



Universidad de La Habana, Cuba

# MANUAL DEL USUARIO DE TC HAVANA Q3

**Programa: Q3**

## **EVALUACIÓN ESTADÍSTICA DE LA DISTRIBUCIÓN DE MOLÉCULAS ALREDEDOR DE UN SISTEMA POLIATÓMICO CENTRAL EN LAS HIPERSUPERFICIES DE MÚLTIPLES MÍNIMOS**

**Q3** es un programa ejecutable de MS-DOS que está diseñado para leer archivos denominados *input.q* que contienen las energías de las celdas generadas (una en cada línea) después de la optimización por MOPAC, y las del sistema de referencia, así como la indicación de cuál fichero contiene la información espacial para las comparaciones entre estructuras con posibilidades de ser redundantes, según los índices de Tanimoto.

### **LA ENTRADA:**

Un archivo nombrado *input.q* debe estar presente en el directorio predefinido y contiene los datos para la corrida. Los formatos de la entrada son amplios y pueden entrarse como datos numéricos separados por comas.

### **Primera línea:**

Título explicativo

### **Segunda línea:**

eref, anum, temp, conv, toind, ifile (formatos 5f15.0, a36)

- *eref* es la energía de referencia (en eV) como suma de las energías totales de las moléculas integrantes aisladas y optimizadas con las mismas opciones MOPAC que los agregados moleculares.
- *anum* es el número de moléculas de referencia que se usa para poder expresar los valores por mol y por molécula de referencia. Implícito: 1. Si es negativo las energías de entrada están en kcal/mol.
- *temp* es la temperatura (en K) a la que se desean los cálculos termodinámicos. Implícito: un rango desde 298 hasta 398 K.
- *conv* es la energía de convergencia de las entalpías molares (en eV). Implícito:  $1.10^{-3}$  eV = 0.0965 kJ/mol.

- `tol i nd` es el nivel de discriminación para el coeficiente de semejanza de Tanimoto (implícito=0.85).
- `i fi l e` es el nombre del fichero del tipo `.rsm` que debe estar en el subdirectorio de corrida.

**Restantes líneas hasta el final:**

Energías totales (en ev) de los agregados moleculares optimizados, en el mismo orden con que aparecen en el archivo `.rsm`.

**LA SALIDA:**

La salida de Q3 consiste en 2 archivos de textos cuyos nombres son `output.q3` y `output.dt3`. La información de los mismos es autoexplicativa en el caso del `output.q3`. El `output.dt3` contiene la misma información en forma de columnas para ser extraídas a programas de hojas de cálculo y gráficos.

**UN EJEMPLO DEL ARCHIVO `input.q`:**

```

Acetylene + formic acid
-1002.99607, 1, , , , c2h2f. rsm
-1002.86347
-1002.86344
-1002.85370
-1002.86348
-1002.85369
-1002.86347
-1002.85371
-1002.86345
-1002.86345
-1002.88616
-1002.85372
-1002.84828
-1002.88605
-1002.84829
-1002.85370
-1002.86342
-1002.86347
-1002.84829
-1002.84826
-1002.84828
-1002.84826
-1002.84826
-1002.86346
-1002.85372
-1002.88604
-1002.84789
-1002.88590
-1002.86339
-1002.85365
-1002.86347
-1002.88617
-1002.84831
-1002.86347
-1002.86340
-1002.84820
-1002.86340
-1002.85372
-1002.86346
-1002.85372
-1002.85365
-1002.85372
-1002.84826
-1002.86346
-1002.86347
-1002.86345
-1002.88500
-1002.86341

```

-1002.88873  
-1002.86347  
-1002.85371  
-1003.07613  
-1003.03307  
-1003.03307  
-1003.07013  
-1003.05016  
-1003.07012  
-1003.07905  
-1003.07906  
-1003.05011  
-1003.07906  
-1003.07906  
-1003.05017  
-1003.05017  
-1003.07607  
-1003.07906  
-1003.07906  
-1003.07906  
-1003.07906  
-1003.03307  
-1003.05016  
-1003.03303  
-1003.07906  
-1003.07906  
-1003.05017  
-1003.05016  
-1003.07899  
-1003.07906  
-1003.07906  
-1003.07007  
-1003.05017  
-1003.07010  
-1003.05016  
-1003.05015  
-1003.05014  
-1003.05015  
-1003.05016  
-1003.03307  
-1003.03307  
-1003.05014  
-1003.07906  
-1003.05015  
-1003.05017  
-1003.07901  
-1003.05016  
-1003.07906  
-1003.05014  
-1003.05016  
-1003.05017  
-1003.07618  
-1003.05017  
-1003.05016

### UN EJEMPLO DEL ARCHIVO *output.q3* CORRESPONDIENTE A LA ENTRADA ANTERIOR:

```
03
Calculation of Thermodynamic Quantities of Association in NVT ensembles
Luis A. Montero, Elsa Sanchez, Universidad de La Habana
Roberto Cruz, ISCTN
La Habana, febrero de 2001

Acetylene + formic acid

Reference energy (kJ/mol):                -96776.306
Number of reference molecules in the cell: 1
Convergence limit in molar enthalpies (kJ/mole): .096
Similarity level of the Tanimoto index:   .850

  de: Relative energy with respect to minimum
  e:  Relative energy with respect to the reference state
  n/N: Relative populations of states
```

q0(i): Boltzmann term of cell i with respect to minimum  
q1(i): Boltzmann term of cell i with respect to the reference state  
p0(i): Partition sum until cell i with respect to minimum  
p1(i): Partition sum until cell i with respect to reference state  
NOTE: Molar values are given with respect to one or one mole of reference molecules.

