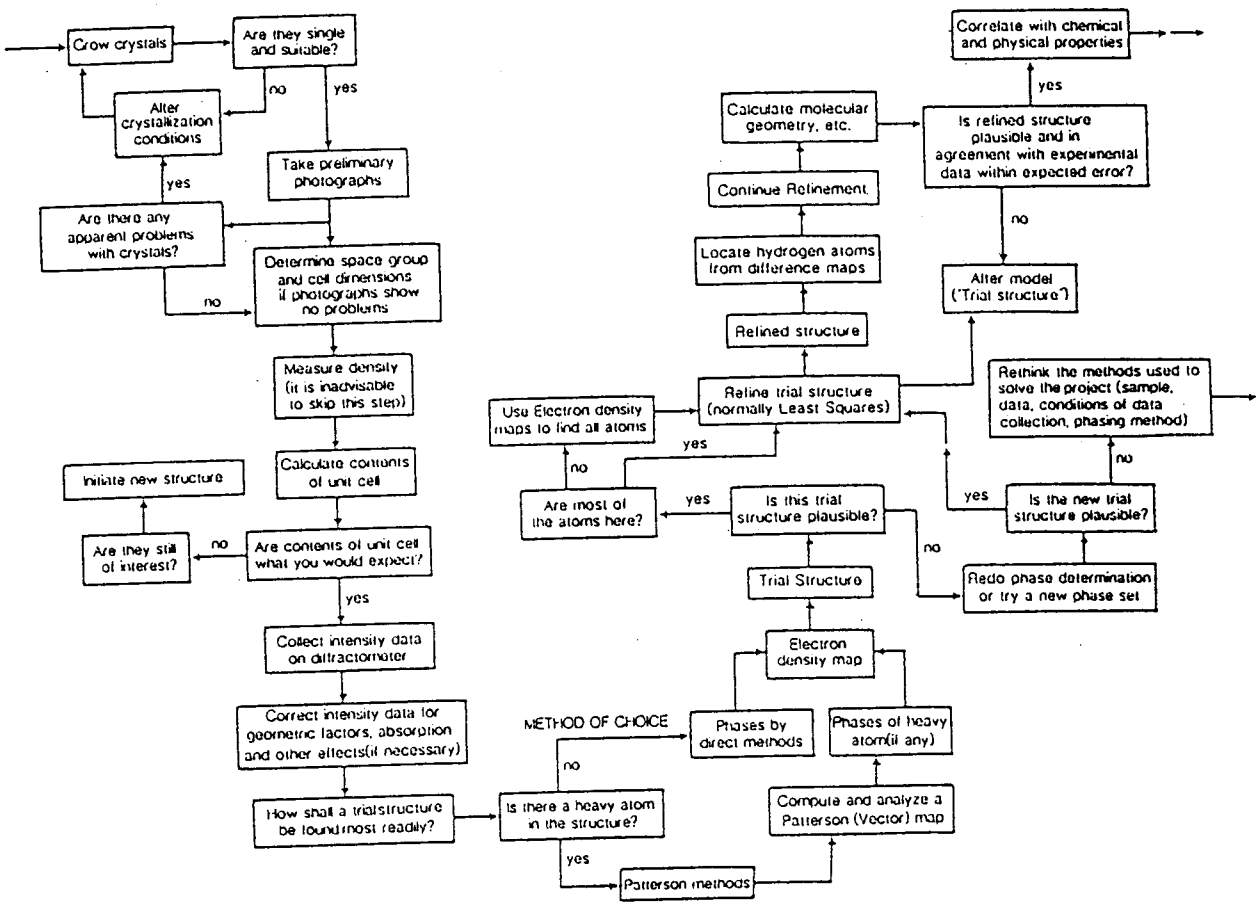
ภาคผนวก

ผนวก ก



แผนภาพแสดงขั้นตอนต่าง ๆ ในการหาโครงสร้างผลึก

โดยเทคนิคการเลี้ยวเบนของรังสีเอกซ์บนผลึกเดี่ยว

ผนวก ข

การคำนวณหาความหนาแน่น

สามารถคำนวณได้จากสูตร

$$D = \text{Mass/Volume}$$

$$= \text{Formular Weight/Molar Volume}$$

$$= \text{Formular Weight/Volume of Formular Unit x N}$$

เมื่อ N = Avogrado Number = 6.02×10^{23}

ดังนั้นในหนึ่งเซลล์หน่วย $D = FW \times Z / U \times W$

เมื่อ U = ปริมาตรของเซลล์หน่วย

Z = จำนวนของ Formular Unit ในเซลล์หน่วย

โดยที่ Formular Unit อาจจะเป็นโมเลกุลหรืออะตอมอื่น ๆ

เนื่องจาก U มีหน่วยเป็นอังสตรอม ($Å^3$) จึงต้องคูณด้วย 10^{-24} เพื่อทำให้ความหนาแน่นมีหน่วยเป็น $g.cm^{-3}$ เมื่อแทนค่า N จะได้

$$D = FW \times Z \times 1.66 / U \qquad g.cm^{-3}$$

ผนวก ค

ระบบผลึก

ระบบผลึกแบ่งออกเป็น 7 ระบบด้วยกัน แต่ละระบบมีการจัดวางแกนผลึกในตำแหน่งที่เหมือนกัน และมีลักษณะของสมมาตรเฉพาะระบบด้วย ลักษณะเฉพาะของแต่ละระบบมีดังนี้

ตารางที่ 1 ระบบผลึก

ระบบผลึก	ด้าน	มุม
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90°, \beta \neq 90°$
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$
Hexagonal	$a = b = c$	$\alpha = \beta = 90°, \gamma = 120°$
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$

ผนวก ง

การคำนวณหาปริมาตรของผลึก

สูตรที่ใช้ในการคำนวณแสดงดังตาราง

ตารางที่ 2 สูตรการคำนวณปริมาตรของผลึก

ระบบผลึก	สูตร
Cubic	$U = a^3$
Tetrahedral	$U = a^2c$
Orthorhobic	$U = abc$
Hexagonal	$U = (3a^2c)/2$ $= 0.866\, a^2c$
Monoclinic	$U = abc.\sin\beta$
Triclicnic	$U = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha.\cos\beta.\cos\gamma$

U = ปริมาตรของผลึก

ผนวก จ

ข้อมูล (Input File) การคำนวณหาโครงสร้างโมเลกลุผลึกของสารประกอบเชิงซ้อน

```
:Step 1     Load Cell Parameter and Diffraction Data
