

# Multistage complexation of fluoride ions by a fluorescent triphenylamine bearing three dimesitylboryl groups: Controlling intramolecular charge transfer

## Supporting Information

Hauke Schmidt,<sup>†</sup> Luisa G. Reuter,<sup>†</sup> Josef Hamacek,<sup>‡</sup> and Oliver S. Wenger<sup>\*,†</sup>

<sup>†</sup>*Georg-August Universität Göttingen, Institut für Anorganische Chemie, Tammannstrasse 4,  
D-37077 Göttingen, Germany*

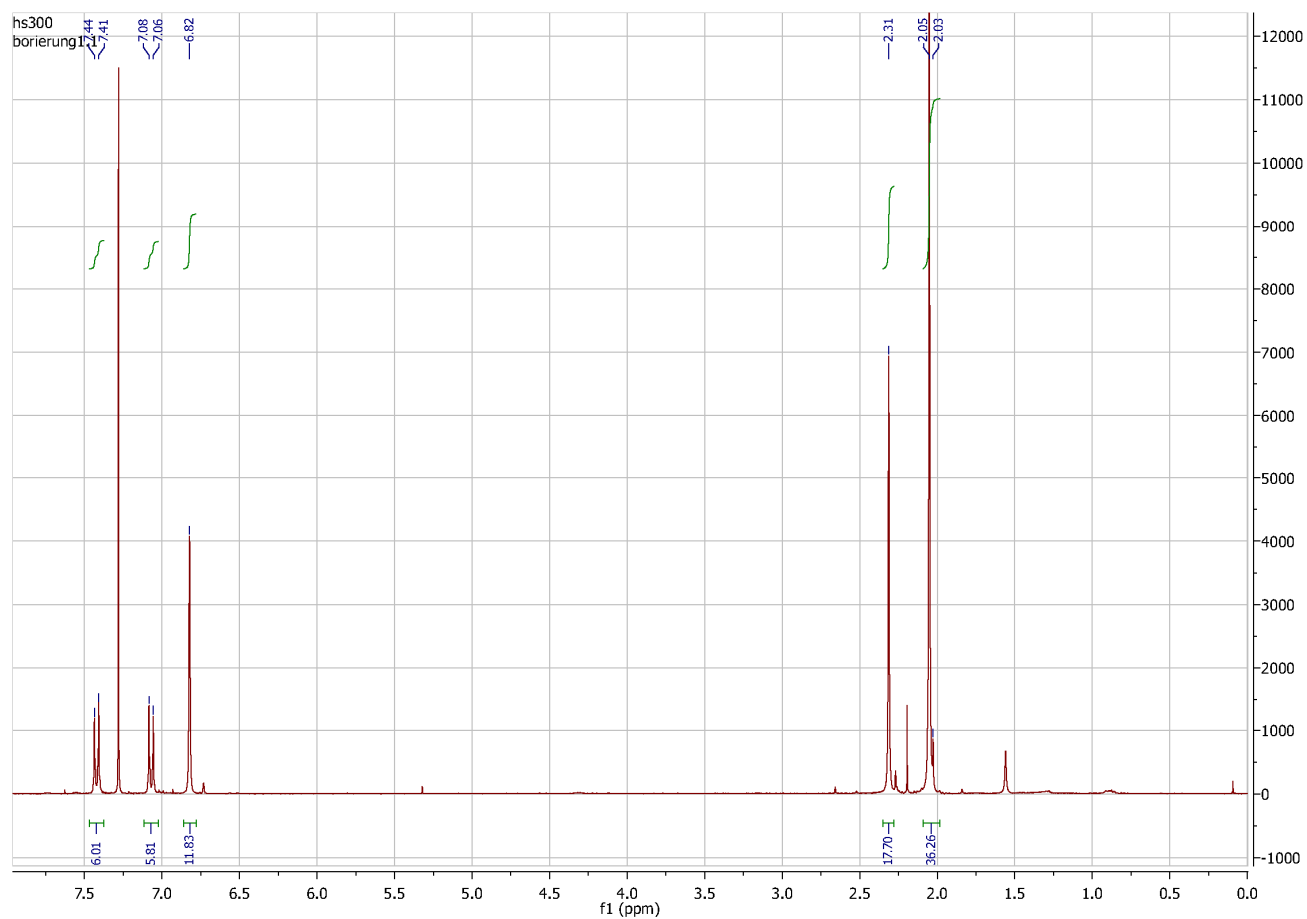
<sup>‡</sup>*Université de Genève, Département de Chimie Minérale, Analytique et Appliquée, 30 quai Ernest-  
Ansermet, CH-1211 Genève 4, Switzerland*

