



บทที่ 6

สูตรและวิธีการผลการทดลอง

ผลการวิจัยเพื่อศึกษาโครงสร้างผลึกของกรดไฮเพอร์นิกด้วยวิธีการเลี้ยวเบนรังสีเอ็กซ์ พบว่าข้อมูลผลึกเบื้องต้นที่จะนำไปใช้ในการคำนวณโครงสร้าง หรือตำแหน่งของอะตอมต่าง ๆ ภายในหนึ่งหน่วยเซลล์ของผลึกนั้น ได้รวบรวมไว้ในตารางที่ 6.1

ตารางที่ 6.1 แสดงข้อมูลทั่วไปของผลึกกรดไฮเพอร์นิก

ระบบผลึก	ออร์โทโรมบิก
หมู่สมมาตรสามมิติ	$P_{2_1^2_1^2_1}$
ค่าคงที่โครงผลึก	$a = 8.1244 \pm 0.0019 \text{ \AA}$ $b = 12.3664 \pm 0.0025 \text{ \AA}$ $c = 27.6717 \pm 0.0077 \text{ \AA}$
μ - สัมประสิทธิ์การดูดกลืนตามเส้น สำหรับรังสีเอ็กซ์ชนิด CuK_α	5.69 (ซม.) ⁻¹
D_m - ความหนาแน่นจากการทดลอง หาโดยวิธีการลอยตัวของผลึกใน ของเหลว โดยมีอัตราส่วนของน้ำ: เอริลีนไกลโคลเป็น 0.10:2.90 โดยปริมาตร	1.120 กรัม (ซม.) ⁻³
D_x - ความหนาแน่นจากการคำนวณ	1.119 กรัม (ซม.) ⁻³
z - จำนวนหน่วยสูตรในหนึ่งหน่วยเซลล์	8 หน่วยสูตร/หน่วยเซลล์

หลังจากรวบรวมข้อมูลความเข้มของรังสีเอ็กซ์ CuK_α ($\lambda = 1.5418 \text{ \AA}$) ที่เลี้ยวเบนออกมาจากผลึกด้วยวิธีฟิล์มซ้อนจากวิธีการแบบไวซ์เชินเบอร์เกอร์จำนวน 1414 จุดแล้ว นำไปกำหนดโครงสร้างผลึกพร้อมกับข้อมูลผลึกทั่วไป ตามตารางที่ 6.1 ด้วยวิธีการผลึกวิทยาแบบตรง โดยการใช้โปรแกรม MULTAN 80 การคำนวณโปรแกรมย่อย NORMAL, MULTAN EXFFT และ SEARCH แสดงไว้ในตารางที่ 6.2, 6.3, 6.4 และ 6.5 ตามลำดับ



