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Original Scientific Paper

Estimation of Properties of Triatomic Molecules from Tabulated Data Using Least-squares Fitting

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This paper shows that it is feasible to make rapid forecasts of data for large numbers of molecules by using least-squares smoothing of tabulated data, though the forecasts are not as precise as those from quantum-chemical computation packages which deal with one molecule at a time. The molecules' properties were chosen to be of value in the plasma and astronomical physics. The work begins with the graphical analysis of critically-analyzed data for ground states of neutral, acyclic, main-group, row 2 to row 6, triatomic molecules to infer a least-squares smoothing equation. The equation is quadratic in a function ($R_1R_2 + R_2R_3$) of the atomic period numbers, quadratic in the group number of the central atom, and cubic in the total number of valence electrons. The coefficients of the equation (some of them zero for some properties) were obtained from high-quality tabulated data for the heat of atomization, ionization potential, log of the partition function at 1000 K, and log of the partial-pressure equilibrium constant for the constituent atoms over the diatomic molecules at 1000 K. The equation and its coefficients were tested by comparison with data, from the same tabulations, for a few molecules not in the original set. Finally, values were forecasted for 164, 145, 107, and 164 additional molecules, for four the properties listed above and in order the same order.

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INTRODUCTION

In spite of the many results produced by experimental groups throughout the world, there exist continual needs for more data on small molecules – especially those pertinent to the spectroscopy of atmospheres of the earth, the planets, and the stars. From time to time, the literature includes lists of molecules for which data are needed.[1,2,3,4]

This paper demonstrates a method that can help fill this gap. It reports a systematic study of tabulated data for neutral, ground-state, acyclic triatomic molecules. The data are smoothed using least-squares methods, the resulting equation is used to forecast new molecular data, and the forecasts are evaluated using data from the same tabulations.

DEFINITIONS

The period number (the principal quantum number of the valence shell) of atom i of any molecule is denoted as R_i and its group number (or valence) as C_i. This work pertains to molecules with atoms for which the range of R_i is from 2 to 7 (where the »row-2 atoms« are Li through Ne) and that of C_i is from 1 to 7 (1, 2, and 13 to 17 in the scheme devised by IUPAC to replace the two different usages of Roman numerals with the letters A and B). This paper deals with acyclic ground-state molecules only; the atoms are designated so that R_2 and C_2 always pertain to the middle of the molecule; each molecular name is written so that the atomic symbols indicate the actual structure.

Three groups of molecules are considered in this paper and should not be confused: the original set of molecules, with known structures and at least one known datum each, used for determination of the smoothing equation; a few additional molecules, with data from the same tabulations, used to test the forecasts; and the forecasted set of molecules for which there were no data in the tabulations and for most of which the structures were unknown.

THE ORIENTATION OF THIS PAPER TO QUANTUM MECHANICS

Ab initio numerical computations based on Schroedinger's equation have unquestionably been very successful in determining quite precise and accurate numerical values for properties of triatomic molecules, one (or one isoelectronic series) at a time.[5,6,7] However, it is not commonly appreciated that there has never appeared any solution of the Schroedinger equation which gives, globally for all diatomic or triatomic molecules, values of some property to a level of precision comparable to the intuitive knowledge common

among experienced researchers[8] (for the heat of atomization, for example, to some 20%). The method described in this paper shows how such values can be obtained with least-squares fitting and prediction.

Gas-phase molecules are assumed to have structures[9,10,11] in no more, and no less, of a sense than that used by the compilers of the tabulated data used in this paper, *i.e.*, as stable structures with their permutation isomers considered as separate entities.

DATA

This paper discusses molecular properties of interest to the plasma and especially to stellar-atmosphere physics. It depends exclusively on critically-analyzed, tabulated data for molecules with known structures. These data are presented in Table I. The table gives the molecular formulae, the group numbers of the central atoms, the total numbers of valence electrons, the function of the period numbers given in Eq. (1) below, and finally the data. The table is sorted by R_1, R_2, and then R_3 (which are not shown).

Total entropies at 298 K (S°_{298}) were obtained from the JANAF Tables of 1974–1982;[12] the average of the few 95% confidence-limit errors given for individual data is approximately 1%, and this value is used where no error is given. Internal entropies at 1000 K were computed by us from S°_{298} using the standard thermodynamic formula with the Sackur-Tetrode constant; the average 95% confidence-limit error for individual data is also approximately 1%. (The results of this computation are not listed.)

Common logarithms of total partition functions at 1000 K (log Q), and common logs of partial-pressure equilibrium constants for the constituent atoms over the diatomic molecules, in N/m^2, at 1000 K (log K_p) were obtained from Sauval.[13] The 95% confidence-limit errors given by Sauval[14] for the »best« values of log Q are in the vicinity of 0.01, that is, from 0.13% to 0.28%. The estimated average 95% confidence-limit error associated with individual values for log K are 10%. Heats of atomization were taken from Gurvich *et al*[15] and are denoted by $\Delta_{at}H$ (Gurvich); the average 95% confidence-limit error associated with individual experimental values is 2.63%. Ionization potentials (IP) were taken from Gurvich;[16] the average 95% confidence-limit error for individual data is 4.23%. Heats of atomization taken from Sauval,[13] denoted by $\Delta_{at}H$ (Sauval) are used for a graphical study in the last section, p. 497. The average 95% confidence-limit error associated with individual values is estimated as being about 20%.

The $S(\text{int})^\circ_{1000}$ and log Q data appear to be linearly related (Figure 1), as would be expected from the argument given in Ref. 17. The average 95% confidence-limit error of 1% pertaining to individual $S(\text{int})^\circ_{1000}$ data fully accounts for the variance of the data from the best-fitting straight line, and

TABLE Ia

Molecular Coordinates, Tabulated Properties, and Errors at 95% Confidence

	Mol.	C_2	n_e	$f(R)$	S°_{298}	Error		Log Q	Log K	Error
						absol.	%	1 kK	1 kK	%
1	C3	4	12	8	56.677	3.00	5.29	5.1455	–47.5418	10
2	BOB	6	12	8	54.405		1.00	4.2389	–41.9141	10
3	FBO	3	16	8	53.705		1.00			
4	NCN	4	14	8	54.035	0.01	0.02	4.3265	–40.6902	15
5	NNO	5	16	8	52.546		1.00	3.8125	–33.6733	10
6	FBF	3	17	8	59.046		1.00	5.1441	–45.3051	10
7	O3	6	18	8	57.080	0.40	0.70	4.7224	–7.3132	10
8	CNN	5	14	8	55.354		1.00	4.2511	–38.1040	10
9	NCO	4	15	8				4.5088	–42.5366	10
10	BeCC	4	10	8				3.9299	–38.3080	10
11	OOF	6	19	8	61.903		1.00	5.7701	–6.6765	10
12	FCF	7	15	8				4.8431	–40.7415	15
13	LiON	6	12	8	58.608		1.00	5.2642	–14.4562	10
14	LiOLi	6	8	8	54.732		1.00	4.6377	–16.4542	10
15	CCO	4	14	8	55.677		1.00	4.9097	–48.7168	10
16	FOF	6	20	8	59.118	0.10	0.17	5.1494	0.8744	10
17	CNC	5	13	8	55.157		1.00	4.5797	–46.7288	10
18	OCO	4	16	8	51.072	0.03	0.06	3.4635	–58.4678	10
19	BeOBe	6	10	8	52.754		1.00	4.0743	–27.8295	10
20	OBO	3	15	8	54.900	0.05	0.09	4.4332	–45.8392	10
21	FCO	4	17	8	59.363		1.00	5.1951	–40.9786	15
22	BCC	4	11	8				3.9918	–40.0505	15
23	ONO	5	17	8	57.343	0.03	0.05	4.7406	–25.0736	10
24	N3	5	15	8	54.100	0.50	0.92	4.2181	–28.7518	10
25	ONF	5	18	8	59.273		1.00	5.1833	–22.0752	10
26	FCF	4	18	8	57.533	0.01	0.02	4.7824	–31.1200	10
27	FNF	5	19	8	59.715		1.00	5.2720	–7.6770	10
28	FBeF	2	16	8	54.360	0.30	0.55	4.2675	–42.7677	10
29	NCF	4	16	8	53.846	0.20	0.37	4.0701	–40.2145	15
30	FOLi	6	14	8	58.775		1.00			
32	NCl	4	16	14	61.479	0.01	0.02			
33	OSO	6	18	12	59.298	0.02	0.03	4.9997	–31.6209	10
34	OClO	7	19	12	61.453		1.00	5.4646	–3.4312	10
35	FMgF	2	16	12	61.280	0.50	0.82	5.6634	–31.6051	10
36	FAlF	3	17	12	63.120		1.00	5.8798	–40.6375	10
37	OAlO	3	15	12	58.608		1.00	5.1102	–28.0314	10
38	FSF	6	20	12	61.565		1.00			
39	FAlO	3	16	12	56.693		1.00			
40	FPF	5	19	12	62.822		1.00	5.6783	–25.9078	10
41	FSiF	4	18	12	61.297	0.10	0.16	5.5013	–39.1014	10
42	OPO	5	17	12	60.607		1.00	5.3462	–35.9125	10
43	OSiO	4	16	12	54.699		1.00	4.1574	–40.5392	10
44	OGeO	4	16	16				4.9958	–27.9017	10
45	FGeF	4	18	16				6.3431	–28.4574	10
46	OSeO	6	18	16				5.3548	–19.9414	10

TABLE Ia (continued)

