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Supplementary Information

Distinct Conformational Preferences of Prolinol and Prolinol Ether Enamines in Solution Revealed by NMR

Markus B. Schmid, Kirsten Zeitler and Ruth M. Gschwind*

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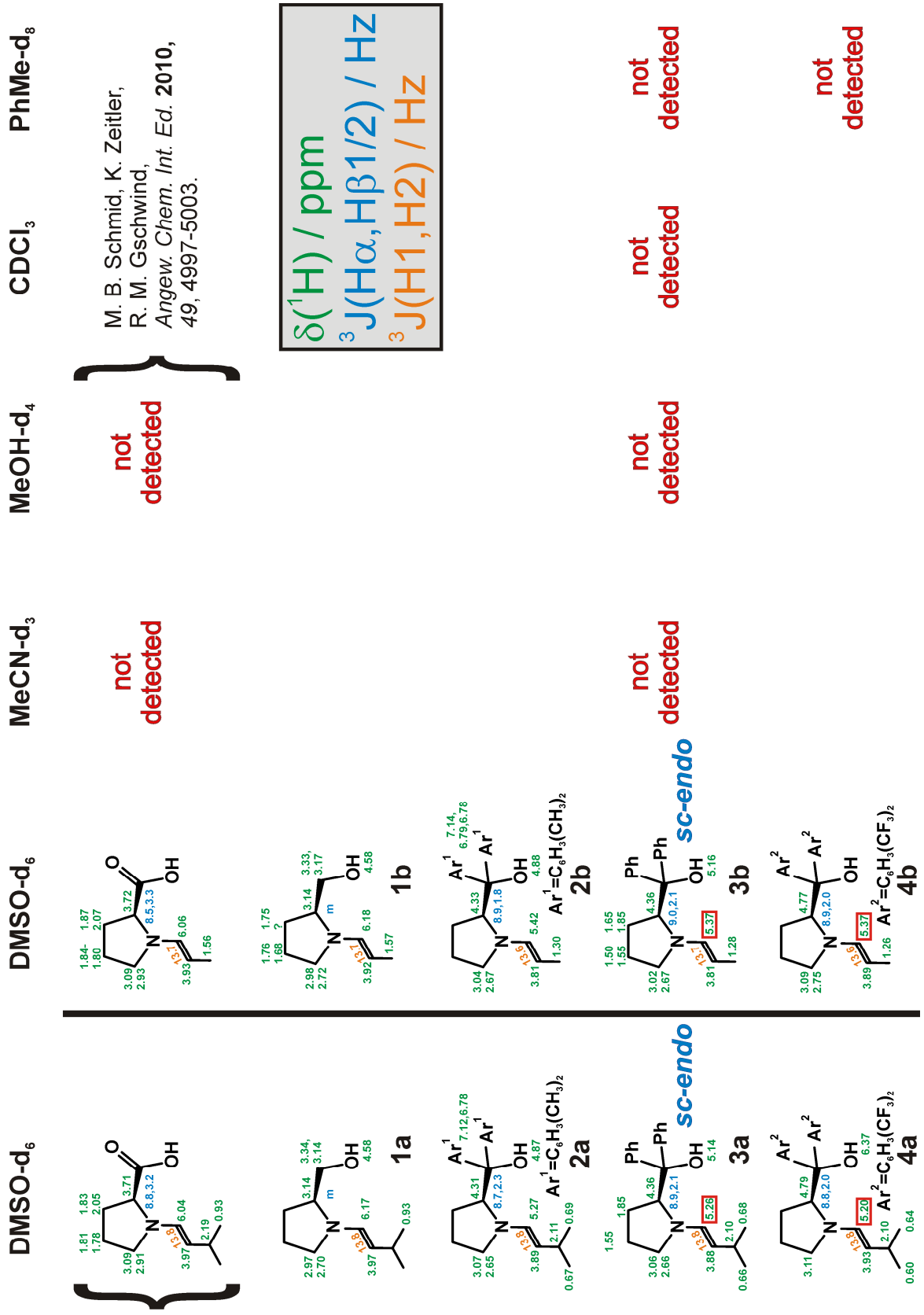
1 Experimental Details

The enamines under investigation were created *in situ* by mixing freshly distilled aldehydes **1** or **2** (30 µmol) with a solution of 100 mol% of one the organocatalysts **3**-**9** in 0.6 mL of a deuterated solvent within a standard 5 mm NMR tube. The NMR tube was transferred to the spectrometer immediately after the preparation of the reaction mixture.