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

ตารางที่ 6.2 (ก) แสดงการคัด JCL เพื่อคำนวณโดยโปรแกรม NORMAL ในระบบ

OS/VS1

```

1 //ZIADJDDI JOB CLASS=1,MSLEVEL=(1,1),MSDCLASS=A,17PROJ=FOLD
2 //ST1 EXEC PGM=ORTVLC,PARM='LET.LIST'
3 //LKED.SYSPRM1 DD SYSOUT=A
4 //LKED.SYSLIM DD DSN=CLP3.CATALOG(NORMAL),DISP=SHR,UNIT=SYSDA,
5 // VOL=SER=VS1KK3
6 //DD.F10.F01 DD SYSOUT=A
7 //FT02F01 DD UNIT=TAPE,VOL=SER=2550,DISP=(OLD,KEEP),LABEL=(,RL),
8 // DCB=(RECFM=V,LRECL=1790)
9 //FT03F01 DD DSN=0032,UNIT=SYSDA,VOL=SER=VS1KK3,DISP=(,PASS),
10 // SPACE=(TRK,(200,10))
11 //FT04F01 DD DSN=0034,UNIT=SYSDA,VOL=SER=VS1KK3,DISP=(,PASS),
12 // SPACE=(TRK,(40,1))
13 //FT05F01 DD DSN=0039,UNIT=SYSDA,VOL=SER=VS1KK3,DISP=(,PASS),
14 // SPACE=(TRK,(40,1))
15 //DD.SYSIN DD *
16 TITLE *** 1-105 * C1342202 ***
17 CELL 3.124 12.556 27.072 90 90 90
18 CONTENTS C 120 H 176 G 16
19 SYM X,Y,Z * 1/2-X,-Y,1/2+Z * 1/2+X,1/2-Y,-Z * -X,1/2+Y,1/2-Z
20 CARD 1
21 (1(,15,F10.0,13))
22 J 0 8 50.90 0
23 C 0 10 33.13 0
24 0 0 12 37.83 0
25 0 0 16 7.03 0
26 0 0 20 9.87 0
27 0 0 22 10.48 0
28 0 0 24 23.16 0
29 0 0 26 18.66 0
30 0 0 34 6.20 0
31 0 1 6 44.08 0
32 0 1 7 6.44 0
33 0 1 8 35.02 0
34 0 1 9 29.29 0
35 0 1 10 20.26 0
36 0 1 11 13.43 0
37 0 1 12 18.71 0
38 0 1 13 7.50 0
39 0 1 14 10.59 0
40 0 1 15 6.12 0
41 0 1 16 12.84 0
42 0 1 17 21.16 0
43 0 1 18 12.83 0
44 0 1 19 9.34 0
45 0 1 20 10.83 0
46 0 1 21 8.41 0
47 0 1 22 9.27 0
48 0 1 23 12.95 0
49 0 1 24 7.11 0
50 0 1 25 12.85 0
51 0 1 27 12.10 0
52 0 1 28 3.64 0
53 0 1 29 7.99 0
54 0 1 30 6.55 0
55 0 1 33 5.92 0
56 0 2 4 34.19 0
57 0 2 5 34.80 0

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58	0	2	6	104.85	0	115	0	4	9	9.85	0
59	0	2	7	24.10	0	116	0	4	10	21.07	0
60	0	2	8	29.25	0	117	0	4	11	21.61	0
61	0	2	9	6.87	0	118	0	4	12	5.82	0
62	0	2	10	30.52	0	119	0	4	13	7.31	0
63	0	2	11	6.29	0	120	0	4	14	9.46	0
64	0	2	12	5.19	0	121	0	4	16	10.41	0
65	0	2	13	7.52	0	122	0	4	18	12.46	0
66	0	2	14	17.42	0	123	0	4	19	13.37	0
67	0	2	15	20.96	0	124	0	4	20	10.47	0
68	0	2	16	9.29	0	125	0	4	21	5.35	0
69	0	2	17	6.93	0	126	0	4	22	5.91	0
70	0	2	18	15.83	0	127	0	4	23	11.26	0
71	0	2	19	8.71	0	128	0	4	28	7.39	0
72	0	2	20	9.01	0	129	0	4	29	6.53	0
73	0	2	21	7.38	0	130	0	4	33	5.70	0
74	0	2	22	12.61	0	131	0	5	1	64.13	0
75	0	2	23	19.39	0	132	0	5	2	4.80	0
76	0	2	24	11.23	0	133	0	5	3	4.99	0
77	0	2	26	7.82	0	134	0	5	4	38.43	0
78	0	2	27	10.15	0	135	0	5	5	93.98	0
79	0	2	28	14.80	0	136	0	5	6	29.00	0
80	0	2	32	6.42	0	137	0	5	7	5.70	0
81	0	3	2	61.90	0	138	0	5	8	57.58	0
82	0	3	3	80.43	0	139	0	5	9	43.67	0
83	0	3	4	24.19	0	140	0	5	10	17.91	0
84	0	3	5	49.27	0	141	0	5	12	16.09	0
85	0	3	6	39.14	0	142	0	5	13	4.43	0
86	0	3	7	28.71	0	143	0	5	14	15.97	0
87	0	3	8	14.24	0	144	0	5	15	23.11	0
88	0	3	9	46.83	0	145	0	5	17	15.35	0
89	0	3	10	37.05	0	146	0	5	18	20.13	0
90	0	3	11	31.69	0	147	0	5	19	25.18	0
91	0	3	12	4.11	0	148	0	5	20	10.21	0
92	0	3	13	17.47	0	149	0	5	21	25.57	0
93	0	3	15	6.13	0	150	0	5	23	8.85	0
94	0	3	16	8.93	0	151	0	5	25	8.42	0
95	0	3	17	11.97	0	152	0	5	28	5.76	0
96	0	3	18	12.06	0	153	0	5	30	7.13	0
97	0	3	19	28.69	0	154	0	6	1	12.13	0
98	0	3	20	10.47	0	155	0	6	2	4.27	0
99	0	3	21	27.52	0	156	0	6	3	19.84	0
100	0	3	22	8.38	0	157	0	6	4	10.99	0
101	0	3	23	16.66	0	158	0	6	5	36.26	0
102	0	3	24	14.08	0	159	0	6	8	15.73	0
103	0	3	26	11.87	0	160	0	6	9	22.82	0
104	0	3	27	16.66	0	161	0	6	12	18.46	0
105	0	3	30	5.70	0	162	0	6	13	15.87	0
106	0	3	34	3.64	0	163	0	6	14	5.82	0
107	0	4	1	11.64	0	164	0	6	15	9.33	0
108	0	4	2	20.78	0	165	0	6	16	8.21	0
109	0	4	3	15.93	0	166	0	6	17	5.68	0
110	0	4	4	12.23	0	167	0	6	18	13.93	0
111	0	4	5	47.50	0	168	0	6	19	16.01	0
112	0	4	6	63.35	0	169	0	6	20	14.68	0
113	0	4	7	52.78	0	170	0	6	21	7.17	0
114	0	4	8	54.69	0	171	0	6	24	5.94	0

172	0	6	25	5.80	0	224	0	9	26	7.31	0
173	0	6	27	10.19	0	230	0	10	1	6.37	0
174	0	7	1	27.83	0	231	0	10	2	5.30	0
175	0	7	2	10.70	0	232	0	10	3	8.00	0
176	0	7	3	16.89	0	233	0	10	4	6.41	0
177	0	7	4	8.90	0	234	0	10	5	12.06	0
178	0	7	5	9.02	0	235	0	10	6	9.66	0
179	0	7	7	12.09	0	236	0	10	7	7.71	0
180	0	7	8	18.13	0	237	0	10	9	18.96	0
181	0	7	9	9.67	0	238	0	10	10	10.32	0
182	0	7	11	31.16	0	239	0	10	11	5.98	0
183	0	7	12	18.65	0	240	0	10	12	8.53	0
184	0	7	13	11.97	0	241	0	10	13	13.11	0
185	0	7	15	11.67	0	242	0	10	14	4.59	0
186	0	7	17	19.40	0	243	0	10	15	5.02	0
187	0	7	18	9.80	0	244	0	10	16	4.14	0
188	0	7	19	14.82	0	245	0	10	17	4.57	0
189	0	7	20	6.00	0	246	0	10	18	10.15	0
190	0	7	21	9.21	0	247	0	10	21	4.52	0
191	0	7	23	4.11	0	248	0	10	23	3.89	0
192	0	7	29	9.27	0	249	0	10	25	6.05	0
193	0	7	30	4.82	0	250	0	10	26	6.14	0
194	0	7	31	3.86	0	251	0	10	27	3.50	0
195	0	8	1	12.26	0	252	0	11	1	7.74	0
196	0	8	2	15.70	0	253	0	11	2	6.24	0
197	0	8	3	12.40	0	254	0	11	3	5.97	0
198	0	8	4	5.06	0	255	0	11	4	9.02	0
199	0	8	6	6.20	0	256	0	11	5	4.60	0
200	0	8	7	7.75	0	257	0	11	6	5.79	0
201	0	8	8	19.88	0	258	0	11	8	6.59	0
202	0	8	9	13.32	0	259	0	11	9	14.13	0
203	0	8	10	7.81	0	260	0	11	10	8.97	0
204	0	8	11	15.35	0	261	0	11	13	8.14	0
205	0	8	13	8.19	0	262	0	11	14	7.91	0
206	0	8	14	6.10	0	263	0	11	16	6.31	0
207	0	8	15	17.64	0	264	0	11	17	7.46	0
208	0	8	16	12.38	0	265	0	11	18	4.40	0
209	0	8	17	5.51	0	266	0	11	24	3.56	0
210	0	8	18	10.68	0	267	0	12	1	4.55	0
211	0	8	19	6.95	0	268	0	12	2	12.39	0
212	0	8	22	6.94	0	269	0	12	3	9.08	0
213	0	8	27	9.80	0	270	0	12	5	8.55	0
214	0	8	28	8.24	0	271	0	12	6	6.19	0
215	0	9	1	18.89	0	272	0	12	7	9.74	0
216	0	9	2	13.56	0	273	0	12	8	6.20	0
217	0	9	3	22.12	0	274	0	12	11	9.86	0
218	0	9	4	6.85	0	275	0	12	13	6.58	0
219	0	9	5	14.52	0	276	0	12	16	6.03	0
220	0	9	6	11.91	0	277	0	12	22	3.58	0
221	0	9	7	14.78	0	278	0	13	3	7.10	0
222	0	9	9	16.03	0	279	0	13	5	9.14	0
223	0	9	10	4.46	0	280	0	13	6	6.85	0
224	0	9	11	12.56	0	281	0	13	10	4.67	0
225	0	9	12	6.50	0	282	0	13	11	6.34	0
226	0	9	14	10.51	0	283	0	13	12	8.43	0
227	0	9	19	6.77	0	284	0	13	13	5.44	0
228	0	9	23	7.89	0	285	0	13	15	8.01	0

286	0	13	19	2.98	0	343	1	1	29	7.55	0
287	0	14	8	9.04	0	344	1	1	30	5.85	0
288	0	14	9	5.94	0	345	1	1	31	6.19	0
289	0	14	11	9.42	0	346	1	1	34	4.75	0
290	0	14	12	5.99	0	347	1	1	35	4.91	0
291	0	14	13	3.52	0	348	1	2	4	52.04	0
292	0	14	15	3.85	0	349	1	2	5	71.34	0
293	0	14	16	4.42	0	350	1	2	6	54.12	0
294	0	15	4	3.58	0	351	1	2	7	49.16	0
295	0	15	5	3.51	0	352	1	2	8	46.01	0
296	0	15	7	5.09	0	353	1	2	9	29.19	0
297	0	15	8	3.76	0	354	1	2	10	44.00	0
298	0	15	10	3.94	0	355	1	2	11	52.73	0
299	0	4	0	42.94	0	356	1	2	12	10.87	0
300	0	6	0	62.99	0	357	1	2	13	29.46	0
301	0	8	0	14.97	0	358	1	2	14	10.48	0
302	0	10	0	21.87	0	359	1	2	15	14.34	0
303	0	12	0	7.08	0	360	1	2	16	23.06	0
304	1	0	6	27.05	0	361	1	2	17	9.81	0
305	1	0	7	45.86	0	362	1	2	18	14.27	0
306	1	0	8	4.06	0	363	1	2	19	12.29	0
307	1	0	9	9.59	0	364	1	2	20	17.75	0
308	1	0	10	14.55	0	365	1	2	21	14.68	0
309	1	0	11	32.05	0	366	1	2	22	12.78	0
310	1	0	12	19.25	0	367	1	2	23	8.99	0
311	1	0	13	15.39	0	368	1	2	24	12.32	0
312	1	0	14	8.68	0	369	1	2	25	7.13	0
313	1	0	17	35.14	0	370	1	2	26	8.74	0
314	1	0	19	5.74	0	371	1	2	29	13.72	0
315	1	0	20	13.70	0	372	1	2	30	6.88	0
316	1	0	23	8.50	0	373	1	3	1	33.91	0
317	1	0	25	13.51	0	374	1	3	2	26.57	0
318	1	0	27	4.97	0	375	1	3	3	24.14	0
319	1	0	28	7.15	0	376	1	3	4	38.25	0
320	1	0	29	8.61	0	377	1	3	5	24.95	0
321	1	0	31	8.54	0	378	1	3	6	36.91	0
322	1	0	33	10.08	0	379	1	3	7	44.99	0
323	1	1	6	47.28	0	380	1	3	8	34.37	0
324	1	1	7	29.79	0	381	1	3	9	24.63	0
325	1	1	8	30.48	0	382	1	3	10	48.14	0
326	1	1	9	16.15	0	383	1	3	11	21.56	0
327	1	1	10	49.30	0	384	1	3	12	21.63	0
328	1	1	11	13.94	0	385	1	3	13	21.10	0
329	1	1	12	29.65	0	386	1	3	14	4.51	0
330	1	1	13	7.87	0	387	1	3	15	28.11	0
331	1	1	14	36.20	0	388	1	3	16	15.83	0
332	1	1	15	15.34	0	389	1	3	17	16.43	0
333	1	1	16	25.74	0	390	1	3	18	17.78	0
334	1	1	17	27.47	0	391	1	3	19	18.36	0
335	1	1	18	16.30	0	392	1	3	20	14.12	0
336	1	1	20	16.51	0	393	1	3	22	12.92	0
337	1	1	21	6.16	0	394	1	3	23	11.50	0
338	1	1	22	10.90	0	395	1	3	24	4.58	0
339	1	1	24	10.09	0	396	1	3	25	16.19	0
340	1	1	25	10.30	0	397	1	3	26	11.13	0
341	1	1	26	11.53	0	398	1	3	27	6.01	0
342	1	1	28	7.13	0	399	1	3	28	6.37	0

400	1	3	29	7.98	0	457	1	6	4	29.98	0
401	1	3	30	7.48	J	458	1	6	5	25.79	J
402	1	3	31	6.84	0	459	1	6	6	21.70	0
403	1	4	1	5.88	0	460	1	6	7	25.46	0
404	1	4	2	51.54	0	461	1	6	8	20.61	J
405	1	4	3	17.70	0	462	1	6	9	15.72	0
406	1	4	4	13.79	0	463	1	6	10	14.77	J
407	1	4	5	27.69	0	464	1	6	11	26.52	J
408	1	4	7	61.93	0	465	1	6	12	10.19	J
409	1	4	8	35.04	0	466	1	6	13	16.04	0
410	1	4	9	35.20	0	467	1	6	14	9.35	0
411	1	4	10	18.72	0	468	1	6	15	11.52	0
412	1	4	11	35.14	0	469	1	6	16	31.59	0
413	1	4	12	28.01	0	470	1	6	18	20.17	0
414	1	4	13	14.78	0	471	1	6	19	22.91	0
415	1	4	14	8.78	0	472	1	6	20	15.13	J
416	1	4	15	24.54	0	473	1	6	21	8.88	0
417	1	4	16	18.50	0	474	1	6	22	8.87	J
418	1	4	17	5.26	0	475	1	6	26	8.95	J
419	1	4	18	16.18	0	476	1	6	28	5.96	0
420	1	4	19	29.83	0	477	1	6	31	4.50	0
421	1	4	20	20.25	0	478	1	7	1	28.99	0
422	1	4	21	11.59	0	479	1	7	2	20.20	0
423	1	4	22	5.42	0	480	1	7	3	10.62	0
424	1	4	23	14.38	0	481	1	7	4	19.62	0
425	1	4	24	17.35	0	482	1	7	5	8.95	0
426	1	4	25	7.08	0	483	1	7	6	9.50	0
427	1	4	26	7.10	0	484	1	7	7	22.05	0
428	1	4	29	6.69	0	485	1	7	8	10.03	J
429	1	4	30	5.72	0	486	1	7	9	17.92	J
430	1	4	32	4.88	0	487	1	7	10	21.74	0
431	1	5	1	30.01	0	488	1	7	11	22.19	0
432	1	5	2	38.05	0	489	1	7	12	14.92	0
433	1	5	3	39.58	0	490	1	7	13	12.94	0
434	1	5	4	14.58	0	491	1	7	14	7.64	0
435	1	5	5	12.43	J	492	1	7	15	13.45	J
436	1	5	6	36.72	0	493	1	7	16	16.81	0
437	1	5	7	11.69	0	494	1	7	17	11.93	0
