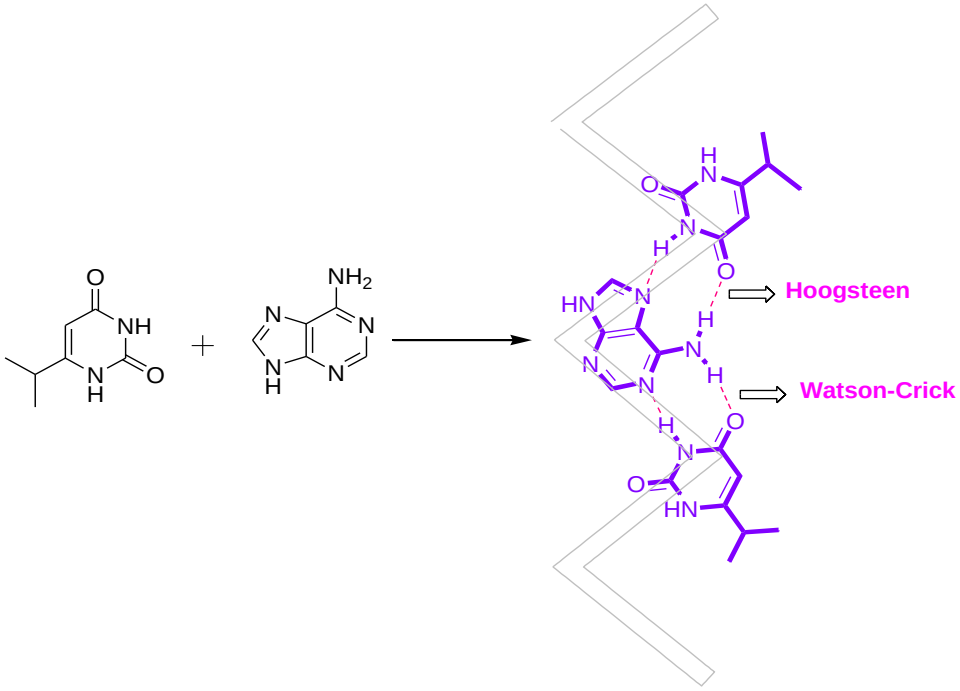
Electronic Supplementary Material (ESI) for RSC Advances

Supplementary Data

K. Radhakrishnan, Laxmi Narayana Burgula, Lal Mohan Kundu

Department of Chemistry, Indian Institute of Technology Guwahati, North Guwahati, Assam-781039, India

**Corresponding author Fax: + 91 361 2582349; Tel: +91 361 2582326; E-mail: lmkundu@iitg.ernet.in*



1. General Information.

2. Procedure for synthesis of 6-isopropyluracil

3. Characterization (^{1}H NMR and XRD data)

1. General Information: Chemicals were purchased from reputed pharmaceuticals and were used without any further purification. Microwave-directed synthesis were carried out in a *Anton Paar Synthos 3000* closed vessel microwave reactor at 600W at about 135°C for variable durations. ^{1}H-NMR (400 MHz) were recorded from a *DRX-400 Varian spectrometer* using DMSO-D_6 as solvent. X-Ray data was obtained from a *Bruker SMART APEX* equipped with a CCD area detector using Mo. The structure was solved by direct method using *SHELLX-97* (Göttingen, Germany).

