) |
| | C(3)-Cr-C(6)-C(7) | |
| 167.80(16) | | |
| | C(2)-Cr-C(6)-C(7) | -23.6(2) |
| | C(1)-Cr-C(6)-C(7) | - |
| 109.47(17) | | |
| | C(8)-Cr-C(6)-C(7) | |
| 28.78(15) | | |
| | C(9)-Cr-C(6)-C(7) | |
| 65.68(16) | | |
| | C(5)-Cr-C(6)-C(7) | 130.9(2) |
| | C(4)-Cr-C(6)-C(7) | |
| 102.68(17) | | |
| | C(3)-Cr-C(6)-C(5) | 36.9(2) |
| | C(2)-Cr-C(6)-C(5) | -154.4(2) |
| | C(1)-Cr-C(6)-C(5) | |
| 119.68(19) | | |
| | C(8)-Cr-C(6)-C(5) | - |
| 102.08(18) | | |
| | C(7)-Cr-C(6)-C(5) | -130.9(2) |
| | C(9)-Cr-C(6)-C(5) | - |
| 65.18(17) | | |

```
          C(4)-Cr-C(6)-C(5)                                  -
28.18(16)
          C(5)-C(6)-C(7)-C(8)                                  2.3(4)
          Cr-C(6)-C(7)-C(8)                                 -53.9(2)
          C(5)-C(6)-C(7)-Cr                                  56.2(2)
          C(3)-Cr-C(7)-C(8)                                  91.1(5)
          C(2)-Cr-C(7)-C(8)                                  -
63.53(19)
          C(1)-Cr-C(7)-C(8)                                 -
154.67(18)
          C(6)-Cr-C(7)-C(8)                                  132.4(2)
          C(9)-Cr-C(7)-C(8)
28.97(15)
          C(5)-Cr-C(7)-C(8)
102.46(18)
          C(4)-Cr-C(7)-C(8)
65.90(16)
          C(3)-Cr-C(7)-C(6)                                  -41.3(5)
          C(2)-Cr-C(7)-C(6)
164.10(17)
          C(1)-Cr-C(7)-C(6)
72.96(18)
          C(8)-Cr-C(7)-C(6)                                 -132.4(2)
          C(9)-Cr-C(7)-C(6)                                 -
103.40(17)
          C(5)-Cr-C(7)-C(6)                                  -
29.91(15)
          C(4)-Cr-C(7)-C(6)                                  -
66.47(15)
          C(6)-C(7)-C(8)-C(9)                                  -0.8(4)
          Cr-C(7)-C(8)-C(9)                                 -54.6(2)
          C(6)-C(7)-C(8)-Cr                                  53.8(2)
          C(3)-Cr-C(8)-C(7)                                 -157.6(2)
          C(2)-Cr-C(8)-C(7)
119.24(19)
          C(1)-Cr-C(8)-C(7)                                  34.5(2)
          C(6)-Cr-C(8)-C(7)                                  -
28.82(16)
          C(9)-Cr-C(8)-C(7)                                 -132.9(2)
          C(5)-Cr-C(8)-C(7)                                  -
65.87(17)
          C(4)-Cr-C(8)-C(7)                                 -
103.18(18)
          C(3)-Cr-C(8)-C(9)                                  -24.8(3)
          C(2)-Cr-C(8)-C(9)                                 -
107.91(17)
          C(1)-Cr-C(8)-C(9)
167.32(16)
          C(6)-Cr-C(8)-C(9)
104.03(16)
          C(7)-Cr-C(8)-C(9)                                  132.9(2)
          C(5)-Cr-C(8)-C(9)
66.98(15)
          C(4)-Cr-C(8)-C(9)
29.67(14)
          C(7)-C(8)-C(9)-C(4)                                  -0.2(4)
```

