Supplementary Material

Different Solvents Yield Different Crystal Forms Through Aromatic, Halogen Bonding and Hydrogen Bonding Competition

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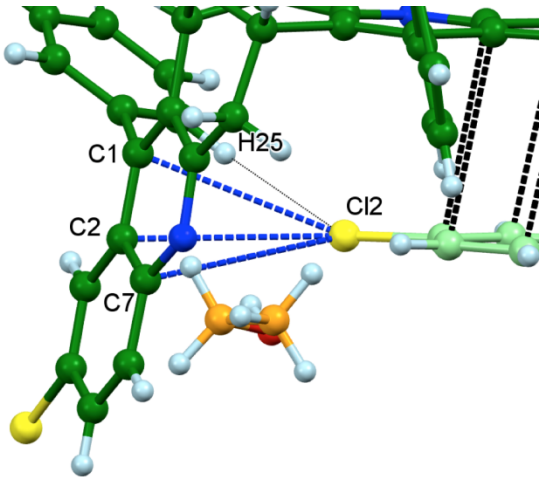
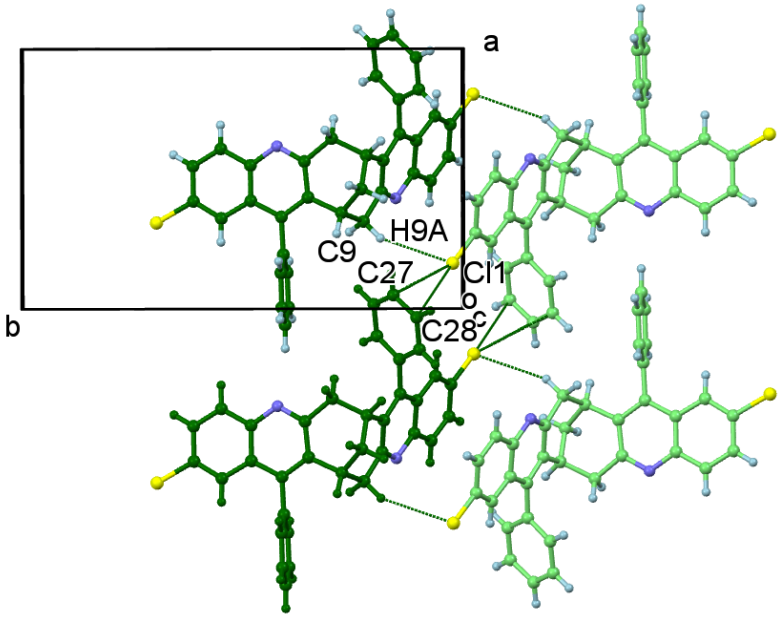




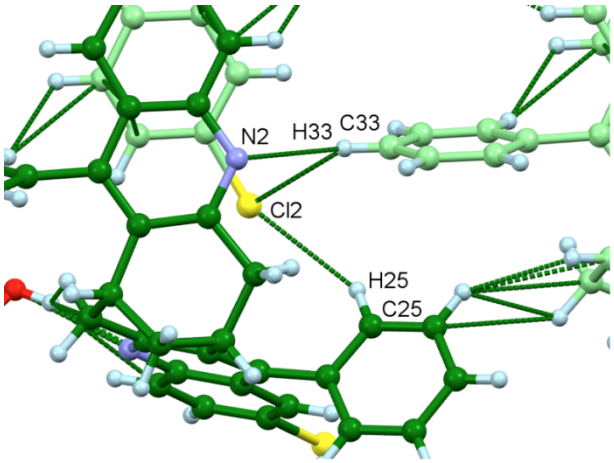


Fig. S1 The alternative, but equivalent, numbering used to designate molecular interactions in the crystal structure of the isostructural inclusion compound (**8**).(ethanol).

