Electronic Supplementary Information for Dalton Transactions

Supplementary data

Synthesis, characterization and optical properties of π-conjugated systems incorporating *closo*-dodecaborate clusters: new potential candidates for two-photon absorption processes

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Synthesis of NC-C_6H_4-C(H)=N-CH_3 (5)

In a typical experiment, 1.30g (0.01mol) of 4-cyanobenzaldehyde are added at r.t. to a large molar excess of an aqueous solution of methylamine (40 wt %). The mixture is kept under stirring during 12h then the title compound was extracted from the aqueous media with diethylether. NC-C_6H_4-C(H)=N-CH_3 (1.14g, 80%) was crystallized from the extracted solution by a slow evaporation of the solvent (Found: C, 74.79; H, 5.44; N, 19.44%. **5** requires C, 74.98; H, 5.59; N, 19.43%). δ_H (CD_3CN) 3.14 (s, 3H, NC**H**$_3$), 7.80 (d, 2H, C_6**H**$_4$), 7.90 (d, 2H, C_6**H**$_4$), 8.38 (s, 1H, N=C**H**); δ_C (CD_2Cl_2) 48.52 (1C, N-**C**H_3), 114.10 (1C, **C**N), 118.91 (1C, NC-**C**$_6H_4$), 128.94 (2C, **C**$_6H_4$), 132.40 (2C, **C**$_6H_4$) 140.67 (1C, HC-**C**$_6H_4$), 160.82 (1C, N=**C**H). DSC analysis: mp 58°C, bp 240°C.