Electronic Supplementary Information

Half-Sandwich Complexes of Iridium and Ruthenium Containing Cysteine-Derived Ligands

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1- Hydrogen bond interactions in 6aSb

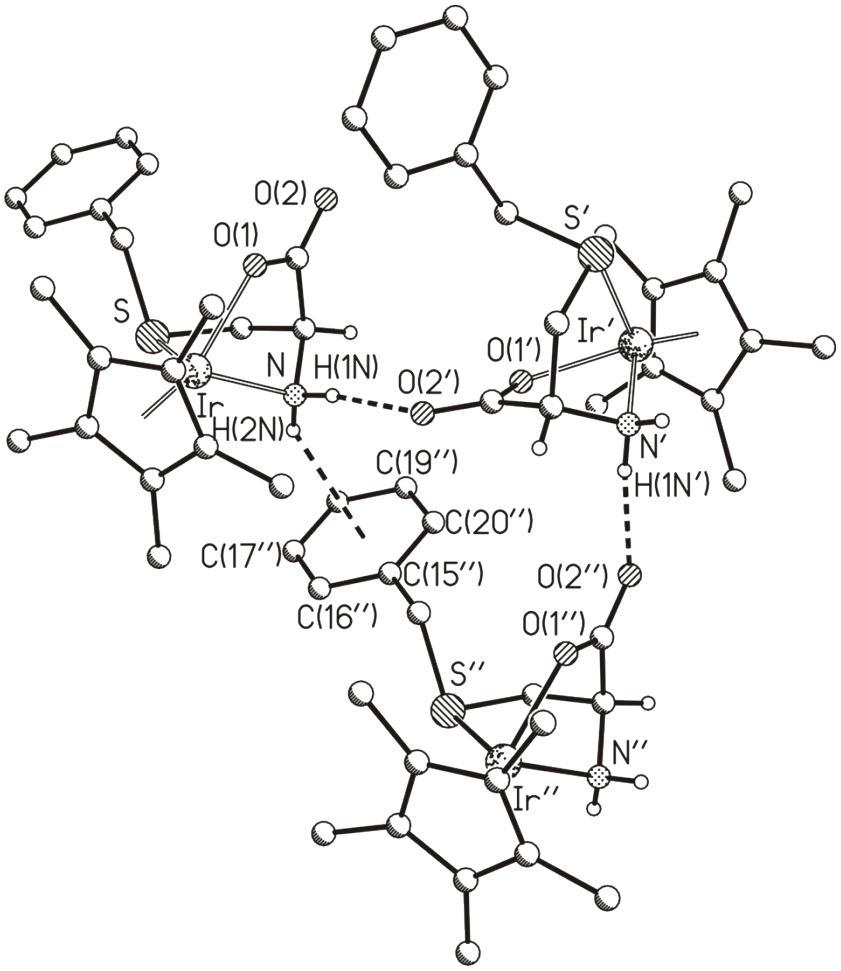


Figure S1. Intermolecular interactions in **6aSb**. Symmetry codes: ') *x* - 1/2, -*y* + 1/2, -*z* + 1; '') *x* - 1, *y*, *z*.

Hydrogen bonds (Å, º): Symmetry code: ') *x* - 1/2, -*y* + 1/2, -*z* + 1.

	D-H	D···A	H···A	D-H···A
N-H(1N)···O(2')	0.90(4)	2.846(4)	1.96(4)	170(4)

N-H ···π interactions (Å, º): Symmetry code: '') *x* - 1, *y*, *z*.

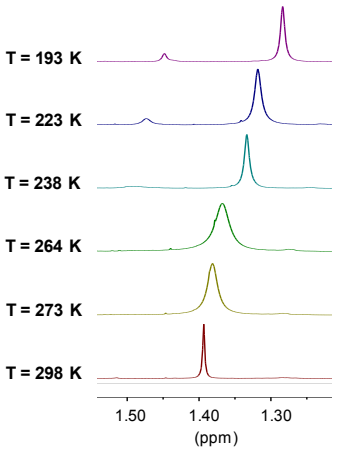
	H···G	H···Ph (plane)	γ	N-H···C	N-H···C (Ph)
N-H(2N)···C(15")/C(20")	2.58(3)	2.54(3)	10.2(6)	C(16"): 2.93(3) C(17"): 2.73(3) C(18"): 2.74(3) C(19"): 2.94(3)	C(15"): 3.10(3) C(20"): 3.11(3)

H···G represents the distance from the H atom to the centroid of the phenyl ring of the reported NH/π interaction. H···Ph is the separation from the H atom to the mean plane of the ring. γ angle: angle between the H-G vector and the normal of the phenyl ring. N-H···C: contact distances between H atom and C atoms under the assumed criterion (3.05 Å). N-H···C(Ph): range of separation between H and the rest of the carbon atoms of the ring.

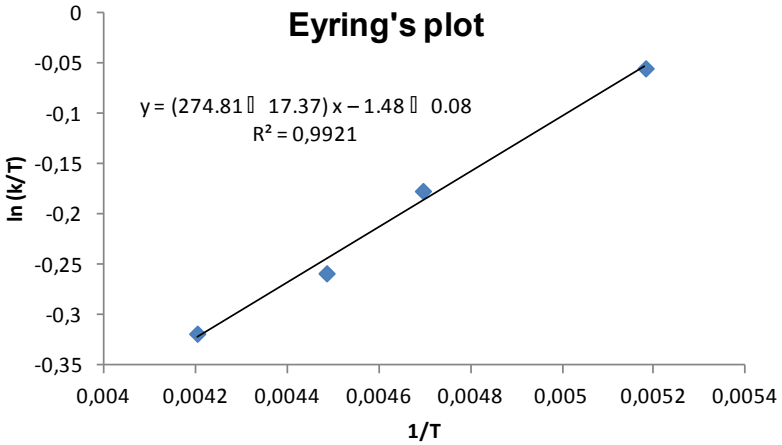
2- Kinetic studies for the epimerization of complex 9a

[**9a**] = 78.61 mM; solvent = CD_2Cl_2

T (K)	k (s^{-1})
193	182,7504
213	178,5546
223	172,2720
238	173,1600



ln (k/T)	1/T
0,005181347	-0,054568901
0,004694836	-0,176397729
0,004484305	-0,258097148
0,004201681	-0,318054651



$\Delta G^{\neq}$ = 12.43 ± 2.28 kcal/mol

$\Delta H^{\neq}$ = - 0.55 ± 0.03 kcal/mol

$\Delta S^{\neq}$ = - 44.3 ± 6.0 cal/K·mol