Chemical Reactivity and Molecular Beam Scattering

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The research program detailed in this final report concerns the measurement of integral cross sections for a large number of molecules. From such cross sections it is possible to determine the so-called van der Waals or C_6 coefficients for the attractive portion of the pair-wise potentials, which follow a $1/r^6$ dependence on the inter-particle distance. We have

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obtained absolute values for total scattering cross sections at velocities well-defined for each of 38 different systems involving Ar and a variety of target molecules, chiefly hydrocarbons. From these scattering cross sections C_6 values for each system were deduced. Using the values of these coefficients obtained from our cross section measurements, we were also able to test a mixing rule recommended by Kramer and Herschbach[1] which allows estimation of force constants between unlike molecules from their interaction with a common partner. 741 such combinations were obtained from our experimental data in conjunction with this mixing rule. With this catalogue of C_6 values and independent experimental investigation of several of the systems, we have evaluated the method as a predictive tool for the estimation of transport and thermodynamic properties which depend upon the attractive forces between molecules.

AFOSR - TR - 76 - 1084

FINAL REPORT

to the

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH

Directorate of Chemical Sciences

for Grant # AFOSR-72-2236

on

Chemical Reactivity and Molecular Beam Scattering

by

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July 31, 1976

A

I. Introduction

When a material system is in gaseous form the average distance between component atoms and molecules is so large that when any two of them collide, they are in relative isolation. Consequently, to explain macroscopic behavior of gaseous systems in terms of microscopic events requires working answers to two primary questions: (1) What is the nature of the two body collisions which are involved? and (2) How do the individual events add up to the macroscopic behavior of a large population? The choice of appropriate summation procedure is the core problem of statistical mechanics. We are concerned here with the first question. Though its answer is most relevant to properties and processes of gaseous systems, two body encounters also provide the basis for first order approximations of the behavior of condensed systems.

The convenient and usual way of describing the interaction between two atoms and molecules is in terms of the potential energy of the system comprising the two particles and its dependence upon the distance between them. There are cases in which such interaction potentials are characterized by repulsive forces at all internuclear distances. Coulomb repulsion between two charged particles of like sign is an example. More generally, however, as in the case of neutral particles, two body potentials have a repulsive branch at small internuclear distances and an attractive branch at large distances. These two branches merge at some intermediate distance to form the so-called potential well. The "depth" of this well is a measure of the strength of the chemical bond between the two particles if they are allowed to give up energy and remain "combined" when they are brought together.

When two particles in a population collide at energies which are high with respect to the depth of the potential well, the dynamics of the collision are

generally governed by the nature of the repulsive part of the potential. When the collision energies are relatively low, it is the attractive part of the potential which dominates the process. At temperatures below about 1500 K most thermodynamic and transport properties of gaseous systems reflect the nature of the attractive portion of the potential. It is possible to infer some features of the interaction potential from such macroscopic properties but most of the details are lost in the averaging consequences of the great numbers of collisions. On the other hand, if full information is available on the interaction potential between potential partners in a population of atoms and molecules, it is possible, in principle, to calculate exactly all the macroscopic transport and thermodynamic properties of the population. Indeed, if enough information is available, it is possible in principle also to describe all possible kinetic behaviour of the population including chemical reactions. Thus, information on the nature of two body interaction potentials is both fundamental and useful. A powerful method for obtaining information on intermolecular potentials is by molecular beam scattering experiments. In such experiments a highly collimated beam of molecules is allowed to intersect a similar beam of "target" molecules at some well defined angle or it is allowed to pass through a scattering chamber containing target gas at a density such that while traversing the chamber, a substantial fraction of the beam molecules will undergo a single collision with one of the target molecules. There are two ways in which the consequences of the resulting collisions with target molecules are examined. In one, a movable detector measures the flux of scattered molecules at various angles with respect to the incident beam. The results are expressed in terms of so-called "differential scattering cross section". It represents the probability that an incident beam of molecules will be scattered in a particular direction.

In the second kind of experiment a stationary detector on the beam axis measures

residual flux on the beam axis after all the scattering has taken place. Clearly, the difference between the initial and final fluxes is a measure of the integral of the differential cross section over all angles. If the angle intercepted by the detector is sufficiently small to be within the minimum observable scattering angle allowed by the uncertainty principle then the resulting integral cross section is known as the total cross section. It represents the cross-sectional area of the sphere within which the centers of two molecules will have to be located if they are to have any observable effect on each other's trajectories. Clearly, differential cross section data contain more information than integral cross section data. But differential measurements are much more difficult to carry out. If integral cross sections are measured at well defined collision energies over a range of such energies the resulting data can provide a fairly detailed description of the attractive part of the intermolecular potential.

The present program has been concerned with measurements of integral cross sections for a wide variety of molecules in order to determine the so-called van der Waals or C_6 coefficients for the attractive portion of the pair wise potential. The C_6 designation stems from the fact that at the relatively large internuclear distances involved in total scattering cross sections for molecules without permanent dipole moments, the attractive force is due to induced-dipole-induced dipole interactions which make the potential energy of the pair decrease as the sixth power of the internuclear distance. Thus C_6 is the coefficient of the $1/r^6$ term in most expressions for intermolecular potential, e.g. the familiar 12-6 or Lennard Jones potential. Originally we planned to obtain relative values of total cross sections over a variety of collision energies. Such measurements provide information about the depth and location of the so-called potential well. As we developed the equipment and our techniques we found that we could obtain absolute values of the total cross section with substantial accuracy and precision. Such absolute values

at a particular and well defined velocity are perhaps the best way of obtaining C_6 values directly but there have been relatively few investigators who have been willing to take the pains necessary to achieve absolute values. Consequently, we devoted much of our effort to obtaining C_6 coefficients for a large number of molecular pairs. We must admit that this slight shift in our objectives was encouraged by difficulties which we encountered in making in situ measurements of beam molecule velocity over a range of velocities during the scattering experiments. We were also stimulated by the desire to test a mixing rule which Kramer and Herschbach had found to be very effective in determining force constants between unlike molecules from their interaction behaviour with a common partner.[1] That is to say, if C_6 is known for the interaction of A with B and A with C, then the mixing rule will predict the C_6 for the interaction of B with C. Thus, if a set of C_6's is obtained for A with a family of molecules, an effective mixing rule would permit the prediction of C_6 for the interaction of any pair of molecules in the family. Clearly, an effective mixing rule together with a set of C_6 values for a particular molecule with a wide variety of collision partners would comprise a very useful predictive tool in the estimation of transport and thermodynamic properties which depend upon the attractive forces between molecules. In what follows we will set forth what we have achieved in developing this tool.

