Supplementary Material (ESI) for Chemical Communications

Supporting Information for

Stereospecific chlorination of β-substituted cyclic alcohols using PPh_3/NCS: factors that control the stereospecificity

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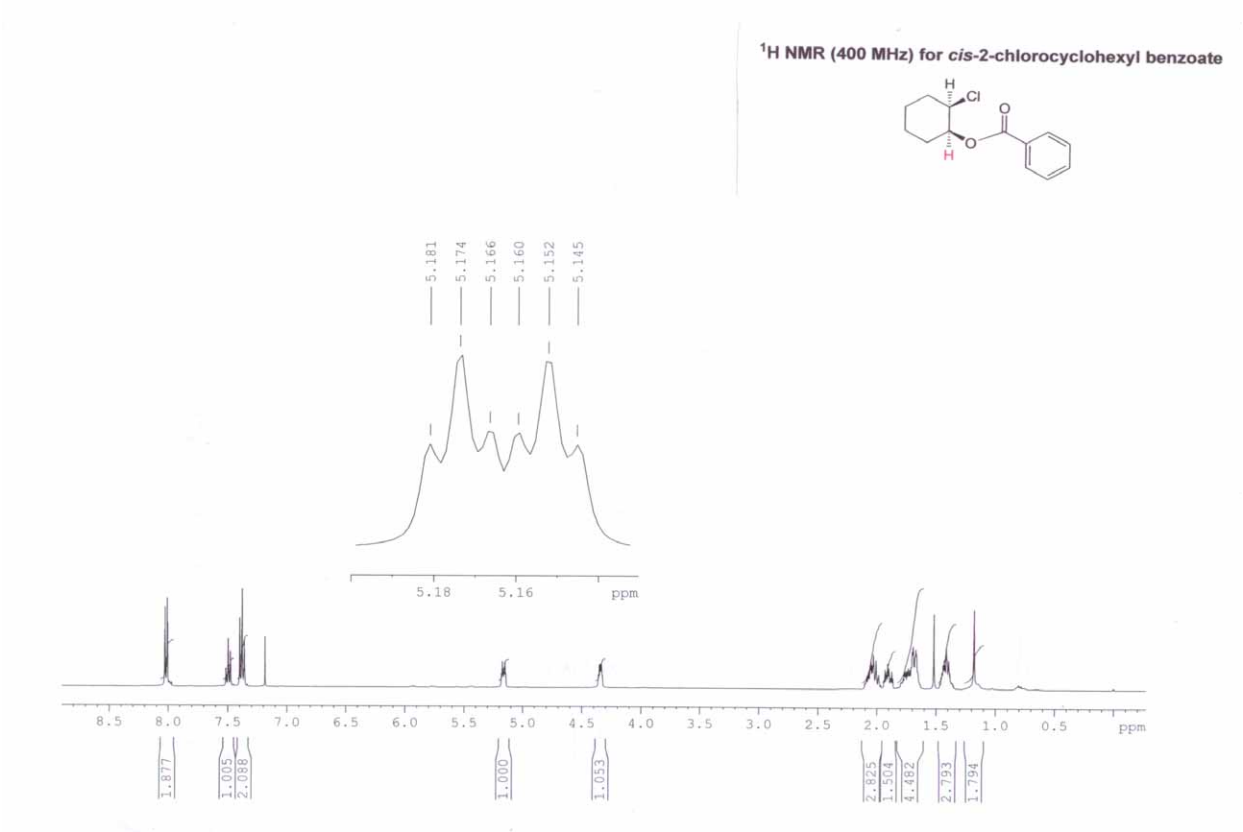
Determination of Stereochemistry by ^{1}H NMR

The stereochemistry of the product chlorides was determined by coupling pattern of methine protons in ^{1}H NMR spectra. All the *cis* chlorides have doublet of triplet (dt) pattern due to one *trans* coupling and two *cis* couplings. Whereas the *trans* chlorides gave triplet of doublet (td) coupling pattern due to two *trans* coupling and one *cis* coupling. This is also confirmed by X-ray structure of selected compounds.

