Electronic Supplementary Material (ESI) for CrystEngComm.

Conformational variation of ligand in mercury halide complexes; high and low Z' structures

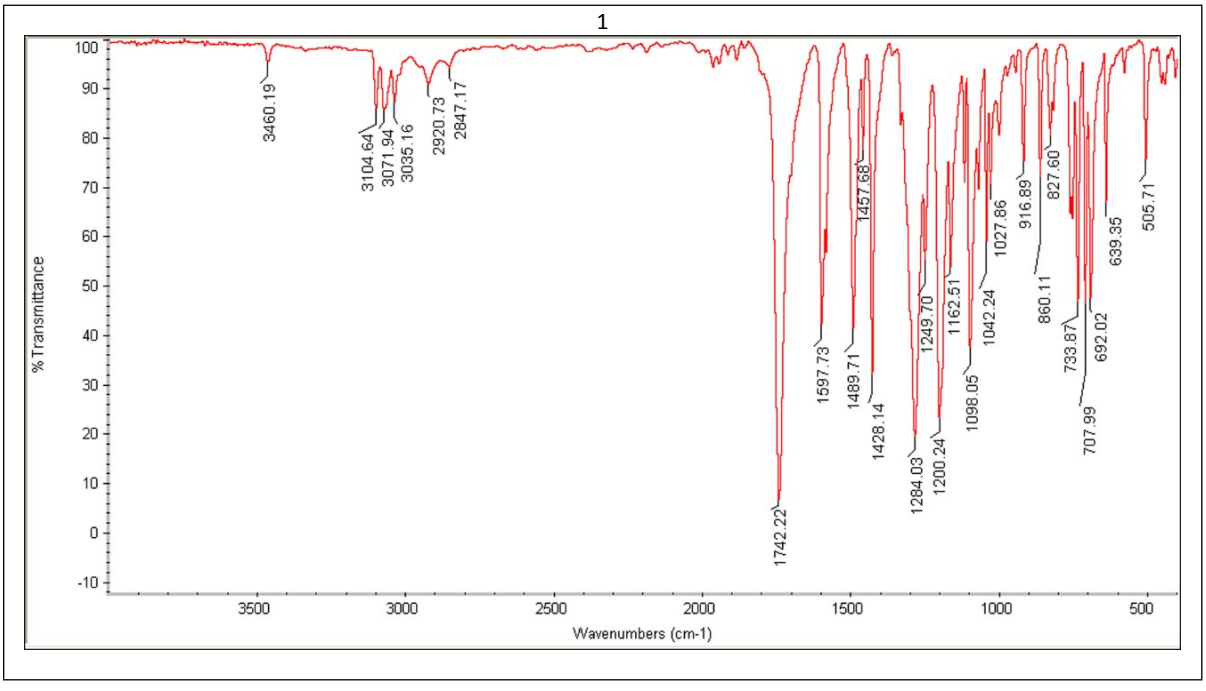
Ali Samie, Alireza Salimi*

Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran

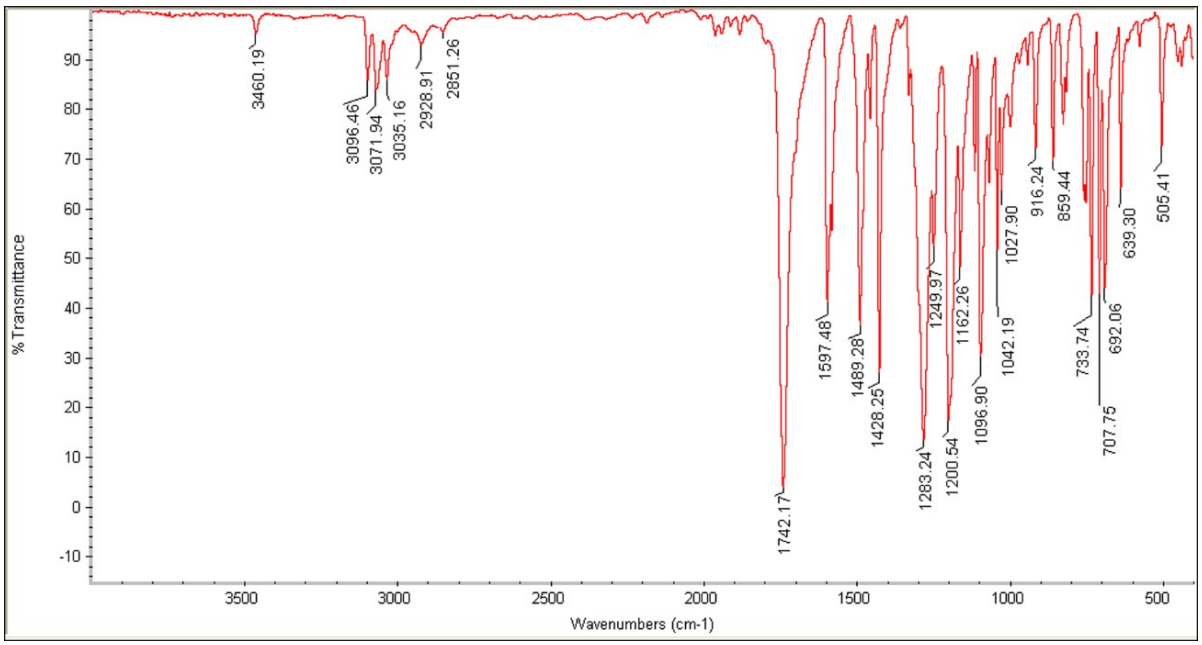
Supporting Information

Contents

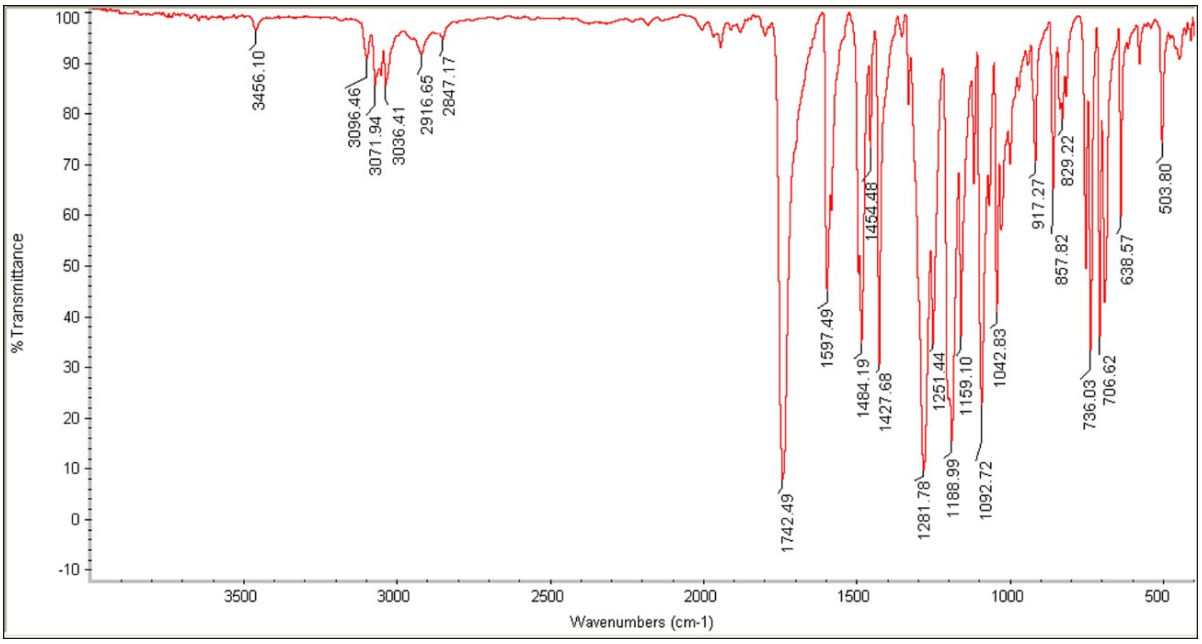
Figure S1. FT-IR transmittance plots for complexes 1-5.



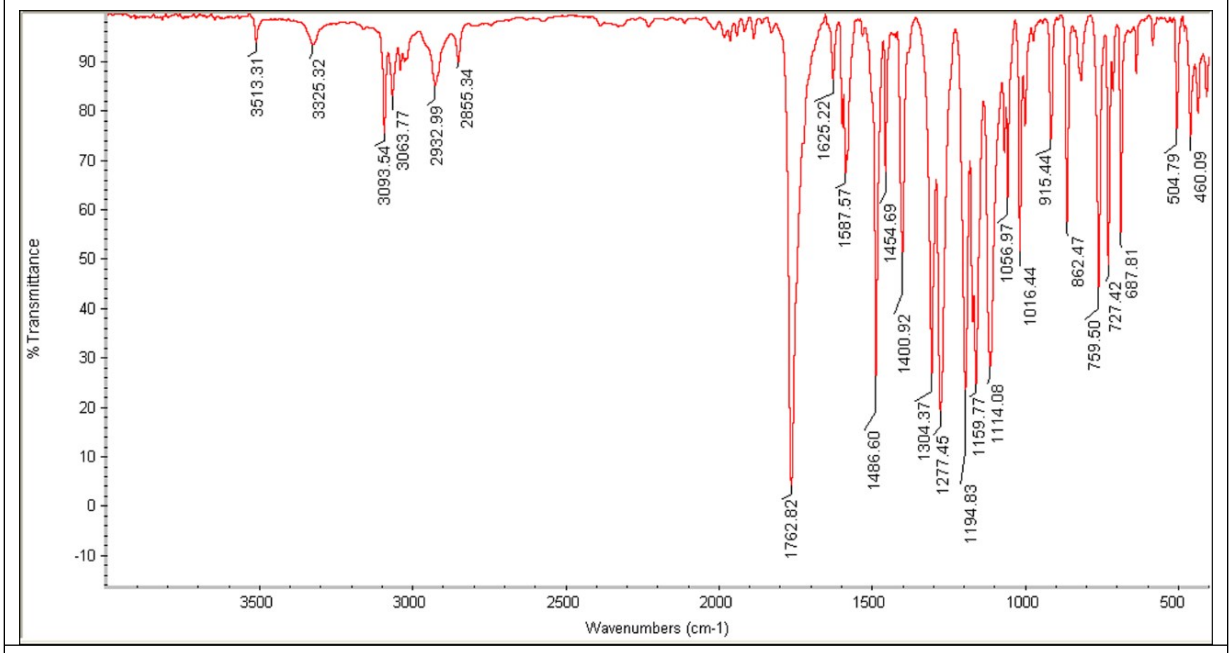
2


3460.19
3096.46
3071.94
3035.16
2928.91
2851.26
1742.17
1597.48
1489.28
1428.25
1283.24
1249.97
1200.54
1162.26
1096.90
1042.19
1027.90
916.24
859.44
733.74
707.75
692.06
639.30
505.41
% Transmittance
Wavenumbers (cm-1)

3


3456.10
3096.46
3071.94
3036.41
2916.65
2847.17
1742.49
1597.49
1484.19
1454.48
1427.68
1281.78
1251.44
1188.99
1159.10
1092.72
1042.83
917.27
857.82
829.22
736.03
706.62
638.57
503.80
% Transmittance
Wavenumbers (cm-1)

4


% Transmittance
Wavenumbers (cm-1)
3513.31
3325.32
3093.54
3063.77
2932.99
2855.34
1762.82
1625.22
1587.57
1486.60
1454.69
1400.92
1304.37
1277.45
1194.83
1159.77
1114.08
1056.97
1016.44
915.44
862.47
759.50
727.42
687.81
504.79
460.09

5

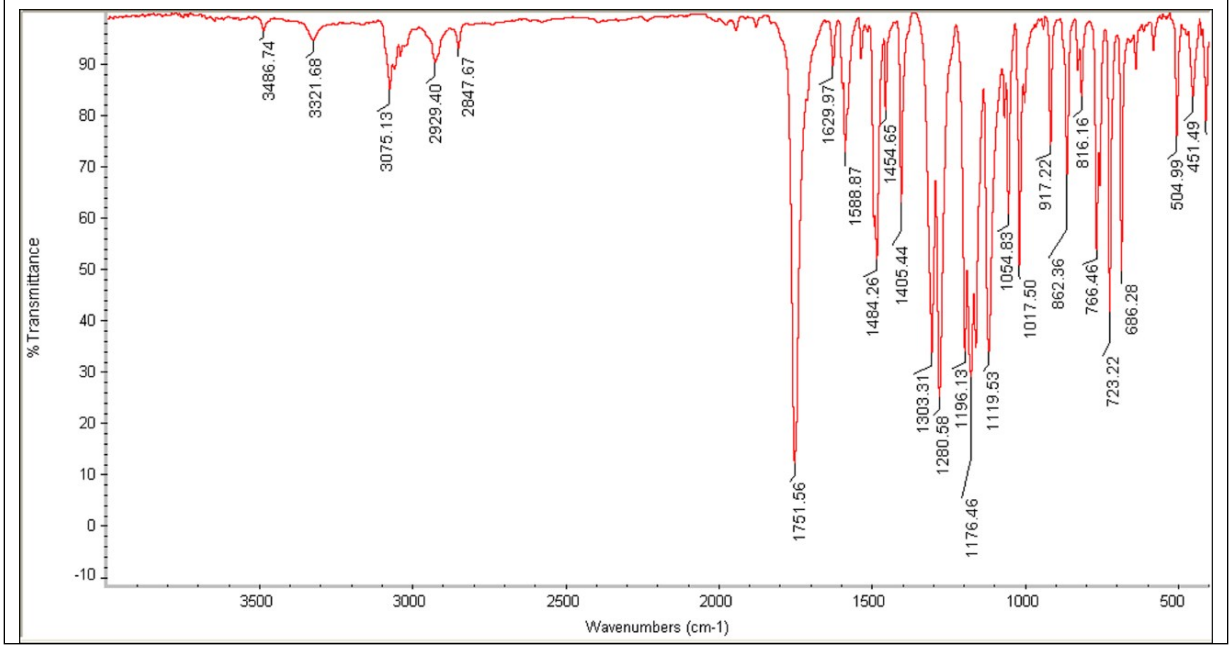

% Transmittance
Wavenumbers (cm-1)
3486.74
3321.68
3075.13
2929.40
2847.67
1751.56
1629.97
1588.87
1484.26
1454.65
1405.44
1303.31
1280.58
1196.13
1176.46
1119.53
1054.83
1017.50
917.22
862.36
816.16
766.46
723.22
686.28
504.99
451.49

Figure S2. CHN-elemental analysis for complexes 1-5.