COMPID      FCUTU
MASTER      NO
TITLE       [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
STARTX
CELL        21.148  13.122  12.274  90.0  90.0  90.0
CELLSD      .002    .002    .007    0     0     0
SGNAME      P 2AC 2AB
CELCON      F    24
CELCON      CU   8
CELCON      S    32
CELCON      C    32
CELCON      N    64
CELCON      H    128
CELCON      O    4
CELCON      SI   4
END
DIFDAT      CAD PRI 50 EXCL INST 4 .0004 OBST 3
ATTENU      19.14
GENSCL      1
END
SORTRF      ORD HKL
END
ADDREF
REDUCE      ITOF RLP4 XRAY
BDFIN       HKL IREL SIGI RCOD
END
FINISH
```

```
:Step 2     Solving Structure
COMPID      FCUTU
MASTER      NO
TITLE       [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
GENEV
END
GENSIN
END
GENTAN
END
FOURR       EMAP
END
PEKPIK      PUNCH
END
MODEL
END
PIG
END
FINISH
```

```
:Step 3
COMPID      FCUTU
MASTER      NO
TITLE       [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
GENEV
END
FOURR       VECT
END
PEKPIK      PUNCH
END
FINISH
```

```
:Step 4      Refining Atom Parameters
COMPID       FCUTU
MASTER       NO
TITLE        [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ADDATM
SCALE        1.9676
ATOM         Cu      .42     .55     .73
END
CRYLSQ       CY 5 AD WS FU 0.8 P1
END
FINISH
```

```
:Step 5
COMPID       FCUTU
MASTER       NO
TITLE        [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ADDATM
SCALE        2.16286     1.00000     PARENT
UOV           .03500                 PARENT
ATOM CU1     .41752   .54732   .73731   .03188   1.00000   .00005   .00008   .00008
UIJ  CU1     .03322   .03557   .02685   .00191   .00043    .00751
END
FOURR        FDIF R2 0
END
PEKPIK       PUNCH
END
FINISH
```