	Mol.	C_2	n_e	$f(R)$	S°_{298}	Error absol.	Error %	Log Q 1 kK	Log K 1 kK	Error %
47	FCaF	2	16	16	65.412	0.50	0.76	6.3360	–36.1193	10
48	OCaO	2	14	16				5.4958	–22.9552	10
49	OSnO	4	16	20				5.4958	–17.5999	10
50	FSrF	2	16	20	69.694	0.50	0.72	6.9545	–35.5242	10
51	OSrO	2	14	20				5.9958	–25.7886	10
52	FSnF	4	18	20						
53	OTeO	6	18	20				5.8232	–16.3234	10
54	OBaO	2	14	24				6.4958	–38.8609	10
55	FPbF	4	18	24	69.928	0.80	1.14	6.8143	–19.6745	10
56	FBaF	2	16	24	71.985	0.50	0.69	7.2304	–38.7872	10
57	ClCO	4	17	10	63.542		1.00			
58	ClBO	3	16	10	56.720		1.00			
59	SCN	4	15	10				4.4958	–26.7193	10
60	SCO	4	16	10				4.2736	–47.2862	10
61	PCC	4	13	10				5.3431	–35.1234	10
62	ClCN	4	16	10	56.459		1.00	4.5180	–39.0037	10
63	ClBeF	2	16	10	58.887		1.00			
64	AlBO	3	12	10						
65	AlCC	4	11	10				4.4918	–26.1385	10
66	ClBF	3	17	10	63.229		1.00			
67	NaCN	4	10	10	58.139		1.00	5.0387	–39.9950	10
68	SiCC	4	12	10	56.553		1.00	5.1649	–42.2809	10
69	ClOLi	6	14	10	61.264		1.00			
70	ClNO	5	18	10	62.517	0.04	0.06			
71	NaOLi	6	8	10	61.270		1.00			
72	SiOSi	6	14	12				5.3431	–34.4827	10
73	SiCSi	4	12	12	57.881		1.00			
74	ClBCl	3	17	12	65.144	0.50	3.50	6.2282	–23.8484	10
75	ClBeCl	2	16	12	60.260	1.00	1.66	5.2425	–25.7440	10
76	SiNSi	5	13	12	61.275		1.00			
77	SCS	4	16	12	56.852	0.02	0.04			
78	AlOAl	6	12	12	61.414	1.50	2.44	5.3531	–30.7423	10
79	ClOCl	6	20	12	64.019		1.00	5.9561	1.9679	10
80	ClCCl	4	18	12	63.392	0.50	0.79	5.8381	–14.6722	10
81	ClBBr	3	17	14	69.056	1.00				
82	SSO	6	18	15	63.796		1.00	5.9093	–21.8569	10
83	ClMgF	2	16	15	62.756		1.00			
84	ClAlO	3	16	15	59.471		1.00			
85	ClAlF	3	17	15	67.586		1.00			
86	AlSAl	6	12	18						
87	ClAlCl	3	17	18	69.146		1.00	6.9547	–23.1390	10
89	ClMgCl	2	16	18	66.184	0.50	0.76	6.4236	–19.3449	10
90	Na3	1	3	18						
92	ClSiCl	4	18	18	67.214		1.00	6.6113	–22.3409	10
93	S3	6	18	18						
94	P3	5	15	18						
95	Si3	4	12	18	64.002		1.00			
96	ClGaCl	3	17	24				7.8431	–24.3805	10

TABLE Ia (continued)

Mol.	C_2	n_e	$f(R)$	S°_{298}	Error absol.	Error %	Log Q 1 kK	Log K 1 kK	Error %
97 ClGeCl	4	18	24				7.8431	–19.3501	10
98 ClCaCl	2	16	24				7.0048	–23.7178	10
99 AlSeAl	6	12	24						
100 ClSnCl	4	18	30						
101 ClSrCl	2	16	30	75.580	1.20	1.59	7.8431	–22.2584	10
102 AlTeAl	6	12	30						
103 ClBaCl	2	16	36	77.826	1.20	1.54	8.4292	–25.2887	10
104 ClPbCl	4	18	36	75.787	0.70	0.92	7.9350	–11.1074	10
105 GeCC	4	12	12				5.4918	–39.7594	10
106 BrBF	3	17	12	65.887		1.00			
107 KCN	4	10	12	60.477		1.00	5.3579	–40.1511	10
108 BrCN	4	16	12	59.334	0.10	0.17			
109 BrNO	5	18	12	65.347		1.00	6.0038	–16.5451	10
110 BrBO	3	16	12	59.463		1.00			
111 GaOGa	6	12	16						
112 BrBeBr	2	16	16	65.439	0.50	0.76			
113 BrBBr	3	17	16	70.402		1.00			
114 GeSiC	4	12	18						
115 BrSiBr	4	18	24						
116 BrMgBr	2	16	24	71.922		1.00			
117 GaSGa	6	12	24						
118 GeGeC	4	12	24						
119 K3	1	3	32						
120 GaSeGa	6	12	32						
121 BrGeBr	4	18	32						
122 BrCaBr	2	16	32	75.200		1.00			
123 Ge3	4	12	32						
124 BrSnBr	4	18	40						
125 BrSrBr	2	16	40	77.270		1.00			
126 GaTeGa	6	12	40						
127 BrPbBr	4	18	48	81.089	0.70	0.86			
128 BrBaBr	2	16	48	81.729		1.00			
129 IBeI	2	16	20	69.649		1.00			
130 IBI	3	17	20	73.964		1.00			
131 InOIn	6	12	20				7.3431	–17.3392	10
132 InSIn	6	12	30						
133 IMgI	2	16	30	75.854	2.00	2.64			
134 IsiI	4	18	30						
135 ICaI	2	16	40	78.263		1.00			
136 TeGaTe	3	15	40						
137 InSeIn	6	12	40						
138 TeInTe	3	15	50						
139 InTeIn	6	12	50						
140 ISrI	2	16	50	81.128		1.00			
141 IPbI	4	18	60	85.908		1.00			
142 IBaI	2	16	60	83.180		1.00			
143 CsOCs	6	8	24	75.998		1.00	7.8075	–4.6097	10
144 Cs3	1	3	72						

TABLE Ib

Molecular Coordinates, Tabulated Properties, and Errors at 95% Confidence

	Mol.	C_2	n_e	$f(R)$	$\Delta_{at}H$	Error		IP	Error	
						absol.	%		absol.	%
1	C3	4	12	8	1302.555	20.0	1.54	11.90	0.60	5.04
2	BOB	6	12	8	1100.000	60.0	5.45			
3	FBO	3	16	8	1477.058	20.0	1.35	13.40	0.50	3.73
4	NCN	4	14	8						
5	NNO	5	16	8	1103.390	0.6	0.05	12.89	0.01	0.08
6	FBF	3	17	8	1216.550	20.0	1.64	8.40	0.20	2.38
7	O3	6	18	8	595.892	2.0	0.34			
8	CNN	5	14	8	1252.821	6.0	0.48			
9	NCO	4	15	8	1251.786	20.0	1.60			
10	BeCC	4	10	8						
11	OOF	6	19	8				12.60	0.20	1.59
12	FCF	7	15	8	1149.645	60.0	5.22			
13	LiON	6	12	8						
14	LiOLi	6	8	8	728.779	6.0	0.82	6.80	0.20	2.94
15	CCO	4	14	8	1382.153	20.0	1.45			
16	FOF	6	20	8	374.578	2.0	0.53	13.70	0.20	1.46
17	CNC	5	13	8				13.00	1.00	7.69
18	OCO	4	16	8	1597.893	0.6	0.04	13.79	0.02	0.15
19	BeOBe	6	10	8				10.50	0.50	4.76
20	OBO	3	15	8	1378.566	20.0	1.45			
21	FCO	4	17	8	1215.243	60.0	4.94			
22	BCC	4	11	8	1200.000	20.0	1.67	10.70	0.50	4.67
23	ONO	5	17	8	927.384	0.6	0.06	9.78	0.05	0.51
24	N3	5	15	8	973.021	6.0	0.62			
25	ONF	5	18	8	857.508	2.0	0.23			
26	FCF	4	18	8	1046.213	6.0	0.57	11.82	0.10	0.85
27	FNF	5	19	8	588.368	6.0	1.02	12.09	0.20	1.65
28	FBeF	2	16	8	1270.796	6.0	0.47	14.70	0.40	2.72
29	NCF	4	16	8	1225.278	20.0	1.63	13.32	0.01	0.08
30	FOLi	6	14	8						
32	NCI	4	16	14				10.87	0.02	0.18
33	OSO	6	18	12	1062.615	0.6	0.06	12.34	0.02	0.16
34	OClO	7	19	12	505.714	6.0	1.19	11.10	1.00	9.01
35	FMgF	2	16	12	1035.448	6.0	0.58	13.50	0.40	2.96
36	FAlF	3	17	12	1151.896	60.0	5.21			
37	OAlO	3	15	12	900.000	20.0	2.22			
38	FSF	6	20	12	720.335	6.0	0.83			
39	FAlO	3	16	12	1221.404	20.0	1.64			
40	FPF	5	19	12	980.113	6.0	0.61			
41	FSiF	4	18	12	1192.217	20.0	1.68	11.00	0.50	4.55
42	OPO	5	17	12	1087.129	6.0	0.55			
43	OSiO	4	16	12	1259.950	20.0	1.59	11.70	0.50	4.27
44	OGeO	4	16	16						
45	FGeF	4	18	16	1095.913	20.0	1.82	11.80	0.20	1.69
46	OSeO	6	18	16				11.50	0.50	4.35

TABLE Ib (continued)

	Mol.	C_2	n_e	$f(R)$	$\Delta_{at}H$	Error		IP	Error	
						absol.	%		absol.	%
47	FCaF	2	16	16	1120.968	6.0	0.54			
48	OCaO	2	14	16						
49	OSnO	4	16	20	834.874	60.0	7.19			
50	FSrF	2	16	20	1098.103	20.0	1.82			
51	OSrO	2	14	20						
52	FSnF	4	18	20	936.910	20.0	2.13	11.50	0.50	4.35
53	OTeO	6	18	20				11.00	0.50	4.55
54	OBaO	2	14	24						
55	FPbF	4	18	24	775.728	6.0	0.77	11.60	0.50	4.31
56	FBaF	2	16	24	1131.968	20.0	1.77			
57	ClCO	4	17	10	1095.158	6.0	0.55			
58	ClBO	3	16	10	1245.403	20.0	1.61			
59	SCN	4	15	10						
60	SCO	4	16	10	1374.591	2.0	0.15	11.18	0.01	0.09
61	PCC	4	13	10				10.90	0.50	4.59
62	ClCN	4	16	10	1168.118	2.0	0.17	12.34	0.01	0.08
63	ClBeF	2	16	10						
64	AlBO	3	12	10				8.50	0.50	5.88
65	AlCC	4	11	10	1069.716	60.0	5.61			
66	ClBF	3	17	10	1037.895	20.0	1.93			
67	NaCN	4	10	10						
68	SiCC	4	12	10	1248.037	20.0	1.60	10.20	0.30	2.94
69	ClOLi	6	14	10						
70	ClNO	5	18	10	782.621	0.6	0.08			
71	NaOLi	6	8	10						
72	SiOSi	6	14	12						
73	SiCSi	4	12	12	1062.519	20.0	1.88	9.20	0.30	3.26
74	ClBCl	3	17	12	861.240	20.0	2.32	7.50	0.20	2.67
75	ClBeCl	2	16	12	921.281	6.0	0.65			
76	SiNSi	5	13	12				9.40	0.30	3.19
77	SCS	4	16	12	1144.845	2.0	0.17	10.07	0.00	0.01
78	AlOAl	6	12	12	1045.000	20.0	1.91	7.70	0.50	6.49
79	ClOCl	6	20	12	405.196	6.0	1.48			
80	ClCCl	4	18	12	725.425	20.0	2.76	13.10	1.00	7.63
81	ClBBr	3	17	14						
82	SSO	6	18	15	839.553	2.0	0.24	10.30	0.30	2.91
83	ClMgF	2	16	15						
84	ClAlO	3	16	15	1043.749	20.0	1.92			
85	ClAlF	3	17	15	1004.241	60.0	5.97			
86	AlSAl	6	12	18	700.000	20.0	2.86	9.00	0.50	5.56
87	ClAlCl	3	17	18	856.586	60.0	7.00			
89	ClMgCl	2	16	18	783.033	6.0	0.77	11.60	0.10	0.86
90	Na3	1	3	18				3.90	0.10	2.56
92	ClSiCl	4	18	18	848.107	6.0	0.71	11.90	0.40	3.36
93	S3	6	18	18	679.355	6.0	0.88	9.68	0.03	0.31
94	P3	5	15	18	732.614	20.0	2.73	10.00	1.00	10.00
95	Si3	4	12	18	702.001	60.0	8.55	8.00	0.50	6.25
96	ClGaCl	3	17	24	750.000	6.0	0.80			