1

Eager 300 Summarize Results

Date : 30/04/2018 at 11:29:31
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-43		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
43	1	AS23	UNK	0.981	6.25	---	

Component name	Element %
Nitrogen%	8.035504341
Carbon%	39.94174576
Hydrogen%	2.606018066
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	8.035504341
Carbon%	39.94174576
Hydrogen%	2.606018066
Sulphur%	0

2

Eager 300 Summarize Results

Date : 30/04/2018 at 11:29:46
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-44		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
44	1	AS27	UNK	0.966	6.25	---	

Component name	Element %
Nitrogen%	3.529394865
Carbon%	38.47299194
Hydrogen%	2.486160994
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	3.529394865
Carbon%	38.47299194
Hydrogen%	2.486160994
Sulphur%	0

3

Eager 300 Summarize Results

Date : 30/04/2018 at 11:30:13
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-46		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
46	1	AS28	UNK	1.03	6.25	---	

Component name	Element %
Nitrogen%	2.993385315
Carbon%	33.39466476
Hydrogen%	2.096810102
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	2.993385315
Carbon%	33.39466476
Hydrogen%	2.096810102
Sulphur%	0

4

Eager 300 Summarize Results

Date : 30/04/2018 at 11:29:31
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-43		

#	Group	Sample Name	Type	Weig.	Pro.F	---	---
43	1	AS23	UNK	0.981	6.25	---	

Component name	Element %
Nitrogen%	8.035504341
Carbon%	39.94174576
Hydrogen%	2.606018066
Sulphur%	0

1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	8.035504341
Carbon%	39.94174576
Hydrogen%	2.606018066
Sulphur%	0

5

Eager 300 Summarize Results

Date : 30/04/2018 at 11:29:56
Method Name : NCHS
Method Filename : Copy of Copy of N C H S-bkp .mth

Filename	AS Method	Vial
Sami-45		

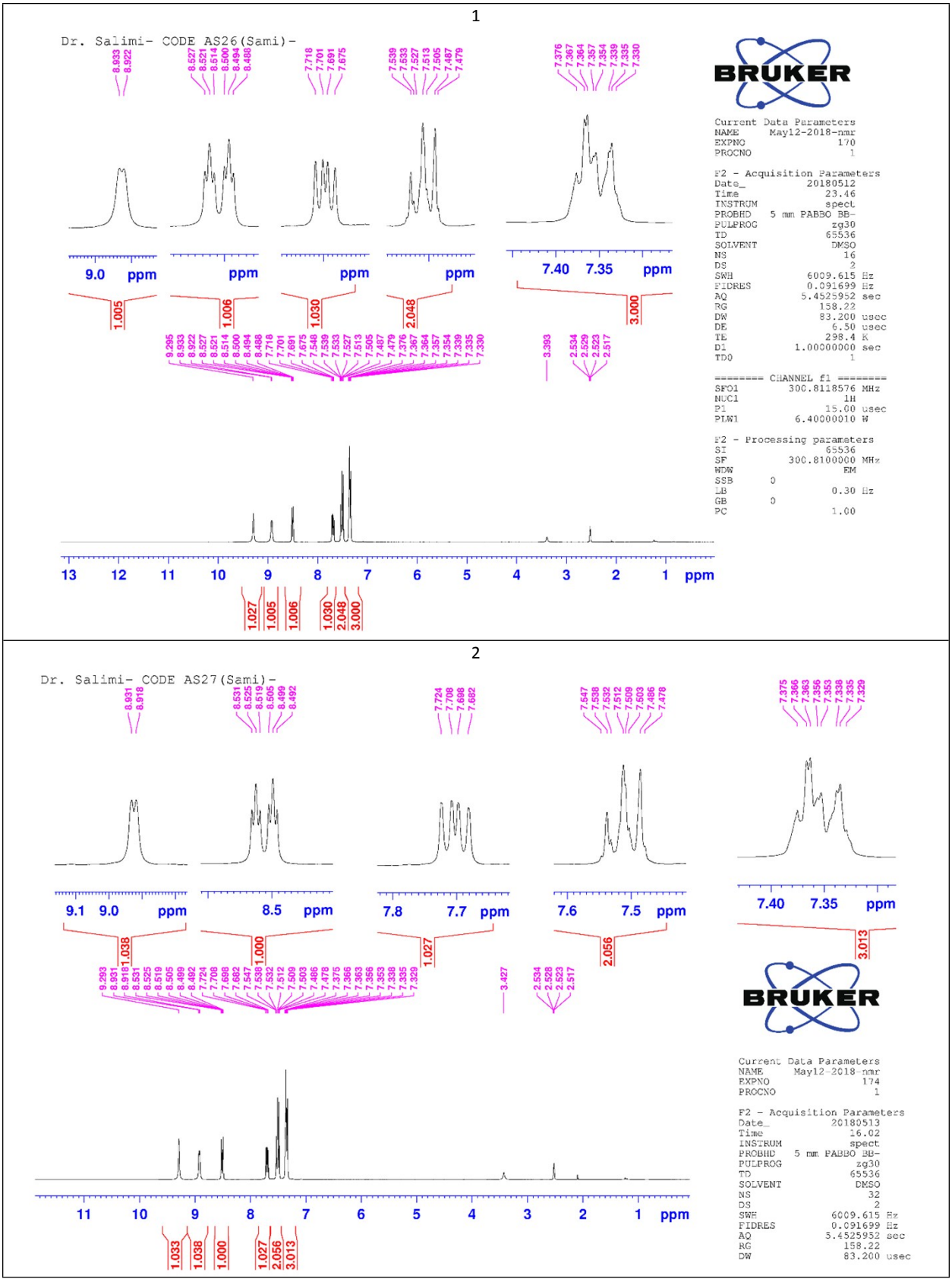
#	Group	Sample Name	Type	Weig.	Pro.F	---	---
45	1	AS24	UNK	0.97	6.25	---	

Component name	Element %
Nitrogen%	7.022572517
Carbon%	35.21708679
Hydrogen%	2.230710745
Sulphur%	0

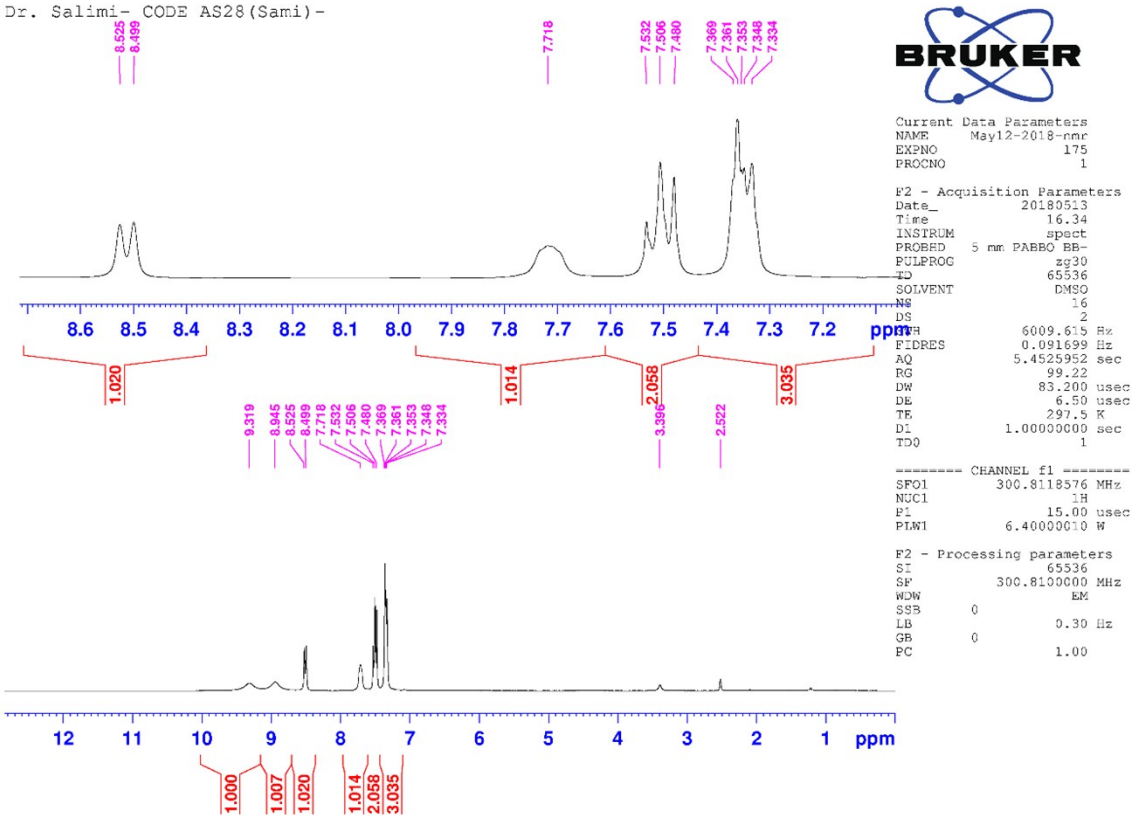
1 Sample(s) in Group No : 1

Component Name	Average
Nitrogen%	7.022572517
Carbon%	35.21708679
Hydrogen%	2.230710745
Sulphur%	0

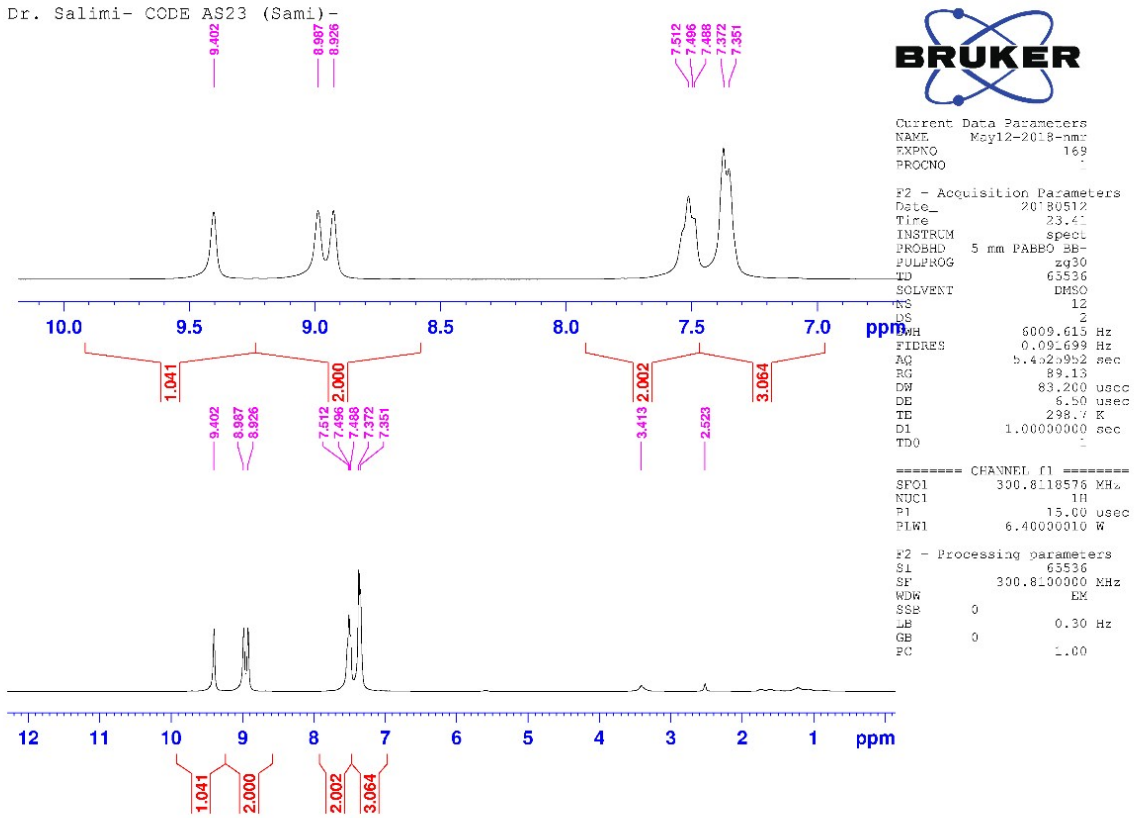
Figure S3. ^{1}H-NMR spectrums for complexes 1-5.