438	1	5	8	33.50	0	495	1	7	18	10.49	0
439	1	5	9	23.23	0	496	1	7	19	5.97	J
440	1	5	10	25.73	0	497	1	7	20	5.97	0
441	1	5	11	10.73	0	498	1	7	21	7.43	J
442	1	5	12	26.73	0	499	1	7	24	5.52	0
443	1	5	13	19.63	J	500	1	7	25	5.89	J
444	1	5	14	14.85	0	501	1	7	27	5.01	0
445	1	5	17	18.15	0	502	1	7	28	6.92	0
446	1	5	18	23.73	J	503	1	8	1	23.01	0
447	1	5	20	10.82	J	504	1	8	2	8.87	J
448	1	5	21	11.77	0	505	1	8	3	21.33	J
449	1	5	22	16.56	0	506	1	8	4	17.70	J
450	1	5	23	13.18	0	507	1	8	5	12.92	J
451	1	5	24	8.80	0	508	1	8	6	15.21	0
452	1	5	30	7.32	0	509	1	8	7	11.45	0
453	1	5	32	6.05	0	510	1	8	8	14.35	0
454	1	6	1	17.63	0	511	1	8	9	18.32	0
455	1	6	2	33.99	0	512	1	8	10	10.90	0
456	1	6	3	28.32	0	513	1	8	13	10.01	0

514	1	3	14	9.44	0	571	1	11	5	10.78	0
515	1	8	15	8.07	0	572	1	11	7	9.46	0
516	1	8	16	8.80	0	573	1	11	8	10.50	0
517	1	8	17	7.70	0	574	1	11	10	7.73	0
518	1	8	18	13.55	0	575	1	11	11	7.69	0
519	1	8	19	5.96	0	576	1	11	12	10.58	0
520	1	8	21	7.75	0	577	1	11	15	5.57	0
521	1	8	24	7.98	0	578	1	11	17	7.94	0
522	1	8	25	6.28	0	579	1	11	18	6.32	0
523	1	8	26	6.08	0	580	1	11	21	5.65	0
524	1	8	27	10.00	0	581	1	11	24	5.50	0
525	1	8	29	5.12	0	582	1	12	1	8.36	0
526	1	8	30	3.63	0	583	1	12	2	7.63	0
527	1	9	1	9.83	0	584	1	12	5	7.34	0
528	1	9	2	13.42	0	585	1	12	6	9.44	0
529	1	9	3	6.55	0	586	1	12	7	7.12	0
530	1	9	4	6.06	0	587	1	12	8	7.89	0
531	1	9	5	5.53	0	588	1	12	9	6.08	0
532	1	9	6	22.06	0	589	1	12	10	7.26	0
533	1	9	7	18.21	0	590	1	12	11	6.37	0
534	1	9	8	8.08	0	591	1	12	14	5.17	0
535	1	9	9	7.16	0	592	1	12	15	5.95	0
536	1	9	10	12.01	0	593	1	12	16	6.23	0
537	1	9	12	13.36	0	594	1	13	2	5.30	0
538	1	9	13	13.12	0	595	1	13	3	5.45	0
539	1	9	14	6.57	0	596	1	13	4	6.77	0
540	1	9	15	5.06	0	597	1	13	5	5.12	0
541	1	9	16	7.82	0	598	1	13	6	8.27	0
542	1	9	17	8.72	0	599	1	13	7	5.59	0
543	1	9	20	7.22	0	600	1	13	11	5.12	0
544	1	9	21	6.16	0	601	1	13	12	6.13	0
545	1	9	23	7.24	0	602	1	13	13	5.64	0
546	1	9	25	5.10	0	603	1	13	14	5.25	0
547	1	9	28	7.46	0	604	1	13	17	5.05	0
548	1	10	1	10.93	0	605	1	13	18	6.15	0
549	1	10	2	15.31	0	606	1	3	0	17.24	0
550	1	10	3	8.62	0	607	1	5	0	44.27	0
551	1	10	4	12.86	0	608	1	6	0	12.64	0
552	1	10	5	21.63	0	609	1	7	0	20.00	0
553	1	10	6	10.24	0	610	1	8	0	28.48	0
554	1	10	7	10.64	0	611	1	10	0	22.32	0
555	1	10	8	7.95	0	612	1	11	0	18.04	0
556	1	10	9	9.88	0	613	2	0	6	20.58	0
557	1	10	11	12.37	0	614	2	0	7	49.22	0
558	1	10	12	10.32	0	615	2	0	8	27.62	0
559	1	10	13	6.22	0	616	2	0	9	14.31	0
560	1	10	14	6.54	0	617	2	0	10	17.91	0
561	1	10	17	5.98	0	618	2	0	11	15.08	0
562	1	10	18	6.02	0	619	2	0	12	37.42	0
563	1	10	21	7.18	0	620	2	0	13	40.35	0
564	1	10	22	10.88	0	621	2	0	14	18.40	0
565	1	10	25	4.65	0	622	2	0	15	14.19	0
566	1	10	27	3.64	0	623	2	0	16	13.92	0
567	1	11	1	14.67	0	624	2	0	17	6.88	0
568	1	11	2	7.13	0	625	2	0	18	26.17	0
569	1	11	3	15.77	0	626	2	0	19	10.58	0
570	1	11	4	7.80	0	627	2	0	20	15.25	0

628	2	0	21	13.67	0	685	2	3	5	29.44	0
629	2	0	24	4.97	0	686	2	3	6	13.09	0
630	2	0	25	8.42	0	687	2	3	7	21.06	0
631	2	0	26	8.61	0	688	2	3	8	10.49	0
632	2	0	29	9.50	0	689	2	3	9	74.15	0
633	2	0	30	6.22	0	690	2	3	10	21.97	0
634	2	0	32	7.37	0	691	2	3	11	22.98	0
635	2	1	6	25.56	0	692	2	3	12	12.84	0
636	2	1	7	21.77	0	693	2	3	13	10.43	0
637	2	1	8	32.77	0	694	2	3	14	22.00	0
638	2	1	9	17.99	0	695	2	3	15	6.80	0
639	2	1	10	17.81	0	696	2	3	16	8.02	0
640	2	1	11	17.07	0	697	2	3	17	11.78	0
641	2	1	12	19.66	0	698	2	3	18	8.37	0
642	2	1	13	10.50	0	699	2	3	19	11.79	0
643	2	1	14	34.37	0	700	2	3	20	3.96	0
644	2	1	15	26.78	0	701	2	3	21	4.64	0
645	2	1	16	11.26	0	702	2	3	22	14.88	0
646	2	1	17	5.40	0	703	2	3	23	9.09	0
647	2	1	18	5.83	0	704	2	3	26	10.82	0
648	2	1	19	11.61	0	705	2	3	27	10.16	0
649	2	1	20	12.81	0	706	2	3	33	5.95	0
650	2	1	24	5.39	0	707	2	4	1	22.02	0
651	2	1	26	9.64	0	708	2	4	2	17.93	0
652	2	1	27	12.83	0	709	2	4	3	25.59	0
653	2	1	28	9.12	0	710	2	4	4	11.62	0
654	2	1	31	5.46	0	711	2	4	5	17.08	0
655	2	1	32	4.75	0	712	2	4	6	26.48	0
656	2	1	33	4.40	0	713	2	4	7	32.55	0
657	2	2	4	41.36	0	714	2	4	8	25.11	0
658	2	2	5	27.18	0	715	2	4	9	6.15	0
659	2	2	6	34.61	0	716	2	4	10	24.06	0
660	2	2	7	34.19	0	717	2	4	11	16.34	0
661	2	2	8	25.05	0	718	2	4	12	20.57	0
662	2	2	9	41.05	0	719	2	4	13	19.77	0
663	2	2	10	20.22	0	720	2	4	14	21.36	0
664	2	2	11	12.45	0	721	2	4	15	14.13	0
665	2	2	12	25.14	0	722	2	4	16	8.48	0
666	2	2	13	14.73	0	723	2	4	17	10.06	0
667	2	2	14	28.09	0	724	2	4	18	20.75	0
668	2	2	15	4.67	0	725	2	4	19	5.59	0
669	2	2	16	10.37	0	726	2	4	20	12.32	0
670	2	2	17	9.45	0	727	2	4	21	10.70	0
671	2	2	18	14.13	0	728	2	4	22	10.30	0
672	2	2	19	14.91	0	729	2	4	23	5.88	0
673	2	2	20	9.49	0	730	2	4	24	10.75	0
674	2	2	21	5.91	0	731	2	4	25	9.57	0
675	2	2	22	5.76	0	732	2	4	26	8.75	0
676	2	2	24	6.48	0	733	2	4	28	5.68	0
677	2	2	26	6.94	0	734	2	4	30	5.66	0
678	2	2	29	5.77	0	735	2	5	1	31.65	0
679	2	2	30	5.15	0	736	2	5	2	18.00	0
680	2	2	31	4.56	0	737	2	5	3	28.02	0
681	2	3	1	15.04	0	738	2	5	4	8.63	0
682	2	3	2	20.82	0	739	2	5	5	6.18	0
683	2	3	3	37.36	0	740	2	5	6	33.22	0
684	2	3	4	30.93	0	741	2	5	7	18.21	0

742	2	5	8	17.47	0	799	2	7	19	5.71	0
743	2	5	9	10.20	0	800	2	7	20	7.05	0
744	2	5	10	15.93	0	801	2	7	21	8.30	0
745	2	5	11	7.29	0	802	2	7	22	6.87	0
746	2	5	12	29.11	0	803	2	7	24	5.33	0
747	2	5	13	10.84	0	804	2	7	27	4.08	0
748	2	5	14	14.84	0	805	2	7	28	3.97	0
749	2	5	15	21.20	0	806	2	8	1	14.78	0
750	2	5	16	4.93	0	807	2	8	2	13.61	0
751	2	5	18	19.24	0	808	2	8	3	5.63	0
752	2	5	19	17.81	0	809	2	8	4	12.36	0
753	2	5	20	13.67	0	810	2	8	5	16.50	0
754	2	5	21	18.66	0	811	2	8	6	7.47	0
755	2	5	22	16.40	0	812	2	8	7	10.93	0
756	2	5	24	4.90	0	813	2	8	8	14.98	0
757	2	5	25	5.66	0	814	2	8	9	15.19	0
758	2	5	27	5.26	0	815	2	8	10	4.68	0
759	2	5	31	4.68	0	816	2	8	11	13.46	0
760	2	6	1	22.66	0	817	2	8	12	9.78	0
761	2	6	2	14.00	0	818	2	8	13	12.10	0
762	2	6	3	13.42	0	819	2	8	14	9.01	0
763	2	6	4	10.76	0	820	2	8	16	7.07	0
764	2	6	5	17.72	0	821	2	8	17	5.91	0
765	2	6	6	11.37	0	822	2	8	18	5.00	0
766	2	6	7	23.02	0	823	2	8	19	7.01	0
767	2	6	8	8.91	0	824	2	8	20	4.44	0
768	2	6	9	20.49	0	825	2	8	23	5.53	0
769	2	6	10	12.37	0	826	2	8	24	4.81	0
770	2	6	11	7.97	0	827	2	8	25	5.07	0
771	2	6	12	18.50	0	828	2	8	26	4.87	0
772	2	6	13	10.54	0	829	2	8	27	7.80	0
773	2	6	14	16.59	0	830	2	8	29	3.68	0
774	2	6	15	6.04	0	831	2	9	1	15.56	0
775	2	6	16	12.84	0	832	2	9	2	21.30	0
776	2	6	17	17.35	0	833	2	9	3	7.83	0
777	2	6	18	16.49	0	834	2	9	4	10.18	0
778	2	6	19	15.98	0	835	2	9	5	8.94	0
779	2	6	20	10.60	0	836	2	9	6	15.31	0
780	2	6	21	4.53	0	837	2	9	7	13.25	0
781	2	6	23	9.99	0	838	2	9	8	13.35	0
782	2	6	26	6.02	0	839	2	9	9	12.60	0
783	2	7	1	22.14	0	840	2	9	10	11.90	0
784	2	7	2	14.11	0	841	2	9	11	11.49	0
785	2	7	3	21.87	0	842	2	9	12	10.54	0
786	2	7	4	20.11	0	843	2	9	13	7.04	0
787	2	7	5	4.77	0	844	2	9	14	5.89	0
788	2	7	6	7.65	0	845	2	9	15	9.13	0
789	2	7	7	10.81	0	846	2	9	16	4.97	0
790	2	7	8	21.35	0	847	2	9	18	5.74	0
791	2	7	9	11.47	0	848	2	9	19	7.89	0
792	2	7	10	11.69	0	849	2	9	21	4.09	0
793	2	7	12	7.39	0	850	2	9	22	4.32	0
794	2	7	14	12.61	0	851	2	9	24	4.56	0
795	2	7	15	13.09	0	852	2	9	25	5.13	0
796	2	7	16	16.88	0	853	2	9	27	5.45	0
797	2	7	17	8.00	0	854	2	10	1	9.92	0
798	2	7	18	7.06	0	855	2	10	3	11.90	0

856	2	10	4	9.15	0	913	3	0	16	23.26	0
857	2	10	5	11.24	0	914	3	0	17	15.63	0
858	2	10	6	10.75	0	915	3	0	18	5.37	0
859	2	10	7	9.06	0	916	3	0	19	4.50	0
860	2	10	8	9.09	0	917	3	0	20	5.45	0
861	2	10	9	8.04	0	918	3	0	22	6.80	0
862	2	10	11	6.49	0	919	3	0	23	6.56	0
863	2	10	12	5.86	0	920	3	0	24	16.40	0
864	2	10	13	6.10	0	921	3	0	25	6.62	0
865	2	10	20	9.82	0	922	3	0	27	10.75	0
866	2	10	21	6.68	0	923	3	0	28	9.15	0
867	2	10	22	5.32	0	924	3	0	30	6.86	0
868	2	10	23	7.02	0	925	3	1	4	29.07	0
869	2	10	26	5.90	0	926	3	1	5	23.36	0
870	2	11	1	7.70	0	927	3	1	6	16.18	0
871	2	11	2	14.08	0	928	3	1	7	14.46	0
872	2	11	4	9.34	0	929	3	1	8	21.92	0
873	2	11	5	5.86	0	930	3	1	9	11.62	0
874	2	11	7	6.45	0	931	3	1	10	5.13	0
875	2	11	8	13.39	0	932	3	1	11	14.59	0
876	2	11	9	8.27	0	933	3	1	12	16.69	0
877	2	11	11	5.98	0	934	3	1	13	12.80	0
878	2	11	13	6.55	0	935	3	1	14	4.40	0
879	2	11	18	7.61	0	936	3	1	15	14.35	0
880	2	11	19	7.07	0	937	3	1	16	14.71	0
881	2	12	1	6.86	0	938	3	1	17	11.72	0
882	2	12	3	10.19	0	939	3	1	18	5.16	0
883	2	12	4	7.46	0	940	3	1	19	10.27	0
884	2	12	7	6.33	0	941	3	1	20	12.31	0
885	2	12	11	6.30	0	942	3	1	21	8.84	0
886	2	12	14	5.80	0	943	3	1	22	5.22	0
887	2	12	18	4.89	0	944	3	1	24	9.12	0
888	2	13	5	5.63	0	945	3	1	25	5.68	0
889	2	13	6	5.65	0	946	3	1	29	5.38	0
890	2	13	9	5.10	0	947	3	1	32	6.59	0
891	2	13	13	5.43	0	948	3	1	33	4.17	0
892	2	14	3	4.49	0	949	3	2	1	51.74	0
893	2	14	9	4.53	0	950	3	2	2	21.03	0
894	2	14	10	4.03	0	951	3	2	3	26.28	0
895	2	3	0	5.41	0	952	3	2	4	26.07	0
896	2	4	0	9.61	0	953	3	2	5	25.93	0
897	2	5	0	6.99	0	954	3	2	6	31.63	0
898	2	6	0	25.94	0	955	3	2	7	16.18	0
899	2	7	0	19.66	0	956	3	2	8	6.51	0
900	2	8	0	4.64	0	957	3	2	9	39.48	0
901	2	10	0	17.53	0	958	3	2	10	17.42	0
902	2	11	0	5.39	0	959	3	2	11	5.62	0
903	2	12	0	8.47	0	960	3	2	12	27.25	0
904	2	13	0	7.41	0	961	3	2	13	16.86	0
905	2	14	0	6.38	0	962	3	2	14	18.81	0
906	3	0	6	17.17	0	963	3	2	15	19.18	0
907	3	0	7	16.62	0	964	3	2	16	11.72	0
908	3	0	8	3.11	0	965	3	2	17	24.73	0
909	3	0	9	7.08	0	966	3	2	18	7.46	0
910	3	0	10	24.33	0	967	3	2	19	7.97	0
911	3	0	11	41.66	0	968	3	2	20	6.10	0
912	3	0	14	9.39	0	969	3	2	21	9.70	0

970	3	2	22	6.29	0	1027	3	5	4	30.30	0
971	3	2	23	10.58	0	1028	3	5	5	23.69	0
972	3	2	24	10.56	0	1029	3	5	6	5.86	0
973	3	2	26	5.94	0	1030	3	5	7	18.73	0
974	3	2	27	5.45	0	1031	3	5	8	13.80	0
975	3	2	29	5.89	0	1032	3	5	9	27.49	0