TABLE Ib (continued)

Mol.	C_2	n_e	$f(R)$	$\Delta_{at}H$	Error		IP	Error	
					absol.	%		absol.	%
97 ClGeCl	4	18	24	778.737	6.0	0.77	10.40	0.50	4.81
98 ClCaCl	2	16	24	901.763	6.0	0.67	10.30	0.10	0.97
99 AlSeAl	6	12	24				9.00	0.50	5.56
100 ClSnCl	4	18	30				10.20	0.50	4.90
101 ClSrCl	2	16	30	885.793	6.0	0.68	9.70	0.10	1.03
102 AlTeAl	6	12	30				10.00	0.50	5.00
103 ClBaCl	2	16	36	905.563	6.0	0.66	9.20	0.10	1.09
104 ClPbCl	4	18	36	608.613	6.0	0.99	10.30	0.50	4.85
105 GeCC	4	12	12				10.10	0.50	4.95
106 BrBF	3	17	12						
107 KCN	4	10	12						
108 BrCN	4	16	12				11.84	0.01	0.08
109 BrNO	5	18	12						
110 BrBO	3	16	12						
111 GaOGa	6	12	16	880.783	20.0	2.27	8.20	0.50	6.10
112 BrBeBr	2	16	16	772.029	20.0	2.59			
113 BrBBr	3	17	16	695.000	20.0	2.88			
114 GeSiC	4	12	18				9.60	0.30	3.13
115 BrSiBr	4	18	24	718.093	6.0	0.84			
116 BrMgBr	2	16	24	668.729	20.0	2.99	10.65	0.15	1.41
117 GaSGa	6	12	24				7.50	0.50	6.67
118 GeGeC	4	12	24				9.30	0.50	5.38
119 K3	1	3	32				3.40	0.10	2.94
120 GaSeGa	6	12	32				7.40	0.50	6.76
121 BrGeBr	4	18	32				9.50	0.50	5.26
122 BrCaBr	2	16	32	298.000	6.0	2.01			
123 Ge3	4	12	32				8.40	0.30	3.57
124 BrSnBr	4	18	40				10.00	0.40	4.00
125 BrSrBr	2	16	40	317.000	20.0	6.31			
126 GaTeGa	6	12	40				7.60	0.50	6.58
127 BrPbBr	4	18	48				10.20	0.50	4.90
128 BrBaBr	2	16	48						
129 IBeI	2	16	20	595.133	20.0	3.36			
130 IBI	3	17	20	545.000	20.0	3.67			
131 InOIn	6	12	20	766.383	20.0	2.61	7.90	0.50	6.33
132 InSIn	6	12	30				7.60	0.50	6.58
133 IMgI	2	16	30	521.133	20.0	3.84	9.57	0.05	0.52
134 IsiI	4	18	30	564.733	20.0	3.54			
135 ICaI	2	16	40	650.703	6.0	0.92			
136 TeGaTe	3	15	40				8.30	0.50	6.02
137 InSeIn	6	12	40				7.50	0.50	6.67
138 TeInTe	3	15	50				8.90	0.50	5.62
139 InTeIn	6	12	50				7.10	0.50	7.04
140 ISrI	2	16	50	644.353	20.0	3.10			
141 IPbI	4	18	60						
142 IBaI	2	16	60	679.163	20.0	2.94	8.10	1.00	12.35
143 CsOCs	6	8	24	540.000	20.0	3.70			
144 Cs3	1	3	72				3.20	0.10	3.13

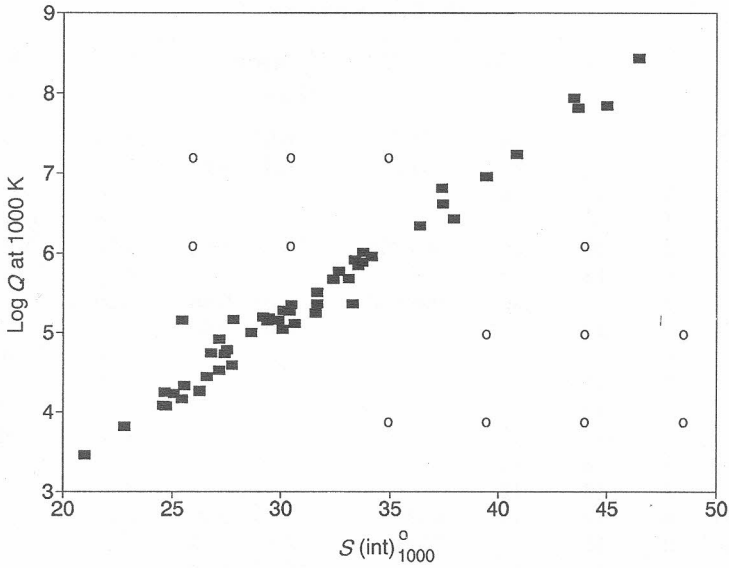

Figure 1. Log Q at 1000 K *vs.* $S(\text{int})^{\circ}_{1000}$. The points which most deviate from the main sequence are C_3 (above abscissa 25.5) and Al_2O (above 33.3).

hence the average 95% confidence-limit error pertaining to individual log Q data is for practical purposes zero. This result (*cf.* Sauval's estimate above) is the sole reason for which S°_{298} and $S(\text{int})_{1000}$ are mentioned in this paper.

There are proportionately far more data for molecules formed from row-2 and row-3 atoms than for heavier molecules. If more data had been available, the ranges of values in the data would probably be extended downward, and possibly even upward (the Malmquist bias). Data were available only for one pair of permutation isomers (#4, NCN, and #8, CNN in Table I); the data are, as expected, somewhat similar. Table II shows the interesting distribution of structures for the molecules whose tabulated data were used.

GRAPHICAL ANALYSIS

It has been shown[17] that data for fixed-group acyclic triatomic molecules are to a good approximation monotonic with respect to the function

$$f(R) = R_1R_2 + R_2R_3 \ . \qquad (1)$$

It was also shown that a quadratic polynomial in $f(R)$ is adequate to obtain a good fit to the central tendency of the monotonicity.

TABLE II

Distribution of molecular structures

(R_1,R_2,R_3)	$C_1 = C_2 = C_3$	$C_1 = C_3$	$C_2 = C_3$	$C_1 \neq C_2 \neq C_3$
(2,2,2)	3	14	6	7
(2,2,5)				1
(2,3,2)		10		1
(2,4,2)		5		
(2,5,2)		5		
(2,6,2)		3		
(3,2,3)		9		
(3,2,4)		1*		
(3,3,2)	1*	3*		
(3,3,3)	3	4	1	
(3,4,3)		5		
(3,5,3)		3		
(3,6,3)		2		
(4,2,2)	1*	1*		4
(4,2,4)		3		
(4,3,2)	1*			
(4,3,4)		3		
(4,4,2)	1*			
(4,4,4)	2	3		
(4,5,4)		3		
(4,6,4)		2		
(5,2,5)		3		
(5,3,5)		3		
(5,4,5)		3		
(5,5,5)		3		
(5,6,5)		2		
(6,2,6)		1		
(6,6,6)	1*			

* $R_1 \neq R_2$; the molecule is not symmetrical.

Triatomic molecules from fixed-row molecules exist at lattice points in a cubical space with coordinates C_1, C_2, and C_3. All such spaces are as is shown in Figure 2. A three-dimensional graph showing molecular data as symbols in the $(R_1,R_2,R_3) = (2,2,2)$ space is shown in Ref. 17.

Plotting of the data as a function of the number of valence electrons n_e requires only a one-dimensional plot. Since

$$n_e = C_1 + C_2 + C_3 \tag{2}$$

increases in the direction parallel to the main diagonal of the C_1,C_2,C_3 space (Figure 2), all the points representing data in the space can be projected

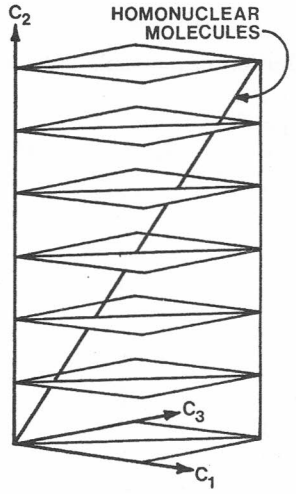

Figure 2. The space C_1,C_2,C_3, where $1 \leq C_i \leq 7$, showing the planes on which molecules with the seven values of C_2 lie. The straight line shows where homonuclear molecules lie in those cases where $R_1 = R_2 = R_3$; it is also the axis perpendicular to all planes of isoelectronic molecules.

onto the diagonal of the space, which then serves as the n_e axis. Furthermore, since n_e is independent of the locations of the three atoms in the molecules, it is possible to plot data points from all the molecules with fixed row numbers whether their structures were known or not. Thus, all molecules, instead of just the molecules with known structure, can be plotted.

Kong[18] plotted relative contractions of the internuclear separations, average bond dissociation energies

$$\overline{D} = [D^\circ_0 (AB - C) + D^\circ_0 (A - BC)] / 2 , \qquad (3)$$

and spectral term symbols both against n_e and against a »triatomic molecular number«, which serves the same role as the atomic number does for atoms and which is piecewise linearly proportional to n_e.

Kong's graphs all show that n_e is a very good independent variable; for example, the graph of bond angles clearly demonstrates Walsh's rules. The graphs for relative contractions of the internuclear separations have maxima at $n_e = 12$ to 14, depending irregularly on the sum of the period numbers, $R_1 + R_2 + R_3$. The graphs for $\overline{D}$ have data points only on the right-hand descent from a non-populated maximum, which Kong states is at $n_e = 12$. Graphs for $S(\text{int})^\circ_{1000}$, log Q, $\Delta_{at}H$, log K, and IP were plotted at this laboratory on the same axis related to n_e. They lead to the same conclusion: n_e is a good independent variable (Figures 3 to 5).

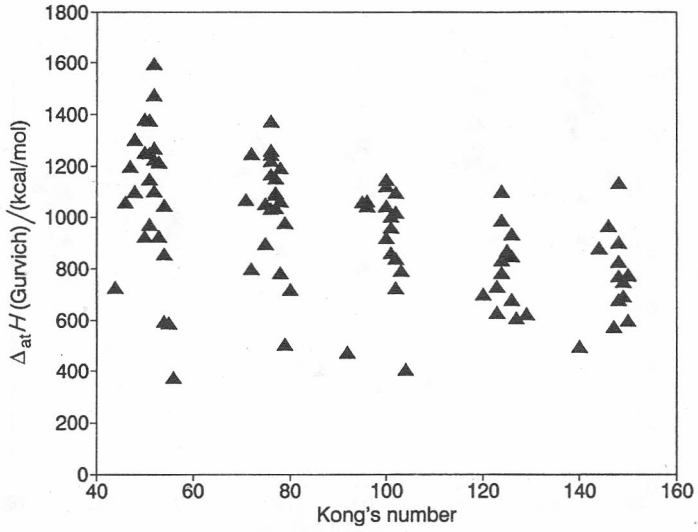

Figure 3. $\Delta_{at}H$ (Gurvich) *vs.* Kong's triatomic molecular number. The highest points in the five swarms of symbols pertain to the following most stable molecules and their abscissae: CO_2, 52; SCO, 76; CS_2, 100; SrF_2, 124; and BaF_2, 148. In the vicinities of these molecules, Kong's number is directly proportional to n_e. All of these molecules, with atoms from different combinations of period numbers, have 16 valence electrons. This phenomenon is evidence of the periodicity of triatomic molecular data.