II. Equipment and Procedures

The essential steps in our experiments comprised: (1) generating a molecular beam by passing the core of a freely expanding supersonic jet through a conical collimating orifice commonly called a skimmer; (2) further collimating the beam and passing it through a scattering box; (3) measuring the intensity of the beam with an ionization gauge detector after it emerged from the scattering box. The intensity I when gas is present in the scattering box and the intensity I_o when

there is no gas in the box are related by Beer's Law:

$$I/I_o = e^{-Qnl}$$

where Q is the total scattering cross section and n is the number density of molecules along the scattering path of length L. From measurements of I, I_o, l and n we obtain Q.

We used a molecular beam apparatus which had been designed and partly built when our laboratory was in Princeton. With the support from the present grant it was completed and put into operation here at Yale. It is a three stage nozzle beam system with separate pumping in the nozzle exhaust, collimating and test chambers respectively, made entirely of stainless steel. We refer to it as our "Minibeam" because it features diffusion pumps only six inches in diameter, as contrasted with the thirty-two inch diameters of our older pumping systems. The advantages of a nozzle beam in scattering experiments include high intensity and narrow velocity distribution of the beam molecules. [2,3] A high intensity is important because in attempting to measure total scattering cross section one wants a very narrow beam and a fairly long distance between the scattering region and the detector so that the effective angular resolution of the apparatus is high, i.e. so that a very small deflection will cause a molecule to miss the detector. The effective resolution in our system is about three quarters of a milliradian. A narrow velocity distribution in the beam is desirable in order to minimize the spread of energies over which the scattering occurrs. In a scattering experiment for the determination of absolute total cross sections the number of target molecules along the scattering path must be precisely known. Therefore, it is almost inevitable that the scattering region must comprise a box of accurately known dimensions containing isotropic low density gas at an accurately known temperature and pressure. Thus, there is always thermal energy spread in the target molecules. (The maximum energy to be associated

with the observed scattering spread is in effect the sum of the energy spreads of the beam and target molecules.) When the beam molecules have a narrow velocity distribution, the corrections for energy spread are much smaller than if the beam had the kind of wide distributions associated with beams from effusive sources.

An important feature of our apparatus is its partnership with PDP 11 computer which AFOSR allowed us to acquire under this grant. It was purchased and incorporated into the system about halfway through the study. This computer not only controlled and operated the beam system, but provided on line processing of the data including the tedious corrections for velocity spread and angular resolution. Because of its ability to process large quantities of data in reasonable time, we were able to increase our precision by averaging results over large numbers of independent measurements. In fact, all the experimental results on total cross sections which we report are averages of at least 48 separate measurements. Implicit in this statement is the fact that after installing the computer, we repeated all the measurements we had made during the first two years of our effort.

Evidence of the precision and accuracy which we are able to achieve is given by our latest determination of the cross section for argon-argon scattering, which is the reference benchmark for all of our measurements. By measuring total cross sections at varying source pressure and extrapolating to zero source pressure, we obtain a value of 342. $\mathring{A}^2$ at a relative velocity of 555 m/s. The best available intermolecular potential for argon-argon, the so-called Barker-Fisher-Watts potential obtained from best fits for a wide range of experimental data of all kinds, predicts a value of 340.6$\mathring{A}^2$ for these conditions. To our knowledge, this agreement is the best that has yet been obtained by anyone. Incidentally, it is noteworthy that the extrapolation to zero pressure became necessary when we learned from other experiments in our laboratory that the dimer population in argon beams from nozzle sources is much higher than previous investigators had believed. Of course, a mass spectro-

meter detector would have eliminated the necessity of extrapolating to zero pressure because it would not "see" dimers when tuned to monomers. On the other hand, rarely can mass spectrometers combine reproducibility and sensitivity as effectively as ionization gauge detectors.

We mentioned in the Introduction that we had had some difficulty in obtaining in situ measurements of beam velocity during scattering experiments. This difficulty arose after we had installed the computer. The programming and interfacing of the computer with velocity distribution measurements by Time-Of-Flight turned out to be more difficult than we had imagined. We now have most of the problems ironed out and in the future, hope to make beam velocity measurements as a routine matter. The inability to make in situ velocity measurements has not been a great inhibition in many cases where we have accurate velocity information from earlier analog experiments in terms of source conditions, especially with relatively simple molecules. Essentially all the results reported here fall in that category and do not suffer from uncertainty in the relative velocity to which the reported cross sections and the derivative C_6 values relate.

A more complete description of the equipment and procedures will be found in the paper "Total Cross Section Measurements for the Scattering of Argon by Aliphatic Hydrocarbons" by T. Nenner, H. Tien and J. B. Fenn which appeared in the Journal of Chemical Physics.

III. Results

As indicated in the Introduction, a primary objective of this work became the testing and implementation of a combination or mixing rule which would make possible the prediction of a large number of C_6 coefficients for molecule pairs from a much smaller number of measurements. In particular, we wanted to increase the scope of a rule which Kramer and Herschbach had found to be most effective. This rule,

first proposed by Molewyn-Hughes can be written:

$$G_{12} = (G_{11} + G_{22})/2$$

where G_{12} is defined by $\alpha_1\alpha_2/C6_{12}$, α being the polarizability, and the subscripts relate to different species. Similarly,

$$G_{23} = G_{12} + G_{13} - G_{11}$$

Thus, we can predict G_{23} from C_6 values obtained from the scattering of species 1 by species 2 and species 3, provided we know something about the polarizability of each species. A straightforward extension of this approach means that with a catalogue of C_6 values obtained from total scattering cross sections for a reference molecule on a variety of target molecules, we can predict C_6 values for all combinations of molecules in the catalog. In our studies thus far we have obtained total scattering cross sections and the derivative C_6 values for argon as a reference molecule on 38 other molecules. This collection of data in combination with the mixing rule gives rise to 741 different C_6 values.

Of course, the question is whether the resulting values are reliable, i.e. does the mixing rule work. In order to answer this question, we also measured total scattering cross sections for another 40 combinations of molecules in the catalogue. At the same time, we calculated C_6 values from polarizabilities using the well known Slater-Kirkwood approximation.[4] We thought it would be valuable to determine the extent to which this approximation might be useful in the absence of any experimental data at all. The Slater-Kirkwood approximation can be written:

$$C_{6_{1\text{-}2}} = \frac{25.1 \times 10^{-60}\ \alpha_1\alpha_2}{(\alpha_1/N_1)^{1/2} + (\alpha_2/N_2)^{1/2}}$$

where N is often taken as the number of outer shell electrons and is sometimes

regarded as an empirical fitting parameter. We have assumed N = 6 for argon. It is the number of outer shell electrons in all the other molecules.

