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CYCLOBIS(PARAQUAT-*p*-PHENYLENE)

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Tue Jan 3 16:49:59 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 112
72 S shells
40 P shells
Number of basis functions: 192
Number of electrons: 192
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-3.5287291	4.3934068	-.8005168
N	2	-3.8140652	3.0556167	-.1674208
C	3	-3.8705833	.4772991	.9114817
C	4	-3.5879944	2.8687354	1.1770335
C	5	-4.1974527	1.9915263	-.9512036
C	6	-4.2363157	.7038361	-.4231073
C	7	-3.6205568	1.5901267	1.7271497
H	8	-3.3680113	3.7541273	1.8049187
H	9	-4.4605022	2.1816760	-2.0100703
H	10	-4.5366252	-.1462516	-1.0636906
H	11	-3.4281693	1.4491909	2.8071074
C	12	-3.6421492	-.8884439	1.4090369
H	13	-4.2166902	4.5535974	-1.6630858
H	14	-3.7625204	5.2078258	-.0759197
C	15	-2.0924733	4.4542324	-1.2365767
N	16	-2.7319823	-3.4138105	2.1894622
H	17	2.5010688	-3.7423525	3.2470515
C	18	-3.7847458	-1.9954245	.5602338
C	19	-3.3211906	-3.2468634	.9571695
H	20	.1462657	-3.8711863	3.9744202
C	21	-3.1691894	-1.1090590	2.7105185
H	22	-4.2482527	-1.8693850	-.4359843
H	23	-3.4055322	-4.1248603	.2874286
C	24	-2.0083690	-4.6963438	2.5110186
H	25	-2.5266043	-5.5519579	2.0187456
C	26	.5783057	4.6005232	-2.0611425
C	27	-1.7342010	4.0725170	-2.5319129
C	28	-1.1169081	4.9616613	-.3747606
C	29	.2113119	5.0344127	-.7848241
C	30	-.4059955	4.1452706	-2.9419737
H	31	-2.5012594	3.7463561	-3.2480971
H	32	-1.3947025	5.3402323	.6188171
H	33	.9601855	5.4692248	-.1082129
H	34	-.1463562	3.8753404	-3.9751294
C	35	2.0086328	4.6967162	-2.5101272
H	36	2.0724864	4.8986505	-3.6047163
H	37	2.5268687	5.5519731	-2.0172356
N	38	2.7320275	3.4138728	-2.1893176
C	39	3.6419718	.8882009	-1.4096209
C	40	3.3236020	3.2470515	-.9581542
C	41	2.7094103	2.3692346	-3.0847777
C	42	3.1665576	1.1085938	-2.7102585
C	43	3.7870431	1.9954245	-.5615860
H	44	3.4099768	4.1252648	-.2889396
H	45	2.3088675	2.5518056	-4.1010336
H	46	3.1355853	.2730370	-3.4341854
H	47	4.2523662	1.8694879	.4338009
C	48	3.8704092	-.4775379	-.9120558
H	49	3.7625648	-5.2079179	.0762060
C	50	3.6196034	-1.5904196	-1.7274153
C	51	4.2369517	-.7039788	.4223248

H	52	4.4617043	-2.1816440	2.0093754
C	53	3.5871670	-2.8689517	-1.1771248
H	54	3.4264662	-1.4495757	-2.8072522
H	55	4.5379392	.1461178	1.0625767
C	56	4.1980863	-1.9915874	.9506299
H	57	3.3666514	-3.7543843	-1.8047598
C	58	3.5287727	-4.3933569	.8006429
N	59	3.8140124	-3.0557022	.1672187
H	60	4.2167788	-4.5533362	1.6632154
C	61	2.0925613	-4.4541179	1.2368559
C	62	-2.7119282	-2.3695681	3.0854267
H	63	-.9596342	-5.4727172	.1104794
H	64	-2.0720033	-4.8976122	3.6057423
C	65	-.5781101	-4.6002473	2.0617969
C	66	1.1172356	-4.9636354	.3760194
C	67	1.7341340	-4.0701909	2.5315078
C	68	.4059955	-4.1428584	2.9417518
C	69	-.2109468	-5.0363049	.7862770
H	70	1.3951624	-5.3438802	-.6168868
H	71	-2.3133565	-2.5522568	4.1024431
H	72	-3.1401627	-.2737809	3.4348511

Point Group = C1 Order = 1 Nsymop = 1
This system has 210 degrees of freedom

Heat of Formation: 1070.937 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	25.97			27.96			30.38		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.062	.089	.217	-.016	-.024	-.058	.002	.004	.008
2	.050	.072	.175	.001	.000	.001	.005	.008	.018
3	.010	.015	.036	.019	.027	.066	.005	.009	.020
4	.067	-.004	.148	.179	.018	-.025	.052	.004	.009
5	.009	.113	.117	-.163	.004	.078	-.042	.013	.032
6	-.008	.088	.053	-.156	.016	.113	-.042	.014	.034
7	.048	-.031	.086	.191	.033	.007	.053	.005	.010
8	.028	-.012	.055	.090	.006	-.023	.026	.000	.000
9	-.001	.050	.038	-.088	-.003	.032	-.023	.005	.012
10	-.010	.036	.005	-.084	.005	.050	-.023	.005	.013
11	.018	-.025	.022	.097	.013	-.005	.027	.001	.001
12	-.010	-.015	-.035	.019	.027	.066	.003	.006	.013
13	.001	.050	.081	-.004	-.020	-.020	.001	-.001	.001
14	.046	.017	.082	-.009	.001	-.027	-.001	.002	.001
15	.030	.043	.105	-.016	-.024	-.058	.002	.004	.010
16	-.050	-.072	-.175	.001	.001	.004	-.005	-.007	-.019
17	-.042	.008	.042	.006	-.075	.005	-.035	.195	-.079
18	-.013	.033	-.096	-.156	.013	.115	-.054	.005	.025
19	-.030	.006	-.159	-.163	-.001	.082	-.058	-.003	.009
20	-.058	-.015	-.011	.006	-.074	.006	-.035	.196	-.079
21	-.027	-.090	-.042	.190	.036	.006	.059	.004	-.007
22	-.001	.026	-.027	-.083	.003	.051	-.028	.003	.013
23	-.010	.013	-.060	-.087	-.004	.033	-.032	-.001	.005
24	-.062	-.089	-.217	-.016	-.023	-.056	-.010	-.014	-.036
25	-.007	-.015	-.094	-.008	.001	-.026	-.008	-.002	-.009
26	-.030	-.044	-.106	-.016	-.023	-.057	.003	.004	.010
27	-.081	.017	.082	.004	-.148	-.016	.017	-.082	.039
28	.112	.026	.023	-.038	.098	-.105	-.013	.089	-.023
29	.081	-.016	-.083	-.038	.098	-.105	-.012	.088	-.023
30	-.111	-.028	-.023	.004	-.148	-.016	.016	-.083	.039
31	-.043	.009	.042	.005	-.071	.004	.008	-.043	.017
32	.058	.013	.012	-.016	.055	-.042	-.007	.044	-.015
33	.042	-.008	-.043	-.016	.056	-.042	-.007	.044	-.015
34	-.058	-.015	-.011	.005	-.071	.004	.008	-.044	.017
35	-.062	-.090	-.218	-.016	-.023	-.057	.002	.003	.008
36	-.040	-.052	-.069	-.005	-.020	-.019	-.001	-.001	.002
37	-.007	-.015	-.094	-.008	.001	-.027	.001	.002	.000
38	-.050	-.072	-.175	.001	.001	.003	.005	.007	.018
39	-.010	-.014	-.035	.019	.028	.066	.006	.008	.020
40	-.031	.006	-.159	-.162	-.001	.081	-.038	-.001	.037