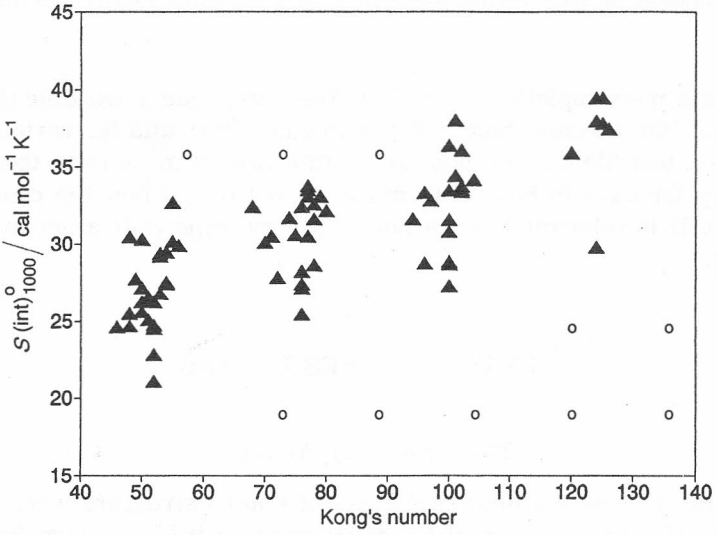

Figure 4. $S(int)^{\circ}_{1000}$ *vs.* Kong's molecular number. The lowest points in the four swarms of symbols pertain to the following molecules and their abscissae: CO_2, 52; SiO_2, 76; CS_2, 100; and CIN, 124. In the domains of the swarms, Kong's number is directly proportional to n_e. As in Figure 4, all these most stable molecules have 16 valence electrons.

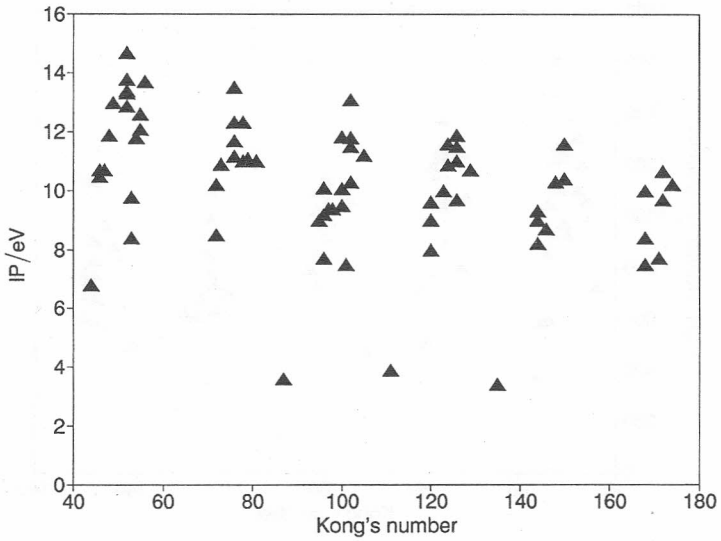

Figure 5. IP *vs.* Kong's natural number. The highest points in the six swarms of symbols pertain to the following molecules and their abscissae: BF_2, 52; MgF_2, 76; CCl_2, 102; $SiCl_2$, 126; PbF_2, 150, and $MgBr_2$, 172. In the domains of the swarms, Kong's number is directly proportional to n_e. These molecules, with atoms from different combinations of period numbers, have 16, 16, 18, 18, 18, and 16 valence electrons, respectively. This fact that not all of these molecules have 16 electrons may be due to the lack of data for even more stable molecules in the third, fourth, and fifth swarms.

The data were replotted with C_2 as the independent variable (Figure 6). The graphs (for various choices of the row numbers and for various properties) have a terrible scatter, but can be interpreted to indicate that there is a tendency for data to have extrema at $C_2 = 4$ (*i.e.,* when the central atom is carbon). It is relevant that carbon is a very important atom in (organic) chemistry.

LEAST SQUARES FITTING

The Smoothing Equation

Data for all the triatomic molecules of known structure were smoothed by the use of a combination of the functions which were suggested by Eqs. (1) and (2) and by the C_2 dependence just described:

$$V(R_1,R_2,R_3,C_1,C_2,C_3) = a + bn_e + cn_e^2 + dn_e^3 + eC_2 + fC_2^2 + g[f(R)] + h[f(R)]^2, \quad (4)$$

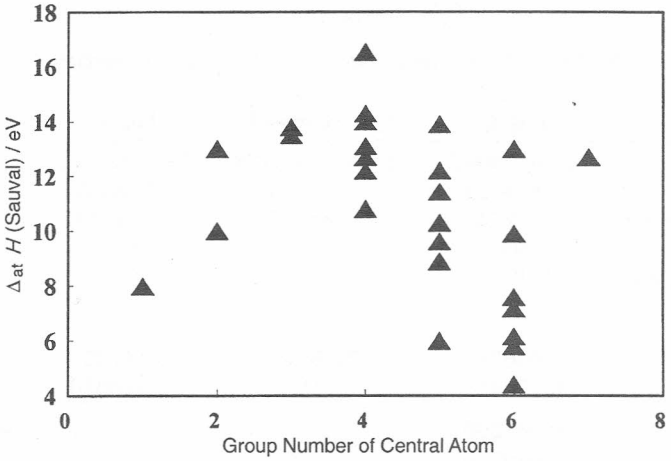

Figure 6. $\Delta_{at}H$ (Sauval) *vs.* the group number of the central atom of the molecule, showing the weak maximum at $C_2 = 4$.

where V stands for values of a property and a through h are coefficients obtained by the smoothing for that property. The »user-defined« fitting was done with PSI-Plot® for Windows® version 5.47. Information concerning the goodness-of-fits is given in Table III. The coefficient of determination (COD) is a measure of the fraction of the total variance accounted for by the model; the correlation (R) is an indication of how much changes in V are related to changes in the dependent variables. The coefficients and σ values in the table are very similar to test results obtained for different sets of molecules and for different numbers of step-wise forward and backward regressions.

Testing Forecasted Data with Tabulated Data

Tables IV through VII show the results of testing the forecasted data against data from the same tabulations (for molecules not in the original set). The first two columns give the forecasted molecular numbers and show the molecules. The asterisks pertain to information in subsequent tables. Columns 3 to 5 give the group number of the central atom, the total number of valence electrons, and the function $f(R)$. The sixth and seventh columns give the forecasted data and the 95% intervals. The remaining columns show the tabulated data and (except for log Q) 95%-confidence errors, the differences between the tabulated data and forecasted data, and the extent to which the 95%-confidence limits of the computed data include the tabulated data (positive for success, negative for failure).

For IP in Table IV, the average difference between the tabulated and the forecasted data (column 8) is 1.09 eV with a Student-t error of 3.20 eV; clearly,

TABLE III

Statistical data from curve fits for four properties

	Log Q	$\Delta_{at}H$ (Gurvich)	Log K_p	IP
Sum sqrt.	17.6359007	2,560,744.9128	5,052.62432	123.802291
COD	0.814581	0.617514	0.592315	0.677227
Correlation R	0.902542	0.785827	0.769739	0.831284
No. of cases	92	88	89	79
Degr. freedom	86	83	85	75
a*	...	...	...	...
b	0.936544	172.58467	–6.14125	1.380395
σ	0.174418	8.71632	0.346010	0.094186
c	–0.087205	...	...	–0.035700
σ	0.019830	...	...	0.004737
d	0.002526	–0.29312	0.011942	...
σ	0.000624	0.02098	0.000890	...
e	–0.048942	...	...	...
σ	0.053425	...	...	...
f	...	4.42003	0.374558	...
σ	...	1.63446	0.082473	...
g	0.225742	–39.23953	0.77764	–0.153773
σ	0.038767	6.29726	0.150108	0.038618
h	–0.002202	0.409551	...	0.001694
σ	0.001014	0.115595	...	0.000624

* No constant terms were necessary.

the average difference is not statistically significant. The forecasted data (column 6) and the appropriate upper or lower error bars (column 7) overlap the tabulated data (positive entries in column 8) in six out of the eight cases. If the tabulated errors of the tabulated data (column 9) are taken into account, then all but one forecasted data are in agreement with the tabulated data, and that one is very close.

For $\Delta_{at}H$ (Gurvich) in Table V, the average difference between the tabulated and the forecasted data is 21 ± 402 kJ mol^{-1}. The forecasted data and the appropriate upper or lower error bars overlap the tabulated data in 15 out of the 18 cases. If the tabulated error of the tabulated data are taken into account, then all of the forecasted data are in agreement.

For log Q in Table VI, the average difference between the tabulated and the forecasted data is 0.069 ± 0.922. The forecasted data with their appropriate upper or lower error bars overlap the tabulated data in nine out of 10 cases. Since the tabulated data have essentially no errors, the one datum marginally outside the error bars of the forecasted datum remains outside.

