Supplementary Materials: Disclosing the Ligand- and Solvent-Induced Changes on the Spin Transition and Optical Properties of Fe(II)-Indazolylpyridine Complexes

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Table S1. Unit Cell Parameters of **3**$[BF4]_2 \cdot 2MeNO_2$ and **3**$[BF4]_2$ Solid State Minima.

Unit cell	*a*	*b*	*c*	*α*	*β*	*γ*
$\mathbf{3}^{HS}[BF4]_2 \cdot 2MeNO_2$	14.27	19.14	14.60	90.0	94.4	90.0
$\mathbf{3}^{LS}[BF4]_2 \cdot 2MeNO_2$	13.78	19.99	13.86	90.0	91.0	90.0
$\mathbf{3}^{HS}[BF4]_2$	14.10	17.99	13.79	90.0	86.5	90.0
$\mathbf{3}^{LS}[BF4]_2$	13.50	19.18	13.74	90.0	91.4	90.0

Table S2. Main absorption (fosc > 0.05) for the five free ligands in the out-out conformation.

1-bip	1,2-bip	2-bip	1-ipp	2-ipp
321 (0.55)	343 (0.19)	349 (0.09)	317 (0.60)	346 (0.10)
313 (0.26)	337 (0.26)	349 (0.12)	302 (014)	323 (0.70)
290 (0.21)	313 (0.53)	328 (0.96)	269 (0.15)	306 (0.15)
282 (0.07)	307 (0.06)	308 (0.46)	258 (0.32)	284 (0.28)
270 (0.19)	290 (0.54)	279 (0.49)	252 (0.36)	270 (0.33)
251 (0.40)	269 (0.11)	260 (0.22)	245 (0.06)	260 (0.05)
250 (0.06)	254 (0.18)	237 (0.13)	233 (0.16)	253 (0.08)
237 (0.19)	250 (0.10)	228 (0.17)	221 (0.15)	245 (0.31)
237 (0.15)	243 (0.12)	225 (0.12)	215 (0.11)	234 (0.05)
221 (0.11)	235 (0.26)	219 (0.73)	213 (0.07)	221 (0.56)
212 (0.29)	222 (0.36)	212 (0.08)	204 (0.35)	204 (0.10)
207 (0.07)	214 (0.08)	205 (0.09)	-	200 (0.12)
205 (0.47)	212 (0.11)	-	-	-
205 (0.23)	209 (0.38)	-	-	-
201 (0.18)	205 (0.05)	-	-	-
-	203 (0.33)	-	-	-

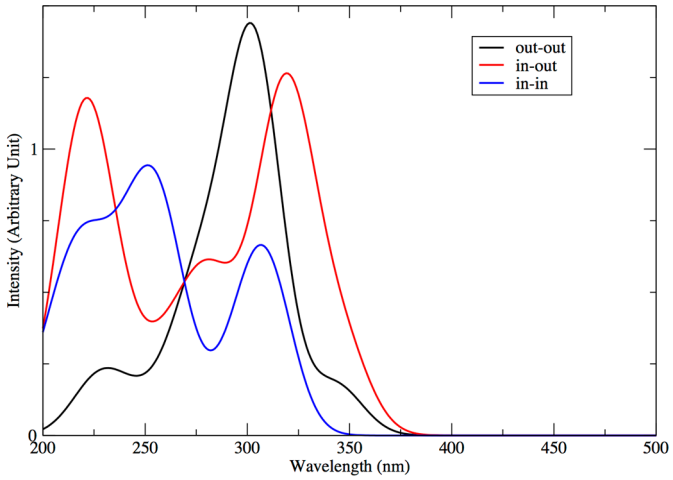

Figure S1. Absorption spectra of the different 2-bip conformers.

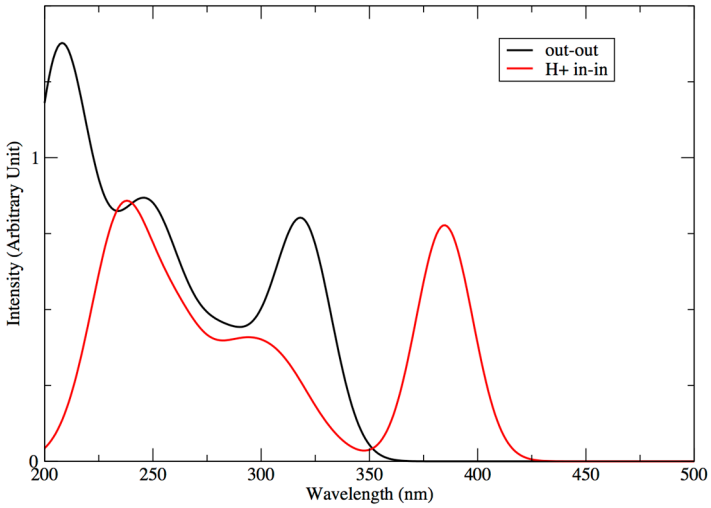

Figure S2. Spectra of *out-out* neutral and *in-in* protonated of 1-bip.

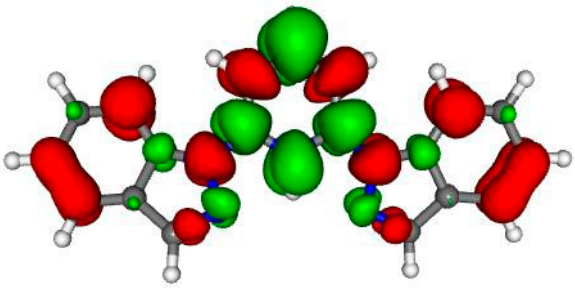

Figure S3. Nature of the lowest absorbing state of the protonated 1-bip ligand.