41	-.045	-.115	-.105	.178	.024	-.027	.049	.017	.004
42	-.026	-.090	-.042	.191	.036	.006	.051	.017	.005
43	-.013	.033	-.096	-.156	.014	.115	-.038	.000	.039
44	-.010	.013	-.060	-.087	-.003	.033	-.021	-.002	.014
45	-.016	-.051	-.032	.090	.008	-.023	.024	.007	-.002
46	-.007	-.037	.001	.096	.015	-.006	.025	.007	-.002
47	-.001	.026	-.027	-.083	.004	.051	-.021	-.002	.016
48	.010	.015	.036	.019	.027	.066	.004	.005	.013
49	.046	.017	.081	-.009	.001	-.027	.002	-.002	-.011
50	.049	-.031	.086	.191	.033	.007	.057	.010	-.009
51	-.009	.088	.053	-.157	.017	.113	-.051	-.003	.027
52	-.002	.050	.038	-.088	-.002	.032	-.030	-.005	.007
53	.067	-.004	.148	.179	.018	-.025	.054	.002	-.024
54	.018	-.025	.022	.097	.013	-.005	.029	.005	-.005
55	-.011	.036	.005	-.084	.005	.050	-.026	-.002	.014
56	.008	.113	.117	-.164	.005	.079	-.056	-.008	.012
57	.028	-.012	.055	.090	.006	-.023	.029	.002	-.013
58	.062	.089	.217	-.017	-.024	-.058	-.009	-.015	-.034
59	.050	.072	.175	.000	.001	.002	-.004	-.008	-.018
60	.001	.050	.081	-.004	-.020	-.020	-.007	-.006	-.007
61	.030	.043	.105	-.017	-.023	-.057	-.013	-.020	-.047
62	-.046	-.115	-.105	.178	.024	-.026	.055	-.002	-.023
63	.042	-.007	-.043	-.017	.059	-.043	.032	-.201	.066
64	-.040	-.052	-.069	-.005	-.020	-.019	.003	-.005	-.010
65	-.030	-.043	-.105	-.016	-.023	-.056	-.013	-.019	-.048
66	.111	.027	.023	-.040	.105	-.107	.057	-.400	.104
67	-.081	.016	.082	.005	-.154	-.013	-.077	.370	-.177
68	-.111	-.029	-.023	.005	-.154	-.012	-.073	.370	-.179
69	.081	-.015	-.083	-.039	.105	-.107	.052	-.401	.105
70	.058	.014	.011	-.017	.059	-.043	.032	-.201	.066
71	-.017	-.051	-.032	.090	.008	-.023	.030	-.001	-.012
72	-.007	-.037	.001	.096	.015	-.005	.030	.002	-.003

Dipole moment: X = .001241 Y = -.002526 Z = .000123
Total Dipole: .002817 Debye

Mulliken Population Analysis

Atom	Occupancy	Charge
C 1	4.094357	-.094357
N 2	4.501211	.498789
C 3	3.984612	.015388
C 4	4.143200	-.143200
C 5	4.143185	-.143185
C 6	4.053638	-.053638
C 7	4.053627	-.053627
H 8	.811286	.188714
H 9	.811287	.188713
H 10	.838537	.161463
H 11	.838538	.161462
C 12	3.985420	.014580
H 13	.866082	.133918
H 14	.866057	.133943
C 15	4.139444	-.139444
N 16	4.500146	.499854
H 17	.869325	.130675
C 18	4.052915	-.052915
C 19	4.144003	-.144003
H 20	.869373	.130627
C 21	4.052858	-.052858
H 22	.838600	.161400
H 23	.811179	.188821
C 24	4.094900	-.094900
H 25	.865983	.134017
C 26	4.139054	-.139054
C 27	4.058082	-.058082
C 28	4.057990	-.057990
C 29	4.058408	-.058408
C 30	4.058447	-.058447
H 31	.869325	.130675

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   H 32      .869345      .130655
   H 33      .869247      .130753
   H 34      .869296      .130704
   C 35     4.094666     -.094666
   H 36      .865976      .134024
   H 37      .866050      .133950
   N 38     4.500863      .499137
   C 39     3.984758      .015242
   C 40     4.143383     -.143383
   C 41     4.143384     -.143384
   C 42     4.053591     -.053591
   C 43     4.053420     -.053420
   H 44      .811198      .188802
   H 45      .811323      .188677
   H 46      .838559      .161441
   H 47      .838520      .161480
   C 48     3.985186      .014814
   H 49      .866003      .133997
   C 50     4.053166     -.053166
   C 51     4.053119     -.053119
   H 52      .811200      .188800
   C 53     4.143721     -.143721
   H 54      .838570      .161430
   H 55      .838579      .161421
   C 56     4.143722     -.143722
   H 57      .811222      .188778
   C 58     4.094760     -.094760
   N 59     4.500522      .499478
   H 60      .865988      .134012
   C 61     4.139087     -.139087
   C 62     4.144076     -.144076
   H 63      .869257      .130743
   H 64      .865957      .134043
   C 65     4.139249     -.139249
   C 66     4.058236     -.058236
   C 67     4.058478     -.058478
   C 68     4.058213     -.058213
   C 69     4.058040     -.058040
   H 70      .869228      .130772
   H 71      .811165      .188835
   H 72      .838610      .161390

Total Charge =  4.000000

Molecule is non-linear

Zero-point vibrational energy is   366.927 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:         384.634 kcal/mol

Translational Entropy:         44.634  cal/mol.K
Rotational Entropy:            38.318  cal/mol.K
Vibrational Entropy:          118.668  cal/mol.K
```

BENZENE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Calculation started: Mon Jan  2 19:59:02 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells:  18
    12 S shells
     6 P shells
```

Number of basis functions: 30
Number of electrons: 30
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	.0000000	.0000000	-2.4860000
C	2	.0000000	.0000000	-1.3910000
C	3	.0000000	.0000000	1.3910000
C	4	1.2050000	.0000000	-.6960000
C	5	-1.2050000	.0000000	-.6960000
C	6	-1.2050000	.0000000	.6960000
C	7	1.2050000	.0000000	.6960000
H	8	2.1530000	.0000000	-1.2430000
H	9	-2.1530000	.0000000	-1.2430000
H	10	-2.1530000	.0000000	1.2430000
H	11	2.1530000	.0000000	1.2430000
H	12	.0000000	.0000000	2.4860000

Point Group = DNH Order = 2 Nsymop = 8
This system has 6 degrees of freedom

Heat of Formation: 23.455 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	355.74 B3u			356.44 Au			619.43 B1g		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.358	.000	.000	.000	.000	.000	.297	.000
2	.000	.452	.000	.000	.000	.000	.000	.279	.001
3	.000	.452	.000	.000	.000	.000	.000	-.279	-.001
4	.000	-.226	.000	.000	.391	.000	.000	-.276	.000
5	.000	-.226	.000	.000	-.391	.000	.000	-.276	.000
6	.000	-.226	.000	.000	.391	.000	.000	.276	.000
7	.000	-.226	.000	.000	-.391	.000	.000	.276	.000
8	.000	-.180	.000	.000	.311	.000	.000	-.301	.000
9	.000	-.180	.000	.000	-.311	.000	.000	-.301	.000
10	.000	-.180	.000	.000	.311	.000	.000	.301	.000
11	.000	-.180	.000	.000	-.311	.000	.000	.301	.000
12	.000	.358	.000	.000	.000	.000	.000	-.297	.000

