Electronic Supplementary Material (ESI) for CrystEngComm.

Polymorphism In Carboxamide Compounds with High-Z' Crystal Structure

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Supporting Information

S0. List of Contents

Figure S1. mass spectroscopy analysis for N-(thiazole-2-yl) pyrazine-2-carboxamide.

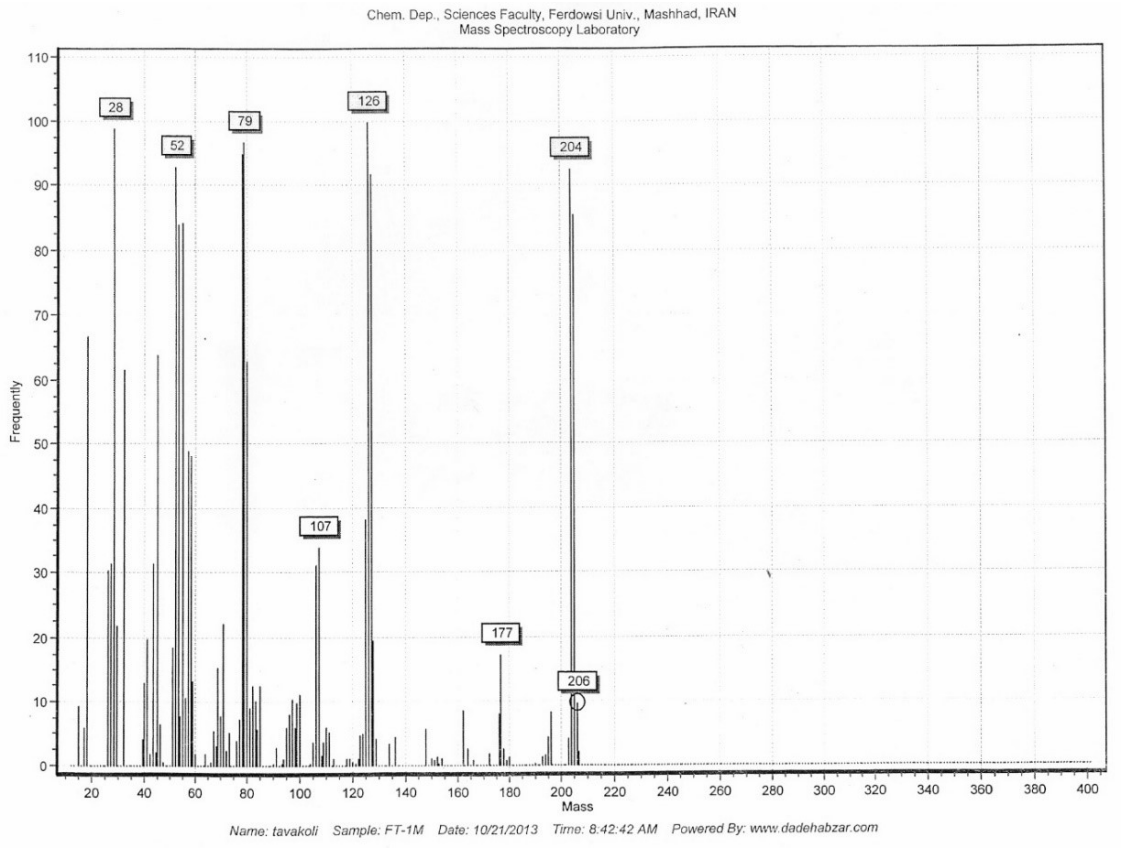

Figure S2. CHN elemental analysis for N-(thiazole-2-yl) pyrazine-2-carboxamide.

```
                    Eager 300 Summarize Results

                              Date : 04/01/2015 at 08:27:27
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                  Method Filename : Copy of Copy of N C H S-bkp .mth

     Filename              AS Method            Vial
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     Component name  Element %
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     Carbon%         48.17142868
     Hydrogen%       2.829131365
     Sulphur%        15.1317749


               1 Sample(s) in Group No : 1
Component Name Average
-------------- --------------
Nitrogen%      27.31689453
Carbon%        48.17142868
Hydrogen%      2.829131365
Sulphur%       15.1317749
```

Figure S3. [1]H-NMR spectrums for N-(thiazole-2-yl) pyrazine-2-carboxamide.

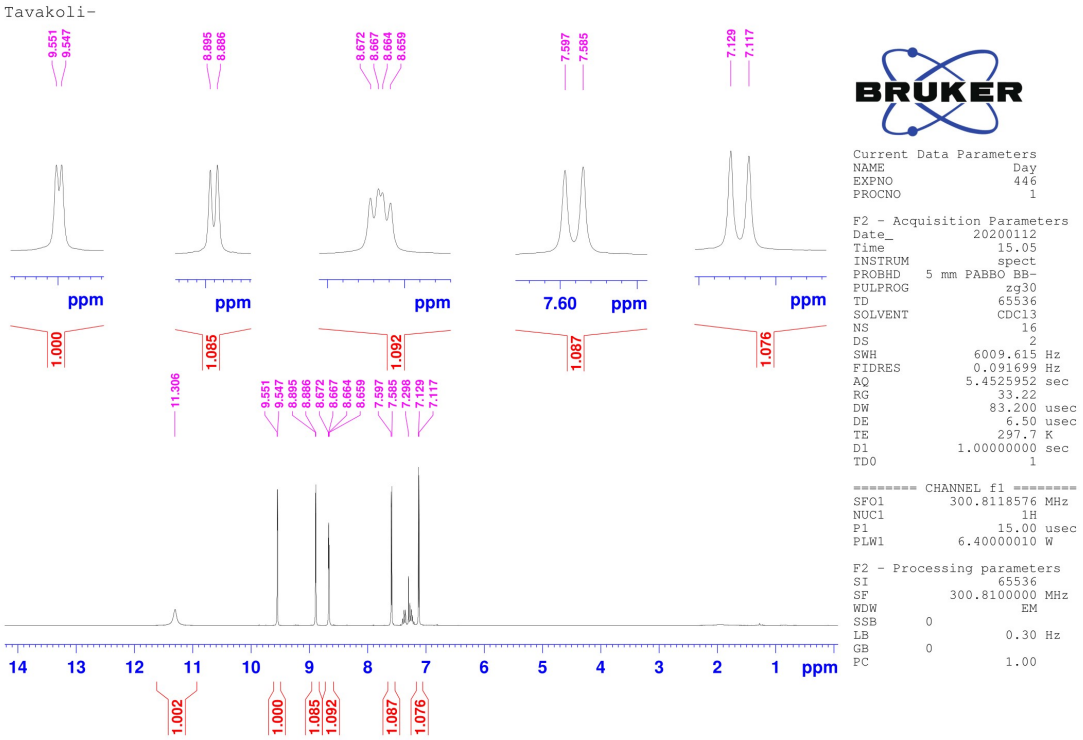


Figure S4. [13]C-NMR spectrums for N-(thiazole-2-yl) pyrazine-2-carboxamide.