The results are summarized in the tables which comprise Section V. In addition to experimental values the tables include all values calculated from the Slater-Kirkwood approximation and from the mixing rule in light of experiments. We have not yet completely digested all of this material, but we will make some observations. First we note that the mixing rule does seem to work for the compounds which we have tested. In general, it gives values within less than five per cent of the experimental value. We would not hesitate, therefore, to use the mixing rule to calculate values of C_6 for practically any combination of molecules in the catalogue. Perhaps more suprising is the effectiveness of the Slater-Kirkwood approximation. It seems in general to give C_6 values which are rarely more than ten per cent in error and are usually much closer. Consequently, we would not hesitate to accept the results of Slater-Kirkwood calculations for any molecules which are not in our catalog but which are reasonably similar in a chemical sense to those in the catalogue. It seems to us that an important consequence of this work is a substantial extension of the possibility of estimating thermodynamic and transport properties where attractive forces play a role and when there is a paucity of experimental data. In essentially all of the interaction potentials which are used in the calculation of these properties the attractive part of the potential is expressed by a term involving the inverse sixth power of the internuclear distance. Our results make it possible to estimate the contribution of that term in more systems with more confidence than has heretofore been possible.

It will have been noted that we hedged a bit in the preceding paragraph by saying that we would not hesitate to use the Slater-Kirkwood or Mixing Rule approximations for "practically" any combination of species. There are some notable exceptions with very small molecules, in particular, helium and hydrogen. In the case of helium the

C_6 value estimated by Slater-Kirkwood is larger than experiment for small target molecules but substantially smaller for large target molecules. The helium atom is so fast and the attractive force is so small that the scattering cross section is due largely to the repulsive part of the potential which is effective at smaller internuclear separations. Consequently, the experimental total cross section does not truly reflect the attractive part of the potential which is what Slater-Kirkwood purports to estimate. For this reason, we can understand why the apparent experimental values of C_6 are smaller than the Slater-Kirkwood values, which is what happens with the smaller molecules as scattering centers. However, with large target molecules the apparent C_6 values from experiment are <u>larger</u> than the Slater-Kirkwood estimates. A similar trend shows up in the case of hydrogen. Because the attractive force is much larger than with helium, the hydrogen scattering is dominated by the attractive part of the potential. Consequently, the agreement between Slater-Kirkwood and experiment is reasonably good in the case of methane. However, as the target molecules become bigger the C_6 from experiment becomes much larger than the C_6 from Slater-Kirkwood. Thus, in the case of both helium and hydrogen, the apparent C_6 relative to the Slater-Kirkwood value increases with increasing size of the target molecule. We have not yet completely rationalized this behavior but we think it may be due to a geometric size effect which has not been hitherto considered. We argue that when the effective diameter of a molecule becomes appreciable relative to the distance of its center of mass from the center of mass of a colliding partner, the average distance over which the induced-dipole induced-dipole interactions occur is less than the internuclear distance. Thus, in the C_6/r^6 term if one inserts the internuclear r the denominator is too big so that the numerator must also appear large. We have made some calculations which give qualitative agreement with what we have observed but much more work is needed before we can draw any quantitative conclusions. We would note in passing that the

same kind of effect is implicit in the well known dependence of van der Waals attraction between a molecule and a surface on r^{-3} where r is the distance from the surface. This dependence on the cube of the distance results from an average of sixth power dependence on internuclear distance for the induced-dipole-induced-dipole interactions over all the surface atoms seen by the approaching gas molecule.

There is another bit of not-quite-finished work which we have carried out. By looking at the polarization of fluorescence from alkali metal dimers in freely expanding jets, Sinha et al found that a substantial fraction of these dimers were aligned so that the plane of rotation was parallel to the jet axis.[5] Korving et al have recently confirmed this observation.[6] It occurred to us that a similar orientation might occur in carbon dioxide molecules being accelerated by a helium carrier gas. Moreover, it seemed likely that aligned molecules would have a smaller scattering cross section than randomly oriented molecules. We therefore undertook some measurements in which we scattered a beam of accelerated carbon dioxide molecules by argon and then under otherwise identical conditions scattered a beam of argon by carbon dioxide molecules. Indeed we found that carbon dioxide scattered by argon (where alignment could occur) showed a total cross section some 7 per cent smaller than argon scattered by carbon dioxide (where alignment could not occur). The problem is that we are not positively certain that the relative velocities were the same in the two cases. Because the velocity dependence of the cross section is appreciable we dare not conclude that we have an alignment effect until we repeat the experiments with in situ measurements of velocity. As we indicated earlier, after having encountered what seemed an almost endless sequence of difficulties in interfacing and programming the computer for TOF velocity measurements, we think we are about ready to succeed. Consequently, we hope to confirm this alignment effect on scattering in the near future.

IV. Publications

Two papers communications have thus far been published:

"Total Cross Section Measurements for the Scattering of Argon by Aliphatic Hydrocarbons," by T. Nenner, H. Tien and J. B. Fenn, Journal of Chemical Physics 63, 5439 (1975)

"Long Range Attractive Forces for Hydrogen-Light Hydrocarbon Pairs," by H. Tien, T. Nenner and J. B. Fenn, AIchE Journal 22, 405 (1976)

In preparation is at least one paper on the mixing rule test and confirmation in which we have measured. If that paper turns out to be too long, we may have to subdivide it. In prospect is a paper on the alignment effect on scattering cross section as well as at least one more paper extending the cross section measurements to additional varieties of collision partners. In particular we are making measurements on aromatic hydrocarbons, and compounds with permanent dipole moments. Although AFOSR sponsorship of this study has ended, its role in our future work in this area is all important and will be duly acknowledged. We would here record our deep appreciation for the support and cooperation which we have enjoyed.

V. Tables

The first table shows a comparison of our values total cross section for argon-argon with these of other investigators. In the remaining tables which comprise this section are listed values of the C_6 van der Waals coefficients which have been obtained from experimental values of total scattering cross sections and from calculations. Each table relates to a particular atom or molecule which appears in the title. The contents of the table are the C_6 values for that atom or molecule paired with each of the atoms and molecules in the left hand column. In general there are three columns of values for C_6. Those in the columns headed "C_6 EXP'T" are based on experimental values of total scattering cross section. Those in the columns headed "C_6 -S-K" are calculated from the Slater-Kirkwood approximation. Those in the columns headed "C_6 - C - R" are from the mixing or combination rule in conjunction with the values from experimental cross sections. In addition, there are columns which show the ratios of the Slater-Kirkwood and mixing rule values to the direct experimental values. The molecular species are identified by their usual chemical symbols. All the hydrocarbons are normal unless there is a suffix "cyclo" or "iso" after the formula. In the case of C_nH_{2n-2} the suffix "yne" indicates an acetylenic linkage and the suffix "diene" indicates two olefinic linkages. In the second table the column heading "POLA" stands for polarizability and the heading "DIPO" indicates dipole moment.