Entry 2 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .89780  
Entry 4 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .97636  
Entry 6 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .96315  
Entry 7 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .92274  
Entry 8 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .88482  
Entry 9 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .97012  
Entry 11 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .95242  
Entry 13 is dismissed because degenerance with respect to entry 10  
Tanimoto index= .95876  
Entry 14 is dismissed because degenerance with respect to entry 12  
Tanimoto index= .93801  
Entry 15 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .98621  
Entry 16 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .91340  
Entry 17 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .94418  
Entry 19 is dismissed because degenerance with respect to entry 18  
Tanimoto index= .92456  
Entry 21 is dismissed because degenerance with respect to entry 18  
Tanimoto index= .92376  
Entry 22 is dismissed because degenerance with respect to entry 12  
Tanimoto index= .89199  
Entry 23 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .97262  
Entry 24 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .85834  
Entry 25 is dismissed because degenerance with respect to entry 10  
Tanimoto index= .94351  
Entry 27 is dismissed because degenerance with respect to entry 10  
Tanimoto index= .94113  
Entry 28 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .94470  
Entry 29 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .87900  
Entry 30 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .95573  
Entry 31 is dismissed because degenerance with respect to entry 10  
Tanimoto index= .98450  
Entry 33 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .94661  
Entry 34 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .91597  
Entry 36 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .99143  
Entry 37 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .92313  
Entry 38 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .91995  
Entry 39 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .89296  
Entry 41 is dismissed because degenerance with respect to entry 3  
Tanimoto index= .95025  
Entry 42 is dismissed because degenerance with respect to entry 18  
Tanimoto index= .92497  
Entry 43 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .91237  
Entry 44 is dismissed because degenerance with respect to entry 1  
Tanimoto index= .97710  
Entry 45 is dismissed because degenerance with respect to entry 1

Tani moto index= .92189  
Entry 47 is dismissed because degenerance wi th respect to entry 1  
Tani moto index= .89039  
Entry 49 is dismissed because degenerance wi th respect to entry 1  
Tani moto index= .98243  
Entry 50 is dismissed because degenerance wi th respect to entry 40  
Tani moto index= .93285  
Entry 56 is dismissed because degenerance wi th respect to entry 54  
Tani moto index= .90776  
Entry 58 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .94484  
Entry 59 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .96954  
Entry 60 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .91217  
Entry 61 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .95574  
Entry 62 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .99726  
Entry 63 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .99877  
Entry 64 is dismissed because degenerance wi th respect to entry 51  
Tani moto index= .99880  
Entry 65 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .98554  
Entry 66 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .95782  
Entry 67 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .91457  
Entry 69 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .94825  
Entry 70 is dismissed because degenerance wi th respect to entry 53  
Tani moto index= .93124  
Entry 71 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .96617  
Entry 72 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .95072  
Entry 73 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .92322  
Entry 74 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .99974  
Entry 75 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .94638  
Entry 76 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .91165  
Entry 77 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .88554  
Entry 78 is dismissed because degenerance wi th respect to entry 54  
Tani moto index= .88541  
Entry 79 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .94347  
Entry 80 is dismissed because degenerance wi th respect to entry 54  
Tani moto index= .92558  
Entry 81 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .95020  
Entry 82 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .96777  
Entry 83 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .97046  
Entry 84 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .93932  
Entry 85 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .96378  
Entry 87 is dismissed because degenerance wi th respect to entry 52  
Tani moto index= .99720  
Entry 88 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .99837  
Entry 89 is dismissed because degenerance wi th respect to entry 57  
Tani moto index= .91391  
Entry 90 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .99864  
Entry 91 is dismissed because degenerance wi th respect to entry 55  
Tani moto index= .93819  
Entry 92 is dismissed because degenerance wi th respect to entry 57

Tanimoto index= .91867  
 Entry 93 is dismissed because degenerance with respect to entry 55  
 Tanimoto index= .99952  
 Entry 94 is dismissed because degenerance with respect to entry 57  
 Tanimoto index= .97696  
 Entry 95 is dismissed because degenerance with respect to entry 55  
 Tanimoto index= .99876  
 Entry 96 is dismissed because degenerance with respect to entry 55  
 Tanimoto index= .94877  
 Entry 97 is dismissed because degenerance with respect to entry 55  
 Tanimoto index= .99814  
 Entry 98 is dismissed because degenerance with respect to entry 51  
 Tanimoto index= .99912  
 Entry 99 is dismissed because degenerance with respect to entry 55  
 Tanimoto index= .99883  
 Entry 100 is dismissed because degenerance with respect to entry 55  
 Tanimoto index= .96423

This set totals 100 counts...