:Step 6

```
COMPID    FCUTU
MASTER    NO
TITLE     [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ADDATM
SCALE     2.16286     1.00000     PARENT
UOV        .03500                 PARENT
ATOM CU1  .41752  .54732  .73731  .03188  1.00000  .00005  .00008  .00008
UIJ  CU1  .03322  .03557  .02685  .00191  .00043   .00751
ATOMC0001      .42507   .53784   .21679
ATOMC0002      .45576   .60970   .57170
ATOMC0003      .49254   .53861   .87493
ATOMC0004      .37810   .39188   .67107
ATOMC0005      .34422   .65868   .81430
ATOMC0006      .39713   .43916   .36958
ATOMC0007      .52995   .53123   .15990
.....atom data omitted brevily.....
ATOMC00041     .17889  1.06466   .47676
ATOMC00042     .28517  1.05258   .43827
ATOMC00043     .17123   .88990   .49547
ATOMC00044     .27885   .87586   .45543
ATOMC00045     .28975   .23980   .48851
END
BONDLA
ATRAD     CU    2.3    1.6
ATRAD     S     1.7    1.2
ATRAD     N     1.5    1.0
ATRAD     C     1.5    1.0
ATRAD     O     1.5    1.0
ATRAD     F     1.5    1.0
ATRAD     H     1.0    0.5
END
PIG
END
FINISH
```