Finally, Table 38 contains preliminary results from new areas which will ultimately be worked into the scheme of Tables 2 through 37.

TABLE I

The comparison of Ar-Ar total cross sections (relative velocity = 669 m/sec).

Source	Value ($Å^2$)
Rothe-Neynaber	298
Swedenburg-Scott	310
Bredewout-Barker-Fisher-Watts	316
Dalgarno-Schiff-Landau-Lifshitz	306
This study	317

TABLE II

THE COMPARISON OF C6 FOR AR-HYDROCARBONS

GAS	C6-S-K	C6-EXP	C-SK/C-EXP	POLA	DIPO
AR	64.7	68.1	.95	1.643	0
N2	76.3	74	1.03	1.74	0
O2	73.2	67	1.09	1.57	0
CO2	115.4	113	1.02	2.59	0
HE	10	5.1	1.96	.2042	0
H2	28.7	46.6	.61	.806	0
CH4	96.9	100.6	.96	2.56	0
C2H6	167.1	173.8	.96	4.39	0
C2H4	152.6	152.3	1	4.1	0
C2H2	116.7	130.9	.89	3.04	0
C3H8	237.6	245.9	.96	6.23	0
C3H6	225.6	226.5	.99	6.02	.35
C3H4	206.7	193	1.07	5.55	.75
C3H4-DIENE	217.3	211.4	1.02	5.98	0
C3H6-CYCLO	215.3	211.4	1.01	5.66	0
C4H10	306.3	325	.94	8.01	0
C4H8-1	295.3	292.6	1	7.83	.37
C4H8-2-CIS	296.6	286.1	1.03	7.88	.37
C4H8-ISO	296.3	289.4	1.02	7.87	.49
C4H6-DIENE	308.1	279.7	1.1	8.56	.49
C4H6-1-YNE	277.9	228.9	1.21	7.41	.8
C5H12	371.6	395.1	.94	9.63	.8
C5H10	357.6	359.3	.99	9.35	.8
C5H8	330.9	327.8	1	8.62	.86
C5H10-CYCLO	346.9	340.4	1.01	8.97	.86
C6H14	451.8	476	.94	11.85	0
C6H12	441.9	448.7	.98	11.72	0
C6H10	415	425.6	.97	10.94	.89
C6H12-CYCLO	414.4	414	1	10.75	0
C7H16	522.8	576.9	.9	13.71	0
C7H14	508.7	560.1	.9	13.43	0
C7H12	486	504.4	.96	12.8	.87
C7H14-CYCLO	497.4	467.6	1.06	13.03	0
C8H18	592.7	660.9	.89	15.53	0
C8H16	578.6	636.8	.9	15.25	0
C8H16-CYCLO	561.6	542.2	1.03	14.87	0

TABLE III

THE COMPARISON OF C6 FOR CO2-HYDROCARBONS

GAS	C6-S-K	C6-C-R	C6-EXPT	C-SK/CEXP	C-CR/CEXP
CO2	209.2	188			
HE	18.4	8.3			
H2	50.5	79			
CH4	171.9	166.5	153	1.12	1.08
C2H6	296.6	287.7	274	1.08	1.04
C2H4	270.1	251.4			
C2H2	207.2	217.7			
C3H8	421.7	407	380	1.11	1.07
C3H6	399.4	374			
C3H4	365.4	317.6			
C3H4-DIENE	383.5	348			
C3H6-CYCLO	382.1	348.3			
C4H10	543.9	538.7	470	1.16	1.14
C4H8-1	523.2	483			
C4H8-2-CIS	525.6	471.7			
C4H8-ISO	525.4	477.3			
C4H6-DIENE	542.9	458.9			
C4H6-1-YNE	491.9	374.8			
C5H12	660	655.2			
C5H10	634.4	594			
C5H8	587.4	541.6			
C5H10-CYCLO	616.3	562.4			
C6H14	801.8	768.5			
C6H12	783.1	741.5			
C6H10	735.6	703.8			
C6H12-CYCLO	736.6	684.4			
C7H16	927.9	958			
C7H14	902.1	929.6			
C7H12	861.6	834.7			
C7H14-CYCLO	883	770.4			
C8H18	1052	1098.2			
C8H16	1026.3	1057			
C8H16-CYCLO	995.7	894			

TABLE IV

THE COMPARISON OF C6 FOR 02-HYDROCARBONS

GAS	C6-S-K	C6-C-R
02	85.5	66
C02	133.6	111.3
HE	11.8	4.9
H2	31.9	46.4
CH4	108.8	98.9
C2H6	187.7	170.8
C2H4	170.7	149.4
C2H2	131.2	128.9
C3H8	266.9	241.6
C3H6	252.6	222.2
C3H4	230.9	189
C3H4-DIENE	242.2	207.1
C3H6-CYCLO	241.8	207.3
C4H10	344.3	319.5
C4H8-1	331	287
C4H8-2-CIS	332.4	280.5
C4H8-ISO	332.3	283.7
C4H6-DIENE	342.7	273.4
C4H6-1-YNE	311	223.5
C5H12	417.9	388.6
C5H10	401.5	352.8
C5H8	371.8	321.7
C5H10-CYCLO	390.2	334.1
C6H14	507.5	467.9
C6H12	495.4	440.4
C6H10	465.3	417.9
C6H12-CYCLO	466.5	406.5
C7H16	587.3	567.8
C7H14	570.8	551.1
C7H12	545.1	495.5
C7H14-CYCLO	558.9	458.2
C8H18	665.9	650.8
C8H16	649.4	626.6
C8H16-CYCLO	629.9	531.5