\*\*\* TEMPERATURE: 298.15 K \*\*\*

E-Eo in cell 40 differs less than .00100 ev with respect to cell 35

Molar functions:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.631504E-04	.136741E+21	.345528E+22	.136741E+21
3	21.743	13.737	13.177	5.616	11.503	.431754E-04	.934890E+20	.236235E+22	.230230E+21
5	21.744	13.738	13.339	8.992	10.658	.431586E-04	.934526E+20	.236143E+22	.323683E+21
10	18.611	10.605	11.957	10.211	8.913	.152721E-03	.330690E+21	.835613E+22	.654373E+21
12	22.266	14.260	12.196	11.922	8.642	.349642E-04	.757091E+20	.191307E+22	.730082E+21
18	22.265	14.259	12.390	13.393	8.397	.349779E-04	.757385E+20	.191382E+22	.805820E+21
20	22.266	14.260	12.551	14.678	8.174	.349642E-04	.757091E+20	.191307E+22	.881529E+21
26	22.304	14.297	12.687	15.811	7.973	.344375E-04	.745686E+20	.188425E+22	.956098E+21
32	22.263	14.257	12.802	16.832	7.784	.350051E-04	.757975E+20	.191531E+22	.103190E+22
35	22.274	14.268	12.902	17.754	7.609	.348556E-04	.754737E+20	.190713E+22	.110737E+22
40	21.748	13.742	12.967	18.645	7.408	.430915E-04	.933072E+20	.235776E+22	.120068E+22
46	18.723	10.717	12.498	19.015	6.829	.145979E-03	.316092E+21	.798726E+22	.151677E+22
48	18.363	10.357	12.082	19.416	6.294	.168786E-03	.365478E+21	.923517E+22	.188225E+22
51	.282	-7.725	-7.656	.261	-7.733	.248255	.537554E+24	.135833E+26	.539436E+24
52	4.436	-3.570	-7.013	3.837	-8.157	.464589E-01	.100599E+24	.254201E+25	.640035E+24
53	4.436	-3.570	-6.546	6.619	-8.519	.464589E-01	.100599E+24	.254201E+25	.740634E+24
54	.861	-7.146	-6.765	9.660	-9.645	.196554	.425604E+24	.107545E+26	.116624E+25
55	2.788	-5.219	-6.543	11.694	-10.029	.903516E-01	.195641E+24	.494360E+25	.136188E+25
57	.000	-8.007	-6.992	13.234	-10.937	.278134	.602251E+24	.152181E+26	.196413E+25
68	4.436	-3.570	-6.825	14.208	-11.061	.464589E-01	.100599E+24	.254201E+25	.206473E+25
86	4.436	-3.570	-6.674	15.111	-11.179	.464589E-01	.100599E+24	.254201E+25	.216533E+25

Partiti on functi on (absol ute): .2165327841E+25

Partiti on functi on (relati ve): .5471513845E+26

Molecul ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.631504E-04	.227050E-03	.573727E-02	.227050E-03
3	21.743	13.737	13.177	5.616	11.503	.431754E-04	.155232E-03	.392253E-02	.382283E-03
5	21.744	13.738	13.339	8.992	10.658	.431586E-04	.155172E-03	.392100E-02	.537455E-03
10	18.611	10.605	11.957	10.211	8.913	.152721E-03	.549090E-03	.138748E-01	.108654E-02
12	22.266	14.260	12.196	11.922	8.642	.349642E-04	.125710E-03	.317654E-02	.121225E-02
18	22.265	14.259	12.390	13.393	8.397	.349779E-04	.125759E-03	.317777E-02	.133801E-02
20	22.266	14.260	12.551	14.678	8.174	.349642E-04	.125710E-03	.317654E-02	.146372E-02
26	22.304	14.297	12.687	15.811	7.973	.344375E-04	.123816E-03	.312869E-02	.158754E-02
32	22.263	14.257	12.802	16.832	7.784	.350051E-04	.125857E-03	.318025E-02	.171340E-02
35	22.274	14.268	12.902	17.754	7.609	.348556E-04	.125319E-03	.316666E-02	.183872E-02
40	21.748	13.742	12.967	18.645	7.408	.430915E-04	.154931E-03	.391491E-02	.199365E-02
46	18.723	10.717	12.498	19.015	6.829	.145979E-03	.524851E-03	.132623E-01	.251850E-02
48	18.363	10.357	12.082	19.416	6.294	.168786E-03	.606853E-03	.153344E-01	.312535E-02

51	.282	-7.725	-7.656	.261	-7.733	.248255	.892574	22.5542	.895699
52	4.436	-3.570	-7.013	3.837	-8.157	.464589E-01	.167038	4.22084	1.06274
53	4.436	-3.570	-6.546	6.619	-8.519	.464589E-01	.167038	4.22084	1.22978
54	.861	-7.146	-6.765	9.660	-9.645	.196554	.706689	17.8571	1.93646
55	2.788	-5.219	-6.543	11.694	-10.029	.903516E-01	.324849	8.20853	2.26131
57	.000	-8.007	-6.992	13.234	-10.937	.278134	1.00000	25.2688	3.26131
68	4.436	-3.570	-6.825	14.208	-11.061	.464589E-01	.167038	4.22084	3.42835
86	4.436	-3.570	-6.674	15.111	-11.179	.464589E-01	.167038	4.22084	3.59539

