

3. DUAL BASES IN CRYSTALLOGRAPHIC COMPUTING

A discussion of the appropriateness of weighted and unweighted means may be found in Taylor & Kennard (1985), which suggests that the unweighted mean might even be preferable if environmental effects are large.

3.1.12. Computation

It has been mentioned that the tensor formulation used in this chapter is particularly amenable to machine computation. As a simple illustration of this point, the following Fortran program will compute the lengths of vectors **X** and **Y** and the angle between them.

```
DIMENSION X(3),Y(3),G(3,3),SUM(3)
READ (5,10)(X(I),I = 1,3)
READ (5,10)(Y(I),I = 1,3)
```

```
      READ (5,10)((G(I,J),J = 1,3),I = 1,3)
10  FORMAT (3F10.5)
      DO 20 I = 1,3
20  SUM(I) = 0
      DO 30 I = 1,3
      DO 30 J = 1,3
      SUM(1) = SUM(1) + X(I) * X(J) * G(I,J)
      SUM(2) = SUM(2) + Y(I) * Y(J) * G(I,J)
      SUM(3) = SUM(3) + X(I) * Y(J) * G(I,J)
30  CONTINUE
      DIST1 = SQRT(SUM(1))
      DIST2 = SQRT(SUM(2))
      ANGLE = 57.296 * ACOS(SUM(3)/(DIST1 * DIST2))
      WRITE (6,10) DIST1,DIST2,ANGLE
      END
```