

Supplementary Material (ESI) for New Journal of Chemistry

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Electronic Supplementary Information for:

An experimental and theoretical investigation of the molecular and electronic structure of 2-amino-4-chloro-6-pyrazolyl-[1,3,5]triazine, forming supramolecular linear tapes in the solid state.

by

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Charts

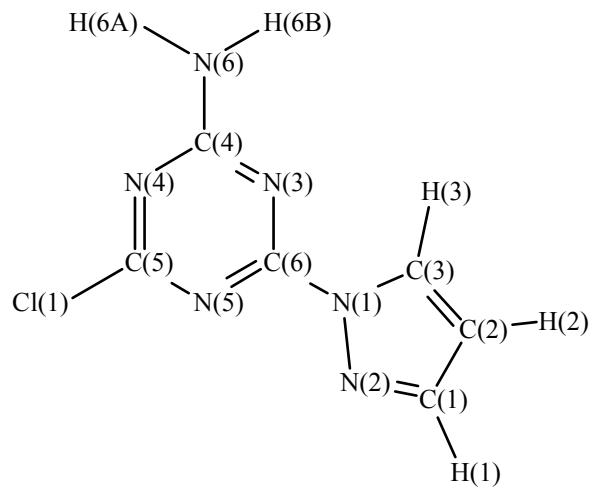


Chart S1

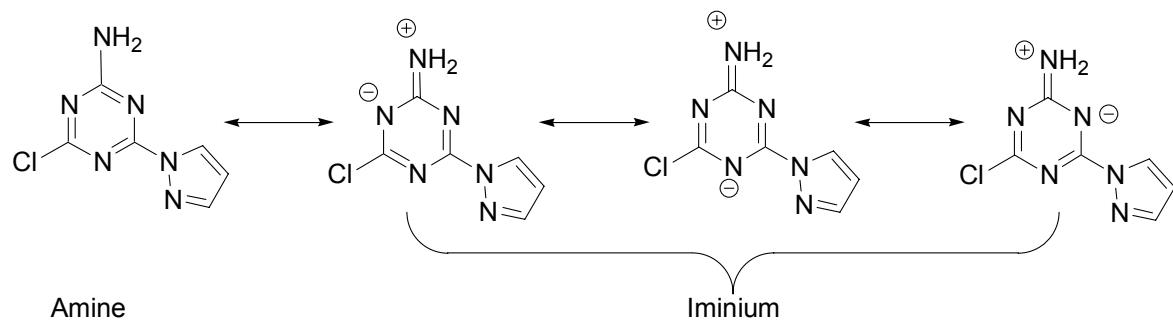
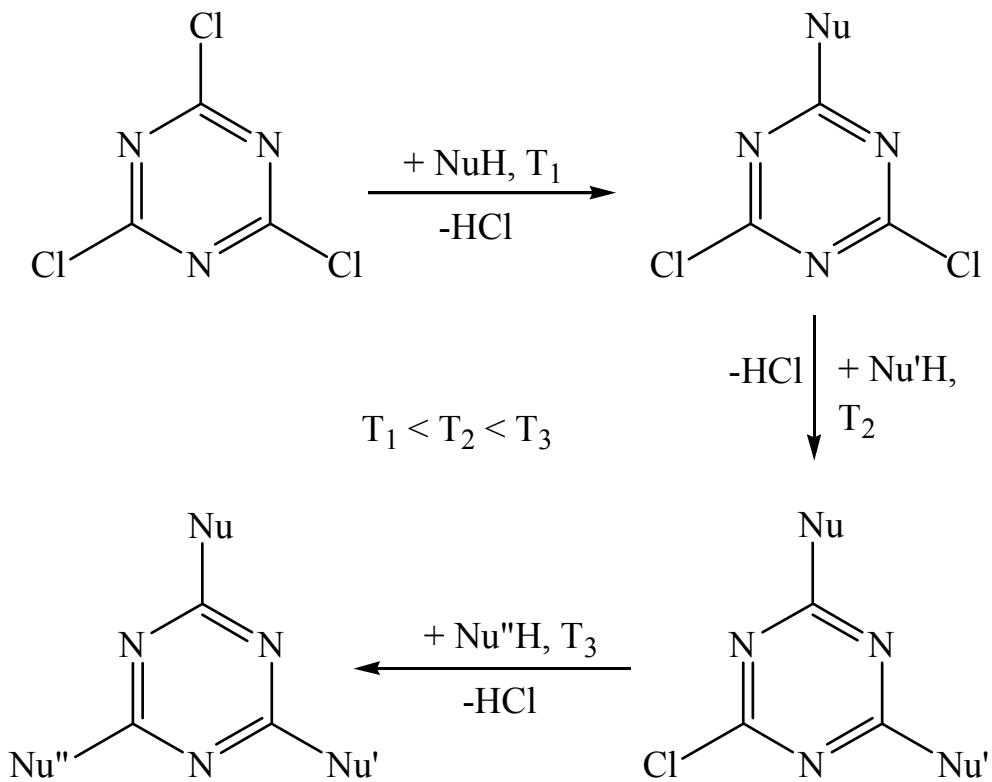