Dipole moment: X = .000000 Y = .000000 Z = .000000
Total Dipole: .000000 Debye

Mulliken Population Analysis

Atom		Occupancy	Charge
H	1	.897904	.102096
C	2	4.102224	-.102224
C	3	4.102224	-.102224
C	4	4.102161	-.102161
C	5	4.102161	-.102161
C	6	4.102161	-.102161
C	7	4.102161	-.102161
H	8	.897776	.102224
H	9	.897776	.102224
H	10	.897776	.102224
H	11	.897776	.102224
H	12	.897904	.102096

Total Charge = .000000

Zero-point vibrational energy is 61.967 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

```
Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:          63.046 kcal/mol

Translational Entropy:         38.979  cal/mol.K
Rotational Entropy:            22.890  cal/mol.K
Vibrational Entropy:            4.977  cal/mol.K
```

TOLUENE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Calculation started: Thu Aug  3 10:02:18 1995
Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  22
  15 S shells
   7 P shells
Number of basis functions:  36
Number of electrons:  36
Use of molecular symmetry enabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	-.0130974	.0000000	-2.9806144
C	2	-.0070018	.0000000	-1.8860269
C	3	.0075758	.0000000	.9043222
C	4	-.0025873	-1.2037355	-1.1891666
C	5	-.0025873	1.2037355	-1.1891666
C	6	.0051432	1.2056960	.2008327
C	7	.0051432	-1.2056960	.2008327
H	8	-.0046581	-2.1523032	-1.7357572
H	9	-.0046581	2.1523032	-1.7357572
H	10	.0105679	2.1553365	.7473449
H	11	.0105679	-2.1553365	.7473449
C	12	-.0004788	.0000000	2.3898558
H	13	-1.0324965	.0000000	2.7667362
H	14	.5012661	.8860238	2.8009014
H	15	.5012661	-.8860238	2.8009014

```
Point Group = CS  Order =  1 Nsymop =  2
This system has  22 degrees of freedom

Heat of Formation:       14.090 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)
```

	38.20 A"			191.01 A'			356.41 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.006	.000	.280	.000	-.002	.000	.011	.000
2	.000	.007	.000	.414	.000	-.005	.000	.015	.000
3	.000	-.031	.000	-.261	.000	.000	.000	-.042	.000
4	.083	.002	-.016	.014	.000	-.002	-.391	.004	-.019
5	-.083	.002	.016	.014	.000	-.002	.391	.004	.019
6	-.082	-.018	.011	-.380	-.001	.000	-.389	-.031	.017
7	.082	-.018	-.011	-.380	.001	.000	.389	-.031	-.017
8	.043	.002	-.008	.024	.000	-.001	-.308	.005	-.011
9	-.043	.002	.008	.024	.000	-.001	.308	.005	.011
10	-.041	-.010	.011	-.179	.000	.000	-.307	-.012	.013
11	.041	-.010	-.011	-.179	.000	.000	.307	-.012	-.013
12	.000	.034	.000	.426	.000	.006	.000	.059	.000
13	.000	.592	.000	.184	.000	.165	.000	.025	.000

```
  14    .490  -.255  -.027     .190  -.001  -.077    -.004   .030  -.023
  15   -.490  -.255   .027     .190   .001  -.077     .004   .030   .023

Dipole moment:  X =   -.037826  Y =    .000000  Z =    .261281
Total Dipole:    .264005 Debye
Zero-point vibrational energy is    79.511 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:          81.694 kcal/mol

Translational Entropy:         39.471  cal/mol.K
Rotational Entropy:            26.952  cal/mol.K
Vibrational Entropy:           13.483  cal/mol.K
```

PHENOL

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Calculation started: Thu Aug  3 10:51:47 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells:  20
    13 S shells
    7 P shells
Number of basis functions:  34
Number of electrons:  36
Use of molecular symmetry enabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	.0321877	.0000000	2.9350776
C	2	.0201197	.0000000	1.8406648
C	3	-.0143424	.0000000	-.9335606
C	4	-1.1946088	.0000000	1.1600287
C	5	1.2166610	.0000000	1.1326758
C	6	1.2126494	.0000000	-.2571126
C	7	-1.2258951	.0000000	-.2278998
H	8	-2.1343304	.0000000	1.7221341
H	9	2.1702423	.0000000	1.6707671
H	10	2.1595073	.0000000	-.8087201
H	11	-2.1803155	.0000000	-.7658745
O	12	-.1127616	.0000000	-2.2985325
H	13	.7672987	.0000000	-2.6539021

```
Point Group = CS  Order =  1 Nsymop =  2
This system has  23 degrees of freedom

Heat of Formation:      -21.672 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)
```

	204.14 A"			285.35 A"			360.83 A"		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	-.287	.000	.000	.061	.000	.000	.011	.000
2	.000	-.416	.000	.000	.086	.000	.000	.011	.000
3	.000	.217	.000	.000	.039	.000	.000	.014	.000
4	.000	.019	.000	.000	.059	.000	.000	-.396	.000
5	.000	.001	.000	.000	-.097	.000	.000	.382	.000
6	.000	.391	.000	.000	-.052	.000	.000	-.397	.000
7	.000	.407	.000	.000	-.049	.000	.000	.394	.000

8	.000	-.005	.000	.000	.038	.000	.000	-.313	.000
9	.000	-.015	.000	.000	-.069	.000	.000	.302	.000
10	.000	.195	.000	.000	-.022	.000	.000	-.311	.000
11	.000	.192	.000	.000	-.049	.000	.000	.297	.000
12	.000	-.551	.000	.000	-.217	.000	.000	-.028	.000
13	.000	-.024	.000	.000	.956	.000	.000	.095	.000

Dipole moment: X = 1.126461 Y = .000000 Z = .185179
Total Dipole: 1.141580 Debye
Zero-point vibrational energy is 65.433 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 67.233 kcal/mol

Translational Entropy: 39.535 cal/mol.K
Rotational Entropy: 26.895 cal/mol.K
Vibrational Entropy: 8.993 cal/mol.K

ANISOLE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Fri Aug 4 10:05:39 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 24
16 S shells
8 P shells
Number of basis functions: 40
Number of electrons: 42
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	.5433721	.0000000	3.3422183
C	2	.3186072	.0000000	2.2711449
C	3	-.2522084	.0000000	-.4486255
C	4	-1.0054683	.0000000	1.8382981
C	5	1.3520527	.0000000	1.3431899
C	6	1.0790923	.0000000	-.0212554
C	7	-1.3029053	.0000000	.4835203
H	8	-1.8185333	.0000000	2.5716496
H	9	2.3925329	.0000000	1.6842535
H	10	1.9091710	.0000000	-.7361727
H	11	-2.3449856	.0000000	.1442685
O	12	-.6712419	.0000000	-1.7647268
C	13	.3206172	.0000000	-2.7607437
H	14	.9509784	-.8959521	-2.7210906
H	15	.9509784	.8959521	-2.7210906
H	16	-.2723035	.0000000	-3.6793929

Point Group = CS Order = 1 Nsymop = 2
This system has 28 degrees of freedom

Heat of Formation: -14.553 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

55.96			170.44			223.64		
A"			A"			A"		
X	Y	Z	X	Y	Z	X	Y	Z

1	.000	-.094	.000	.000	-.195	.000	.000	-.218	.000
2	.000	-.170	.000	.000	-.303	.000	.000	-.303	.000
3	.000	.197	.000	.000	.184	.000	.000	.149	.000
4	.000	-.225	.000	.000	.019	.000	.000	-.008	.000
5	.000	.088	.000	.000	-.077	.000	.000	.072	.000
6	.000	.274	.000	.000	.232	.000	.000	.314	.000
7	.000	-.042	.000	.000	.291	.000	.000	.306	.000
8	.000	-.122	.000	.000	.004	.000	.000	-.020	.000
9	.000	.043	.000	.000	-.050	.000	.000	.028	.000
10	.000	.139	.000	.000	.130	.000	.000	.138	.000
11	.000	-.023	.000	.000	.140	.000	.000	.149	.000
12	.000	.523	.000	.000	-.249	.000	.000	-.458	.000
13	.000	-.520	.000	.000	-.056	.000	.000	-.036	.000
14	-.137	-.242	.111	.308	.209	.223	-.204	-.163	-.235
15	.137	-.242	-.111	-.308	.209	-.223	.204	-.163	.235
16	.000	-.170	.000	.000	-.458	.000	.000	.375	.000