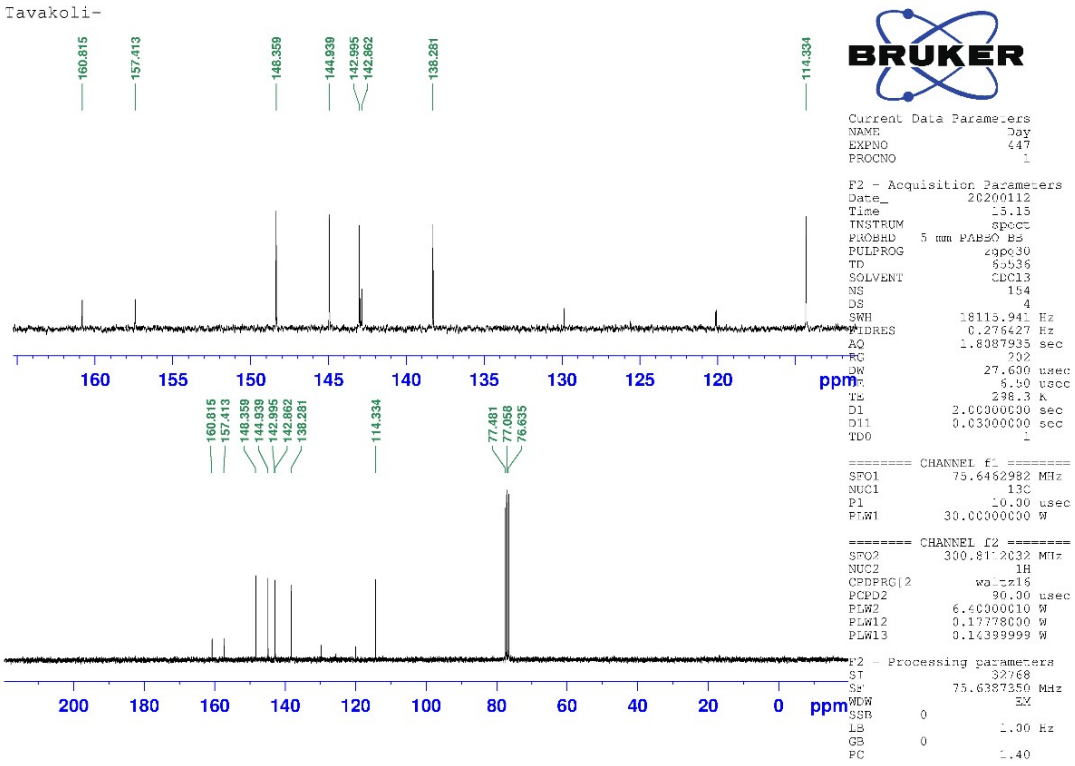


Figure S5. The overlay of symmetry independent molecules of **I** (a), **II** (b), and **III** (c).

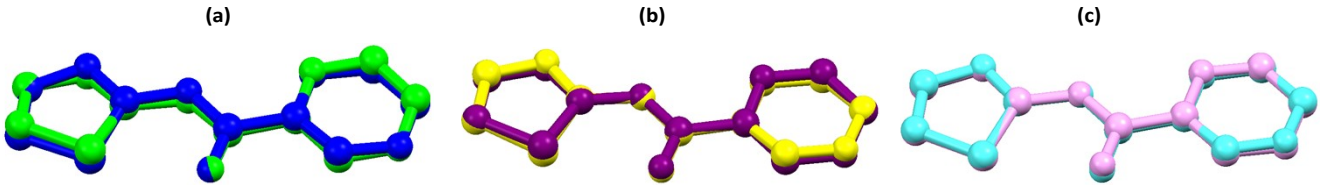


Figure S6. Overlay of PXRD plots for **I**, **II** and **III**.

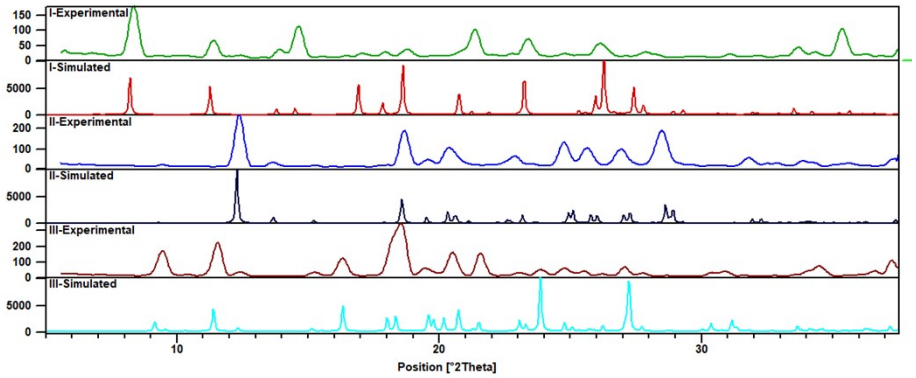


Figure S7. Overlay of FT-IR plots for **I**, **II** and **III**.