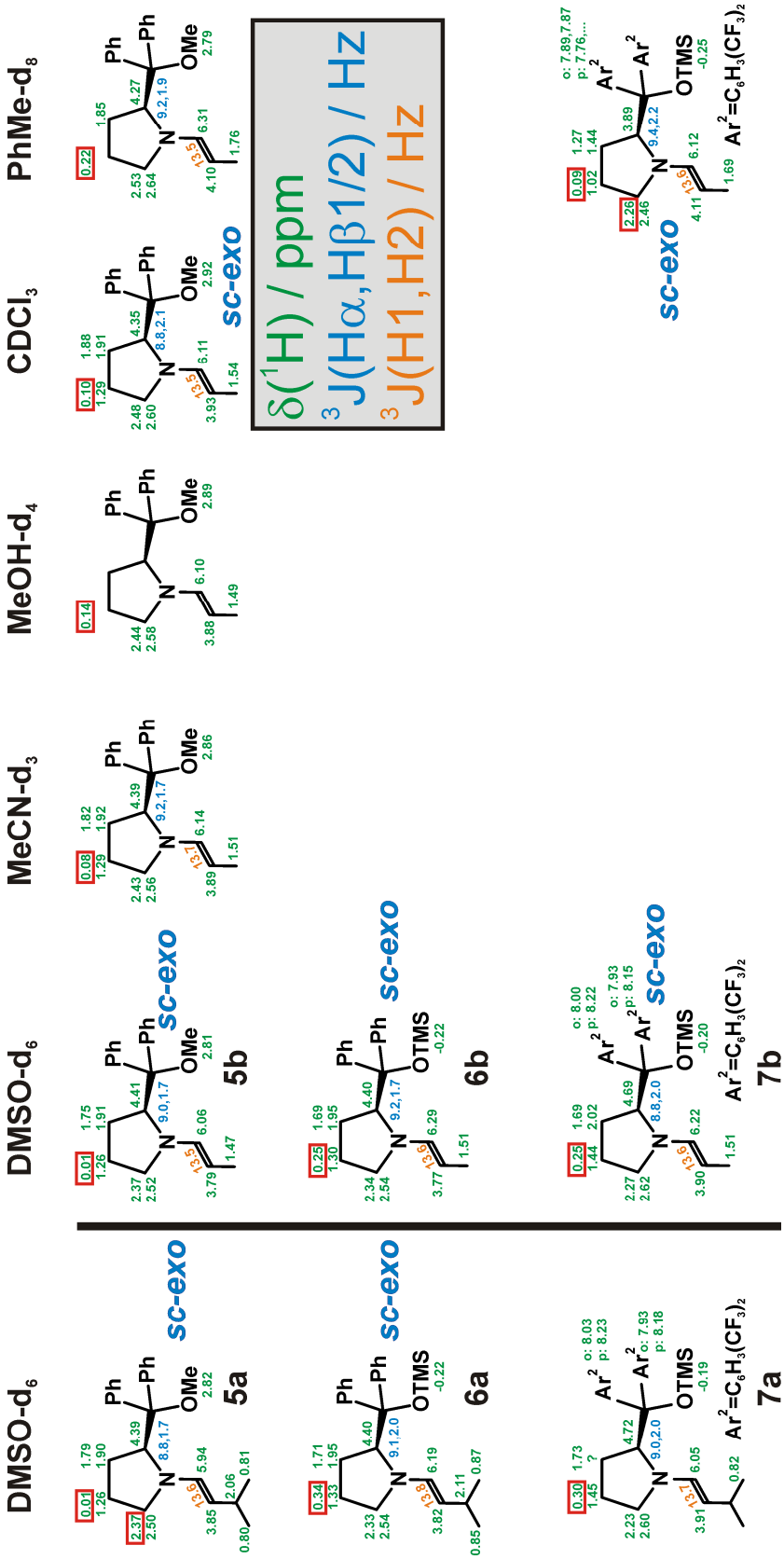
NMR measurements were performed at 300 K on a Bruker Avance DRX 600 (600.13 MHz) and on a Bruker Avance III 600 (600.25 MHz) spectrometer, the latter equipped with a TCI cryoprobe with z-gradient (53.5 G/cm). ^{1}H,^{1}H-NOESY spectra were recorded using a mixing time of 700 ms. NMR data were processed and evaluated with Bruker´s TOPSPIN 2.1.

