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2,4-Dimethyl-3-phenyl-[2'-methyl-3'-chloro]-7-chloro-8-methyl-1,3-diaza-2,4-diboranaphtalene Tricarbonylchromium Complexes

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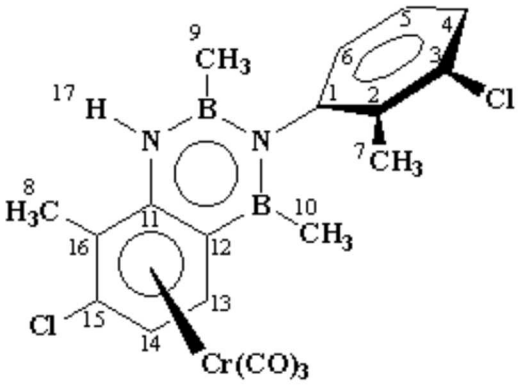
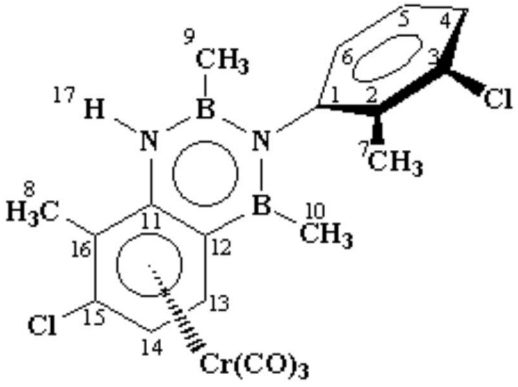


isomer 1



isomer 2

All reactions were carried out under dry nitrogen using Schlenk techniques. 2,4–Dimethyl-3-phenyl-[2'-methyl-3'-chloro]-7-chloro-8-methyl-1,3-diaza-2,4-diboranaphtalene tricarbonylchromium complexes were obtained by a classical method [1]. A solution of ligand (0.3 g, 0.907 mmol) and $Cr(CO)_6$ (0.3 g, 1.36 mmol) in 30 mL of dibutyl ether and 5 mL of THF was heated under reflux for 48 h under vigorous stirring. A strong yellow color shows the formation of the complex. After cooling and filtration through silica gel, the solution was evaporated to dryness. The crude product is a mixture of two isomers (0.19 g, 45%, Mp: 165°C). Reaction with $Cr(CO)_3$ gives exclusively the compounds with $Cr(CO)_3$ h^6-bonded to the benzo part of the molecule [2]. The two isomers were separated by silica gel chromatography with diethyl ether/hexane mixture (25/75).
Isomer 1, Mp:180-182°C; isomer 2, Mp:176-178 °C.

^{1}H (500 MHz) and ^{13}C NMR (125 MHz) chemical shifts for isomer 1 and isomer 2

	isomer 1		isomer 2		Δ
	δ (^{1}H)	δ (^{13}C)	δ (^{1}H)	δ (^{13}C)	$\delta_1 - \delta_2$
1		147.25		147.18	+0.07
2		133.20		132.41	+0.79
3		136.17		135.85	+0.32
4	7.29	127.73	7.28	127.75	-0.02
5	7.13	127.85	7.13	127.82	+0.03
6	6.84	126.41	6.84	127.10	-0.69
7	2.11	15.61	2.12	15.92	-0.31
8	2.48	14.78	2.46	14.76	+0.02
9	0.23	1.01	0.22	1.01	-
10	0.42	1.71	0.4	1.71	-
11		127.48		127.43	+0.05
12		79.50		79.50	
13	5.86	98.59	5.88	98.71	-0.12
14	5.25	88.14	5.23	88.02	+0.12
15		119.33		119.53	-0.20
16		91.87		91.65	+0.22
17	5.97		5.92		
CO		233.39		233.51	

References

1. Mahaffy, C. A. L.; Pauson, P. L. *Inorg. Synth.* **1979**, *19*, 154.
2. Allaoud, S.; Karim, A.; Mortreux, A.; Petit, F.; Frange, B. *J. Organomet. Chem.* **1989**, *89*, 379.

Sample availability: available from the authors and MDPI.