Supplementary Materials

Completion of Crystallographic Data for the Series of 4-Halogenated-1*H*-Pyrazoles: Crystal Structure Determination of 4-Iodo-1*H*-Pyrazole and Spectroscopic Comparison

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Table S1. Crystal data refinement parameters for 4-I-pzH in the $P2_1ab$ space group.

	4-I-pzH
Formula	$C_3H_3IN_2$
$D_{calc.}$/g cm^{-3}	2.561
μ/mm^{-1}	6.21
M_r	193.97
T/K	170
Crystal System	Orthorhombic
Space group	$P2_1ab$ (No. 29)
a/Å	5.5309(6)
b/Å	6.9477(8)
c/Å	13.0940(14)
V/Å^3	503.16(10)
Z	4
Measured Refl.	7789
Independent Refl.	1239
R_{int}	0.028
Parameters	55
[a]GooF	1.16
[b]wR_2	0.148
[c]R_1	0.069

[a] GooF = $[\sum[w(F_o^2 - F_c^2)^2]/(N_o - N_v)]^{1/2}$ $(N_o = number\ of\ observations, N_v = number\ of\ variables)$

[b] $wR_2 = \sum||F_o| - |F_c||/\sum|F_o|$

[c] $R_1 = [(\sum w(F_o^2 - F_c^2)^2 / \sum|F_o|^2)]^{1/2}$

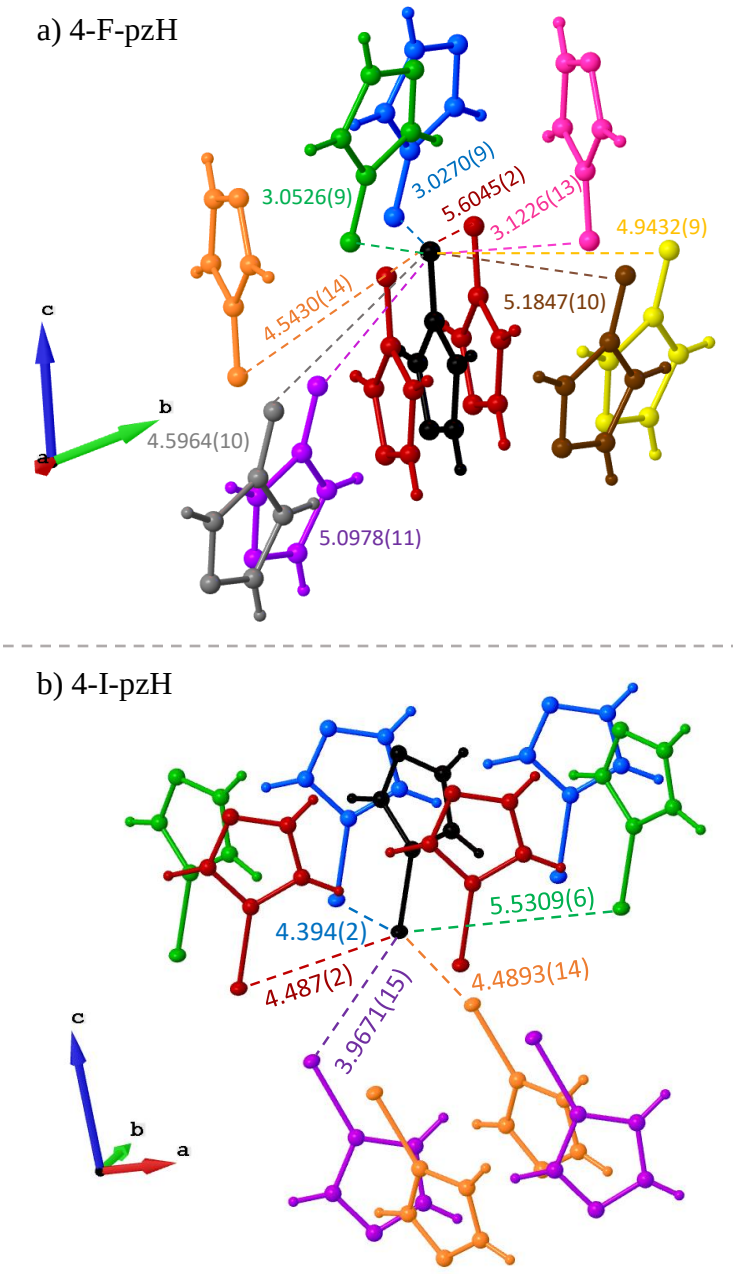

Figure S1. Perspective view showing nearest neighbors of the central molecule (black) for (a) 4-F-pzH and (b) 4-I-pzH. Individual molecules and their corresponding distance from the central molecule are color coded to match.