:Step 7

COMPID FCUTU

MASTER NO

TITLE [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4

ADDATM

SCALE 2.16286 1.00000 PARENT

UOV .03500 PARENT

ATOM CU1	.41752	.54732	.73731	.03188	1.00000	.00005	.00008	.00008
UIJ CU1	.03322	.03557	.02685	.00191	.00043	.00751		
ATOM S11	.45576	.60970	.57170	.03153	1.00000	.00011	.00016	.00017
UIJ S11	.04438	.03141	.01880	-.00326	.00447	-.00111		
ATOM C11	.47925	.73363	.59593	.03672	1.00000	.00044	.00064	.00071
UIJ C11	.05231	.03396	.02388	-.01153	.00731	-.00101		
ATOM N111	.48325	.79616	.51431	.07102	1.00000	.00052	.00058	.00070
UIJ N111	.13820	.03750	.03736	-.02043	.01364	.00674		
ATOM N112	.49324	.76559	.69319	.04930	1.00000	.00040	.00054	.00064
UIJ N112	.07538	.03298	.03954	-.01590	-.00785	-.01466		
ATOM S12	.49254	.53861	.87493	.03773	1.00000	.00010	.00019	.00018
UIJ S12	.03313	.05399	.02607	.00836	-.00457	.00483		
ATOM C12	.56783	.52400	.82263	.04166	1.00000	.00035	.00065	.00081
UIJ C12	.02081	.04585	.05833	.00369	-.01194	.01597		
ATOM N121	.57784	.51581	.72099	.06875	1.00000	.00035	.00076	.00068
UIJ N121	.03164	.12035	.05428	.00434	.00986	.03587		
ATOM N122	.61511	.51430	.89331	.07079	1.00000	.00037	.00071	.00083
UIJ N122	.03841	.08735	.08661	-.00189	-.01555	.02766		
ATOM S13	.37810	.39188	.67107	.03391	1.00000	.00011	.00016	.00019
UIJ S13	.04226	.03279	.02667	-.00681	.00151	.00347		
ATOM C13	.34363	.30778	.75974	.04218	1.00000	.00044	.00067	.00073
UIJ C13	.05136	.04348	.03171	-.00899	-.00217	.00845		
ATOM N131	.34643	.32011	.86574	.06248	1.00000	.00045	.00063	.00067
UIJ N131	.08701	.05531	.04512	-.01067	.02278	-.00074		
ATOM N132	.31506	.22778	.71851	.07806	1.00000	.00050	.00068	.00072
UIJ N132	.11524	.06642	.05253	-.05104	.01042	.00338		
ATOM S14	.34422	.65868	.81430	.03654	1.00000	.00011	.00018	.00018
UIJ S14	.04328	.04249	.02385	.01367	.00023	.00286		
ATOM C14	.31389	.74063	.71859	.03819	1.00000	.00040	.00063	.00074
UIJ C14	.03793	.03551	.04113	.00381	-.00767	.00468		
ATOM N141	.31844	.72228	.61282	.04623	1.00000	.00037	.00059	.00058
UIJ N141	.05721	.05998	.02149	.02105	.00222	.00708		

```
ATOM N142  .28410   .82326   .75057   .06936  1.00000  .00046  .00066  .00070
UIJ  N142  .09562   .06719   .04525   .04713   .00691  .00764
ATOM Cu2   .42507   .53784   .21679   .03628  1.00000  .00005  .00008  .00009
UIJ  Cu2   .03598   .03985   .03300   .00188 -.00245   .00490
ATOM S21   .39713   .43916   .36958   .03770  1.00000  .00011  .00016  .00018
UIJ  S21   .04968   .03147   .03194   .00659   .01256  .00592
.....atom data omitted brevily.....
ATOM Si    .22919   .96991   .46624   .02856  1.00000  .00010  .00019  .00018
UIJ  Si    .02685   .04416   .01469   .00664   .00151  .00282
ATOM F1    .21252   .95893   .33223   .03809  1.00000  .00022  .00037  .00036
UIJ  F1    .04477   .05090   .01860 -.00079  -.00386 -.00210
ATOM F2    .24542   .98033   .60151   .05239  1.00000  .00024  .00047  .00038
UIJ  F2    .04872   .09502   .01344   .00939  -.00071  .00485
ATOM F3    .17889  1.06466   .47676   .09424  1.00000  .00038  .00049  .00048
UIJ  F3    .15761   .08459   .04052   .07226  -.02484 -.02477
ATOM F4    .28517  1.05258   .43827   .11633  1.00000  .00032  .00070  .00050
UIJ  F4    .08477   .22091   .04332 -.10117  -.00653  .02661
ATOM F5    .17123   .88990   .49547   .10258  1.00000  .00038  .00059  .00051
UIJ  F5    .13053   .13036   .04686 -.07766   .02417 -.01390
ATOM F6    .27885   .87586   .45543   .16475  1.00000  .00048  .00074  .00050
UIJ  F6    .23685   .22863   .02878   .20073   .00335  .00436
ATOM O     .28975   .23980   .48851   .16518   .50000  .00124  .00166  .00232
UIJ  O     .19433   .10797   .19324 -.06012  -.06849 -.00785
END
CRYLSQ     CY 5 AD WS FU 0.8 P1
END
BONDLA
ATRAD      CU    2.3   1.6
ATRAD      S     1.7   1.2
ATRAD      N     1.5   1.0
ATRAD      C     1.5   1.0
ATRAD      O     1.5   1.0
ATRAD      F     1.5   1.0
ATRAD      H     1.0   0.5
END
PIG
END
FINISH
```

