**Supporting Information**

Selective functionalization of carbonyl closo-decaborate [2-B10H9CO]¯ with building block properties via Grignard reagents

Nadine Mahfouz,1,2 Fatima Abi-Ghaida,1,\* Wael Kotob,1 Ahmad Mehdi,2,\* and Daoud Naoufal1,\*

1 Inorganic and Organometallic Coordination Chemistry Laboratory LCIO, Lebanese University, Faculty of Sciences, Lebanon, dnaoufal@ul.edu.lb, fghaida@ul.edu.lb

2 Institut Charles Gerhardt ICGM, Université de Montpellier, CNRS, ENSCM, Montpellier, 34090, France, ahmad.mehdi@umontpellier.fr

**\*** Correspondence: fghaida@ul.edu.lb , ahmad.mehdi@umontpellier.fr, dnaoufal@ul.edu.lb

**Table of Content**

[**1.** **11B NMR spectra for all compounds with carbonyl-closodecaborate(1)** 2](#_Toc139472166)

[**2.** **Product (PPh4)(MgBr)[2-B10H9C(O)CH2CH3] (2)** 3](#_Toc139472167)

[**2.1.** **1H NMR Spectra** 3](#_Toc139472168)

[**2.2.** **13C NMR spectra** 4](#_Toc139472169)

[**2.3.** **31P NMR spectra** 5](#_Toc139472170)

[**2.4.** **Mass spectrometry ESI/MS** 6](#_Toc139472171)

[**3.** **Product (PPh4) (MgBr)[2-B10H9C(O)(CH2)4CH3] (3)** 6](#_Toc139472172)

[**3.1.** **1H NMR Spectra** 6](#_Toc139472173)

[**3.2.** **13C NMR Spectra** 7](#_Toc139472174)

[**3.3.** **31P NMR spectra** 8](#_Toc139472175)

[**3.4.** **Mass spectrometry ESI/MS** 8](#_Toc139472176)

[**4.** **Product (PPh4) (MgCl)[2-B10H9C(O)C3H7] (4)** 9](#_Toc139472177)

[**4.1.** **1H NMR spectra** 9](#_Toc139472178)

[**4.2.** **13C NMR spectra** 10](#_Toc139472179)

[**4.3.** **31P NMR spectra** 11](#_Toc139472180)

[**4.4.** **Mass spectrometry ESI/MS** 11](#_Toc139472181)

[**5.** **Product (PPh4) (MgCl)[2-B10H9C(O)CH2CH=CH2] (5)** 12](#_Toc139472182)

[**5.1.** **13C NMR spectra** 12](#_Toc139472183)

[**5.2.** **31P NMR spectra** 13](#_Toc139472184)

[**5.3.** **Mass spectrometry ESI/MS** 13](#_Toc139472185)

[**6.** **Product (PPh4) (MgBr)[2-B10H9C(O)CH=CH2] (6)** 14](#_Toc139472186)

[**6.1.** **13C NMR spectra** 14](#_Toc139472187)

[**6.2.** **31P NMR spectra** 15](#_Toc139472188)

[**6.3.** **Mass spectrometry ESI/MS** 15](#_Toc139472189)

[**7.** **Product (PPh4) (MgBr)[2-B10H9C(O)C≡CCH3] (7)** 16](#_Toc139472190)

[**7.1.** **31P NMR spectra** 16](#_Toc139472191)