TABLE V

THE COMPARISON OF C6 FOR N2-HYDROCARBONS

GAS	C6-S-K	C6-C-R	C6-EXPT	C-SK/CEXP	C-CR/CEXP
N2	91.1	80.5	82	1.11	0.98
O2	88	72.9	79	1.11	0.92
CO2	138	123			
HE	12.1	5.5			
H2	33.5	51.2			
CH4	113.8	109.2	116	0.98	0.95
C2H6	196.2	188.6	197	1.00	0.96
C2H4	178.8	165.1			
C2H2	137.1	142.4			
C3H8	279	266.8	283	1.01	0.95
C3H6	264.3	245.5			
C3H4	241.9	208.9			
C3H4-DIENE	253.9	228.8			
C3H6-CYCLO	252.8	229.1			
C4H10	359.8	353	331	1.09	1.07
C4H8-1	346.2	317.1			
C4H8-2-CIS	347.8	309.9			
C4H8-ISO	347.7	313.5			
C4H6-DIENE	359.6	302.2			
C4H6-1-YNE	325.6	247.1			
C5H12	436.6	429.2			
C5H10	419.8	389.7			
C5H8	388.6	355.5			
C5H10-CYCLO	407.7	369.1			
C6H14	530.5	516.8			
C6H12	518.2	486.6			
C6H10	486.8	461.7			
C6H12-CYCLO	487.2	449			
C7H16	613.9	627.1			
C7H14	596.9	608.7			
C7H12	570.1	547.4			
C7H14-CYCLO	584.2	586.3			
C8H18	696	718.7			
C8H16	679.1	692			
C8H16-CYCLO	658.9	587.3			

TABLE VI

THE COMPARISON OF C6 FOR HE-HYDROCARBONS

GAS	C6-S-K	C6-C-R	C6-EXPT	C-SK/CEXP	C-CR/CEXP
HE	1.6	.5	0.64	2.59	0.78
H2	4.3	3			
CH4	14.8	7.7	8.7	1.70	0.88
C2H6	25.6	13.2	18.4	1.39	0.71
C2H4	23.2	11.9	14.7	1.58	0.86
C2H2	17.9	9.6			
C3H8	36.4	18.7	36.3	0.95	0.48
C3H6	34.4	17.5	27.8	1.13	0.49
C3H4	31.4	15.4			
C3H4-DIENE	32.9	16.8			
C3H6-CYCLO	33	16.4			
C4H10	46.9	24.4	50.7	0.97	0.48
C4H8-1	45.1	22.7			
C4H8-2-CIS	45.3	22.5			
C4H8-ISO	45.3	22.6	41.8	1.08	0.54
C4H6-DIENE	46.6	22.8			
C4H6-1-YNE	42.3	19			
C5H12	57	29.6	77.9	0.82	2.52
C5H10	54.7	27.6	68.9	0.79	0.40
C5H8	50.7	25.3			
C5H10-CYCLO	53.2	26.3			
C6H14	69.2	36	98.1	0.71	0.37
C6H12	67.5	34.5			
C6H10	63.4	32.5			
C6H12-CYCLO	63.6	31.8			
C7H16	80.1	42.8			
C7H14	77.8	41.7			
C7H12	74.3	38.4			
C7H14-CYCLO	76.2	36.9			
C8H18	90.8	48.8			
C8H16	88.5	47.4			
C8H16-CYCLO	85.8	42.5			

TABLE VII

THE COMPARISON OF C6 FOR H2-HYDROCARBONS

GAS	C6-S-K	C6-C-R	C6-EXPT	C-SK/CEXP	C-CR/CEXP
H2	12.8	37.8			
CH4	43.1	67.5	48	0.93	1.40
C2H6	74.3	116.9	116	0.67	1.00
C2H4	68	100.2			
C2H2	51.8	91			
C3H8	105.7	165.1	187	0.58	0.90
C3H6	100.5	149.5			
C3H4	92.2	124.2			
C3H4-DIENE	97.1	136.7			
C3H6-CYCLO	95.8	139.2			
C4H10	136.2	220.5	242	0.58	0.90
C4H8-1	131.5	192.7			
C4H8-2-CIS	132.1	186.6			
C4H8-ISO	132.1	189.6			
C4H6-DIENE	137.8	176.6			
C4H6-1-YNE	123.9	142.3			
C5H12	165.1	269.3			
C5H10	159.1	239			
C5H8	147.2	217.3			
C5H10-CYCLO	154.2	225.5			
C6H14	200.9	321.8			
C6H12	196.7	298			
C6H10	184.8	284.3			
C6H12-CYCLO	184.1	275.6			
C7H16	232.5	397.1			
C7H14	226.4	384.2			
C7H12	216.3	338.5			
C7H14-CYCLO	221.2	303.9			
C8H18	263.5	457.1			
C8H16	257.4	437			
C8H16-CYCLO	250	354.2			

TABLE VIII

THE COMPARISON OF C6 FOR CH4-HYDROCARBONS

GAS	C6-S-K	C6-C-R	C6-EXPT	C-SK/CEXP	C-CR/CEXP
CH4	145.4	149.1	144	1.01	1.03
C2H6	250.6	257.4	2244	1.03	1.05
C2H4	229	226.3	214	1.07	1.06
C2H2	174.9	193.1			
C3H8	356.2	364.2	344	1.03	1.06
C3H6	338.4	336.3	312	1.07	1.08
C3H4	310.3	287.6			
C3H4-DIENE	326.5	314.7			
C3H6-CYCLO	322.9	313.9			
C4H10	459.2	480.8	468	0.98	1.03
C4H8-1	442.9	434.6			
C4H8-2-CIS	445	425.5			
C4H8-ISO	444.9	430.1	416	1.07	1.03
C4H6-DIENE	463	417.8			
C4H6-1-YNE	417.1	342.7			
C5H12	557	584.1	573	0.97	1.02
C5H10	536.2	533	521	1.03	1.02
C5H8	496.2	486.5			
C5H10-CYCLO	520	505.3			
C6H14	677.4	704.5	697	0.97	1.01
C6H12	662.8	665.6			
C6H10	622.5	630.8			
C6H12-CYCLO	621.1	614			
C7H16	783.8	851.7			
C7H14	762.9	827.3			
C7H12	728.9	747.2			
C7H14-CYCLO	745.8	695.8			
C8H18	888.6	975.3			
C8H16	867.7	940.6			
C8H16-CYCLO	842.4	806.2			

TABLE IX

THE COMPARISON OF C6 FOR C2H6-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C2H6	431.9	444.4
C2H4	394.7	390.6
C2H2	301.4	333.5
C3H8	614	628.8
C3H6	583.3	580.4
C3H4	534.7	496.3
C3H4-DIENE	562.6	543
C3H6-CYCLO	556.5	541.8
C4H10	791.6	830.2
C4H8-1	763.3	750
C4H8-2-CIS	767	734.3
C4H8-ISO	766.7	742.2
C4H6-DIENE	797.9	720.5
C4H6-1-YNE	718.8	590.9
C5H12	960	1008.7
C5H10	924.1	920.1
C5H8	855.2	839.7
C5H10-CYCLO	896.3	872.1
C6H14	1167.5	1216.4
C6H12	1142.3	1148.9
C6H10	1072.9	1069
C6H12-CYCLO	1070.6	1059.9
C7H16	1351	1471.1
C7H14	1314.9	1428.8
C7H12	1256.3	1290
C7H14-CYCLO	1285.4	1200.5
C8H18	1531.6	1684.6
C8H16	1495.5	1624.4
C8H16-CYCLO	1451.9	1391.1