:Step 8

```
COMPID    FCUTU
MASTER    NO
TITLE     [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ADDATM
SCALE     2.16286     1.00000     PARENT
UOV        .03500                 PARENT
ATOM CU1  .41752   .54732   .73731   .03188  1.00000  .00005  .00008  .00008
UIJ  CU1  .03322   .03557   .02685   .00191   .00043  .00751
ATOM S11  .45576   .60970   .57170   .03153  1.00000  .00011  .00016  .00017
UIJ  S11  .04438   .03141   .01880  -.00326   .00447 -.00111
ATOM C11  .47925   .73363   .59593   .03672  1.00000  .00044  .00064  .00071
UIJ  C11  .05231   .03396   .02388  -.01153   .00731 -.00101
.....atom data omitted brevily.....
ATOM Si   .22919   .96991   .46624   .02856  1.00000  .00010  .00019  .00018
UIJ  Si   .02685   .04416   .01469   .00664   .00151  .00282
ATOM F1   .21252   .95893   .33223   .03809  1.00000  .00022  .00037  .00036
UIJ  F1   .04477   .05090   .01860  -.00079  -.00386 -.00210
ATOM F2   .24542   .98033   .60151   .05239  1.00000  .00024  .00047  .00038
UIJ  F2   .04872   .09502   .01344   .00939  -.00071  .00485
ATOM F3   .17889  1.06466   .47676   .09424  1.00000  .00038  .00049  .00048
UIJ  F3   .15761   .08459   .04052   .07226  -.02484 -.02477
ATOM F4   .28517  1.05258   .43827   .11633  1.00000  .00032  .00070  .00050
UIJ  F4   .08477   .22091   .04332  -.10117  -.00653  .02661
ATOM F5   .17123   .88990   .49547   .10258  1.00000  .00038  .00059  .00051
UIJ  F5   .13053   .13036   .04686  -.07766   .02417 -.01390
ATOM F6   .27885   .87586   .45543   .16475  1.00000  .00048  .00074  .00050
UIJ  F6   .23685   .22863   .02878   .20073   .00335  .00436
ATOM O    .28975   .23980   .48851   .16518   .50000  .00124  .00166  .00232
UIJ  O    .19433   .10797   .19324  -.06012  -.06849 -.00785
END
FOURR     FDIF R2 0
END
PEKPIK    PUNCH
PLIMIT    .15 *3 40
END
FINISH
```

:Step 9

```
COMPID    FCUTU
MASTER    NO
TITLE     [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
BONDAT    PC
CALCAT    TETCHN  0.95 N12 C13 C14 H13A H13B
CALCAT    TETCHN  0.95 C13 C14 N15 H14A H14B
CALCAT    TRIGON  0.95 C14 N15 C11 H15
CALCAT    TRIGON  0.95 C21 N22 C23 H22
CALCAT    TETCHN  0.95 N22 C23 C24 H23A H23B
CALCAT    TETCHN  0.95 C23 C24 N25 H24A H24B
CALCAT    TRIGON  0.95 C24 N25 C21 H25
CALCAT    TRIGON  0.95 C31 N32 C33 H32
CALCAT    TETCHN  0.95 N32 C33 C34 H33A H33B
CALCAT    TETCHN  0.95 C33 C34 N35 H34A H34B
CALCAT    TRIGON  0.95 C34 N35 C31 H35
CALCAT    TRIGON  0.95 C41 N42 C43 H42
CALCAT    TETCHN  0.95 N42 C43 C44 H43A H43B
CALCAT    TETCHN  0.95 C43 C44 N45 H44A H44B
CALCAT    TRIGON  0.95 C44 N45 C41 H45
CALCAT    TRIGON  0.95 C51 N52 C53 H52
CALCAT    TETCHN  0.95 N52 C53 C54 H53A H53B
CALCAT    TETCHN  0.95 C53 C54 N55 H54A H54B
CALCAT    TRIGON  0.95 C54 N55 C51 H55
CALCAT    TRIGON  0.95 C61 N62 C63 H62
CALCAT    TETCHN  0.95 N62 C63 C64 H63A H63B
CALCAT    TETCHN  0.95 C63 C64 N65 H64A H64B
CALCAT    TRIGON  0.95 C64 N65 C61 H65
END
FINISH
```