976	3	3	1	23.08	0	1033	3	5	10	17.09	0
977	3	3	2	13.13	0	1034	3	5	11	8.12	0
978	3	3	3	21.84	0	1035	3	5	12	16.31	0
979	3	3	4	30.60	0	1036	3	5	13	11.00	0
980	3	3	5	7.82	0	1037	3	5	14	16.79	0
981	3	3	6	22.43	0	1038	3	5	15	9.10	0
982	3	3	7	25.02	0	1039	3	5	16	18.17	0
983	3	3	8	17.25	0	1040	3	5	17	9.11	0
984	3	3	9	23.38	0	1041	3	5	18	12.65	0
985	3	3	10	21.42	0	1042	3	5	19	17.39	0
986	3	3	11	36.54	0	1043	3	5	20	14.30	0
987	3	3	12	13.27	0	1044	3	5	21	10.60	0
988	3	3	13	12.25	0	1045	3	5	22	12.86	0
989	3	3	14	12.13	0	1046	3	5	23	5.90	0
990	3	3	16	15.13	0	1047	3	5	27	5.87	0
991	3	3	17	12.96	0	1048	3	5	29	5.49	0
992	3	3	18	7.32	0	1049	3	6	1	5.84	0
993	3	3	19	9.24	0	1050	3	6	2	4.29	0
994	3	3	20	13.16	0	1051	3	6	3	11.20	0
995	3	3	21	10.95	0	1052	3	6	4	19.88	0
996	3	3	22	16.14	0	1053	3	6	5	21.71	0
997	3	3	28	7.57	0	1054	3	6	6	22.10	0
998	3	3	29	5.28	0	1055	3	6	7	26.92	0
999	3	3	31	6.23	0	1056	3	6	8	9.71	0
1000	3	4	1	34.26	0	1057	3	6	9	12.09	0
1001	3	4	2	27.34	0	1058	3	6	10	12.37	0
1002	3	4	3	36.29	0	1059	3	6	11	15.70	0
1003	3	4	4	32.50	0	1060	3	6	12	7.06	0
1004	3	4	5	33.60	0	1061	3	6	13	7.51	0
1005	3	4	6	31.14	0	1062	3	6	14	14.63	0
1006	3	4	7	39.27	0	1063	3	6	15	6.07	0
1007	3	4	8	7.21	0	1064	3	6	16	11.53	0
1008	3	4	9	16.40	0	1065	3	6	17	10.02	0
1009	3	4	10	19.76	0	1066	3	6	18	12.56	0
1010	3	4	11	12.71	0	1067	3	6	19	11.37	0
1011	3	4	12	22.31	0	1068	3	6	20	13.21	0
1012	3	4	13	10.39	0	1069	3	6	21	6.30	0
1013	3	4	14	9.09	0	1070	3	6	22	5.63	0
1014	3	4	17	13.69	0	1071	3	6	24	7.14	0
1015	3	4	18	16.76	0	1072	3	6	29	7.29	0
1016	3	4	19	16.74	0	1073	3	7	1	12.59	0
1017	3	4	20	12.44	0	1074	3	7	2	7.35	0
1018	3	4	21	6.32	0	1075	3	7	3	21.37	0
1019	3	4	22	12.34	0	1076	3	7	4	17.26	0
1020	3	4	23	11.06	0	1077	3	7	5	22.62	0
1021	3	4	24	4.78	0	1078	3	7	6	20.10	0
1022	3	4	26	5.42	0	1079	3	7	7	15.29	0
1023	3	4	28	7.26	0	1080	3	7	8	13.14	0
1024	3	5	1	11.87	0	1081	3	7	9	13.31	0
1025	3	5	2	23.24	0	1082	3	7	10	9.25	0
1026	3	5	3	7.36	0	1083	3	7	11	11.27	0

1084	3	7	12	6.01	0	1141	3	11	2	11.05	0
1085	3	7	13	16.89	0	1142	3	11	4	8.11	0
1086	3	7	14	21.38	0	1143	3	11	5	5.68	0
1087	3	7	15	11.21	0	1144	3	11	7	8.03	0
1088	3	7	16	14.81	0	1145	3	11	8	8.86	0
1089	3	7	17	15.64	0	1146	3	11	9	9.58	0
1090	3	7	19	10.64	0	1147	3	11	13	6.52	0
1091	3	7	21	7.32	0	1148	3	11	15	6.46	0
1092	3	7	24	6.40	0	1149	3	11	16	5.30	0
1093	3	7	25	6.31	0	1150	3	11	17	5.23	0
1094	3	8	1	13.13	0	1151	3	11	18	5.35	0
1095	3	8	2	16.61	0	1152	3	11	19	4.21	0
1096	3	8	3	23.20	0	1153	3	11	22	4.71	0
1097	3	8	4	8.97	0	1154	3	11	23	4.65	0
1098	3	8	5	13.09	0	1155	3	12	3	9.78	0
1099	3	8	6	9.32	0	1156	3	12	4	8.51	0
1100	3	8	7	9.22	0	1157	3	12	14	7.04	0
1101	3	8	8	14.00	0	1158	3	12	19	5.76	0
1102	3	8	9	12.87	0	1159	3	12	20	6.30	0
1103	3	8	10	6.11	0	1160	3	2	0	42.84	0
1104	3	8	11	5.00	0	1161	3	3	0	14.42	0
1105	3	8	12	21.57	0	1162	3	4	0	5.16	0
1106	3	8	13	14.74	0	1163	3	5	0	38.97	0
1107	3	8	14	15.58	0	1164	3	6	0	14.61	0
1108	3	8	15	8.21	0	1165	3	7	0	11.54	0
1109	3	8	16	6.36	0	1166	3	8	0	13.36	0
1110	3	8	25	6.87	0	1167	3	9	0	6.57	0
1111	3	8	27	5.27	0	1168	3	11	0	7.82	0
1112	3	9	1	13.15	0	1169	3	12	0	7.47	0
1113	3	9	2	28.00	0	1170	4	0	4	43.62	0
1114	3	9	3	13.74	0	1171	4	0	5	16.84	0
1115	3	9	4	11.40	0	1172	4	0	6	8.56	0
1116	3	9	5	5.56	0	1173	4	0	7	21.60	0
1117	3	9	6	5.13	0	1174	4	0	8	3.37	0
1118	3	9	7	10.65	0	1175	4	0	9	3.18	0
1119	3	9	8	10.19	0	1176	4	0	10	9.53	0
1120	3	9	9	13.37	0	1177	4	0	11	10.08	0
1121	3	9	10	7.49	0	1178	4	0	12	18.71	0
1122	3	9	11	14.82	0	1179	4	0	13	18.00	0
1123	3	9	14	5.99	0	1180	4	0	14	5.39	0
1124	3	9	17	5.11	0	1181	4	0	17	10.07	0
1125	3	9	23	4.63	0	1182	4	0	18	13.81	0
1126	3	9	25	4.59	0	1183	4	0	20	17.19	0
1127	3	9	26	5.97	0	1184	4	0	21	13.38	0
1128	3	9	27	4.09	0	1185	4	0	24	9.75	0
1129	3	10	1	22.78	0	1186	4	0	26	7.12	0
1130	3	10	2	22.79	0	1187	4	0	32	3.87	0
1131	3	10	5	11.08	0	1188	4	1	3	20.04	0
1132	3	10	6	7.51	0	1189	4	1	4	25.04	0
1133	3	10	7	5.74	0	1190	4	1	5	21.04	0
1134	3	10	8	10.09	0	1191	4	1	6	19.16	0
1135	3	10	9	8.89	0	1192	4	1	7	15.02	0
1136	3	10	12	5.66	0	1193	4	1	8	10.69	0
1137	3	10	15	6.03	0	1194	4	1	9	12.92	0
1138	3	10	18	6.44	0	1195	4	1	10	8.89	0
1139	3	10	25	4.50	0	1196	4	1	11	15.10	0
1140	3	11	1	5.24	0	1197	4	1	12	4.14	0

1198	4	1	13	18.16	0	1255	4	3	13	5.55	0
1199	4	1	14	10.50	0	1256	4	3	14	16.84	0
1200	4	1	15	13.62	0	1257	4	3	15	9.64	0
1201	4	1	16	8.95	0	1258	4	3	16	10.20	0
1202	4	1	17	7.59	0	1259	4	3	17	9.75	0
1203	4	1	18	12.10	0	1260	4	3	18	8.50	0
1204	4	1	19	8.27	0	1261	4	3	19	6.00	0
1205	4	1	20	15.20	0	1262	4	3	20	14.09	0
1206	4	1	21	4.66	0	1263	4	3	22	7.24	0
1207	4	1	23	5.77	0	1264	4	3	23	5.02	0
1208	4	1	24	10.81	0	1265	4	3	24	5.61	0
1209	4	1	25	7.00	0	1266	4	3	28	5.13	0
1210	4	1	26	8.39	0	1267	4	3	31	5.14	0
1211	4	1	27	8.69	0	1268	4	4	1	31.25	0
1212	4	1	29	4.31	0	1269	4	4	2	15.37	0
1213	4	1	30	5.88	0	1270	4	4	3	9.26	0
1214	4	1	32	3.34	0	1271	4	4	4	8.80	0
1215	4	2	1	43.95	0	1272	4	4	5	16.69	0
1216	4	2	2	18.29	0	1273	4	4	6	33.48	0
1217	4	2	3	27.67	0	1274	4	4	7	9.65	0
1218	4	2	4	16.21	0	1275	4	4	8	12.64	0
1219	4	2	5	30.29	0	1276	4	4	9	4.68	0
1220	4	2	6	11.69	0	1277	4	4	10	21.40	0
1221	4	2	7	11.59	0	1278	4	4	11	15.62	0
1222	4	2	8	6.15	0	1279	4	4	12	17.17	0
1223	4	2	9	11.14	0	1280	4	4	13	14.30	0
1224	4	2	10	11.73	0	1281	4	4	14	6.24	0
1225	4	2	12	11.82	0	1282	4	4	15	15.46	0
1226	4	2	13	11.42	0	1283	4	4	16	8.95	0
1227	4	2	14	5.56	0	1284	4	4	17	12.74	0
1228	4	2	15	12.81	0	1285	4	4	18	6.23	0
1229	4	2	16	6.81	0	1286	4	4	19	17.67	0
1230	4	2	18	6.31	0	1287	4	4	20	7.83	0
1231	4	2	19	7.05	0	1288	4	4	21	9.48	0
1232	4	2	20	5.46	0	1289	4	4	24	5.10	0
1233	4	2	21	8.16	0	1290	4	4	28	4.27	0
1234	4	2	22	5.78	0	1291	4	4	29	5.01	0
1235	4	2	23	4.66	0	1292	4	5	1	14.14	0
1236	4	2	25	10.30	0	1293	4	5	2	21.02	0
1237	4	2	26	8.87	0	1294	4	5	3	16.18	0
1238	4	2	27	4.41	0	1295	4	5	4	18.69	0
1239	4	2	28	6.22	0	1296	4	5	5	14.09	0
1240	4	2	29	7.24	0	1297	4	5	6	7.92	0
1241	4	2	30	5.50	0	1298	4	5	7	11.14	0
1242	4	2	32	3.39	0	1299	4	5	8	26.69	0
1243	4	3	1	30.18	0	1300	4	5	9	20.90	0
1244	4	3	2	40.75	0	1301	4	5	11	10.30	0
1245	4	3	3	25.23	0	1302	4	5	12	19.89	0
1246	4	3	4	19.26	0	1303	4	5	15	4.30	0
1247	4	3	5	6.80	0	1304	4	5	14	7.11	0
1248	4	3	6	24.71	0	1305	4	5	15	10.11	0
1249	4	3	7	10.90	0	1306	4	5	16	12.26	0
1250	4	3	8	7.55	0	1307	4	5	17	15.78	0
1251	4	3	9	13.57	0	1308	4	5	18	4.47	0
1252	4	3	10	15.05	0	1309	4	5	19	7.26	0
1253	4	3	11	16.05	0	1310	4	5	20	8.58	0
1254	4	3	12	10.54	0	1311	4	5	21	9.98	0

1312	4	5	22	8.85	0	1369	4	8	21	4.84	0
1313	4	5	25	5.27	0	1370	4	8	23	4.69	0
1314	4	5	25	7.49	0	1371	4	8	24	4.13	0
1315	4	5	29	5.73	0	1372	4	8	27	3.94	0
1316	4	5	30	3.85	0	1373	4	9	1	5.44	0
1317	4	6	1	11.72	0	1374	4	9	2	6.81	0
1318	4	6	3	15.97	0	1375	4	9	3	17.37	0
1319	4	6	4	5.41	0	1376	4	9	4	18.39	0
1320	4	6	5	12.66	0	1377	4	9	5	15.45	0
1321	4	6	6	18.23	0	1378	4	9	6	9.37	0
1322	4	6	7	10.64	0	1379	4	9	7	6.09	0
1323	4	6	8	24.03	0	1380	4	9	8	7.57	0
1324	4	6	10	9.74	0	1381	4	9	9	14.18	0
1325	4	6	11	10.32	0	1382	4	9	10	12.42	0
1326	4	6	12	15.69	0	1383	4	9	11	12.40	0
1327	4	6	13	18.16	0	1384	4	9	14	5.43	0
1328	4	6	14	10.72	0	1385	4	9	15	10.42	0
1329	4	6	15	14.54	0	1386	4	9	19	4.43	0
1330	4	6	16	12.37	0	1387	4	9	21	4.95	0
1331	4	6	17	19.86	0	1388	4	9	25	3.58	0
1332	4	6	18	9.92	0	1389	4	10	1	14.17	0
1333	4	6	19	8.17	0	1390	4	10	2	8.18	0
1334	4	6	20	7.49	0	1391	4	10	3	6.63	0
1335	4	6	21	5.38	0	1392	4	10	4	5.35	0
1336	4	6	22	8.94	0	1393	4	10	5	5.52	0
1337	4	6	23	5.46	0	1394	4	10	6	11.28	0
1338	4	7	1	5.04	0	1395	4	10	8	10.21	0
1339	4	7	2	9.41	0	1396	4	10	9	9.15	0
1340	4	7	3	8.12	0	1397	4	10	10	4.97	0
1341	4	7	4	6.13	0	1398	4	10	12	7.73	0
1342	4	7	5	11.25	0	1399	4	10	16	3.95	0
1343	4	7	7	7.40	0	1400	4	10	17	6.17	0
1344	4	7	8	10.00	0	1401	4	10	18	5.41	0
1345	4	7	9	22.32	0	1402	4	10	19	4.42	0
1346	4	7	10	19.36	0	1403	4	10	22	4.14	0
1347	4	7	11	12.42	0	1404	4	10	23	2.79	0
1348	4	7	14	6.62	0	1405	4	11	1	7.69	0
1349	4	7	15	20.53	0	1406	4	11	2	13.80	0
1350	4	7	17	9.71	0	1407	4	11	3	4.56	0
1351	4	7	20	6.97	0	1408	4	11	4	7.64	0
1352	4	7	21	4.75	0	1409	4	11	5	5.33	0
1353	4	8	1	5.72	0	1410	4	11	6	4.50	0
1354	4	8	2	13.84	0	1411	4	11	7	5.26	0
1355	4	8	3	13.36	0	1412	4	11	8	6.25	0
1356	4	8	4	13.43	0	1413	4	11	9	5.15	0
1357	4	8	5	13.51	0	1414	4	11	11	6.84	0
1358	4	8	6	18.54	0	1415	4	11	16	5.03	0
1359	4	8	7	14.81	0	1416	4	11	18	4.33	0
1360	4	8	8	9.82	0	1417	4	11	21	3.49	0
1361	4	8	9	5.44	0	1418	4	12	3	4.39	0
1362	4	8	11	12.77	0	1419	4	12	5	4.42	0
1363	4	8	12	20.28	0	1420	4	12	6	4.77	0
1364	4	8	13	11.31	0	1421	4	12	10	6.69	0
1365	4	8	14	5.80	0	1422	4	12	11	5.05	0
1366	4	8	17	6.78	0	1423	4	12	12	4.89	0
1367	4	8	18	4.89	0	1424	4	12	13	4.54	0
1368	4	8	19	4.77	0	1425	4	12	18	4.41	0
						1426	4	2	0	39.22	0
						1427	4	3	0	7.24	0
						1428	4	4	0	6.59	0
						1429	4	5	0	25.93	0
						1430	4	6	0	20.41	0
						1431	4	7	0	3.71	0
						1432	4	8	0	16.28	0
						1433	4	9	0	10.13	0
						1434	4	11	0	12.25	0
						1435	4	12	0	6.45	0
						1436	1	0	0	-99.	0
						1437	14				
						1438	11				

ตารางที่ 6.2 (ข) แสดงผลการคำนวณจากโปรแกรม NORMAL

PROGRAM TO NORMALISE STRUCTURE FACTORS

VERSION JAN 1983

TITLE

*** H-105 * C15H22O2 ***

DIRECT CELL A = 8.124 B = 12.366 C = 27.672 ALPHA = 90.00 BETA = 90.00 GAMMA = 90.00

PHI = 0.000000 * H**2 + 0.001635 * H * K + 0.000026 * L**2 + 0.000000 * H * K * L + 0.000000 * H * L + 0.000000 * K * L

THE STRUCTURE IS NONCENTROSYMMETRIC

4 GENERAL EQUIVALENT POSITIONS

LATTICE IS OF TYPE P

X Y Z
 1/2 - X - Y 1/2 + Z
