

Supporting Information

Formation of quaternary centres by copper catalysed asymmetric conjugate addition to β -substituted cyclopentenones with the aid of a quantitative structure-selectivity relationship

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X-ray Crystallography

Low temperature, single crystal X-ray diffraction data for **L26** (*S*)-amine.HCl and **L28** (*S*)-amine.HCl salts were collected with a (Rigaku) Oxford Diffraction SuperNova A diffractometer at 150 K. Raw frame data were collected and reduced using CrysAlisPro. The structure was solved *ab initio* using SuperFlip^[1] and refined using CRYSTALS.^[2] Further details about the refinement are documented in the CIF. The crystallographic data have been deposited with the CCDC as entries 1818574 and 1818575.

Table 1. Summary of X-ray crystallographic data

Compound Number	L26 -(<i>S</i>)-amine.HCl salt	L28 -(<i>S</i>)-amine.HCl salt
Moiety Formula	C ₂₄ H ₃₀ NCl	C ₂₂ H ₂₀ F ₆ NCl
CCDC	1818574	1818575
Space Group	P 2 ₁ 2 ₁ 2 ₁	P 2 ₁
a [Å]	8.33200(10)	11.4023(2)
b [Å]	11.3877(2)	8.44600(10)
c [Å]	22.1875(4)	12.1680(2)
α [°]	90	90
β [°]	90	117.387(2)
γ [°]	90	90
V [Å ³]	2105.20(6)	1040.49(3)
Z	4	2
T [K]	150	150
Total Reflections	16356	11013
R _{int}	0.0385	0.0213
Reflections, Restraints, Parameters (I > 3.0/σ(I))	4368, 452, 309	4285, 565, 345
Min. and Max. Residual Density, [eÅ ⁻³]	-0.18, 0.28	-0.42, 0.41
R ₁ (I > 2σ(I))	0.0317	0.0357
wR ₂	0.0796	0.0937
Absolute Struct. (Flack param.)	-0.007(12)	-0.007(15)

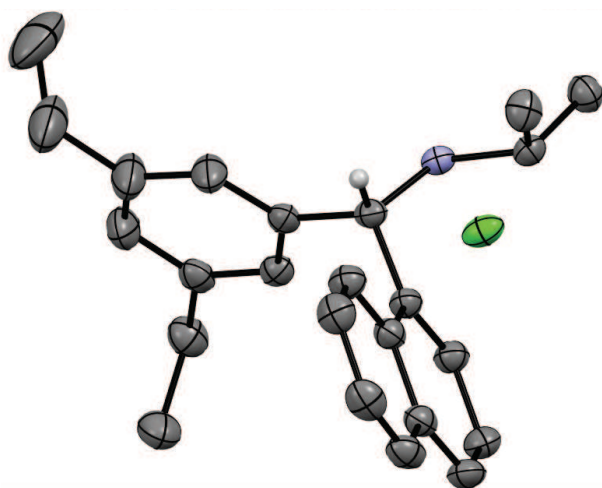


Figure 1: Solid state structure of **L26-(S)-amine.HCl** salt. Displacement ellipsoid plots are drawn at 50% probability. Hydrogen atoms (except at the stereocentre) and disordered components are omitted for clarity.

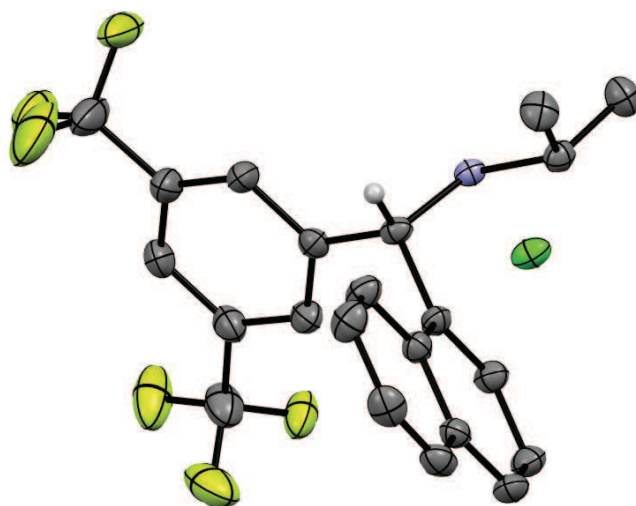


Figure 2: Solid state structure of **L28-(S)-amine.HCl** salt. Displacement ellipsoid plots are drawn at 50% probability. Hydrogen atoms (except at the stereocentre) and disordered components are omitted for clarity.

[1] L. Palatinus & G. Chapuis, *J. Appl. Cryst.*, **2007**, *40*, 786–790.

[2] a) P. W. Betteridge, J. R. Carruthers, R. I. Cooper, K. Prout, & D. J. Watkin, *J. Appl. Cryst.*, **2003**, *36*, 1487;
b) R. I. Cooper, A. L. Thompson & D. J. Watkin, *J. Appl. Cryst.* **2010**, *43*, 1100–1107.