**A New Thermodynamic Prediction Method and its Application to Chemical Weapons**

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**Abstract:** A relatively new thermodynamic property prediction method will be very briefly presented. The starting point is the quantum mechanics calculation of the surface charge on each molecule. This calculation has to be done only once for each molecule and then stored for all future use in all thermodynamic calculations. Our available data base contains more than 2200 molecules. Since the qm calculation is molecule specific, and unlike simple group contribution methods the method can distinguish between isomers (important for toxicity and drug effectiveness studies), and can be used when group-group interaction parameters (as in UNIFAC) are unavailable. The examples I will use today deal with chemical warfare agents for which group contribution methods are inapplicable, and the agents are too hazardous for laboratory measurements.



**Biography:** **Stanley I. Sandler** is the H. B. DuPont Professor of Chemical and Biomolecular Engineering at the University of Delaware, where he has been a faculty member for 50 years. He received the B.Ch.E. at the City College of New York and the University of Minnesota. He has been, or is, a visiting professor U. California Berkeley, Imperial College (London), Universities of Queensland and Melbourne (both in Australia) and the National University of Singapore. He is the previous editor of the AIChE Journal, and the author of more than 400 research papers and several widely used textbooks (including one in its 5th edition) in the general area of thermodynamics.

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