 1/2 + X 1/2 - Y - Z
 - X 1/2 + Y 1/2 - Z

3

UNIT CELL CONTENTS

ATOM	NUMBER IN CELL	ATOMIC NUMBER	SCATTERING FACTOR CONSTANTS	FF = A1*EXP(A*FMCI) + B0*EXPI(B*FMCI) + CC1
C	120	6	2.112 7.827	2.467 27.650 1.417
H	176	1	0.388 7.151	0.601 30.180 0.308
O	16	8	4.197 6.327	2.219 22.150 1.978

NUMBER OF ATOMS IN ASYMMETRIC UNIT = 24.00

OUTPUT FOR MULTAN 236 LARGEST C'S AND 100 SMALLEST E'S

NUMBER OF REFLECTIONS = 1414

MAXIMUM |SIN(THETA)/LAMBDA|**2 = 0.3054

NUMBER OF POINTS ON WILSON PLOT = 14

LEAST SQUARES PLOT

RANGE	F(0) + (S.PITH/LAMBDA)**2	NUMBER	MEAN RHO	MEAN I	MEAN EXPL 2*0*0*0*0**2	CSBYE	WILSON
1	0.0000	489	0.0398	1120.8	0.4500	0.7129	0.7129
2	0.0250	900	0.0606	736.6	0.4200	0.8676	0.8676
3	0.0579	1051	0.0875	396.5	0.3275	1.1162	1.1162
4	0.0869	1046	0.1154	247.7	0.2716	1.3036	1.3036
5	0.1158	1007	0.1419	172.0	0.2640	1.3319	1.3319
6	0.1448	993	0.1734	168.5	0.2731	1.2980	1.2980
7	0.1737	936	0.2012	132.3	0.2440	1.4107	1.4107
8	0.2027	912	0.2285	90.9	0.1856	1.6641	1.6641
9	0.2316	607	0.2576	64.2	0.1452	1.9205	1.9205
10	0.2606	594	0.2890	46.8	0.1150	2.1624	2.1624
11	0.2895	462	0.2175	37.5	0.1022	2.2912	2.2912
12	0.3185	354	0.2444	34.9	0.0972	2.3305	2.3305
13	0.3475	293	0.2708	27.0	0.0790	2.5379	2.5379
14	0.3764	157	0.3934	22.6	0.0677	2.6511	2.6511

NORMAL EQUATIONS

C.394E+01 * SLCPH + 0.172E+04 * INTERCEPT = 0.300E+04

0.172E+04 * SLCPH + 0.959E+04 * INTERCEPT = 0.143E+05

SLCPH = 9.1126

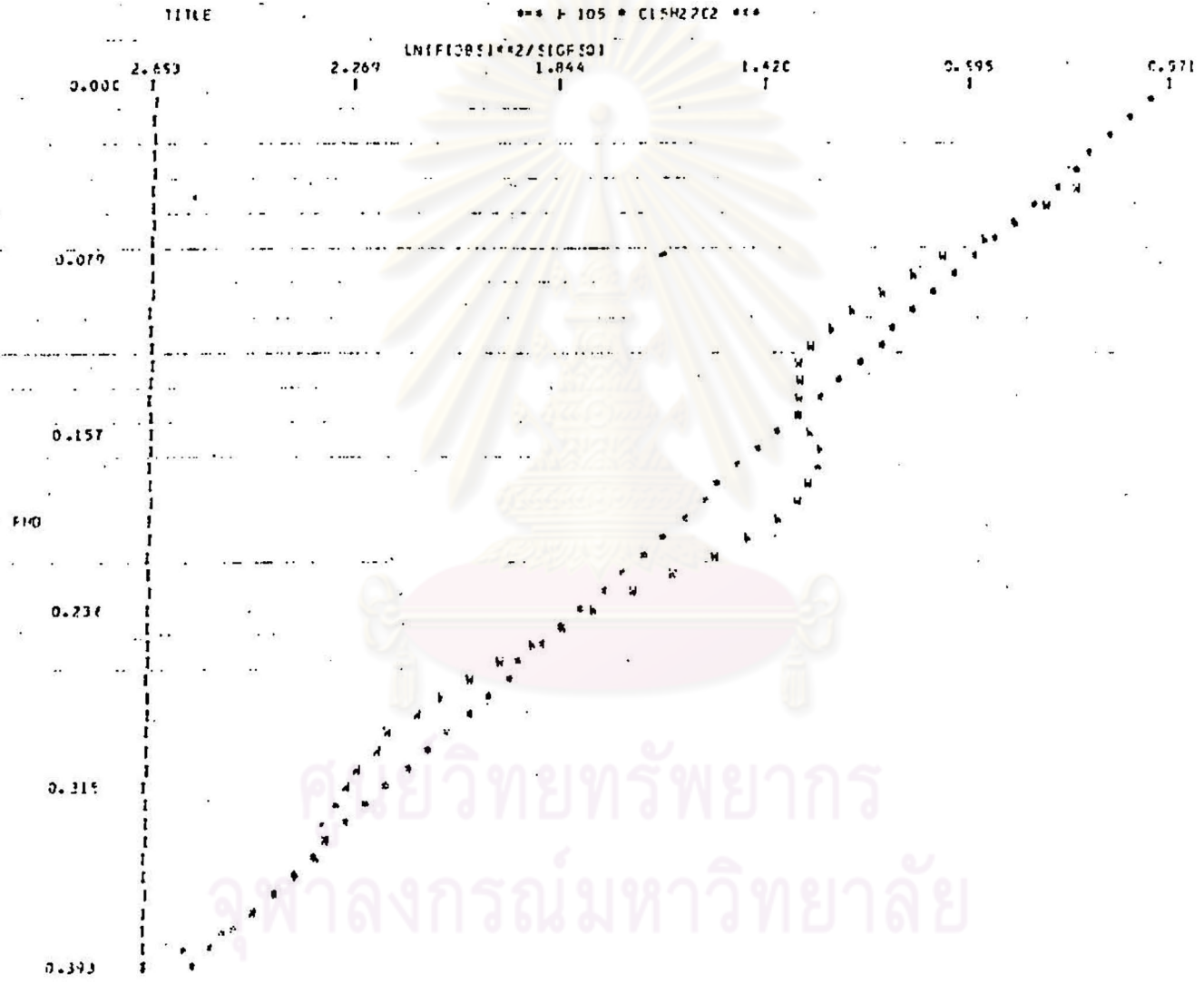
INTERCEPT = 0.5711

TEMPERATURE FACTOR (R) = 2.5563

SCALE = 1.7702

F.(ABSOLUTE)**2 = SCALE*F(COBSERVED)**2

PLCI OF WILSON AND TEPYE CURVES AND LEAST SQUARES STRAIGHT LINE



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

AVERAGE E**2 ACCORDING TO APPROPRIATE INDEX SPECIFIC PERCENT RECALCULATING

PARITY GROUPS									
E**2	ALL	EEE	EE	E	CC1	CC	CC	CC	CC
NUMBER	4846	686	524	622	514	600	528	636	572

FINAL STATISTICS

DISTRIBUTION OF E**2 WITH SIGNIFICANT DIFFERENCE										
SIGN/LAM	0.0000	0.1273	0.1913	0.2547	0.3183	0.3820	0.4457	0.5093	0.5730	0.6367
E**2	0.0000	1.0805	0.1857	1.0327	1.0203	0.9609	1.0224	0.9994	1.0092	0.9399
NUMBER	0	14	171	410	673	788	902	890	588	440

AVERAGE VALUES

AVERAGE	ALL DATA	EXPERIMENTAL				THEORETICAL		
		HCL	CKL	HCL	HFO	ACENTRIC	CENTRIC	HYPERCENTRIC
MUD(E)	0.921	0.921	0.943	0.883	0.941	0.886	0.799	0.718
E**2	1.000	0.984	1.106	0.993	1.122	1.000	1.000	1.000
E**3	1.217	1.163	1.562	1.291	1.529	1.229	1.596	1.516
E**4	1.665	1.523	2.415	1.855	2.156	2.000	2.000	4.500
E**5	2.556	2.196	5.100	2.855	3.276	3.273	6.383	12.260
E**6	4.407	3.473	11.349	4.610	5.014	6.000	15.000	27.500
MUD(E**2 1)	0.576	0.544	0.742	0.735	0.815	0.726	0.958	1.145
(E**2 1)**2	0.666	0.555	1.402	0.877	0.934	1.000	2.000	3.500
(E**2 1)**3	1.410	0.856	5.623	1.022	0.815	2.000	8.000	26.000
(MUD(E**2 1))**3	1.648	1.372	6.115	1.455	1.280	2.415	8.691	25.700
WEIGHTED SAMPLE SIZE	4846	4064	436	156	76			

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

WEIGHTED CUMULATIVE PROBABILITY DISTRIBUTION

Z	ALL DATA	EXPERIMENTAL					THEORETICAL		
		HKL	CKL	HOL	HRC	ACENTRIC	CENTRIC	HYPERCENTRIC	
0.1	0.025	0.017	0.056	0.090	0.105	0.055	0.249	0.369	
0.2	0.068	0.055	0.112	0.179	0.227	0.111	0.345	0.463	
0.3	0.127	0.116	0.201	0.255	0.342	0.255	0.416	0.527	
0.4	0.209	0.162	0.269	0.325	0.342	0.320	0.473	0.574	
0.5	0.272	0.258	0.332	0.423	0.342	0.353	0.526	0.612	
0.6	0.350	0.342	0.377	0.436	0.395	0.421	0.561	0.643	
0.7	0.434	0.426	0.481	0.474	0.421	0.503	0.597	0.670	
0.8	0.505	0.503	0.515	0.532	0.447	0.551	0.629	0.654	
0.9	0.555	0.566	0.550	0.577	0.474	0.552	0.657	0.711	
1.0	0.620	0.627	0.604	0.607	0.521	0.622	0.683	0.732	
1.2	0.736	0.720	0.705	0.692	0.575	0.655	0.727	0.765	
1.4	0.783	0.750	0.757	0.744	0.659	0.752	0.743	0.791	
1.6	0.824	0.844	0.791	0.801	0.684	0.758	0.794	0.813	
1.8	0.876	0.887	0.828	0.844	0.737	0.825	0.827	0.832	
2.0	0.902	0.915	0.854	0.846	0.737	0.865	0.843	0.846	
2.2	0.921	0.920	0.864	0.855	0.814	0.869	0.862	0.863	
2.4	0.942	0.951	0.897	0.897	0.842	0.905	0.879	0.875	
2.6	0.954	0.961	0.922	0.923	0.895	0.922	0.892	0.886	
2.8	0.967	0.972	0.933	0.936	0.921	0.929	0.905	0.896	
3.0	0.974	0.989	0.952	0.946	0.924	0.950	0.917	0.905	
3.2	0.977	0.982	0.960	0.949	1.000	0.959	0.926	0.912	
3.4	0.981	0.985	0.968	0.962	1.000	0.967	0.925	0.910	
3.6	0.982	0.987	0.955	0.974	1.000	0.972	0.942	0.926	
3.8	0.986	0.989	0.955	0.957	1.000	0.978	0.946	0.932	
4.0	0.991	0.994	0.963	1.000	1.000	0.982	0.954	0.932	
WEIGHTED SAMPLE SIZE	4845	4064	536	156	76				

DISTRIBUTION OF NUMBER OF P'S AGT. LIMIT

P	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5
NO.	1022	660	485	325	201	102	225	156	112	77	50	39	27	16	6	4	4	3	2

ศูนย์วิจัยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

286 LARGEST E VALUES WRITTEN TO CONTROL FILE

CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E
1	0	5	5	2.752	2	2	3	9	2.703	3	0	2	6	2.656	4	0	5	8	2.371	5	1	6	10	2.184
7	0	4	6	2.070	8	2	5	2	2.057	5	0	5	21	2.042	10	0	5	1	2.037	11	0	3	21	2.035
13	4	4	6	2.019	14	0	2	28	2.016	15	4	8	12	2.016	16	0	2	27	2.012	17	4	6	17	1.999
15	0	4	3	1.990	20	0	3	19	1.979	21	3	3	11	1.978	22	2	0	18	1.975	23	4	3	2	1.964
25	4	7	15	1.917	26	4	0	4	1.907	27	1	4	7	1.906	28	0	3	2	1.897	29	2	10	2	1.882
31	2	0	13	1.856	32	4	5	8	1.850	33	4	6	8	1.818	34	4	11	2	1.773	35	0	5	9	1.318
37	1	0	17	1.617	38	0	4	7	1.613	39	1	2	29	1.603	40	2	5	12	1.787	41	3	10	1	1.776
43	0	3	27	1.753	44	4	2	0	1.741	45	2	1	14	1.729	46	3	5	0	1.713	47	4	4	1	1.707
49	1	10	22	1.702	50	1	3	25	1.700	51	1	2	11	1.651	52	5	7	9	1.662	53	2	5	10	1.679
55	3	8	12	1.671	56	4	4	19	1.670	57	3	5	9	1.666	58	1	2	10	1.658	59	0	10	5	1.656
61	1	6	15	1.652	62	1	1	17	1.643	63	4	9	4	1.641	64	2	10	20	1.626	65	0	6	27	1.625
67	1	0	23	1.626	68	1	4	24	1.626	69	7	5	22	1.621	70	0	2	23	1.620	71	2	7	14	1.619
72	0	14	8	1.610	73	0	6	5	1.610	74	2	5	21	1.604	75	4	11	0	1.602	76	4	3	25	1.601
76	3	0	24	1.583	77	2	2	17	1.582	78	2	0	12	1.576	79	1	2	15	1.573	80	4	2	0	1.572
85	2	1	27	1.567	86	1	2	5	1.559	87	4	7	10	1.554	88	0	2	26	1.552	89	1	9	6	1.552
91	1	7	11	1.546	92	4	8	6	1.543	93	0	9	3	1.541	94	4	10	1	1.539	95	1	10	5	1.532
97	1	11	0	1.524	98	0	5	18	1.521	99	2	11	8	1.518	100	3	0	3	1.516	101	2	6	7	1.512
103	4	5	12	1.509	104	3	5	19	1.509	105	1	7	1	1.509	106	4	0	20	1.503	107	3	2	1	1.507
109	2	2	5	1.506	110	2	5	18	1.503	111	1	9	28	1.502	112	1	1	14	1.500	113	2	4	5	1.494
116	4	4	10	1.490	117	0	3	2	1.470	118	0	4	5	1.469	119	0	2	7	1.469	120	2	5	1	1.467
121	2	0	7	1.484	122	1	6	18	1.474	123	4	2	25	1.473	124	1	1	10	1.471	125	4	2	5	1.469
127	0	3	15	1.462	128	1	11	3	1.460	129	2	10	0	1.460	130	2	5	6	1.458	131	2	6	27	1.457
133	1	4	20	1.454	134	3	0	16	1.452	135	4	6	11	1.451	136	2	5	15	1.445	137	2	7	3	1.443
139	0	10	19	1.435	140	2	7	8	1.433	141	0	11	9	1.432	142	0	13	12	1.426	143	0	8	8	1.425
145	1	6	11	1.423	146	4	6	0	1.421	147	4	5	9	1.416	148	0	0	24	1.416	149	1	5	2	1.415
151	3	2	22	1.408	152	1	5	22	1.407	153	2	1	15	1.407	154	3	5	4	1.405	155	1	4	2	1.404
157	2	11	2	1.394	158	0	0	26	1.393	159	1	9	7	1.393	160	4	9	9	1.389	161	2	5	11	1.386
163	1	5	12	1.385	164	2	7	16	1.391	165	1	2	10	1.379	166	2	6	18	1.379	167	1	4	11	1.375
169	4	2	26	1.372	170	0	10	13	1.366	171	2	5	19	1.365	172	0	13	15	1.364	173	0	3	26	1.359
175	2	4	14	1.358	176	1	7	10	1.357	177	0	1	27	1.354	178	2	3	26	1.354	179	0	5	4	1.352
181	1	3	15	1.346	182	0	13	6	1.345	183	3	5	22	1.345	184	0	3	23	1.345	185	1	2	17	1.342
187	2	0	32	1.335	188	1	11	1	1.339	189	4	5	5	1.337	190	4	6	6	1.337	191	2	2	27	1.335
193	1	5	23	1.334	194	1	5	6	1.333	195	1	5	8	1.332	196	0	7	3	1.330	197	4	9	13	1.329
199	3	0	27	1.327	200	0	6	19	1.326	201	4	5	17	1.325	202	1	4	15	1.324	203	4	3	0	1.322
205	0	2	10	1.321	206	0	7	12	1.321	207	1	7	7	1.320	208	1	6	2	1.319	209	4	10	6	1.319
211	4	6	22	1.319	212	0	9	26	1.313	213	2	4	6	1.311	214	4	3	20	1.317	215	2	8	14	1.316
217	2	4	7	1.310	218	1	2	0	1.307	219	3	5	16	1.308	220	3	2	0	1.307	221	0	12	5	1.305
223	0	9	1	1.304	224	2	4	12	1.302	225	1	1	16	1.302	226	2	10	26	1.299	227	2	6	12	1.298
229	4	2	27	1.293	230	4	9	3	1.291	231	2	6	7	1.291	232	0	10	26	1.291	233	1	8	1	1.291
235	2	1	29	1.287	236	4	5	2	1.289	237	3	6	20	1.289	238	4	6	15	1.283	239	2	10	23	1.285
241	0	6	22	1.319	242	2	11	18	1.277	243	4	4	12	1.271	244	6	2	3	1.267	245	3	6	6	1.266
247	2	3	22	1.262	248	4	6	12	1.261	249	4	10	6	1.261	250	0	7	19	1.259	251	2	6	9	1.257
253	3	12	20	1.253	254	2	2	14	1.253	255	3	11	9	1.252	256	0	2	27	1.252	257	1	5	1	1.251
259	0	12	7	1.245	260	1	4	12	1.249	261	4	1	26	1.249	262	2	6	23	1.247	263	4	2	14	1.247
265	0	3	5	1.246	266	2	8	14	1.246	267	1	11	17	1.245	268	4	6	7	1.245	269	1	5	2	1.243
271	1	3	29	1.238	272	2	5	20	1.237	273	1	8	18	1.236	274	0	10	0	1.235	275	1	7	10	1.234
277	0	5	30	1.231	278	4	0	13	1.227	279	1	6	25	1.227	280	4	0	24	1.227	281	4	4	15	1.227
283	5	7	16	1.223	284	3	4	1	1.229	285	3	5	5	1.220	286	2	7	1	1.220					

33 SMALLEST E VALUES WRITTEN TO CONTROL FILE

CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E
1	3	0	6	0.122	2	1	0	8	0.122	3	0	1	7	0.122	4	1	4	0	0.127	5	2	3	0	0.133
7	0	5	3	0.172	8	0	3	12	0.142	9	0	0	0	0.169	10	4	0	0	0.191	11	4	0	0	0.191
13	0	2	12	0.212	14	0	2	9	0.219	15	3	1	10	0.224	16	0	5	7	0.225	17	1	3	14	0.221
19	3	0	2	0.245	20	1	0	9	0.252	21	2	2	3	0.255	22	0	5	5	0.257	23	3	2	11	0.262
25	0	5	13	0.264	26	1	0	9	0.265	27	2	5	0	0.284	28	4	1	12	0.282	29	2	4	5	0.285
31	0	1	15	0.282	32	0	1	12	0.282	33	2	2	15	0.283										

ตารางที่ 6.3 (ก) แสดงการสัต์ JCL เพื่อคำนวณโดยโปรแกรม MULTAN ในระบบ OS/VS1