TABLE IV

Comparison of forecasted and tabulated ionization potentials

Molecule	Address			Forecasted		Tabulated		Differences	
	C_2	n_e	$f(R)$	Values	95% error	Values	95% error	Values	Within error of forecast?
3 TeAlTe*	3	15	30	9.57	2.53	6.50	0.50	3.07	–0.54
15 FbrF*	7	21	16	11.20	2.65	11.20	0.50	0.00	2.65
26 FCIF*	7	21	12	11.63	2.64	11.00	0.50	0.63	2.01
29 GaOF*	6	16	12	11.34	2.52	9.50	0.50	1.84	0.68
31 GaOTe*	6	15	18	10.44	2.51	7.70	0.50	2.74	–0.23
32 GeOGe*	6	14	16	10.29	2.52	8.70	1.00	1.59	0.92
35 TeGeTe*	4	16	40	9.48	2.54	10.80	0.50	–1.32	1.23
36 FIF*	7	21	20	10.83	2.66	10.70	1.00	0.13	2.53

TABLE V

Comparison of forecasted and tabulated heats of atomization ($\Delta_{at}H$ / eV)

Molecule	Address			Forecasted		Tabulated		Differences	
	C_2	n_e	$f(R)$	Values	95% error	Values	95% error	Values	Within error of forecast?
1 IAlI*	3	17	30	646	354	592	60	55	299
2 SAlS*	3	15	18	986	351	630	60	356	–6
11 OBeO*	2	14	8	1306	356	926	20	380	–24
14 BrAlBr*	3	17	24	749	352	723	60	26	326
18 BrCBr*	4	18	16	804	350	597	60	207	144
24 Cl3*	7	21	18	121	389	623	60	–502	–113
25 ClPCl*	5	19	18	585	356	607	6	–22	334
28 FGaF*	3	17	16	931	350	960	60	–29	379
32 GeOGe*	6	14	16	930	356	967	20	–36	320
34 SGeS*	4	16	24	785	351	828	60	–43	308
38 ClInCl*	3	17	30	646	354	700	60	–54	300
39 FInF*	3	17	20	833	351	870	6	–37	314
43 KOK*	6	8	16	549	368	496	20	53	314
51 NaONa*	6	8	12	660	364	476	6	184	179
60 OPbO*	4	16	24	785	351	679	60	105	246
61 SPbS*	4	16	36	610	356	625	60	–16	341
63 RbORb*	6	8	20	452	372	515	20	–63	309
70 ClSiF*	4	18	15	830	350	1020	20	–190	160

For log K_p in Table VII, the average difference between the tabulated and the forecasted data is 3.74 ± 17.55. The forecasted data and the appropriate upper or lower error bars overlap the tabulated data in 15 out of 17

TABLE VI

Comparison of forecasted and tabulated log Q at 1000 K

Molecule	Address			Forecasted		Tabulated		Differences	
	C_2	n_e	$f(R)$	Values	95% error	Values	95% error	Values	Within error of forecast?
9 BaOBa*	6	10	24	7.08	1.11	7.34	10.00	0.26	0.85
11 OBeO*	2	14	8	4.58	1.04	4.50	10.00	–0.09	0.95
21 CCS*	4	14	10	4.86	1.01	5.34	10.00	0.48	0.52
23 CaOCa*	6	10	16	5.97	1.08	5.84	10.00	–0.13	0.95
30 OGaO*	3	15	16	5.93	1.02	6.00	10.00	0.07	0.95
32 GeOGe*	6	14	16	5.78	1.06	5.84	10.00	0.07	0.99
48 MgOMg*	6	10	12	5.32	1.06	5.34	10.00	0.03	1.03
53 PCN*	4	14	10	4.86	1.02	4.50	10.00	–0.36	0.65
54 POC*	6	15	15	5.63	1.05	4.50	10.00	–1.13	–0.08
56 PNO*	5	16	10	4.88	1.02	5.00	10.00	0.12	0.90

TABLE VII

Comparison of forecasted and tabulated log K at 1000 K

Molecule	Address			Forecasted		Tabulated		Differences	
	C_2	n_e	$f(R)$	Values	95% error	Values	95% error	Values	Within error of forecast?
5 OAsO*	5	17	16	–23.86	16.34	–28.11	10.00	–4.25	12.09
9 BaOBa*	6	10	24	–17.24	17.74	–27.98	10.00	–10.74	7.00
11 OBeO*	2	14	8	–45.46	16.67	–27.61	10.00	17.84	–1.17
13 OBiO*	5	17	24	–17.62	16.66	–13.86	10.00	3.77	12.89
21 CCS*	4	14	10	–39.40	16.39	–29.84	10.00	9.55	6.84
23 CaOCa*	6	10	16	–23.48	17.12	–18.73	10.00	4.75	12.37
25 ClPCl*	5	19	18	–11.35	16.64	–16.05	10.00	–4.70	11.94
28 FGaF*	3	17	16	–29.86	16.40	–33.48	10.00	–3.62	12.78
30 OGaO*	3	15	16	–35.95	16.38	–17.81	10.00	18.14	–1.76
32 GeOGe*	6	14	16	–27.22	16.71	–32.50	10.00	–5.29	11.43
53 PCN*	4	14	10	–39.40	16.39	–32.01	10.00	7.38	9.01
54 PCO*	4	15	10	–38.00	16.37	–36.68	10.00	1.32	15.05
56 PNO*	5	16	10	–32.16	16.33	–22.32	10.00	9.84	6.49
60 OPbO*	4	16	24	–24.61	16.56	–8.09	10.00	16.53	0.03
66 OSbO*	5	17	20	–20.74	16.45	–18.46	10.00	2.28	14.17
68 SiCN*	4	13	10	–39.79	16.43	–36.84	10.00	2.94	13.48
69 SiCO*	4	14	10	–39.40	16.39	–41.51	10.00	–2.11	14.28

cases. If the tabulated error of the tabulated data are taken into account, then all of the forecasted data are in agreement with the tabulated data.

For log Q, the systematic error of 0.069 in the logarithm converts to a systematic error of 1.02% in Q. For log K_p, the systematic error of 3.78 corresponds to a systematic error of 164% in K_p.

FORECASTING DATA FOR MOLECULES WITH NO TABULATED DATA

Forecasts

Tables VIII to XI show the results of predictions, from Eq. (4), for the forecasted molecules. The first column gives a forecasted molecular number for a ready comparison between tables IV to XI. The formula for the asymmetric molecule is given in the next column, arranged alphabetically by the first atomic symbol, followed by the symmetric form (if any) or by other asymmetric forms. An asterisk denotes the most stable structure of the molecules, when it is known. Prediction errors at 95% confidence are given.

Discussion

The random errors shown in the tables for $\Delta_{at}H$ (Gurvich) and especially for IP are larger than those which can be obtained with reasonably-priced computer packages such as Gaussian-94. For comparison, however, it is noted that a much more sophisticated attempt to obtain least- squares fits for D_e (the »dissociation energy« from the bottom of the potential curve) of large numbers of diatomic molecules resulted in 74% errors (at 50% confidence).[19,20]

A stereographical study of the locations, in the space $f(R),C_2,n_e$, of the predicted and of the originally-fitted molecules showed that molecules whose forecasted data differ from the tabulated data by more than the 95%-confidence intervals of the predictions are not widely distant from the swarm of original data.

Figure 7 shows contours of constant log Q at *1000 K* for $(R_1,R_2,R_3) = (2,2,2)$, obtained from Eq. (4), plotted on the plane $C_1 = C_3$ in Figure 2. These contours are actually sheets which extend in and out of the bounding surfaces of the cubical volume in Figure 2. The figure also shows where some isoelectronic sequences (dotted lines) and adjacent-DIM molecular sequences[17] (solid lines) cross the plane. The orientations of these lines with respect to the contours show why data for molecules in these series are roughly constant, as described in Ref. 17: both sets of lines climb past the contours relatively slowly on the plane of the graphs. Similar contours for $\Delta_{at}H$

TABLE VIII

Forecasted values of ionization potential (IP/eV) with some control values

Molecule		Address			Forecasted	
		C_2	n_e	$f(R)$	Values	95% error
2	AISS	6	15	15	10.74	2.51
	SAIS*	3	15	15	10.74	2.51
3	AITeTe	6	15	40	9.21	2.54
	TeAITe*	3	15	30	9.57	2.53
4	AsCC	4	13	12	10.30	2.53
	CAsC	5	13	16	9.88	2.52
6	BBS	3	12	10	10.05	2.54
	BSB	6	12	12	9.81	2.54
7	BSS	6	15	15	10.74	2.51
	SBS	3	15	12	11.06	2.52
8	BSiSi	4	11	15	8.93	2.54
	SiBSi	3	11	12	9.26	2.54
9	BaBaO	2	10	48	6.73	2.59
	BaOBa*	6	10	24	7.51	2.55
10	BaCC	4	10	16	8.20	2.54
	CBaC	2	10	24	7.51	2.55
11	BeOO	6	14	8	11.20	2.55
	OBeO*	2	14	8	11.20	2.55
12	BeSiSi	4	10	15	8.30	2.54
	SiBeSi	2	10	12	8.63	2.54
15	BrFF	7	21	12	11.63	2.64
	FBrF*	7	21	16	11.20	2.65
16	BrOO	6	19	12	11.73	2.55
	OBrO	7	19	16	11.30	2.55
17	CBB	3	10	8	9.11	2.56
	BCB	4	10	8	9.11	2.56
18	CBrBr	7	18	24	10.55	2.54
	BrCBr*	4	18	16	11.24	2.53
19	CCCI	4	15	10	11.30	2.53
	CCIC	7	15	12	11.06	2.52
20	CCGa	4	11	12	9.26	2.54
	CGaC	3	11	16	8.83	2.54
21	CCS*	4	14	10	10.95	2.53
	CSC	6	14	12	10.72	2.52
22	CaCC	4	10	12	8.63	2.54
	CCaC	2	10	16	8.20	2.54
23	CaCaO	2	10	24	7.51	2.55
	CaOCa*	6	10	16	8.20	2.54
24	CI3*	7	21	18	11.01	2.66
25	CICIP	7	19	18	11.11	2.56
	CIPCI*	5	19	18	11.11	2.56
26	CIFF	7	21	10	11.87	2.64
	FCIF*	7	21	12	11.63	2.64
27	CsOO	6	13	16	9.88	2.52
	OCsO	1	13	24	9.18	2.53
29	GaFO	7	16	12	11.34	2.52
	GaOF*	6	16	12	11.34	2.52
	OGaF	3	16	16	10.91	2.51
30	GaOO	6	15	12	11.0	2.52
	OGaO*	3	15	16	10.64	2.51
31	GaOTe*	6	15	18	10.44	2.51
	GaTeO	6	15	30	9.57	2.53
	OGaTe	3	15	28	9.68	2.52
32	GeGeO	4	14	24	9.60	2.52
	GeOGe*	6	14	16	10.29	2.52
33	GeGeSi	4	12	28	8.43	2.54
	GeSiGe	4	12	24	8.70	2.54
34	GeSS	6	16	21	10.45	2.51
	SGeS*	4	16	24	10.22	2.52
35	GeTeTe	6	16	45	9.43	2.55
	TeGeTe*	4	16	40	9.48	2.54
36	IFF	7	21	14	1.41	2.65
	FIF*	7	21	20	10.83	2.66
37	IOO	6	19	14	11.51	2.55
	OIO*	7	19	20	10.93	2.56
40	InOO	6	15	14	10.84	2.51
	OInO*	3	15	20	10.26	2.51
41	KFF	7	15	12	11.06	2.53
	FKF	1	15	16	10.64	2.51
42	KKNa	1	3	28	0.83	2.64
	KNaK	1		24	1.10	2.62
43	KKO	1	8	12	7.15	2.54
	KOK*	6	8	16	6.72	2.55
44	KNaNa	1	3	21	1.33	2.60
	NaKNa	1	3	24	1.10	2.62

TABLE VIII (continued)