Representative ^{1}H NMR spectrum for *cis*-chloride



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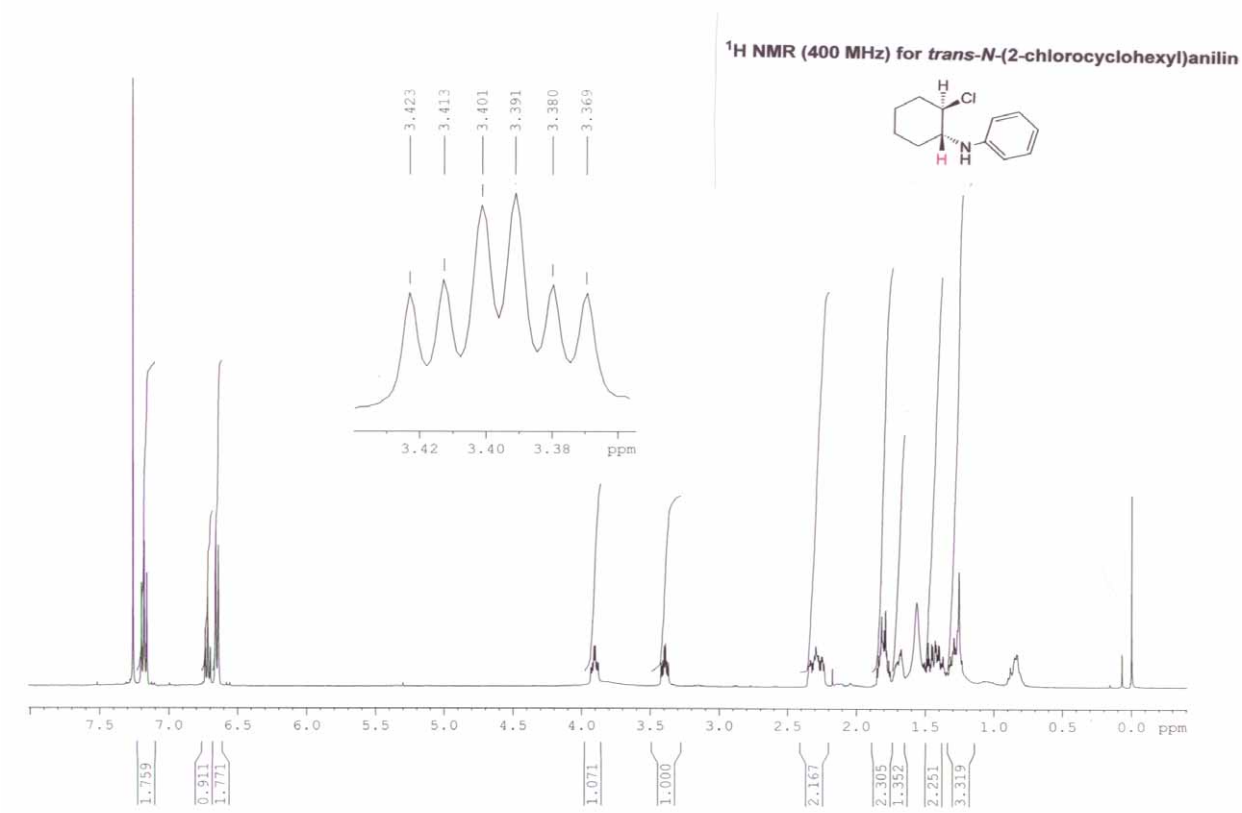
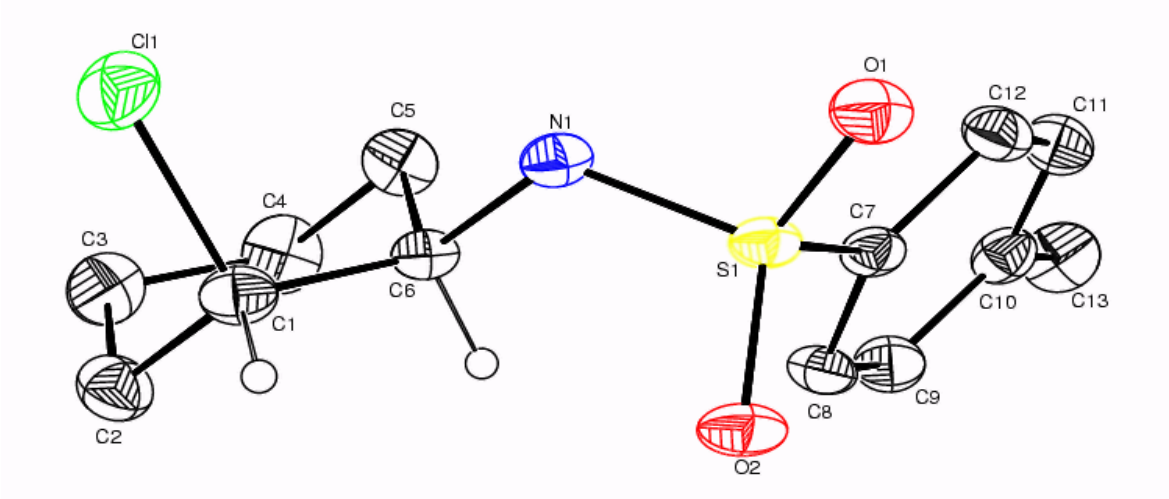
Representative ^{1}H NMR spectrum for *trans*-chloride