```

1 //ZIAD1134 JOB CLASS=T,MSGLEVEL=(1,1),MSGCLASS=A,TPRU1=HOLD
2 //ST1 EXEC FORVLS,PARM='LET,LIST'
3 //LKED.SYSPRINT DD SYSOUT=A
4 //LKED.SYSLOAD DD DSN=666JSET(S00PGM),DISP=(,PASS),UNIT=SYSOA,
5 // SPACE=(TRK,(50,20,1),RLSE)
6 //LKED.SYSLIM DD DSN=COPY.XTALCJ(MULTAN),DISP=SHR,UNIT=SYSOA,
7 // VOL=SER=VS1WK2
8 //SD.FT05F01 DD SYSOUT=A
9 //FT02F01 DD UNIT=TAPE,VOL=SER=2006,DISP=(OLD,KEEP),LABEL=(,NL),
10 // DCB=(RECFM=V,LRECL=1706)
11 //FT03F01 DD UNIT=TAPE,VOL=SER=0327,DISP=(OLD,KEEP),LABEL=(,NL),
12 // DCB=(RECFM=V,LRECL=1769)
13 //FT04F01 DD UNIT=TAPE,VOL=SER=2330,DISP=(OLD,KEEP),LABEL=(,NL),
14 // DCB=(RECFM=V,LRECL=1769)
15 //SYSIN DD *
16 TESTCASE MULTAN
17
18 /*
19 //

```

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

ตารางที่ 6.3 (ข) แสดงผลการคำนวณจากโปรแกรม NORMAL

MULTIPLY PA-1 :

SET UP STANDARD RELATIONSHIPS

VERSION

JJA

1972

STANDARD RELATIONSHIPS

THE TOTAL NUMBER OF PHASE RELATIONSHIPS IS 5297

CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E	CODE	H	K	L	E
146	0	0	24	2.416	151	0	0	26	1.371	177	0	1	27	1.354	3	0	2	2.455	102	0	2	21	1.320	254	0	2	27	1.312	
14	0	2	28	2.016	116	0	3	2	1.471	22	0	3	3	1.245	265	0	3	3	1.246	117	0	3	3	1.427	205	0	3	3	1.331
20	0	3	15	1.474	11	0	3	21	2.035	104	0	2	23	1.345	234	0	3	24	1.797	171	0	3	26	1.255	14	0	3	27	2.212
117	0	4	5	1.465	7	0	4	6	2.371	23	0	4	7	1.813	179	0	4	0	1.580	170	0	5	1	2.037	179	0	5	4	1.352
1	0	5	5	1.252	6	0	5	8	2.371	25	0	5	7	1.418	127	0	5	15	1.467	54	0	5	18	1.521	33	0	5	17	1.262
5	0	5	21	2.042	277	0	5	30	1.231	36	0	6	3	1.817	74	0	6	5	1.617	262	0	6	5	1.225	207	0	6	17	1.326
241	0	6	20	1.277	65	0	6	27	1.535	196	0	7	1	1.310	12	0	7	11	2.032	206	0	7	12	1.321	56	0	7	17	1.426
250	0	7	19	1.255	77	0	7	29	1.521	142	0	8	8	1.425	126	0	8	15	1.468	43	0	8	27	1.752	33	0	8	23	1.512
223	0	7	1	1.306	71	0	9	3	1.541	212	0	9	26	1.276	274	0	10	12	1.456	59	0	10	5	1.656	170	0	10	13	1.366
125	0	10	19	1.435	232	0	10	26	1.291	141	0	11	9	1.432	132	0	12	2	1.456	259	0	12	7	1.246	123	0	12	11	1.426
221	0	13	5	1.205	182	0	13	6	1.345	142	0	13	12	1.426	172	0	13	15	1.364	73	0	14	8	1.610	42	0	14	11	1.332
37	0	7	17	1.817	254	0	10	31	1.250	07	1	0	33	1.626	124	0	10	10	1.471	112	1	1	14	1.350	225	1	1	16	1.302
162	1	1	17	1.642	64	1	2	5	1.559	218	1	2	5	1.309	252	1	2	3	1.255	145	1	2	10	1.276	51	1	2	11	1.251
29	1	2	29	1.202	162	1	3	7	1.316	26	1	2	19	1.656	02	1	3	15	1.573	181	1	3	15	1.346	50	1	3	35	1.700
271	1	3	29	1.237	155	1	4	2	1.406	27	1	4	7	1.506	167	1	4	11	1.375	260	1	4	12	1.249	202	1	4	15	1.324
18	1	4	19	1.560	133	1	4	20	1.494	60	1	4	24	1.626	144	1	5	0	1.423	257	1	5	1	1.251	267	1	5	2	1.240
149	1	5	3	1.415	194	1	5	6	1.333	154	1	5	3	1.322	163	1	5	12	1.385	145	1	5	17	1.342	53	1	5	13	1.270
152	1	5	22	1.407	193	1	5	23	1.334	208	1	6	2	1.319	145	1	6	11	1.423	5	1	6	16	2.184	122	1	6	13	1.474
61	1	6	15	1.652	219	1	6	26	1.229	105	1	7	1	1.505	207	1	7	7	1.320	176	1	7	10	1.276	50	1	7	11	1.546
275	1	7	16	1.234	54	1	8	0	1.677	223	1	8	1	1.251	273	1	8	18	1.276	49	1	8	27	1.550	89	1	8	16	1.562
159	1	9	7	1.393	111	1	9	28	1.302	66	1	10	0	1.677	95	1	10	5	1.532	47	1	10	22	1.702	97	1	10	0	1.274
180	1	11	1	1.334	121	1	11	3	1.469	267	1	11	17	1.245	121	2	0	7	1.494	81	2	0	12	1.576	31	2	0	13	1.556
22	2	0	18	1.575	120	2	0	29	1.434	167	2	0	32	1.335	45	2	1	14	1.727	153	2	1	15	1.407	84	2	1	27	1.567
235	2	1	28	1.289	109	2	2	9	1.506	102	2	2	14	1.512	2	2	3	9	2.761	254	2	3	14	1.252	247	2	2	22	1.262
178	2	3	26	1.254	151	2	3	27	1.335	217	2	4	7	1.310	175	2	4	14	1.253	78	2	4	18	1.558	120	2	5	6	1.456
40	2	5	12	1.787	126	2	5	15	1.445	110	2	5	18	1.503	171	2	5	19	1.365	75	2	5	21	1.604	69	2	5	22	1.621
270	2	6	0	1.239	231	2	6	7	1.291	251	2	6	9	1.257	227	2	6	12	1.253	266	2	6	14	1.246	156	2	6	17	1.400
166	2	6	16	1.375	150	2	6	19	1.433	262	2	6	23	1.247	286	2	7	1	1.227	276	2	7	3	1.221	140	2	7	8	1.433
164	2	7	16	1.281	121	2	7	27	1.457	72	2	9	2	1.618	124	2	10	0	1.460	64	2	10	20	1.636	239	2	10	23	1.285
226	2	10	26	1.299	157	2	11	2	1.394	59	2	11	8	1.518	242	2	11	18	1.275	204	2	12	3	1.322	49	2	12	11	1.704
124	3	0	16	1.452	74	3	0	24	1.503	159	3	0	27	1.327	228	3	0	28	1.254	220	3	2	0	1.307	107	3	2	1	1.507
108	3	2	9	1.507	180	3	2	12	1.352	60	3	2	17	1.582	21	3	3	11	1.478	151	3	3	22	1.408	284	3	4	1	1.223
148	3	4	3	1.326	240	3	4	4	1.282	113	3	4	5	1.494	213	3	4	6	1.319	60	3	4	7	1.552	224	3	4	12	1.202
46	3	5	0	1.712	154	3	5	4	1.406	263	3	5	5	1.220	57	3	5	9	1.666	215	3	5	16	1.206	104	3	5	15	1.505
272	3	5	20	1.237	180	3	5	22	1.345	245	3	6	5	1.246	101	3	6	7	1.512	237	3	6	20	1.298	137	3	6	2	1.442
64	3	7	9	1.568	216	3	7	6	1.315	186	3	7	13	1.342	71	3	7	14	1.619	213	3	7	16	1.223	179	3	7	17	1.498
100	3	8	3	1.514	55	3	8	12	1.671	215	3	8	14	1.316	8	3	9	2	2.057	141	3	9	11	1.286	41	3	10	1	1.176
29	3	10	2	1.862	255	3	11	5	1.252	253	3	12	20	1.253	26	4	0	4	1.509	278	4	0	12	1.229	105	4	0	20	1.500
246	4	0	21	1.264	280	4	0	24	1.227	6	4	1	24	2.100	261	4	1	26	1.243	210	4	1	27	1.315	44	4	2	0	1.741
74	4	2	1	1.561	244	4	2	3	1.259	125	4	2	5	1.449	123	4	2	25	1.473	165	4	2	24	1.272	229	4	2	25	1.253
168	4	3	1	1.373	23	4	2	2	1.564	203	4	3	6	1.323	263	4	3	14	1.247	214	4	3	20	1.217	47	4	4	1	1.707
13	4	4	6	2.019	115	4	4	10	1.490	243	4	4	12	1.271	281	4	4	15	1.227	56	4	4	15	1.679	83	4	5	0	1.572
224	4	5	2	1.288	32	4	5	8	1.850	147	4	5	9	1.416	103	4	5	12	1.509	201	4	5	17	1.322	146	4	6	3	1.371
190	4	6	6	1.337	263	4	6	7	1.245	23	4	6	8	1.818	135	4	6	11	1.451	248	4	6	12	1.261	114	4	6	13	1.452
236	4	6	15	1.284	17	4	6	17	1.979	211	4	6	22	1.319	52	4	7	9	1.682	67	4	7	10	1.554	25	4	7	15	1.517
222	4	8	0	1.304	52	4	8	6	1.543	244	4	8	7	1.246	14	4	8	12	2.014	225	4	8	3	1.251	63	4	8	5	1.641
189	4	9	5	1.337	160	4	9	9	1.309	152	4	9	10	1.334	197	4	9	11	1.371	174	4	9	15	1.358	76	4	10	1	1.519
205	4	10	6	1.319	249	4	10	8	1.261	76	4	11	0	1.602	34	4	11	2	1.618										

THE TOTAL NUMBER OF PHASE RELATIONSHIPS IS 5297

THE NUMBER OF PHASE RELATIONSHIPS SAVED IS 2228

THE MINIMAL VALUE OF KAPPA IS 0.60

FILE

*** 0105 * C15-2202 ***

SIGNAL RESULTS AND CONVERGENCE

REFLECTIONS REQUESTED FOR STARTING SET APE

NSPEC = 0

NOEN = 0

MAXI = 0

*** SIGNAL RESULTS ***

PHASE ACCEPTED IF PROBABILITY GREATER THAN 0.65 AND NUMBER OF CONVERGENT POINTS IS GREATER THAN 3

CODE	H	K	L	E	PHI	PROB	%C	CODE	H	K	L	E	PHI	PROB	%C	CODE	H	K	L	E	PHI	PROB	%C
1	0	2	5	2.00	180	0.500	0	7	0	4	8	2.07	180	0.525	1	14	0	2	29	2.07	180	0.525	2
19	0	4	8	1.98	180	0.500	0	22	2	0	18	1.98	180	0.500	0	21	4	0	4	1.91	180	0.491	2
36	0	6	0	1.82	180	0.237	11	44	4	2	0	1.78	360	0.579	4	73	0	14	9	1.61	180	0.520	0
81	2	0	12	1.58	180	0.548	3	83	0	8	28	1.55	360	0.573	3	106	4	0	23	1.51	180	0.520	0
129	2	10	0	1.46	180	0.611	11	132	0	12	2	1.45	180	0.500	0	135	0	10	19	1.44	180	0.516	0
143	0	8	8	1.42	180	0.519	1	146	4	6	0	1.42	180	0.656	5	148	0	0	24	1.42	180	0.520	2
158	0	0	26	1.39	350	0.561	3	187	2	0	32	1.34	360	0.573	3	222	4	8	0	1.33	350	0.545	2
232	0	10	26	1.29	180	0.500	0	241	0	6	20	1.28	360	0.527	2	270	2	6	0	1.24	360	0.577	0
274	0	10	0	1.22	180	0.194	13	243	4	0	24	1.23	180	0.511	2								

MAXIMUM NUMBER OF SPTS REQUIRED = 65

TABLE OF ESTIMATED ALPHA'S

CODE	ALPHA	MK	CODE	ALPHA	MK	CODE	ALPHA	MK	CODE	ALPHA	MK	CODE	ALPHA	MK	CODE	ALPHA	MK	CODE	ALPHA	MK	CODE	ALPHA	MK
1	95.7	7	2	71.5	1	3	47.1	13*	4	27.4	7	5	28.3	1	6	19.5	1	7	22.6	13*	8	25.1	1
9	14.3	7	10	20.1	7	11	19.5	7	12	15.6	7	13	22.3	1*	14	13.5	13*	15	16.5	1*	16	11.7	7
17	16.2	1	18	22.1	1	19	22.1	13*	20	12.7	7	21	22.7	1	22	11.7	13*	23	15.0	1	24	24.1	1
25	13.3	1	26	11.9	13*	27	24.7	1	28	19.1	7	29	14.5	1	30	9.9	7	31	10.9	7	32	12.5	1
33	11.7	1*	34	10.5	1	35	13.4	7	36	7.2	13*	37	5.5	7	38	13.1	12	39	12.2	1	40	12.7	1
41	14.1	1	42	6.2	13	43	7.3	13	44	7.6	13*	45	13.5	1	46	7.2	7	47	13.3	1	48	3.0	1
49	8.7	1	50	5.5	1	51	20.8	1	52	10.7	1	53	10.9	1	54	6.5	7	55	10.6	1	56	7.7	1
57	12.7	1	58	17.1	1	59	4.0	13	60	12.4	1	61	8.9	1	62	11.4	1	63	7.6	1	64	7.1	1*
65	2.0	12	66	3.7	7	67	2.4	7	68	6.3	1	69	9.6	1	70	6.5	12	71	6.7	1	72	10.7	1
73	4.3	13*	74	7.7	13	75	11.5	1	76	2.3	13	77	4.7	7	78	10.2	1*	79	5.4	13	80	7.2	1
81	6.4	13*	82	9.8	1	83	5.8	12	84	7.6	1	85	6.1	1	86	15.1	1	87	6.2	1	88	4.3	12*
89	7.6	1	90	5.5	1	91	8.6	1	92	7.6	1*	93	7.5	7	94	6.1	1	95	5.3	1	96	4.6	7
97	2.6	7	98	6.8	7	99	4.5	1	100	6.4	1	101	5.8	1	102	5.9	1*	103	4.5	1	104	5.8	1
105	9.7	1	106	3.7	13*	107	11.2	1	108	7.7	1	109	8.0	1	110	6.3	1	111	5.2	1	112	10.0	1
113	7.0	1	114	4.3	1	115	7.4	1*	116	7.3	7	117	4.3	12	118	6.1	1	119	9.5	7	120	2.0	7
121	5.2	7	122	5.2	1	123	5.0	1	124	12.8	1	125	6.4	1	126	4.9	13	127	4.2	7	128	5.6	1
129	2.8	13*	130	6.0	1	131	2.1	1	132	4.1	13*	133	6.5	1	134	2.7	13	135	2.4	1	136	6.3	1
137	4.8	1	138	2.2	12	139	2.8	13*	140	5.6	1	141	3.7	7	142	2.2	7	143	4.5	13*	144	2.6	1
145	5.8	1	146	2.6	12*	147	5.6	1	148	2.7	13*	149	5.3	1	150	4.5	1	151	4.5	1	152	4.2	7
153	7.7	1	154	5.5	1	155	6.8	1	156	5.7	1	157	4.2	1	158	1.9	12*	159	6.5	1	160	4.0	7
161	5.1	1	162	7.4	1	163	4.8	1	164	3.8	1	165	5.9	1	166	4.8	1*	167	7.0	1	168	4.3	1
169	2.9	1*	170	5.3	12	171	3.7	1	172	1.4	7	173	1.8	7	174	4.3	1	175	2.8	1*	176	7.1	1
177	5.1	7	178	2.2	1	179	4.3	7	180	5.6	1	181	4.0	1	182	1.6	7	183	3.2	1	184	4.2	7
185	4.3	1	186	2.9	1	187	0.3	13*	188	3.3	1	189	2.3	1	190	3.8	1*	191	2.4	1	192	3.1	1
193	2.7	1	194	2.6	1	195	5.2	1	196	4.3	7	197	3.6	1	198	4.1	1	199	1.6	7	200	1.5	12
201	2.6	1	202	3.4	1	203	3.9	1	204	1.7	1	205	3.2	7	206	3.1	7	207	4.1	1	208	6.3	1
209	3.0	1*	210	3.1	1	211	2.3	1*	212	1.8	7	213	5.0	1	214	4.1	1	215	1.8	1	216	2.8	1
217	3.7	1	218	4.5	1	219	2.8	1	220	1.9	7	221	1.1	7	222	1.8	13*	223	3.2	7	224	3.0	1
225	5.6	1	226	2.9	1*	227	4.4	1*	228	1.7	12	229	1.4	1	230	1.5	1	231	2.9	1	232	2.2	12*
232	6.3	1	233	2.3	7	234	3.2	1	235	1.8	1	236	1.8	1	237	1.3	1	238	2.2	1	239	2.2	1
241	0.9	13*	242	2.0	1	243	3.1	1*	244	4.5	1	245	2.9	1	246	1.2	7	247	3.2	1	248	1.7	1*
249	1.1	1*	250	2.2	7	251	1.7	1	252	3.7	1	253	0.6	1	254	3.1	1	255	2.1	1	256	2.1	13
257	3.2	1	258	0.9	7	259	2.5	13	260	3.0	1	261	1.8	1	262	2.6	1	263	2.6	1	264	3.7	1
265	2.1	7	266	2.5	1*	267	1.6	1	268	3.5	1	269	2.5	1	270	1.3	13*	271	1.0	1	272	2.8	1
273	1.9	1	274	0.6	13*	275	3.1	1	276	3.8	1	277	1.7	7	278	2.1	7	279	0.5	1	280	0.6	13*
281	2.1	1	282	1.3	13	283	1.7	1	284	2.5	1	285	2.7	1	286	2.8	1						

TITLE

*** H 105 * C15H22C2 ***

CONVERGENCE MAPPING

MILTAZ HAS DIFFICULTY IN FINDING GOOD ORIGIN DEFINING REFLECTIONS PLEASE LOOK CRITICALLY AT THE CONVERGENCE RESULTS

INITIAL CONVERGENCE LISTING FINAL STAGES ONLY GC REFLECTIONS

CCCE	H	K	L	ALFEST	CONTRIBUTORS																			
105	1	7	1	1.25	24	8	0	1.02	31	23	0	0.80	105	32	12	0.70	153	5	0	0.78				
24	4	2	1	1.10	23	10	0	1.21	119	32	12	0.90												
23	4	2	2	1.01	32	3	0	1.61																
32	4	5	0	0.90																				
89	1	9	4	2.10	26	8	0	1.02	27	10	12	1.01	86	12	0	0.82	106	25	12	0.75	167	1	12	1.16
10	0	5	1	1.65	59	37	0	1.00	58	51	0	0.55	145	124	0	0.71	167	124	12	0.69	176	51	12	0.78
100	3	2	9	2.16	53	2	12	1.17	12	8	0	1.05	80	19	12	0.79	86	26	12	0.75	107	15	12	0.75
					53	52	0	0.71																
60	3	2	17	2.15	51	12	0	0.90	44	37	0	0.84	01	24	0	0.75	86	81	0	0.65	145	12	12	0.70
					154	11	0	0.76	195	2	0	0.97												
37	1	0	17	2.24	51	3	0	1.35	59	16	0	1.01	154	25	0	0.69	167	7	0	0.86	177	124	0	0.61
					195	35	12	0.74																
20	0	3	15	2.26	19	12	0	1.33	112	86	12	0.77	124	39	0	0.69	177	19	12	0.49	195	51	0	0.75
					233	52	12	0.72																
39	1	2	25	1.99	51	22	12	1.01	53	12	0	1.03	78	52	0	0.61	145	78	12	0.69	153	112	0	0.64
					195	11	12	0.97																
233	1	8	1	2.22	27	7	0	0.85	27	19	0	0.61	195	2	12	0.79	80	13	12	0.72	78	13	12	0.69
					44	41	12	0.67	53	35	12	0.65	124	12	12	0.65	113	13	12	0.45				
195	1	5	3	1.97	107	2	12	0.93	13	8	0	0.52	51	28	12	0.71	112	7	0	0.69	85	28	0	0.66
					177	18	0	0.60	153	27	12	0.60	154	26	0	0.67								
19	0	4	9	2.03	29	12	0	1.27	61	51	0	0.92	101	41	0	0.89	107	101	0	0.75	124	32	0	0.62
44	4	2	0	2.05	13	3	0	1.56	52	35	0	0.89	101	17	12	0.64	112	66	12	0.69	147	117	0	0.61
112	3	4	5	2.11	112	2	12	1.00	107	3	0	1.00	27	15	0	0.96	58	25	0	0.79	81	27	0	0.75
					102	61	0	0.62																
12	4	7	5	2.12	20	12	0	1.07	51	8	0	0.58	58	41	12	0.83	78	2	12	1.24	154	86	0	0.62
78	2	4	18	2.10	61	41	0	0.73	61	7	0	0.87	81	13	0	0.85	101	51	0	0.69	107	61	0	0.67
					153	28	0	0.71	177	2	12	1.00												
177	0	1	27	1.83	11	3	0	1.22	5	7	0	0.66	11	7	12	0.95	25	15	12	0.97				
61	1	6	17	2.13	58	2	0	1.27	101	81	0	0.66	112	1	0	1.25	115	58	0	0.66	124	35	0	0.74
115	0	3	9	2.11	22	2	0	1.39	25	13	0	0.56	101	8	0	0.77	124	18	0	0.72	176	18	12	0.67
					225	27	12	0.62																
101	3	6	7	1.80	41	7	0	0.93	66	15	0	0.75	102	27	0	0.73	107	7	0	0.79	112	75	12	0.61
					145	22	0	0.71	145	26	12	0.69												
41	3	10	1	1.78	51	15	12	1.01	154	1	12	1.26	176	2	12	1.11								
124	3	5	4	1.84	85	7	0	1.31	8	7	12	1.00	51	25	0	0.75	124	13	0	0.70	107	23	0	0.67

22	2	C	18	1.85	153	18	12	0.65	167	27	12	C.67	167	60	0	0.75								
16	0	3	27	1.64	16	2	12	1.44	225	51	12	0.74	225	167	12	C.69	167	124	0	0.67	176	51	0	0.78
9	0	5	21	1.61	58	51	12	0.95	112	27	12	C.58	145	124	2	C.72	112	28	12	C.60	124	11	12	C.65
51	1	2	11	1.68	75	58	0	0.75	88	7	12	0.91	107	61	0	0.67								
176	1	7	10	1.75	176	75	12	0.62	86	1	0	1.15	26	27	0	0.82	167	11	0	C.63				
167	1	4	11	1.74	18	2	C	1.21	86	3	0	0.75	124	11	12	C.69	147	8	C	C.67	112	28	12	C.65
					225	1	12	C.97																
26	4	0	4	1.80	25	12	0	1.24	107	86	12	0.75	147	1	0	1.47								
25	4	7	15	1.37	13	11	C	1.32	147	3	0	1.21	29	15	0	0.95	81	75	0	0.60				
147	4	5	9	1.37	15	11	12	C.57	27	8	12	0.93	124	2	C	1.02	145	15	C	C.72				
107	3	2	1	1.56	60	3	0	1.11	86	13	0	0.79	86	7	C	C.77	225	1	12	1.01				
145	1	6	11	1.80	8	2	12	1.35	98	11	12	C.60	225	66	12	0.69								
11	0	3	21	1.54	81	2	12	1.48	112	27	12	0.57	225	3	0	C.56	225	7	12	C.75				
58	1	3	10	1.68	86	1	0	1.51	153	86	12	0.61												
86	1	2	5	C.81	102	18	12	0.78	112	2	0	1.08												
102	2	2	14	1.67	2	1	0	2.27																
13	4	4	6	1.01	15	7	0	1.61	153	2	12	1.31	153	75	12	0.74								
7	0	4	6	1.05	153	2	C	1.15	153	75	0	0.78												
153	2	1	15	1.12	7	2	0	1.73																
81	2	0	12	1.86	78	2	0	1.33	27	18	12	C.55	60	18	C	C.64	75	35	C	C.77				
27	1	4	7	1.49	112	75	C	C.77	124	28	12	C.69	225	2	12	1.15	225	35	12	C.75				
225	1	1	16	1.09	60	7	12	0.99	124	2	12	C.45	26	18	C	C.61								
26	C	3	7	C.92	35	3	0	1.57																
35	C	5	5	C.85	40	6	C	1.33	124	18	0	0.89												
124	1	1	10	1.23	19	2	0	1.35	15	8	12	1.02												
7	2	3	5	C.89	75	11	12	1.19																
75	2	5	21	1.74	18	F	C	1.09	112	60	0	0.66												
15	4	8	12	1.03	60	18	C	1.13	112	8	0	1.04												
112	1	1	14	1.31	19	1	C	1.61																
60	3	4	7	1.24	8	1	12	1.05																
12	0	7	11	1.34	3	1	0	2.93																

CONVERGENCE HAS REJECTED THE FOLLOWING 50 REFLEXIONS FROM THE PHASE DETERMINATION PROCESS

CODE	H	K	L	MK	CODE	H	K	L	MK	CODE	H	K	L	MK	CODE	H	K	L	MK	CODE	H	K	L	MK
256	0	2	27	13	291	4	4	15	1	278	4	C	13	7	176	2	3	26	1	120	2	C	29	7
242	2	11	18	1	255	3	11	9	1	273	1	E	12	1	230	4	9	3	1	193	1	5	23	1
234	0	3	24	7	158	0	0	26	13*	165	4	2	26	19	65	C	6	27	13	212	0	9	26	7
261	4	1	26	1	234	4	5	2	1	222	4	8	0	13*	283	3	7	16	1	277	C	5	20	7
248	4	6	12	1*	240	3	4	4	1	251	2	C	9	1	274	2	12	3	1	197	3	0	27	7
182	0	13	5	7	219	3	8	14	1	237	3	6	20	1	200	C	6	19	13	226	4	2	29	1
238	4	6	15	1	270	2	6	C	13*	282	0	6	9	13	246	4	0	21	7	245	4	10	8	1*
271	1	3	29	1	258	1	0	31	7	241	0	6	20	13*	253	3	12	20	1	274	C	10	0	13*
279	1	6	26	1	187	2	0	22	13*															

THE NUMBER OF RELATIONSHIPS ACCEPTED IS 1914

TITLE *** H 105 * C15H22O2 *** CONVERGENCE RESULTS

THE NUMBER OF ORIGIN DEFINING REFLECTIONS IS 2

ORIGIN FIXING REFLECTIONS

CODE	H	K	L	PHI	PK	CODE	H	K	L	PHI	PK	CODE	H	K	L	PHI	PK
1	0	5	5	90	7	5	1	6	16	45	1	6	2	5	2	45	1

THE PHASE OF THE 3 9 2 REFLECTION CAN HAVE THE TWO VALUES 45 AND 315 DEGREES

OTHER REFLECTIONS IN STARTING SET

CODE	H	K	L	PK	CODE	H	K	L	PK	CODE	H	K	L	PK	CODE	H	K	L	PK
3	0	2	6	13	18	1	4	15	1	53	1	5	18	1					

THE ENANTIOMORPH IS FIXED BY THE 1 6 16 REFLECTION

MAGIC INTEGER REPRESENTATION (PHI IN) * MIN(PK) OF UNKNOWN GENERAL PHASES IN STARTING SET

CODE	H	K	L	PHI IN	CODE	H	K	L	MIN(PK)	CODE	H	K	L	PHI IN	CODE	H	K	L	PHI IN
18	1	4	15	3	53	1	5	18	2										

NUMBER OF SETS TO BE GENERATED = 56

TITLE *** H 105 * C15H22O2 *** SET UP PSI ZERO RELATIONSHIPS

THE 33 WEAKEST REFLECTIONS TAKE PART IN 1773 RELATIONSHIPS

PSI ZERO FIGURE OF MERIT TO BE CALCULATED USING 33 REFLECTIONS AND 1773 RELATIONSHIPS

TITLE

*** 3 103 * C15H272 ***

NUMBER OF PHASE SETS ALREADY DEVELOPED IS 0

THE EARLY FIGURES OF MULTI ARE NOT TO BE APPLIED

SET	FIGURES OF MULTI		UNCERTAIN	STARTING PHASES	SET PHASES GENERATED BY PROGRAM					
	ANS	PSI/CFC			RESID	1	3	5	8	18
1	1.4254	1.282	37.03	0	50	360	45	45	39	26
2	1.4904	1.656	40.05	0	90	360	45	45	116	77
3	1.7675	1.007	45.80	0	90	360	45	45	193	129
4	1.6855	1.675	44.16	0	90	360	45	45	270	180
5	0.9105	1.345	122.05	195	50	360	45	45	247	231
6	1.9153	2.366	51.74	0	50	360	45	45	64	283
7	1.7727	1.455	43.77	0	90	360	45	45	141	234
8	1.9155	2.080	52.45	0	50	360	45	45	219	26
9	1.6155	1.515	44.23	0	90	360	45	45	296	77
10	1.7606	1.101	35.53	0	50	360	45	45	13	129
11	1.9032	1.945	52.61	0	90	360	45	45	90	180
12	0.9160	1.652	139.56	195	90	360	45	45	167	231
13	1.9077	2.308	51.77	0	50	360	45	45	244	283
14	1.6161	1.860	49.05	0	90	360	45	45	321	334
15	0.9371	2.364	122.02	195	50	180	45	45	39	26
16	0.9379	1.147	130.08	203	50	180	45	45	116	77
17	1.3722	0.455	31.43	0	90	180	45	45	193	129
18	2.2623	2.532	63.73	0	50	180	45	45	270	180
19	1.7356	1.489	47.18	0	90	180	45	45	347	231
20	1.7690	1.465	47.92	0	50	180	45	45	64	283
21	1.7664	1.670	46.16	0	50	180	45	45	141	334
22	0.9878	0.560	175.20	158	90	180	45	45	215	76
23	0.9065	1.101	156.44	201	90	180	45	45	296	77
24	1.7550	1.501	41.95	0	90	180	45	45	13	129
25	1.6329	1.718	42.66	0	50	180	45	45	50	100
26	1.6258	1.752	42.01	0	90	180	45	45	167	231
27	2.1750	2.452	61.85	0	90	180	45	45	244	283
28	2.1334	2.542	61.28	0	50	180	45	45	321	334
29	1.4087	1.375	36.20	0	90	360	45	315	35	26
30	1.9160	2.473	52.62	0	50	360	45	315	116	77
31	0.9858	1.151	155.95	157	90	360	45	315	193	129
32	1.6357	1.500	41.67	0	50	360	45	315	270	180
33	1.7023	1.860	45.13	0	50	360	45	315	347	231
34	1.6467	1.454	45.21	0	90	360	45	315	64	283
35	1.5949	1.979	41.96	0	50	360	45	315	141	334
36	1.6121	1.481	42.45	0	90	360	45	315	219	26
37	1.5861	1.451	40.98	0	50	360	45	315	296	77
38	0.9849	1.121	166.79	157	90	360	45	315	13	129
39	1.9721	1.534	52.42	0	90	360	45	315	90	180
40	1.5948	1.332	41.01	0	50	360	45	315	167	231
41	1.6617	1.454	44.25	0	90	360	45	315	244	283
42	1.0770	2.068	52.60	0	50	360	45	315	321	334
43	1.8766	1.825	48.71	0	90	180	45	315	39	26
44	1.7835	1.632	46.70	0	90	180	45	315	116	77
45	1.7415	1.057	33.52	0	50	180	45	315	193	129
46	2.1432	2.274	59.43	0	90	180	45	315	270	180
47	1.5940	2.080	43.63	0	50	180	45	315	347	231
48	0.9872	1.059	145.54	207	50	180	45	315	64	283
49	0.9872	1.078	125.96	196	50	180	45	315	141	334
50	2.0313	1.719	50.49	0	50	180	45	315	219	26
51	2.2344	2.071	61.16	0	90	180	45	315	256	77
52	1.7412	1.462	45.52	0	50	180	45	315	13	129
53	1.7564	2.170	59.76	0	90	180	45	315	90	180
54	1.7779	1.596	47.67	0	50	180	45	315	167	231
55	0.9855	1.119	145.01	200	50	180	45	315	244	283
56	0.9855	1.067	121.82	185	90	180	45	315	321	334

TITLE

*** H 105 * C 1542202 ***

SUMMARY OF FIGURES OF MERIT OUTPUT BY TANGENT FORMULA

	ADS FCM	PSI ZFCO	PESID
MAXIMUM VALUE	2.2622	2.671	63.73
MINIMUM VALUE	1.2415	0.059	33.43
RELATIVE HEIGHTS (OFF COMBINED FCM)	0.60	1.20	1.20

NUNSET	ADS FCM	PSI ZFCO	PESID	COMBINED FCM
1	1.4299	1.322	37.03	1.7607
2	1.4904	1.051	40.05	2.0171
3	1.7735	1.007	45.00	1.5567
4	1.6897	1.675	44.17	1.6609
6	1.9193	2.266	57.14	1.0101
7	1.6737	1.659	63.77	1.6767
9	1.9165	2.080	52.42	1.2122
9	1.6194	1.719	44.23	1.4485
10	1.3606	1.100	25.22	2.1456
11	1.9837	1.545	52.61	1.3290
13	1.7097	2.308	51.77	1.0841
16	1.6181	1.860	45.05	1.4153
17	1.7225	0.059	33.43	2.4202
18	2.2622	2.532	63.73	0.2520
19	1.7396	1.585	47.38	1.3597
20	1.7680	1.965	47.52	1.3715
21	1.7484	1.670	46.16	1.4721
24	1.7570	1.401	43.55	1.8562
25	1.5529	1.311	42.66	1.6149
26	1.6758	1.793	42.01	1.6265
27	2.1759	2.642	61.85	0.6363
28	2.1354	2.512	61.28	0.4581
29	1.4087	1.379	36.20	1.9889
30	1.9160	2.432	52.42	0.9792
32	1.6357	1.560	43.47	1.7084
33	1.7073	1.860	45.13	1.5084
34	1.6467	1.654	44.21	1.6452
35	1.5155	1.555	40.56	1.7889
36	1.6121	1.681	42.55	1.6533
37	1.5661	1.651	40.50	1.7325
38	1.9321	1.934	52.32	1.5111
40	1.5448	1.322	41.01	1.9107
41	1.6617	1.854	44.29	1.5195
42	1.8970	2.068	52.00	1.2015
43	1.8266	1.825	48.71	1.4707
46	1.7879	1.832	46.70	1.5207
49	1.3415	1.057	38.57	2.0000
48	2.1427	2.374	59.43	0.3186
47	1.5840	2.000	49.71	1.4660
50	2.0212	1.715	50.45	1.2165
51	2.2346	2.671	63.73	0.6042
52	1.7412	1.662	45.52	1.6456
53	1.7504	2.170	50.36	1.1214
54	1.7779	1.557	47.07	1.6316

ตารางที่ 6.4 (ก) แสดงการขีด JCL เพื่อคำนวณโดยโปรแกรม EXFFT ในระบบ OS/VS1