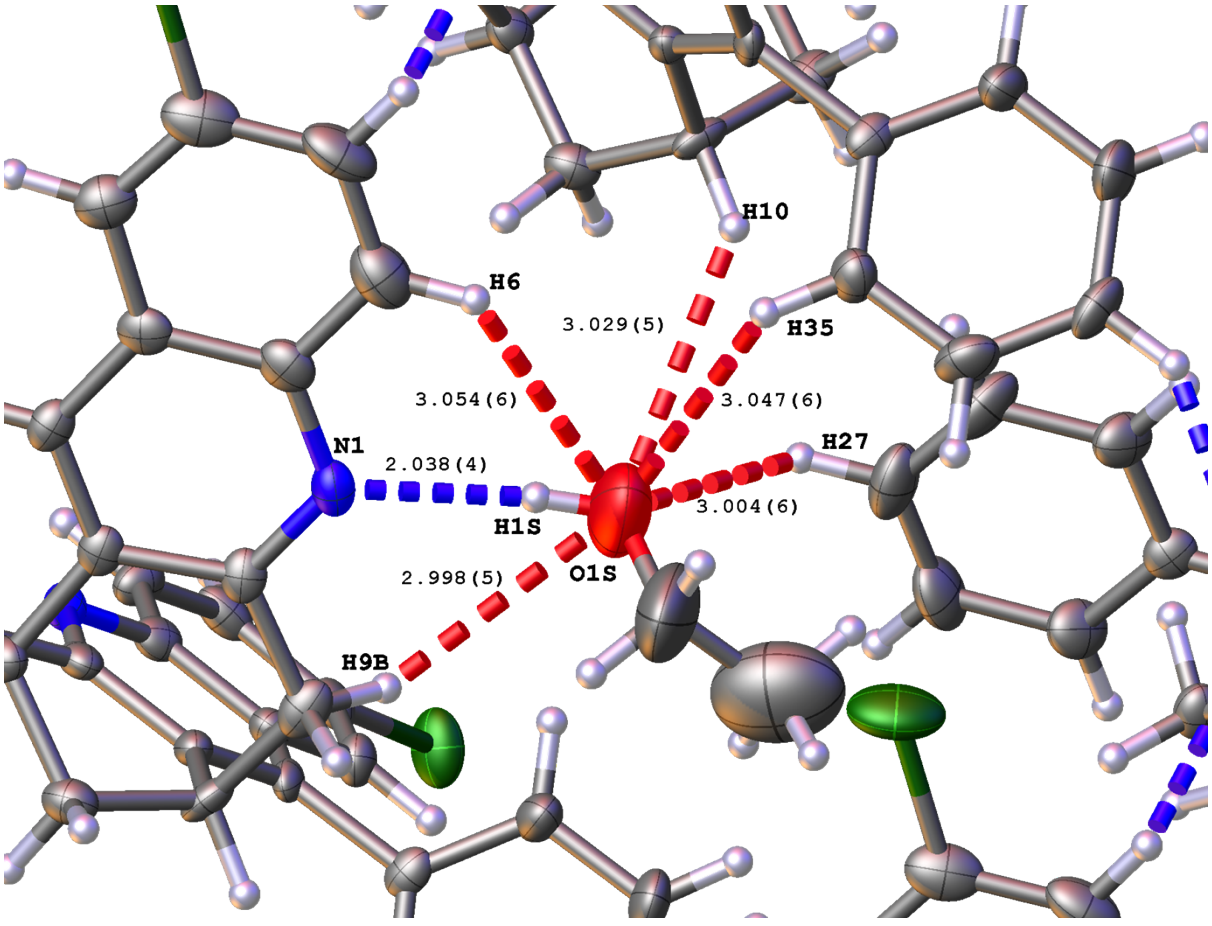


Fig. S2 The spectrum of host-guest hydrogen bonding interactions present in (**8**).(ethanol). This comprises the N···H-O strong hydrogen bond (blue) and five C-H···O weak hydrogen bonds (red).