Parti ti on functi on (absol ute): 3.595388835

Parti ti on functi on (relati ve): 90.85099918

E-Eo (kJ/mol): -6.673622074

S (j /K mol): 15.11087562

(A-Eo) (kJ/mol): -11.17892964

\*\*\* TEMPERATURE: 323.15 K \*\*\*

Mol ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.115753E-03	.261699E+21	.515083E+22	.261699E+21
3	21.743	13.737	13.184	5.638	11.362	.815023E-04	.184263E+21	.362672E+22	.445963E+21
5	21.744	13.738	13.346	9.014	10.433	.814730E-04	.184197E+21	.362542E+22	.630160E+21
10	18.611	10.605	12.019	10.410	8.655	.261447E-03	.591090E+21	.116340E+23	.122125E+22
12	22.266	14.260	12.267	12.150	8.340	.670880E-04	.151675E+21	.298531E+22	.137292E+22
18	22.265	14.259	12.465	13.635	8.059	.671121E-04	.151729E+21	.298638E+22	.152465E+22
20	22.266	14.260	12.627	14.926	7.804	.670880E-04	.151675E+21	.298531E+22	.167633E+22
26	22.304	14.297	12.764	16.060	7.574	.661550E-04	.149566E+21	.294379E+22	.182590E+22
32	22.263	14.257	12.879	17.079	7.360	.671603E-04	.151838E+21	.298853E+22	.197773E+22
35	22.274	14.268	12.977	17.997	7.162	.668955E-04	.151240E+21	.297674E+22	.212897E+22
40	21.748	13.742	13.038	18.874	6.939	.813561E-04	.183933E+21	.362022E+22	.231291E+22
46	18.723	10.717	12.581	19.283	6.350	.250781E-03	.566974E+21	.111593E+23	.287988E+22
48	18.363	10.357	12.173	19.706	5.804	.286724E-03	.648235E+21	.127587E+23	.352812E+22
51	.282	-7.725	-7.596	.452	-7.742	.239867	.542301E+24	.106737E+26	.545829E+24
52	4.436	-3.570	-6.893	4.225	-8.258	.511033E-01	.115536E+24	.227402E+25	.661365E+24
53	4.436	-3.570	-6.399	7.093	-8.691	.511033E-01	.115536E+24	.227402E+25	.776902E+24
54	.861	-7.146	-6.668	9.972	-9.890	.193375	.437190E+24	.860489E+25	.121409E+25
55	2.788	-5.219	-6.451	11.989	-10.325	.943992E-01	.213421E+24	.420061E+25	.142751E+25
57	.000	-8.007	-6.913	13.488	-11.271	.266384	.602251E+24	.118537E+26	.202976E+25
68	4.436	-3.570	-6.733	14.505	-11.420	.511033E-01	.115536E+24	.227402E+25	.214530E+25
86	4.436	-3.570	-6.571	15.442	-11.561	.511033E-01	.115536E+24	.227402E+25	.226084E+25

Parti ti on functi on (absol ute): .2260836864E+25

Parti ti on functi on (relati ve): .4449839417E+26

Mol ecul ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.115753E-03	.434535E-03	.855263E-02	.434535E-03
3	21.743	13.737	13.184	5.638	11.362	.815023E-04	.305958E-03	.602194E-02	.740493E-03
5	21.744	13.738	13.346	9.014	10.433	.814730E-04	.305848E-03	.601978E-02	.104634E-02
10	18.611	10.605	12.019	10.410	8.655	.261447E-03	.981467E-03	.193175E-01	.202781E-02
12	22.266	14.260	12.267	12.150	8.340	.670880E-04	.251847E-03	.495691E-02	.227965E-02
18	22.265	14.259	12.465	13.635	8.059	.671121E-04	.251937E-03	.495869E-02	.253159E-02
20	22.266	14.260	12.627	14.926	7.804	.670880E-04	.251847E-03	.495691E-02	.278344E-02
26	22.304	14.297	12.764	16.060	7.574	.661550E-04	.248344E-03	.488798E-02	.303178E-02
32	22.263	14.257	12.879	17.079	7.360	.671603E-04	.252118E-03	.496226E-02	.328390E-02
35	22.274	14.268	12.977	17.997	7.162	.668955E-04	.251124E-03	.494269E-02	.353502E-02
40	21.748	13.742	13.038	18.874	6.939	.813561E-04	.305409E-03	.601114E-02	.384043E-02
46	18.723	10.717	12.581	19.283	6.350	.250781E-03	.941425E-03	.185294E-01	.478186E-02
48	18.363	10.357	12.173	19.706	5.804	.286724E-03	.107635E-02	.211851E-01	.585821E-02
51	.282	-7.725	-7.596	.452	-7.742	.239867	.900456	17.7230	.906314
52	4.436	-3.570	-6.893	4.225	-8.258	.511033E-01	.191841	3.77586	1.09815
53	4.436	-3.570	-6.399	7.093	-8.691	.511033E-01	.191841	3.77586	1.29000
54	.861	-7.146	-6.668	9.972	-9.890	.193375	.725926	14.2879	2.01592
55	2.788	-5.219	-6.451	11.989	-10.325	.943992E-01	.354372	6.97485	2.37029

57	.000	-8.007	-6.913	13.488	-11.271	.266384	1.00000	19.6823	3.37029
68	4.436	-3.570	-6.733	14.505	-11.420	.511033E-01	.191841	3.77586	3.56213
86	4.436	-3.570	-6.571	15.442	-11.561	.511033E-01	.191841	3.77586	3.75398

Parti ti on functi on (absol ute): 3.753975480  
Parti ti on functi on (relati ve): 73.88674664

E-Eo (kJ/mol): -6.570991645  
S (j /K mol): 15.44151784  
(A-Eo) (kJ/mol): -11.56091813