Molecule	Address			Forecasted	
	C_2	n_e	$f(R)$	Values	95% error
45 KOO	6	13	12	10.30	2.53
OKO	1	13	16	9.88	2.52
46 LiOO	6	13	8	10.78	2.54
OLiO	1	13	8	10.78	2.55
47 MgCC	4	10	10	8.86	2.55
CMgC	2	10	12	8.63	2.54
48 MgMgO	2	10	15	8.30	2.54
MgOMg*	6	10	12	8.63	2.54
49 MgOO	6	14	10	10.95	2.53
OMgO	2	14	12	10.72	2.52
50 NaFF	7	14	10	10.95	2.54
FNaF	1	15	12	11.06	2.52
51 NaNaO	1	8	15	8.83	2.55
NaONa*	6	9	12	7.15	2.54
52 NaOO	6	13	10	10.54	2.53
ONaO	1	13	12	10.30	2.53
53 PCN*	4	14	10	10.95	2.53
PNC	5	14	10	10.95	2.53
CPN	5	14	12	10.72	2.52
54 PCO*	4	15	10	11.30	2.53
POC	6	15	15	10.74	2.53
CPO	5	15	12	11.06	2.51
55 PCIF	7	19	16	11.40	2.55
PFCI	7	19	12	11.73	2.55
FPCI	5	19	15	11.40	2.55
56 PNO*	5	16	10	11.57	2.52
PON	6	16	10	11.57	2.52
NPO	5	16	12	11.34	2.52
57 PPC	5	14	15	10.39	2.52
PCP	4	14	12	10.72	2.52
58 PPO	5	16	15	11.01	2.51
POP	6	16	12	11.34	2.52
59 PbBrCI	7	18	36	9.92	2.56
PbCIBr	7	18	30	10.17	2.56
CIPbBr	4	18	42	9.79	2.57
60 PbOO	6	16	16	10.91	2.51
OPbO*	4	16	24	10.22	2.52
61 PbSS	6	16	27	10.01	2.52
SPbS*	4	16	36	9.59	2.54
62 RbOO	6	13	14	10.08	2.52
ORbO	1	13	20	9.50	2.52
63 RbRbO	1	8	35	5.44	2.59
RbORb*	6	8	20	6.35	2.56
64 SFP	7	18	12	11.67	2.53
SPF	5	18	15	11.34	2.53
PSF	6	18	15	11.34	2.53
67 SeCC	4	14	12	10.72	2.52
CSeC	6	14	16	10.29	2.52
68 SiCN*	4	13	10	10.54	2.54
SiNC	5	13	10	10.54	2.54
CSiN	4	13	15	9.98	2.52
69 SiCO*	4	14	10	10.95	2.53
SiOC	6	14	10	10.95	2.53
CSiO	4	14	12	10.72	2.52
70 SiCiF	7	18	15	11.34	2.53
SiFCI	7	18	12	11.67	2.53
CISiF*	4	18	15	11.34	2.53
71 SiNO	5	15	10	11.30	2.53
SiON	6	15	10	11.30	2.53
NSiO	4	15	12	11.06	2.52
72 SiSS	6	16	18	10.72	2.51
SSiS	4	16	18	10.72	2.51
73 SnCICI	7	18	24	10.55	2.54
CiSnCI*	4	18	30	10.17	2.56
74 SnSS	6	16	24	10.22	2.52
SSnS	4	16	30	9.84	2.53
75 SrSrO	2	10	35	6.91	2.57
SrOSr	6	10	20	7.83	2.55
76 TIOO	6	15	16	10.64	2.51
OTIO	3	15	24	9.94	2.52

TABLE IX

Forecasted Heats of Atomization ($\Delta_{at}H$ / eV)

	Molecule	Address			Forecasted	
		C_2	n_e	$f(R)$	Values	95% error
1	AlII	7	17	40	365	382
	IAlI*	3	17	30	646	354
2	AlSS	6	15	18	867	356
	SAlS*	3	15	18	986	351
3	AlTeTe	6	15	40	528	372
	TeAlTe*	3	15	30	752	354
4	AsCC	4	13	12	1117	352
	CAsC	5	13	16	967	354
5	AsOO	6	17	12	923	353
	OAsO*	5	17	16	861	349
6	BBS	3	12	10	1173	354
	BSB	6	12	12	994	359
7	BSS	6	15	15	944	354
	SBS	3	15	12	1148	351
8	BSiSi	4	11	15	941	354
	SiBSi	3	11	12	1057	354
9	BaBaO	2	10	48	477	379
	BaOBa*	6	10	24	569	371
10	BaCC	4	10	16	839	356
	CBaC	2	10	24	710	361
11	BeOO	6	14	8	1165	357
	OBeO*	2	14	8	1306	356
12	BeSiSi	4	10	15	866	355
	SiBeSi	2	10	12	1003	355
13	BiOO	6	17	16	812	353
	OBiO*	5	17	24	678	353
14	BrBrAl	7	17	28	501	371
	BrAlBr*	3	17	24	749	352
15	BrFF	7	21	12	282	385
	FBrF*	7	21	16	171	387
16	BrOO	6	19	12	698	358
	OBrO	7	19	16	530	368
17	CBB	3	10	8	1105	355
	BCB	4	10	8	1074	354
18	CBrBr	7	18	24	476	370
	BrCBr*	4	18	16	804	350
19	CCCl	4	15	10	1177	350
	CClC	7	15	12	972	363
20	CCGa	4	11	12	1026	353
	CGaC	3	11	16	946	355
21	CCS*	4	14	10	1190	351
	CSC	6	14	12	1041	355
22	CaCC	4	10	12	950	354
	CCaC	2	10	16	892	356
23	CaCaO	2	10	24	710	361
	CaOCa*	6	10	16	751	364
24	Cl3*	7	21	18	121	389
25	ClClP	7	19	18	479	369
	ClPCl*	5	19	18	585	356
26	ClFF	7	21	10	342	384
	FClF*	7	21	12	282	385
27	CsOO	6	13	19	844	352
	OCsO	1	13	24	890	357
28	GaFF	7	17	12	866	361
	FGaF*	3	17	16	931	350
29	GaFO	7	16	12	933	362
	GaOF*	6	16	12	990	353
	OGaF	3	16	16	998	350
30	GaOO	6	15	12	1029	354
	OGaO*	3	15	16	1037	350
31	GaOTe*	6	15	18	867	356
	GaTeO	6	15	30	633	363
	OGaTe	3	15	28	783	354
32	GeGeO	4	14	24	836	354
	GeOGe*	6	14	16	930	356
33	GeGeSi	4	12	28	717	360
	GeSiGe	4	12	24	789	358
34	GeSS	6	16	21	759	356
	SGeS*	4	16	24	785	351
35	GeTeTe	6	16	45	468	379
	TeGeTe*	4	16	40	577	360
36	IFF	7	21	14	225	386
	FIF*	7	21	20	73	391
37	IOO	6	19	25	386	356
	OIO*	7	19	26	310	356
38	InClCl	7	17	24	573	368
	ClInCl*	3	17	30	646	354
39	InFF	7	17	14	809	362
	FInF*	3	17	20	833	351
40	InOO	6	15	21	798	353
	OInO*	3	15	18	986	350

TABLE IX (continued)

Molecule	Address			Forecasted	
	C_2	n_e	$f(R)$	Values	95% error
41 KFF	7	15	22	719	353
FKF	1	15	16	1072	350
42 KKNa	1	3	28	-271	379
KNaK	1	3	24	-199	375
43 KKO	1	8	12	814	355
KOK*	6	8	16	549	368
44 KNaNa	1	3	21	-137	372
NaKNa	1	3	24	-199	375
45 KOO	6	13	19	844	352
OKO	1	13	16	1072	355
46 LiOO	6	13	19	844	352
OLiO	1	13	8	1307	358
47 MgCC	4	10	10	1011	354
CMgC	2	10	12	1003	355
48 MgMgO	2	10	15	919	356
MgOMg*	6	10	12	862	361
49 MgOO	6	14	10	1102	356
OMgO	2	14	12	1182	353
50 NaFF	7	14	21	753	353
FNaF	1	15	12	1183	354
51 NaNaO	1	8	15	730	357
NaONa*	6	8	12	660	364
52 NaOO	6	13	19	844	352
ONaO	1	13	12	1183	355
53 PCN *	4	14	10	1190	351
PNC	5	14	10	1150	351
CPN	5	14	12	1090	352
54 PCO *	4	15	10	1177	350
POC	6	15	15	944	354
CPO	5	15	12	1077	350
55 PClF	7	19	15	556	367
PFCl	7	19	12	641	366
FPCl	5	19	15	662	355
56 PNO *	5	16	10	1099	350
PON	6	16	10	1050	353
NPO	5	16	12	1039	349
57 PPC	5	14	15	1005	352
PCP	4	14	12	1129	351
58 PPO	5	16	15	954	349
POP	6	16	12	990	353
59 PbBrCl	7	18	42	257	364
PbClBr	7	18	36	301	379
ClPbBr	4	18	30	519	374
60 PbOO	6	16	16	879	353
OPbO*	4	16	24	785	351
61 PbSS	6	16	27	642	360
SPbS*	4	16	36	610	356
62 RbOO	6	13	14	972	352
ORbO	1	13	20	974	356
63 RbRbO	1	8	35	356	365
RbORb*	6	8	20	452	372
64 SFP	7	18	12	769	354
SPF	5	18	15	790	362
PSF	6	18	15	742	351
65 SNO	5	17	10	1032	350
SON	6	17	10	984	353
NSO	6	17	12	923	353
66 SbOO	6	17	14	866	353
OSbO*	5	17	20	763	351
67 SeCC	4	14	12	1129	351
CSeC	6	14	16	930	356
68 SiCN*	4	13	10	1177	352
SiNC	5	13	10	1138	353
CSiN	4	13	15	1033	352
69 SiCO*	4	14	10	1190	351
SiOC	6	14	10	1102	356
CSiO	4	14	12	1129	351
70 SiClF	7	18	15	685	363
SiFCl	7	18	12	769	362
ClSiF*	4	18	15	830	350
71 SiNO	5	15	10	1138	351
SiON	6	15	10	1089	354
NSiO	4	15	12	1117	349
72 SiSS	6	16	18	829	354
SSiS	4	16	18	917	349
73 SnClCl	7	18	24	476	370
ClSnCl*	4	18	30	519	362
74 SnSS	6	16	24	697	358
SSnS	4	16	30	682	354
75 SrSrO	2	10	35	545	365
SrOSr	6	10	20	654	368
76 TlOO	6	15	16	918	355