:Step 10

COMPID FCUTU

MASTER NO

TITLE [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4

ADDATM

SCALE 2.16286 1.00000 PARENT

UOV .03500 PARENT

ATOM CU1	.41752	.54732	.73731	.03188	1.00000	.00005	.00008	.00008
UIJ CU1	.03322	.03557	.02685	.00191	.00043	.00751		
ATOM S11	.45576	.60970	.57170	.03153	1.00000	.00011	.00016	.00017
UIJ S11	.04438	.03141	.01880	-.00326	.00447	-.00111		
ATOM C11	.47925	.73363	.59593	.03672	1.00000	.00044	.00064	.00071
UIJ C11	.05231	.03396	.02388	-.01153	.00731	-.00101		
ATOM N111	.48325	.79616	.51431	.07102	1.00000	.00052	.00058	.00070
UIJ N111	.13820	.03750	.03736	-.02043	.01364	.00674		
ATOM N112	.49324	.76559	.69319	.04930	1.00000	.00040	.00054	.00064
UIJ N112	.07538	.03298	.03954	-.01590	-.00785	-.01466		
ATOM S12	.49254	.53861	.87493	.03773	1.00000	.00010	.00019	.00018
UIJ S12	.03313	.05399	.02607	.00836	-.00457	.00483		

.....atom data omitted brevily.....

ATOM SI	.22919	.96991	.46624	.02856	1.00000	.00010	.00019	.00018
UIJ SI	.02685	.04416	.01469	.00664	.00151	.00282		
ATOM F1	.21252	.95893	.33223	.03809	1.00000	.00022	.00037	.00036
UIJ F1	.04477	.05090	.01860	-.00079	-.00386	-.00210		
ATOM F2	.24542	.98033	.60151	.05239	1.00000	.00024	.00047	.00038
UIJ F2	.04872	.09502	.01344	.00939	-.00071	.00485		
ATOM F3	.17889	1.06466	.47676	.09424	1.00000	.00038	.00049	.00048
UIJ F3	.15761	.08459	.04052	.07226	-.02484	-.02477		
ATOM F4	.28517	1.05258	.43827	.11633	1.00000	.00032	.00070	.00050
UIJ F4	.08477	.22091	.04332	-.10117	-.00653	.02661		
ATOM F5	.17123	.88990	.49547	.10258	1.00000	.00038	.00059	.00051
UIJ F5	.13053	.13036	.04686	-.07766	.02417	-.01390		
ATOM F6	.27885	.87586	.45543	.16475	1.00000	.00048	.00074	.00050
UIJ F6	.23685	.22863	.02878	.20073	.00335	.00436		
ATOM O	.28975	.23980	.48851	.16518	.50000	.00124	.00166	.00232
UIJ O	.19433	.10797	.19324	-.06012	-.06849	-.00785		