Dipole moment: X = 1.018347 Y = .000000 Z = -.372999
Total Dipole: 1.084508 Debye
Zero-point vibrational energy is 82.069 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 84.793 kcal/mol

Translational Entropy: 39.949 cal/mol.K
Rotational Entropy: 27.920 cal/mol.K
Vibrational Entropy: 16.027 cal/mol.K

ANILINE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Aug 3 12:16:45 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 21
14 S shells
7 P shells
Number of basis functions: 35
Number of electrons: 36
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	-.0551138	-.3581809	-2.9381162
C	2	-.0346788	-.2272094	-1.8518120
C	3	.0172639	.1092967	.9164363
C	4	-1.2250093	-.1634853	-1.1349502
C	5	1.1816032	-.1246198	-1.1848360
C	6	1.2165879	.0414596	.1933728
C	7	-1.2082030	.0022181	.2436055
H	8	-2.1826507	-.2442343	-1.6596279
H	9	2.1188195	-.1748149	-1.7487570
H	10	2.1829656	.1213281	.7049025
H	11	-2.1546128	.0511190	.7948100
N	12	.0416898	.3863826	2.3190602
H	13	.8773614	.0507454	2.7442208
H	14	-.7639815	.0234000	2.7782478

Point Group = C1 Order = 1 Nsymop = 1
This system has 36 degrees of freedom

Heat of Formation: 21.295 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	196.20 A			230.26 A			357.99 A		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.005	.285	-.032	-.003	.000	.000	.004	.000	.000
2	-.008	.420	-.043	.002	.000	.000	.008	.000	.000
3	.004	-.223	.031	.022	.000	.000	-.016	.000	.000
4	.000	-.001	.006	.002	.086	.002	.008	-.388	.039
5	.001	-.001	.006	.005	-.086	-.002	-.006	.388	-.039
6	.009	-.391	.053	.013	-.035	-.003	-.007	-.391	.055
7	.006	-.391	.053	.012	.036	.003	-.022	.390	-.054
8	.000	.013	.000	-.001	.054	-.002	.008	-.305	.031
9	.000	.013	.000	.001	-.054	.002	-.003	.305	-.031
10	.004	-.195	.025	.008	-.010	-.009	.001	-.306	.040
11	.003	-.195	.025	.008	.010	.009	-.010	.306	-.040
12	-.010	.459	-.115	-.195	-.003	.004	.017	.000	.000
13	-.002	.194	.023	.246	.633	-.083	.029	.043	-.014
14	-.003	.194	.024	.270	-.625	.072	.031	-.042	.013

Dipole moment: X = .031648 Y = -1.138588 Z = .620028
Total Dipole: 1.296849 Debye

Molecule is non-linear

Zero-point vibrational energy is 73.032 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy:	.889	kcal/mol
Rotational Enthalpy:	.889	kcal/mol
Vibrational Enthalpy:	74.938	kcal/mol
Translational Entropy:	39.503	cal/mol.K
Rotational Entropy:	26.927	cal/mol.K
Vibrational Entropy:	9.673	cal/mol.K

t-BUTYLBENZENE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Mon Jan 2 20:09:36 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 34
24 S shells
10 P shells
Number of basis functions: 54
Number of electrons: 54
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-.0349865	.0000135	-1.4440135
C	2	-.0319865	.0000135	.0729865
C	3	.0550135	.0000135	2.8699865
C	4	-.0039865	-1.2019865	.7829865
C	5	-.0029865	1.2020135	.7829865
C	6	.0370135	1.2030135	2.1719865
C	7	.0370135	-1.2019865	2.1719865
H	8	-.0149865	-2.1509865	.2259865

H	9	-.0139865	2.1510135	.2249865
H	10	.0560135	2.1530135	2.7149865
H	11	.0550135	-2.1519865	2.7159865
H	12	.0860135	.0000135	3.9639865
C	13	1.4240135	.0000135	-1.9100135
C	14	-.7419865	1.2390135	-1.9950135
C	15	-.7409865	-1.2399865	-1.9940135
H	16	-.3279865	2.1620135	-1.5560135
H	17	-1.8159865	1.2230135	-1.7660135
H	18	-.6339865	1.3050135	-3.0850135
H	19	-.3259865	-2.1619865	-1.5570135
H	20	-.6339865	-1.3059865	-3.0850135
H	21	-1.8149865	-1.2259865	-1.7650135
H	22	1.9580135	-.8849865	-1.5420135
H	23	1.9570135	.8870135	-1.5430135
H	24	1.4930135	.0000135	-3.0060135

Point Group = C1 Order = 1 Nsymop = 1
This system has 66 degrees of freedom

Heat of Formation: .321 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	41.10			124.42			170.21		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.021	.000	-.093	.000	.004	.000	.041	.000
2	.001	.047	.000	-.332	.000	.004	.001	.071	.000
3	-.002	-.030	.000	.425	-.001	-.020	-.002	-.072	.000
4	.322	.027	-.038	-.271	-.001	.000	-.028	.034	-.051
5	-.319	.028	.038	-.274	.001	.000	.030	.034	.050
6	-.331	-.013	.041	.132	.000	-.012	.051	-.040	.054
7	.330	-.013	-.041	.134	-.001	-.013	-.053	-.041	-.055
8	.158	.015	-.024	-.128	.000	.001	-.005	.017	-.027
9	-.157	.015	.024	-.130	.001	.001	.006	.016	.026
10	-.172	-.008	.021	.075	.000	-.004	.029	-.020	.029
11	.172	-.008	-.021	.076	.000	-.005	-.029	-.020	-.030
12	-.001	-.017	.000	.246	.000	-.009	-.001	-.036	.000
13	.000	-.326	-.001	.045	-.001	.404	.000	.013	-.001
14	.275	.140	-.081	.062	-.001	-.187	.012	-.010	-.121
15	-.276	.140	.082	.060	.002	-.185	-.012	-.010	.124
16	.115	.022	-.019	-.032	-.001	-.006	-.114	.003	.066
17	.073	.098	-.051	-.005	-.010	-.161	-.029	-.077	-.192
18	.110	.029	-.021	.126	.011	-.043	.159	.056	-.016
19	-.116	.022	.019	-.033	.001	-.005	.120	.003	-.070
20	-.111	.029	.021	.124	-.011	-.043	-.165	.059	.017
21	-.073	.098	.051	-.005	.011	-.160	.030	-.081	.199
22	-.054	-.117	.025	-.017	.001	.165	.129	.252	.410
23	.054	-.117	-.026	-.018	.001	.159	-.129	.251	-.410
24	.000	-.131	.000	.104	-.004	.123	.000	-.492	.000

Dipole moment: X = .039200 Y = .000586 Z = -.294534
Total Dipole: .297132 Debye

Mulliken Population Analysis

Atom	Occupancy	Charge
C 1	3.995008	.004992
C 2	4.067930	-.067930
C 3	4.106746	-.106746
C 4	4.109592	-.109592
C 5	4.109763	-.109763
C 6	4.098223	-.098223
C 7	4.098335	-.098335
H 8	.886670	.113330
H 9	.886720	.113280
H 10	.898371	.101629
H 11	.898462	.101538
H 12	.897788	.102212