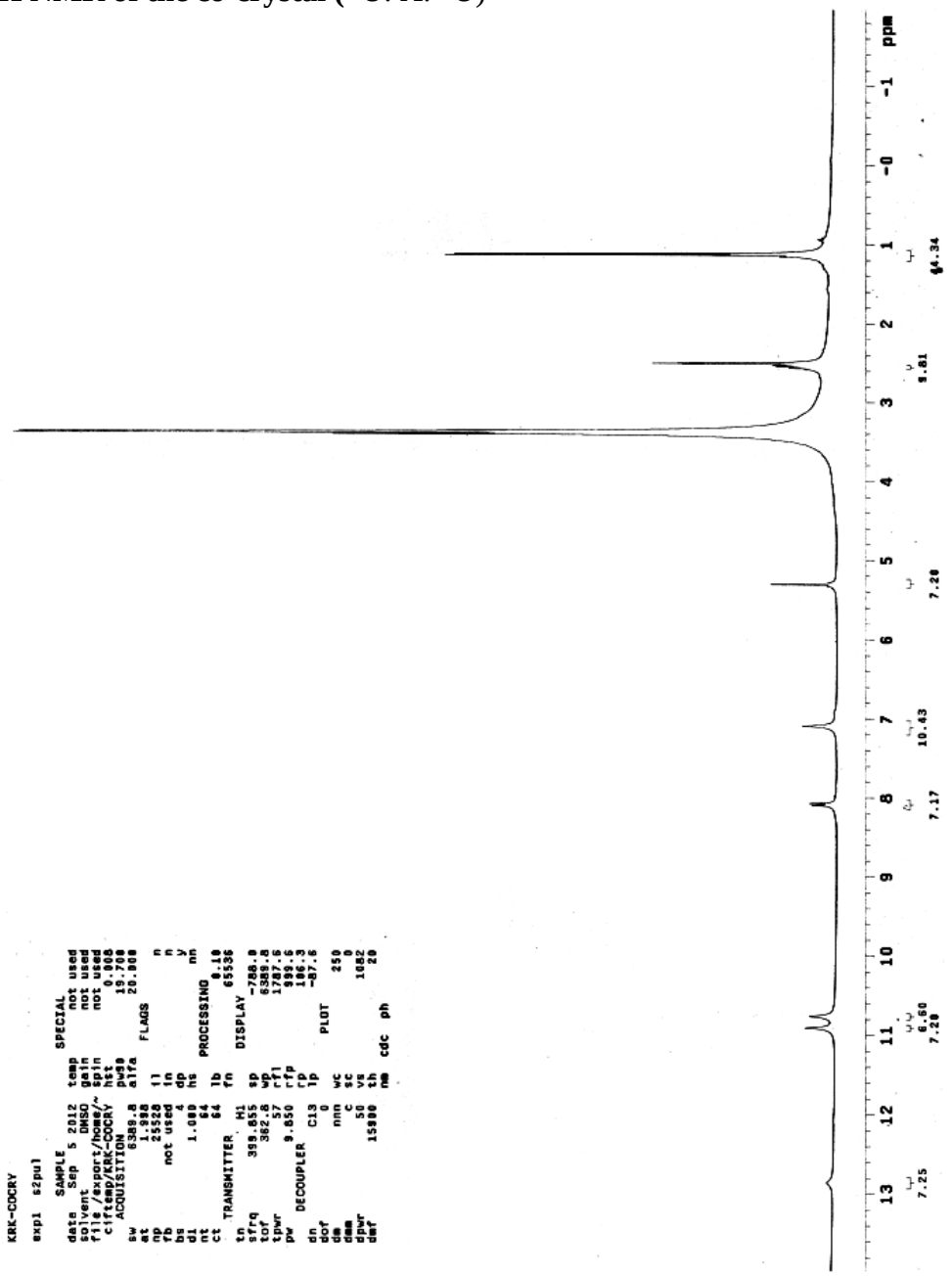
2. General Procedure: Methylisobutyryl acetate (144.1 mg, 1mmol) was taken in a reactor vessel and mixed thoroughly with urea (90.0 mg, 1.5mmol). The reaction vessel was closed immediately and irradiated with microwave radiation at 135°C for 7 minutes. The reaction mixture was cooled and the compound was purified by column chromatography. **Yield:** 79%.

Synthesis using $BF_3.Et_2O$ as Lewis acid: Methylisobutyryl acetate (144.1 mg, 1mmol) was taken in a reactor vessel with $BF_3.Et_2O$ (141.9 mg, 1mmol), and mixed thoroughly with urea (90.0 mg, 1.5mmol). The reaction vessel was closed immediately and irradiated with microwave radiation at 135°C for 3 minutes. The reaction mixture was cooled and the compound was further purified by column chromatography. **Yield:** 87**%**