E-mail: [oliver.wenger@chemie.uni-goettingen.de](mailto:oliver.wenger@chemie.uni-goettingen.de)

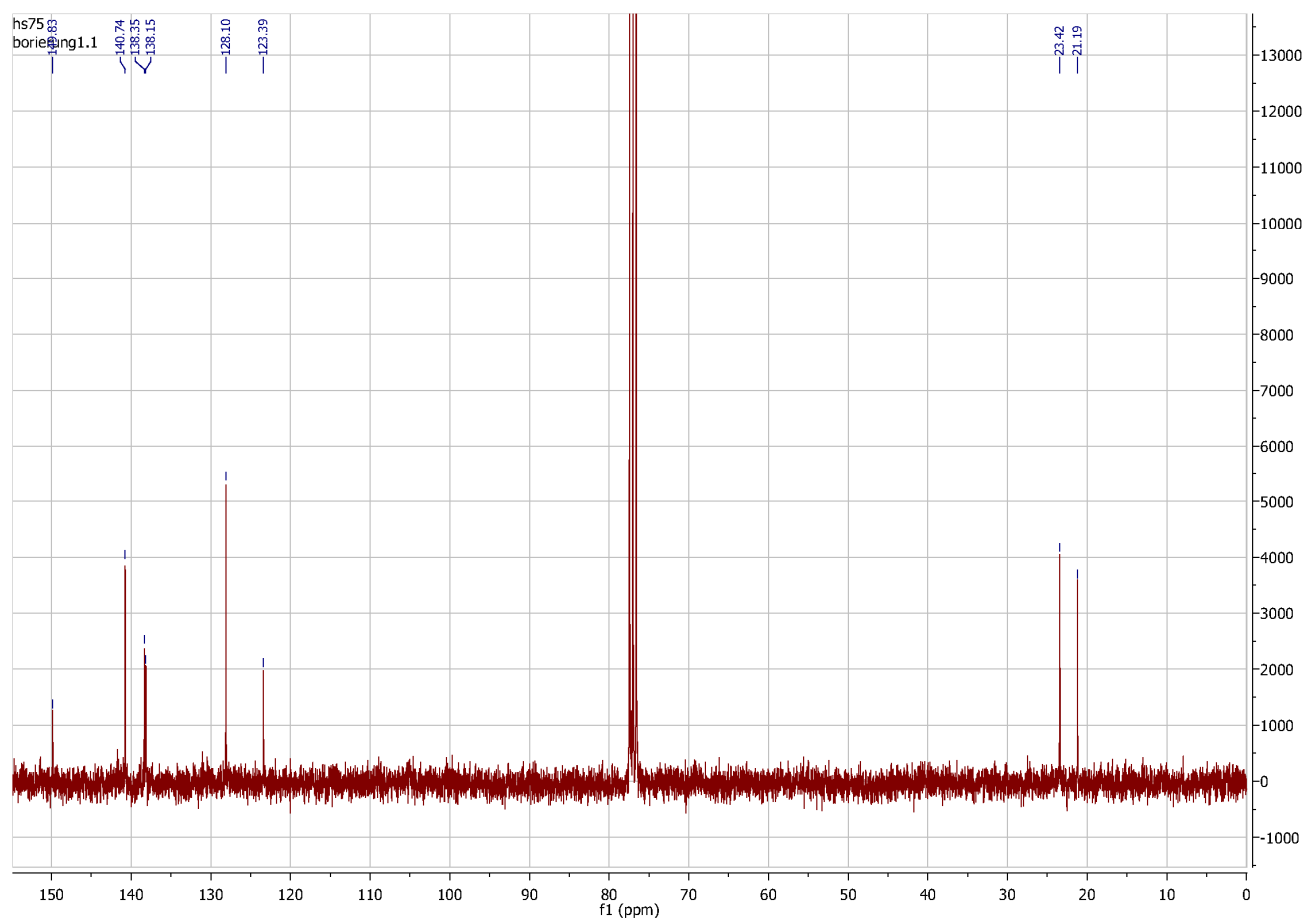
## Contents

<sup>1</sup> H NMR spectrum of molecule NB <sub>3</sub> in CDCl <sub>3</sub>	S2
<sup>13</sup> C NMR spectrum of molecule NB <sub>3</sub> in CDCl <sub>3</sub>	S3
<sup>11</sup> B NMR spectra	S4