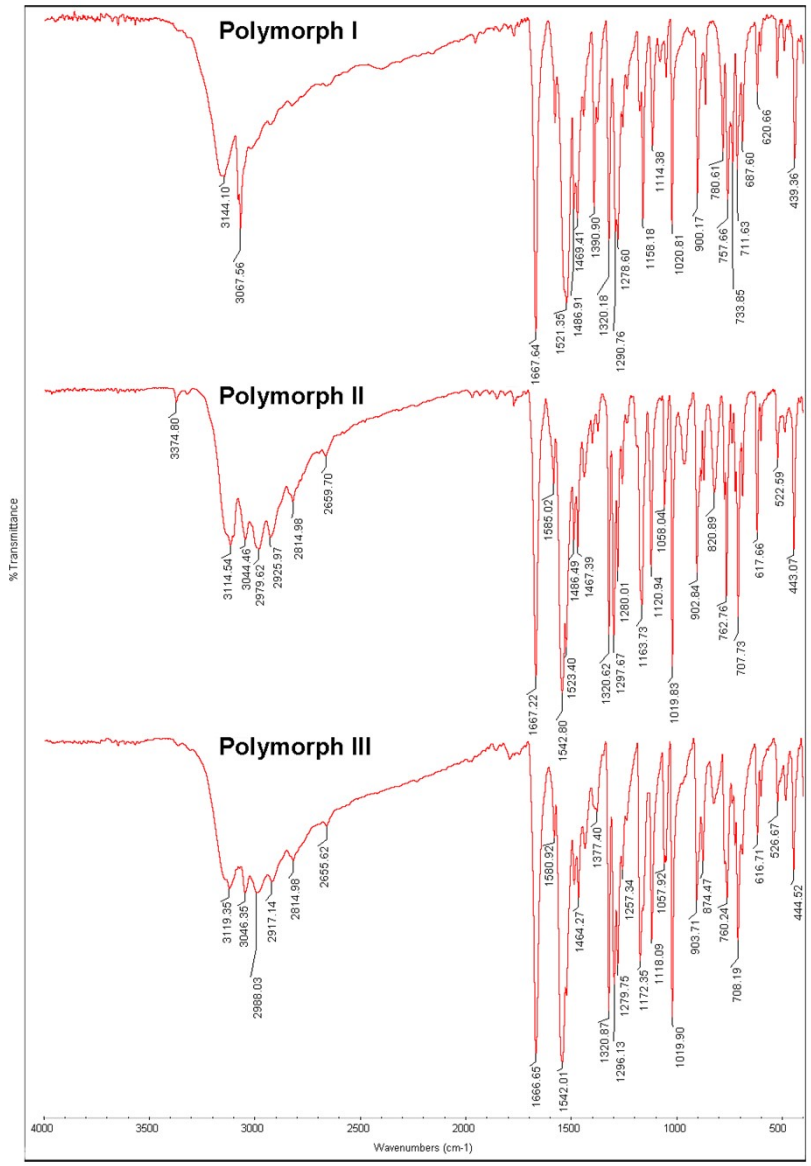


Figure S8. Overlay of TGA plots for **I**, **II** and **III**.

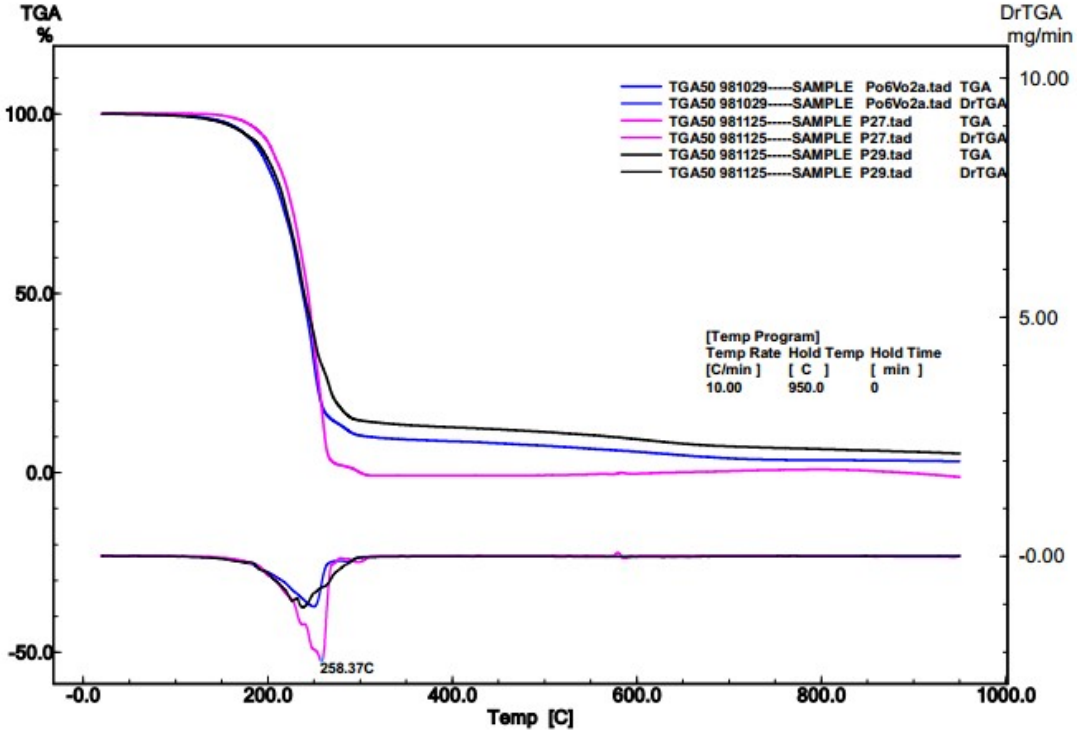


Figure S9. Overlay of DSC plots for **II** and **III**.

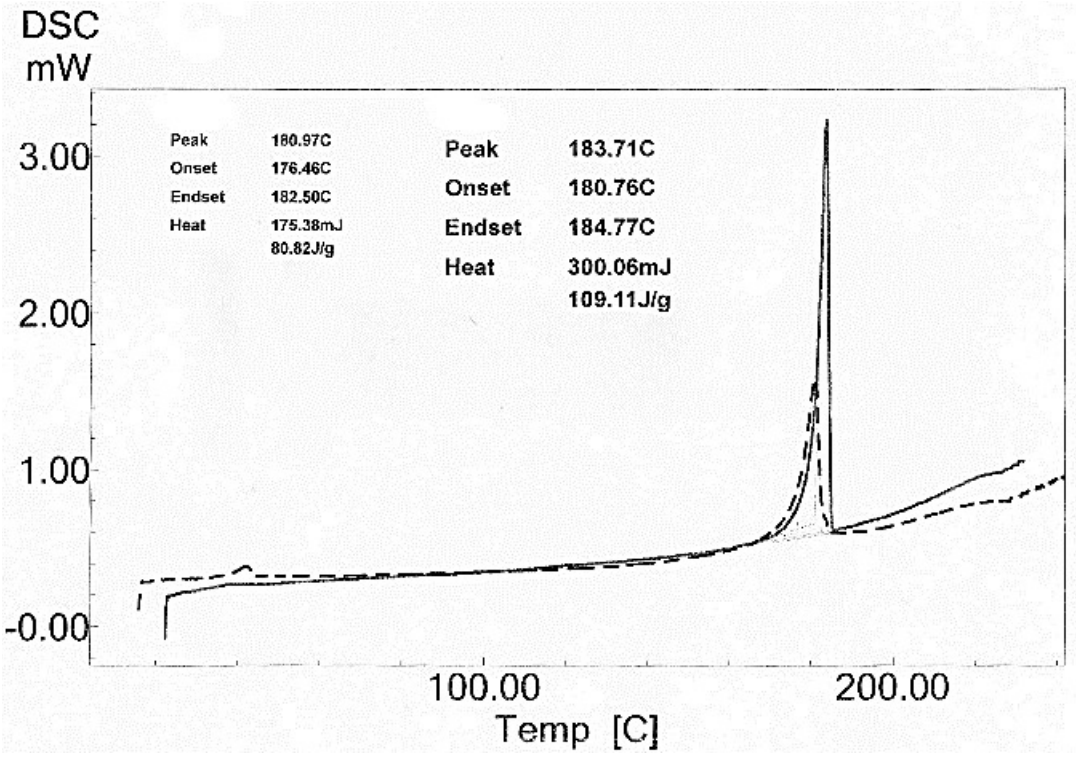
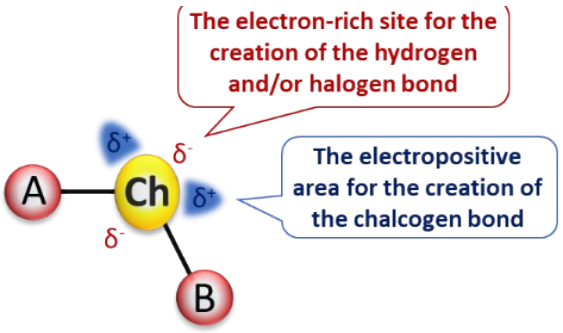


Figure S10. Schematic representation of the electron density around a chalcogen atom.