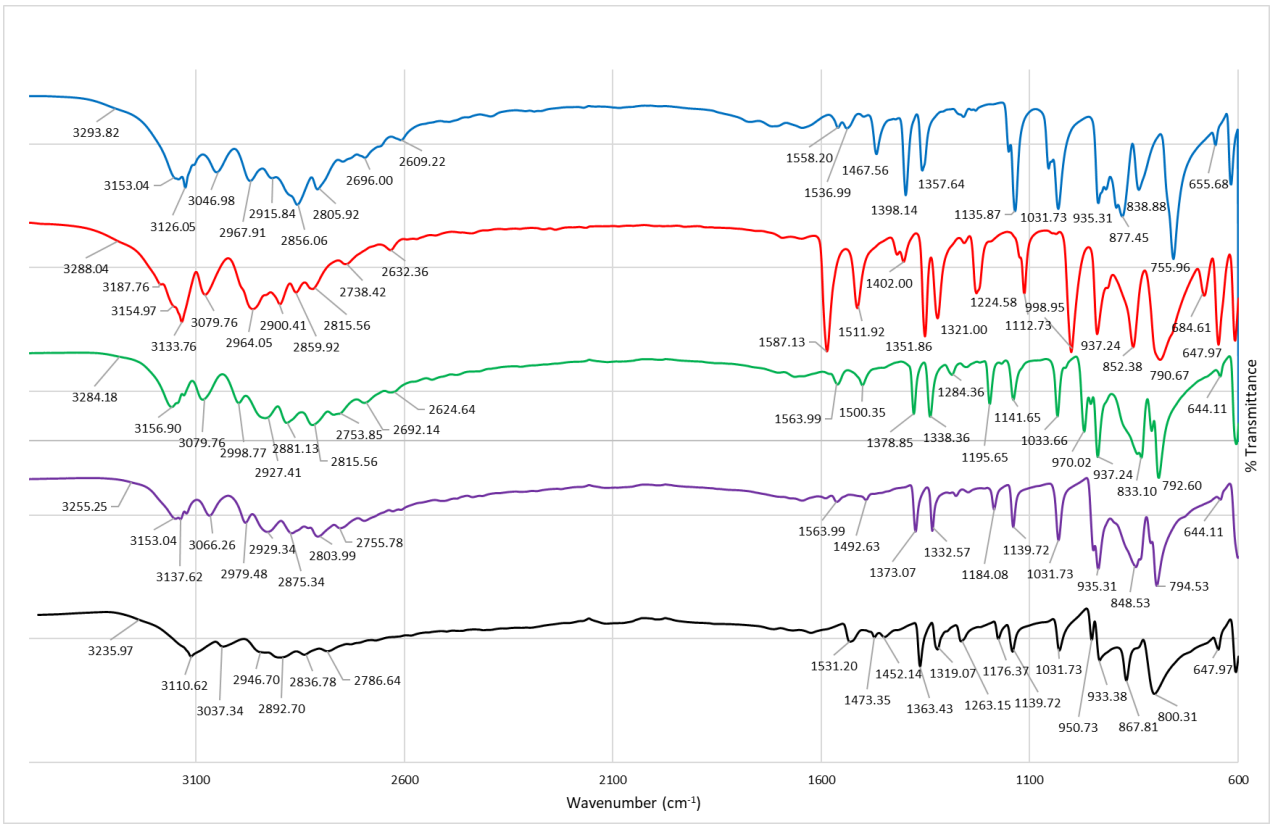

Figure S2. Annotated IR spectra of simple pyrazole and 4-X-pyrazole (where X = F, Cl, Br, I).