ATOM H111a	.47684	.77823	.45179	.10400	1.00000	.00000	.00000	.00000
ATOM H111b	.49440	.86776	.51918	.10400	1.00000	.00000	.00000	.00000
ATOM H112a	.51185	.81269	.69973	.07400	1.00000	.00000	.00000	.00000
ATOM H112b	.48861	.71621	.76700	.07400	1.00000	.00000	.00000	.00000
ATOM H121a	.54979	.55291	.67085	.11300	1.00000	.00000	.00000	.00000
ATOM H121b	.62381	.53801	.70099	.11300	1.00000	.00000	.00000	.00000
ATOM H122a	.59800	.52542	.96167	.11100	1.00000	.00000	.00000	.00000
ATOM H122b	.64426	.45731	.89265	.11100	1.00000	.00000	.00000	.00000
ATOM H131a	.33310	.24530	.87960	.09600	1.00000	.00000	.00000	.00000
ATOM H131b	.31286	.36058	.90227	.09600	1.00000	.00000	.00000	.00000
ATOM H132a	.28411	.17189	.76159	.12000	1.00000	.00000	.00000	.00000
ATOM H132b	.29399	.21370	.64802	.12000	1.00000	.00000	.00000	.00000
ATOM H141a	.30658	.77919	.56923	.07400	1.00000	.00000	.00000	.00000
ATOM H141b	.35270	.67981	.58789	.07400	1.00000	.00000	.00000	.00000
ATOM H142a	.27272	.88305	.69259	.10100	1.00000	.00000	.00000	.00000
ATOM H142b	.27270	.81360	.83989	.10100	1.00000	.00000	.00000	.00000
ATOM H211a	.50522	.31248	.22339	.09200	1.00000	.00000	.00000	.00000
ATOM H211b	.44796	.24362	.25011	.09200	1.00000	.00000	.00000	.00000
ATOM H212a	.43066	.30073	.51421	.11700	1.00000	.00000	.00000	.00000
ATOM H212b	.46590	.20720	.44670	.11700	1.00000	.00000	.00000	.00000
ATOM H221a	.65990	.59760	.31260	.06900	1.00000	.00000	.00000	.00000
ATOM H221b	.66036	.55463	.20190	.06900	1.00000	.00000	.00000	.00000
ATOM H222a	.51154	.54325	.39521	.08600	1.00000	.00000	.00000	.00000
ATOM H222b	.57587	.57188	.42770	.08600	1.00000	.00000	.00000	.00000
ATOM H231a	.30470	.88846	.17298	.07900	1.00000	.00000	.00000	.00000
ATOM H231b	.32950	.89020	.29430	.07900	1.00000	.00000	.00000	.00000
ATOM H232a	.34645	.78556	.03465	.08400	1.00000	.00000	.00000	.00000
ATOM H232b	.39770	.69760	.08840	.08400	1.00000	.00000	.00000	.00000
ATOM H241a	.22455	.49364	.18839	.09500	1.00000	.00000	.00000	.00000
ATOM H241b	.30652	.47011	.24477	.09500	1.00000	.00000	.00000	.00000
ATOM H242a	.21468	.56945	.02035	.11100	1.00000	.00000	.00000	.00000
ATOM H242b	.22730	.48590	.00000	.11100	1.00000	.00000	.00000	.00000