Ch: O, S, Se, Te, and Po; **A, B**: C, N, etc.

Table S1. Intermolecular interactions geometrical parameters and energies for all of the polymorphs.

Dimers	Energy (kcal.mole^{-1})	Interactions	B*···A (Å)	D···A (Å)	<D-B*···A	Symmetry operation
			***P*$_{bca}$**			
Dimer 1I-SR	-7.55	$Cg_{thia}\cdots Cg_{pz}$	3.683	-	9	-
Dimer 2I-SI	-7.47	$N_1\cdots N_6\text{-}H_{6n}$	2.4278(4)	3.1125(5)	161	-0.5+x, 2.5-y, 1-z
Dimer 2I-SI	-7.47	$N_5\cdots N_2\text{-}H_{2n}$	2.2180(3)	3.1128(5)	160	-0.5+x, 2.5-y, 1-z
Dimer 2I-SI	-7.47	$N_7\cdots C_2\text{-}H_2$	2.5719(4)	3.2858(5)	134	-0.5+x, 2.5-y, 1-z
Dimer 2I-SI	-7.47	$N_3\cdots C_{10}\text{-}H_{10}$	2.5404(4)	3.2059(4)	129	-0.5+x, 2.5-y, 1-z
Dimer 3I-SI	-5.04	$Cg_{thia}\cdots Cg_{pz}$	3.979	-	10	-
Dimer 3I-SI	-5.04	$Cg_{pz}\cdots C_{12}\text{-}N_6$	3.713	-	11	-
Dimer 4I-SI	-3.37	$O_1\cdots C_{15}\text{-}H_{15}$	2.6183(5)	3.2269(6)	124	x, y, z
Dimer 4I-SI	-3.37	$S_1\cdots C_{15}\text{-}H_{15}$	3.0316(4)	3.9589(6)	174	x, y, z
Dimer 5I-SR	-3.35	$C_{16}\text{-}H_{16}\cdots Cg_{thia}$	3.130	-	173	-
Dimer 6I-SI	-2.94	$C_7\text{-}H_7\cdots O_2$	2.6636(5)	3.3367(5)	130	x, 2.5-y, 0.5+z
Dimer 6I-SI	-2.94	$C_7\text{-}H_7\cdots S_2$	3.0291(4)	3.9570(6)	175	x, 2.5-y, -0.5+z
Dimer 7I-SR	-1.60	$C_{11}\text{-}H_{11}\cdots N_8$	2.5538(4)	3.4139(5)	154	0.5+x, y, 0.5-z
Dimer 8I-SR	-1.47	$C_3\text{-}H_3\cdots N_4$	2.4620(3)	3.3707(5)	166	-0.5+x, 2.5-y, 1-z
			P*2$_1$/*c			
Dimer 1II-SR	-6.96	$C_8\text{-}H_8\cdots N_3$	2.6056(4)	3.2409(6)		-x, 0.5+y, 1.5-z
Dimer 1II-SR	-6.96	$C_7\text{-}H_7\cdots N_1$	2.5082(4)	3.2262(7)		-x, 0.5+y, 1.5-z
Dimer 1II-SR	-6.96	$N_2\text{-}H_{2n}\cdots N_4$	2.1869(3)	3.0065(5)		-x, -0.5+y, 1.5-z
Dimer 2II-SR	-6.80	$C_{15}\text{-}H_{15}\cdots N_5$	2.5783(4)	3.2701(5)		1-x, 0.5+y, 1.5-z
Dimer 2II-SR	-6.80	$C_{16}\text{-}H_{16}\cdots N_7$	2.5674(4)	3.2105(6)		1-x, 0.5+y, 1.5-z
Dimer 2II-SR	-6.80	$N_6\text{-}H_{6n}\cdots N_8$	2.2020(3)	3.0195(5)	159	1-x, -0.5+y, 1.5-z
Dimer 3II-SR	-6.74	$C_4\text{-}N_2\cdots Cg_{pz}$	4.485	-	17	-
Dimer 4II-SR	-6.17	$C_{12}\text{-}N_6\cdots Cg_{pz}$	4.730	-	14	-
Dimer 5II-SR	-5.42	$C_4\text{-}N_2\cdots Cg_{thia}$	3.322	-	7	-
Dimer 6II-SR	-4.91	$C_{12}\text{-}N_6\cdots Cg_{thia}$	3.452	-	7	-
Dimer 7II-SR	-2.49	$Cg_{pz}\cdots Cg_{pz}$	3.820	-	0	-
Dimer 8II-SI	-1.25	$C_9\text{-}S_2\cdots S_1$	3.7431(6)	4.8648(8)	121	x, 1.5-y, 0.5+z
Dimer 8II-SI	-1.25	$C_{12}\text{-}O_2\cdots S_1$	3.5139(8)	4.4799(8)	138	x, 1.5-y, 0.5+z
Dimer 9II-SI	-0.86	$C_{10}\text{-}H_{10}\cdots S_1$	2.8838(4)	3.7915(6)	165	x, y, z
Dimer 9II-SI	-0.86	$C_{10}\text{-}H_{10}\cdots O_1$	2.6040(5)	3.3281(5)	135	x, y, z
			***P*2$_1$**			
Dimer 1III-SI	-7.42	$C_7\text{-}H_7\cdots N_5$	2.5649(1)	3.2451(1)	129	x, y, z
Dimer 1III-SI	-7.42	$C_8\text{-}H_8\cdots N_7$	2.4755(1)	3.1649(1)	129	x, y, z
Dimer 1III-SI	-7.42	$N_6\text{-}H_{6n}\cdots N_4$	2.1231(1)	2.9684(1)	161	x, y, z
Dimer 2III-SR	-6.20	$C_4\text{-}N_2\cdots Cg_{pz}$	3.578	-	6	-
Dimer 2III-SR	-6.20	$C_4\text{-}N_2\cdots Cg_{thia}$	3.710	-	4	-
Dimer 3III-SI	-3.75	$Cg_{thia}\cdots Cg_{pz}$	3.698	-	7	-
Dimer 4III-SR	-3.15	$C_9\text{-}S_2\cdots S_2$	3.7627(1)	4.0522(2)	162	-1-x, 0.5+y, -1-z
Dimer 4III-SR	-3.15	$C_9\text{-}S_2\cdots O_2$	3.3108(2)	4.5265(2)	152	-1-x, -0.5+y, -1-z
Dimer 5III-SR	-2.41	$C_1\text{-}S_1\cdots S_1$	3.6940(1)	4.9677(2)	135	-1-x, -0.5+y, -z
Dimer 5III-SR	-2.41	$C_1\text{-}S_1\cdots O_1$	3.2786(2)	4.9597(3)	162	-1-x, -0.5+y, -z
Dimer 6III-SR	-1.22	$C_2\text{-}H_2\cdots Cg_{thia}$	3.534	-	141	-

B: H (for hydrogen bond), S (for chalcogen bond), N (for amide···π), and Cg (for π···π interaction).