\*\*\* TEMPERATURE: 348.15 K \*\*\*

Molar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.193965E-03	.456268E+21	.725053E+22	.456268E+21
3	21.743	13.737	13.189	5.655	11.221	.140056E-03	.329456E+21	.523537E+22	.785723E+21
5	21.744	13.738	13.351	9.031	10.207	.140009E-03	.329346E+21	.523362E+22	.111507E+22
10	18.611	10.605	12.072	10.569	8.393	.413205E-03	.971989E+21	.154458E+23	.208706E+22
12	22.266	14.260	12.327	12.330	8.034	.116909E-03	.275006E+21	.437010E+22	.236206E+22
18	22.265	14.259	12.529	13.825	7.715	.116948E-03	.275097E+21	.437156E+22	.263716E+22
20	22.266	14.260	12.692	15.119	7.428	.116909E-03	.275006E+21	.437010E+22	.291217E+22
26	22.304	14.297	12.829	16.253	7.170	.115399E-03	.271454E+21	.431366E+22	.318362E+22
32	22.263	14.257	12.943	17.269	6.930	.117026E-03	.275281E+21	.437448E+22	.345890E+22
35	22.274	14.268	13.040	18.183	6.709	.116597E-03	.274273E+21	.435847E+22	.373318E+22
40	21.748	13.742	13.097	19.049	6.465	.139823E-03	.328907E+21	.522665E+22	.406208E+22
46	18.723	10.717	12.651	19.492	5.865	.397534E-03	.935126E+21	.148600E+23	.499721E+22
48	18.363	10.357	12.250	19.938	5.309	.450160E-03	.105892E+22	.168272E+23	.605613E+22
51	.282	-7.725	-7.506	.721	-7.757	.232282	.546399E+24	.868281E+25	.552456E+24
52	4.436	-3.570	-6.756	4.633	-8.369	.552986E-01	.130080E+24	.206709E+25	.682535E+24
53	4.436	-3.570	-6.246	7.548	-8.874	.552986E-01	.130080E+24	.206709E+25	.812615E+24
54	.861	-7.146	-6.565	10.277	-10.143	.190180	.447362E+24	.710901E+25	.125998E+25
55	2.788	-5.219	-6.358	12.268	-10.629	.977450E-01	.229927E+24	.365376E+25	.148990E+25
57	.000	-8.007	-6.832	13.727	-11.611	.256025	.602251E+24	.957035E+25	.209216E+25
68	4.436	-3.570	-6.641	14.777	-11.786	.552986E-01	.130080E+24	.206709E+25	.222224E+25
86	4.436	-3.570	-6.471	15.738	-11.951	.552986E-01	.130080E+24	.206709E+25	.235231E+25

Parti ti on functi on (absol ute): .2352314624E+25  
Parti ti on functi on (relati ve): .3738052606E+26

Molecul ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.193965E-03	.757603E-03	.120390E-01	.757603E-03
3	21.743	13.737	13.189	5.655	11.221	.140056E-03	.547040E-03	.869299E-02	.130464E-02
5	21.744	13.738	13.351	9.031	10.207	.140009E-03	.546858E-03	.869010E-02	.185150E-02
10	18.611	10.605	12.072	10.569	8.393	.413205E-03	.161393E-02	.256468E-01	.346543E-02
12	22.266	14.260	12.327	12.330	8.034	.116909E-03	.456629E-03	.725628E-02	.392206E-02
18	22.265	14.259	12.529	13.825	7.715	.116948E-03	.456782E-03	.725870E-02	.437884E-02
20	22.266	14.260	12.692	15.119	7.428	.116909E-03	.456629E-03	.725628E-02	.483547E-02
26	22.304	14.297	12.829	16.253	7.170	.115399E-03	.450732E-03	.716257E-02	.528620E-02
32	22.263	14.257	12.943	17.269	6.930	.117026E-03	.457086E-03	.726354E-02	.574329E-02
35	22.274	14.268	13.040	18.183	6.709	.116597E-03	.455414E-03	.723696E-02	.619870E-02
40	21.748	13.742	13.097	19.049	6.465	.139823E-03	.546129E-03	.867852E-02	.674483E-02
46	18.723	10.717	12.651	19.492	5.865	.397534E-03	.155272E-02	.246742E-01	.829755E-02
48	18.363	10.357	12.250	19.938	5.309	.450160E-03	.175827E-02	.279405E-01	.100558E-01
51	.282	-7.725	-7.506	.721	-7.757	.232282	.907262	14.4173	.917317
52	4.436	-3.570	-6.756	4.633	-8.369	.552986E-01	.215989	3.43227	1.13331
53	4.436	-3.570	-6.246	7.548	-8.874	.552986E-01	.215989	3.43227	1.34930
54	.861	-7.146	-6.565	10.277	-10.143	.190180	.742816	11.8041	2.09211
55	2.788	-5.219	-6.358	12.268	-10.629	.977450E-01	.381779	6.06684	2.47389
57	.000	-8.007	-6.832	13.727	-11.611	.256025	1.00000	15.8910	3.47389
68	4.436	-3.570	-6.641	14.777	-11.786	.552986E-01	.215989	3.43227	3.68988
86	4.436	-3.570	-6.471	15.738	-11.951	.552986E-01	.215989	3.43227	3.90587

Parti ti on functi on (absol ute): 3.905868468



Parti ti on functi on (relative): 62.06798043

E-Eo (kJ/mol): -6.471443183  
S (j /K mol): 15.73827625  
(A-Eo) (kJ/mol): -11.95072406

