Supporting Information for

Experimental verification and theoretical analysis of the possibility of forming ytterbium imido complexes based on aniline with bulky benzhydryl substituents

Valentina A. Melnikova,[a] Nikolay V. Somov,[b] Vladimir A. Dodonov[a]*

[a] G. A. Razuvaev Institute of Organometallic Chemistry, Russian Academy of Sciences, 49 ul. Tropinina, 603137 Nizhny Novgorod, Russian Federation. Fax: +7 (831) 462 7497. E-mail: dodonov@iomc.ras.ru

[b] N. I. Lobachevsky State University of Nizhny Novgorod, 23 prosp. Gagarina, 603022 Nizhny Novgorod, Russian Federation. Fax: +7 (831) 462 3085. E-mail: somov@phys.unn.ru

Assignment of the ^{1}H NMR signals for compound 2 (partial)

^{1}H NMR (400 MHz, THF-d_8) δ:

- 6.91 (br s, 17H), 6.71 (br s, 3H), 6.38 (br s, 3H), 6.07 (br s, 6H), 5.76 (br s, 2H), 5.51 (br s, 1H) — aromatic protons (Ar–H), a set of overlapping broadened signals.
- 4.78 (br s, 4H), 4.74 (br s, 2H) — benzylic protons (CH in Ph_2CH fragments / benzylic CH) (broadened and partially overlapping).
- 2.86 (br s, 3H) — CH_3 (methyl group).

All ^{1}H signals are significantly broadened over the range −50 to +50 °C; no ^{13}C–^{1}H cross-peaks are observed in the HSQC/HMQC spectra. The broadening is likely caused by chemical exchange (conformational/coordination rearrangements, slow exchange of K^+ cations). Therefore, unambiguous positional assignment (assignment of individual protons/positions in the aromatic rings) is not possible; only a group assignment is given.

^{13}C NMR spectrum (101 MHz, THF-d^8) δ 155.6 (C Ar), 146.8 (C Ar), 146.1 (C Ar), 145.0 (C Ar), 134.9 (C Ar), 132.5 (CH Ar), 130.4 (CH Ar), 129.7 (CH Ar), 128.5 (CH Ar), 127.8 (CH Ar), 127.2 (CH Ar), 127.1 (CH Ar), 127.0 (CH Ar), 126.2 (CH Ar), 124.7 (CH Ar), 124.6 (CH Ar), 123.4 (CH Ar), 116.5 (C Ar), 114.9 (CH Ar), 101.7 (CH Ar), 94.0 (CPh_2), 53.6 ($CHPh_2$), 20.3 (CH_3).