C 13	4.112269	-.112269
C 14	4.118774	-.118774
C 15	4.118822	-.118822
H 16	.953529	.046471
H 17	.954259	.045741
H 18	.955522	.044478
H 19	.953574	.046426
H 20	.955669	.044331
H 21	.954277	.045723
H 22	.955637	.044363
H 23	.955776	.044224
H 24	.958285	.041715

Total Charge = .000000

Molecule is non-linear

Zero-point vibrational energy is 133.208 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy:	.889	kcal/mol
Rotational Enthalpy:	.889	kcal/mol
Vibrational Enthalpy:	137.594	kcal/mol
Translational Entropy:	40.593	cal/mol.K
Rotational Entropy:	29.433	cal/mol.K
Vibrational Entropy:	25.773	cal/mol.K

THIOPHENOL

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Aug 3 14:12:18 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 20
13 S shells
7 P shells
Number of basis functions: 34
Number of electrons: 36
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
H 1	-.0196072	.0000000	3.3746092
C 2	-.0096277	.0000000	2.2799059
C 3	.0156892	.0000000	-.5120272
C 4	-1.2072686	.0000000	1.5711529
C 5	1.1993266	.0000000	1.5932986
C 6	1.2144090	.0000000	.2032068
C 7	-1.1978340	.0000000	.1823042
H 8	-2.1616262	.0000000	2.1081779
H 9	2.1442702	.0000000	2.1465427
H 10	2.1748093	.0000000	-.3254619
H 11	-2.1425314	.0000000	-.3756612
S 12	-.0798884	.0000000	-2.2665669
H 13	1.1947316	.0000000	-2.5701839

Point Group = CS Order = 1 Nsymop = 2
This system has 23 degrees of freedom

Heat of Formation: 27.670 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	154.09 A"			183.85 A"			262.26 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.236	.000	.000	-.165	.000	-.109	.000	-.012
2	.000	.362	.000	.000	-.247	.000	-.148	.000	-.038
3	.000	-.334	.000	.000	.163	.000	.425	.000	.003
4	.000	.007	.000	.000	-.058	.000	-.023	.000	-.259
5	.000	.075	.000	.000	.027	.000	-.013	.000	.204
6	.000	-.311	.000	.000	.264	.000	.310	.000	.181
7	.000	-.390	.000	.000	.172	.000	.293	.000	-.227
8	.000	.022	.000	.000	-.042	.000	-.040	.000	-.135
9	.000	.059	.000	.000	.008	.000	-.040	.000	.122
10	.000	-.142	.000	.000	.135	.000	.115	.000	.101
11	.000	-.186	.000	.000	.073	.000	.122	.000	-.133
12	.000	.442	.000	.000	-.044	.000	-.501	.000	.124
13	.000	-.440	.000	.000	-.869	.000	-.141	.000	-.169

Dipole moment: X = 1.156162 Y = .000000 Z = 1.075477
Total Dipole: 1.579038 Debye
Zero-point vibrational energy is 60.344 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 62.539 kcal/mol

Translational Entropy: 40.002 cal/mol.K
Rotational Entropy: 27.767 cal/mol.K
Vibrational Entropy: 11.763 cal/mol.K

THIOANISOLE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b

Calculation started: Fri Feb 23 09:02:20 1996
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 24
16 S shells
8 P shells
Number of basis functions: 40
Number of electrons: 42
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
S	1	-.3530396	-.1056825	-1.8475573
C	2	.0285858	.1300529	-.1449602
C	3	.7066313	.7194103	2.5011789
C	4	-.1658299	-.8167065	.8603769
C	5	.5670338	1.3785702	.1869435
C	6	.9029410	1.6688573	1.5020766
C	7	.1723486	-.5215386	2.1768652
H	8	-.5865722	-1.8011460	.6222465
H	9	.7227766	2.1283297	-.5989377
H	10	1.3236576	2.6482626	1.7527582
H	11	.0154843	-1.2723450	2.9583012
H	12	.9722717	.9501557	3.5377556
C	13	-1.0069067	-1.7789734	-1.9773898
H	14	-.2911364	-2.5511511	-1.6731391
H	15	-1.2446900	-1.9410809	-3.0364436

```
    H  16    -1.9260324    -1.9333489    -1.4007002

Point Group = C1  Order =  1 Nsymop =  1
This system has  42 degrees of freedom

Heat of Formation:       23.243 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)
```

	36.54			145.70			174.49		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	.432	-.164	-.074	.209	-.079	-.037	-.287	.109	.052
2	.095	-.037	-.016	-.232	.090	.039	.259	-.102	-.042
3	-.096	.037	.017	.287	-.112	-.049	-.288	.114	.049
4	.256	-.099	-.043	-.215	.083	.035	.309	-.120	-.049
5	-.162	.063	.028	-.274	.107	.047	.277	-.109	-.048
6	-.251	.097	.043	.007	-.003	-.001	-.052	.021	.007
7	.157	-.061	-.027	.088	-.035	-.016	.024	-.007	-.001
8	.135	-.052	-.023	-.113	.044	.019	.133	-.052	-.022
9	-.086	.033	.015	-.131	.051	.023	.129	-.051	-.023
10	-.130	.050	.022	.012	-.005	-.002	-.046	.018	.007
11	.082	-.032	-.014	.056	-.022	-.010	-.003	.002	.002
12	-.050	.019	.009	.180	-.070	-.031	-.195	.077	.033
13	-.517	.195	.087	-.004	.000	.006	-.063	.025	.003
14	-.233	-.037	-.015	-.169	.000	.397	-.142	.028	.347
15	-.230	.087	.038	.399	-.153	-.065	.345	-.128	-.060
16	-.137	.177	.077	-.232	.153	-.326	-.219	.108	-.293

```
Molecule is non-linear

Zero-point vibrational energy is    79.942 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:          83.115 kcal/mol

Translational Entropy:         40.360  cal/mol.K
Rotational Entropy:            28.650  cal/mol.K
Vibrational Entropy:           19.677  cal/mol.K
```

p-XYLENE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Calculation started: Mon Jan  2 20:12:14 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells:  26
    18 S shells
     8 P shells
Number of basis functions:  42
Number of electrons:  42
Use of molecular symmetry enabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	.0090690	2.1550000	-1.2399310
H	2	.4850690	-.8860000	-3.2979310
H	3	.4920690	.8860000	3.2980690
C	4	-.0139310	.0000000	-2.8839310

C	5	.0060690	.0000000	1.3990690
H	6	.0090690	-2.1550000	-1.2399310
H	7	.4850690	.8860000	-3.2979310
H	8	-1.0479310	.0000000	-3.2549310
H	9	.4920690	-.8860000	3.2980690
C	10	-.0079310	.0000000	2.8850690
C	11	.0030690	.0000000	-1.3989310
C	12	.0080690	-1.2050000	.6940690
C	13	.0080690	1.2050000	.6940690
C	14	.0060690	1.2050000	-.6949310
C	15	.0060690	-1.2050000	-.6949310
H	16	.0120690	-2.1550000	1.2400690
H	17	.0120690	2.1550000	1.2400690
H	18	-1.0419310	.0000000	3.2570690