\*\*\* TEMPERATURE: 373.15 K \*\*\*

Molar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.302608E-03	.738394E+21	.974910E+22	.738394E+21
3	21.743	13.737	13.194	5.669	11.079	.223322E-03	.544930E+21	.719477E+22	.128332E+22
5	21.744	13.738	13.356	9.045	9.981	.223253E-03	.544761E+21	.719253E+22	.182808E+22
10	18.611	10.605	12.118	10.697	8.127	.612798E-03	.149529E+22	.197425E+23	.332337E+22
12	22.266	14.260	12.379	12.474	7.724	.188683E-03	.460407E+21	.607880E+22	.378378E+22
18	22.265	14.259	12.583	13.976	7.368	.188742E-03	.460550E+21	.608069E+22	.424433E+22
20	22.266	14.260	12.747	15.272	7.048	.188683E-03	.460407E+21	.607880E+22	.470474E+22
26	22.304	14.297	12.884	16.406	6.762	.186409E-03	.454857E+21	.600552E+22	.515959E+22
32	22.263	14.257	12.996	17.419	6.497	.188859E-03	.460836E+21	.608447E+22	.562043E+22
35	22.274	14.268	13.092	18.329	6.253	.188214E-03	.459263E+21	.606370E+22	.607969E+22
40	21.748	13.742	13.146	19.185	5.987	.222975E-03	.544083E+21	.718359E+22	.662378E+22
46	18.723	10.717	12.711	19.659	5.376	.591086E-03	.144231E+22	.190430E+23	.806609E+22
48	18.363	10.357	12.318	20.125	4.808	.663783E-03	.161970E+22	.213851E+23	.968579E+22
51	.282	-7.725	-7.378	1.075	-7.779	.225390	.549974E+24	.726137E+25	.559660E+24
52	4.436	-3.570	-6.598	5.070	-8.490	.590734E-01	.144145E+24	.190317E+25	.703805E+24
53	4.436	-3.570	-6.083	7.999	-9.068	.590734E-01	.144145E+24	.190317E+25	.847950E+24
54	.861	-7.146	-6.455	10.583	-10.404	.187026	.456362E+24	.602540E+25	.130431E+25
55	2.788	-5.219	-6.259	12.540	-10.939	.100508	.245249E+24	.323805E+25	.154956E+25
57	.000	-8.007	-6.748	13.960	-11.958	.246814	.602251E+24	.795159E+25	.215181E+25
68	4.436	-3.570	-6.549	15.034	-12.159	.590734E-01	.144145E+24	.190317E+25	.229596E+25
86	4.436	-3.570	-6.373	16.012	-12.348	.590734E-01	.144145E+24	.190317E+25	.244010E+25

Parti ti on functi on (absolute): .2440103700E+25

Parti ti on functi on (relative): .3221696415E+26

Molecul ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.302608E-03	.122606E-02	.161878E-01	.122606E-02
3	21.743	13.737	13.194	5.669	11.079	.223322E-03	.904821E-03	.119465E-01	.213088E-02
5	21.744	13.738	13.356	9.045	9.981	.223253E-03	.904540E-03	.119427E-01	.303542E-02
10	18.611	10.605	12.118	10.697	8.127	.612798E-03	.248283E-02	.327811E-01	.551825E-02
12	22.266	14.260	12.379	12.474	7.724	.188683E-03	.764476E-03	.100935E-01	.628273E-02
18	22.265	14.259	12.583	13.976	7.368	.188742E-03	.764714E-03	.100966E-01	.704744E-02
20	22.266	14.260	12.747	15.272	7.048	.188683E-03	.764476E-03	.100935E-01	.781192E-02
26	22.304	14.297	12.884	16.406	6.762	.186409E-03	.755260E-03	.997179E-02	.856718E-02
32	22.263	14.257	12.996	17.419	6.497	.188859E-03	.765189E-03	.101029E-01	.933237E-02
35	22.274	14.268	13.092	18.329	6.253	.188214E-03	.762576E-03	.100684E-01	.100949E-01
40	21.748	13.742	13.146	19.185	5.987	.222975E-03	.903416E-03	.119279E-01	.109984E-01
46	18.723	10.717	12.711	19.659	5.376	.591086E-03	.239487E-02	.316197E-01	.133932E-01
48	18.363	10.357	12.318	20.125	4.808	.663783E-03	.268941E-02	.355085E-01	.160826E-01
51	.282	-7.725	-7.378	1.075	-7.779	.225390	.913197	12.0570	.929279
52	4.436	-3.570	-6.598	5.070	-8.490	.590734E-01	.239344	3.16009	1.16862
53	4.436	-3.570	-6.083	7.999	-9.068	.590734E-01	.239344	3.16009	1.40797
54	.861	-7.146	-6.455	10.583	-10.404	.187026	.757761	10.0048	2.16573
55	2.788	-5.219	-6.259	12.540	-10.939	.100508	.407220	5.37658	2.57295
57	.000	-8.007	-6.748	13.960	-11.958	.246814	1.00000	13.2031	3.57295
68	4.436	-3.570	-6.549	15.034	-12.159	.590734E-01	.239344	3.16009	3.81229
86	4.436	-3.570	-6.373	16.012	-12.348	.590734E-01	.239344	3.16009	4.05164

Parti ti on functi on (absolute): 4.051636632

Parti ti on functi on (relative): 53.49421506

E-Eo (kJ/mol): -6.372886423  
S (j /K mol): 16.01166156

(A-Eo) (kJ/mol):