3


Dr. Salimi- CODE AS28(Sami)-
8.525
8.499
7.718
7.532
7.506
7.480
7.369
7.361
7.353
7.348
7.334
BRUKER
Current Data Parameters
NAME May12-2018-nmr
EXPNO 175
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180513
Time 16.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4525952 sec
RG 99.22
DW 83.200 usec
DE 6.50 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.8118576 MHz
NUC1 1H
P1 15.00 usec
PLW1 6.40000010 W
F2 - Processing parameters
SI 65536
SF 300.8100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 ppm
1.020
1.014
2.058
3.035
9.319
8.945
8.525
8.499
7.718
7.532
7.506
7.480
7.369
7.361
7.353
7.348
7.334
3.398
2.522
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.007
1.020
1.014
2.058
3.035

4


Dr. Salimi- CODE AS23 (Sami)-
9.402
8.987
8.926
7.512
7.496
7.488
7.372
7.351
BRUKER
Current Data Parameters
NAME May12-2018-nmr
EXPNO 169
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180512
Time 23.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 12
DS 2
SWH 6009.615 Hz
FIDRES 0.091699 Hz
AQ 5.4529952 sec
RG 89.13
DW 83.200 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 300.8118576 MHz
NUC1 1H
P1 15.00 usec
PLW1 6.40000010 W
F2 - Processing parameters
SI 65536
SF 300.8100000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 ppm
1.041
2.000
2.002
3.064
9.402
8.987
8.926
7.512
7.496
7.488
7.372
7.351
3.413
2.523
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.041
2.000
2.002
3.064

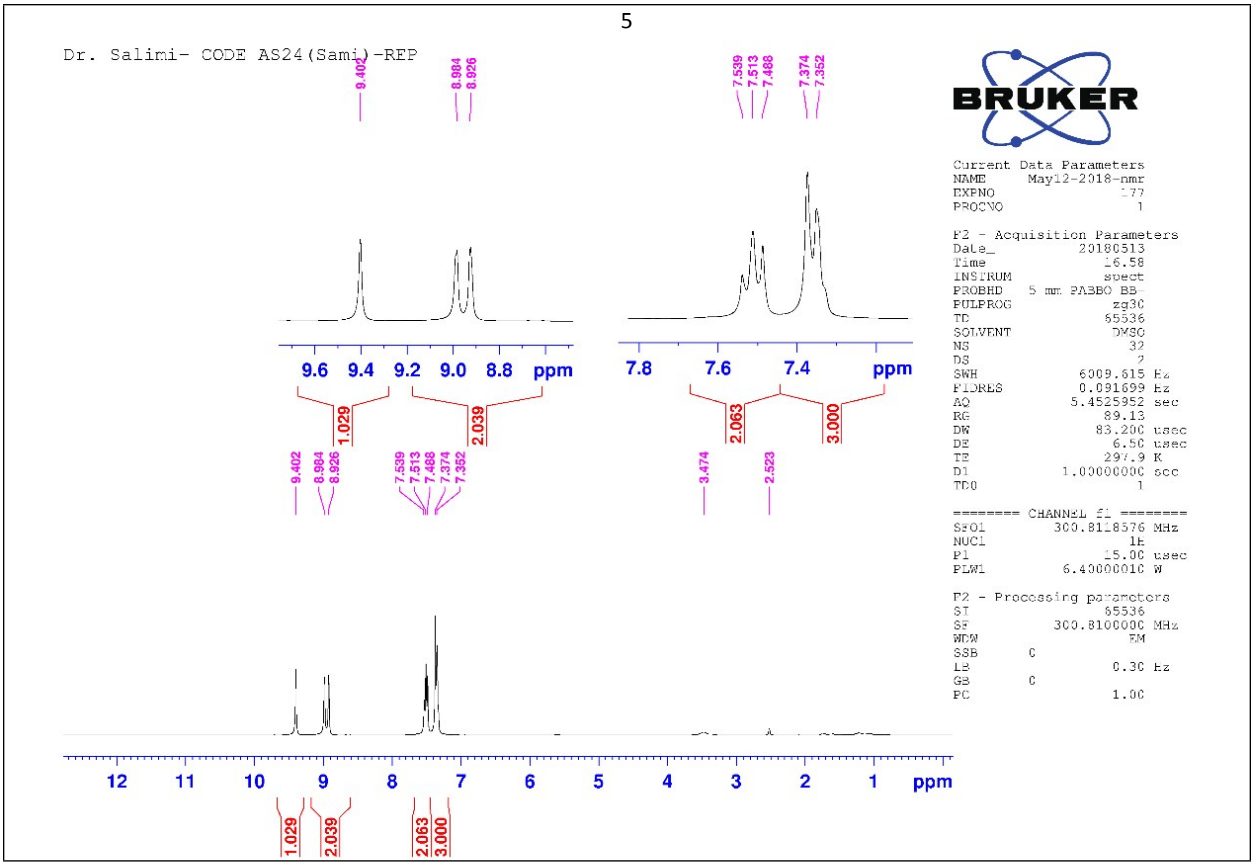
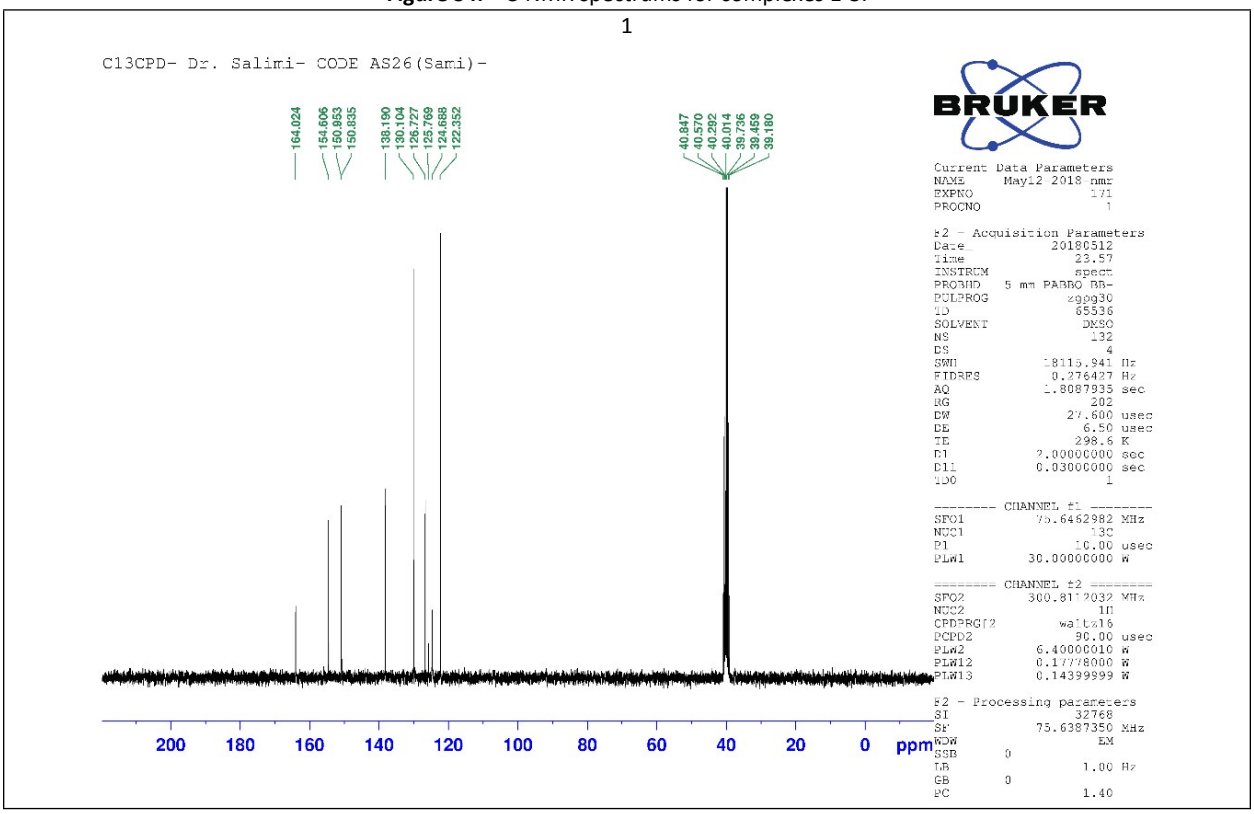
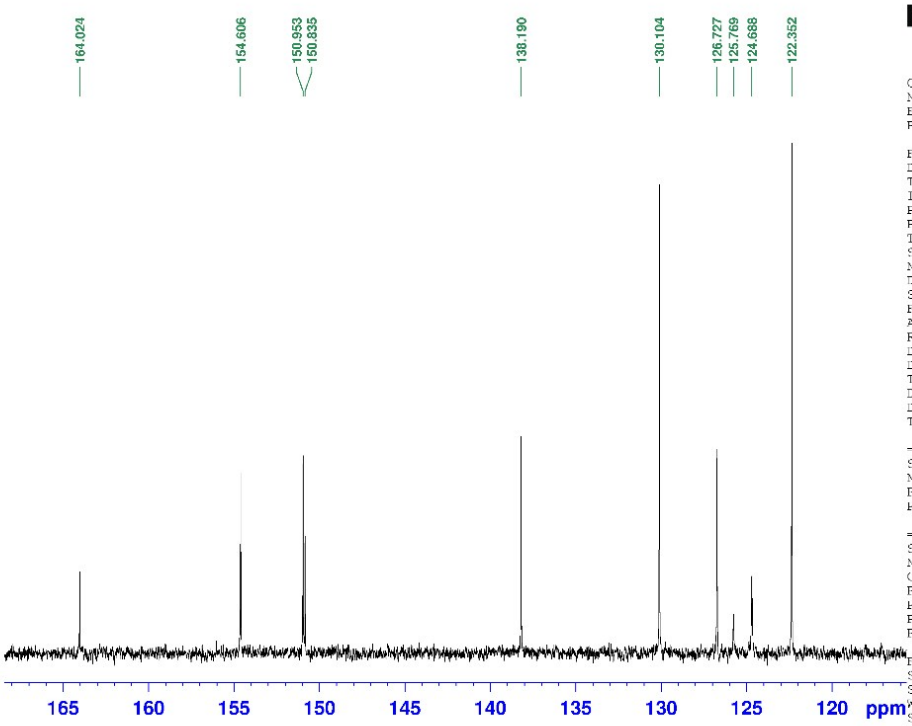


Figure S4. ^{13}C-NMR spectrums for complexes 1-5.



1 expand

C13CPD- Dr. Salimi- CODE AS26(Sami)-

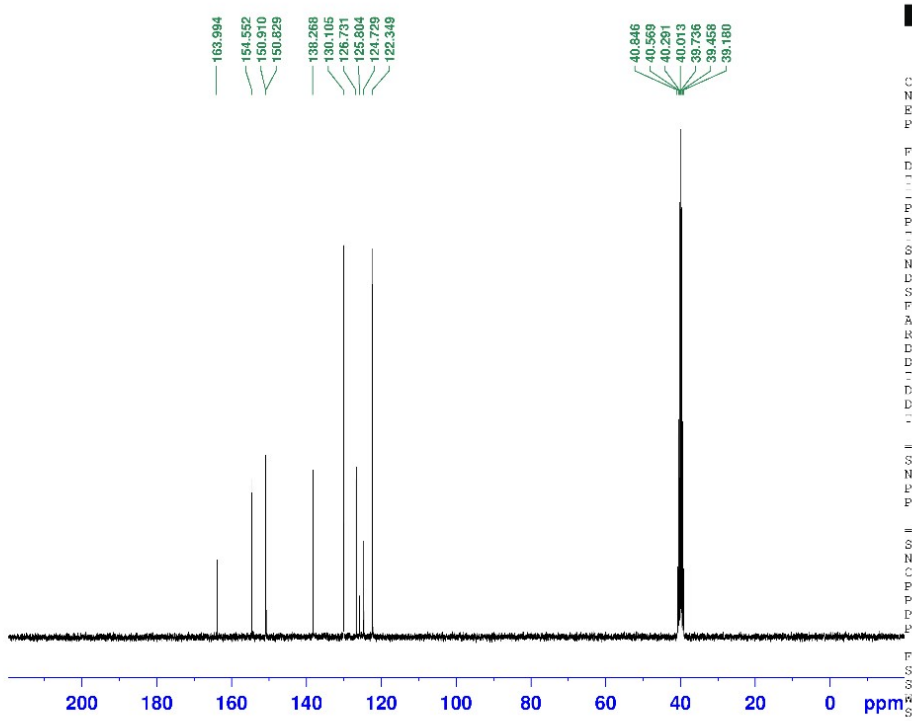


BRUKER

```
Current Data Parameters
NAME      May12-2018-nmr
EXPNO               171
PROCNO                1

F2 - Acquisition Parameters
Date_          20180512
Time              23.57
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                  132
DS                    4
SWH           18115.941 Hz
FIDRES        0.276427 Hz
AQ            1.8087935 sec
RG                  202
DW             27.600 usec
DE              6.50 usec
TE              298.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        75.6462982 MHz
NUC1               13C
P1               10.00 usec
PLW1       30.00000000 W

======== CHANNEL f2 ========
SFO2       300.8112032 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        6.40000010 W
PLW12       0.17778000 W
PLW13       0.14399999 W

F2 - Processing parameters
SI                32768
SF         75.6387350 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

2

Dr. Salimi- CODE AS27(Sami)-

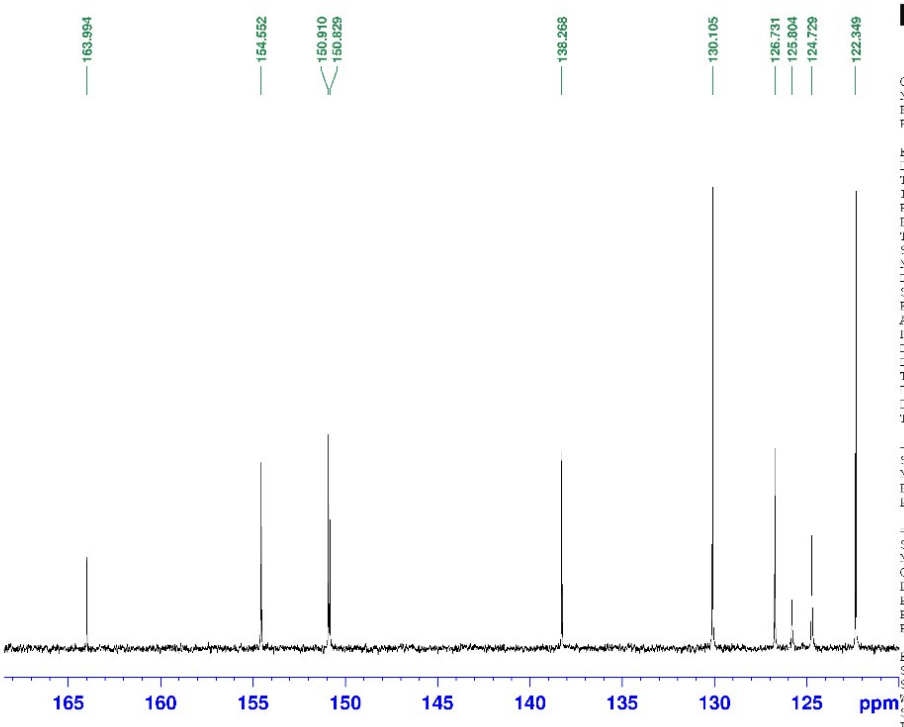


BRUKER

