

## Electronic Supplementary Information

### Solvent dependent asymmetric hydrogenation with self-assembled catalysts: a combined catalytic, NMR- and IR-study

Ivan A. Shuklov,<sup>a</sup> Natalia V. Dubrovina,<sup>b\*</sup> Enrico Barsch,<sup>a,c</sup> Ralf Ludwig,<sup>a,c</sup> Dirk Michalik,<sup>a</sup> Armin Börner<sup>a,b\*</sup>

Contribution from: <sup>a</sup>Leibniz-Institut für Katalyse an der Universität Rostock e.V., A.-Einstein-Str. 29a, 18059 Rostock (Germany). Fax: (+49)381-1281-5202. E-mail: [natalia.dubrovina@uni-rostock.de](mailto:natalia.dubrovina@uni-rostock.de), [armin.boerner@catalysis.de](mailto:armin.boerner@catalysis.de).

<sup>b</sup>Institut für Chemie der Universität Rostock, A.-Einstein-Str. 3a, 18059 Rostock (Germany).

<sup>c</sup>Institut für Chemie der Universität Rostock, Dr.-Lorenz-Weg 1, 18059 Rostock (Germany).

## Experimental

### NMR-Study

<sup>31</sup>P NMR spectra were recorded on a AVANCE 500 spectrometer at 162.0 MHz. The <sup>31</sup>P chemical shifts are referenced to 85% H<sub>3</sub>PO<sub>4</sub> as external standard.

### IR-Study

The IR measurements were performed with a Bruker Vertex 70 FTIR-spectrometer. The spectrometer was purged continuously with dry air during the experiments in order to minimize contributions from atmospheric water vapor. A L.O.T.-Oriel variable-temperature cell equipped with CaF<sub>2</sub> windows and an optical pathlength 0.05 mm was used. Temperatures were maintained with an external Haake DC-30/K-20 cryostat and were monitored with a NiCrNi-thermocouple attached directly to the cell. For each spectrum 75 scans at a spectral resolution of 0.5 cm<sup>-1</sup> were recorded. Subtraction of the solvent's, instrument's and cell window's optical response was carried out by using reference spectra of the solvent spectra obtained at the same temperatures as the sample spectra.

In the literature, up to now IR-studies of the tautomeric system 2-hydroxypyridine/2-pyridone in TFE were unknown. For IR-spectra in MeOH and chlorinated alkanes (CHCl<sub>3</sub>), see: S. Castillo, J. Favrot, T. Bourssou, J. F. Brazier, M. T. Boisdon, A. Zwick, *Spectrochimica Acta* **1994**, 50A, 1121-1139; D. Schioeberg, G. Zundel, *J. Chem. Soc., Faraday Trans. 2* **1973**, 69, 771-81.

### Ab-initio-calculations at the B3LYP level

Ab-initio-calculations at the B3LYP level were performed within Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels,

M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.