| | | |
|---|---|---|
| | Cr-C(8)-C(9)-C(4) | -54.97(19) |
| | C(7)-C(8)-C(9)-C(11) | -179.9(2) |
| | Cr-C(8)-C(9)-C(11) | 125.2(2) |
| | C(7)-C(8)-C(9)-Cr | 54.8(2) |
| | C(5)-C(4)-C(9)-C(8) | -0.5(3) |
| | C(10)-C(4)-C(9)-C(8) | -177.7(2) |
| | Cr-C(4)-C(9)-C(8) | 54.49(19) |
| | C(5)-C(4)-C(9)-C(11) | 179.3(2) |
| | C(10)-C(4)-C(9)-C(11) | 2.1(3) |
| | Cr-C(4)-C(9)-C(11) | -125.7(2) |
| | C(5)-C(4)-C(9)-Cr | -55.0(2) |
| | C(10)-C(4)-C(9)-Cr | 127.8(2) |
| | C(3)-Cr-C(9)-C(8) | 164.26(16) |
| | C(2)-Cr-C(9)-C(8) | 73.20(18) |
| | C(1)-Cr-C(9)-C(8) | -43.7(5) |
| | C(6)-Cr-C(9)-C(8) | -64.55(16) |
| | C(7)-Cr-C(9)-C(8) | -28.34(16) |
| | C(5)-Cr-C(9)-C(8) | -101.14(17) |
| | C(4)-Cr-C(9)-C(8) | -131.1(2) |
| | C(3)-Cr-C(9)-C(4) | -64.60(16) |
| | C(2)-Cr-C(9)-C(4) | -155.66(15) |
| | C(1)-Cr-C(9)-C(4) | 87.5(5) |
| | C(8)-Cr-C(9)-C(4) | 131.1(2) |
| | C(6)-Cr-C(9)-C(4) | 66.60(15) |
| | C(7)-Cr-C(9)-C(4) | 102.81(16) |
| | C(5)-Cr-C(9)-C(4) | 30.00(14) |
| | C(3)-Cr-C(9)-C(11) | 50.1(2) |
| | C(2)-Cr-C(9)-C(11) | -40.9(2) |
| | C(1)-Cr-C(9)-C(11) | -157.8(4) |
| | C(8)-Cr-C(9)-C(11) | -114.1(3) |
| | C(6)-Cr-C(9)-C(11) | -178.7(2) |
| | C(7)-Cr-C(9)-C(11) | -142.5(2) |
| | C(5)-Cr-C(9)-C(11) | 144.7(2) |
| | C(4)-Cr-C(9)-C(11) | 114.7(3) |
| | C(5)-C(4)-C(10)-O(6) | -103.1(3) |
| | C(9)-C(4)-C(10)-O(6) | 74.1(3) |
| | Cr-C(4)-C(10)-O(6) | 165.12(17) |
| | C(5)-C(4)-C(10)-C(14) | 16.5(4) |
| | C(9)-C(4)-C(10)-C(14) | -166.3(3) |
| | Cr-C(4)-C(10)-C(14) | -75.3(3) |
| | C(12)-O(4)-C(11)-O(5) | 69.6(3) |
| | C(12)-O(4)-C(11)-C(9) | -167.0(3) |
| | C(13)-O(5)-C(11)-O(4) | 56.9(3) |
| | C(13)-O(5)-C(11)-C(9) | -64.9(3) |

| | |
|---|---|
| C(8)-C(9)-C(11)-O(4) | -16.0(3) |
| C(4)-C(9)-C(11)-O(4) | 164.2(2) |
| Cr-C(9)-C(11)-O(4) | 73.4(3) |
| C(8)-C(9)-C(11)-O(5) | 107.7(2) |
| C(4)-C(9)-C(11)-O(5) | -72.1(3) |
| Cr-C(9)-C(11)-O(5) | -162.86(15) |