TABLE X

THE COMPARISON OF C6 FOR C2H4-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C2H4	360.9	344.5
C2H2	275.4	291.7
C3H8	561.1	552.8
C3H6	533.3	511.5
C3H4	489	439.2
C3H4-DIENE	514.6	480.2
C3H6-CYCLO	508.6	477.8
C4H10	723.4	728.6
C4H8-1	697.8	661.3
C4H8-2-CIS	701.1	648.4
C4H8-ISO	700.9	655
C4H6-DIENE	730	639.6
C4H6-1-YNE	657.3	526
C5H12	877.2	884.8
C5H10	844.6	810
C5H8	781.6	739.7
C5H10-CYCLO	819	768.3
C6H14	1067	1068.3
C6H12	1044.2	1011.7
C6H10	980.7	958.1
C6H12-CYCLO	978.2	933
C7H16	1234.7	1288.5
C7H14	1201.8	1252.1
C7H12	1148.3	1134.1
C7H14-CYCLO	1174.7	1060.8
C8H18	1399.7	1474.5
C8H16	1366.8	1423.4
C8H16-CYCLO	1327.1	1228.2

TABLE XI

THE COMPARISON OF C6 FOR C2H2-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C2H2	210.4	252
C3H8	428.5	471.8
C3H6	407	433.8
C3H4	373.1	368.8
C3H4-DIENE	392.4	404
C3H6-CYCLO	388.3	404.8
C4H10	552.4	624.2
C4H8-1	532.7	560.3
C4H8-2-CIS	535.2	547.4
C4H8-ISO	535	553.8
C4H6-DIENE	556.5	533.2
C4H6-1-YNE	501.5	435.7
C5H12	670	759.2
C5H10	644.9	688.8
C5H8	596.8	628.2
C5H10-CYCLO	625.5	652.3
C6H14	814.8	913.9
C6H12	797.1	859.9
C6H10	748.7	816.1
C6H12-CYCLO	747.2	793.6
C7H16	942.8	1109.6
C7H14	917.6	1076.9
C7H12	876.7	967.7
C7H14-CYCLO	897	894.2
C8H18	1068.8	1271.8
C8H16	1043.6	1224.4
C8H16-CYCLO	1013.1	1037.4

TABLE XII

THE COMPARISON OF C6 FOR C3H8-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C3H8	872.8	889.8
C3H6	829.1	821.3
C3H4	760.1	702.4
C3H4-DIENE	799.6	768.6
C3H6-CYCLO	79 1	766.8
C4H10	1125.2	1174.6
C4H8-1	1085.1	1061.4
C4H8-2-CIS	1090.2	1039.2
C4H8-ISO	1089.8	1050.4
C4H6-DIENE	1134	1020
C4H6-1-YNE	1021.8	836.6
C5H12	1364.7	1427.2
C5H10	1313.6	1302
C5H8	1215.7	1158.3
C5H10-CYCLO	1274.1	1234.2
C6H14	1659.6	1721.1
C6H12	1623 7	1625.9
C6H10	1525.1	1541
C6H12-CYCLO	1521.9	1499.8
C7H16	1920.5	2081.3
C7H14	1869.1	2021.5
C7H12	1785.8	1825.3
C7H14-CYCLO	1827.2	1699.1
C8H18	2177.1	2383.3
C8H16	2125.8	2298.2
C8H16-CYCLO	2063.8	1968.9

TABLE XIII

THE COMPARISON OF C6 FOR C3H6-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C3H6	787.9	759.6
C3H4	722.5	651.6
C3H4-DIENE	760.3	712.6
C3H6-CYCLO	751.5	709.4
C4H10	1068.9	1082.9
C4H8-1	1031	982
C4H8-2-CIS	1036	962.5
C4H8-ISO	1035.6	972.4
C4H6-DIENE	1078.5	948.6
C4H6-1-YNE	971.1	779.6
C5H12	1296.3	1315.1
C5H10	1248	1203.1
C5H8	1154.9	1098.6
C5H10-CYCLO	1210.2	1141
C6H14	1576.6	1587.5
C6H12	1542.9	1502.7
C6H10	1449.1	1423.3
C6H12-CYCLO	1445.5	1385.8
C7H16	1824.5	1915.7
C7H14	1775.8	1861.4
C7H12	1696.8	1685
C7H14-CYCLO	1735.8	1574.5
C8H18	2068.3	2192.5
C8H16	2019.7	2116.1
C8H16-CYCLO	1961	1823.3

TABLE XIV

THE COMPARISON OF C6 FOR C3H4-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C3H4	662.6	561.7
C3H4-DIENE	697.4	613.7
C3H6-CYCLO	689	608.9
C4H10	979.9	924.4
C4H8-1	945.4	842.8
C4H8-2-CIS	949.9	827.6
C4H8-ISO	949.6	835.4
C4H6-DIENE	989.4	820.7
C4H6-1-YNE	890.5	676.6
C5H12	1188.3	1121.8
C5H10	1144.2	1030.7
C5H8	1058.8	941.8
C5H10-CYCLO	1109.3	978.3
C6H14	1445.4	1356
C6H12	1414.6	1287.6
C6H10	1328.7	1218.3
C6H12-CYCLO	1325	1187.1
C7H16	1672.6	1631.2
C7H14	1628.1	1586
C7H12	1555.7	1441.1
C7H14-CYCLO	1591.3	1354.7
C8H18	1896.1	1865.5
C8H16	1851.7	1802.8
C8H16-CYCLO	1797.9	1567.2

TABLE XV

THE COMPARISON OF C6 FOR C3H4-DIENE-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C3H4-DIENE	734.1	670.6
C3H6-CYCLO	724.8	665.8
C4H10	1030.8	1011.9
C4H8-1	994.7	921.5
C4H8-2-CIS	999.5	904.6
C4H8-ISO	999.1	913.3
C4H6-DIENE	1041.7	895.9
C4H6-1-YNE	937.1	738.1
C5H12	1250	1228.1
C5H10	1203.7	1127.4
C5H8	1113.3	1030
C5H10-CYCLO	1166.9	1069.9
C6H14	1520.5	1484.1
C6H12	1488.4	1408.4
C6H10	1398	1332.9
C6H12-CYCLO	1393.6	1298.5
C7H16	1759.5	1786.5
C7H14	1712.9	1736.7
C7H12	1636.8	1576.9
C7H14-CYCLO	1674	1480.5
C8H18	1994.6	2043.3
C8H16	1943.1	1974.2
C8H16-CYCLO	1891.6	1713.2