Spartan ´06 (http://www.wavefun.com) was employed for the structure models displayed in Figure 4B. The structures were refined with the help of molecular mechanics conformer distribution calculations (MMFF force field).

2 NMR Characterization of Enamines

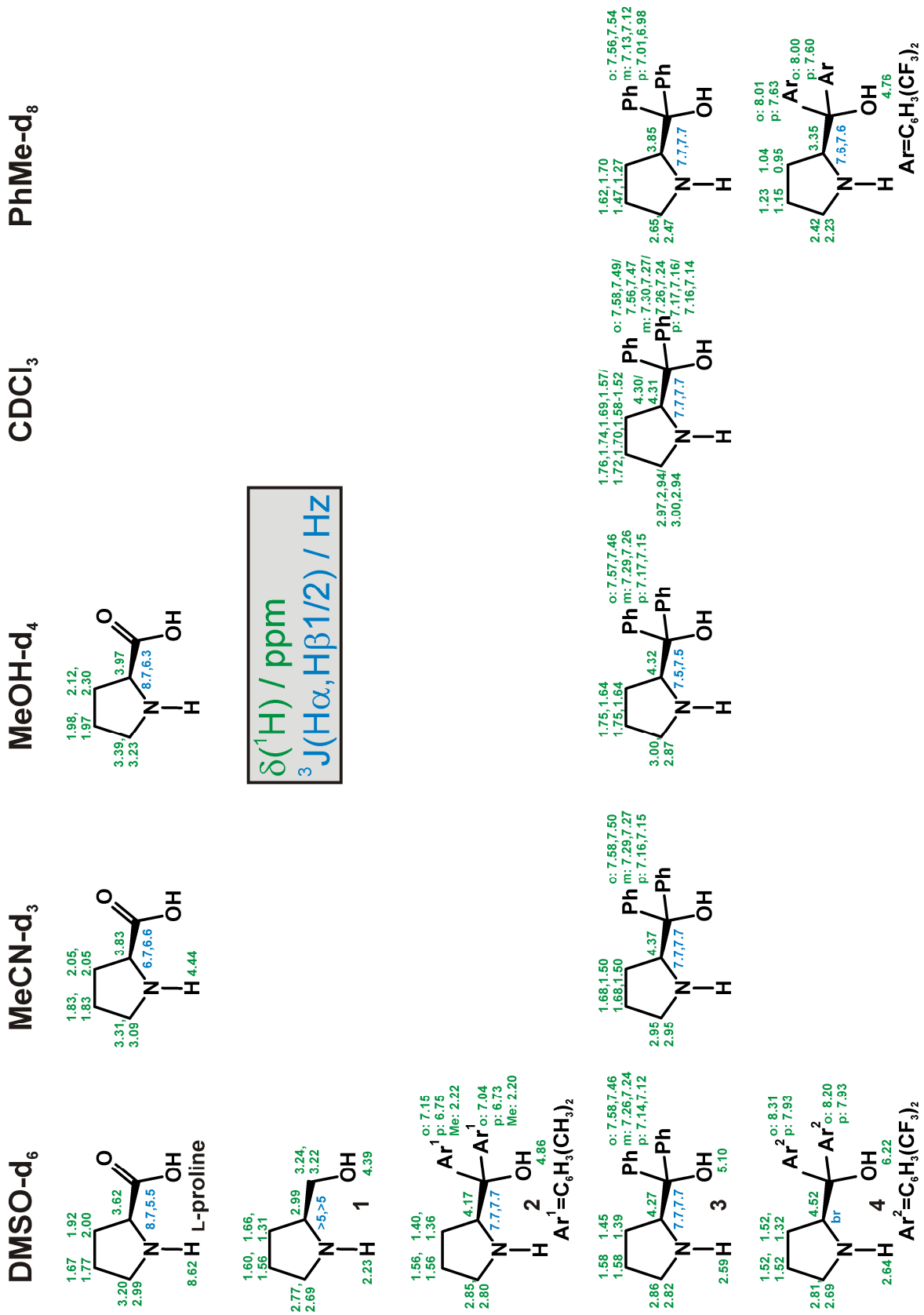


Scheme S1 Overview of the prolinol enamines, relevant ^{1}H chemical shifts and coupling constants.
(Note: Chemical shifts of Hβ1, Hγ1 and Hδ1 are listed below those of Hβ2, Hγ2, Hδ2.)