```
Current Data Parameters
NAME      May12-2018-nmr
EXPNO               173
PROCNO                1

F2 - Acquisition Parameters
Date_          20180513
Time              16.26
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT            DMSO
NS                  336
DS                    4
SWH           18115.941 Hz
FIDRES        0.276427 Hz
AQ            1.8087935 sec
RG                  202
DW             27.600 usec
DE              6.50 usec
TE              298.0 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        75.6462982 MHz
NUC1               13C
P1               10.00 usec
PLW1       30.00000000 W

======== CHANNEL f2 ========
SFO2       300.8112032 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        6.40000010 W
PLW12       0.17778000 W
PLW13       0.14399999 W

F2 - Processing parameters
SI                32768
SF         75.6387350 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

2 expand

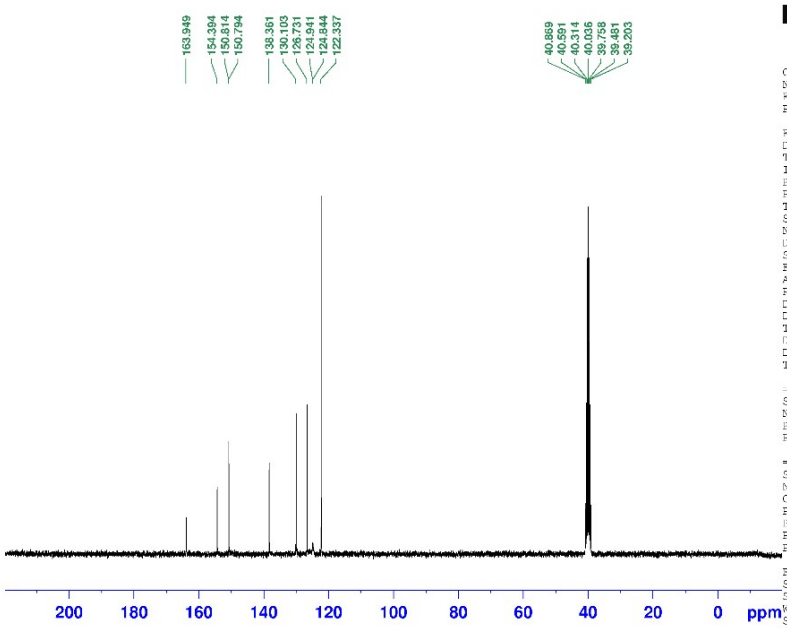
Dr. Salimi- CODE AS27(Sami)-




```
Current Data Parameters
NAME          May12_2018_nmr
EXPNO                   173
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180513
Time                   16.26
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                       336
DS                         4
SWH                18115.941 Hz
FIDRES              0.276427 Hz
AQ                  1.8087935 sec
RG                       202
DW                    27.600 usec
DE                     6.50 usec
TE                    298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1               75.6462982 MHz
NUC1                      13C
P1                      10.00 usec
PLW1               30.00000000 W

======== CHANNEL f2 ========
SFO2              300.8112032 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2               6.40000010 W
PLW12              0.17778000 W
PLW13              0.14399999 W

F2 - Processing parameters
SI                       32768
SF                 75.6387350 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

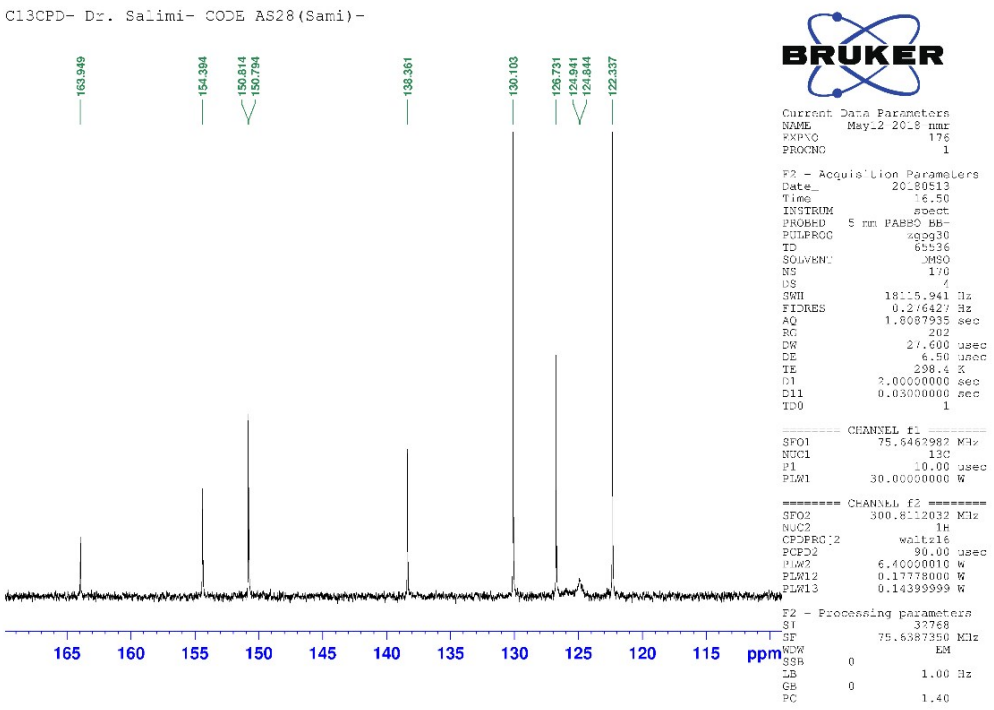
3

C13CPD- Dr. Salimi- CODE AS28(Sami)-

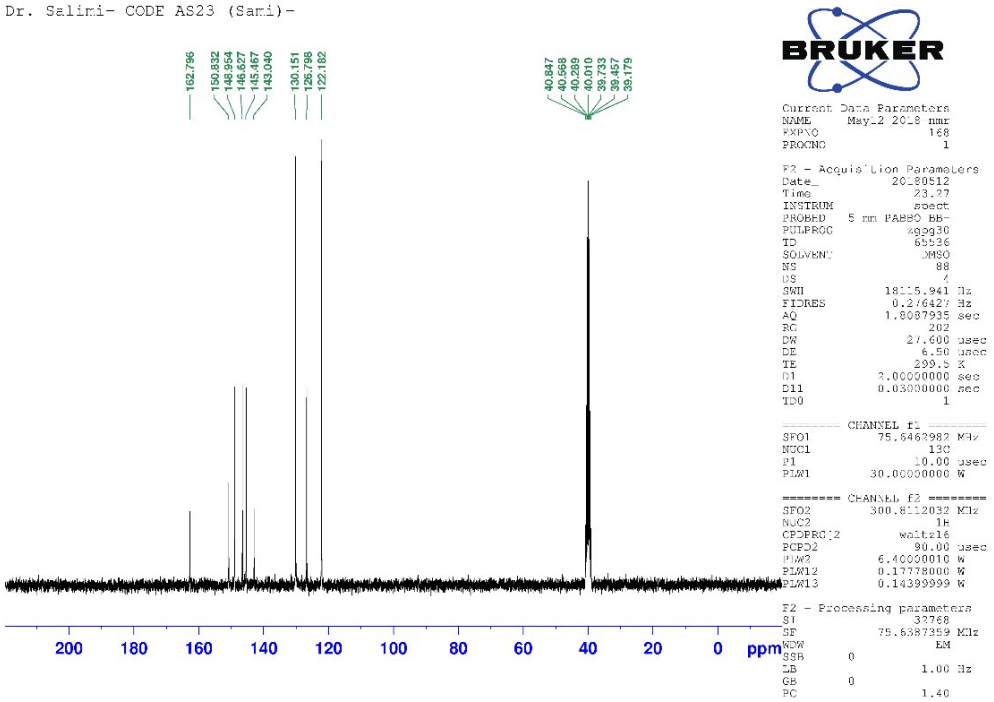



```
Current Data Parameters
NAME          May_2 2018 nmr
EXPNO                   176
PROCNO                    1

F2 - Acquisition Parameters
Date_               20180513
Time                   16.50
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                       170
DS                         4
SWH                18115.941 Hz
FIDRES              0.276427 Hz
AQ                  1.8087935 sec
RG                       202
DW                    27.600 usec
DE                     6.50 usec
TE                    298.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1               75.6462982 MHz
NUC1                      13C
P1                      10.00 usec
PLW1               30.00000000 W

======== CHANNEL f2 ========
SFO2              300.8112032 MHz
NUC2                       1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2               6.40000010 W
PLW12              0.17778000 W
PLW13              0.14399999 W

F2 - Processing parameters
SI                       32768
SF                 75.6387350 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

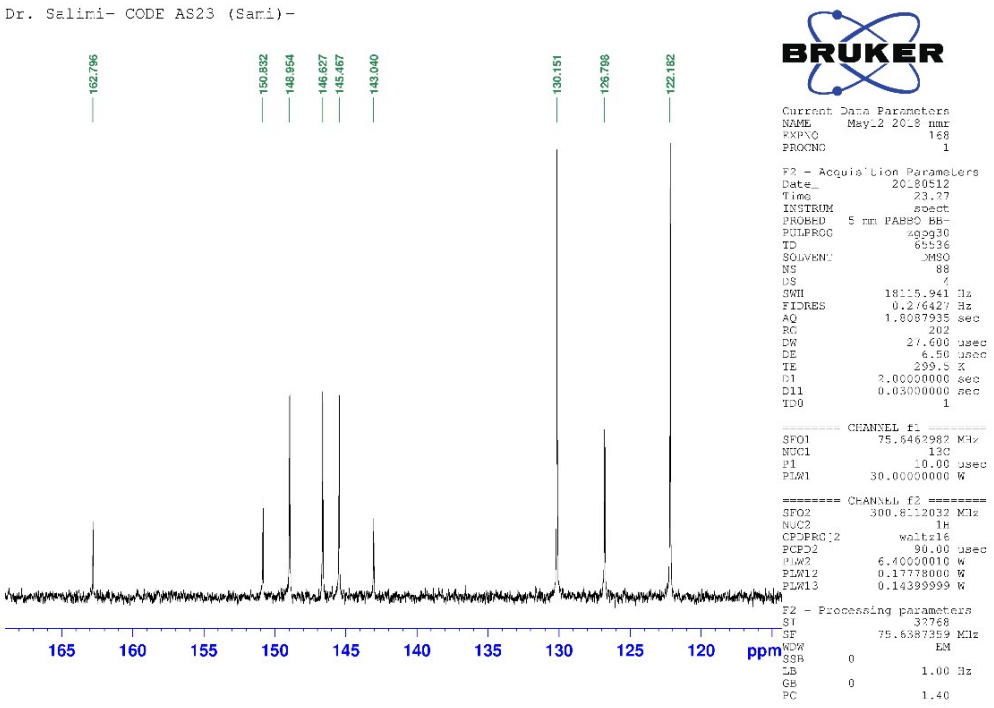
3 expand


C13CPD- Dr. Salimi- CODE AS28(Sami)-
163.949
154.394
150.814
150.794
138.361
130.103
126.731
124.941
124.844
122.337
165 160 155 150 145 140 135 130 125 120 115 ppm
BRUKER
Current Data Parameters
NAME May_2 2018 nmr
EXPNO 176
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180513
Time 16.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 170
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 75.6462982 MHz
NUC1 13C
P1 10.00 usec
PLW1 30.00000000 W
CHANNEL f2
SFO2 300.8112032 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 6.40000010 W
PLW12 0.17778000 W
PLW13 0.14399999 W
F2 - Processing parameters
SI 32768
SF 75.6387350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4


Dr. Salimi- CODE AS23 (Sami)-
162.796
150.832
148.954
146.627
145.467
143.040
130.151
126.798
122.182
40.847
40.568
40.289
40.010
39.733
39.457
39.179
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME May_2 2018 nmr
EXPNO 168
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180512
Time 23.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 88
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 75.6462982 MHz
NUC1 13C
P1 10.00 usec
PLW1 30.00000000 W
CHANNEL f2
SFO2 300.8112032 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 6.40000010 W
PLW12 0.17778000 W
PLW13 0.14399999 W
F2 - Processing parameters
SI 32768
SF 75.6387359 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

4 expand


Dr. Salimi- CODE AS23 (Sami)-
162.796
150.832
148.954
146.627
145.467
143.040
130.151
126.788
122.182
165
160
155
150
145
140
135
130
125
120
ppm
BRUKER
Current Data Parameters
NAME May_2 2018 nmr
EXPNO 168
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180512
Time 23.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 88
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.6462982 MHz
NUC1 13C
P1 10.00 usec
PLW1 30.00000000 W
======== CHANNEL f2 ========
SFO2 300.8112032 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 6.40000010 W
PLW12 0.17778000 W
PLW13 0.14399999 W
F2 - Processing parameters
SI 32768
SF 75.6387359 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