Table S2. Intramolecular interactions geometrical parameters in **I**, **II**, and **III**.

Polymorph	Interactions	B*···A (Å)	<D-B···A (°)
I			
	C_3-S_1…O_1	2.6532 (5)	164.280 (13)
	C_{11}-S_2…O_2	2.6562 (5)	162.858 (13)
	N_2-H_{2n}…N_3	2.3770 (4)	102.595 (15)
	N_6-H_{6n}…N_7	2.5043 (4)	103.391 (19)
II			
	C_3-S_1…O_1	2.7037 (7)	161.786 (9)
	C_{11}-S_2…O_2	2.7000 (5)	162.251 (11)
	N_2-H_{2n}…N_3	2.3831 (7)	106.158 (15)
	N_6-H_{6n}…N_7	2.3514 (5)	107.617 (19)
III			
	C_3-S_1…O_1	2.7168 (1)	162.028 (2)
	C_{11}-S_2…O_2	2.6987 (2)	162.356 (3)
	N_2-H_{2n}…N_3	2.3813 (1)	106.383 (4)
	N_6-H_{6n}…N_7	2.3914 (1)	106.295 (4)

B: H (for hydrogen bond) and S (for chalcogen bond)

Table S3. The results of CSD-study.

- **i. Compound**
- **ii. Number of polymorphs**
- **iii. Ref code**
- **iv. Polymorphs**
- **v. Ref. Number**
- **vi. Space group**
- **vii. Z'**
- **viii. Number of rmsd**
- **ix. Involved Polymorphs in rmsd-[r]-crystal Calculation**
- **x. Max rmsd-[r]-crystal**

i	ii	iii	iv	v	vi	vii	viii	ix	x
1	2	ABIZAP	1	ABIZAP 00	$P\bar{1}$	2	1	ABIZAP 00-01	0.0599
			2	ABIZAP 01	$P2_1/n$	2			
2	2	AHADAQ	3	AHADAQ 00	$P1$	4	2	AHADAQ 00-01	0.0976
			4	AHADAQ 01	$Fdd2$	2			
3	2	AHEGEZ	5	AHEGEZ 00	$P2_1/n$	2	3	AHEGEZ 00-01	0.3204
			6	AHEGEZ 01	$P\bar{1}$	2			
4	2	AMUQOQ	7	AMUQOQ 00	$P2_1$	2	4	AMUQOQ 00-01	0.2084
			8	AMUQOQ 01	$P2_12_12_1$	2			
5	3	ANONEX	9	ANONEX 00	$P1$	2	5	ANONEX 00-01	0.4100
			10	ANONEX 01	$P1$	2	6	ANONEX 00-02	0.6807
			11	ANONEX 02	$P1$	2	7	ANONEX 01-02	0.6792
6	2	ASITEC	12	ASITEC 00	$Pbca$	3	8	ASITEC 00-01	2.3474
			13	ASITEC 01	$P2_1/c$	2			
7	2	AWICEQ	14	AWICEQ 00	$P2_1/n$	2	9	AWICEQ 00 - 01	0.0489
			15	AWICEQ 01	$P2_1/n$	2			
8	2	AZESEE	16	AZESEE 00	$P2_1/c$	2	10	AZESEE 00-01	0.5329
			17	AZESEE 01	$P2_1/n$	2			
9	2	BAJYIU	18	BAJYIU 01	$P\bar{1}$	2	11	BAJYIU 01-02	0.0235
			19	BAJYIU 02	$P\bar{1}$	2			
10	2	BEDVAK	20	BEDVAK 00	$P\bar{1}$	4	12	BEDVAK 00-01	0.4690
			21	BEDVAK 01	$P\bar{1}$	2			
11	2	BEDVEO	22	BEDVEO 00	$P\bar{1}$	4	13	BEDVEO 00-01	0.4765
			23	BEDVEO 01	$P\bar{1}$	2			
12	4	BENZIE	24	BENZIE 01	$P\bar{1}$	3	14	BENZIE 01-02	0.2546
			25	BENZIE 02	$P2_1/c$	1.5	15	BENZIE 01-03	0.3197
			26	BENZIE 03	$P2_1/n$	4.5	16	BENZIE 01-04	0.2664
			27	BENZIE 04		4.5	17	BENZIE 02-03	0.3542