Chart S2

Scheme



Scheme S1

Table

Experimental (XRD data) and calculated (DFT) bond lengths (\AA) and angles (deg) of **1**.

	Expt.	Calcd.		Expt.	Calcd.
Cl(1)–C(5)	1.736(1)	1.752	C(6)–N(1)	1.400(2)	1.402
N(5)–C(5)	1.323(2)	1.328	C(3)–C(2)	1.354(3)	1.373
N(5)–C(6)	1.336(2)	1.339	C(3)–N(1)	1.364(2)	1.379
N(4)–C(5)	1.307(2)	1.324	C(1)–N(2)	1.321(2)	1.327
N(4)–C(4)	1.357(2)	1.355	C(1)–C(2)	1.390(3)	1.424
N(3)–C(6)	1.319(2)	1.335	N(1)–N(2)	1.3560(2)	1.368
N(3)–C(4)	1.351(2)	1.347	N(6)–H(6A)	0.848	1.012
C(4)–N(6)	1.321(2)	1.353	N(6)–H(6B)	0.840	1.012
C(5)–N(5)–C(6)	111.5(1)	112.3	N(4)–C(5)–Cl(1)	116.5(1)	115.7
C(5)–N(4)–C(4)	113.1(1)	112.7	N(5)–C(5)–Cl(1)	114.3(1)	115.6
C(6)–N(3)–C(4)	113.5(1)	113.5	C(2)–C(3)–N(1)	106.3(2)	106.3
N(6)–C(4)–N(3)	117.8(2)	117.6	N(2)–C(1)–C(2)	112.5(2)	112.5
N(6)–C(4)–N(4)	117.6(2)	116.8	C(3)–C(2)–C(1)	105.4(2)	104.7
N(3)–C(4)–N(4)	124.6(1)	125.7	N(2)–N(1)–C(3)	112.0(1)	112.4
N(3)–C(6)–N(5)	128.0(1)	127.1	N(2)–N(1)–C(6)	121.0(1)	121.7
N(3)–C(6)–N(1)	116.4(1)	115.6	C(3)–N(1)–C(6)	126.9(1)	125.9
N(5)–C(6)–N(1)	115.6(1)	117.3	C(4)–N(6)–H(6A)	117.71	118.2
C(1)–N(2)–N(1)	103.7(2)	103.9	C(4)–N(6)–H(6B)	116.21	118.9
N(4)–C(5)–N(5)	129.3(1)	128.6			