```
1 //ZIAD1034 JOB CLASS=T,MSGLEVEL=(1,1),MSGCLASS=A,TYPROJ=FOLO
2 //ST1 EXEC FORIVLG,PARM='LET,LIST'
3 //LKED.SYSPRINT DD SYSOUT=A
4 //LKED.SYSL400 DD DSN=EQGJSET(900PGM),DISP=(,PASS),UNIT=SYSDA,
5 // SPACE=(TRK,(50,20,1),RLSE)
6 //LKED.SYSLIN DD DSN=CUP1.XTAL03J(EXFFT),DISP=SI,UNIT=SYSDA,
7 // VOL=SER=VS1WK1
8 //DD.FT05F001 DD SYSOUT=A
9 //FT05F001 DD UNIT=TAPE,VOL=SER=2556,DISP=(OLD,KEEP),LABEL=(,IL),
10 // JCB=(RECFM=V,LRECL=1796)
11 //FT04F001 DD UNIT=TAPE,VOL=SER=3100,DISP=(OLD,KEEP),LABEL=(,IL),
12 // JCB=(RECFM=V,LRECL=1796)
13 //FT08F001 DD UNIT=TAPE,VOL=SER=0327,DISP=(OLD,KEEP),LABEL=(,IL),
14 // JCB=(RECFM=V,LRECL=1796)
15 //SYSIN DD *
16
17 /*
18 //
```

ตารางที่ 6.4 (ข) แสดงผลการคำนวณจากโปรแกรม EXFFT

```

FAST FOURIER TRANSFORM                                VERSION JAN 1980
-----
TITLE                                *** P.105 'C15H22O2' ***
-----
NPTS  ET      ABS RM      PSI ZFC      RESID
17      1.2725      C.86      33.42
-----
GRID SPACING IS APPROXIMATELY C.333 ANGSTROMS
-----
UNIT CELL PARAMETERS      A      B      C      ALPHA      BETA      GAMMA
                           8.124    12.266    27.672    90.0      90.0      90.0
-----
MAXIMUM INDICES           H      K      L
                           4      14     32
-----
NUMBER OF GRID POINTS    NX      NY      NZ
IN FOURIER MAP           24     40     90
-----
FOURIER MAP FACT TO BE PRINTED
-----
NUMBER OF INDEPENDENT REFLECTIONS INPUT = 284
NUMBER OF REFLECTIONS IN ONE HEMISPHERE = 944
SCALE = 2.923

```

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

ตารางที่ 6.5 (ก) แสดงการขีด JCL เพื่อคำนวณโดยโปรแกรม SEARCH ในระบบ OS/VS1