Point Group = CS Order = 1 Nsymop = 2
This system has 27 degrees of freedom

Heat of Formation: 4.740 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	21.30 A"			45.47 A"			123.38 A'		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.040	.010	.009	-.044	.000	.006	-.090	.000	.000
2	.490	.253	.024	-.003	.005	-.004	.187	.000	.056
3	.021	-.018	.003	.490	-.253	-.025	.186	.000	-.056
4	.000	-.039	.000	.000	.017	.000	.475	.000	-.008
5	.000	.000	.000	.000	-.031	.000	-.071	.000	.001
6	-.040	.010	-.009	.044	.000	-.006	-.090	.000	.000
7	-.490	.253	-.024	.003	.005	.004	.187	.000	.056
8	.000	-.594	.000	.000	.011	.000	.182	.000	-.123
9	-.021	-.018	-.003	-.490	-.253	.025	.186	.000	-.056
10	.000	-.015	.000	.000	.040	.000	.473	.000	.007
11	.000	.031	.000	.000	-.002	.000	-.073	.000	-.001
12	-.080	.003	-.012	.082	-.020	-.007	-.255	.000	.000
13	.080	.003	.012	-.082	-.020	.007	-.255	.000	.000
14	.078	.020	.008	-.085	-.004	.012	-.256	.000	.000
15	-.078	.020	-.008	.085	-.004	-.012	-.256	.000	.000
16	-.042	.000	-.006	.041	-.010	-.009	-.089	.000	.000
17	.042	.000	.006	-.041	-.010	.009	-.089	.000	.000
18	.000	.020	.000	.000	.593	.000	.181	.000	.122

Dipole moment: X = -.075464 Y = .000000 Z = .001483
Total Dipole: .075478 Debye

Mulliken Population Analysis

Atom	Occupancy	Charge
H 1	.895523	.104477
H 2	.956002	.043998
H 3	.956011	.043989
C 4	4.063537	-.063537
C 5	4.081095	-.081095
H 6	.895523	.104477
H 7	.956002	.043998
H 8	.953335	.046665
H 9	.956011	.043989
C 10	4.063209	-.063209
C 11	4.080788	-.080788
C 12	4.099647	-.099647
C 13	4.099647	-.099647
C 14	4.099555	-.099555
C 15	4.099555	-.099555
H 16	.895610	.104390
H 17	.895610	.104390
H 18	.953342	.046658

Total Charge = .000000

Zero-point vibrational energy is 97.012 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy:	.889	kcal/mol
Rotational Enthalpy:	.889	kcal/mol
Vibrational Enthalpy:	100.338	kcal/mol
Translational Entropy:	39.894	cal/mol.K
Rotational Entropy:	27.955	cal/mol.K
Vibrational Entropy:	23.181	cal/mol.K

1,4-DICHLOROBENZENE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Mon Jan 2 19:56:23 1995
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 20
12 S shells
8 P shells
Number of basis functions: 36
Number of electrons: 42
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
Cl	1	.0000000	.0000000	3.0650000
C	2	.0000000	.0000000	1.3800000
C	3	.0000000	.0000000	-1.3800000
C	4	-1.2130000	.0000000	.6950000
C	5	1.2130000	.0000000	.6950000
C	6	1.2130000	.0000000	-.6950000
C	7	-1.2130000	.0000000	-.6950000
H	8	-2.1570000	.0000000	1.2520000
H	9	2.1570000	.0000000	1.2520000
H	10	2.1570000	.0000000	-1.2520000
H	11	-2.1570000	.0000000	-1.2520000
Cl	12	.0000000	.0000000	-3.0650000

Point Group = DNH Order = 2 Nsymop = 8
This system has 6 degrees of freedom

Heat of Formation: 10.112 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	93.71			216.95			279.91		
	B3u			B2u			B2g		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.505	.000	-.510	.000	.000	.000	-.224	.000
2	.000	-.185	.000	.270	.000	.000	.000	.454	.000
3	.000	-.185	.000	.270	.000	.000	.000	-.454	.000
4	.000	-.310	.000	.277	.000	-.017	.000	.309	.000
5	.000	-.310	.000	.277	.000	.017	.000	.309	.000
6	.000	-.310	.000	.277	.000	-.017	.000	-.309	.000
7	.000	-.310	.000	.277	.000	.017	.000	-.309	.000
8	.000	-.097	.000	.080	.000	-.004	.000	.161	.000
9	.000	-.097	.000	.080	.000	.004	.000	.161	.000
10	.000	-.097	.000	.080	.000	-.004	.000	-.161	.000
11	.000	-.097	.000	.080	.000	.004	.000	-.161	.000
12	.000	.505	.000	-.510	.000	.000	.000	.224	.000

```
Dipole moment:  X =     .000000  Y =     .000000  Z =     .000000
Total Dipole:     .000000 Debye

Mulliken Population Analysis

     Atom     Occupancy      Charge
     ----    -----------  -----------

     Cl 1      6.928469      .071531
     C  2      4.128608     -.128608
     C  3      4.128608     -.128608
     C  4      4.090755     -.090755
     C  5      4.090755     -.090755
     C  6      4.090755     -.090755
     C  7      4.090755     -.090755
     H  8       .880707      .119293
     H  9       .880707      .119293
     H 10       .880707      .119293
     H 11       .880707      .119293
     Cl12      6.928469      .071531

Total Charge =    .000000

Zero-point vibrational energy is     50.562 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:          53.065 kcal/mol

Translational Entropy:         40.845  cal/mol.K
Rotational Entropy:            26.528  cal/mol.K
Vibrational Entropy:           13.862  cal/mol.K
```

HYDROQUINONE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 4.0.2b

Calculation started: Fri Feb 23 10:15:49 1996
Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  22
  14 S shells
   8 P shells
Number of basis functions:  38
Number of electrons:  42
Use of molecular symmetry disabled
Molecular charge:   0
Spin multiplicity:  1

                Cartesian Coordinates (Angstroms)
     Atom          X             Y             Z
     ----    ------------- ------------- -------------

     O   1      -.0039723     -.0428728    -2.7469992
     C   2      -.0060535      .0192020    -1.3772501
     C   3       .0027133     -.0209751     1.3893815
     C   4       .0857382    -1.2077371     -.7071289
     C   5      -.0933861     1.2249569     -.6682409
     C   6      -.0891004     1.2059796      .7192507
     C   7       .0900412    -1.2267138      .6803827
     H   8       .1535225    -2.1438054    -1.2728373
     H   9      -.1650673     2.1826718    -1.1967061
     H  10      -.1568966     2.1420316     1.2849838
     H  11       .1616327    -2.1844294     1.2088543
     O  12       .0012416      .0411792     2.7591258
```

```
    H  13      -.0724022       .8444724     -3.0761075
    H  14       .0658466      -.8464357      3.0882733

Point Group = C1  Order =  1 Nsymop =  1
This system has  36 degrees of freedom

Heat of Formation:       -66.063 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

             135.04                  249.96                  257.23
               A                       A                       A
        X      Y      Z        X      Y      Z        X      Y      Z
   1    .555   .041  -.001     .274   .021  -.001    -.159  -.013   .001
   2   -.062  -.005   .000    -.122  -.009   .000     .044   .004   .000
   3   -.062  -.005   .000     .121   .009   .000     .047   .004   .000
   4   -.277  -.020   .001    -.136  -.010   .000    -.042  -.003   .000
   5   -.275  -.020   .001    -.022  -.002   .000    -.004   .000   .000
   6   -.277  -.020   .001     .137   .010   .000    -.039  -.003   .000
   7   -.275  -.020   .001     .022   .002   .000    -.004   .000   .000
   8   -.099  -.007   .000    -.064  -.005   .000    -.040  -.003   .000
   9   -.103  -.008   .000    -.015  -.001   .000     .001   .000   .000
  10   -.099  -.007   .000     .065   .005   .000    -.038  -.003   .000
  11   -.103  -.008   .000     .015   .001   .000     .001   .000   .000
  12    .555   .041  -.001    -.270  -.019   .000    -.166  -.012   .000
  13    .113   .008   .000    -.628  -.048   .001     .675   .051  -.002
  14    .112   .008   .000     .613   .044  -.001     .690   .050  -.002