					$P2_1/n$		18	BENZIE 02-04	0.3007
							19	BENZIE 03-04	0.3536
13	2	BETJAL	28	BETJAL 00	$P\bar{1}$	2	20	BETJAL 00-01	1.0126
			29	BETJAL 01	$P\bar{1}$	2			
14	2	BUFNEV	30	BUFNEV 00	$P\bar{1}$	2	21	BUFNEV 00 - 01	0.1030
			31	BUFNEV 01	$P\bar{1}$	2			
15	2	BIPCOS	32	BIPCOS 00	$P4_12_12$	4	22	BIPCOS 00-01	0.1225
			33	BIPCOS 01	$P1$	8			
16	2	CARZIF	34	CARZIF 03	Pn	8	23	CARZIF 03 - 07	0.8406
			35	CARZIF 07	$P2_12_12_1$	2			
17	2	CHOLEC	36	CHOLEC 01	$P2_1$	2	24	CHOLEC 01-03	0.6340
			37	CHOLEC 03	$P2_1$	4			
18	2	CLPHOL	38	CLPHOL 12	$P2_1/c$	2	25	CLPHOL 12-13	0.0100
			39	CLPHOL 13	$P2_1/c$	2			
19	2	CRESOL	40	CRESOL 01	$P2_1/c$	2	26	CRESOL 01-02	0.0321
			41	CRESOL 02	$C2/c$	3			
20	2	CUKHUM	42	CUKHUM 00	$Pbca$	2	27	CUKHUM 00-01	0.3304
			43	CUKHUM 01	$P2_1/c$	4			
21	2	CUNKUS	44	CUNKUS 00	$P2_1/n$	2	28	CUNKUS 00-01	0.7978
			45	CUNKUS 01	$P\bar{1}$	6			
22	2	CYACAC	46	CYACAC 00	$P\bar{1}$	2	29	CYACAC 00-01	0.0604
			47	CYACAC 01	$P2_1/c$	3			
23	2	DCLNAP	48	DCLNAP 01	$Pb2_1a$	2	30	DCLNAP 01-02	0.0324
			49	DCLNAP 02	$P\bar{1}$	2			
24	2	DOKNOI	50	DOKNOI 00	$Pca2_1$	2	31	DOKNOI 00-01	0.6188
			51	DOKNOI 01	$P\bar{1}$	2			
25	2	DOVGEC	52	DOVGEC 00	$P2_1$	2	32	DOVGEC 00-01	0.8815
			53	DOVGEC 01	$P2_1$	2			
26	2	DPGUAN	54	DPGUAN 00	$P112_1/b$	2	33	DPGUAN 00-01	0.2150
			55	DPGUAN 01	$P2_12_12_1$	2			
27	2	DUQJOP	56	DUQJOP 00	$P2_1$	4	34	DUQJOP 00-01	0.823
			57	DUQJOP 01	$P2_1/n$	2			
28	2	DUXSUK	58	DUXSUK 00	$P2_1/c$	3	35	DUXSUK 00-05	0.0640
			59	DUXSUK 05	$P2_1/c$	3			
29	2	EBIDUP	60	EBIDUP 01	$P2_1/n$	4	36	EBIDUP 00 - 01	0.5103
			61	EBIDUP 00	$P2_1/c$	2			
30	2	EPOPDO	62	EPOPDO 00	$P2_1/c$	2	37	EPOPDO 00-01	0.0312
			63	EPOPDO 01	$P2_1/c$	2			
31	2	EVAZEG	64	EVAZEG 00	$C2/c$	2	38	EVAZEG 00-01	0.8580
			65	EVAZEG 01	$P2_1/n$	2			
32	2	EWAMAR	66	EWAMAR 00	$I\bar{4}$	2	39	EWAMAR 00-01	0.0415
			67	EWAMAR 01	$P2_12_12_1$	8			
33	2	EWAZOT	68	EWAZOT 00	$P\bar{1}$	2	40	EWAZOT 00-01	0.4299
			69	EWAZOT 01	$P\bar{1}$	2			
34	2	FACCOB	70	FACCOB 01	$P2_1/b11$	2	41	FACCOB 01-02	0.0724
			71	FACCOB 02	$P2_1/c$	3			
35	2	FEGHAA	72	FEGHAA 06	$P2_1$	2	42	FEGHAA 06-07	0.7573
			73	FEGHAA 07	$P2_1$	2			
36	2	FEXRIK	74	FEXRIK 00	$P2_1$	2	43	FEXRIK 00-01	0.2831
			75	FEXRIK 01	$P\bar{1}$	4			
37	2	FIHNUH	76	FIHNUH 00	$P2_1$	2	44	FIHNUH 00-01	0.3109
			77	FIHNUH 01	$P2_1/c$	2			
38	2	FINQIF	78	FINQIF 00	$P2_1$	4	45	FINQIF 00-01	0.1476
			79	FINQIF 01	$P\bar{1}$	3			
39	2	GADSIO	80	GADSIO 00	$P2_1/c$	2	46	GADSIO 00-01	0.1106
			81	GADSIO 01	$P2_1/n$	2			
40	2	GINKIZ	82	GINKIZ 00	$P2_1/c$	2	47	GINKIZ 00-01	0.7377
			83	GINKIZ 01	$P\bar{1}$	2			
41	2	GOCJIT	84	GOCJIT 00	$P2_1$	2	48	GOCJIT 00-01	0.5086
			85	GOCJIT 01	$P2_1/n$	3			
42	2	GUJNAA	86	GUJNAA 00	$P2_1$	2	49	GUJNAA 00-01	0.2550
			87	GUJNAA 01	$P\bar{1}$	3			
43	2	GUMXAO	88	GUMXAO 00	$P2_1/c$	2	50	GUMXAO 00-02	0.5164
			89	GUMXAO 02	$P\bar{1}$	2			
44	2	HIRYIR	90	HIRYIR 00	$P2_1/c$	2	51	HIRYIR 00-01	0.1920
			91	HIRYIR 01	$C2/c$	2			
45	2	HUDHUK	92	HUDHUK 00	Cc	2	52	HUDHUK 00-01	0.2128
			93	HUDHUK 01	$P\bar{1}$	2			

46	2	HUKHUQ	94	HUKHUQ 00	$P2_1/n$	6	53	HUKHUQ 00 - 01	0.8252
			95	HUKHUQ 01	$P2_1/c$	2			
47	2	IBIJAF	96	IBIJAF 00	$I2/a$	2	54	IBIJAF 00-01	0.1627
			97	IBIJAF 01	$P1$	4			
48	2	IDOBAG	98	IDOBAG 00	$P\bar{1}$	3	55	IDOBAG 00-01	0.8226
			99	IDOBAG 01	$P2_1/c$	2			
49	2	ISAZOS	100	ISAZOS 00	$C2/c$	3	56	ISAZOS 00 - 01	0.8536
			101	ISAZOS 01	$C2/c$	3			
50	2	ISUNAL	102	ISUNAL 00	$P\bar{1}$	2	57	ISUNAL 00-01	0.4994
			103	ISUNAL 01	$P2_1/c$	2			
51	2	JECXOH	104	JECXOH 00	$P2_1/c$	2	58	JECXOH 00	0.4708
			105	JECXOH 01	$P\bar{1}$	2			
52	2	JETLEA	106	JETLEA 00	$Pca2_1$	2	59	JETLEA 00-01	0.0965
			107	JETLEA 01	$P2_1$	2			
53	2	JIMVUW	108	JIMVUW 00	$P2_1$	2	60	JIMVUW 00-01	0.0320
			109	JIMVUW 01	$P2_1/a$	2			
54	2	JOWPAO	110	JOWPAO 00	$P\bar{1}$	2	61	JOWPAO 00-01	0.3305
			111	JOWPAO 01	$Pbc2_1$	2			
55	2	KAMCOQ	112	KAMCOQ 00	$P2_1/c$	2	62	KAMCOQ 00-01	0.7557
			113	KAMCOQ 01	$P\bar{1}$	2			
56	2	KASSOM	114	KASSOM 00	$P2_1/a$	2	63	KASSOM 00-01	0.6712
			115	KASSOM 01	$P\bar{1}$	2			
57	4	KELNIA	116	KELNIA 00	$P2_1$	2	64	KELNIA 00-01	1.0228
			117	KELNIA 01	P1	2	65	KELNIA 00-06	1.0569
			118	KELNIA 06	$P2_1$	2	66	KELNIA 00-07	1.0443
			119	KELNIA 07	$P1$	2	67	KELNIA 01-06	1.0681
							68	KELNIA 01-07	1.0556
							69	KELNIA 06-07	1.0170
58	2	KETDUI	120	KETDUI 00	$P2_1$	2	70	KETDUI 00-01	0.6453
			121	KETDUI 01	$P2_12_12_1$	2			
59	2	KUCYOY	122	KUCYOY 00	$P2_1$	2	71	KUCYOY 00-01	1.0953
			123	KUCYOY 01	$P2_1$	2			
60	2	KUPMUE	124	KUPMUE 00	$P\bar{1}$	4	72	KUPMUE 00-01	0.1134
			125	KUPMUE 01	$P2_1$	4			
61	2	LAFKAE	126	LAFKAE 00	$P\bar{1}$	2	73	LAFKAE 00-01	0.0596
			127	LAFKAE 01	$P\bar{1}$	2			
62	2	LAJZON	128	LAJZON 00	$P2_1/c$	2	74	LAJZON 00-01	0.0891
			129	LAJZON 01	$P2_1/n$	2			
63	2	LEQPIH	130	LEQPIH 00	$P2_1$	2	75	LEQPIH 00-01	0.1496
			131	LEQPIH 01	$P\bar{1}$	2			
64	2	LEZPAH	132	LEZPAH 00	$Pca2_1$	2	76	LEZPAH 00-01	0.1127
			133	LEZPAH 01	$P2_1/c$	2			
65	2	LISLEU	134	LISLEU 02	$P2_1$	2	77	LISLEU 02-03	0.9306
			135	LISLEU 03	$P2_1$	4			
66	2	LOQQEN	136	LOQQEN 00	$P\bar{1}$	2	78	LOQQEN 00-01	0.0236
			137	LOQQEN 01	$P2_1$	2			
67	2	LUKXAQ	138	LUKXAQ 00	$P2_1$	2	79	LUKXAQ 00-01	0.3205
			139	LUKXAQ 01	$P2_1$	2			
68	2	MEDLUE	140	MEDLUE 00	$Pbca$	2	80	MEDLUE 00-01	0.1294
			141	MEDLUE 01	$P2_1/n$	2			
69	2	MELXEG	142	MELXEG 00	$P2_1$	3	81	MELXEG 00-01	1.3333
			143	MELXEG 01	$P2_12_12_1$	2			
70	2	MERHOG	144	MERHOG 00	$P2_12_12$	2	82	MERHOG 00-01	0.5113
			145	MERHOG 01	$C2$	2			
71	2	MOKYER	146	MOKYER 00	$C2/c$	2	83	MOKYER 00-01	0.0092
			147	MOKYER 01	$Pbca$	2			
72	2	MOVXIF	148	MOVXIF 00	$P\bar{1}$	4	84	MOVXIF 00-01	0.3518
			149	MOVXIF 01	$P\bar{1}$	2			
73	2	NAKQOG	150	NAKQOG 00	$P2_1/c$	2	85	NAKQOG 00-01	0.0386
			151	NAKQOG 01	$Pna2_1$	2			
74	2	NEMLOG	152	NEMLOG 00	$P2_1/n$	2	86	NEMLOG 00-02	1.2661
			153	NEMLOG 02	$P2_1/c$	2			
75	3	NENNUP	154	NENNUP 01	$P\bar{1}$	2	87	NENNUP 01-02	0.1281
			155	NENNUP 02	$P2_1/c$	2			
76	4	NIMRIK	156	NIMRIK 01	$P\bar{1}$	3	88	NIMRIK 01-08	0.0955
			157	NIMRIK 08	$C2/c$	6			
77	2	OBARIV	158	OBARIV 00	$P2_1$	4	89	OBARIV 00-01	1.1009
			159	OBARIV 01	$P1$	2	90	OBARIV 00-04	0.5715