5

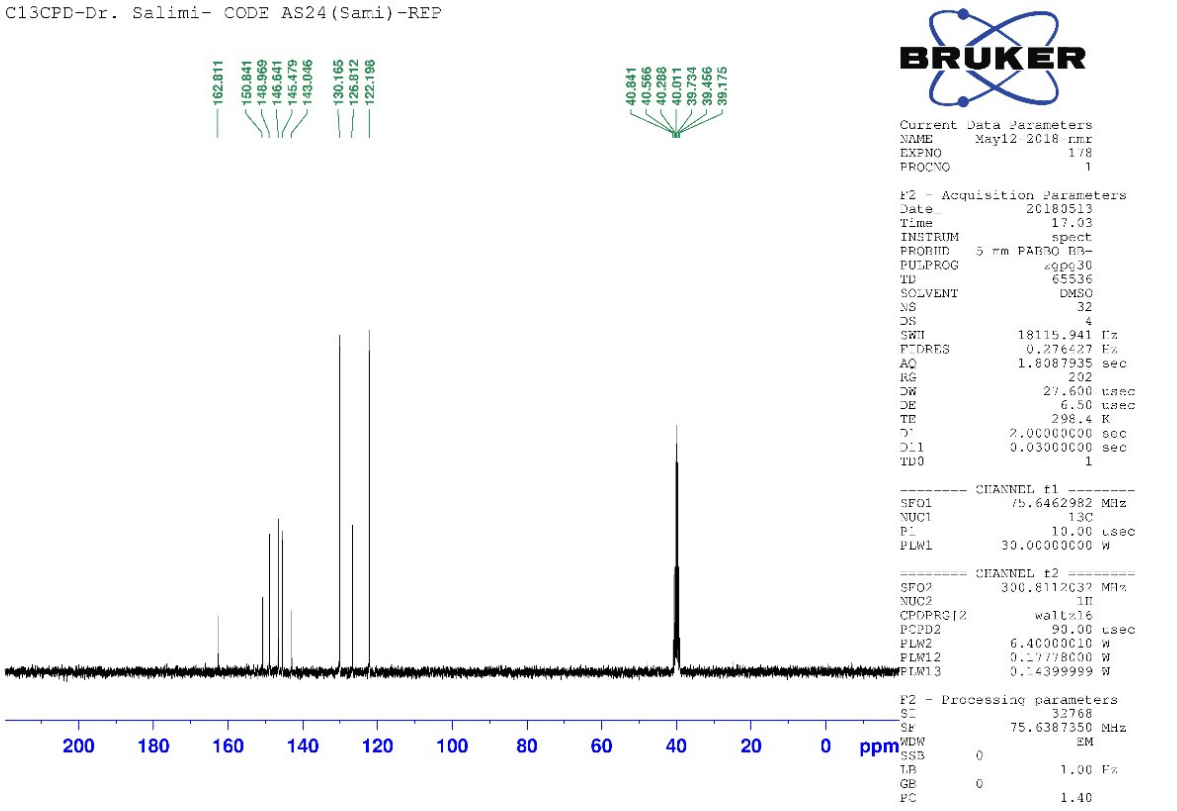

C13CPD-Dr. Salimi- CODE AS24(Sami)-REP
162.811
150.841
148.969
146.641
145.479
143.046
130.165
126.812
122.198
40.841
40.566
40.288
40.011
39.734
39.456
39.175
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME May12 2018 nmr
EXPNO 178
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180513
Time 17.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 32
DS 4
SWH 18115.941 Hz
FIDRES 0.276427 Hz
AQ 1.8087935 sec
RG 202
DW 27.600 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.6462982 MHz
NUC1 13C
P1 10.00 usec
PLW1 30.00000000 W
======== CHANNEL f2 ========
SFO2 300.8112032 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 6.40000010 W
PLW12 0.17778000 W
PLW13 0.14399999 W
F2 - Processing parameters
SI 32768
SF 75.6387350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S5. TGA plots for complexes 1-5.

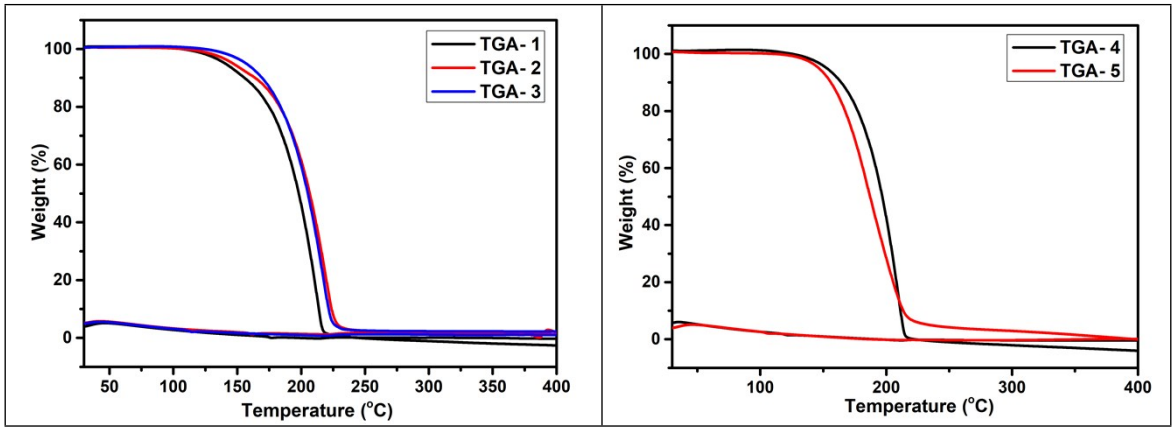


Figure S6. DSC plots for complexes 1-5.

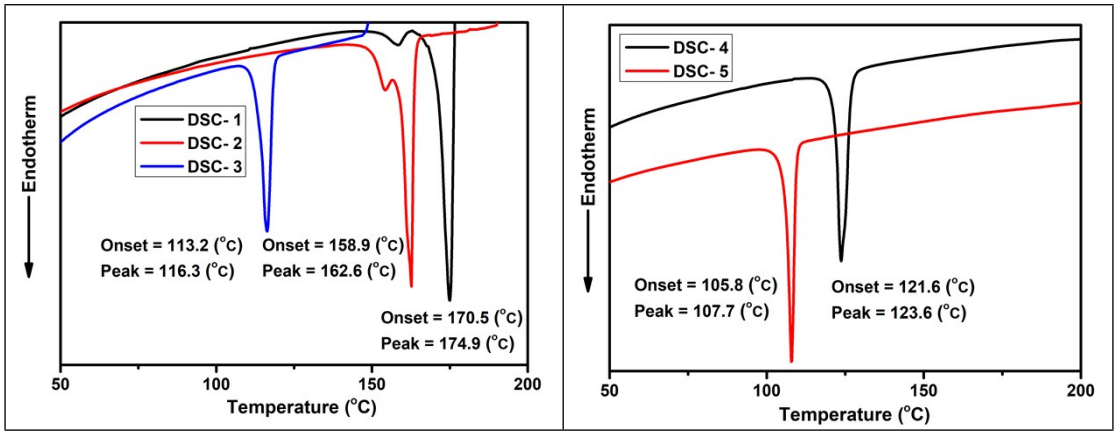
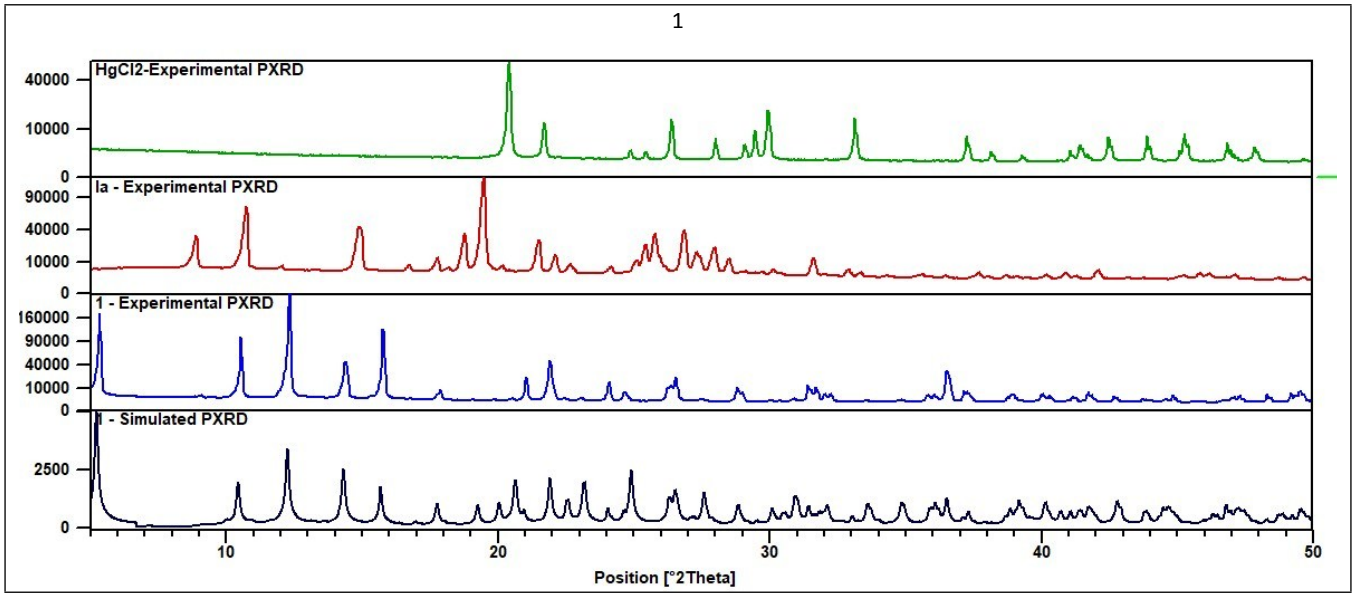
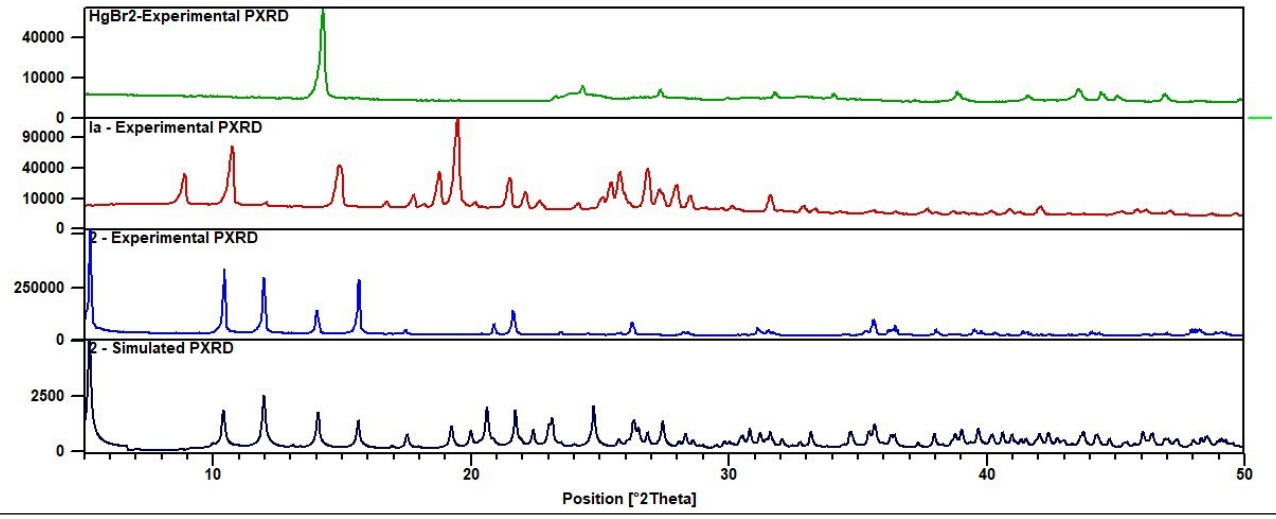


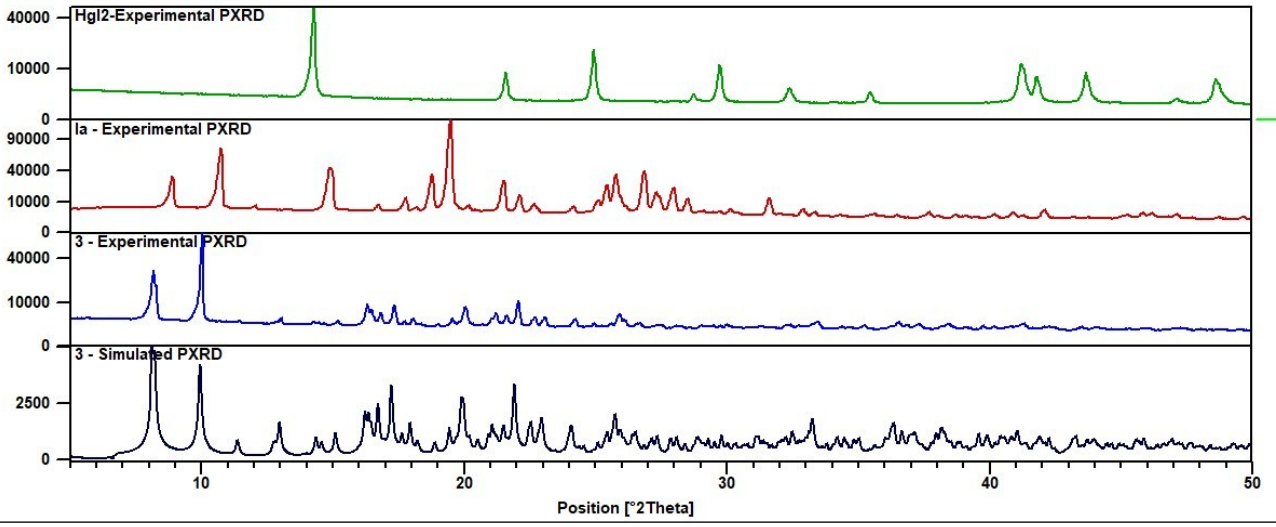
Figure S7. PXRD patterns for complexes 1-5.