Table S1

Figures

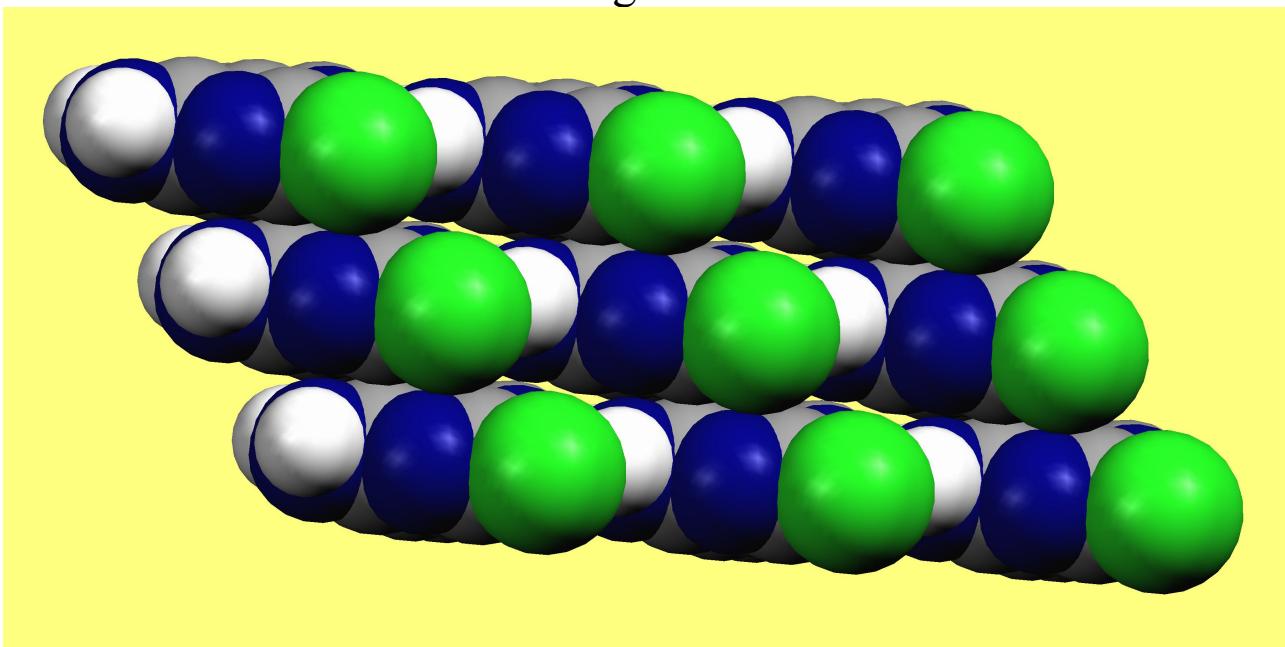


Figure S1

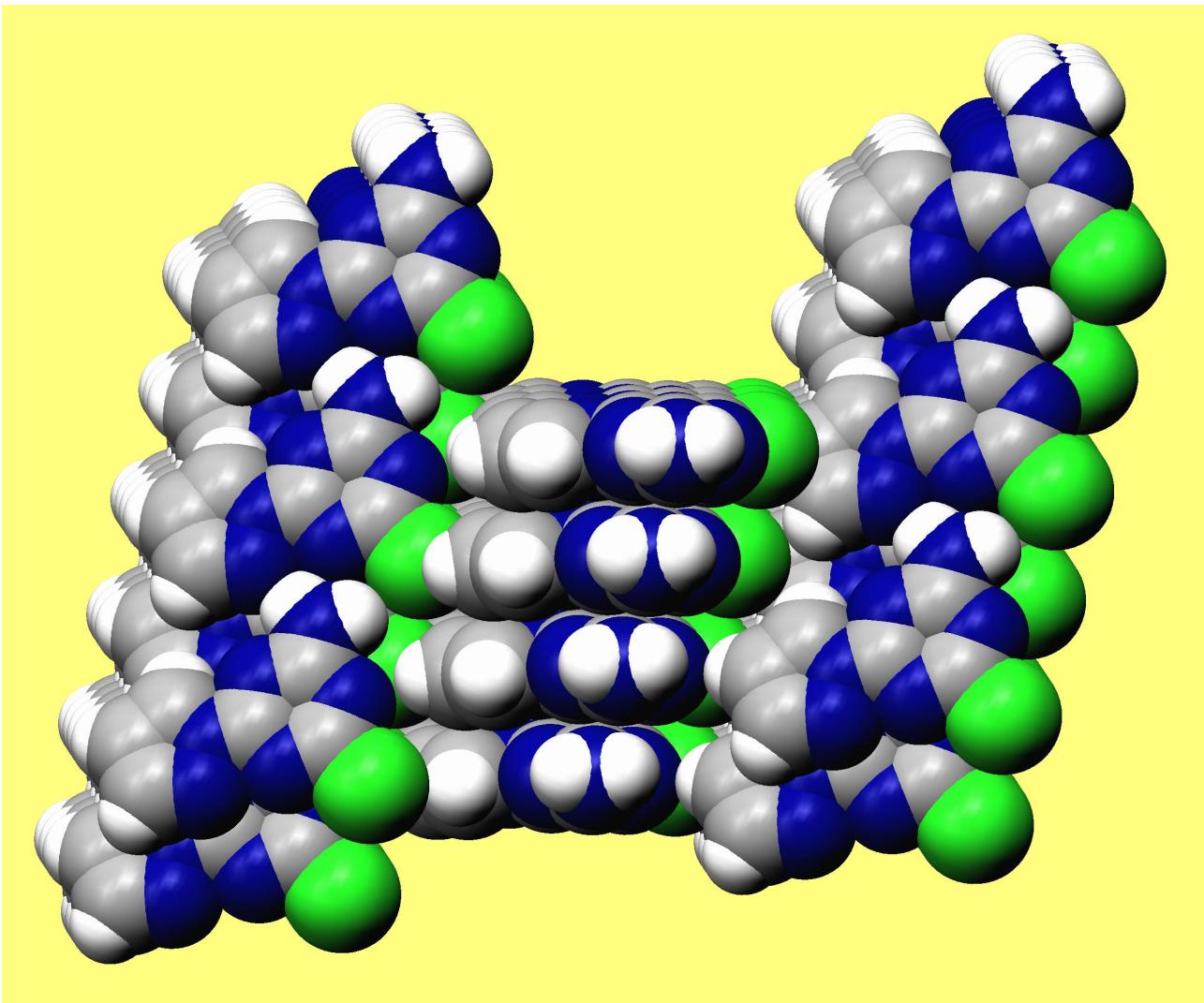


Figure S2

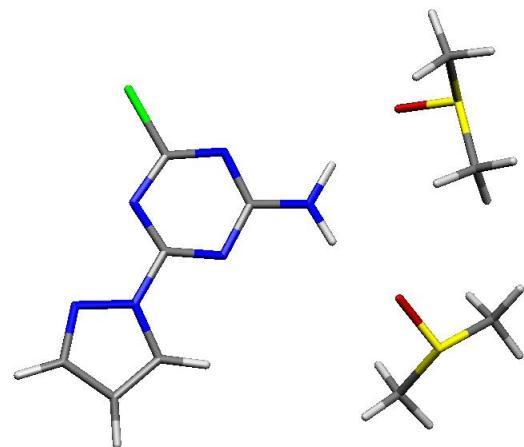