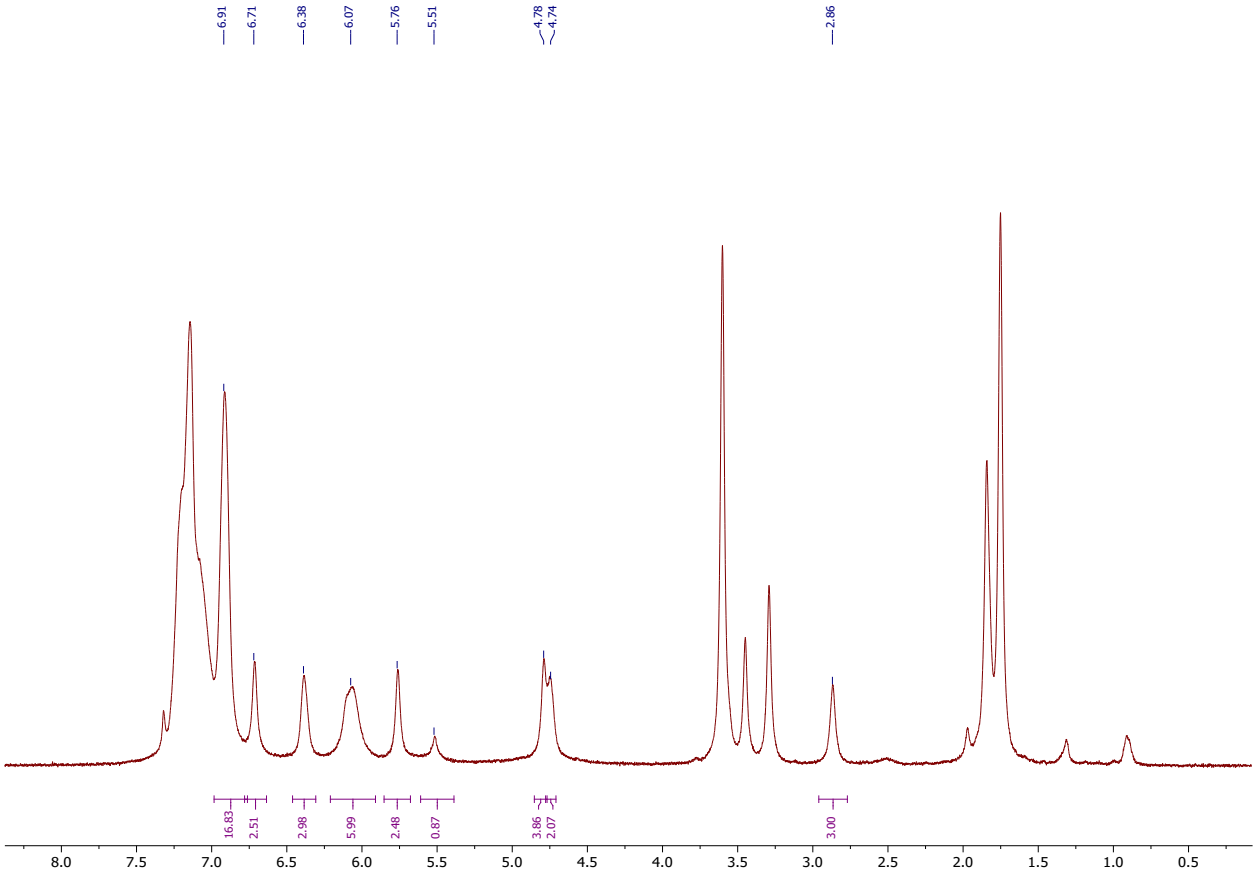

Figure S1. ^{1}H NMR spectrum of compound **2** (THF-d^8, 25°C, 400 MHz)