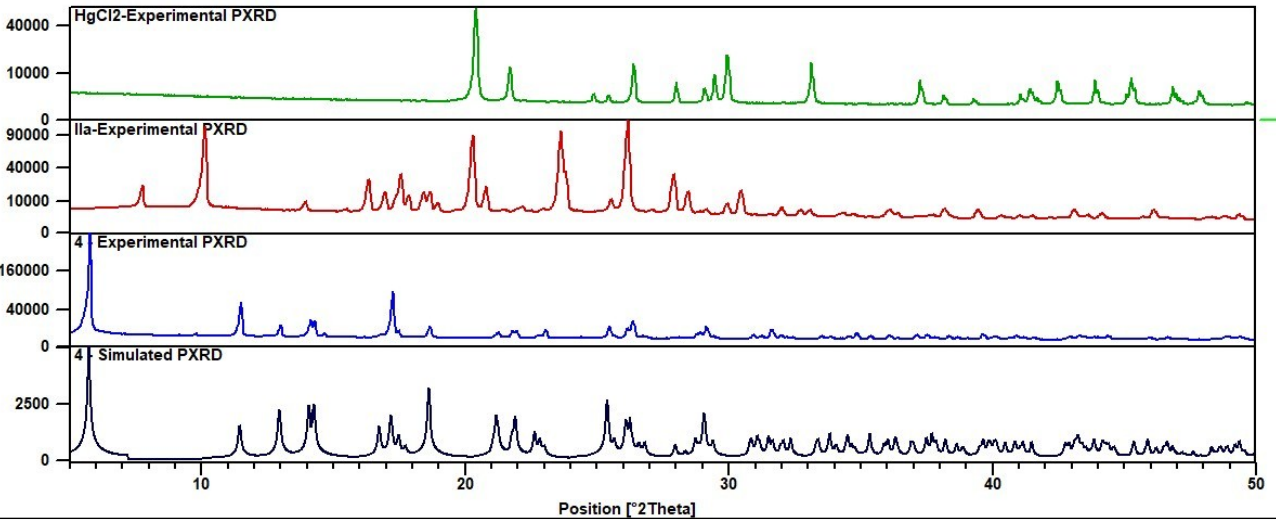
2


HgBr2-Experimental PXRD
40000
10000
0
Ia - Experimental PXRD
90000
40000
10000
0
2 - Experimental PXRD
250000
0
2 - Simulated PXRD
2500
0
10
20
30
40
50
Position [°2Theta]

3


HgI2-Experimental PXRD
40000
10000
0
Ia - Experimental PXRD
90000
40000
10000
0
3 - Experimental PXRD
40000
10000
0
3 - Simulated PXRD
2500
0
10
20
30
40
50
Position [°2Theta]

4


HgCl2-Experimental PXRD
40000
10000
0
IIa-Experimental PXRD
90000
40000
10000
0
4 Experimental PXRD
160000
40000
0
4 - Simulated PXRD
2500
0
10
20
30
40
50
Position [°2Theta]

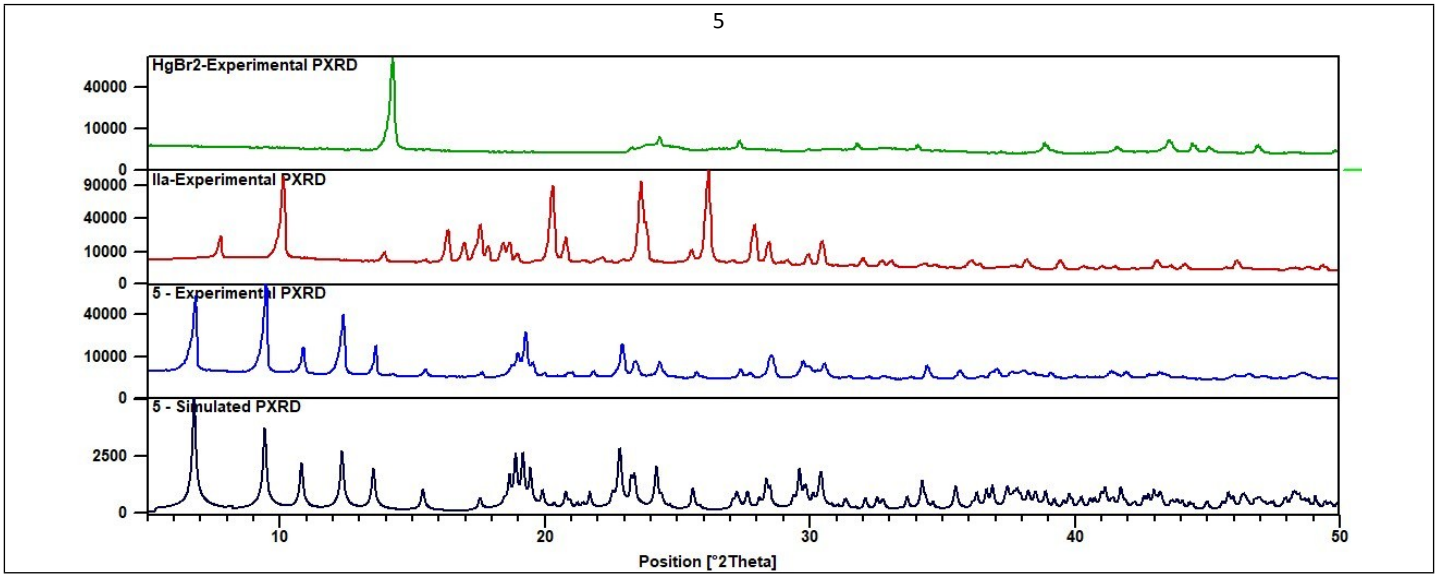
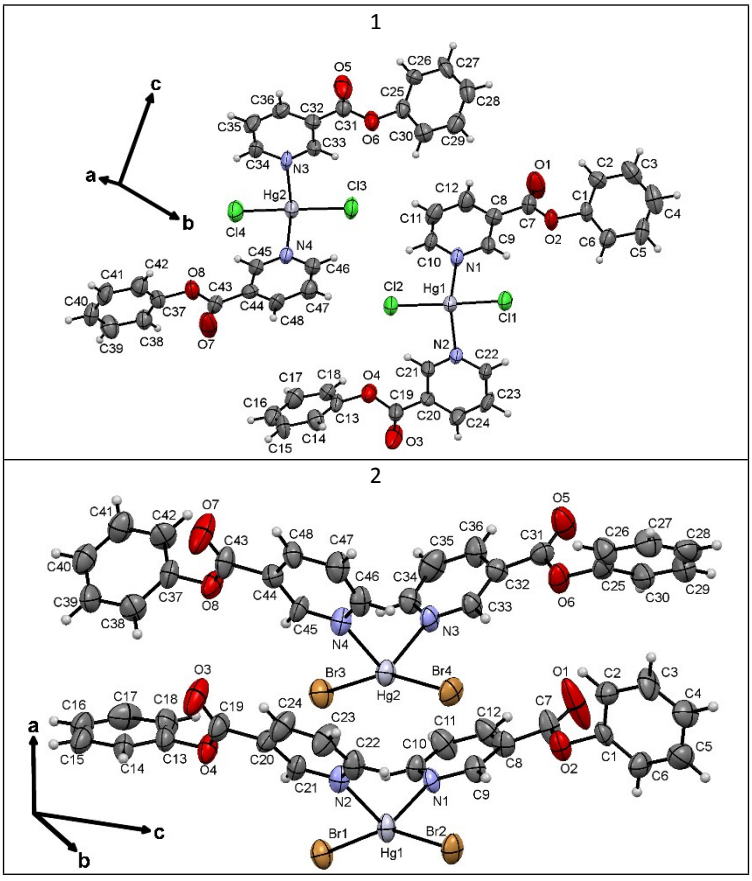


Figure S8. atom numbering and ortep diagram with 50% probablity for complexes 1-5.



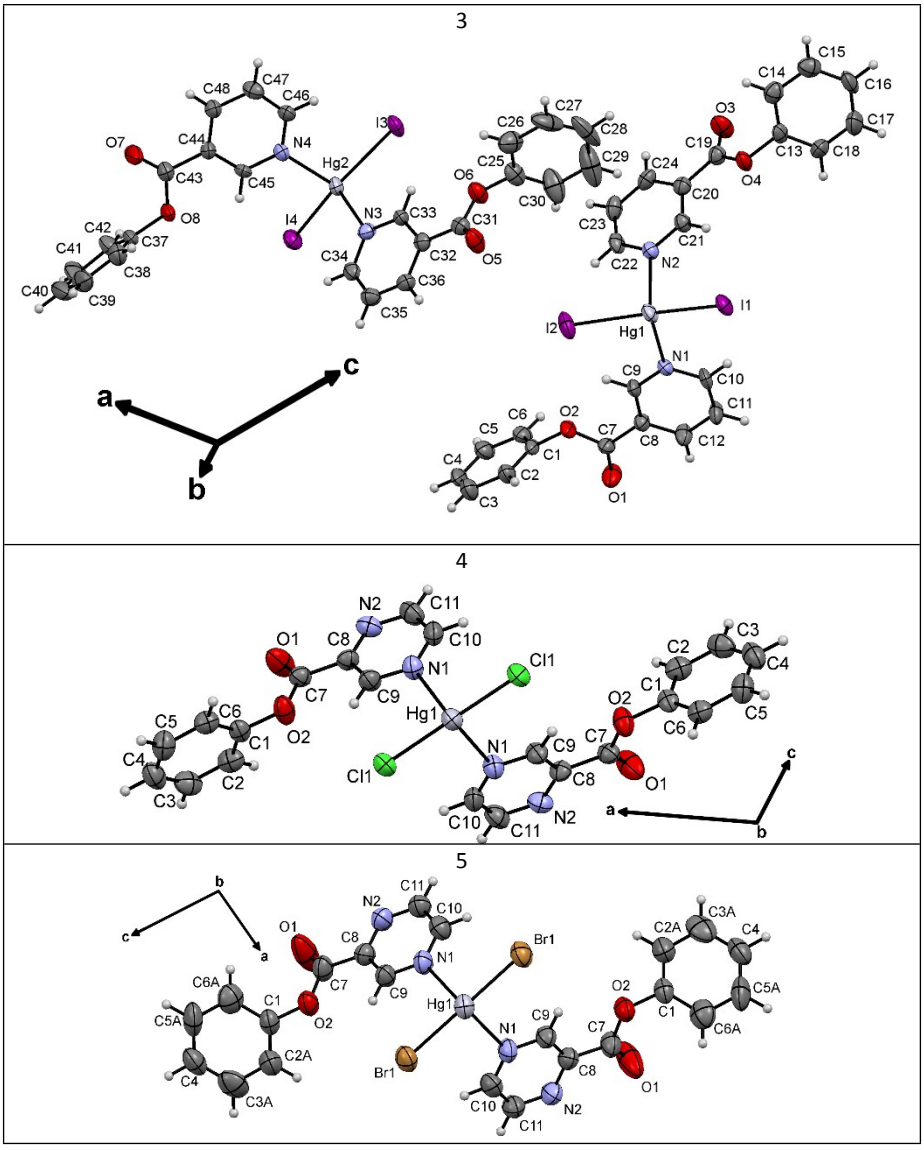


Table S1. Intermolecular interactions geometrical parameters and energies for complex 1.

Dimers (Complex 1)	Energy (kcal/mol)	Interactions	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation
Dimer1 (SI)	-18.55	$C_{21}–H_{21}\cdots Cl_3$	3.128(3)	3.41(1)	100	1-x, 1-y, -z
		$C_9–H_9\cdots Cl_4$	3.178(3)	3.43(1)	98	1-x, 1-y, -z
Dimer2 (SI)	-8.16	$C_{35}–H_{35}\cdots Cl_1$	2.920(3)	3.81(1)	161	x, -1+y, z
Dimer3 (SI)	-7.28	$C_{10}–H_{10}\cdots Cl_3$	2.897(3)	3.49(1)	123	x, y, z
Dimer4 (SI)	-4.85	$C_{27}–H_{27}\cdots O_3$	2.71(1)	3.39(1)	131	1+x, y, 1+z
Dimer5 (SI)	-4.83	$C_3–H_3\cdots O_7$	2.69(1)	3.50(1)	146	x, 1+y, 1+z
Dimer6 (SI)	-2.64	$C_{29}–H_{29}\cdots O_1$	2.68(1)	3.56(1)	159	1+x, y, z
Energy for SI Molecules	-43.67					
Dimer7 (SR)	-7.60	$C_{47}–H_{47}\cdots Cl_3$	3.043(3)	3.91(1)	156	2-x, 1-y, -z
Dimer8 (SR)	-8.60	$C_{22}–H_{22}\cdots Cl_1$	3.009(3)	3.52(1)	116	2-x, 2-y, -z
Dimer9 (SR)	-3.35	$C_5–H_5\cdots O_3$	2.66(1)	3.51(2)	153	1-x, 2-y, -z
Energy for SR Molecules	-19.54					

Table S2. Intermolecular interactions geometrical parameters and energies for complex 2.

Dimers (Complex 2)	Energy (kcal/mol)	Interactions	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation
Dimer1 (SI)	-19.18	C_9–H_9···Br_4	3.194(2)	3.49(1)	101	x, y, z
		C_{21}–H_{21}···Br_3	3.239(2)	3.54(1)	101	x, y, z
Dimer2 (SI)	-7.58	C_{35}–H_{35}···Br_1	2.957(2)	3.87(2)	161	1-x, -y, 1-z
Dimer3 (SI)	-6.96	C_{22}–H_{22}···Br_4	3.004(2)	3.62(1)	124	1-x, 1-y, 1-z
		C_{46}–H_{46}···Br_2	3.109(2)	3.68(1)	120	1-x, 1-y, 1-z
Dimer4 (SI)	-4.85	C_{15}–H_{15}···O_7	2.57(1)	3.42(1)	149	1-x, -y, -z
Dimer5 (SI)	-4.47	C_{29}–H_{29}···O_1	2.64(1)	3.35(1)	132	2-x, 1-y, 2-z
Dimer6 (SI)	-2.48	C_{27}–H_{27}···O_3	2.71(1)	3.62(1)	161	2-x, 1-y, 1-z
Energy for SI Molecules	-45.47					
Dimer7 (SR)	-7.72	C_{10}–H_{10}···Br_1	3.086(2)	3.64(1)	119	-x, -y, 1-z
Dimer8 (SR)	-6.86	C_{47}–H_{47}···Br_4	3.061(2)	3.95(1)	157	2-x, 1-y, 1-z
Dimer9 (SR)	-6.54	C_{34}–H_{34}···Br_3	3.047(2)	3.62(1)	121	1-x, -y, 1-z
Dimer10 (SR)	-3.38	C_{17}–H_{17}···O_1	2.74(1)	3.59(2)	150	1-x, -y, 1-z
Energy for SR Molecules	-24.51					

Table S3. Intermolecular interactions geometrical parameters and energies for complex 3.

