

# **ANSYS Chemkin-Pro Getting Started Guide**



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# **Getting Started With Chemkin Manual**

**Annelies Wilder-Smith** 

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carbon monoxide and hydrocarbon or alternate fuels Readers looking for guidance to the current knowledge we have in this area will find a broad outline and extensive references to the review and archival literature in Chapter 1 where the essential **Computer Generated Physical Properties** Stan features of combustion chemistry modeling are surveyed Bumble, 1999-06-01 Computer Generated Physical Properties offers the environmental scientist a basis to predict the properties of molecules and reengineer them to remove those properties that are harmful to the environment This technology is currently used in other fields and is now becoming popular in the environmental engineering field because of its pollution prevention and waste reduction capabilities This book interdisciplinary in scope treats the physical properties of matter as generated by computers It covers a wide variety of topics pointing towards synthesizing new molecules to substitute for reactants intermediaries and products in industrial processes with better physical and environmental properties than the original The author achieves this with a spreadsheet program called SYNPROPS that operates on a PC computer with optimization features A radar type graph one for each property visually sorts the various groups in order of their contribution to the property creating the necessity for a computer to obtain answers for the structure of the optimum molecules for substitution or synthesis The author discusses applications to biologically active molecules without side effects including antineoplatic drugs Additionally he demonstrates model compounds and the applications of SYNPROPS optimization and substitution This book has everything you need to know about deriving properties and combinational chemistry from molecular structure Light Water Reactor Safety Research Program Sandia National Laboratories, 1981-10

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