Figure S3. Calculated geometry of **1** + 2 molecules of DMSO

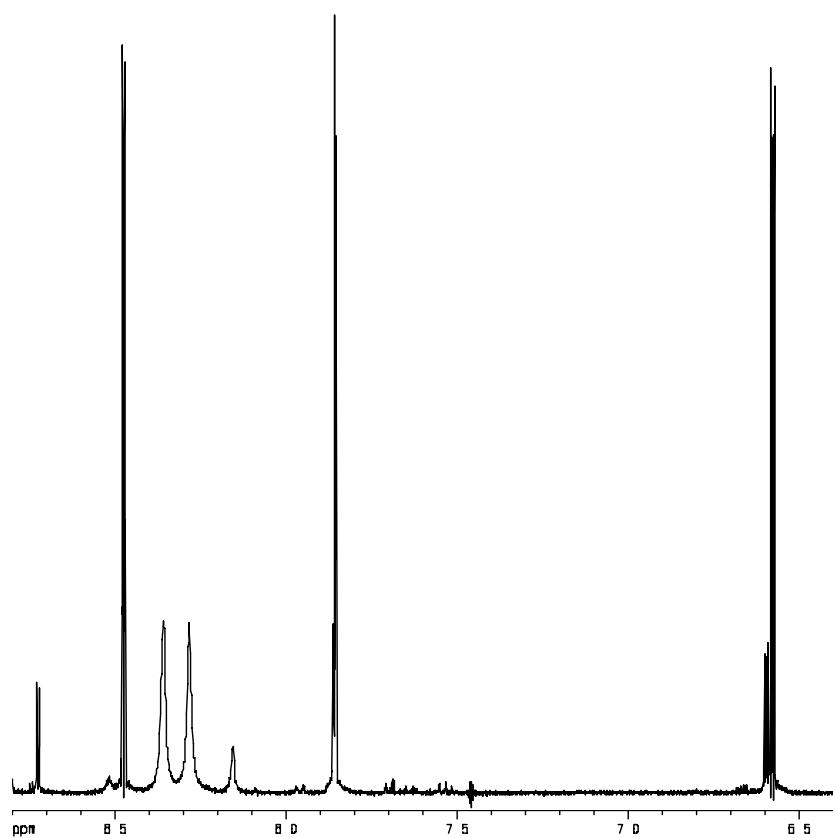


Figure S4. ^1H NMR spectrum of **1**.