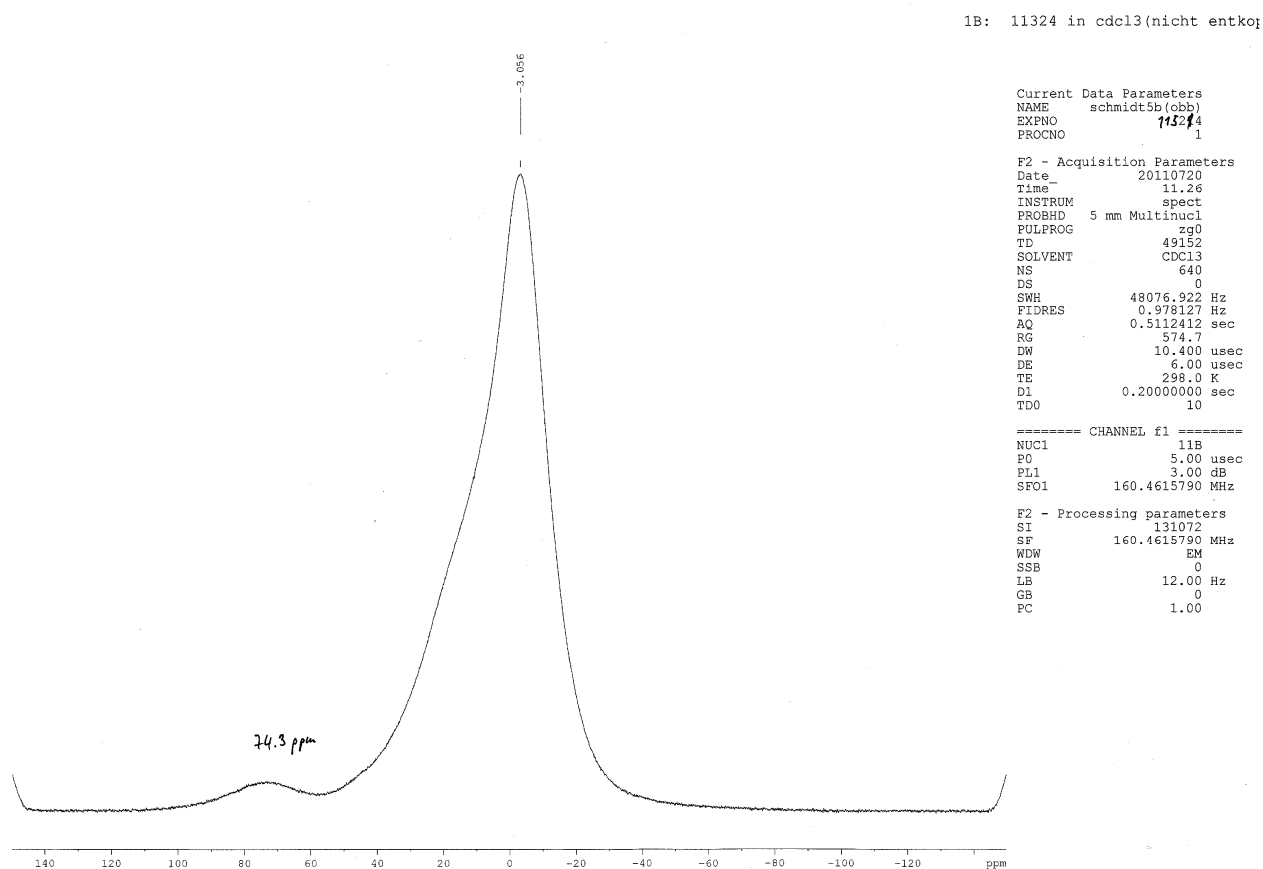
# $^1\text{H}$ NMR spectrum of molecule $\text{NB}_3$ in $\text{CDCl}_3$