TABLE XVI

THE COMPARISON OF C6 FOR C3H6-CYCLO-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C3H6-CYCLO	717	662.5
C4H10	1019.8	1010.8
C4H8-1	983.5	917.1
C4H8-2-CIS	988.2	899.1
C4H8-ISO	987.8	908.3
C4H6-DIENE	1028	886.6
C4H6-1-YNE	926.1	728.8
C5H12	1236.9	1227.5
C5H10	1193.7	1123.4
C5H8	1101.9	1025.9
C5H10-CYCLO	1154.8	1065.6
C6H14	1504.2	1481.9
C6H12	1471.7	1403.2
C6H10	1382.3	1328.9
C6H12-CYCLO	1379.3	1294
C7H16	1740.7	1787.8
C7H14	1694.1	1737.2
C7H12	1618.6	1573.1
C7H14-CYCLO	1656.1	1470.8
C8H18	1973.3	2046
C8H16	1926.8	1974.9
C8H16-CYCLO	1870.6	1703.1

TABLE XVII

THE COMPARISON OF C6 FOR C4H10-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C4H10	1450.7	1551.6
C4H8-1	1398.9	1399.3
C4H8-2-CIS	1405.5	1369
C4H8-ISO	1405	1384.2
C4H6-DIENE	1461.9	1340.6
C4H6-1-YNE	1317.2	1098.3
C5H12	1759.5	1885.8
C5H10	1693.6	1717.5
C5H8	1567.4	1567.2
C5H10-CYCLO	1642.6	1627.6
C6H14	2139.7	2273
C6H12	2093.3	2144.6
C6H10	1966.2	2033.5
C6H12-CYCLO	1962.1	1978.6
C7H16	2476	2752
C7H14	2409.7	2672.4
C7H12	2302.3	2409.4
C7H14-CYCLO	2355.8	2237.8
C8H18	2806.9	3152.3
C8H16	2740.7	3038.3
C8H16-CYCLO	2660.7	2594

TABLE XVIII

THE COMPARISON OF C6 FOR C4H8-1-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C4H8-1	1349.2	1269.5
C4H8-2-CIS	1355.7	1244.5
C4H8-ISO	1355.2	1257.2
C4H6-DIENE	1410.9	1227.1
C4H6-1-YNE	1270.7	1008.8
C5H12	1696.5	1699.2
C5H10	1633.3	1555.1
C5H8	1511.5	1420.1
C5H10-CYCLO	1583.9	1475
C6H14	2363.3	2051.4
C6H12	2019	1942.4
C6H10	1896.3	1839.6
C6H12-CYCLO	1891.8	1791.3
C7H16	2387.7	2474.9
C7H14	2323.9	2404.9
C7H12	2220.4	2177.6
C7H14-CYCLO	2271.7	2035.9
C8H18	2706.7	2832.3
C8H16	2643.1	2733.9
C8H16-CYCLO	2566.2	2357.5

TABLE XIX

THE COMPARISON OF C6 FOR C4H8-2-CIS-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C4H8-2-CIS	1362.2	1220.9
C4H8-ISO	1361.7	1233
C4H6-DIENE	1417.8	1206.6
C4H6-1-YNE	1276.8	993.1
C5H12	1704.6	1662
C5H10	1641	1523.5
C5H8	1518.7	1391.6
C5H10-CYCLO	1591.4	1445.5
C6H14	2073.1	2007.5
C6H12	2028.6	1903.1
C6H10	1905.4	1801.7
C6H12-CYCLO	1900.8	1754.8
C7H16	2399	2419.1
C7H14	2335	2351.3
C7H12	2231.1	2132.1
C7H14-CYCLO	2282.5	1997.8
C8H18	2719.6	2767.7
C8H16	2655.7	2672.8
C8H16-CYCLO	2578.4	2312.4

TABLE XX

THE COMPARISON OF C6 FOR C4H8-ISO-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C4H8-ISO	1361.2	1245.4
C4H6-DIENE	1417.3	1217.4
C4H6-1-YNE	1276.3	1001.4
C5H12	1704	1680.6
C5H10	1640.5	1539.5
C5H8	1518.1	1406.1
C5H10-CYCLO	1590.8	1460.5
C6H14	2072.4	2029.6
C6H12	2027.9	1923
C6H10	1904.7	1820.8
C6H12-CYCLO	1900.1	1773.3
C7H16	2398.2	2446.9
C7H14	2334.2	2378
C7H12	2230.3	2155.1
C7H14-CYCLO	2281.7	2017.4
C8H18	2718.7	2799.8
C8H16	2654.8	2703.3
C8H16-CYCLO	2577.5	2335.5

TABLE XXI

THE COMPARISON OF C6 FOR C4H6-DIENE-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C4H6-DIENE	1478.3	1202.3
C4H6-1-YNE	1329.4	993.6
C5H12	1772.7	1625.9
C5H10	1707.2	1498.8
C5H8	1579.8	1370.1
C5H10-CYCLO	1654.9	1423.4
C6H14	2156.5	1967.5
C6H12	2111.2	1872.7
C6H10	1983	1770.6
C6H12-CYCLO	1976.3	1725.9
C7H16	2495.5	2361.3
C7H14	2429.6	2296.9
C7H12	2321.7	2093
C7H14-CYCLO	2374.1	1976.3
C8H18	2828.9	2698.7
C8H16	2763	2610.7
C8H16-CYCLO	2633.1	2284.7

TABLE XXII

THE COMPARISON OF C6 FOR C4H6-1-YNE-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C4H6-1-YNE	1196.8	822.8
C5H12	1597.4	1331.4
C5H10	1538	1230.7
C5H8	1423.3	1125.6
C5H10-CYCLO	1491.3	1169.4
C6H14	1943	1612.6
C6H12	1901.5	1538
C6H10	1785.9	1453.1
C6H12-CYCLO	1781.3	1417.1
C7H16	2248.4	1931.5
C7H14	2188.5	1879.5
C7H12	2091.1	1716.9
C7H14-CYCLO	2139.1	1627.3
C8H18	2548.8	2206.5
C8H16	2489.1	2136.3
C8H16-CYCLO	2416.7	1880