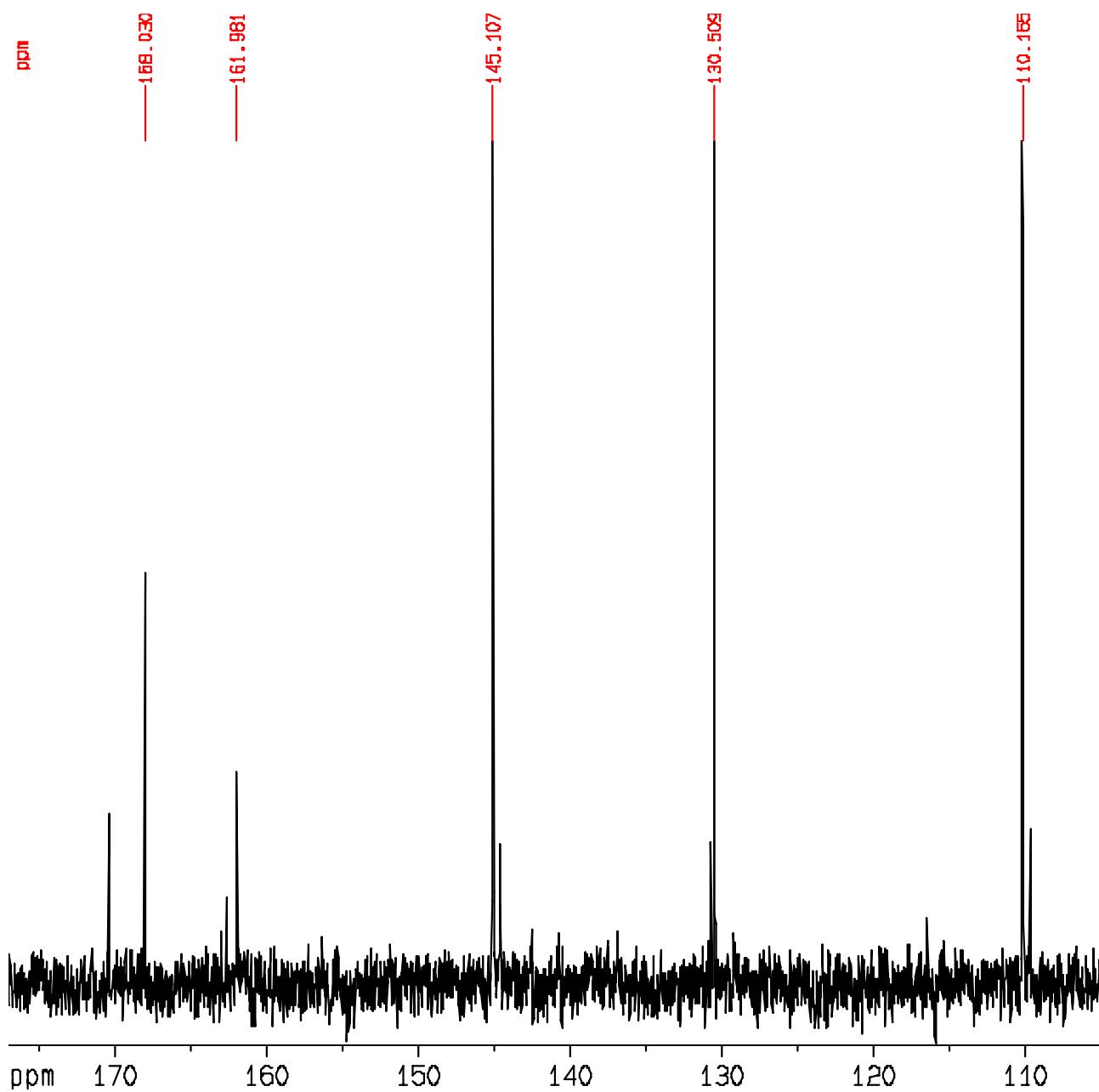


Figure S5. ^{13}C NMR spectrum of **1**.