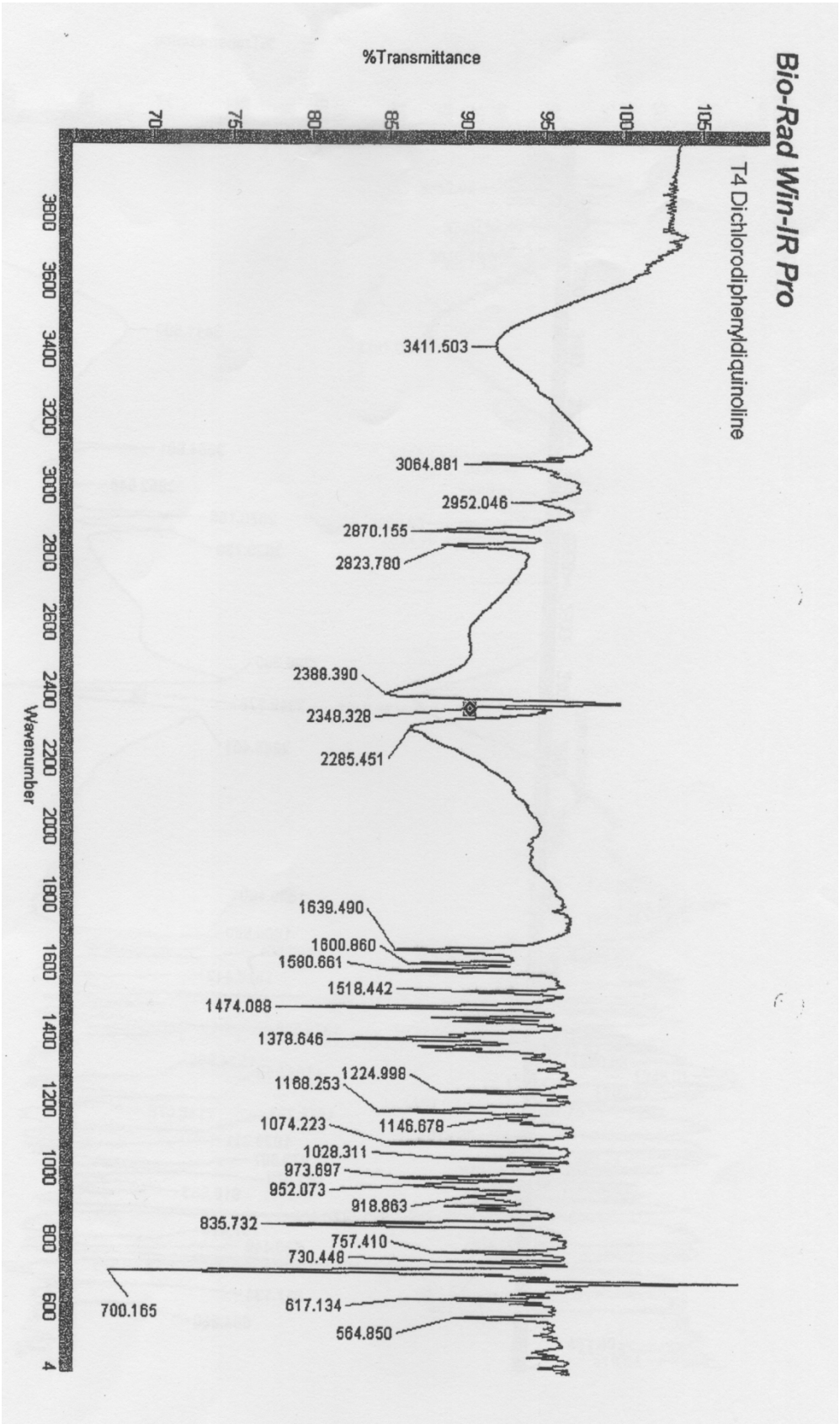
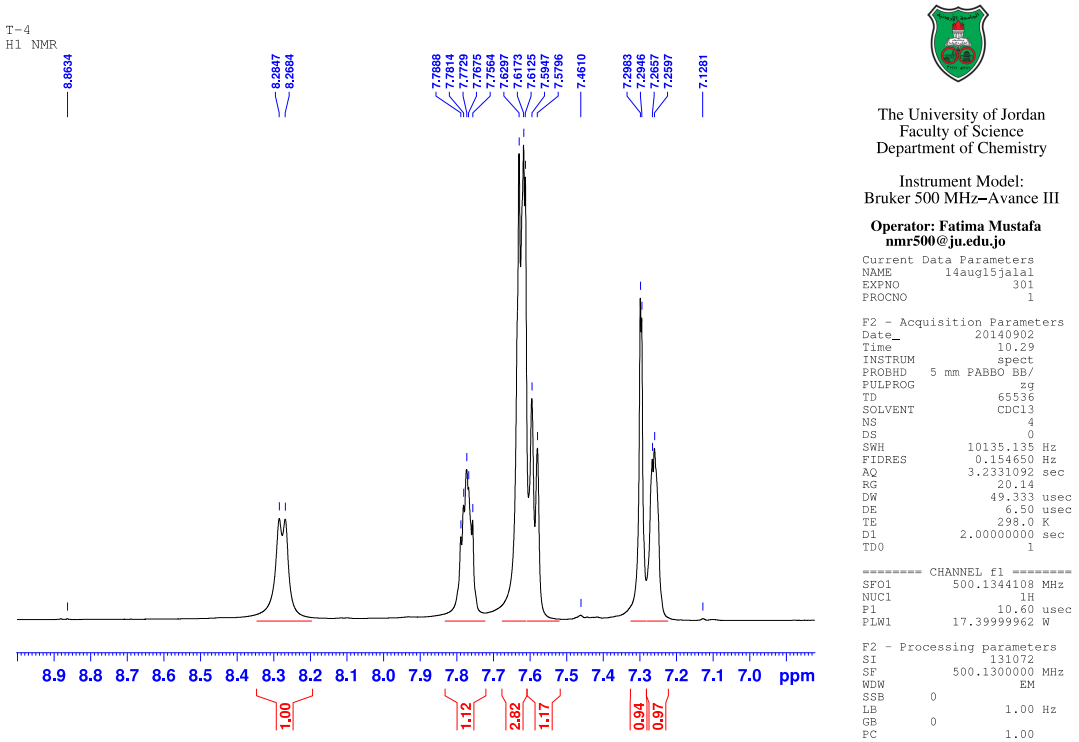


