J. Braz. Chem. Soc., Vol. 16, No. 4, 1, 2005.
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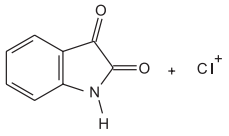
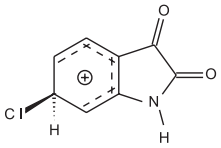
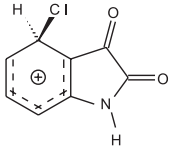
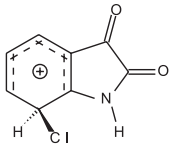
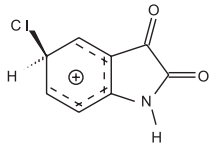
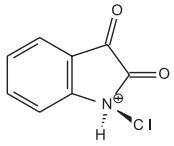
0103 - 5053 $6.00+0.00

Table S1. Enthalpy differences (298 K, 1 atm) for single Cl^+ of isatin at several positions

Species	ΔH^{298} (kcal mol^{-1})[a]	Species	ΔH^{298} (kcal mol^{-1})[a]
	190.4		21.8
	23.5		4.4
	0.0		23.1

[a] Performed at the B3LYP/6-31++G** level, taking into account zero-point energy and thermal expansion correction. All calculations were performed with the Gaussian 98 package.

Table S2. Enthalpy differences (298 K, 1 atm) for protonation of TICA

Reaction	ΔH^{298} (kcal mol^{-1})[a]
$H_3SO_4^+ + TICA \rightarrow H_2SO_4 + H\text{-}TICA^+$	-12.0
$2\ H_3SO_4^+ + TICA \rightarrow 2\ H_2SO_4 + H_2\text{-}TICA^{+2}$	77.6
$3\ H_3SO_4^+ + TICA \rightarrow H_2SO_4 + H_3\text{-}TICA^{+3}$	235.9

[a] Performed at the B3LYP/6-31++G** level, taking into account zero-point energy and thermal expansion correction. All calculations were performed with the Gaussian 98 package.