Dimers (Complex 3)	Energy (kcal/mol)	Interactions	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation
Dimer1 (SI)	-7.40	C_{14}–H_{14}···I_4	3.301(1)	4.25(1)	175	x, 1.5-y, 0.5+z
Dimer2 (SI)	-5.36	C_{11}–H_{11}···O_5	2.57(1)	3.45(2)	155	1-x, -0.5+y, 1.5-z
		C_{12}–H_{12}···Cg_{Ph3}	3.064		129	1-x, -0.5+y, 1.5-z
Dimer3 (SI)	-5.00	C_{23}–H_{23}···O_7	2.50(1)	3.43(2)	169	2-x, -0.5+y, 1.5-z
Dimer4 (SI)	-4.92	C_{47}–H_{47}···Cg_{Ph1}	3.296		112	-1+x, 1.5-y, -0.5+z
Dimer5 (SI)	-3.00	C_{35}–H_{35}···O_1	2.83(1)	3.76(1)	165	1-x, 2-y, 1-z
Dimer6 (SI)	-2.14	C_{11}···C_{42}		3.49(1)		-1+x, y, z
Dimer7 (SI)	-1.95	C_{15}···C_{48}		3.38(1)		2-x, 2-y, 2-z
Energy for SI Molecules	-29.78					
Dimer8 (SR)	-17.21	C_{42}–H_{42}···Cg_{Ph3}	3.491		151	2-x, -½+y, 1.5-z
Dimer9 (SR)	-15.75	C_2–H_2···Cg_{Ph2}	3.345		141	1-x, -0.5+y, 1.5-z
Dimer10 (SR)	-6.02	C_{18}–H_{18}···Cg_{Ph1}	2.672		143	x, 1.5-y, -0.5+z
Dimer11 (SR)	-5.57	C_{40}–H_{40}···I_4	3.238(1)	4.06(1)	146	2-x, 2-y, 1-z
Dimer12 (SR)	-3.89	C_3–H_3···I_2	3.097(1)	3.87(1)	140	1-x, 2-y, 1-z
Dimer13 (SR)	-2.52	C_{41}–H_{41}···I_3	3.002(1)	3.83(1)	147	x, 1.5-y, -0.5+z
Energy for SR Molecules	-50.96					

Table S4. Intermolecular interactions geometrical parameters and energies for complex 4.

Dimers (Complex 4)	Energy (kcal/mol)	Interactions	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation
Dimer1	-7.16	C_3–H_3···O_1	2.55(1)	3.48(1)	166	x, -y, -0.5+z
Dimer2	-16.26	C_{11}–H_{11}···Cl_1	2.934(3)	3.84(1)	160	-x, 1-y, 1-z
Dimer3	-6.58	C_{10}–H_{10}···Cl_1	2.983(3)	3.69(1)	133	-x, 2-y, 1-z
Energy for SR Molecules	-29.99					

Table S5. Intermolecular interactions geometrical parameters and energies for complex 5.

Dimers (Complex 5)	Energy (kcal/mol)	Interactions	H···A/Å	D···A/Å	∠D–H···A/°	Symmetry Operation
Dimer1	-6.06	C_{11}–H_{11}···O_1	2.76(1)	3.37(1)	123	1.5-x, 0.5+y, 0.5-z
Dimer2	-15.80	C_9–H_9···Br_1	3.502(2)	3.60(1)	88	x, -1+y, z
		C_{10}–H_{10}···Br_1	3.39(2)	3.56(1)	96	1-x, -1+y, 0.5-z
Dimer3	-3.71	C_4–H_4··· Br_1	3.361(2)	4.03(1)	130	1-x, -1-y, -z
Energy for SR Molecules	-25.57					

Figure S9. representation of the interactions between SR molecules of complex 1 with calculated energy of dimers; (i)2-x, 1-y, -z, (ii)2-x, 2-y, -z, (iii)1+x, y, z.

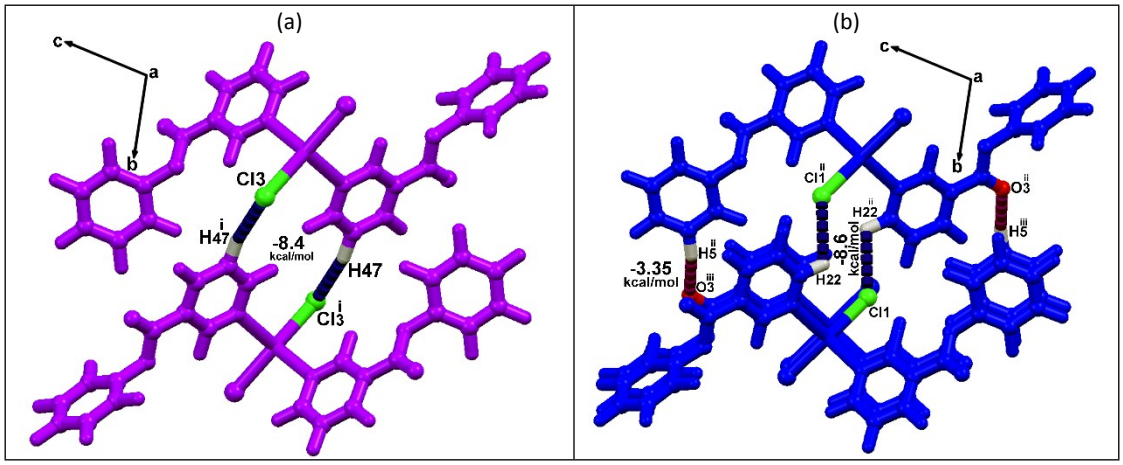


Figure S10. representation of the interactions between SR molecules of complex 2 with calculated energy of dimers; (i)-x, -y, 1-z, (ii)1-x, -y, 1-z (iii)2-x, 1-y, 1-z.

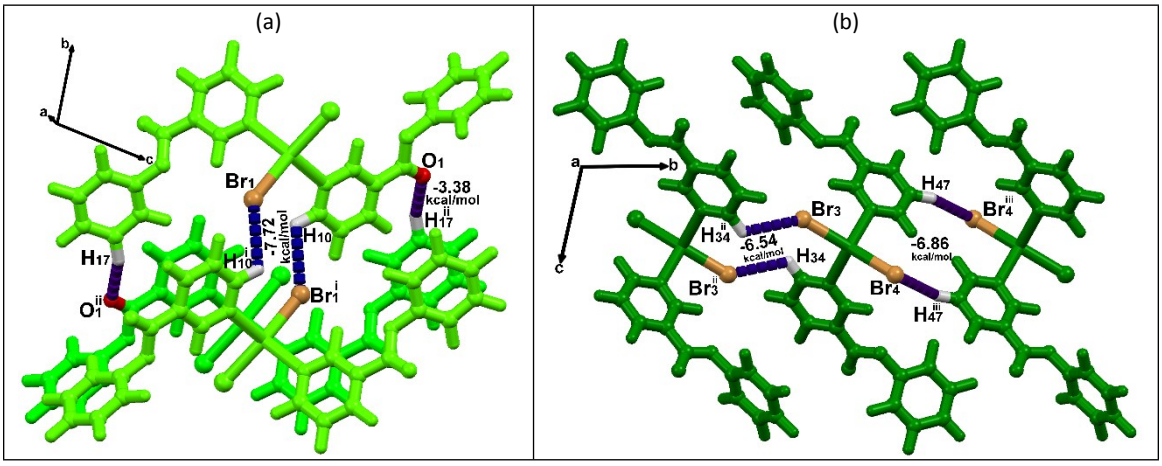


Figure S11. representation of the interactions between SR molecules of complex 3 with calculated energy of dimers; (i)2-x, 2-y, 2-z, (ii)2-x, ½+y, 1.5-z, (iii)x, 1.5-y, ½+z, (iv)1-x, 2-y, 1-z, (v)x, 2.5-y, -½+z.

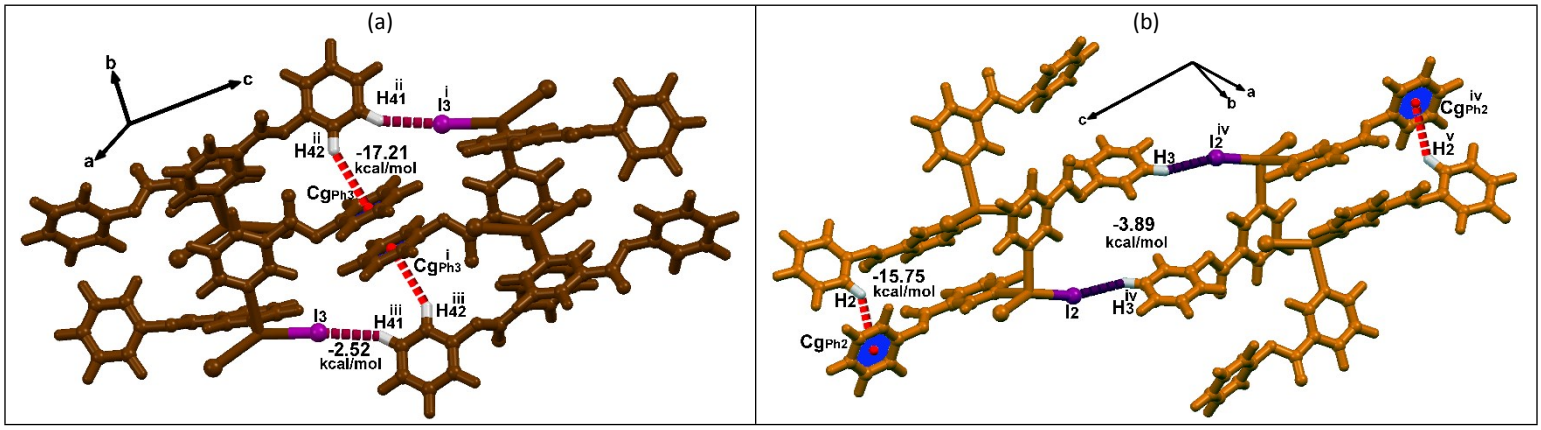


Figure S12. overlay between SI molecules in the asymmetric unit for high Z' complexes of 1-3.

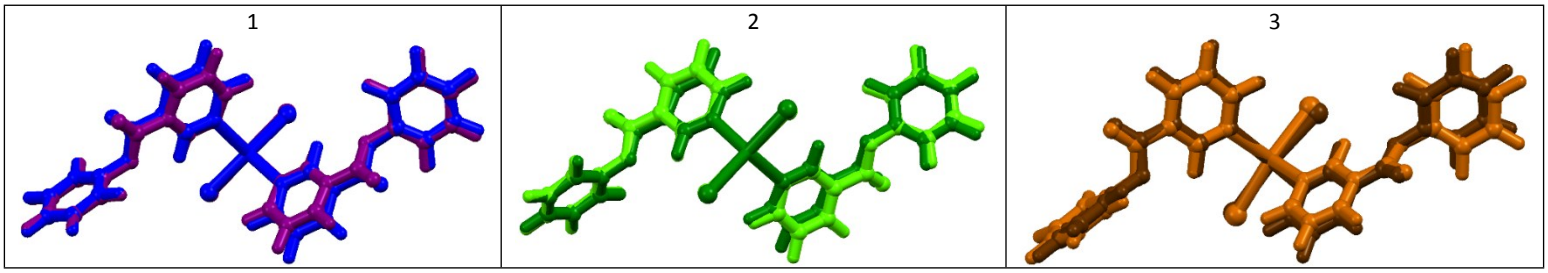


Figure S13. C–H···X–M/O/π interactions for each monomer of complexes 1-3 in asymmetric unit by Hirshfeld Surface Analysis.

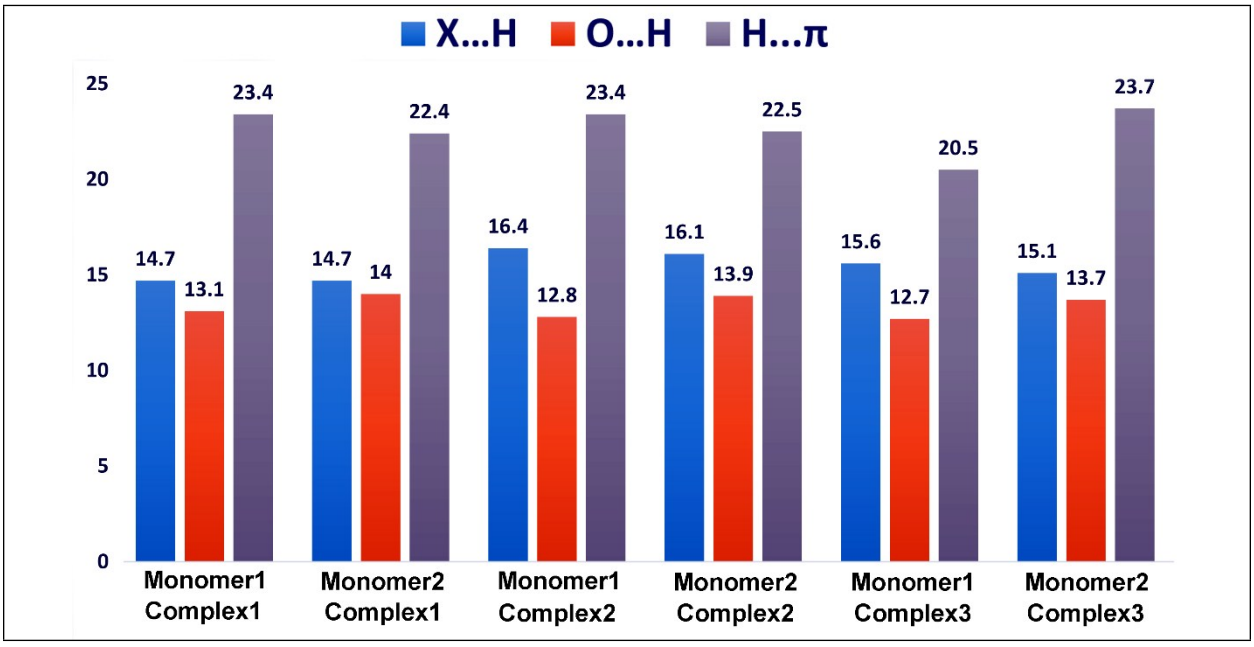


Figure S14. C−H···X−M/O/π interactions for complexes 1-5 by Hirshfeld Surface Analysis.