-12.34763793

\*\*\* TEMPERATURE: 398.15 K \*\*\*

Molar functions:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.445564E-03	.112487E+22	.126302E+23	.112487E+22
3	21.743	13.737	13.199	5.680	10.937	.335156E-03	.846134E+21	.950053E+22	.197100E+22
5	21.744	13.738	13.361	9.056	9.755	.335059E-03	.845888E+21	.949776E+22	.281689E+22
10	18.611	10.605	12.159	10.801	7.858	.863188E-03	.217920E+22	.244684E+23	.499609E+22
12	22.266	14.260	12.424	12.591	7.411	.286183E-03	.722498E+21	.811232E+22	.571859E+22
18	22.265	14.259	12.630	14.098	7.017	.286267E-03	.722708E+21	.811468E+22	.644130E+22
20	22.266	14.260	12.794	15.395	6.665	.286183E-03	.722498E+21	.811232E+22	.716380E+22
26	22.304	14.297	12.931	16.527	6.350	.282949E-03	.714332E+21	.802063E+22	.787813E+22
32	22.263	14.257	13.042	17.538	6.060	.286434E-03	.723130E+21	.811941E+22	.860126E+22
35	22.274	14.268	13.137	18.445	5.793	.285517E-03	.720815E+21	.809343E+22	.932207E+22
40	21.748	13.742	13.187	19.292	5.506	.334668E-03	.844902E+21	.948670E+22	.101670E+23
46	18.723	10.717	12.763	19.793	4.882	.834494E-03	.210676E+22	.236550E+23	.122737E+23
48	18.363	10.357	12.377	20.278	4.303	.930326E-03	.234870E+22	.263715E+23	.146224E+23
51	.282	-7.725	-7.207	1.517	-7.811	.219092	.553119E+24	.621050E+25	.567741E+24
52	4.436	-3.570	-6.416	5.541	-8.623	.624597E-01	.157686E+24	.177052E+25	.725427E+24
53	4.436	-3.570	-5.908	8.453	-9.274	.624597E-01	.157686E+24	.177052E+25	.883112E+24
54	.861	-7.146	-6.335	10.895	-10.673	.183942	.464381E+24	.521414E+25	.134749E+25
55	2.788	-5.219	-6.155	12.812	-11.256	.102781	.259481E+24	.291350E+25	.160697E+25
57	.000	-8.007	-6.659	14.191	-12.309	.238553	.602251E+24	.676217E+25	.220923E+25
68	4.436	-3.570	-6.454	15.281	-12.538	.624597E-01	.157686E+24	.177052E+25	.236691E+25
86	4.436	-3.570	-6.274	16.269	-12.751	.624597E-01	.157686E+24	.177052E+25	.252460E+25

Partiti on functi on (absol ute): .2524596665E+25

Partiti on functi on (relati ve): .2834657635E+26

Molecul ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.445564E-03	.186777E-02	.209717E-01	.186777E-02
3	21.743	13.737	13.199	5.680	10.937	.335156E-03	.140495E-02	.157750E-01	.327273E-02
5	21.744	13.738	13.361	9.056	9.755	.335059E-03	.140454E-02	.157704E-01	.467727E-02
10	18.611	10.605	12.159	10.801	7.858	.863188E-03	.361843E-02	.406283E-01	.829569E-02
12	22.266	14.260	12.424	12.591	7.411	.286183E-03	.119966E-02	.134700E-01	.949536E-02
18	22.265	14.259	12.630	14.098	7.017	.286267E-03	.120001E-02	.134739E-01	.106954E-01
20	22.266	14.260	12.794	15.395	6.665	.286183E-03	.119966E-02	.134700E-01	.118950E-01
26	22.304	14.297	12.931	16.527	6.350	.282949E-03	.118610E-02	.133177E-01	.130811E-01
32	22.263	14.257	13.042	17.538	6.060	.286434E-03	.120071E-02	.134818E-01	.142818E-01
35	22.274	14.268	13.137	18.445	5.793	.285517E-03	.119687E-02	.134386E-01	.154787E-01
40	21.748	13.742	13.187	19.292	5.506	.334668E-03	.140291E-02	.157521E-01	.168816E-01
46	18.723	10.717	12.763	19.793	4.882	.834494E-03	.349814E-02	.392777E-01	.203798E-01
48	18.363	10.357	12.377	20.278	4.303	.930326E-03	.389986E-02	.437883E-01	.242796E-01
51	.282	-7.725	-7.207	1.517	-7.811	.219092	.918418	10.3121	.942698
52	4.436	-3.570	-6.416	5.541	-8.623	.624597E-01	.261827	2.93983	1.20452
53	4.436	-3.570	-5.908	8.453	-9.274	.624597E-01	.261827	2.93983	1.46635
54	.861	-7.146	-6.335	10.895	-10.673	.183942	.771074	8.65775	2.23743
55	2.788	-5.219	-6.155	12.812	-11.256	.102781	.430852	4.83768	2.66828
57	.000	-8.007	-6.659	14.191	-12.309	.238553	1.00000	11.2282	3.66828
68	4.436	-3.570	-6.454	15.281	-12.538	.624597E-01	.261827	2.93983	3.93011
86	4.436	-3.570	-6.274	16.269	-12.751	.624597E-01	.261827	2.93983	4.19193