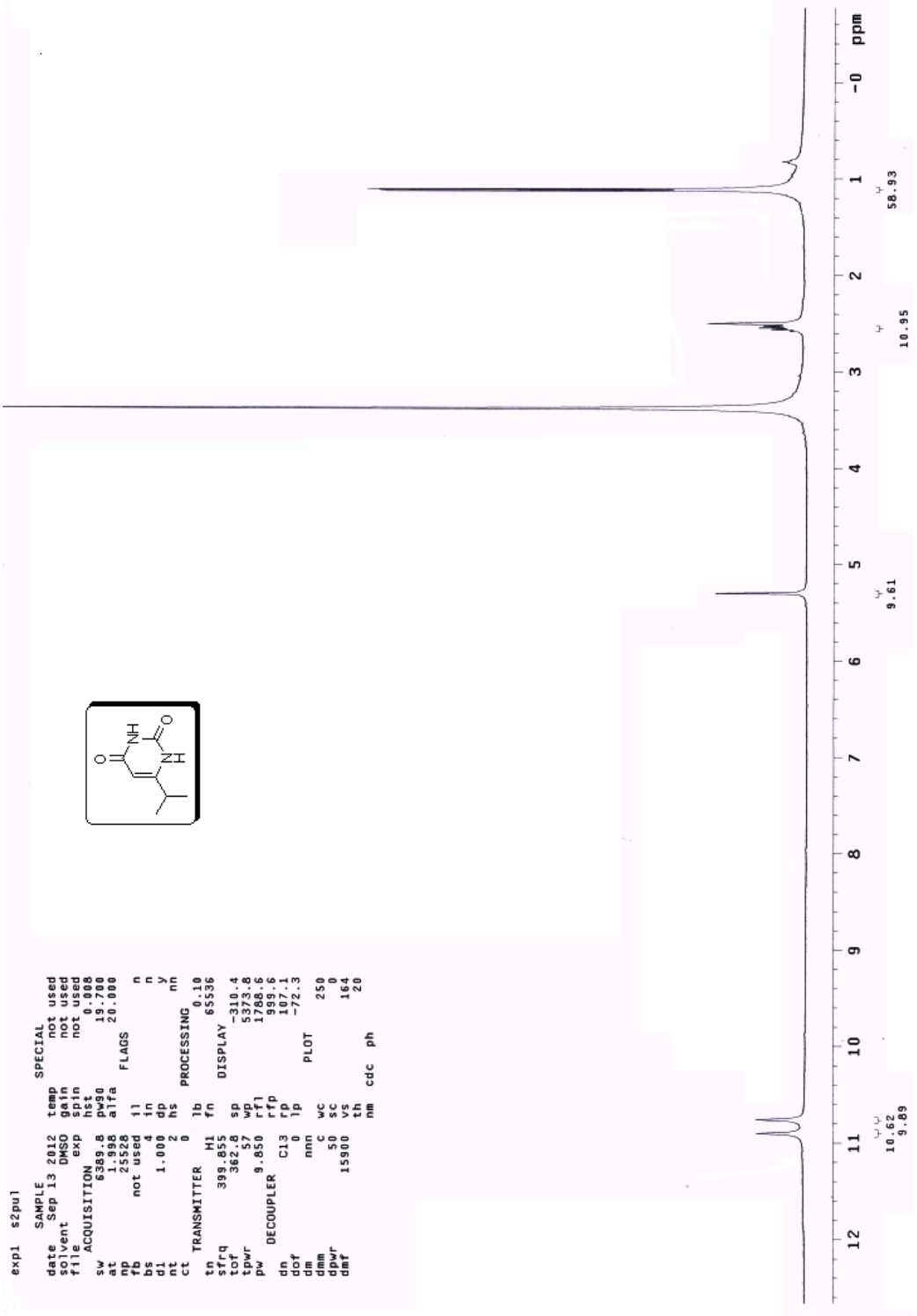
3. Characterization

^{1}H NMR and XRD data