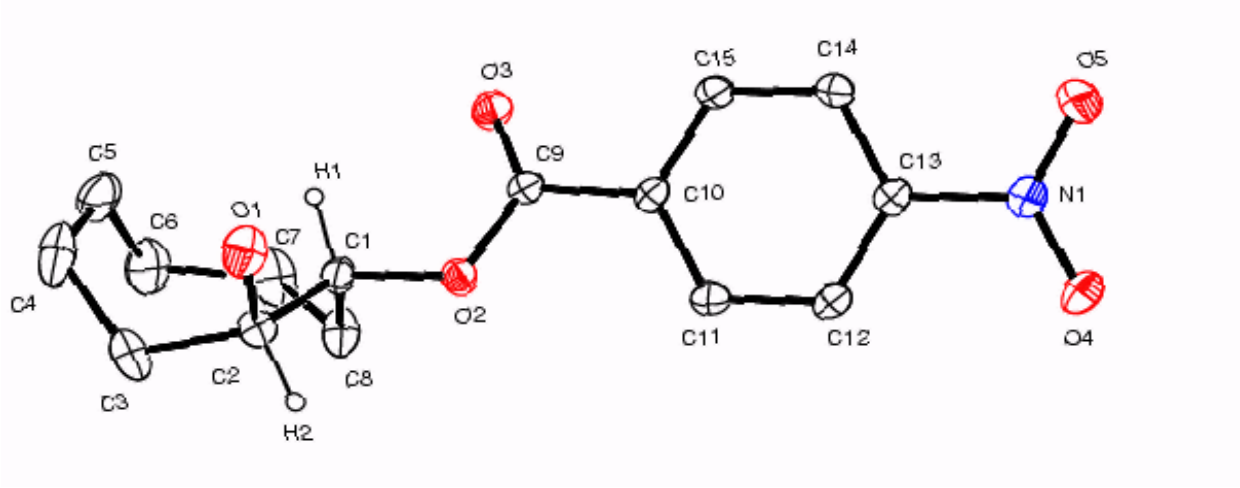
X-ray crystal structure of *cis*-*N*-(2-chlorocyclohexyl)-4-methylbenzenesulfonamide. (30% Probability).