TABLE XXIII

THE COMPARISON OF C6 FOR C5H12-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C5H12	2133.9	2292.3
C5H10	2054	2086.3
C5H8	1900.9	1903.5
C5H10-CYCLO	1992.2	1976.8
C6H14	2595	2762.3
C6H12	2538.8	2605
C6H10	2384.5	2470.4
C6H12-CYCLO	2379.8	2403.5
C7H16	3002.9	3346.1
C7H14	2922.5	3248.9
C7H12	2792.1	2927.5
C7H14-CYCLO	2857.1	2716.4
C8H18	3404.3	3833.3
C8H16	3323.9	3693.8
C8H16-CYCLO	3226.9	3149.3

TABLE XIV

THE COMPARISON OF C6 FOR C5H10-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C5H10	1977.2	1906.3
C5H8	1829.8	1740.3
C5H10-CYCLO	1917.6	1807.5
C6H14	2498	2517.4
C6H12	2444.1	2380.8
C6H10	2295.5	2255.6
C6H12-CYCLO	2290.6	2195.9
C7H16	2890.6	3040.6
C7H14	2813.3	2954
C7H12	2687.9	2671
C7H14-CYCLO	2750.2	2491.7
C8H18	3277	3480.8
C8H16	3199.8	3358.2
C8H16-CYCLO	3106.5	2886.2

TABLE XXV

THE COMPARISON OF C6 FOR C5H8-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C5H8	1693.4	1589
C5H10-CYCLO	1774.7	1650.3
C6H14	2311.8	2297.2
C6H12	2261.8	2173.6
C6H10	2124.4	2059
C6H12-CYCLO	2119.9	2004.6
C7H16	2675.2	2773.5
C7H14	2603.6	2694.7
C7H12	2487.5	2437.9
C7H14-CYCLO	2545.3	2276.1
C8H18	3032.7	3174.6
C8H16	2961.2	3063.4
C8H16-CYCLO	2874.9	2636.2

TABLE XXVI

THE COMPARISON OF C6 FOR C5H10-CYCLO-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C5H10-CYCLO	1860	1714.1
C6H14	2422.7	2385.7
C6H12	2370.2	2257.5
C6H10	2226.1	2138.5
C6H12-CYCLO	2221.8	2082
C7H16	2803.6	2880.1
C7H14	2728.4	2798.3
C7H12	2606.7	2531.9
C7H14-CYCLO	2667.4	2364.3
C8H18	3178.3	3296.6
C8H16	3103.2	3181.2
C8H16-CYCLO	3012.6	2738.2

TABLE XXVII

THE COMPARISON OF C6 FOR C6H14-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C6H14	3155.8	3330.1
C6H12	3087.6	3143.4
C6H10	2900.1	2980.1
C6H12-CYCLO	2893.9	2900
C7H16	3651.9	4030.1
C7H14	3554.2	3913.8
C7H12	3395.8	3530.6
C7H14-CYCLO	3474.6	3281.8
C8H18	4140	4615.7
C8H16	4042.4	4449.6
C8H16-CYCLO	3924.5	3803.7

TABLE XXVIII

THE COMPARISON OF C6 FOR C6H12-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C6H12	3021.2	2973.4
C6H10	2837.7	2816.9
C6H12-CYCLO	2831	2742.4
C7H16	3573	3796.2
C7H14	3477.6	3688.1
C7H12	3322.7	3335.5
C7H14-CYCLO	3399.4	3112.3
C8H18	4050.5	4345.5
C8H16	3955.2	4192.8
C8H16-CYCLO	3840.1	3605.2

TABLE XXIX

THE COMPARISON OF C6 FOR C6H10-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C6H10	2665.3	2069.3
C6H12-CYCLO	2659	2598.3
C7H16	3355.9	3601.4
C7H14	3266.3	3493.4
C7H12	3120.8	3161.3
C7H14-CYCLO	3192.9	2946.2
C8H18	3804.4	4123.2
C8H16	3714.9	3977.2
C8H16-CYCLO	3606.8	3413.3

TABLE XXX

THE COMPARISON OF C6 FOR C6H12-CYCLO-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C6H12-CYCLO	2654	2529.4
C7H16	3348.8	3593.1
C7H14	3259	3483.2
C7H12	3113.6	3076.8
C7H14-CYCLO	3186.2	2869.8
C8H18	3796.4	4010.2
C8H16	3706.7	3868.9
C8H16-CYCLO	3598.4	3324.3

TABLE XXXI

THE COMPARISON OF C6 FOR C7H16-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C7H16	4226	4887.6
C7H14	4112.9	4744.5
C7H12	3929.6	4269.1
C7H14-CYCLO	4020.7	3952.7
C8H18	4790.8	5600.8
C8H16	4677.8	5394.4
C8H16-CYCLO	4541.4	4584.3

TABLE XXXII

THE COMPARISON OF C6 FOR C7H14-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C7H14	4003	4606
C7H12	3824.6	4146.6
C7H14-CYCLO	3913.1	3842.2
C8H18	4662.5	5436.3
C8H16	4552.8	5236.8
C8H16-CYCLO	4420.1	4455.6

TABLE XXXIII

THE COMPARISON OF C6 FOR C7H12-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C7H12	3654.2	3744.5
C7H14-CYCLO	3738.7	3486.1
C8H18	4454.7	4888.4
C8H16	4349.9	4714.2
C8H16-CYCLO	4223.2	4039.5

TABLE XXXIV

THE COMPARISON OF C6 FOR C7H14-CYCLO-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C7H14-CYCLO	3825.5	3269.3
C8H18	4558.1	4521.7
C8H16	4450.6	4367.7
C8H16-CYCLO	4320.8	3783.8

TABLE XXXV

THE COMPARISON OF C6 FOR C8H18-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C8H18	5431.1	6418.9
C8H16	5303	6181
C8H16-CYCLO	5148.3	5245

TABLE XXXVI

THE COMPARISON OF C6 FOR C8H16-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C8H16	5178.1	5954.1
C8H16-CYCLO	5027.2	5065

TABLE XXXVII

THE COMPARISON OF C6 FOR C8H16-CYCLO-HYDROCARBONS

GAS	C6-S-K	C6-C-R
C8H16-CYCLO	4880.8	4380

TABLE XXXVIII

Preliminary results for other systems.

Ar - halogenated hydrocarbons

Gas	Q exp., $\AA^2$
CH_3Cl	506
CH_3Br	546
C_2H_5Cl	586

H_2-rare gases

Gas	C_6 exp., a.u.	C_6 S-K, a.u.
He	2.21	4.49
Ne	3.53	9.68
Kr	57.59	43.92
Xe	81.35	63.11