Supporting information for:

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The First Nonempirical Circular Dichroism Determination of the Absolute Configuration of *N*-Phthalimidosulfoximines Based on Exciton Coupling Mechanism and a Correlation with the Absolute Configuration of Chiral Sulfoxides

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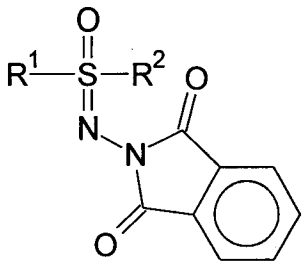

1

	R^1	R^2
1a	4-MeC_6H_4	Me
1b	4-MeC_6H_4	Et
1c	4-MeC_6H_4	*n*-Pr
1d	4-MeC_6H_4	*i*-Pr
1e	4-MeC_6H_4	*t*-Bu
1f	Ph	Me

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Experimental Section

All melting points are uncorrected. NMR spectra were recorded on a Bruker 200AC spectrometer and are reported in δ units using tetramethylsilane. All optical rotation measurements were determined on a Perkin-Elmer 241M photopolarimeter. N-Aminophthalimide and lead tetraacetate were obtained from Aldrich.

Optically active sulfoxides (2a-g): p-Tolyl alkyl sulfoxides **2a-e** were prepared by literature methods[1,2] using diastereomerically pure O-menthyl p-toluenesulfinate as a substrate and had the following optical rotation values: **2a**, $[\alpha]_D$=+140.2 (acetone); **2b**, $[\alpha]_D$=+203.0 (acetone); **2c**, $[\alpha]_D$=-171.6 (acetone); **2d**, $[\alpha]_D$=-163.0 (acetone); **2e**, $[\alpha]_D$=+142.8 (acetone).

Similarly, methyl phenyl sulfoxide **2f**, $[\alpha]_D$=+104.6 (EtOH) and methyl α-naphthyl sulfoxide **2g**, $[\alpha]_D$=+230.0 (acetone), were prepared starting from O-diacetone-glucose methanesulfinate.[3]

Preparation of N-phthalimidosulfoximines 1a-g

The optically active sulfoxide **2** (1 mmol) and N-aminophthalimide (1.2 mmol) were dissolved in dry $CHCl_3$ and lead tetraacetate (1.5 mmol) in portionts was added to the clear solution. After complete addition the slurry was stirred at room temperature for 12 hrs, then water (150 ml) was added and the organic layer separated. The water phase was extracted again with $CHCl_3$ (2x30 ml). The combined organic solutions were dried, filtered and concentrated in vacuo leaving a solid which was purified by chromatography on a silica gel column (approximately 60 g of silica gel) employing petroleum ether – acetone (10:3) or diethyl ether as eluents. Optical rotations of the isolated N-phthalimido sulfoximines **1** are collected in Table 2 and the remainig analytical and NMR data are given below:

(R)-**1a**: yield 71%; mp 143-145°C; Anal. Calcd for $C_{16}H_{14}N_2O_3S$: C, 61.13; H, 4.49; N, 8.91; S, 10.20. Found: C, 61.44; H, 4.57; N, 9.33; S, 10.49. NMR ($CDCl_3$) δ 2.42 (s, CH_3Ar); 3.33 [s, CH_3S(O)(NNPht)]; 7.35-8.12 (m, 8HAr)

(R)-**1b**: yield 60.9%; mp 63-65°C; Anal. Calcd for $C_{17}H_{16}N_2O_3S$: C, 62.17; H, 4.91; N, 8.54; S, 9.77. Found: C, 62.43; H, 4.99; N, 8.90; S, 10.12. NMR ($CDCl_3$) δ 1.31 (t, J=7.33 Hz, -CH_2CH_3), 2.43 (s, CH_3-Ar); 3.31-3.67 (ABX_3 system, CH_2-CH_3); 7.62-7.82 (m, 8HAr)

(S)-**1c**: yield 43.8%; mp 118-120°C; Anal. Calcd for $C_{18}H_{18}N_2O_3S$: C, 63.14; H, 5.30; N, 8.18, S, 9.36. Found: C, 63.43; H, 5.47; N, 8.48; S, 9.66. NMR ($CDCl_3$) δ 0.98 (t, J=7.44 Hz, $CH_3CH_2CH_2$); 1.60-2.00 (ABC_5 system, CH_2-CH_2-CH_3); 2.43 (s, CH_3Ar); 3.23-3.62 (ABC_2 system, CH_2-CH_2CH_3); 7.60-7.80 (m, 8HAr)