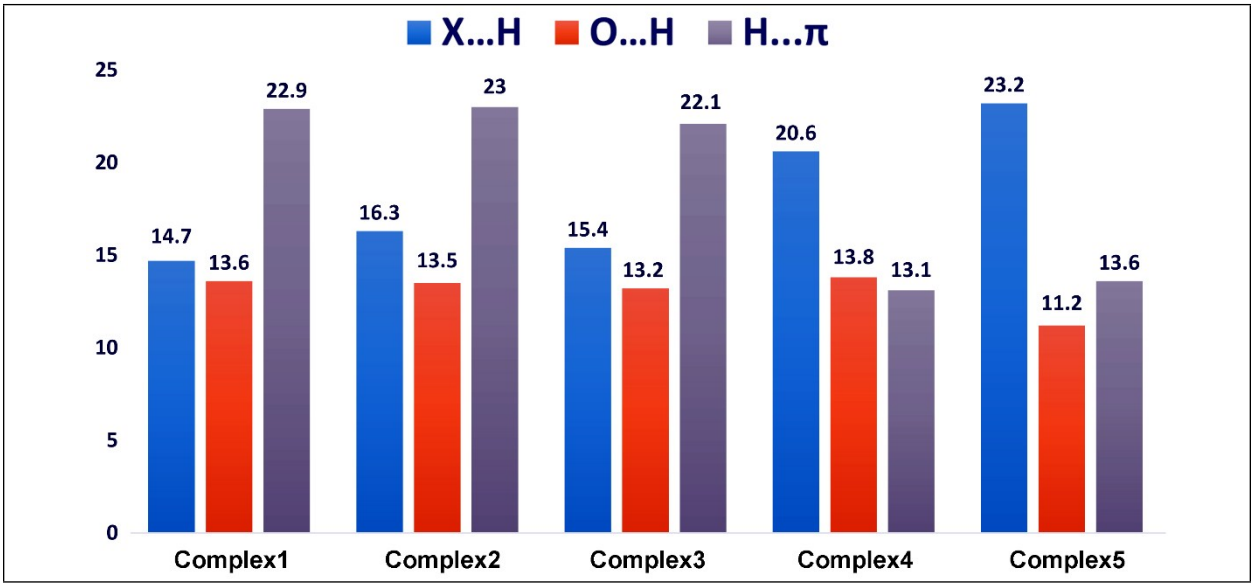


Figure S15. the structure of **(a)** REHLAT01, **(b)** REHLAT, **(c)** TEFYEK.

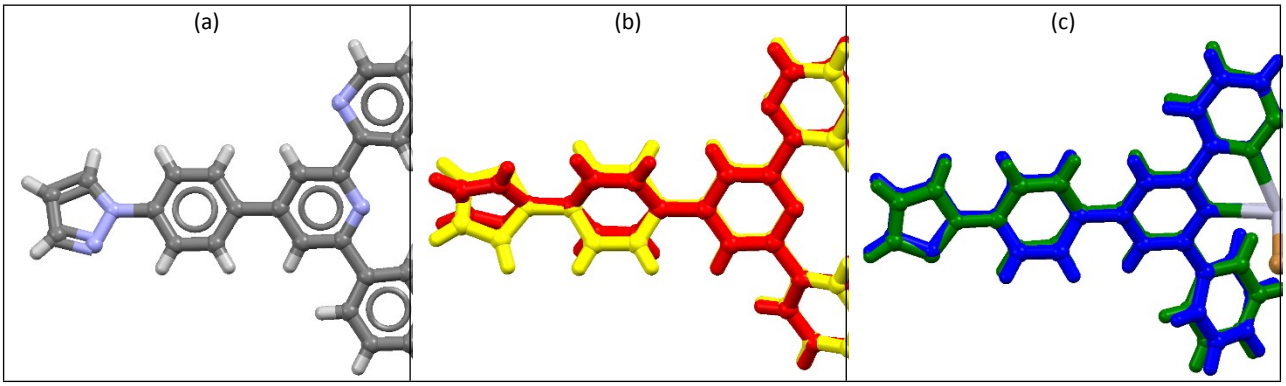


Table S6. high and low Z' pairs in CSD study.

No.	Refcode	rmsd	τ	No.	Refcode	rmsd	τ	No.	Refcode	rmsd	τ
1	ACACCR	0.16	×	41	DILWIE	0.22	×	81	HISZOA	0.431	✓
2	ACACMN	0.2	×	42	DIQPIE	0.754	✓	82	HIYVUG	0.278	✓
3	ACACMO	0.17	×	43	DOCQIV	0.105	×	83	HMCTST	0.063	×
4	AJAHAW	0.25	✓	44	DOVPAF	0.091	✓	84	IBEFUR	0.248	✓
5	ALACAC	0.14	×	45	DOZCIF	0.008	✓	85	IBIRAM	0.234	✓
6	AMOPIB	0.86	✓	46	DUCMOE	0.933	✓	86	IBUZOW	1.06	✓
7	AMOTIH	0.76	✓	47	DUYYIG	0.121	✓	87	IHAMAG	0.85	✓
8	AVETIE	0.16	✓	48	DUZDAF	0.154	✓	88	IHOLEW	0.119	✓
9	AVOZIV	0.06	×	49	ECERIP	0.121	✓	89	ILUNEI	0.149	✓
10	AXEYUY	0.39	✓	50	ECUSAW	0.428	✓	90	INUTUH	0.103	✓
11	AXIYIP	0.41	✓	51	EKABEY	0.423	✓	91	IRUMEN	0.388	✓
12	AZFAPD	0.5	✓	52	ELUREI	0.036	✓	92	ISIVIQ	0.52	✓
13	BABQIF	0.22	✓	53	EMEQAO	0.196	✓	93	ISULOY	0.326	✓
14	BADDAM	0.16	✓	54	ETCMSN	0.454	✓	94	IYANUR	0.323	✓
15	BATFEI	0.23	✓	55	ETEDUC	0.367	✓	95	JADGAW	0.389	×
16	BATLAK	1.11	✓	56	EVUCIH	0.671	✓	96	JAXVIN	0.305	✓
17	BEZHET	0.12	×	57	FAKHUU	0.249	✓	97	JEHZOL	0.115	✓
18	BICLUU	0.37	✓	58	FECWAL	0.35	✓	98	JETWOU	0.42	✓
19	BIMCEF	0.13	✓	59	FEROCA	0.08	×	99	JISPAD	0.16	✓
20	BIPHHG	0.14	✓	60	FEROCE	0.008	×	100	JIXFAY	0.915	✓
21	BIWZOY	0.07	×	61	FERWEE	0.547	✓	101	JIXFIG	0.118	✓
22	BMOMPY	0.14	✓	62	FEXWIO	0.645	✓	102	JOJYOX	0.541	✓
23	BOSVOU	0.1	×	63	FEZZAN	0.318	✓	103	JOWLEM	0.449	✓
24	BOTQOQ	0.51	✓	64	FIBZOH	0.2	×	104	JUDLOJ	0.2	✓
25	BOWXAM	0.5	✓	65	FIMVOO	0.1	✓	105	KARHIU	0.533	✓
26	BURGAW	0.11	✓	66	FITLAV	0.433	✓	106	KEMCOW	0.211	✓
27	BUZJEL	0.2	✓	67	FODSIA	0.061	✓	107	KEPMIZ	0.117	✓
28	BZQXPD	0.001	×	68	FODTOJ	0.35	✓	108	KIFKOZ	0.218	✓
29	CALHAZ	0.1	✓	69	FODZIH	0.3	✓	109	KOCPID	0.176	✓
30	CAQQEQ	0.24	×	70	FUCPAU	0.77	✓	110	KOSWOE	0.159	✓
31	CEZYEN	0.076	✓	71	FUGDAM	0.09	×	111	KUDGIZ	0.038	×
32	COCTFT	0.145	✓	72	GADWEN	0.025	✓	112	KUQMAL	0.34	✓
33	COZMUB	0.545	✓	73	GAFMUW	0.09	×	113	KUSFAG	0.0334	✓
34	CYPTIS	0.287	✓	74	GAXGOB	0.11	✓	114	LAGLEL	0.38	✓
35	DABMUO	0.2	✓	75	GEDJEE	0.0715	×	115	LAKMOZ	0.246	✓
36	DAQQOD	0.64	✓	76	GITXEM	0.26	×	116	LALMAM	0.55	✓
37	DCCPTI	0.33	×	77	GOBBEG	0.444	✓	117	LARVUV	0.042	×
38	DEHJOP	0.092	×	78	GPTANI	0.241	✓	118	LAVSOR	0.2934	✓
39	DEXLOJ	0.536	✓	79	GULLUW	0.289	✓	119	QUHWAT	0.227	✓
40	DIFCAW	0.308	×	80	HEFHOP	0.15	✓	120	RABFAX	0.148	✓

No.	Refcode	rmsd	τ	No.	Refcode	rmsd	τ	No.	Refcode	rmsd	τ
121	LEKSEB	0.28	✓	161	RARJIE	0.15	✓	201	WIJXAO	0.189	✓
122	LITKOO	0.454	✓	162	REDMAP	0.265	✓	202	WOKRAP	0.45	✓
123	LUBJEX	0.516	✓	163	RIGHOG	0.37	✓	203	WOLMIT	0.45	✓
124	LUWSUS	0.473	✓	164	SAKMAS	0.178	✓	204	WOPDAG	0.24	✓
125	LUZNEB	0.53	✓	165	SAXDAW	0.122	✓	205	XEXXIJ	0.48	✓
126	MADHUV	0.754	✓	166	SEMYAM	0.157	×	206	XIKFON	0.086	✓
127	MEBBAY	0.389	✓	167	SETHIK	0.35	✓	207	XIRFIP	0.8	✓
128	MEWBIB	0.194	✓	168	SMOHGB	1.06	✓	208	XITJEQ	0.17	✓
129	MIGBOU	0.273	×	169	SUDFAY	0.75	✓	209	XOFQOZ	0.102	✓
130	MIGCUB	0.0547	✓	170	TAHDOV	0.121	✓	210	XOMFEL	0.27	×
131	MOFORM	0.0202	×	171	TAPIFE	0.31	✓	211	XOVBOZ	0.154	✓
132	MOXESA	0.0957	×	172	TAXJUY	0.26	✓	212	XUGREX	0.27	✓
133	MPEIWC	0.14	✓	173	TCACTC	0.215	✓	213	XUHREY	0.62	✓
134	MUVSUR	0.274	✓	174	THUCUA	0.8	✓	214	YADWOP	0.47	✓
135	NAFZOJ	0.264	✓	175	TIFGOE	0.52	✓	215	YAFYOU	0.343	✓
136	NELXAF	0.43	✓	176	TIKHEA	0.18	✓	216	YICKOL	0.154	✓
137	NESLIH	0.7	✓	177	TIVLOZ	0.112	✓	217	YIQPIY	2.19	✓
138	NOXLET	0.222	✓	178	TIVPAP	0.18	✓	218	YOHBOM	0.085	×
139	NOYWOP	0.0364	✓	179	TOLSCU	3.123	✓	219	YOSJAR	0.13	×
140	NUYBUG	1.95	✓	180	TTPCUC	1.147	✓	220	YUBJEK	0.17	✓
141	NUYZUE	1.1	✓	181	TUKTUQ	0.128	✓	221	YUJJOD	0.3	✓
142	OBODIT	0.375	✓	182	UBUKAD	0.353	✓	222	ZAGMIG	0.12	✓
143	OMILOL	0.477	✓	183	UJEYEO	0.31	×	223	ZEPPAL	0.37	✓
144	OMUQUJ	0.13	✓	184	UKEVEL	0.22	✓	224	ZEWSIF	0.097	✓
145	OPORIV	0.086	✓	185	VAFXUV	0.2	✓	225	ZEWXOO	0.06	×
146	ORAREF	0.086	×	186	VALCAO	0.92	✓	226	ZOQVIK	0.28	✓
147	OROKEM	0.56	✓	187	VASTAK	0.1	✓	227	ZUJSEE	0.894	✓
148	OWEFED	0.11	✓	188	VAZWEY	0.86	✓	228	ZZZTWE	0.0774	×
149	PBPHCY	0.07	×	189	VEJHUP	0.32	✓				
150	PCSTIB	0.58	✓	190	VEPQAI	0.67	✓				
151	PELVIM	1.321	✓	191	VEZFOX	0.182	✓				
152	PIHVUY	0.341	✓	192	VIQZAY	0.45	✓				
153	PIKVIQ	0.6703	✓	193	VOLCOQ	0.043	✓				
154	PNTRCU	0.176	✓	194	VUDVEW	0.08	✓				
155	PORKOX	0.352	✓	195	VUWLOO	0.724	✓				
156	QATMON	0.3	×	196	WAMTUZ	0.38	✓				
157	QIYMIV	0.1465	✓	197	WEHZEO	0.13	✓				
158	QUHWAT	0.286	✓	198	WENDOI	0.31	✓				
159	RABFAX	0.15	✓	199	WEQZAT	3.04	✓				
160	RAGWON	0.265	✓	200	WIBCUF	0.486	✓				