TABLE X

Forecasted values of log Q at 1000 K

	Molecule	Address			Forecasted			Molecule	Address			Forecasted	
		C_2	n_e	$f(R)$	Values	95% error			C_2	n_e	$f(R)$	Values	95% error
2	AlSS	6	15	18	6.09	1.07	29	GaFO	7	16	12	5.14	1.05
	SAlS*	3	15	18	6.23	1.02	30	GaOO	6	15	12	5.13	1.04
3	AlTeTe	6	15	40	8.25	1.42		OGaO*	3	15	16	5.93	1.02
	TeAlTe*	3	15	30	7.67	1.06	31	GaOTe*	6	15	18	6.09	1.07
4	AsCC	4	13	12	5.24	1.01		GaTeO	6	15	30	7.53	1.12
	CAsC	5	13	16	5.85	1.03		OGaTe	3	15	28	7.48	1.04
5	AsOO	6	17	12	5.32	1.03	32	GeGeO	4	14	24	6.98	1.04
	OAsO*	5	17	16	6.02	1.02		GeOGe*	6	14	16	5.78	1.06
6	BBS	3	12	10	4.99	1.03	33	GeGeSi	4	12	28	7.51	1.06
	BSB	6	12	12	5.20	1.03		GeSiGe	4	12	24	7.06	1.05
7	BSS	6	15	15	5.63	1.05	34	GeSS	6	16	21	6.57	1.07
	SBS	3	15	12	5.27	1.01		SGeS*	4	16	24	7.04	1.03
8	BSiSi	4	11	15	5.86	1.04	35	GeTeTe	6	16	45	8.51	1.77
	SiBSi	3	11	12	5.41	1.04		TeGeTe*	4	16	40	8.41	1.38
9	BaOO	2	10	48	8.89	2.03	37	OIO*	7	19	26	7.79	1.09
	BaOBa*	6	10	24	7.08	1.11	40	InOO	6	15	14	5.46	1.05
10	BaCC	4	10	16	6.07	1.07		OInO	3	15	20	6.51	1.02
	CBaC	2	10	24	7.27	1.11	45	OKO	1	13	16	6.05	1.05
11	BeOO	6	14	8	4.39	1.03	46	OLiO	1	13	8	4.66	1.08
	OBeO*	2	14	8	4.58	1.04	47	MgCC	4	10	10	5.06	1.05
12	BeSiSi	4	10	15	5.91	1.07		CMgC	2	10	12	5.51	1.09
	SiBeSi	2	10	12	5.51	1.09	48	MgMgO	2	10	15	6.01	1.10
13	BiOO	6	17	16	5.97	1.04		MgOMg*	6	10	12	5.32	1.06
	OBiO*	5	17	24	7.13	1.04	49	MGOO	6	14	10	4.76	1.03
16	OBrO	7	19	16	6.45	1.03		OMgO	2	14	12	5.31	1.02
17	CBB	3	10	8	4.73	1.07	52	ONaO	1	13	12	5.39	1.06
	BCB	4	10	8	4.69	1.06	53	PCN*	4	14	10	4.86	1.02
19	CClC	7	15	12	5.08	1.07		PNC	5	14	10	4.81	1.01
20	CCGa	4	11	12	5.36	1.03		CPN	5	14	12	5.17	1.02
	CGaC	3	11	16	6.07	1.05	54	POC*	6	15	15	5.63	1.05
21	CCS*	4	14	10	4.86	1.01		POC	6	15	15	5.63	1.01
	CSC	6	14	12	5.12	1.04		CPO	5	15	12	5.17	1.00
22	CaCC	4	10	12	5.41	1.06	56	PNO*	5	16	10	4.88	1.02
	CCaC	2	10	16	6.17	1.10		PON	6	16	10	4.83	1.03
23	CaCaO	2	10	24	7.27	1.11		NPO	5	16	12	5.23	1.02
	CaOCa*	6	10	16	5.97	1.08	57	PPC	5	14	15	5.67	1.03
27	OCsO	1	13	24	7.15	1.07		PCP	4	14	12	5.21	1.01

TABLE X (continued)

Molecule	Address			Forecasted		Molecule	Address			Forecasted	
	C_2	n_e	$f(R)$	Values	95% error		C_2	n_e	$f(R)$	Values	95% error
58 PPO	5	16	15	5.73	1.03	72 SiSS	6	16	18	6.15	1.06
POP	6	16	12	5.19	1.04	SSiS	4	16	18	6.24	1.02
60 PbOO	6	16	16	5.84	1.05	74 SnSS	6	16	24	6.95	1.08
OPbO	4	16	24	7.04	1.03	SSnS	4	16	30	7.69	1.06
61 PbSS	6	16	27	7.29	1.09	75 SrSrO	2	10	35	8.33	1.21
SPbS	4	16	36	8.17	1.19	SrOSr	6	10	20	6.56	1.10
62 ORbO	1	13	20	6.63	1.06	76 TlOO	6	15	16	5.78	1.06
64 SFP	7	18	12	5.48	1.03	OTlO	3	15	24	7.03	1.03
PSF	6	18	15	6.03	1.02						
65 SNO	5	17	10	5.01	1.03						
SON	6	17	10	4.96	1.01						
NSO	6	17	12	5.32	1.03						
66 SbOO	6	17	14	5.65	1.03						
OSbO*	5	17	20	6.61	1.03						
67 SeCC	4	14	12	5.21	1.01						
CSeC	6	14	16	5.78	1.06						
68 SiCN	4	13	10	4.89	1.01						
SiNC	5	13	10	4.84	1.01						
CSiN	4	13	15	5.74	1.02						
69 SiCO	4	14	10	4.86	1.01						
SiOC	6	14	10	4.76	1.03						
CSiO	4	14	12	5.21	1.01						
71 SiNO	5	15	10	4.82	1.02						
SiON	6	15	10	4.77	1.03						
NSiO	4	15	12	5.22	1.01						

(Sauval) are shown in Figure 8. Contours of IP based on Eq. (4) are strictly parallel to isoelectronic sequences (Table III), *i.e.,* strictly dependent on the number of valence electrons in the molecular orbitals. In Figures 7 and 8, it is the dependence on C_2 which causes the contours to be more complicated.

The contour lines shown in these figures are low-level approximations, obtained from smoothed data only. The figures in Laurenzi's papers[5–7] show the much more resolved contours are obtained (for several different isoelectronic series of diatomic molecules) when it is possible to use *ab initio* computations.

TABLE XI

Forecasted values of log K

	Molecule	Address			Forecasted	
		C_2	n_e	$f(R)$	Values	95% error
1	AlII	7	17	40	3.86	19.52
	IAlI*	3	17	30	–18.94	16.95
2	AlSS	6	15	18	–24.26	16.70
	SAlS*	3	15	18	–34.39	16.40
3	AlTeTe	6	15	40	–7.10	18.96
	TeAlTe*	3	15	30	–25.03	17.01
4	AsCC	4	13	12	–38.23	16.40
	CAsC	5	13	16	–31.73	16.52
5	AsOO	6	17	12	–22.86	16.48
	OAsO*	5	17	16	–23.86	16.34
6	BBS	3	12	10	–41.87	16.51
	BSB	6	12	12	–30.19	16.78
7	BSS	6	15	15	–26.60	16.59
	SBS	3	15	12	–39.07	16.42
8	BSiSi	4	11	15	–33.95	16.52
	SiBSi	3	11	12	–38.91	16.49
9	BaBaO	2	10	48	–10.52	19.97
	BaOBa*	6	10	24	–17.24	17.74
10	BaCC	4	10	16	–30.98	16.59
	CBaC	2	10	24	–29.24	16.94
11	BeOO	6	14	8	–33.46	16.60
	OBeO*	2	14	8	–45.46	16.67
12	BeSiSi	4	10	15	–31.76	16.55
	SiBeSi	2	10	12	–38.60	16.54
13	BiOO	6	17	16	–19.74	16.54
	OBiO*	5	17	24	–17.62	16.66
14	BrBrAl	7	17	28	–.50	17.93
	BrAlBr*	3	17	24	–23.62	16.57
15	BrFF	7	21	12	9.37	17.92
	FBrF*	7	21	16	12.49	18.04
16	BrOO	6	19	12	–11.90	16.71
	OBrO	7	19	16	–3.91	17.23
17	CBB	3	10	8	–39.85	16.52
	BCB	4	10	8	–37.22	16.49
18	CBrBr	7	18	24	–3.79	17.58
	BrCBr*	4	18	16	–22.41	16.40
19	CCCl	4	15	10	–38.00	16.37
	CClC	7	15	12	–24.07	17.02
20	CCGa	4	11	12	–36.29	16.47
	CGaC	3	11	16	–35.79	16.53
21	CCS*	4	14	10	–39.40	16.39
	CSC	6	14	12	–30.34	16.61
22	CaCC	4	10	12	–34.10	16.49
	CCaC	2	10	16	–35.48	16.58
23	CaCaO	2	10	24	–29.24	16.94
	CaOCa*	6	10	16	–23.48	17.12
24	Cl3*	7	21	18	14.05	18.13
25	ClClP	7	19	18	–2.35	17.32
	ClPCl*	5	19	18	–11.35	16.64
26	ClFF	7	21	10	7.81	17.90
	FClF*	7	21	12	9.37	17.92
27	CsOO	6	13	16	–27.61	16.40
	OCsO	1	13	24	–34.49	16.79
28	GaFF	7	17	12	–17.98	16.92
	FGaF*	3	17	16	–29.86	16.40
29	GaFO	7	16	12	–21.60	16.95
	GaOF*	6	16	12	–26.47	16.48
	OGaF	3	16	16	–33.48	16.37
30	GaOO	6	15	12	–28.94	16.53
	OGaO*	3	15	16	–35.95	16.38
31	GaOTe*	6	15	18	–24.26	16.70
	GaTeO	6	15	30	–14.90	17.64
	OGaTe	3	15	28	–26.59	16.85
32	GeGeO	4	14	24	–28.48	16.69
	GeOGe*	6	14	16	–27.22	16.71
33	GeGeSi	4	12	28	–25.21	17.19
	GeSiGe	4	12	24	–28.33	16.87
34	GeSS	6	16	21	–19.45	16.79
	SGeS*	4	16	24	–24.61	16.56
35	GeTeTe	6	16	45	–0.73	19.65
	TeGeTe*	4	16	40	–12.13	18.14
36	IFF	7	21	14	10.93	17.97
	FIF*	7	21	20	15.61	18.24
37	IOO	6	19	14	–10.34	16.73
	OIO	7	19	20	–0.79	17.44
38	InClCl	7	17	24	–8.62	17.00
	ClInCl*	3	17	30	–18.94	17.45
39	InFF	7	17	14	–16.42	16.40
	FInF*	3	17	20	–26.74	16.60
40	InOO	6	15	14	–27.38	16.57
	OInO	3	15	20	–32.83	16.44
41	KFF	7	15	12	–24.07	16.40
	FKF	1	15	16	–38.95	16.50

TABLE XI (continued)