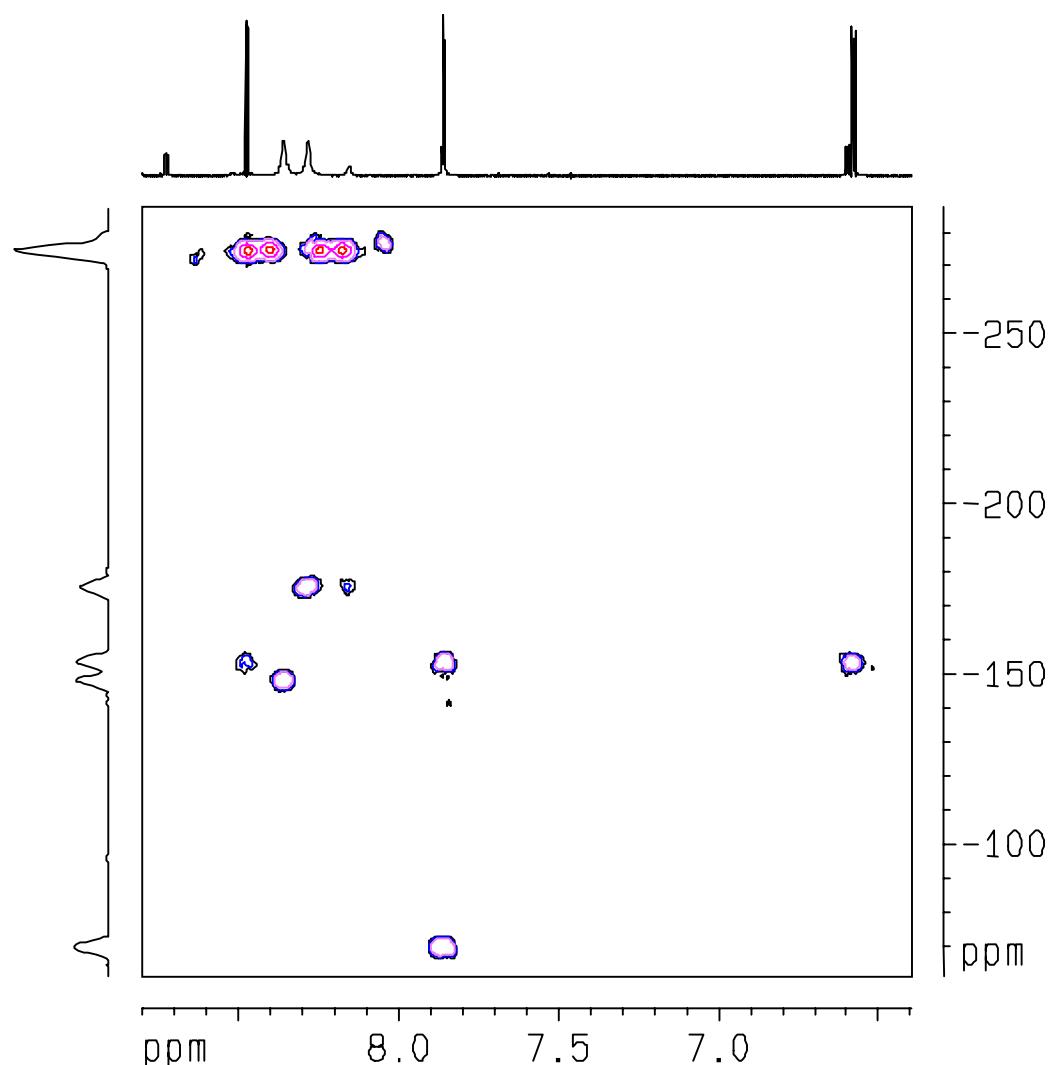


Figure S6. $^1\text{H}, ^{15}\text{N}$ HMBC NMR spectrum of **1**.