(S)-**1d**; yield 48%; mp 118-121°C; Anal. Calcd for $C_{18}H_{18}N_2O_3S$: C, 63.14; H, 5.30; N, 8.18; S, 9.36. Found: C, 62.99; H, 5.17; N, 7.99; S, 9.66. NMR ($CDCl_3$) δ 1.43 (dd, J=6.82 Hz, $(CH_3)_2$CH); 2.42 (s, CH_3-Ar); 3.69 [sep]=6.82 Hz, $CH(CH_3)_2$]; 7.33-8.07 (m, 8HAr)

(R)-**1e**: yield 73%; mp 147-155°C (decomp); Anal. Calcd for $C_{19}H_{20}N_2O_3S$: C, 64.02; H, 5.66; N, 7.86; S, 9.00. Found: C, 64.27; H, 5.73; N, 7.95; S, 9.40. NMR ($CDCl_3$) δ 1.542 (s, $(CH_3)_3$C); 2.168 9s, CH_3-Ar); 7.31-8.10 (m, 8HAr)

(R)-**1f**[4]: yield 52.3%; mp 110-113°C; Anal. Calcd for $C_{15}H_{12}N_2O_3S$: C, 59.98; H, 4.03; N, 9.33; S, 10.68. Found: C, 60.27; H, 4.09; N, 9.65; S, 10.95. NMR ($CDCl_3$) δ 3.36 [s, CH_3S(O)(NNPhth)]; 7.55-8.29 (m, 9HAr)

(R)-**1g**: yield 48%; mp 185-188°C (decomp); Anal. Calcd for $C_{19}H_{14}N_2O_3S$: C, 65.12; H, 4.03; N, 7.99; s, 9.15. Found: C, 65.43; H, 4.12; N, 8.07; S, 9.47. NMR ($CDCl_3$) δ 3.48 [s, CH_3S(O)(NNPhth)]; 7.62-9.42 (m, 11HAr)

References

1. Mislow, K., Green, M.M., Laur, P., Melillo, J.P., Simons, T., Ternay Jr., A.L. *J. Am. Chem. Soc.* 1965, **87**, 1958.
2. Drabowicz, J., Bujnicki, B., Mikołajczyk, M. *J. Org. Chem.* 1982, **47**, 3325.
3. Fernandez, I., Khiar, N., Llera, J.M., Alcudia, F. *J. Org. Chem.* 1992, **57**, 6789.
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Chiroptical properties of **1a-1f**. Cotton effects shown in bold numbers are used for absolute configuration determination

	$\Delta\varepsilon$ (nm), in CH_3CN				$[\alpha]_D$ ($CHCl_3$)
(*R*)-**1a**	-0.5 (343)	-0.7 (276)	**-14.4 (232)**	-14.9 (198)	-159.5
	+0.7 (302)	-0.7 (269)	**+7.4 (215)**		
		+0.2 (257)			
(*R*)-**1b**	-0.6 (344)	-0.8 (276)	**-14.5 (235)**	-13.4 (199)	-125.8
	+0.8 (302)	-0.8 (269)	**+6.8 (216)**		
		+0.8 (256)			
(*S*)-**1c**	+0.5 (345)	+0.8 (276)	**+11.3 (235)**	+11.5 (196)	+142.7
	-0.7 (303)	+0.8 (269)	**-6.5 (216)**		
		-0.3 (256)			
(*S*)-**1d**	+0.6 (347)	+0.9 (276)	**+14.2 (233)**	+14.7 (196)	+169.6
	-1.1 (303)	+0.7 (269)	**-6.7 (217)**		
		-0.9 (254)			
(*R*)-**1e**	-0.6 (346)	-0.8 (276)	**-16.7 (232)**	-23.0 (196)	-150.9
	+1.3 (303)	-0.7 (269)	**+12.6 (215)**		
		+0.7 (256)			
(*R*)-**1f**[a]	-0.6 (346)	-1.3 (275)	**-12.6 (233)**	-15.6 (190)	-157.0
	+0.7 (302)	-1.3 (268)	**+9.1 (214)**		
		+1.4 (252)			

[a] data corrected to 100% e.e.

The CD spectra measured in acetonitrile solutions are in full qualitative agreement with the CD spectra obtained in methanol solution, indicating little solvent effect on the rotamer population.