## Table 1. Crystal data and structure refinement for 3a'

| | |
|---|---|
| Empirical formula | C14 H16 Cr O6 |
| Formula weight | 332.27 |
| Temperature | 293(2) K |
| Wavelength | 0.70930 Å |
| Crystal system, space group | Monoclinic, P21/n |
| Unit cell dimensions | a = 13.639(1) Å<br>b = 8.994(1) Å<br>c = 13.74(1)Å<br>β = 113.594 (7) ° |
| Volume | 1544.6(3) $A^3$ |
| Z, Calculated density | 4, 1.429 $Mg/m^3$ |
| Absorption coefficient | 0.763 $mm^{-1}$ |
| F(000) | 688 |
| Crystal size | 0.4 x 0.35 x 0.30 mm |
| Theta range for data collection | 1.77 to 24.90°. |
| Limiting indices | -16<=h<=14, 0<=k<=10, 0<=l<=16 |
| Reflections collected / unique | 2710 / 2710 [R(int) = 0.0000] |
| Completeness to theta = 24.90 | 99.9 % |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 2710 / 0 / 254 |
| Goodness-of-fit on $F^2$ | 1.087 |
| Final R indices [I>2sigma(I)] | R1 = 0.0289, wR2 = 0.0838 |
| R indices (all data) | R1 = 0.0350, wR2 = 0.0861 |
| Largest diff. peak and hole | 0.210 and -0.381 e. $Å^{-3}$ |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Cr | 4872(1) | 11472(1) | 1929(1) | 32(1) |
| O(1) | 3205(2) | 12554(2) | -130(1) | 76(1) |
| O(2) | 4131(2) | 13697(2) | 3117(2) | 70(1) |
| O(3) | 6302(2) | 13888(2) | 1754(2) | 93(1) |
| O(4) | 2868(1) | 8981(2) | -120(1) | 49(1) |
| O(5) | 2874(1) | 7199(2) | 1114(1) | 51(1) |
| O(6) | 3872(2) | 10435(2) | 4082(1) | 55(1) |
| C(1) | 3842(2) | 12130(2) | 659(2) | 46(1) |
| C(2) | 4402(2) | 12824(2) | 2657(2) | 45(1) |
| C(3) | 5758(2) | 12950(3) | 1816(2) | 54(1) |
| C(4) | 4440(1) | 9553(2) | 2728(1) | 34(1) |
| C(5) | 5499(2) | 10018(2) | 3354(2) | 39(1) |
| C(6) | 6276(2) | 10122(3) | 2929(2) | 44(1) |
| C(7) | 6003(2) | 9732(2) | 1857(2) | 41(1) |
| C(8) | 4963(2) | 9283(2) | 1220(2) | 35(1) |
| C(9) | 4161(1) | 9207(2) | 1645(1) | 32(1) |
| C(10) | 3665(2) | 9363(3) | 3268(2) | 43(1) |
| C(11) | 3041(2) | 8716(2) | 938(2) | 38(1) |
| C(12) | 1766(3) | 8891(6) | -829(3) | 82(1) |
| C(13) | 3561(3) | 6180(3) | 897(3) | 74(1) |
| C(14) | 3823(3) | 7829(3) | 3780(3) | 64(1) |

Table 3. Bond lengths [Å] and angles [°] for **3a'**.

| | |
|---|---|
| Cr-C(2) | 1.845(2) |
| Cr-C(1) | 1.845(2) |
| Cr-C(3) | 1.845(2) |
| Cr-C(6) | 2.219(2) |
| Cr-C(8) | 2.2216(19) |
| Cr-C(5) | 2.222(2) |
| Cr-C(9) | 2.2225(18) |
| Cr-C(7) | 2.228(2) |
| Cr-C(4) | 2.2467(18) |
| O(1)-C(1) | 1.150(3) |
| O(2)-C(2) | 1.157(3) |
| O(3)-C(3) | 1.149(3) |
| O(4)-C(11) | 1.396(2) |
| O(4)-C(12) | 1.429(3) |
| O(5)-C(11) | 1.420(2) |
| O(5)-C(13) | 1.426(4) |
| O(6)-C(10) | 1.418(3) |