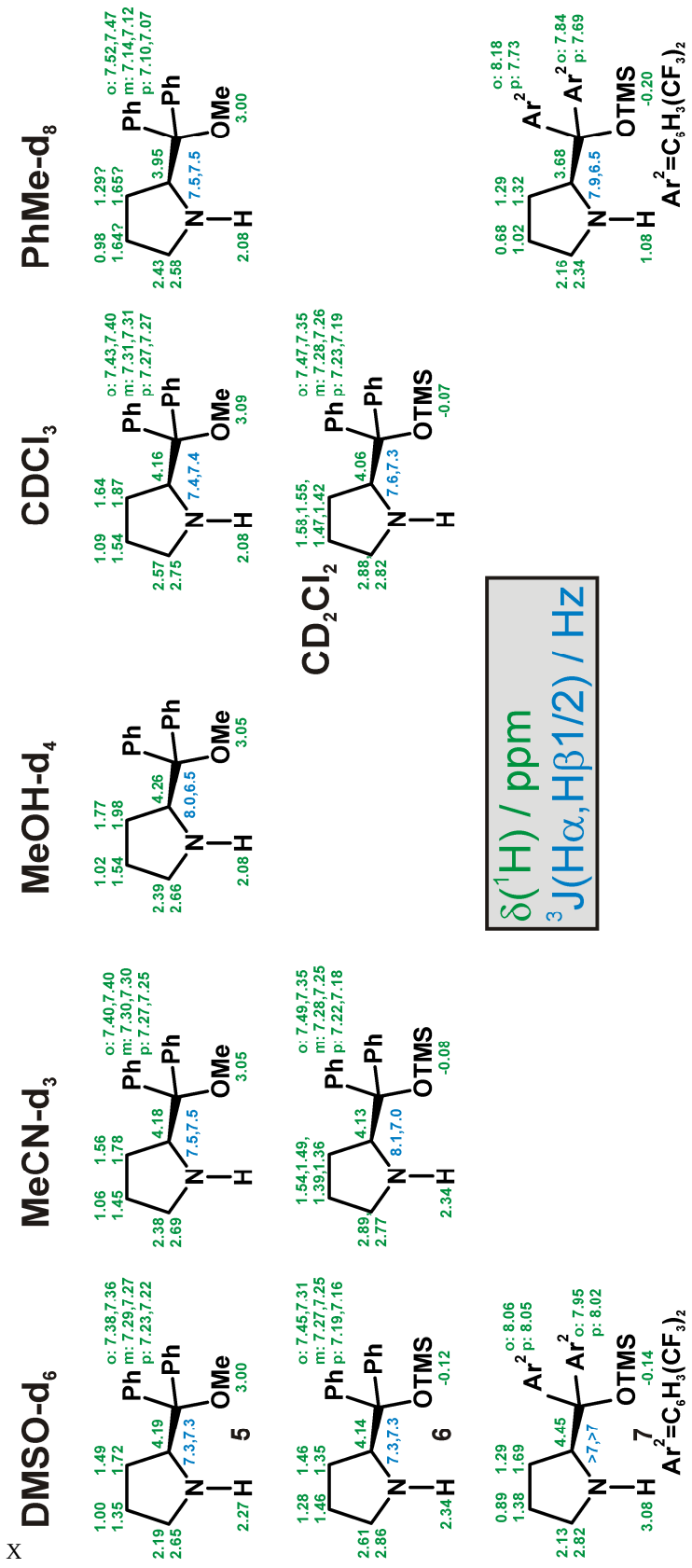


Scheme S2 Overview of the prolinol ether enamines, relevant ^{1}H chemical shifts and coupling constants. (Note: Chemical shifts of Hβ1, Hγ1 and Hδ1 are listed below those of Hβ2, Hγ2, Hδ2.)

2 NMR Characterization of Organocatalysts



Scheme S3 ^{1}H chemical shift assignment and relevant coupling constants of the prolinol organocatalysts.
(Note: Chemical shifts of Hβ1, Hγ1 and Hδ1 are listed below those of Hβ2, Hγ2, Hδ2.)



Scheme S4 ^{1}H chemical shift assignment and relevant coupling constants of the prolinol ether organocatalysts. (Note: Chemical shifts of Hβ1, Hγ1 and Hδ1 are listed below those of Hβ2, Hγ2, Hδ2.