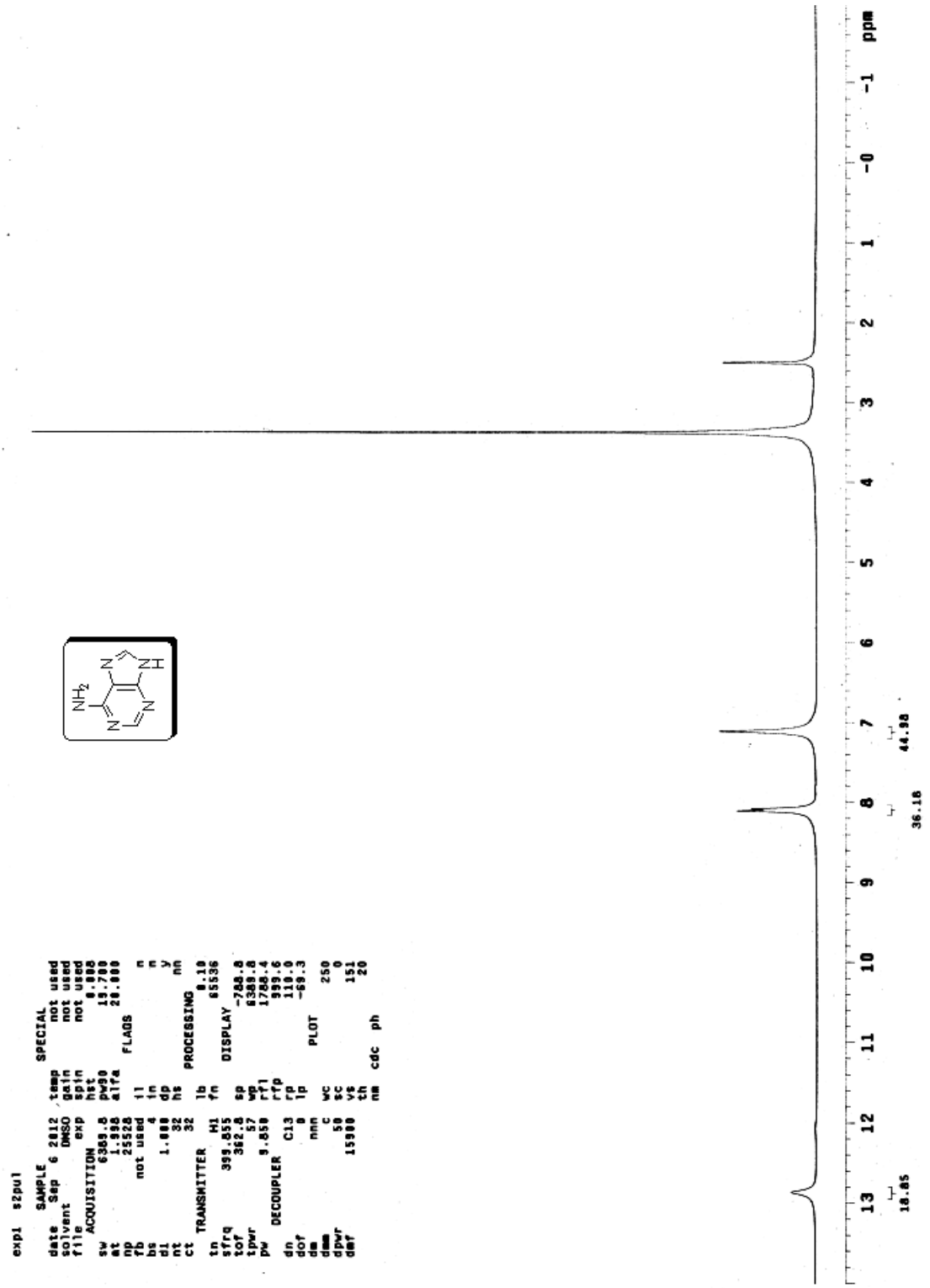
^{1}H NMR of the co-crystal (^{ip}U: A: ^{ip}U)



^{1}H NMR of isopropyl uracil:



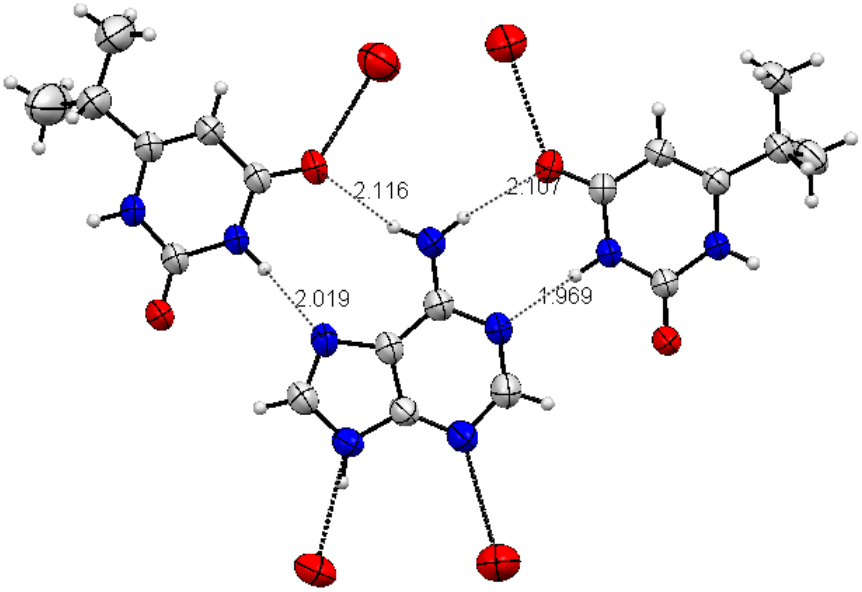
^{1}H NMR of adenine:



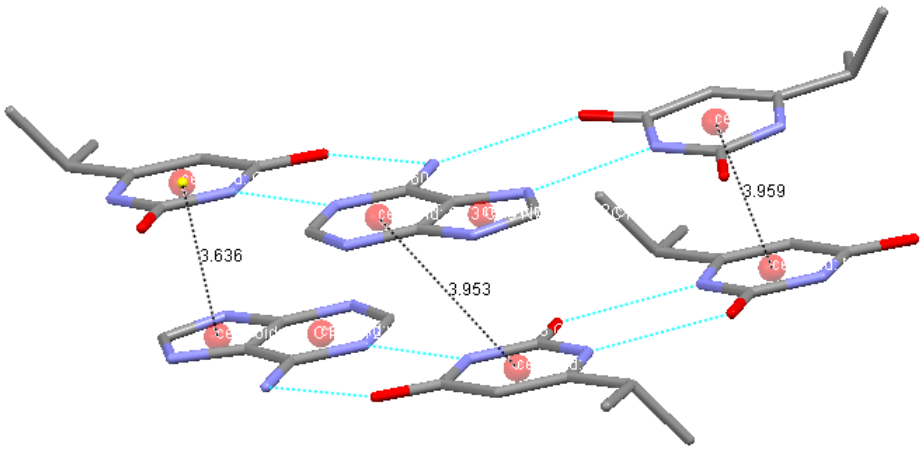
X-ray crystallographic data:

The crystal structure of the 2:1 complex obtained from 6-isopropyl (^{ip}U) uracil and adenine in methanol/water mixture (2:1):

Table 2: Crystallographic data of the ^{ip}U: A: ^{ip}U complex	
Chemical formula	2(C7 H10 N2 O2), C5 H5 N5, 4(O)
Formula Mass	507.48
Temperature/K	296(2)
Crystal system	'Triclinic'
Space group	'P-1 '
a/Å	10.8173(19)
b/Å	11.0856(19)
c/Å	13.235(2)
α/°	89.971(10)
β/°	69.525(10)
γ/°	63.586(11)
Unit cell volume/Å	1308.7(4)
Z	2
μ (mm-1)	0.102
ϱcalcd (g cm-3)	0.972
No. of reflections measured	4584
No. of independent reflections	2733
Final R1 values (I > 2σ(I))	0.0645
Final wR(F2) values (I > 2σ(I))	0.1749
Final R1 values (all data)	0.0890
Final wR(F2) values (all data)	0.1892
Goodness of fit (F^2)	0.892



ORTEP diagram of the ^{ip}U: A: ^{ip}U co-crystal showing the H-bond distances



Pi-pi interactions in the ^{ip}U: A: ^{ip}U co-crystal