Fig. S3 The IR spectrum of the host molecule **8**.



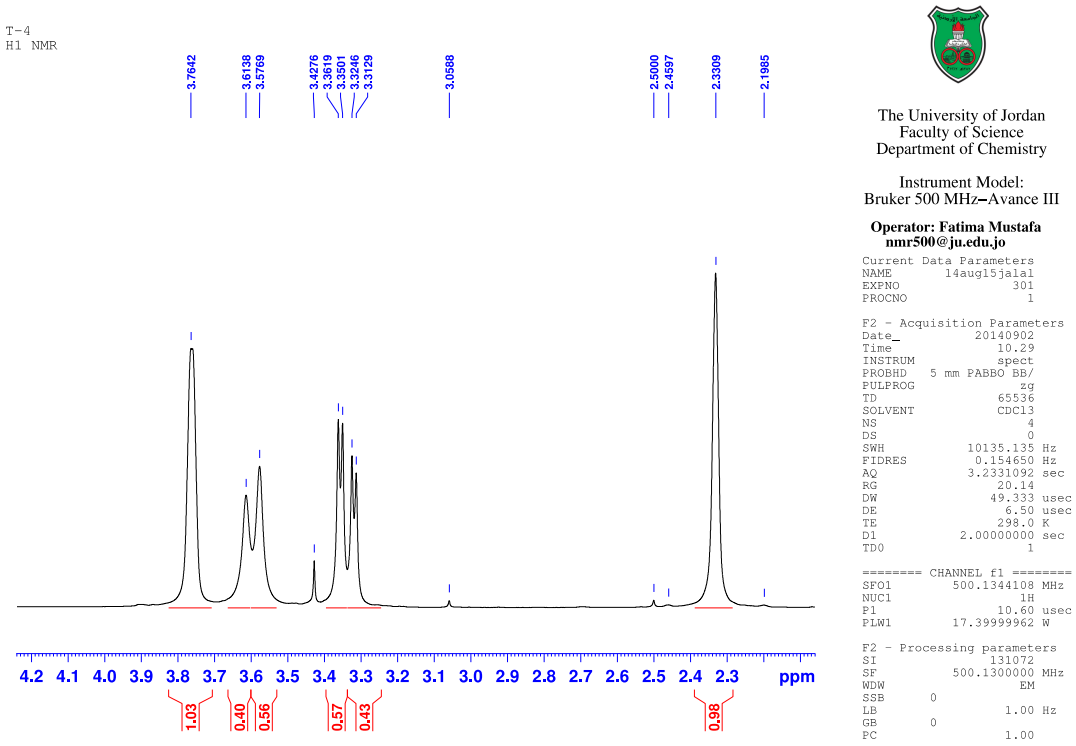
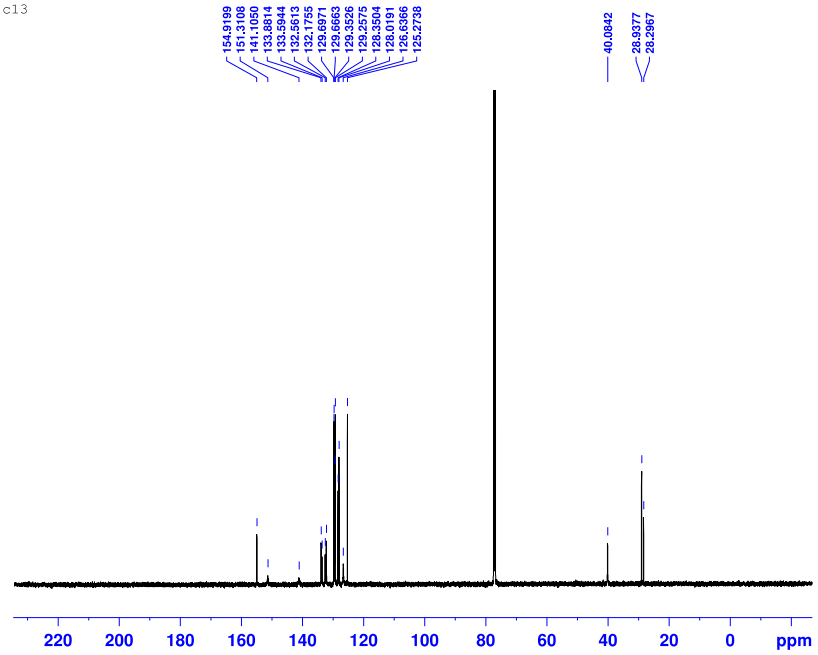