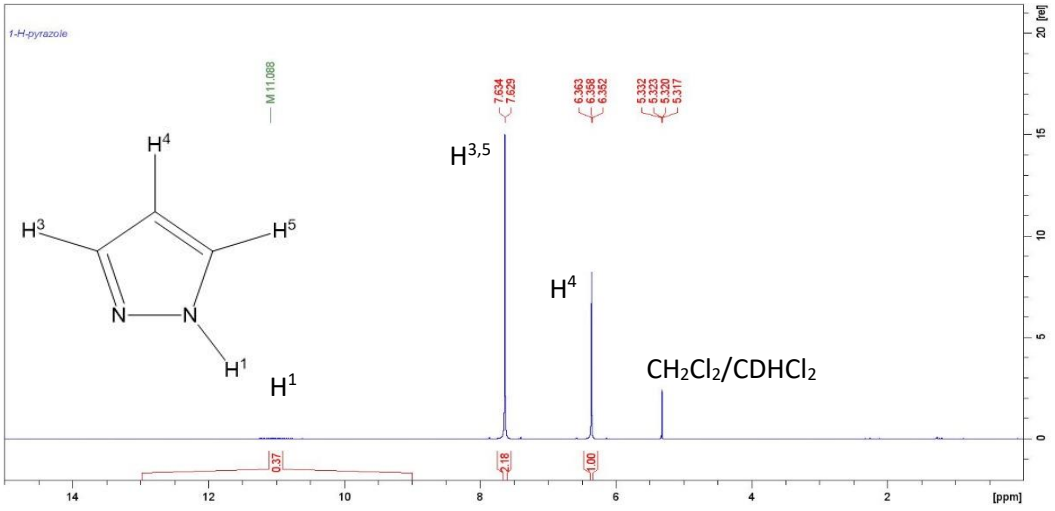

Figure S3. Full 400 MHz ^{1}H NMR spectrum of 4-F-pyrazole in CD_2Cl_2

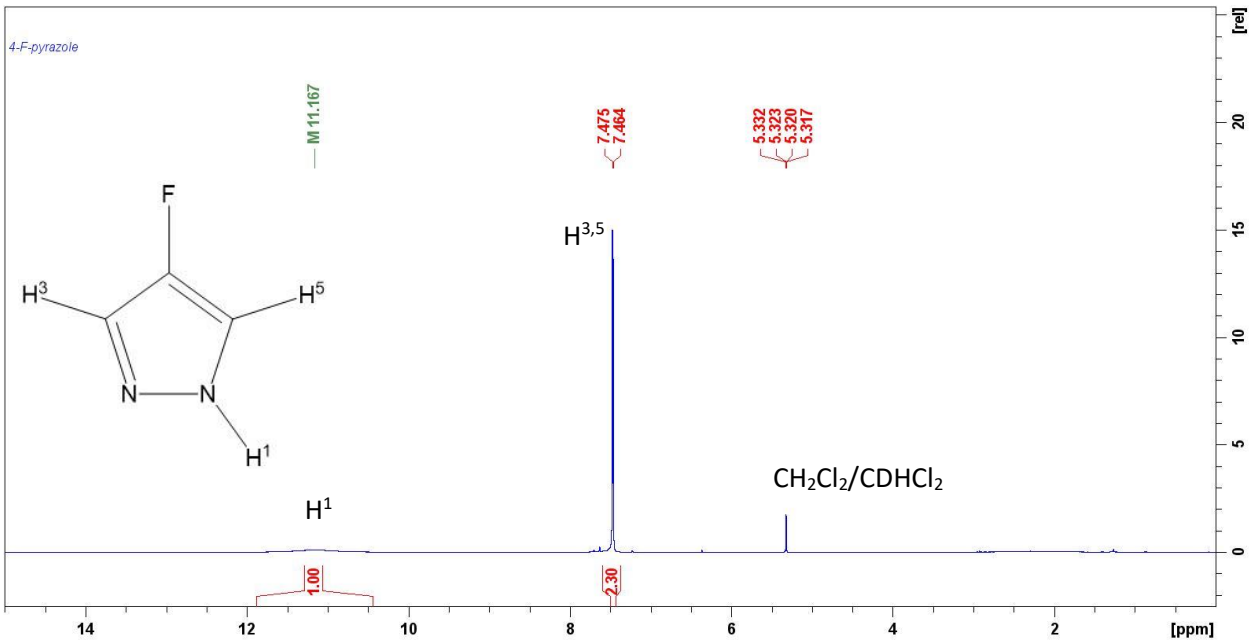

Figure S4. Full 400 MHz ^{1}H NMR