| | |
|---|---|
| O(6)-H(6O) | 0.65(3) |
| C(4)-C(9) | 1.415(3) |
| C(4)-C(5) | 1.417(3) |
| C(4)-C(10) | 1.524(2) |
| C(5)-C(6) | 1.402(3) |
| C(5)-H(5) | 0.89(2) |
| C(6)-C(7) | 1.412(3) |
| C(6)-H(6) | 0.90(2) |
| C(7)-C(8) | 1.396(3) |
| C(7)-H(7) | 0.83(2) |
| C(8)-C(9) | 1.432(2) |
| C(8)-H(8) | 0.93(2) |
| C(9)-C(11) | 1.511(3) |
| C(10)-C(14) | 1.524(4) |
| C(10)-H(10) | 0.99(2) |
| C(11)-H(11) | 0.91(2) |
| C(12)-H(12A) | 0.89(4) |
| C(12)-H(12B) | 0.88(4) |
| C(12)-H(12C) | 0.94(4) |
| C(13)-H(13A) | 1.01(4) |
| C(13)-H(13B) | 0.98(4) |
| C(13)-H(13C) | 0.87(4) |
| C(14)-H(14A) | 0.98(3) |
| C(14)-H(14B) | 0.95(3) |
| C(14)-H(14C) | 0.88(3) |
| C(2)-Cr-C(1) | 90.20(9) |
| C(2)-Cr-C(3) | 87.29(10) |
| C(1)-Cr-C(3) | 88.03(11) |
| C(2)-Cr-C(6) | 115.21(9) |
| C(1)-Cr-C(6) | 154.49(9) |
| C(3)-Cr-C(6) | 90.81(10) |
| C(2)-Cr-C(8) | 156.09(8) |
| C(1)-Cr-C(8) | 91.39(8) |
| C(3)-Cr-C(8) | 116.60(9) |
| C(6)-Cr-C(8) | 66.48(8) |
| C(2)-Cr-C(5) | 90.30(9) |
| C(1)-Cr-C(5) | 154.30(9) |
| C(3)-Cr-C(5) | 117.66(10) |
| C(6)-Cr-C(5) | 36.81(7) |
| C(8)-Cr-C(5) | 78.18(8) |
| C(2)-Cr-C(9) | 118.53(8) |
| C(1)-Cr-C(9) | 90.82(8) |
| C(3)-Cr-C(9) | 154.16(9) |
| C(6)-Cr-C(9) | 79.33(8) |
| C(8)-Cr-C(9) | 37.60(6) |
| C(5)-Cr-C(9) | 66.56(7) |
| C(2)-Cr-C(7) | 152.17(9) |
| C(1)-Cr-C(7) | 117.49(9) |
| C(3)-Cr-C(7) | 90.75(10) |
| C(6)-Cr-C(7) | 37.03(8) |
| C(8)-Cr-C(7) | 36.57(8) |
| C(5)-Cr-C(7) | 66.18(7) |
| C(9)-Cr-C(7) | 67.01(7) |
| C(2)-Cr-C(4) | 91.47(8) |
| C(1)-Cr-C(4) | 117.32(9) |
| C(3)-Cr-C(4) | 154.63(10) |
| C(6)-Cr-C(4) | 66.87(7) |

