Appendix I. A BASIC Computer Program for Calculating Interatomic Distances and Angles and Torsion Angles from Crystal Coordinates

The program transforms the crystal coordinates to Cartesian coordinates by applying Eqs. 5.30 and finds the torsion angle $\omega(ABCD) = \omega(IJKL)$ by applying Eqs. 5.35 and 5.36. The input consists of the unit-cell dimensions (line 20) and the crystal coordinates of the atoms, which are assigned code numbers $I = 1$ to N (line 46). The input is terminated by writing $I = 0$. Each torsion angle required has to be requested separately by specifying the code numbers of the four atoms concerned: interatomic distances and angles are then printed in addition to the torsion angle. If torsion angles are not required, the code numbers of only three atoms need to be specified; if only a distance is required then code numbers of only two atoms suffice. A sample output follows.

App. I   Program

```
4    PRINT
5    PRINT "MOLECULAR GEOMETRY"
10   DIM X[60],Y[60],Z[60]
15   PRINT "A,B,C,ALPHA,BETA,GAMMA"
20   INPUT A1,A2,A3,W1,W2,W3
21   PRINT
25   LET P=3.14159/180
30   LET C1= COS (W1*P)
31   LET C2= COS (W2*P)
32   LET C3= COS (W3*P)
33   LET S3= SIN (W3*P)
35   LET M6=(C1-C3*C2)/S3
37   LET V= SQR (1-C1*C1-C2*C2-C3*C3+2*C1*C2*C3)
39   LET M9=V/S3
45   PRINT "I,X(I),Y(I),Z(I), I=0 FOR LAST ATOM"
46   INPUT I,X[I],Y[I],Z[I]
47   PRINT
48   IF I= 0 GOTO  75
49   LET U=A1*X[I]+A2*Y[I]*C3+A3*Z[I]*C2
50   LET V=A2*Y[I]*S3+A3*Z[I]*M6
51   LET W=A3*Z[I]*M9
52   LET X[I]=U
55   LET Y[I]=V
57   LET Z[I]=W
58   GOTO  46
75   PRINT "BOND LENGTH: I1,I2,0,0"
76   PRINT "BOND ANGLE : I1,I2,I3,0"
77   PRINT "TORSION ANGLE: I1,I2,I3,I4"
85   INPUT T1,T2,T3,T4
86   PRINT
```

Appendix I

```
100    LET E[1]=X[T2]-X[T1]
105    LET E[2]=Y[T2]-Y[T1]
110    LET E[3]=Z[T2]-Z[T1]
115    LET F=1
120    LET D1= SQR (E[1]*E[1]+E[2]*E[2]+E[3]*E[3])
121    LET D=D1
125    GOSUB  325
133    IF T3= 0 GOTO  499
135    LET E[4]=X[T3]-X[T2]
140    LET E[5]=Y[T3]-Y[T2]
145    LET E[6]=Z[T3]-Z[T2]
150    LET F=4
155    LET D2= SQR (E[4]*E[4]+E[5]*E[5]+E[6]*E[6])
156    LET D=D2
160    GOSUB  325
165    LET C4=-(E[1]*E[4]+E[2]*E[5]+E[3]*E[6])
170    LET S4= SQR (1-C4*C4)
175    LET A4= ATN (S4/C4)/P
176    IF A4> 0 GOTO  180
177    LET A4=A4+180
180    IF T4= 0 GOTO  497
185    LET E[7]=X[T4]-X[T3]
190    LET E[8]=Y[T4]-Y[T3]
195    LET E[9]=Z[T4]-Z[T3]
200    LET F=7
205    LET D3= SQR (E[7]*E[7]+E[8]*E[8]+E[9]*E[9])
210    LET D=D3
215    GOSUB  325
220    LET C5=-(E[4]*E[7]+E[5]*E[8]+E[6]*E[9])
225    LET S5= SQR (1-C5*C5)
230    LET A5= ATN (S5/C5)/P
231    IF A5> 0 GOTO  250
232    LET A5=A5+180
250    LET U1=(E[2]*E[6])-(E[3]*E[5])
252    LET U2=(E[3]*E[4])-(E[1]*E[6])
254    LET U3=(E[1]*E[5])-(E[2]*E[4])
256    LET V1=(E[5]*E[9])-(E[6]*E[8])
258    LET V2=(E[6]*E[7])-(E[4]*E[9])
260    LET V3=(E[4]*E[8])-(E[5]*E[7])
265    LET C6=(U1*V1+U2*V2+U3*V3)/(S4*S5)
270    LET S6=(E[1]*V1+E[2]*V2+E[3]*V3)/(S4*S5)
275    LET A6= ATN (S6/C6)/P
280    IF A6> 0 GOTO  290
281    IF S6< 0 GOTO  300
282    LET A6=A6+180
284    GOTO  300
290    IF C6> 0 GOTO  300
292    LET A6=A6-180
299    PRINT
300    PRINT " T("T1;T2;T3;T4;") ="A6
301    PRINT " W("T2;T3;T4;")     ="A5
302    PRINT " D("T3;T4;")        ="D3
305    GOTO  497
325    FOR J=F TO F+2
327      LET E[J]=E[J]/D
329    NEXT J
331    RETURN
496    PRINT
497    PRINT " W("T1;T2;T3;")     ="A4
498    PRINT " D("T2;T3;")        ="D2
499    PRINT " D("T1;T2;")        ="D1
510    PRINT
```

```
512  GOTO  85
515  END
```

```
BASIC?
*READY
RUN

MOLECULAR GEOMETRY
A,B,C,ALPHA,BETA,GAMMA
? 7.877? 7.210? 7.891? 105.56? 116.25? 79.84
I,X(I),Y(I),Z(I),  I=0 FOR LAST ATOM
? 1? -.1361? .1572? -.0717
? 2? -.0963? .1157? .1184
? 3? .0920? .0109? .2083
? 4? -.1955? .3344? -.1057
? 5? -.2272? .4046? -.2806
? 6? -.2182? .1553? .2003
? 7? -.4167? .2445? .1235
? 8? .2174? .0656? .3903
? 9? .2034? .2392? .5396
? 10? .1361? -.1572? .0717
? 11? .0963? -.1157? -.1184
? 12? -.0920? -.0109? -.2083
? 0? 0? 0? 0
BOND LENGTH: I1,I2,0,0
BOND ANGLE : I1,I2,I3,0
TORSION ANGLE: I1,I2,I3,I4
? 12? 1? 2? 3
 T( 12   1   2   3  ) = 46.2811
 W( 1   2   3 )       = 114.158
 D( 2   3 )           = 1.49519
 W( 12   1   2 )      = 114.083
 D( 1   2 )           = 1.49324
 D( 12   1 )          = 1.49442

? 1? 2? 3? 10
 T( 1   2   3   10 ) =-46.3004
 W( 2   3   10 )      = 114.124
 D( 3   10 )          = 1.49442
 W( 1  2   3 )       = 114.158
 D( 2   3 )           = 1.49519
 D( 1   2 )           = 1.49324

? 2? 3? 10? 11
 T( 2   3   10   11 ) = 46.2653
 W( 3   10   11 )     = 114.083
 D( 10   11 )         = 1.49324
 W( 2   3   10 )      = 114.124
 D( 3   10 )          = 1.49442
 D( 2   3 )           = 1.49519
```