Appendixes

Computer Programs

The following appendixes contain subroutines for calculating scattering by a homogeneous sphere (BHMIE), a coated sphere (BHCOAT), and a normally illuminated infinite cylinder (BHCYL), together with their calling programs and sample calculations. A brief description accompanies each program. The final versions of the programs were tested on the CDC 7600 computer at the Los Alamos Scientific Laboratory. Although we tried to write the programs in standard Fortran so that they can be run on most computers, it is likely that they will have to be modified slightly. For example, the first statement in each calling program is not executable by many Fortran compilers; also, input, output, and format statements may have to be changed. Major changes, although unlikely, may be necessary.

We aimed at simplicity and lucidity rather than programming elegance so that users will be able to easily adapt these programs to their own needs. To this end Fortran variables were chosen to resemble or suggest the corresponding variables in the sections where the underlying theory is developed and discussed. The logic of the programs should be evident without prolonged study: there are no clever, but obscure, shortcuts. Little effort was made to optimize the programs; they are neither the best nor the brightest. A lifetime could be devoted to refining them, making them faster and more efficient, and extending the range of their applicability.

Any program will, if extended beyond its proper limits, give unreliable or nonsensical results. The programs described below are most likely to give trouble either for very small or very large size parameters. Computations based on exact theories, however, are often unnecessary in such extremes: Rayleigh theory is a good approximation for very small particles, and geometrical optics combined with diffraction theory is a good approximation for very large particles. To call for the exact theory in these instances is to call for an elephant gun to shoot a mouse.

The programs should not be used without an attitude of healthy skepticism. We tested them as much as possible, but they undoubtedly contain hidden flaws. In the following appendixes we discuss criteria that the programs were required to satisfy. Some of them are obvious: the extinction efficiency must not be less than the scattering efficiency, and both must be nonnegative; others are more subtle.

Each program is composed of two parts: a calling program, which requires as input refractive indices, particle size, and wavelength; and a subroutine—the workhorse—which computes scattering coefficients, scattering matrix elements, and efficiencies. The possible combinations of input and output variables are almost countless. Therefore, we have included calling programs merely to point the way to how the subroutines might be grafted onto calling programs more suited to the users' needs.