Electronic energy and standard Gibbs free energy for the conformers of each compound optimized at the B97-3c level of theory and lying within 1 kcal/mol from the ground conformer (highlighted in orange). The electronic energy and standard Gibbs free energy of the ground conformers optimized at the TPSSh level of theory are also quoted for comparison.

	B97-3c			TPSSh	
	Electronic energy (Eh)	G° (Eh)	G° - G°min (kcal/mol)	Electronic energy (Eh)	G° (Eh)
CoL.001	-2381.67939347883	-2381.38895907	0.00	-2382.30506027118	-2382.01271513
CoLpy.001	-2629.86557773221	-2629.49310691	0.37		
CoLpy.010	-2629.86648148943	-2629.49369973	0.00	-2630.73774160234	-2630.36221829
CoLpy.012	-2629.86628976642	-2629.49352229	0.11		
CoLpy2cis.002	-2878.05252005451	-2877.59758530	0.16		
CoLpy2cis.003	-2878.05287162491	-2877.59784742	0.00	-2879.17252245147	-2878.71295488
CoLpy2cis.004	-2878.05124989715	-2877.59679029	0.66		
CoLpy2cis.007	-2878.05318057563	-2877.59764715	0.13		
CoLpy2trans.001	-2878.05262317449	-2877.59700358	0.42		
CoLpy2trans.004	-2878.05343220078	-2877.59766855	0.00	-2879.17234504063	-2878.71259957
py	-248.16619606987	-248.10557102	0.00	-248.40962770746	-248.34799261