| | |
|---|---|
| C(8)-Cr-C(4) | 66.73(7) |
| C(5)-Cr-C(4) | 36.98(8) |
| C(9)-Cr-C(4) | 36.91(7) |
| C(7)-Cr-C(4) | 78.68(7) |
| C(11)-O(4)-C(12) | 113.2(2) |
| C(11)-O(5)-C(13) | 114.71(19) |
| C(10)-O(6)-H(6O) | 105(3) |
| O(1)-C(1)-Cr | 179.3(2) |
| O(2)-C(2)-Cr | 178.1(2) |
| O(3)-C(3)-Cr | 178.7(2) |
| C(9)-C(4)-C(5) | 118.88(16) |
| C(9)-C(4)-C(10) | 122.70(17) |
| C(5)-C(4)-C(10) | 118.33(17) |
| C(9)-C(4)-Cr | 70.62(10) |
| C(5)-C(4)-Cr | 70.55(11) |
| C(10)-C(4)-Cr | 133.81(13) |
| C(6)-C(5)-C(4) | 121.57(18) |
| C(6)-C(5)-Cr | 71.49(12) |
| C(4)-C(5)-Cr | 72.47(11) |
| C(6)-C(5)-H(5) | 121.8(14) |
| C(4)-C(5)-H(5) | 116.5(14) |
| Cr-C(5)-H(5) | 125.7(14) |
| C(5)-C(6)-C(7) | 119.37(19) |
| C(5)-C(6)-Cr | 71.70(11) |
| C(7)-C(6)-Cr | 71.83(12) |
| C(5)-C(6)-H(6) | 120.2(14) |
| C(7)-C(6)-H(6) | 120.4(14) |
| Cr-C(6)-H(6) | 130.5(14) |
| C(8)-C(7)-C(6) | 120.18(18) |
| C(8)-C(7)-Cr | 71.46(11) |
| C(6)-C(7)-Cr | 71.14(12) |
| C(8)-C(7)-H(7) | 122.5(16) |
| C(6)-C(7)-H(7) | 117.3(16) |
| Cr-C(7)-H(7) | 127.9(17) |
| C(7)-C(8)-C(9) | 120.61(18) |
| C(7)-C(8)-Cr | 71.96(12) |
| C(9)-C(8)-Cr | 71.24(10) |
| C(7)-C(8)-H(8) | 121.1(12) |
| C(9)-C(8)-H(8) | 118.3(12) |
| Cr-C(8)-H(8) | 130.3(12) |
| C(4)-C(9)-C(8) | 119.34(17) |
| C(4)-C(9)-C(11) | 121.14(16) |
| C(8)-C(9)-C(11) | 119.49(16) |
| C(4)-C(9)-Cr | 72.47(10) |
| C(8)-C(9)-Cr | 71.17(10) |
| C(11)-C(9)-Cr | 129.66(13) |
| O(6)-C(10)-C(4) | 110.53(18) |
| O(6)-C(10)-C(14) | 107.7(2) |
| C(4)-C(10)-C(14) | 109.26(18) |
| O(6)-C(10)-H(10) | 109.5(14) |
| C(4)-C(10)-H(10) | 111.6(14) |
| C(14)-C(10)-H(10) | 108.1(14) |
| O(4)-C(11)-O(5) | 111.69(16) |
| O(4)-C(11)-C(9) | 108.99(15) |
| O(5)-C(11)-C(9) | 111.17(17) |
| O(4)-C(11)-H(11) | 107.7(13) |
| O(5)-C(11)-H(11) | 103.7(13) |

| | |
|---|---|
| C(9)-C(11)-H(11) | 113.4(13) |
| O(4)-C(12)-H(12A) | 109(3) |
| O(4)-C(12)-H(12B) | 107(3) |
| H(12A)-C(12)-H(12B) | 115(4) |
| O(4)-C(12)-H(12C) | 112(3) |
| H(12A)-C(12)-H(12C) | 102(3) |
| H(12B)-C(12)-H(12C) | 113(3) |
| O(5)-C(13)-H(13A) | 115.7(19) |
| O(5)-C(13)-H(13B) | 114(2) |
| H(13A)-C(13)-H(13B) | 99(3) |
| O(5)-C(13)-H(13C) | 107(2) |
| H(13A)-C(13)-H(13C) | 112(3) |
| H(13B)-C(13)-H(13C) | 109(3) |
| C(10)-C(14)-H(14A) | 109.0(17) |
| C(10)-C(14)-H(14B) | 110.8(18) |
| H(14A)-C(14)-H(14B) | 118(3) |
| C(10)-C(14)-H(14C) | 110(2) |
| H(14A)-C(14)-H(14C) | 105(3) |
| H(14B)-C(14)-H(14C) | 104(3) |