Crystallographic data for *cis*-*N*-(2-chlorocyclohexyl)-4-methylbenzenesulfonamide:

C_{13} H_{18} Cl N O_2 S, M = 287.79, Triclinic, a = 6.7769(4), b = 9.7641(8), c = 11.4462(8) A^{o}, α = 76.916(5), β = 80.416(4), γ = 74.897(4) , V = 707.58(9), T = 273(2) K, space group P-1, Z = 2, μ = 0.411 mm^{-1}, R_{int} = 0.0280 (for 4438 measured reflections), $R1$ = 0.0626 [for 1996 unique reflections with I > 2σ(I)], wR2 = 0.1733 (for all 2382 unique reflections), CCDC 621755

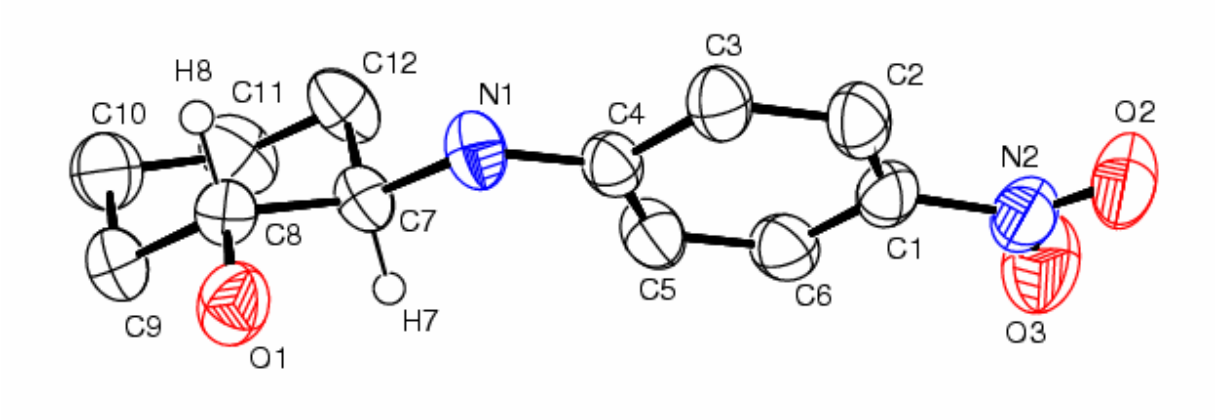
X-ray crystal structures of *trans*-2-hydroxycyclooctyl-4-nitrobenzoate. 30% Probability



Crystallographic data for *trans*-2-hydroxycyclooctyl-4-nitrobenzoate. 30% Probability

$C_{15}H_{19}NO_5$, M = 293.31, Triclinic, a = 7.2564(6), b = 7.4017(5) , c = 15.5988(13) A^o, α = 88.923(5), β = 85.403(5), γ = 62.334(4), V = 739.47(10), T = 293(2) K, space group P-1, Z = 2, μ = 0.099 mm^{-1}, R_{int} = 0.0237 (for 9003 measured reflections), $R1$ = 0.0826 [for 2033 unique reflections with I > 2σ(I)], wR2 = 0.2637 (for all 2530 unique reflections), CCDC 621756.

X-ray crystal structures of *trans*-2-(4-nitrophenylamino)cyclohexanol (30% Probability)



Crystallographic data for *trans*-2-(4-nitrophenylamino)cyclohexanol

C_{12} H_{16} N_2 O_3, M = 236.27, Monoclinic, a = 18.6930(18), b = 9. 9424(8), c = 14.9984(16) A^o, β = 122.342(10), V = 2355.1(4), T = 273(2) K, space group C2/c, Z = 8, μ = 0.097 mm^{-1}, R_{int} = 0.0220 (for 16937 measured reflections), $R1$ = 0.0526 [for 2723 unique reflections with I > 2σ(I)], wR2 = 0.1973 (for all 4148 unique reflections), CCDC 622916.