```
1 //ZIAD7733 JOB CLASS=T,MSGLEVEL=(1,1),MSGCLASS=A,TYPRUN=HOLD
2 //ST1 EXEC POF1JLS,PARM='LET.LIST'
3 //LKED.SYSPRINT DD SYSOUT=A
4 //LKED.SYSL100 DD DSN=66G0SET(250P3M),DISP=(,PASS),UNIT=SYSDA,
5 // SPACE=(TRK,(50,20,1),RLSE)
6 //LKED.SYSLIN DD DSN=CUP1.XTALOBJ(SEARCH),DISP=(R,UNIT=SYSJA,
7 // VOL=SER=VSLWK3
8 //GD.FT03F01 DD SYSOUT=A
9 //FT03F01 DD UNIT=TAPE,VOL=SER=2556,DISP=(OLD,KEEP),LABEL=(,NL),
10 // DCB=(RECFM=V,LRECL=1795)
11 //FT03F01 DD UNIT=TAPE,VOL=SER=0327,DISP=(OLD,KEEP),LABEL=(,NL),
12 // DCB=(RECFM=V,LRECL=1795)
13 //SYSIN DD *
14
15 /*
16 //
```

ตารางที่ 6.5 (ข) แสดงผลการคำนวณจากโปรแกรม SEARCH

PEAK SEARCH AND INTERPRETATION

VERSION JUN 1990

TITLE

*** F 105 4 C15M22E2 ***

SET NO. 17

NUMBER OF ATOMS TO BE FOUND IS 24

NUMBER OF ATOMIC POSITIONS INPUT FROM CARDS IS 0

NUMBER OF HEAVY ATOMS IN ASYMMETRIC UNIT IS 0

NUMBER OF PEAKS TO BE CONSIDERED IS DECIDED BY PROGRAM

STEREOCHEMICAL CRITERIA

MINIMUM BONDING DISTANCE = 1.10
 MAXIMUM BONDING DISTANCE = 1.95
 MINIMUM BOND ANGLE = 85.0
 MAXIMUM BOND ANGLE = 145.0

INTERATOMIC DISTANCES ARE OMITTED WHEN LESS THAN 2.40

NO BOND SEQUENCES TO BE INPUT

NUMBER OF PROJECTIONS TO BE OUTPUT IS DECIDED BY PROGRAM

UNIT CELL PARAMETERS

A = 8.124
 B = 12.304
 C = 27.677
 ALPHA = 90.00
 BETA = 90.00
 GAMMA = 90.00

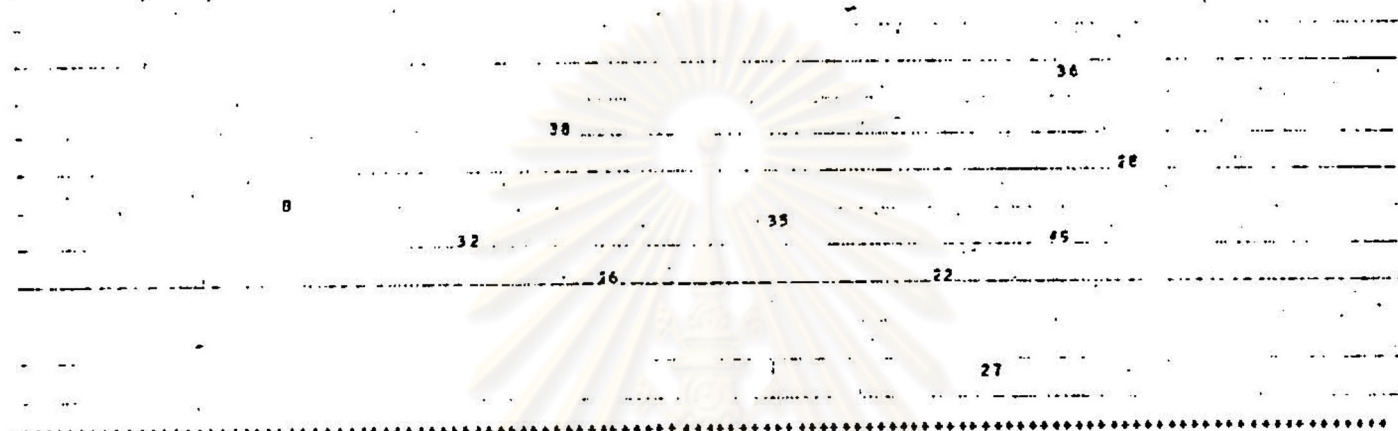
NONCENTROSYMMETRIC SPACE GROUP SYMMETRY OPERATORS WITH LATTICE TYPE P

1	1.	0.	0.	0.0000	0.	0.	1.	0.0000	0.	0.	0.	1.0000
2	1.	0.	0.	0.5000	0.	0.	1.	0.0000	0.	0.	0.	1.0000
3	1.	0.	0.	0.5000	0.	0.	1.	0.0000	0.	0.	0.	1.0000
4	1.	0.	0.	0.0000	0.	0.	1.	0.0000	0.	0.	0.	1.0000

** SINCE SPACE GROUP SYMMETRY PERMITS, ONLY HALF THE MAP WILL BE SEARCHED **

TITLE *** H 105 * C15H22O2 *** SET NO. 17 CLUSTER 5

PLOT OF PEAKS ON LEAST SQUARES PLANE SCALE = 2.50 CM/A



TITLE *** H 105 * C15H22O2 *** SET NO. 17 CLUSTER 5

PLOT OF PEAKS ON PLANE ORTHOGONAL TO LEAST AND MOST SQUARES PLANES SCALE = 2.50 CM/A



INTERPRETATION OF CLUSTER 5 STARTING WITH PEAK NUMBER 22

PEAK	22	26	27	28	32	35	38
FRAGMENTS TO	27	32	22	22	26	22	32
FRAGMENTS TO	28	35			38	28	
FRAGMENTS TO	35						
FRAGMENT	1	1	1	1	1	1	1

NO. OF PEAKS IN EACH FRAGMENT 7

ศูนย์วิทยุทรัพยากร
 วิทยาลัยเกษตรและเทคโนโลยี

TITLE		*** P 105 * C15H22C2 ***			PEAK COORDINATES	
PEAK	HEIGHT	X	Y	Z	CLUSTER NUMBER	
1	1509	C.755C	C.0766	C.5533	1	
2	1324	C.5468	C.2256	C.21C5	0	
3	1115	0.0469	0.2324	C.9A84	0	
4	1117	C.7851	C.2544	C.17C4	0	
5	955	C.9942	0.2443	C.357C	2	
6	866	0.7015	0.07C9	0.2270	2	
7	861	C.7113	C.2417	C.3553	4	
8	812	0.3235	C.66C3	C.42C4	5	
9	8C2	C.4531	0.1137	0.9460	0	
10	765	C.25C1	0.2513	0.3873	4	
11	764	0.7113	C.12C6	C.85EE	6	
12	763	0.7205	0.0973	0.10C0	7	
13	755	C.2021	0.0745	0.7768	8	
14	707	0.7912	C.6543	C.6621	8	
15	689	0.2967	0.2114	C.1686	0	
16	666	C.66C7	C.0255	0.2666	3	
17	65C	C.6597	C.1641	C.3172	4	
18	639	0.6706	0.1192	C.0684	7	
19	630	C.5366	C.2215	0.3194	4	
20	62C	C.6216	C.6559	C.2767	2	
21	601	C.8224	0.4265	0.4422	4	
22	555	C.3370	0.4293	0.5554	5	
23	557	C.5371	C.0355	0.5976	0	
24	591	0.7933	0.0761	C.9112	6	
25	5EE	0.4625	0.2456	0.3534	4	
26	580	C.7391	C.2245	C.4984	5	
27	578	0.3304	C.5253	C.5284	5	
28	574	C.4545	0.4765	0.6130	5	
29	545	C.5577	C.1423	C.9C21	6	
30	518	C.623C	C.10F1	C.522C	1	
31	513	C.6271	C.1733	0.9525	6	
32	51C	C.2964	C.156C	C.4623	5	
33	5C7	0.4152	0.1007	C.8113	6	
34	5C2	C.4527	C.0963	0.7666	5	
35	501	0.3842	C.22C8	C.52C7	5	
36	500	0.5521	0.4251	0.6015	5	
37	454	0.1232	0.0070	C.4899	0	
38	486	C.4951	C.2217	C.4642	5	
39	491	0.7026	0.1873	C.6886	8	
40	46C	C.2832	C.1623	C.3455	4	
41	475	C.7085	C.3512	C.421C	4	
42	477	0.7228	C.2070	C.3532	4	
43	46E	C.7935	C.2541	0.0238	0	
44	463	C.5776	C.4227	C.4328	4	
45	44E	C.2674	C.3449	C.7697	8	
46	447	C.5456	0.1269	0.7174	8	
47	440	C.553C	C.1510	0.3128	2	
48	436	0.3458	0.07C5	C.7264	8	
49	435	C.2950	C.4060	0.5161	5	
50	432	C.651C	C.1753	C.7225	8	
51	430	1.0399	0.1247	C.8564	6	

TOTAL NUMBER OF PEAKS IN EACH CLUSTER 2 3 2 1 10 5 2 5

TITLE		*** H 101 * C15H22O2 ***		TABLE OF INTERPEAK DISTANCES			
FROM	TO	DIST					
1	30	1.72					
2	4	2.29	15	2.35			
4	2	2.29					
5	7	2.30	47	1.72			
6	16	1.52	20	2.13			
7	5	2.30	17	1.49	19	1.76	25 2.02 42 1.26
8	32	1.67					
10	25	1.57	40	1.45			
11	24	1.01	29	2.01	21	1.84	
12	18	1.15					
13	33	2.00	34	2.07	45	1.42	48 2.17
14	39	1.64	50	2.39			
15	2	2.35					
16	6	1.52					
17	7	1.45	15	1.50	20	2.27	25 2.29 47 2.07
18	12	1.15	42	2.31			
19	7	1.76	17	1.50	25	1.16	40 2.23
20	6	2.13	17	2.27	47	1.21	
21	41	1.29	42	2.19	44	2.01	
22	27	1.45	28	1.94	35	1.61	36 2.16 45 1.72
23	33	2.38					
24	11	1.01	25	1.55	21	1.67	
25	7	2.02	10	1.97	17	2.39	15 1.16 40 1.66
26	32	1.79	25	1.87	38	2.28	
27	22	1.45					
28	22	1.94	36	1.06	49	1.55	
29	13	2.01	24	1.49	31	1.79	51 1.61
30	1	1.72	22	2.38	38	2.49	
31	11	1.84	24	1.67	29	1.79	
32	6	1.67	26	1.39	38	1.83	
33	13	2.00	34	1.27	45	1.37	
34	13	2.07	22	1.27	45	0.93	46 1.62 48 2.02
35	22	1.61	26	1.87	38	2.22	
36	22	2.16	28	1.56	49	2.14	
38	26	2.28	10	2.40	32	1.83	35 2.22
39	14	1.94	46	1.65	50	0.95	
40	10	1.45	19	2.73	25	1.66	
41	21	1.25	42	1.32	44	1.44	
42	7	1.76	21	2.19	41	1.22	44 2.25
43	15	2.11					
44	21	2.01	41	1.44	42	2.23	
45	12	1.42	22	1.36	34	0.93	40 2.30 48 1.46
46	34	1.62	35	1.55	45	2.30	50 1.20
47	5	1.72	17	2.07	20	1.21	
48	13	2.17	34	2.02	45	1.46	
49	27	1.72	28	1.55	36	2.14	
50	14	2.35	35	0.95	46	1.33	
51	27	1.61					



TABLE OF BOND ANGLES (IN DEGREES) AMONG PEAKS IN ABOVE TABLE (CLOSER TOGETHER THAN 1.6Å)

17	7	19	54	17	7	42	167	19	7	42	120	24	11	31	64	7	17	19	72	7	15	17	53
7	19	25	85	17	15	25	128	27	22	28	101	27	22	35	113	27	22	45	125	28	27	35	127
28	22	49	50	35	22	49	121	11	24	25	59	11	24	31	82	29	24	31	67	19	25	40	113
32	26	35	117	22	28	36	87	22	28	45	58	36	28	49	108	24	25	31	55	24	27	51	128
31	29	51	174	11	31	24	33	11	31	29	67	24	21	29	55	8	22	26	167	8	32	38	104
26	32	38	89	34	32	45	41	33	34	45	76	33	24	46	157	45	34	46	126	22	25	26	124
14	39	46	94	14	39	50	106	46	39	50	52	10	40	25	78	21	41	42	114	21	41	44	94
42	41	44	111	7	42	41	170	12	45	33	51	13	45	24	122	13	45	48	97	22	42	24	63
33	45	48	172	34	45	48	113	34	46	39	151	34	46	50	116	39	46	50	25	5	47	20	165
22	49	28	72	39	50	46	93																

DISTANCES BETWEEN ATOMS IN DIFFERENT ASYMMETRIC UNITS

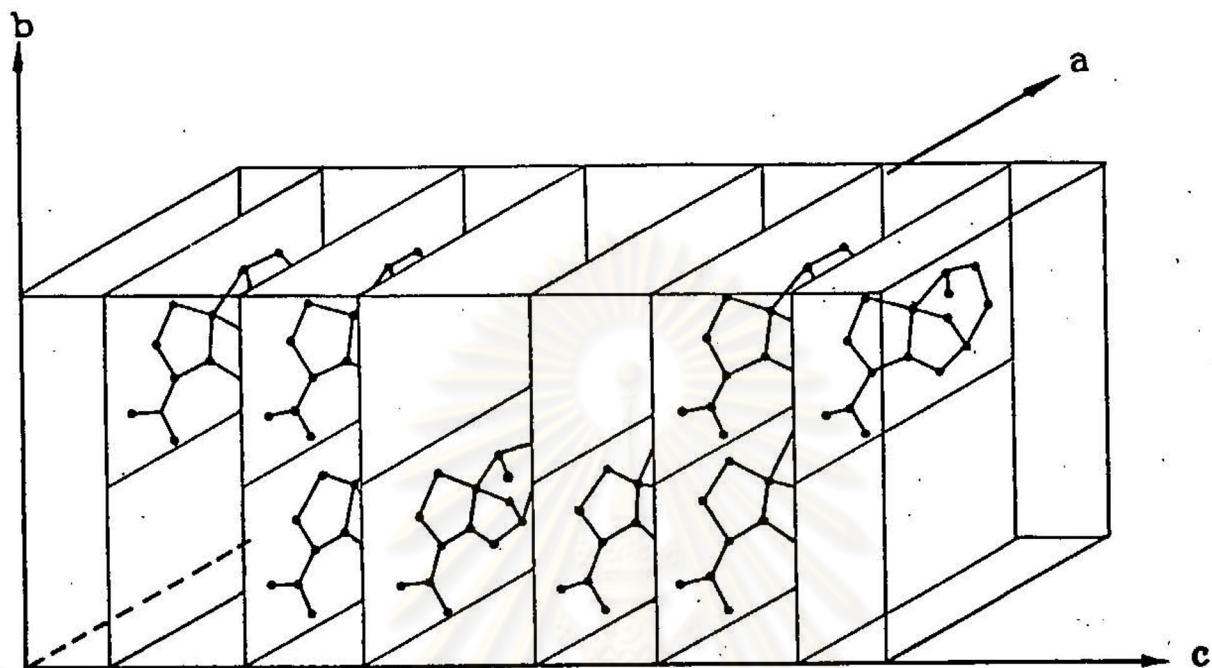
FROM	TO SYMM	X	Y	Z	DIST	FROM	TO SYMM	X	Y	Z	DIST	FROM	TO SYMM	X	Y	Z	DIST					
1	441	3	0.00	0.00	1.001	2.33	3	311	1	1.00	0.00	0.001	2.17	3	431	1	1.00	0.00	1.001	2.25		
3	431	3	1.00	0.00	1.001	2.05	4	311	3	0.00	0.00	1.001	2.12	4	511	3	1.00	0.00	1.001	2.25		
5	101	1	1.00	0.00	0.001	2.24	5	391	3	0.00	0.00	1.001	2.27	7	451	3	0.00	0.00	1.001	2.20		
8	361	3	1.00	0.00	1.001	2.27	5	271	4	1.00	1.00	1.001	2.15	9	371	2	0.00	0.00	0.001	2.00		
9	451	3	1.00	1.00	1.001	2.26	10	391	3	1.00	0.00	1.001	2.27	11	271	4	1.00	1.00	1.001	2.40		
11	261	4	1.00	1.00	1.001	2.35	17	491	3	0.00	0.00	1.001	2.19	21	231	3	0.00	0.00	1.001	2.12		
22	241	4	1.00	1.00	1.001	2.24	24	271	4	1.00	1.00	1.001	2.02	24	491	4	1.00	1.00	1.001	2.32		
26	301	3	1.00	0.00	1.001	2.34	26	281	3	1.00	0.00	1.001	2.32	26	411	3	1.00	0.00	1.001	2.10		
27	311	4	1.00	1.00	1.001	2.25	31	451	1	0.00	0.00	1.001	2.23	27	441	2	1.00	0.00	1.001	2.25		
39	401	3	0.00	0.00	1.001	1.96																

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

ผลการคำนวณจากโปรแกรม MULTAN พบว่าโปรแกรมไม่สามารถหาเซตของจุดสะท้อนเริ่มต้นที่ดีได้ ดังแสดงในตารางที่ 6.3 (ข) อาจเป็นเพราะจุดสะท้อนที่สังเกตได้จากภาพถ่ายแบบไวซ์เซ็นเบอร์ักมีจำนวนน้อยเกินไป หรือข้อมูลความเข้มที่ใช้ในการคำนวณไม่ถูกต้องเพราะวิธีการรวบรวมข้อมูลความเข้มมีโอกาสที่จะเกิดการผิดพลาดได้มาก จากสภาพของข้อมูลความเข้มที่มีอยู่ การคำนวณโปรแกรม MULTAN ปรากฏว่าให้เซตที่ 17 เป็นเซตของเฟลล์ที่มีเลยความถูกต้องสูงที่สุด หลังจากนำเซตที่ 17 มาคำนวณแผนภาพ E และหาตำแหน่งอะตอมในหนึ่งหน่วยเซลล์ ปรากฏผลว่ากลุ่มหมายเลข 4 มีตำแหน่งที่น่าจะเป็นอะตอมที่เข้ากลุ่มกันมากที่สุด คือ 10 ตำแหน่ง เลือกตำแหน่งที่น่าจะเป็นอะตอมในกลุ่มหมายเลข 4 บางส่วนที่คิดว่าถูกต้องที่สุดนำไปคำนวณแผนภาพความหนาแน่นอิเล็กตรอน เพื่อหาตำแหน่งอะตอมอื่นเพิ่ม

กรณีโครงสร้างของผลึกกรดไฮเพอร์นิค จะวางตัวกันอย่างใดในหนึ่งหน่วยเซลล์นั้น พิจารณาได้จากแผนภาพแพทเทอร์สัน สัมมาตรสัมมิติ และตำแหน่งที่คิดว่าน่าจะเป็นอะตอมมากที่สุด จากกลุ่มหมายเลข 4 ของผลการคำนวณโดยโปรแกรม MULTAN ซึ่งผลจากการพิจารณาพบว่า โครงสร้างโมเลกุลของผลึกกรดไฮเพอร์นิคน่าจะวางตัวในแนวขนานกับแกน a และมีระยะห่างระหว่างระนาบตั้งเช่นที่แสดงในรูปที่ 6.1 ซึ่งเป็นการบรรจุโมเลกุลทั้ง 8 ของกรดไฮเพอร์นิคที่มีความเป็นไปได้สูง





รูปที่ 6.1 ภาพการบรรจุโมเลกุลทั้ง 8 ของกรดไฮเพอริคที่คาดว่าจะจะเป็น

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