			160	OBARIV 04	$P1$	4	91	OBARIV 01-04	1.0518
78	2	ONITAN	161	ONITAN 02	$P2_1/n$	2	92	ONITAN 02-03	0.0418
			162	ONITAN 03	$P2_1/c$	2			
79	2	PAMTAY	163	PAMTAY 00	$P\bar{1}$	3	93	PAMTAY 00-01	0.1199
			164	PAMTAY 01	$P6_1$	3			
80	2	PEJCAJ	165	PEJCAJ 00	$P2_1/c$	2	94	PEJCAJ 00-01	0.2495
			166	PEJCAJ 01	$P2_1/n$	2			
81	2	PILRAG	167	PILRAG 00	$Pna21$	2	95	PILRAG 00-01	0.0699
			168	PILRAG 01	$P2_1/c$	2			
82	2	PINCOL	169	PINCOL 01	$P6_5$	2	96	PINCOL 01-02	1.1804
			170	PINCOL 02	$C2/c$	3			
83	2	PODQIJ	171	PODQIJ 00	$C2/c$	2	97	PODQIJ 00-01	0.5350
			172	PODQIJ 01	Cc	2			
84	2	PUVVUX	173	PUVVUX 00	$P2_1/a$	2	98	PUVVUX 00-01	0.0266
			174	PUVVUX 01	$Pca2_1$	2			
85	2	PYDSYD	175	PYDSYD 10	P2/c	2	99	PYDSYD 10-11	0.0807
			176	PYDSYD 11	$P2_1/c$	2			
86	2	QIDVII	177	QIDVII 00	$P\bar{1}$	2	100	QIDVII 00-01	1.4472
			178	QIDVII 01	$P2_12_12_1$	2			
87	2	QIJTOS	179	QIJTOS 00	$P2_1$	2	101	QIJTOS 00-01	0.5401
			180	QIJTOS 01	$P2_1$	2			
88	2	QIXZAY	181	QIXZAY 02	$P2_1/n$	2	102	QIXZAY 02-03	0.0760
			182	QIXZAY 03	$P2_1/c$	2			
89	2	QUBPIN	183	QUBPIN 00	$P1$	2	103	QUBPIN 00-02	0.0517
			184	QUBPIN 02	$P1$	2			
90	3	QUZREJ	185	QUZREJ 00	$P\bar{1}$	2	104	QUZREJ 00-02	0.2302
			186	QUZREJ 02	$P\bar{1}$	2	105	QUZREJ 00-03	0.2522
			187	QUZREJ 03	$P\bar{1}$	2	106	QUZREJ 02-03	0.2050
91	2	REKJOH	188	REKJOH 00	$P2_1$	8	107	REKJOH 00-01	0.0733
			189	REKJOH 01	$P2_1/c$	4			
92	3	REZQOF	190	REZQOF 00	$P2_1$	3	108	REZQOF 00-02	0.1006
			191	REZQOF 02	$P\bar{1}$	6	109	REZQOF 00-03	0.0807
			192	REZQOF 03	$P2_1/c$	3	110	REZQOF 02-03	0.0840
93	2	RIFMUQ	193	RIFMUQ 00	$P2_1$	2	111	RIFMUQ 00-01	0.1031
			194	RIFMUQ 01	$P2_1$	2			
94	2	RITBED	195	RITBED 00	$P\bar{1}$	2	112	RITBED 00-01	0.4595
			196	RITBED 01	$P2_1/c$	2			
95	2	RIVFAE	197	RIVFAE 00	$P\bar{1}$	3	113	RIVFAE 00-01	0.3375
			198	RIVFAE 01	$P\bar{1}$	2			
96	2	ROFVAK	199	ROFVAK 00	$P2_1/c$	2	114	ROFVAK 00-01	0.1148
			200	ROFVAK 01	$P\bar{1}$	2			
97	2	SAPVAI	201	SAPVAI 00	$P2_1$	4	115	SAPVAI 00-01	0.3889
			202	SAPVAI 01	$P2_12_12_1$	2			
98	2	SIDHOD	203	SIDHOD 00	$Pca2_1$	2	116	SIDHOD 00-01	0.2381
			204	SIDHOD 01	$P2_1/c$	2			
99	3	SOBPEE	205	SOBPEE 00	$P\bar{1}$	2	117	SOBPEE 00-01	0.1248
			206	SOBPEE 01	$P\bar{1}$	2	118	SOBPEE 00-02	0.2843
			207	SOBPEE 02	$P\bar{1}$	2	119	SOBPEE 01-02	0.2638
100	2	SOBSUX	208	SOBSUX 00	$I4_1/a$	2	120	SOBSUX 00-01	0.1312
			209	SOBSUX 01	$P2_1/n$	2			
101	2	SUZYES	210	SUZYES 00	$P2_1/c$	2	121	SUZYES 00-01	0.3091
			211	SUZYES 01	$P2_1$	4			
102	2	TAJVAC	212	TAJVAC 00	$C2/c$	2	122	TAJVAC 00-01	0.3394
			213	TAJVAC 01	$P\bar{1}$	4			
103	2	TAJVIK	214	TAJVIK 00	$P\bar{3}$	1.17	123	TAJVIK 00-01	0.8570
			215	TAJVIK 01	$P\bar{1}$	2.5			
104	2	TAPZIT	216	TAPZIT 01	Pn	4	124	TAPZIT 01-02	0.0421
			217	TAPZIT 02	$P2_1/c$	2			
105	3	TAWRIT	218	TAWRIT 01	$P\bar{1}$	2	126	TAWRIT 00-02	0.6755
			219	TAWRIT 02	$P2_1/n$	2	127	TAWRIT 01-02	0.1524
106	2	TELRAG	220	TELRAG 00	$P\bar{1}$	2	128	TELRAG 00-02	0.6231
			221	TELRAG 02	$P\bar{1}$	2			
107	2	TEMBES	222	TEMBES 00	$P2_1/c$	3	129	TEMBES 00-01	0.0297
			223	TEMBES 01	$Pca2_1$	2			
108	2	TINBIB	224	TINBIB 00	$P2_12_12_1$	2	130	TINBIB 00-01	0.9332
			225	TINBIB 01	$P2_1$	2			
109	2	TIVXUS	226	TIVXUS 00	$P2_1$	2	131	TIVXUS 00-01	0.0191