Partiti on functi on (absol ute): 4.191931813

Partiti on functi on (relati ve): 47.06768288

E-Eo (kJ/mol): -6.273500020

S (j /K mol): 16.26944038

(A-Eo) (kJ/mol): -12.75117771

\*\*\* TEMPERATURE: 423.15 K \*\*\*

## Molar functions:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.625614E-03	.163047E+22	.158697E+23	.163047E+22
3	21.743	13.737	13.203	5.690	10.795	.478575E-03	.124726E+22	.121398E+23	.287774E+22
5	21.744	13.738	13.365	9.065	9.529	.478444E-03	.124692E+22	.121365E+23	.412466E+22
10	18.611	10.605	12.194	10.888	7.587	.116556E-02	.303768E+22	.295663E+23	.716233E+22
12	22.266	14.260	12.464	12.688	7.095	.412477E-03	.107500E+22	.104632E+23	.823733E+22
18	22.265	14.259	12.671	14.198	6.663	.412590E-03	.107529E+22	.104660E+23	.931263E+22
20	22.266	14.260	12.835	15.495	6.279	.412477E-03	.107500E+22	.104632E+23	.103876E+23
26	22.304	14.297	12.971	16.626	5.936	.408089E-03	.106356E+22	.103519E+23	.114512E+23
32	22.263	14.257	13.082	17.634	5.620	.412817E-03	.107588E+22	.104718E+23	.125271E+23
35	22.274	14.268	13.175	18.538	5.331	.411573E-03	.107264E+22	.104402E+23	.135997E+23
40	21.748	13.742	13.223	19.379	5.022	.477919E-03	.124555E+22	.121232E+23	.148453E+23
46	18.723	10.717	12.808	19.903	4.386	.112907E-02	.294257E+22	.286406E+23	.177878E+23
48	18.363	10.357	12.429	20.405	3.794	.125067E-02	.325949E+22	.317253E+23	.210473E+23
51	.282	-7.725	-6.990	2.046	-7.856	.213302	.555907E+24	.541075E+25	.576954E+24
52	4.436	-3.570	-6.209	6.046	-8.767	.654890E-01	.170677E+24	.166124E+25	.747631E+24
53	4.436	-3.570	-5.718	8.915	-9.491	.654890E-01	.170677E+24	.166124E+25	.918309E+24
54	.861	-7.146	-6.203	11.217	-10.949	.180941	.471568E+24	.458987E+25	.138988E+25
55	2.788	-5.219	-6.041	13.088	-11.579	.104641	.272716E+24	.265440E+25	.166259E+25
57	.000	-8.007	-6.564	14.423	-12.667	.231084	.602251E+24	.586183E+25	.226484E+25
68	4.436	-3.570	-6.354	15.523	-12.923	.654890E-01	.170677E+24	.166124E+25	.243552E+25
86	4.436	-3.570	-6.172	16.517	-13.161	.654890E-01	.170677E+24	.166124E+25	.260620E+25

Parti ti on functi on (absol ute): .2606199044E+25

Parti ti on functi on (rel ati ve): .2536665591E+26

## Molecul ar functi ons:

i	de(i) kJ/mol	e(i) kJ/mol	E-Eo kJ/mol	S J/K.mol	A-Eo kJ/mol	n(i)/N	q0(i)	q1(i)	p0(i)
1	20.801	12.794	12.794	.000	12.794	.625614E-03	.270730E-02	.263507E-01	.270730E-02
3	21.743	13.737	13.203	5.690	10.795	.478575E-03	.207100E-02	.201574E-01	.477830E-02
5	21.744	13.738	13.365	9.065	9.529	.478444E-03	.207043E-02	.201519E-01	.684873E-02
10	18.611	10.605	12.194	10.888	7.587	.116556E-02	.504387E-02	.490930E-01	.118926E-01
12	22.266	14.260	12.464	12.688	7.095	.412477E-03	.178497E-02	.173734E-01	.136776E-01
18	22.265	14.259	12.671	14.198	6.663	.412590E-03	.178546E-02	.173782E-01	.154630E-01
20	22.266	14.260	12.835	15.495	6.279	.412477E-03	.178497E-02	.173734E-01	.172480E-01
26	22.304	14.297	12.971	16.626	5.936	.408089E-03	.176598E-02	.171886E-01	.190140E-01
32	22.263	14.257	13.082	17.634	5.620	.412817E-03	.178643E-02	.173877E-01	.208004E-01
35	22.274	14.268	13.175	18.538	5.331	.411573E-03	.178105E-02	.173354E-01	.225815E-01
40	21.748	13.742	13.223	19.379	5.022	.477919E-03	.206816E-02	.201298E-01	.246496E-01
46	18.723	10.717	12.808	19.903	4.386	.112907E-02	.488595E-02	.475559E-01	.295356E-01
48	18.363	10.357	12.429	20.405	3.794	.125067E-02	.541217E-02	.526778E-01	.349477E-01
51	.282	-7.725	-6.990	2.046	-7.856	.213302	.923048	8.98421	.957995
52	4.436	-3.570	-6.209	6.046	-8.767	.654890E-01	.283399	2.75838	1.24139
53	4.436	-3.570	-5.718	8.915	-9.491	.654890E-01	.283399	2.75838	1.52479
54	.861	-7.146	-6.203	11.217	-10.949	.180941	.783009	7.62118	2.30780
55	2.788	-5.219	-6.041	13.088	-11.579	.104641	.452827	4.40746	2.76063
57	.000	-8.007	-6.564	14.423	-12.667	.231084	1.00000	9.73320	3.76063
68	4.436	-3.570	-6.354	15.523	-12.923	.654890E-01	.283399	2.75838	4.04403
86	4.436	-3.570	-6.172	16.517	-13.161	.654890E-01	.283399	2.75838	4.32743

Parti ti on functi on (absol ute): 4.327427362

Parti ti on functi on (rel ati ve): 42.11971496

E-Eo (kJ/mol): -6.171800327

S (j /K mol): 16.51713598

(A-Eo) (kJ/mol): -13.16102642