	Molecule	Address			Forecasted	
		C_2	n_e	$f(R)$	Values	95% error
42	KKNa	1	3	28	4.12	17.80
	KNaK	1	3	24	1.00	17.40
43	KKO	1	8	24	−23.91	17.20
	KOK*	6	8	16	−17.03	16.80
44	KNaNa	1	3	21	−1.34	17.30
	NaKNa	1	3	24	1.00	17.50
45	KOO	6	13	12	−30.73	16.40
	OKO	1	13	16	−40.73	16.59
46	LiOO	6	13	8	−33.85	16.60
	OLiO	1	13	8	−46.97	16.76
47	MgCC	4	10	10	−35.66	16.48
	CMgC	2	10	12	−38.60	16.54
48	MgMgO	2	10	15	−36.26	16.56
	MgOMg*	6	10	12	−26.60	16.94
49	MgOO	6	14	10	−31.90	16.60
	OMgO	2	14	12	−42.34	16.54
50	NaFF	7	14	10	−27.02	16.40
	FNaF	1	15	12	−42.07	16.61
51	NaNaO	1	8	15	−30.93	16.50
	NaONa*	6	8	12	−20.15	17.08
52	NaOO	6	13	10	−32.29	16.40
	ONaO	1	13	12	−43.85	16.62
53	PCN*	4	14	10	−39.40	16.39
	PNC	5	14	10	−36.02	16.39
	CPN	5	14	12	−34.46	16.40
54	PCO*	4	15	10	−38.00	16.37
	POC	6	15	15	−26.60	16.59
	CPO	5	15	12	−33.07	16.36
55	PClF	7	19	15	−4.69	16.58
	PFCl	7	19	12	−7.03	17.20
	FPCl	5	19	15	−13.69	17.12
56	PNO*	5	16	10	−32.16	16.33
	PON	6	16	10	−28.03	16.48
	NPO	5	16	12	−30.60	16.31
57	PPC	5	14	15	−32.12	16.42
	PCP	4	14	12	−37.84	16.36
58	PPO	5	16	15	−28.26	16.32
	POP	6	16	12	−26.47	16.48
59	PbBrCl	7	18	42	10.25	18.43
	PbClBr	7	18	36	5.57	18.94
	ClPbBr	4	18	30	−11.49	18.18
60	PbOO	6	16	16	−23.35	16.56
	OPbO*	4	16	24	−24.61	16.56
61	PbSS	6	16	27	−14.77	17.24
	SPbS*	4	16	36	−15.25	17.62
62	RbOO	6	13	14	−29.17	16.40
	ORbO	1	13	20	−37.61	16.64
63	RbRbO	1	8	35	−15.33	18.40
	RbORb*	6	8	20	−13.91	17.00
64	SFP	7	18	12	−13.15	16.58
	SPF	5	18	15	−19.81	16.40
	PSF	6	18	15	−15.69	16.96
65	SNO	5	17	10	−28.54	16.48
	SON	6	17	10	−24.42	16.34
	NSO	6	17	12	−22.86	16.48
66	SbOO	6	17	14	−21.30	16.50
	OSbO*	5	17	20	−20.74	16.45
67	SeCC	4	14	12	−37.84	16.36
	CSeC	6	14	16	−27.22	16.71
68	CSiN	4	13	15	−35.89	16.42
	SiCN*	4	13	10	−39.79	16.43
	SiNC	5	13	10	−36.41	16.45
69	SiCO*	4	14	10	−39.40	16.39
	SiOC	6	14	10	−31.90	16.60
	CSiO	4	14	12	−37.84	16.36
70	SiFCl	7	18	12	−13.15	16.96
	SiClF	7	18	15	−10.81	17.04
	ClSiF*	4	18	15	−23.19	16.40
71	SiNO	5	15	10	−34.63	16.35
	SiON	6	15	10	−30.50	16.53
	NSiO	4	15	12	−36.44	16.33
72	SiSS	6	16	18	−21.79	16.63
	SSiS	4	16	18	−29.29	16.33
73	SnClCl	7	18	24	−3.79	17.58
	ClSnCl*	4	18	30	−11.49	17.05
74	SnSS	6	16	24	−17.11	16.99
	SSnS	4	16	30	−19.93	16.99
75	SrSrO	2	10	35	−20.66	18.01
	SrOSr	6	10	20	−20.36	17.39
76	TlOO	6	15	16	−25.82	16.62
	OTlO	3	15	24	−29.71	16.60

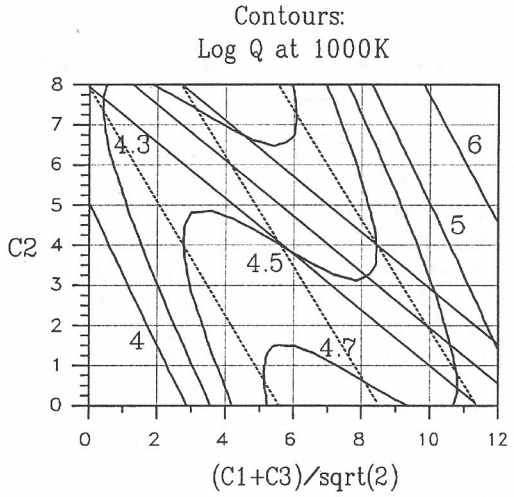

Figure 7. Log Q at 1000 K countours on the vertical plane containing the isoelectronic axis in Figure 2, for $R_1 = R_2 = R_3 = 2$. Since Eq. (4) contains no dependence on R_2-R_1 or R_3-R_1, the contour lines extend unchanged, as sheets, to the edges of the cube in Figure 2. Dotted lines show where planes containing isoelectronic molecules interesect the vertical plane. Solid lines show where planes containing adjacent-DIM-isoelectronic molecules intersect the plane. The lines also serve as end-views of planes extending to the edges of the cube.

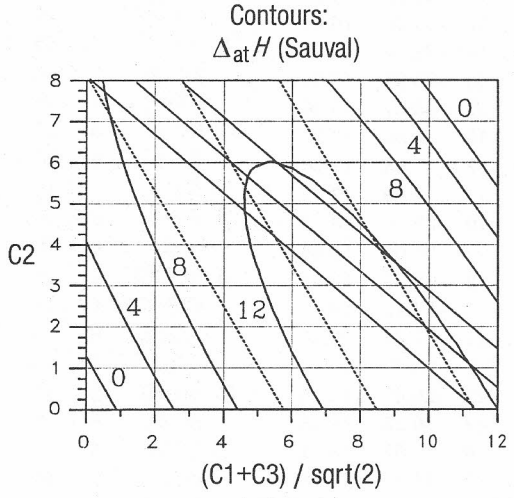

Figure 8. Same as in Figure 7, but for $\Delta_{at}H$ (Sauval).

SUMMARY

A statistical analysis of quality tabulated data for four properties of neutral, ground-state, acyclic, main-group triatomic molecules has revealed that they show periodic behavior, that they can be reasonably well fitted by a simple equation, and that this equation can be used to forecast data for other molecules by the hundred. A few data from the tables have allowed testing of the forecasts, and certainly additional data exist in the literature.

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REFERENCES

1. H. R. Johnson and A. J. Sauval, *Astron. Astrophys.* Suppl. Ser. **49** (1982) 77–87.
2. P. L. Smith, *Atomic Molecular Data Required for Ultraviolet and Optical Astrophysics*, Harvard College Observatory, Cambridge, MA, 1989.
3. U. G. Jorgensen, *Revista Mexicana de Astronomia y Astrofisica* **23** (1991) 49–62.
4. N. Grevesse, A. Noels, and A. J. Sauval, *Laboratory and Astronomical High Resolution Spectra,* ASP Conference Series **81** (1995) 74–87.
5. B. J. Laurenzi, *J. Chem. Phys.* **74** (1981) 1840–1851.
6. B. J. Laurenzi and M. F. Mall, *Int. J. Quantum Chem.* **30** (1986) 51–75.
7. B. J. Laurenzi and D. R. Gaylord, *Int. J. Quantum Chem.* **44** (1992) 17–43.
8. C. E. Wulfman, private communication.
9. H. Primas, *Chemistry, Quantum Mechanics and Reductionism: Perspectives in Theoretical Chemistry,* Springer-Verlag, Berlin, Germany, 1983.
10. V. V. Nefedova, A. I. Boldyrev, and J. Simons, *J. Chem. Phys.* **98** (1993) 8801–8809.
11. A. I. Boldyrev, in: *Structure and Dynamics of Non-Rigid Molecular Systems*, Kluwer Academic Publishers, Dordrecht, The Netherlands, 1995, pp. 1–45.
12. D. R. Stull and H. Prophet, JANAF *Thermochemical Tables,* Office of Standard Reference Data, National Bureau of Standards, U. S. Government Printing Office, Washington, DC 1971. M. W. Chase et al, *J. Phys. Chem. Ref. Data* **3** (1974) 311–480; **4** (1975) 1–175; **7** (1978) 793–940; **11** (1982) 695–940.
13. A. J. Sauval and J. B. Tatum [computations for triatomic molecules done at the same time as those for diatomic molecules, the latter being used in *Astrophys. J. Suppl.* **56** (1984) 193–209].
14. A. J. Sauval, private communication, 1986.
15. L. V. Gurvich (Ed.), *Thermodinamicheskie Svoistva Individual'nikh Veschestv,* Vols. 1–4, Nauka, Moscow, 1978, 1979, 1981, 1982.
16. L. V. Gurvich, G. V. Karachevtzev, V. N. Kondrat'ev, Yu. A. Lebedev, V. A. Medvedev, V. K. Potapov and Yu. S. Khodeev, *Energii Razryva Khimicheskikh Svyazei. Potentialy Ionizatzii i Srodsvo k Electronu*, Nauka, Moscow, 1974. [An earlier edition was translated into English: V. I. Vedeneev, L. V. Gurvich, V. N. Kondrat'ev and Ya. L. Frankevich, *Bond Energies, Ionization Potentials, and Electron Affinities*, St. Martins, New York, 1966.]

17. R. Cavanaugh, R. Marsa, J. Roberton, and R. Hefferlin, *J. Mol. Struct.*, **382** (1996) 137–145.
18. F. A. Kong, in: R. Hefferlin, *Periodic Systems of Molecules and Their Relation to the Systematic Analysis of Molecular Data,* The Edwin Mellen Press, Lewiston, New York, 1989, pp. 396–413.
19. J. L. Gazquez and R. G. Parr, *Chem. Phys. Lett.* **66** (1979) 419–422.
20. R. Hefferlin, *Periodic Systems and Their Relation to the Systematic Analysis of Molecular Data*, The Edwin Mellen Press, Lewiston, NY 1989, pp. 18, 216.

SAŽETAK

Procjena svojstava troatomnih molekula iz tabličnih podataka s pomoću metode najmanjih kvadrata

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Ovaj rad prvi put pokazuje da je moguće načiniti brze prognoze rezultata za velik broj molekula izglađivanjem tabuliranih podataka metodom najmanjih kvadrata; predviđanja ipak nisu tako precizna poput onih dobivenih kvantno-kemijskim proračunima u kojima se svaka molekula obrađuje posebno. Odabrana su takva molekulska svojstva koja se koriste u fizici plazme i u astrofizici. Rad započinje grafičkom analizom izabranih podataka za osnovna stanja neutralnih, acikličkih troatomnih molekula sastavljenih od atoma glavne skupine (od 2. do 6. periode) koji se unose u jednadžbu za izglađivanje metodom najmanjih kvadrata. Jednadžba je kvadratna ($R_1R_2 + R_2R_3$) funkcija atomskog broja i grupnog broja centralnog atoma, a kubna funkcija ukupnog broja valentnih elektrona. Koeficijenti jednadžbe (neki su jednaki i ništici) dobiveni su iz najboljih podataka za toplinu atomizacije, ionizacijski potencijal, logaritam particijskog koeficijenta pri 1000 K i za logaritam konstante ravnoteže pri 1000 K. Jednadžba i njezini koeficijenti testirani su prema podacima iz iste baze podataka, i to na nekoliko molekula kojih nije bilo u početnom skupu. Na kraju su navedena svojstva predviđena za 164, 145, 107 i 164 dodatnih molekula.