**$^{13}\text{C}$  NMR spectrum of molecule  $\text{NB}_3$  in  $\text{CDCl}_3$**

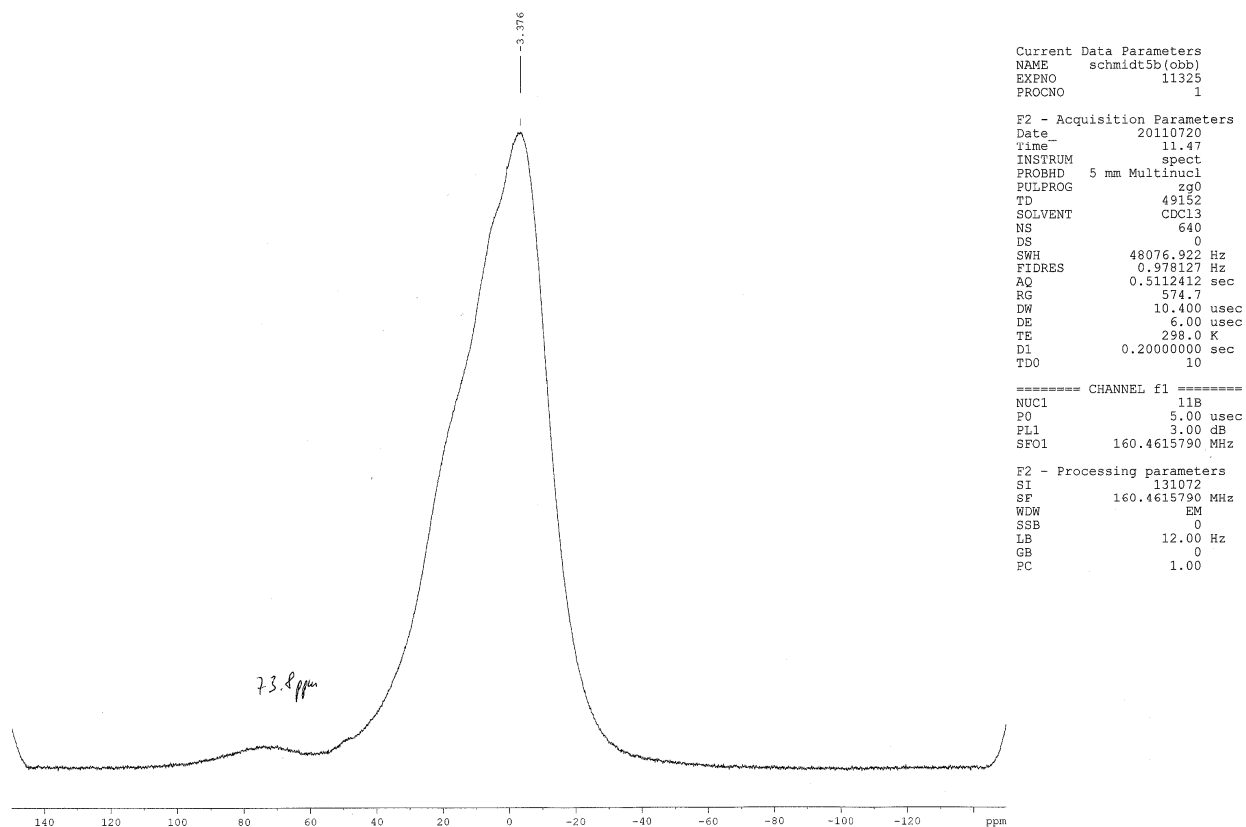


# <sup>11</sup>B-NMR spectra of molecule NB<sub>3</sub>



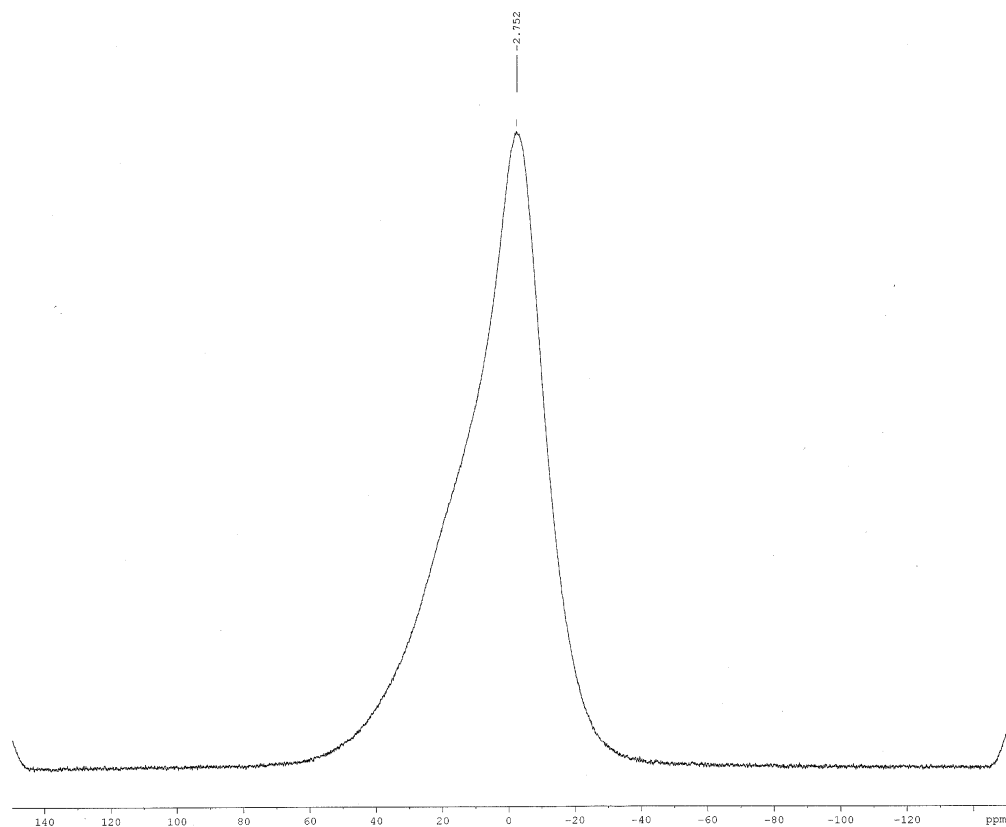
<sup>11</sup>B-NMR spectrum of tris(4-(dimesitylboryl)phenyl)amine in CDCl<sub>3</sub>. The intense signal around 3 ppm is due to boron contained in the glass of the NMR tube, see spectrum on page S6.

1B: 11325 in cdcl3(nicht entko)



<sup>11</sup>B-NMR spectrum of tris(4-(dimesitylboryl)phenyl)amine in CDCl<sub>3</sub> after addition of 1 equivalent of tetrabutylammonium fluoride. The intense signal around 3 ppm is due to boron contained in the glass of the NMR tube, see spectrum on page S6. The spectrum here contains an additional signal (noticeable as a shoulder to the 3 ppm signal) between 5 and 10 ppm, which is assigned to boron sites with bound fluoride.

//8: vergleich in cdcl3(nicht entl)



```

Current Data Parameters
NAME      schmidt5b(obb)
EXPNO     10000
PROCNO    1

F2 - Acquisition Parameters
Date_     20110720
Time      12.24
INSTRUM   spect
PROBHD    5 mm Multinucl
PULPROG   zg0
TD        49152
SOLVENT   CDCl3
NS        640
DS        0
SWH       48076.922 Hz
FIDRES    0.978127 Hz
AQ        0.5112412 sec
RG        574.7
DW        10.400 usec
DE        6.00 usec
TE        298.0 K
D1        0.20000000 sec
TD0       10

===== CHANNEL f1 =====
NUC1      11B
P0        5.00 usec
PL1       3.00 dB
SFO1      160.4615790 MHz

F2 - Processing parameters
SI        131072
SF        160.4615790 MHz
WDW       EM
SSB       0
LB        12.00 Hz
GB        0
PC        1.00

```

$^{11}\text{B}$ -NMR spectrum of the empty NMR tube used for the measurements shown in the spectra on pages S4 and S5.