Dipole moment:  X =   -.005940  Y =   -.000379  Z =    .000090
Total Dipole:    .005952 Debye

Molecule is non-linear

Zero-point vibrational energy is    68.767 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:          71.365 kcal/mol

Translational Entropy:         40.003  cal/mol.K
Rotational Entropy:            27.893  cal/mol.K
Vibrational Entropy:           13.732  cal/mol.K
```

1,4-DIMETHOXYBENZENE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Calculation started: Mon Dec 19 11:03:27 1994
Run type: Geometry optimization
Numerical Frequency
Model: RHF/PM3
Number of shells:  30
    20 S shells
    10 P shells
Number of basis functions:  50
Number of electrons:  54
Use of molecular symmetry disabled
Molecular charge:   0
Spin multiplicity:  1

              Cartesian Coordinates (Angstroms)
    Atom         X             Y             Z
    ----   ------------- ------------- -------------

    O   1       .7701153       .0241992    -2.6662850
    C   2       .3921943      -.0396291    -1.3342095
    C   3      -.4767064       .0412415     1.2965834
```

C	4	.1865469	-1.2360081	-.6364421
C	5	.1613264	1.1965822	-.7206434
C	6	-.2763515	1.2360948	.5975559
C	7	-.2454108	-1.1982619	.6797992
H	8	.3665777	-2.1964796	-1.1416469
H	9	.3183186	2.1291922	-1.2744224
H	10	-.4566859	2.2086918	1.0692655
H	11	-.4066772	-2.1315005	1.2314942
O	12	-.9045939	-.0583358	2.6084962
C	13	1.4159401	-1.1157081	-3.1807864
C	14	-1.1542733	1.1395088	3.2993537
H	15	.9176610	-2.0553145	-2.8980943
H	16	2.4604940	-1.1509333	-2.8527738
H	17	1.3625567	-.9636439	-4.2612312
H	18	-1.4671203	.7793526	4.2831911
H	19	-1.9595028	1.7254248	2.8409785
H	20	-.2562700	1.7609063	3.3954254

Point Group = C1 Order = 1 Nsymop = 1
This system has 54 degrees of freedom

Heat of Formation: -51.899 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	40.44			67.78			115.03		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	.012	-.036	-.006	-.365	-.126	-.126	.409	.090	.093
2	-.062	-.012	-.023	-.174	-.036	-.057	-.072	.052	-.043
3	-.169	-.006	-.060	.063	-.003	.014	-.047	.005	-.034
4	-.029	-.010	-.009	-.308	-.034	-.090	-.198	.038	-.105
5	-.176	-.013	-.066	.060	-.026	-.001	-.231	.039	-.074
6	-.232	-.010	-.084	.183	-.008	.042	-.223	.014	-.071
7	-.082	-.007	-.027	-.200	-.020	-.058	-.181	.014	-.099
8	.017	-.002	.005	-.129	-.009	-.042	-.079	.012	-.040
9	-.064	-.005	-.024	.044	-.009	.005	-.084	.014	-.022
10	-.093	-.003	-.034	.111	.001	.028	-.088	.001	-.022
11	-.016	-.001	-.004	-.088	-.004	-.023	-.059	.001	-.036
12	-.317	-.004	-.109	.304	.020	.091	.452	-.022	.124
13	.294	.064	.138	.433	.173	.197	.022	-.140	.142
14	.567	.017	.176	-.080	.018	-.046	.043	-.046	.025
15	.127	-.004	.039	.260	-.014	.080	-.198	.022	-.114
16	.076	.082	.077	.115	.236	.110	-.054	-.246	.215
17	.114	-.003	.036	.153	-.013	.047	.213	.057	.045
18	.198	.006	.062	-.024	.008	-.013	.149	-.018	.049
19	.209	.143	.150	-.049	-.058	-.049	-.107	-.142	.054
20	.264	-.131	-.002	-.066	.065	-.004	-.065	.114	-.094

Dipole moment: X = .332062 Y = .031222 Z = .255889
Total Dipole: .420380 Debye

Mulliken Population Analysis

Atom	Occupancy	Charge
O 1	6.191356	-.191356
C 2	3.954285	.045715
C 3	3.944071	.055929
C 4	4.145195	-.145195
C 5	4.099400	-.099400
C 6	4.149712	-.149712
C 7	4.103293	-.103293
H 8	.882468	.117532
H 9	.881937	.118063
H 10	.885211	.114789
H 11	.881315	.118685
O 12	6.188918	-.188918
C 13	3.953442	.046558
C 14	3.948848	.051152
H 15	.968508	.031492

```
     H 16      .974335      .025665
     H 17      .951209      .048791
     H 18      .950594      .049406
     H 19      .972829      .027171
     H 20      .973073      .026927

Total Charge =    .000000

Molecule is non-linear

Zero-point vibrational energy is   102.168 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:         106.561 kcal/mol

Translational Entropy:         40.679  cal/mol.K
Rotational Entropy:            29.529  cal/mol.K
Vibrational Entropy:           27.863  cal/mol.K
```

p-PHENYLENEDIAMINE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7
Calculation started: Thu Aug  3 14:39:52 1995
Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  24
  16 S shells
   8 P shells
Number of basis functions:  40
Number of electrons:  42
Use of molecular symmetry enabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
N	1	2.8268461	.0000000	.0930169
C	2	1.3976069	.0000000	-.0071489
C	3	-1.3976069	.0000000	.0071489
C	4	.6933055	-1.2114821	-.0040136
C	5	.6933055	1.2114821	-.0040136
C	6	-.6933055	1.2114821	.0040136
C	7	-.6933055	-1.2114821	.0040136
H	8	1.2296565	-2.1679437	-.0071340
H	9	1.2296565	2.1679437	-.0071340
H	10	-1.2296565	2.1679437	.0071340
H	11	-1.2296565	-2.1679437	.0071340
N	12	-2.8268461	.0000000	-.0930169
H	13	-3.2174137	-.8198644	.3162784
H	14	-3.2174137	.8198644	.3162784
H	15	3.2174137	-.8198644	-.3162784
H	16	3.2174137	.8198644	-.3162784

```
Point Group = CNH Order =  2 Nsymop =  4
This system has  12 degrees of freedom

Heat of Formation:       19.489 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

            126.60                  211.00                  216.45
              Bu                      Au                      Bg
```

	X	Y	Z	X	Y	Z	X	Y	Z
1	.037	.000	-.509	.000	.157	.000	.000	-.134	.000
2	-.007	.000	.060	.000	-.024	.000	.000	.011	.000
3	-.007	.000	.060	.000	-.024	.000	.000	-.011	.000
4	-.006	.001	.269	.005	-.018	.022	.011	.004	.084
5	-.006	-.001	.269	-.005	-.018	-.022	-.011	.004	-.084
6	-.006	.001	.269	.005	-.018	.022	-.011	-.004	-.084
7	-.006	-.001	.269	-.005	-.018	-.022	.011	-.004	.084
8	-.001	.000	.102	-.003	-.008	.021	.009	.005	.043
9	-.001	.000	.102	.003	-.008	-.021	-.009	.005	-.043
10	-.001	.000	.102	-.003	-.008	.021	-.009	-.005	-.043
11	-.001	.000	.102	.003	-.008	-.021	.009	-.005	.043
12	.037	.000	-.509	.000	.157	.000	.000	.134	.000
13	-.038	.000	-.183	-.006	-.180	-.451	.000	-.186	-.444
14	-.038	.000	-.183	.006	-.180	.451	.000	-.186	.444
15	-.038	.000	-.183	.006	-.180	.451	.000	.186	-.444
16	-.038	.000	-.183	-.006	-.180	-.451	.000	.186	.444

