

This Week's Citation Classic

Monchick L & Mason E A. Transport properties of polar gases.

J. Chem. Phys. **35**:1676-97, 1961.

[Applied Physics Lab., Johns Hopkins University, Silver Spring, MD and
Institute for Molecular Physics, University of Maryland, College Park, MD]

Physical arguments were used to construct an approximation that enabled the calculation of viscosity, diffusivity, and heat conductivity of polar gases with the computing ability of the time. The full numerical calculation, while no longer quite impossible, is usually still impractical. [The SCI[®] indicates that this paper has been cited over 280 times since 1961.]

Louis Monchick
Johns Hopkins University
Applied Physics Laboratory
Laurel, MD 20810
and
E.A. Mason
Department of Chemistry
Brown University
Providence, RI 02912

January 5, 1981

"By the late 1950s the transport properties of nonpolar gases seemed well in hand, but polar gases were a different story. The permanent dipoles made the intermolecular forces strongly dependent on the relative orientations of the molecules, so that a collision trajectory was extremely difficult to compute. Although the basic kinetic theory existed, the collision dynamics was far too complicated for the computers of the day. Incidentally, it is *still* too complicated, in that a full calculation is difficult enough to be infeasible in practice, although not impossible. The obvious trick of first averaging over orientations to produce an effective spherical interaction threw the baby out with the bath water.

"The trick that did work, described in this paper, grew out of our earlier independent work on gas properties at very high temperatures, a subject of

great interest at that time. Monchick had just calculated the collision integrals for an exponential repulsion potential, and Mason had just worked on the kinetic theory for dissociated gases, where multiple interactions occur between valence-unsaturated atoms, which depend on the relative orientations of the electron spins. The latter problem had shown that the correct procedure was to calculate collision integrals for each spin orientation, then average the integrals over all possible orientations. This result suggested a feasible approximation for polar molecules—first calculate the collision integrals for fixed relative orientation, and then average. Presumably, in each collision only the orientation around the distance of closest approach would dominate.

"Thus a collaboration was born—'How hard would it be to calculate the collision integrals for a polar Stockmayer potential with fixed orientation?' 'Not quite like duck soup, but close to it.' There was no reason for the collaboration other than mutual interest and the fun of attacking a long-standing problem. We never had any official institutional connection, and were not even especially close geographically. But this paper was the first result of a collaboration that lasted over ten years and resulted in some 18 journal articles^{1,2} (in which the authors' names appeared in idiosyncratic order).

"Why has this work held up so well for 20 years? We suspect the following: (a) Success in correlating a wealth of experimental data, (b) Physical attractiveness and mathematical tractability of the model. (c) Lack of anything better. ('The game may be crooked, but it's the only one in town.') (d) Recent improved justification for its premises—it is the classical limit of the currently-popular infinite-order-sudden (IOS) approximation of quantum scattering theory."

1. Mason E A & Monchick L. Heat conductivity of polyatomic and polar gases. *J. Chem. Phys.* **36**:1622-39, 1962.
2. Ferziger J H & Kaper H G. *Mathematical theory of transport processes in gases*. Amsterdam: North Holland, 1972. 579 p.