			227	TIVXUS 01	$P2_1/n$	2			
110	2	TOLPHO	228	TOLPHO 10	$P2_1/c$	3	132	TOLPHO 10-11	0.1537
			229	TOLPHO 11	$P\bar{1}$	2			
111	2	TPPHSE	230	TPPHSE 01	$P\bar{1}$	2	133	TPPHSE 01-02	0.0507
			231	TPPHSE 02	$P2_1/c$	2			
112	2	UHENUQ	232	UHENUQ 00	$P\bar{1}$	6	134	UHENUQ 00-01	0.2945
			233	UHENUQ 01	$C2/c$	3			
113	2	UNEWIU	234	UNEWIU 00	$P\bar{1}$	4	135	UNEWIU 00-01	0.3719
			235	UNEWIU 01	$P2_1/n$	2			
114	2	UXIZAD	236	UXIZAD 00	Pbca	3	136	UXIZAD 00-01	0.2197
			237	UXIZAD 01	$P2_1/c$	2			
115	2	VAXZIF	238	VAXZIF 00	$C2/c$	2	137	VAXZIF 00-01	0.215
			239	VAXZIF 01	$P\bar{1}$	2			
116	2	VIMJIM	240	VIMJIM 00	$P2_1/c$	2	138	VIMJIM 00-01	0.1697
			241	VIMJIM 01	$P2_1/c$	2			
117	2	VIZHIW	242	VIZHIW 00	$P2_1/n$	2	139	VIZHIW 00-02	0.3463
			243	VIZHIW 01	Cc	1.5			
118	3	VUXZEU	244	VUXZEU 00	$P2_1/c$	2	140	VUXZEU 00-01	0.1989
			245	VUXZEU 01	$P2_1/c$	2	141	VUXZEU 00-02	0.4028
			246	VUXZEU 02	$I4_1/a$	2	142	VUXZEU 01-02	0.2238
119	2	WELHEA	247	WELHEA 01	$P\bar{1}$	2	143	WELHEA 01-02	0.1333
			248	WELHEA 02	$C2/c$	2			
120	2	WITDEK	249	WITDEK 00	$P\bar{1}$	2	144	WITDEK 00-01	0.2242
			250	WITDEK 01	$P\bar{1}$	2			
121	2	XELLOP	251	XELLOP 00	$P\bar{1}$	2	145	XELLOP 00-01	0.0645
			252	XELLOP 01	$P2_1$	3			
122	2	XILQOY	253	XILQOY 00	$P2_1/c$	2	146	XILQOY 00-01	1.4053
			254	XILQOY 01	$P\bar{1}$	2			
123	2	XIMMEL	255	XIMMEL 00	$P2_1$	2	147	XIMMEL 00-01	0.8720
			256	XIMMEL 01	$P2/c$	2			
124	2	XOCFOK	257	XOCFOK 00	$C2/c$	2	148	XOCFOK 00-01	0.2349
			258	XOCFOK 01	$C2/c$	1.5			
125	2	YAJPUV	259	YAJPUV 00	$C2/c$	2	149	YAJPUV 00-02	0.0297
			260	YAJPUV 02	$Pbca$	2			
126	2	YASFIJ	261	YASFIJ 00	$P2_1/n$	2	150	YASFIJ 00 - 01	0.7869
			262	YASFIJ 01	$P2_1/n$	2			
127	2	YAXWAX	263	YAXWAX 00	$P\bar{1}$	3	151	YAXWAX 00-01	0.0305
			264	YAXWAX 01	$P2_1/c$	2			
128	2	YIRXAZ	265	YIRXAZ 00	$P\bar{1}$	2	152	YIRXAZ 00-01	0.7580
			266	YIRXAZ 01	$P\bar{1}$	2			
129	2	YUHTEA	267	YUHTEA 00	$P2_1$	4	153	YUHTEA 00-04	0.0804
			268	YUHTEA 04	$Pna2_1$	4			
130	3	ZZZAUS	269	ZZZAUS 20	$P2_1/c$	3	154	ZZZAUS 20-21	0.1504
			270	ZZZAUS 21	$Pbca$	2	155	ZZZAUS 20-22	0.1866
			271	ZZZAUS 22	$P\bar{1}$	2	156	ZZZAUS 21-22	0.1575
131	2	ZZZJIQ	272	ZZZJIQ 01	$P\bar{1}$	4	157	ZZZJIQ 01-02	0.2090
			273	ZZZJIQ 02	$P2_1/n$	2			
132	2	ZZZMUC	274	ZZZMUC 08	$P2_1/a$	2	158	ZZZMUC 08-09	0.0988
			275	ZZZMUC 09	$Pca2_1$	2			
133	3	ZZZVXQ	276	ZZZVXQ 02	$P3_1$	12	159	ZZZVXQ 02-03	0.3778
			277	ZZZVXQ 03	$P\bar{1}$	6	160	ZZZVXQ 02-04	
			278	ZZZVXQ 04	$P6_5$	3	161	ZZZVXQ 03-04	0.2902