spectrum of 4-F-pyrazole in CD_2Cl_2

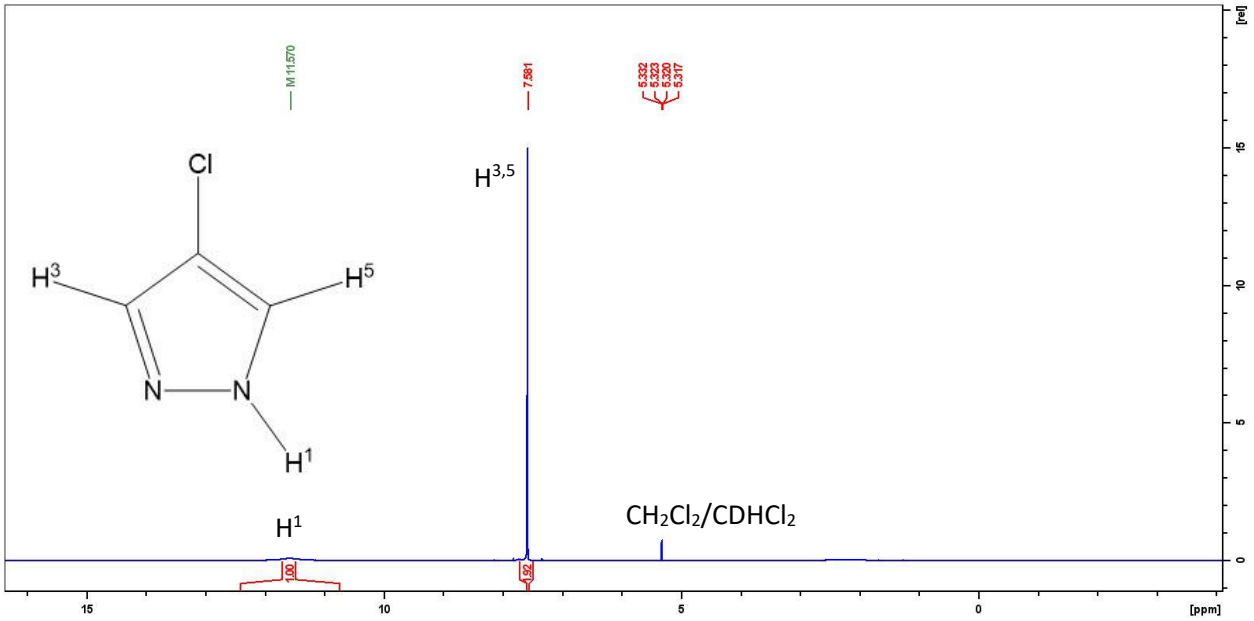

Figure S5. Full 400 MHz ^{1}H NMR spectrum of 4-Cl-pyrazole in CD_2Cl_2

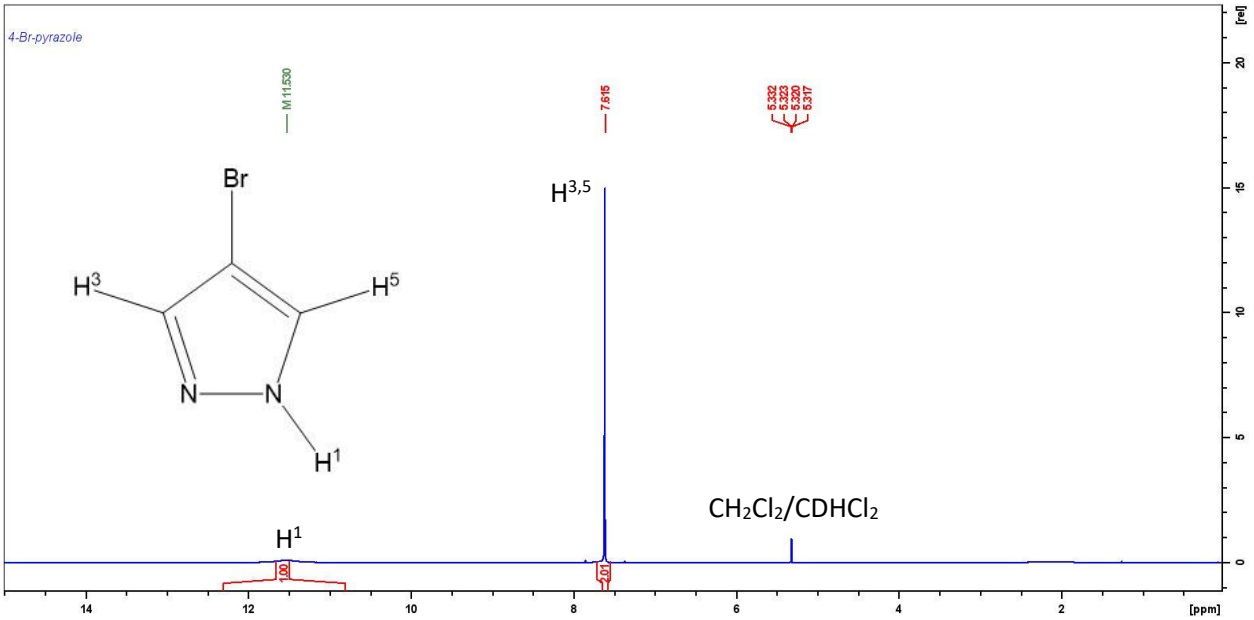

