1 SUMMARY

This subroutine applies the **Schmidt orthogonalisation process** to N vectors in M dimensional space, N ≤ M. The vectors are to be specified as adjacent columns of a matrix and the first vector need not be the first column of the matrix. The subroutine ensures that the resultant vectors are orthonormal to the full accuracy of the computer.

ATTRIBUTES — **Version:** 1.0.0. **Types:** `MC06A, MC06AD` **Calls:** `SDOT/DDOT.` **Original date:** September 1963. **Origin:** W.H.O. Osbourne, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

```
CALL MC06A (A,M,N1,N2,IA)
```

The double precision version

```
CALL MC06AD (A,M,N1,N2,IA)
```

`A` is a two dimensional `REAL` (`DOUBLE PRECISION` in the D version) array, with first dimension `IA,` whose components are the components of the vectors. The N vectors are

```
(A(1,J), A(2,J), ..., A(M,J)),     J = N1, N1 + 1, ..., N2
```

so that `N = N2 – N1 + 1.` The subroutine will overwrite the original vectors with the required ones.

`M` is an `INTEGER` giving the dimension of the space.

`N1` is an `INTEGER` giving the index of the first vector.

`N2` is an `INTEGER` giving the index of the last vector.

`IA` is an `INTEGER` giving the first dimension of the array `A,` so that in the calling routine there must be a statement of the form

```
DIMENSION  A(IA, )
```

3 GENERAL INFORMATION

Use of common: None

Workspace: Internal workspace `S` of dimension 100.

Input/output: None.

Restrictions:

N2 ≤ 100.

This arises because of the private working array `S(100),` and it can therefore be altered by a recompilation with a changed dimension statement.