Table 4. Anisotropic displacement parameters ($A^2$ x $10^3$) for **3a′**. 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 | 32(1) | 32(1) | 33(1) | -2(1) | 15(1) | -3(1) |
| O(1) | 94(1) | 59(1) | 50(1) | 9(1) | 2(1) | 22(1) |
| O(2) | 86(1) | 54(1) | 84(1) | -16(1) | 48(1) | 10(1) |
| O(3) | 97(2) | 77(1) | 126(2) | -16(1) | 68(2) | -47(1) |
| O(4) | 48(1) | 56(1) | 37(1) | 2(1) | 11(1) | -17(1) |
| O(5) | 63(1) | 35(1) | 64(1) | -2(1) | 34(1) | -16(1) |
| O(6) | 59(1) | 72(1) | 43(1) | 5(1) | 28(1) | 26(1) |
| C(1) | 57(1) | 33(1) | 46(1) | -2(1) | 18(1) | 2(1) |
| C(2) | 47(1) | 40(1) | 49(1) | -1(1) | 21(1) | -1(1) |
| C(3) | 57(1) | 50(1) | 64(1) | -7(1) | 34(1) | -14(1) |
| C(4) | 36(1) | 34(1) | 36(1) | 7(1) | 19(1) | 8(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(5) | 41(1) | 47(1) | 30(1) | 3(1) | 14(1) | 7(1) |
| C(6) | 29(1) | 55(1) | 44(1) | 2(1) | 11(1) | 5(1) |
| C(7) | 37(1) | 47(1) | 46(1) | 2(1) | 25(1) | 4(1) |
| C(8) | 42(1) | 32(1) | 37(1) | -1(1) | 22(1) | 0(1) |
| C(9) | 38(1) | 25(1) | 36(1) | 2(1) | 19(1) | 1(1) |
| C(10) | 40(1) | 58(1) | 38(1) | 5(1) | 23(1) | 5(1) |
| C(11) | 42(1) | 33(1) | 42(1) | -1(1) | 21(1) | -7(1) |
| C(12) | 63(2) | 104(3) | 56(2) | 8(2) | -1(2) | -30(2) |
| C(13) | 98(3) | 34(1) | 101(2) | -5(1) | 51(2) | -6(1) |
| C(14) | 85(2) | 63(2) | 67(2) | 11(1) | 53(2) | -3(2) |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(5) | 5633(17) | 10300(20) | 4015(18) | 44(6) |
| H(6) | 6952(19) | 10400(20) | 3347(18) | 45(6) |
| H(7) | 6475(18) | 9810(30) | 1626(18) | 46(6) |
| H(8) | 4773(15) | 9010(20) | 512(17) | 30(5) |
| H(10) | 2910(20) | 9440(30) | 2755(19) | 52(6) |
| H(11) | 2521(17) | 9200(20) | 1070(16) | 35(5) |
| H(12A) | 1410(30) | 9620(50) | -680(30) | 106(16) |
| H(12B) | 1540(30) | 8000(50) | -770(30) | 104(13) |
| H(12C) | 1670(30) | 9130(50) | -1530(40) | 123(14) |
| H(13A) | 3650(30) | 6340(30) | 210(30) | 89(11) |
| H(13B) | 4320(30) | 6260(40) | 1390(30) | 89(11) |
| H(13C) | 3340(30) | 5290(40) | 940(30) | 99(11) |
| H(14A) | 4530(20) | 7780(30) | 4360(20) | 69(8) |
| H(14B) | 3630(20) | 7070(40) | 3260(20) | 71(9) |
| H(14C) | 3370(30) | 7710(30) | 4090(30) | 81(9) |
| H(6O) | 3530(20) | 10960(30) | 3870(20) | 48(9) |

****THE END****