Figure S6. Full 400 MHz ^{1}H NMR spectrum of 4-Br-pyrazole in CD_2Cl_2

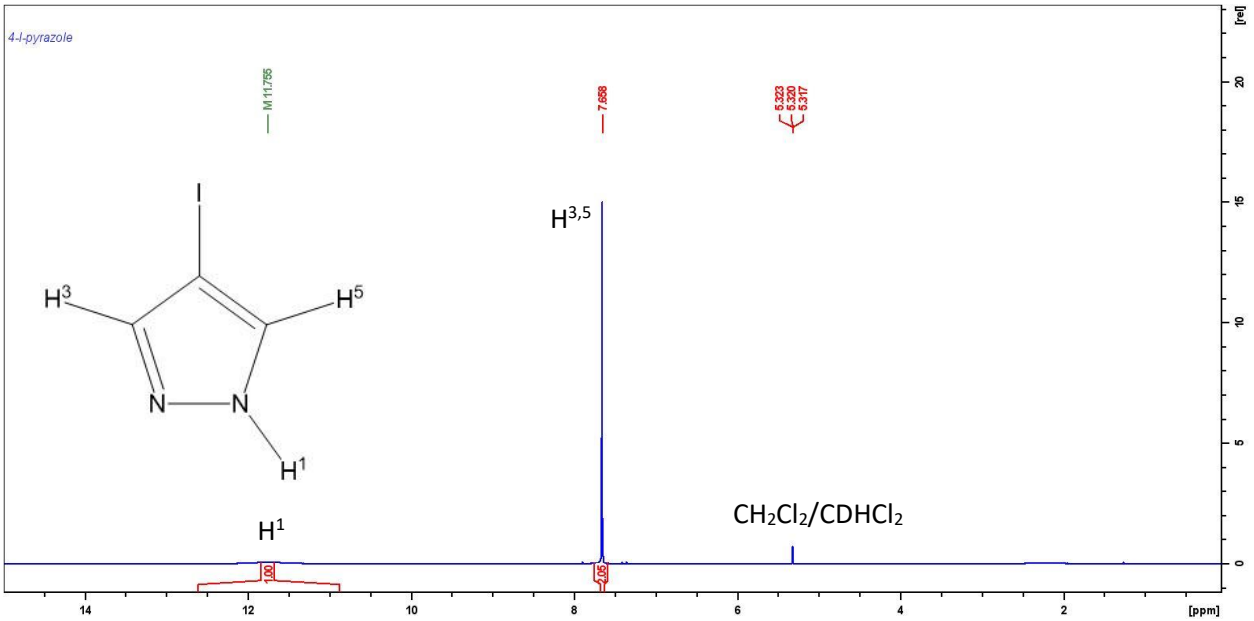

Figure S7. Full 400 MHz ^{1}H NMR spectrum of 4-I-pyrazole in CD_2Cl_2