Fig. S4 The ^{1}H NMR spectrum of the host molecule **8**.

t4
c13



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Department of Chemistry

Instrument Model:
Bruker 500 MHz–Avance III

Operator: Fatima Mustafa
nmr500@ju.edu.jo


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Current Data Parameters
NAME         14aug15jalal
EXPNO                 302
PROCNO                  1

F2 - Acquisition Parameters
Date_            20140902
Time                10.41
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2048
DS                     4
SWH            32894.738 Hz
FIDRES             0.501934 Hz
AQ               0.9961472 sec
RG                  202.06
DW                 15.200 usec
DE                  6.50 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1           125.7708561 MHz
NUC1                   13C
P1                   10.60 usec
PLW1           17.39999962 W

======== CHANNEL f2 ========
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           17.37800026 W
PLW12           0.36307999 W
PLW13           0.22982000 W

F2 - Processing parameters
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WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
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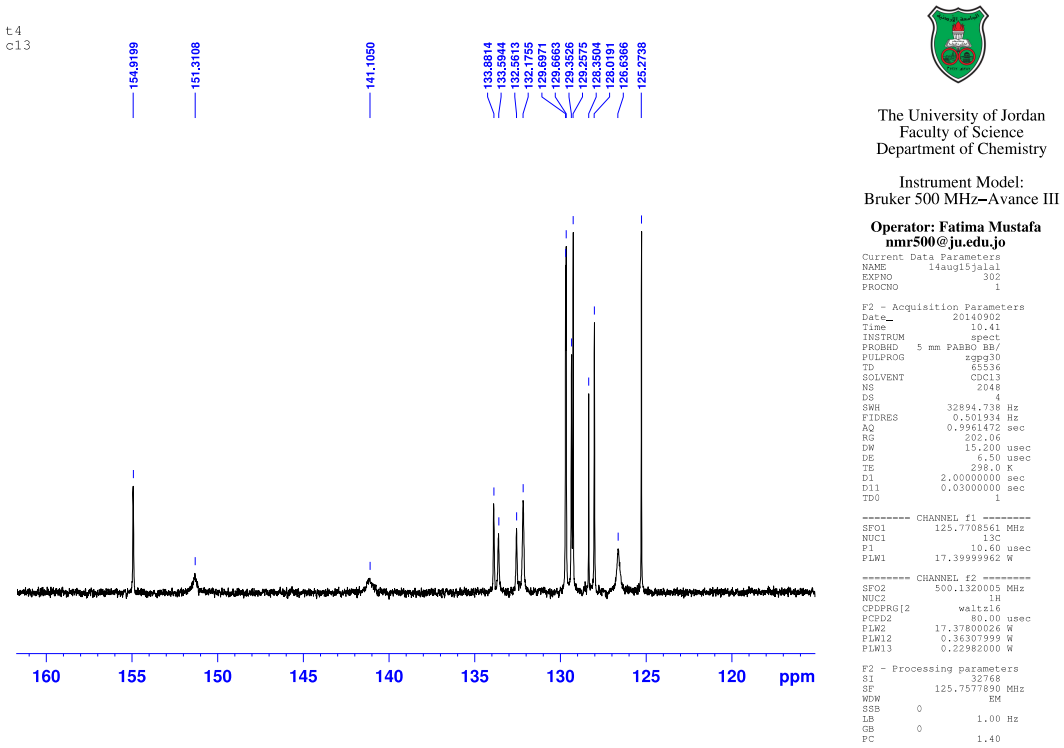

Fig. S5 ^{13}C NMR spectrum of **8**. The three broad signals at 151.31, 141.11 and 126.64 δ indicate a slow conformational equilibrium occurring on the NMR timescale. This phenomenon is relatively common for bridged molecules of limited flexibility at laboratory temperature.