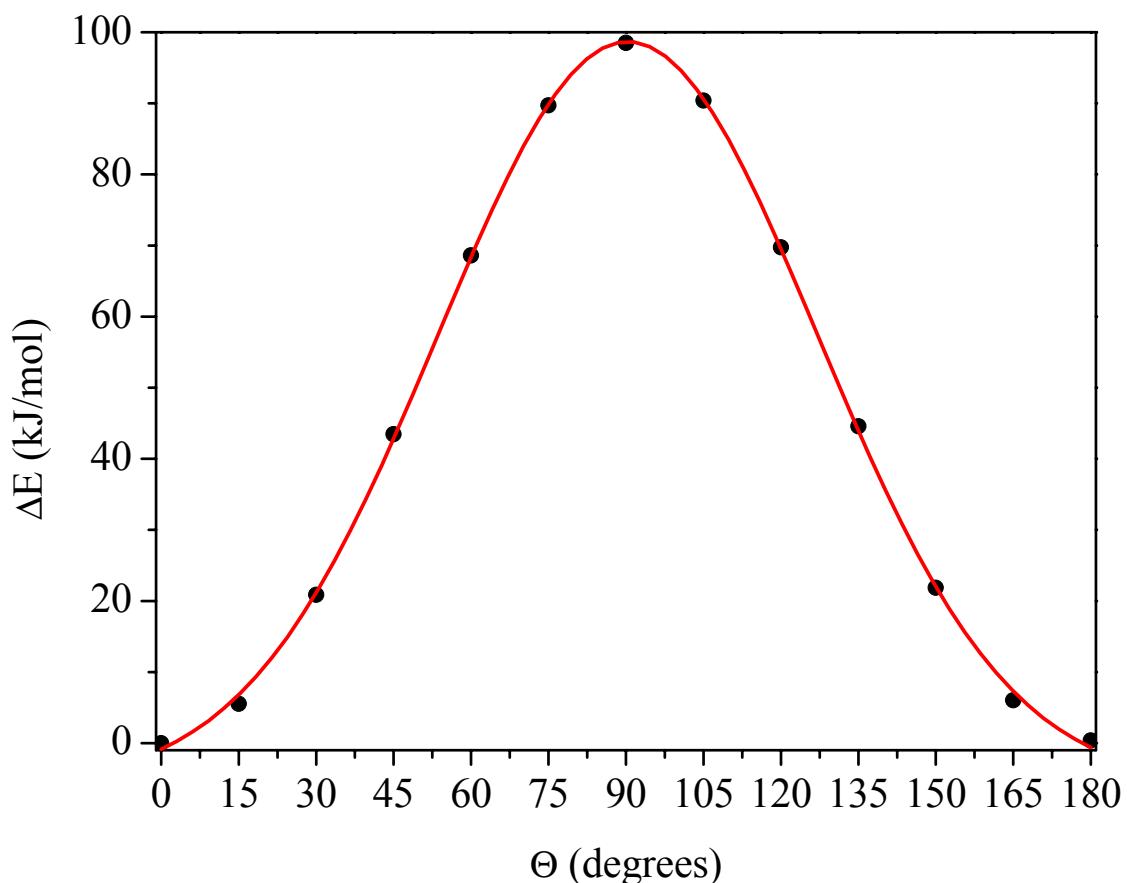


Figure S7

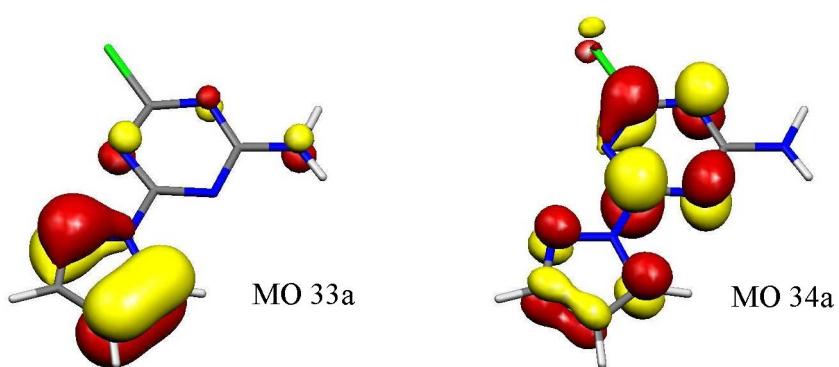


Figure S8. Contour plots of HOMO (33a) and LUMO (34a) of 1.