# **11B NMR spectra for all compounds with carbonyl-closodecaborate(1)**



**Fig. S 1. 11B NMR spectrum for all compounds with carbonyl-closodecaborate (1)**

# **Product (PPh4)(MgBr)[2-B10H9C(O)CH2CH3] (2)**

## **1H NMR Spectra**

**1H NMR** (δ ppm, DMSO-d6): 0.65 (3 H, d, CH3), 2.23 (2 H, quadruplet, CH2), 7.5-7.8 (20 H, m, H of PPh4+).



**Fig. S 2. 1H NMR spectrum of Product (2) in DMSO-d6**

## **13C NMR spectra**

**13C NMR** (δ ppm, DMSO-d6): 157.30 (a), 135.52 (g), 134.88 (f), 130.45 (e), 118.73(d), 8.65 (b), 1.13 (c).



**Fig. S 3. 13C NMR Spectrum of product (2). Attributed carbons (a to g) are annotated on the structure**

## **31P NMR spectra**

**31P NMR** (DMSO-d6): 22.59



**Fig. S 4. 31P NMR spectrum of product (2)**

## **Mass spectrometry ESI/MS**



**Fig. S 5. ESI/MS spectra of the product (2)**

# **Product (PPh4) (MgBr)[2-B10H9C(O)(CH2)4CH3] (3)**

## **1H NMR Spectra**

**1H NMR** (δ ppm, DMSO-d6): 0.75 (3H, t, CH3), 1.10 (2H, sextuplet, CH2), 1.25 (4H, quintuplet, 2CH2), 2.15 (2H, t, CH2), 7.5-7.8 (20H, m, H of PPh4+)



**Fig. S 6. 1H NMR spectrum of Product 2 in DMSO-d6**

## **13C NMR Spectra**

**13C NMR** (δ ppm, DMSO-d6): 166.35 (a), 135.52 (g), 134.88 (f), 130.45 (e), 118.73(d),32.10 (b), 24.18 (c), 22.72 (h), 14.32 (i).



**Fig. S 7. 13C NMR Spectrum of product (3). Attributed carbons (a to i) are annotated on the structure**

## **31P NMR spectra**

**31P NMR** (DMSO-d6): 22.13



**Fig. S 8. 31P spectrum of the product (3)**

## **Mass spectrometry ESI/MS**

Mass spectrometry m/z (3) = 216



**Fig. S 9. Mass spectrometry ESI/MS of the product (3)**

# **Product (PPh4) (MgCl)[2-B10H9C(O)C3H7] (4)**

## **1H NMR spectra**

**1H NMR** (δ ppm, DMSO-d6): 0.68 (6H, d, 2CH3), 2.65 (1H, septuplet, CH), 7.51-8.04 (20H, m, H of PPh4+)



**Fig. S 10. 1H NMR spectrum of Product (4) in DMSO-d6**

## **13C NMR spectra**

**13C NMR** (δ ppm, DMSO-d6): 135.75 (g), 135.29 (f), 130.91 (e),118.71 (d), 19.59 (c).



**Fig. S 11. 13C NMR Spectrum of product (4). Attributed carbons (a to g) are annotated on the structure**

## **31P NMR spectra**

**31P NMR** (DMSO-d6): 22.59



**Fig. S 12. 31P NMR spectrum of the product (4)**

## **Mass spectrometry ESI/MS**

**Mass spectrometry (ESI):** m/z (4) = 188



**Fig. S 13. Mass spectrometry ESI/MS of the product (4)**

# **Product (PPh4) (MgCl)[2-B10H9C(O)CH2CH=CH2] (5)**

## **13C NMR spectra**

**13C NMR** (δ ppm, DMSO-d6): 135.87(g), 135.09 (h), 131.03(f),130.84 (e), 118.61 (d), 117.69 (c), 45.959 (b)



**Fig. S 14.** **13C NMR Spectrum of product (5). Attributed carbons (a to h) are annotated on the structure**

## **31P NMR spectra**

**31P NMR** (DMSO-d6): 21.64



**Fig. S 15. 31P NMR spectrum of product (5)**

## **Mass spectrometry ESI/MS**

**Mass spectrometry (ESI):** m/z (5)= 185



**Fig. S 16. Mass spectrometry ESI/MS of the product (5)**

# **Product (PPh4) (MgBr)[2-B10H9C(O)CH=CH2] (6)**

## **13C NMR spectra**

**13C NMR** (δ ppm, DMSO-d6): 175.56 (a), 135.95(b), 135.10(g),134.90(f), 130.91(c),118.72, 117.65(d)



**Fig. S 17. 13C NMR Spectrum of product (6). Attributed carbons (a to g) are annotated on the structure**

## **31P NMR spectra**

**31P NMR** (DMSO-d6): 22.14.



**Fig. S 18. 31P NMR Spectrum of the product (6)**

## **Mass spectrometry ESI/MS**

**Mass spectrometry (ESI):** m/z (6) = 172.



**Fig. S 19. Mass spectrometry ESI/MS of the product (6)**

# **Product (PPh4) (MgBr)[2-B10H9C(O)C≡CCH3] (7)**

## **31P NMR spectra**

**31P NMR** (DMSO-d6): 22.13.



**Fig. S 20. 31P NMR spectrum of the product (7)**