END

CRYLSQ CY 1 BD AD WS FU 0.6 LR 10.0 P1 RX

NOREF H

END

```
BONDLA    BRAC
ATRAD     CU  2.3  1.6
ATRAD     S   1.7  1.2
ATRAD     N   1.5  1.0
ATRAD     C   1.5  1.0
ATRAD     O   1.5  1.0
ATRAD     F   1.5  1.0
ATRAD     H   1.0  0.5
END
ABSORB    GAUSS FREL
REMARK    R=.053 BEFORE ABSORB
DIFF      C C C C
ORIENT    20  0  0   1.607 -52.21 0 14 0 4.814 37.93
FACEML    0  -1  0    .15
FACEML    1   0  0    .11
FACEML   -1   0  0    .11
FACEML    1   1  0    .14
FACEML   -1   1  0    .145
FACEML    0   0  1    .19
FACEML    0   0 -1    .19
END
FC
END
PIG
PRESET    BOND 10 ROTN 5 SEXT
RADII     F   1.3
RADII     CU  1.6
RADII     S   1.2
RADII     N   1.0
RADII     C   1.0
RADII     O   1.0
RADII     H   0.36
END
FINISH
```

```
:Step 11    Plot Molecule
COMPID      FCUTU
MASTER      NO
TITLE       [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
LSQPL
PLANE
DEFINE      S11  C11  N111  N112
NONDEF      CU1
PLANE
DEFINE      S12  C12  N121  N122
NONDEF      CU1
PLANE
DEFINE      S13  C13  N131 N132
NONDEF      CU1
PLANE
DEFINE      S14  C14  N141 N142
NONDEF      CU1
PLANE
DEFINE      S21  C21  N211 N212
NONDEF      CU2
PLANE
DEFINE      S22  C22  N221 N222
NONDEF      CU2
PLANE
DEFINE      S23  C23  N231 N232
NONDEF      CU2
PLANE
DEFINE      S24  C24  N241 N242
NONDEF      CU2
END
```

```
ORTEP     AUTO MOLE SPHE
VSC       1  6   1   6   5  .5  2.7  .03
VSC       1  6   7   36  5  .5  2.5  .03
VSC       7  42  1   6   5  .5  2.5  .03
VSC       1  42  1   42  1  .5  2.0  .03
VSC       1  42  43  78  1  .5  1.2  .001
SYMBOL    [Cu(tu)4]2[SiF6]H2O Cu2C8H32F6SiON16S8
PLOTP     12 12 0 0.5
ELLIPS    5 1.0 .20 -.20 .10
GENINS    SYMB
END
PREVUE
END
PLOTX     POSTL PRE
END
PLOT
COLOR     NOCOL NOFIL
STARTP    VDU
END
FINISH
```

```
:Step 12    Plot Molecule (Non Hydrogen Atom)
COMPID      FCUTU
MASTER      NO
TITLE       [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ORTEP       AUTO MOLE EXCL
VSC         1  6   1  6   5  .5  2.7  .03
VSC         1  6   7  36  5  .5  2.5  .03
VSC         7  42  1  6   5  .5  2.5  .03
VSC         1  42  1  42  1  .5  2.0  .03
VSC         1  42  43 78  1  .5  1.2  .001
PLOTP       12 12 0 0.4
GENINS      SYMB
ELLIPS      5 1.0 .20 -.20 .15
SEQ         REPLACE 6
INST        501 1 555 1 1 555 1 3 555 1 1 555 1 5 555 1 1
SEQ         PRECEDE 7
INST        502 3 55  1 -82
END
PLOT
COLOR       NOCOL NOFIL
STARTP      DOT *3 8 8
END
FINISH
```

```
:Step 13    Plot Cell (Non Hydrogen Atom)
COMPID      FCUTU
MASTER      NO
TITLE       [Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ORTEP       AUTO CELL EXCL
VSC         1  6   1   6   5  .5  2.7  .03
VSC         1  6   7   36  5  .5  2.5  .03
VSC         7  42  1   6   5  .5  2.5  .03
VSC         1  42  1   42  1  .5  2.0  .03
VSC         1  42  43  78  1  .5  1.2  .001
PLOTP       12 12  0 0.4   AB  *8 90
ELLIPS      5  1.0 .20   -.20  .15
SEQ         REPLACE 5
INST        401 1 555 1 -42  555  1  13  565 1 -18 565 1 37 565 1 -42 565 1
INST        401 3 565 1   5  565  1
INST        401 1 554 2 -42  554  2   7  564 2 -12 564 2 19 555 2 -24 555 2
INST        401 3 555 2  -6  555  2
INST        401 1 666 3 -42  666  3  13  656 3 -18 656 3 37 656 3 -42 656 3
INST        401 3 656 3   5  656  3
INST        401 1 656 4 -42  656  4   7  646 4 -12 646 4 19 655 4 -24 655 4
INST        401 3 655 4  -6  655  4
END
FINISH
```

:Step 14

COMPID	FCUTU
MASTER	NO
TITLE	[Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
	Structure Factor Amplitudes (10Fo,10Fc,10sigFo)
	C4 H16 Cu F3 N8 S4 Si0.5.1/4(H2O)
LISTFC	ORD HKL NFL WIDTH 118 LIN 85
END	
FINISH	

:Step 15

COMPID	FCUTU
MASTER	NO
TITLE	[Cu(tu)4]2[SiF6]1/2H2O, P212121, Z = 4
ATABLE	
END	
FINISH	