The Hydroboration Reaction as a Key for a Straightforward Synthesis

of New MRI-NCT agents

Paolo Boggio, Antonio Toppino, Simonetta Geninatti-Crich, Diego Alberti, Domenica Marabello, Claudio Medana, Cristina Prandi, Paolo Venturello, Silvio Aime, Annamaria Deagostino.

Table of contents

| Figure 1 ¹ H, ¹³ C, DEPT, ¹¹ B of hexadecyldecaborane (3) | 2 |
|---|----|
| Figure 2 ¹ H, ¹³ C, DEPT, ¹¹ B of <i>C</i> -(2-hydroxy)-ethyl- <i>C</i> '-H-4-(hexadecyl)- <i>ortho</i> -carborane (5a) | 4 |
| Figure 3 ¹ H, ¹³ C, DEPT, ¹¹ B of <i>C</i> -(2-hydroxy)-ethyl- <i>C</i> '-H-9-(hexadecyl)- <i>ortho</i> -carborane (5b) | 6 |
| Figure 4 ¹ H, ¹³ C, DEPT of <i>C</i> -(carboxymethyl)- <i>C</i> '-H-4-(hexadecyl)- <i>o</i> -carborane (6a) | 8 |
| Figure 5 ¹ H, ¹³ C, DEPT of <i>C</i> -(carboxymethyl)- <i>C</i> '-H-9-(hexadecyl)- <i>o</i> -carborane (6b) | 10 |
| Figure 6 ¹ H, ¹³ C, DEPT of <i>C</i> -[<i>ter</i> -butylDOTAMA-C ₆]-acetamido- <i>C</i> '-H-4-(hexadecyl)- <i>o</i> -carborane (7a) | 12 |
| Figure 7 ¹ H, ¹³ C, DEPT, ¹¹ B of <i>C</i> -[<i>ter</i> -butylDOTAMA-C ₆]-acetamido- <i>C</i> '-H-9-(hexadecyl)- <i>o</i> -carborane (7b) | 14 |
| Figure 8 ¹ H, ¹³ C, DEPT of <i>C</i> -[benzylDOTAMA-C ₆]-acetamido- <i>C</i> '-H-4-(hexadecyl)- <i>o</i> -carborane (8a) | 16 |
| Figure 9 ¹ H, ¹³ C, DEPT of <i>C</i> -[benzylDOTAMA-C ₆]-acetamido- <i>C</i> '-H-9-(hexadecyl)- <i>o</i> -carborane (8b) | 18 |
| Figure 10 ¹ H, ¹³ C, DEPT of C-[DOTAMA-C ₆]-acetamido-C'-H-4-(hexadecyl)-o-carborane (9a) | 20 |
| Figure 11 ¹ H, ¹³ C, DEPT of <i>C</i> -[DOTAMA-C ₆]-acetamido- <i>C</i> '-H-9-(hexadecyl)- <i>o</i> -carborane (9b) | 24 |
| Figure 12 Effect of HP β CD concentration on the R _{10bs} values (21,5 MHz) for PB01a and PB01b | 27 |
| Figure 13 Determination of the Critical Micellar Concentration (CMC) of PB01a and PB01b | 28 |



Figure 1 ¹H, ¹³C, DEPT, ¹¹B of hexadecyldecaborane ($\frac{3}{4}$)



ω

Figure 2¹H, ¹³C DEPT, ¹¹B of *C*-(2-hydroxy)-ethyl-*C*'-H-4-(hexadecyl)-*ortho*-carborane (**5a**)





л



Figure 3 ¹H, ¹³C DEPT, ¹¹B of *C*-(2-hydroxy)-ethyl-*C*'-H-9-(hexadecyl)-*ortho*-carborane (5b)



 \checkmark









Figure 5¹H, ¹³C, DEPT of *C*-(carboxymethyl)-*C*'-H-4-(hexadecyl)-*o*-carborane (6b)

























Figure 10¹H, ¹³C, DEPT of *C*-[DOTAMA-C₆]-acetamido-*C*'-H-4-(hexadecyl)-*o*-carborane (9a)

















Figure 12 Effect of HP β CD concentration on the R_{1obs} values (21,5 MHz) for PB01a and PB01b



Figure 13 Determination of the Critical Micellar Concentration (CMC) of PB01a and PB01b by measuring the longitudinal water proton relaxation rates ($R_{1 obs}$) of solutions containing decreasing amounts of complex.