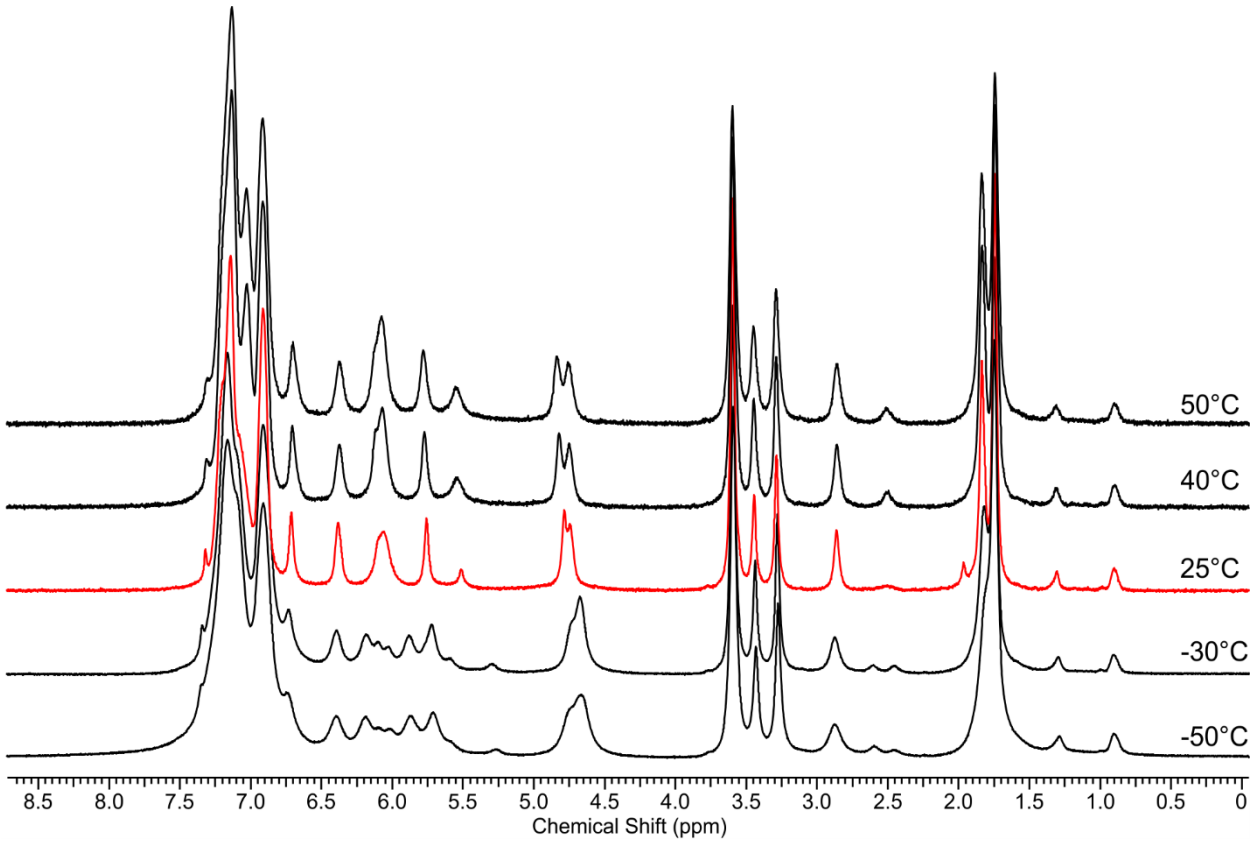

Figure S2. Variable-temperature ^{1}H NMR spectrum of compound **2** (THF-d^{8}, 400 MHz).

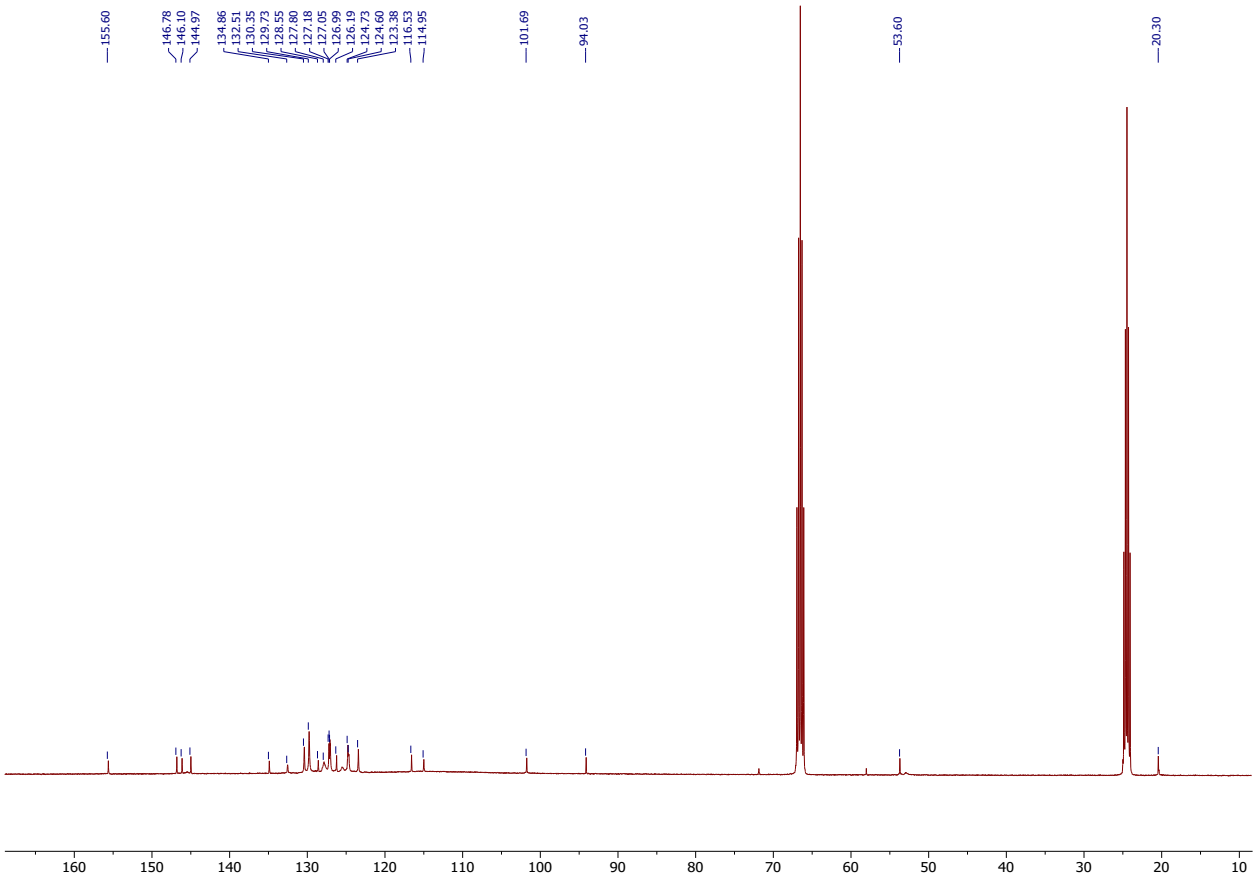

Figure S3. ^{13}C NMR spectrum of compound **2** (THF-d^{8}, 25°C, 101 MHz)