Dipole moment: X = .000000 Y = .000000 Z = .000000
Total Dipole: .000000 Debye
Zero-point vibrational energy is 84.071 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 86.858 kcal/mol

Translational Entropy: 39.949 cal/mol.K
Rotational Entropy: 26.552 cal/mol.K
Vibrational Entropy: 14.992 cal/mol.K

1,4-DIMERCAPTOBENZENE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 22
14 S shells
8 P shells
Number of basis functions: 38
Number of electrons: 42
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
S	1	-.0751927	.0000000	3.1543131
C	2	.0163379	.0000000	1.4015531
C	3	-.0163379	.0000000	-1.4015531
C	4	-1.1968023	.0000000	.7074291
C	5	1.2122910	.0000000	.6801523
C	6	1.1968023	.0000000	-.7074291
C	7	-1.2122910	.0000000	-.6801523
H	8	-2.1419941	.0000000	1.2651360
H	9	2.1754357	.0000000	1.2045555
H	10	2.1419941	.0000000	-1.2651360
H	11	-2.1754357	.0000000	-1.2045555
S	12	.0751927	.0000000	-3.1543131
H	13	-1.2001879	.0000000	-3.4551435
H	14	1.2001879	.0000000	3.4551435

Point Group = CNH Order = 2 Nsymop = 4

This system has 13 degrees of freedom

Heat of Formation: 32.001 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	85.16 Au			174.19 Bg			179.05 Au		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.510	.000	.001	-.181	.000	.000	-.094	.000
2	.000	-.176	.000	-.001	.109	.000	.000	.014	.000
3	.000	-.176	.000	-.001	-.109	.000	.000	.014	.000
4	.000	-.306	.000	-.001	.148	.000	.000	-.025	.000
5	.000	-.304	.000	-.001	-.012	.000	.000	-.031	.000
6	.000	-.306	.000	-.001	-.148	.000	.000	-.025	.000
7	.000	-.304	.000	-.001	.012	.000	.000	-.031	.000
8	.000	-.101	.000	.000	.084	.000	.000	-.008	.000
9	.000	-.101	.000	.000	-.012	.000	.000	-.015	.000
10	.000	-.101	.000	.000	-.084	.000	.000	-.008	.000
11	.000	-.101	.000	.000	.012	.000	.000	-.015	.000
12	.000	.510	.000	.001	.181	.000	.000	-.094	.000
13	.000	.045	.000	.000	-.653	.000	.000	.699	.000
14	.000	.045	.000	.000	.653	.000	.000	.699	.000

Dipole moment: X = .000000 Y = .000000 Z = .000000

Total Dipole: .000000 Debye

Zero-point vibrational energy is 58.678 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 62.030 kcal/mol

Translational Entropy: 40.763 cal/mol.K
Rotational Entropy: 27.945 cal/mol.K
Vibrational Entropy: 19.316 cal/mol.K

p-CHLOROANILINE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b

Calculation started: Sat Feb 24 14:54:35 1996
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 22
14 S shells
8 P shells
Number of basis functions: 38
Number of electrons: 42
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
Cl	1	.0000000	.0000000	-2.6749884
C	2	.0000000	.0000000	-.9865628
C	3	.0000000	.0000000	1.7900338
C	4	-1.2117113	.0000000	-.2996198
C	5	1.2117113	.0000000	-.2996198
C	6	1.2183053	.0000000	1.0862618
C	7	-1.2183053	.0000000	1.0862618

H	8	-2.1535858	.0000000	-.8589004
H	9	2.1535858	.0000000	-.8589004
H	10	2.1743368	.0000000	1.6224110
H	11	-2.1743368	.0000000	1.6224110
N	12	.0000000	.0000000	3.1886838
H	13	-.8547036	.0000000	3.6832324
H	14	.8547036	.0000000	3.6832324

Point Group = CNV Order = 2 Nsymop = 4
This system has 13 degrees of freedom

Heat of Formation: 18.626 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	-851.25			107.08			256.68		
	B1			B1			B2		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	-.001	.000	.000	-.462	.000	-.560	.000	.000
2	.000	.004	.000	.000	.214	.000	.377	.000	.000
3	.000	-.140	.000	.000	.023	.000	.062	.000	.000
4	.000	.012	.000	.000	.325	.000	.321	.000	-.098
5	.000	.012	.000	.000	.326	.000	.321	.000	.098
6	.000	-.019	.000	.000	.242	.000	.142	.000	.135
7	.000	-.019	.000	.000	.242	.000	.142	.000	-.135
8	.000	.006	.000	.000	.117	.000	.113	.000	-.064
9	.000	.006	.000	.000	.117	.000	.113	.000	.064
10	.000	-.007	.000	.000	.080	.000	.019	.000	.077
11	.000	-.007	.000	.000	.080	.000	.019	.000	-.077
12	.000	.470	.000	.000	-.535	.000	-.370	.000	.000
13	.000	-.616	.000	.000	-.206	.000	-.146	.000	-.079
14	.000	-.616	.000	.000	-.207	.000	-.146	.000	.079

Dipole moment: X = .000000 Y = .000000 Z = 2.743968
Total Dipole: 2.743968 Debye

1 imaginary frequencies ignored

Zero-point vibrational energy is 66.114 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 68.630 kcal/mol

Translational Entropy: 40.431 cal/mol.K
Rotational Entropy: 27.243 cal/mol.K
Vibrational Entropy: 13.505 cal/mol.K

p-CHLOROPHENOL

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b

Calculation started: Sat Feb 24 15:22:29 1996
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 21
13 S shells
8 P shells
Number of basis functions: 37
Number of electrons: 42
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
Cl	1	-.1103419	-.0091237	-2.6398710
C	2	-.0353650	-.0092084	-.9546202
C	3	.0884046	-.0130098	1.8058228
C	4	-.0218372	-1.2238696	-.2697694
C	5	.0127211	1.2021390	-.2709013
C	6	.0750338	1.2076024	1.1167675
C	7	.0402321	-1.2339667	1.1157845
H	8	-.0601309	-2.1645418	-.8301138
H	9	.0012666	2.1450424	-.8284601
H	10	.1121379	2.1607284	1.6566387
H	11	.0507214	-2.1821707	1.6651189
O	12	.1472837	-.0967900	3.1694814
H	13	.1775224	.7864043	3.5156691

Point Group = C1 Order = 1 Nsymop = 1
This system has 33 degrees of freedom

Heat of Formation: -28.390 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	113.63			260.20			279.03		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.464	.007	.021	-.008	-.562	.010	.098	-.001	-.004
2	.226	-.003	-.010	.006	.387	.003	-.203	.003	.009
3	.016	.000	-.001	.001	.053	-.004	.195	-.003	-.009
4	.341	-.005	-.015	.000	.324	-.104	-.061	.001	.003
5	.334	-.005	-.015	.010	.327	.106	-.192	.003	.009
6	.231	-.003	-.010	.008	.137	.145	.146	-.002	-.007
7	.239	-.003	-.011	-.004	.133	-.144	.163	-.002	-.007
8	.125	-.002	-.006	-.002	.116	-.069	-.023	.000	.001
9	.120	-.002	-.005	.005	.116	.068	-.110	.002	.005
10	.072	-.001	-.003	.004	.018	.080	.088	-.001	-.004
11	.072	-.001	-.003	-.003	.018	-.077	.070	-.001	-.003
12	-.575	.008	.025	-.007	-.384	-.035	-.393	.006	.017
13	-.150	.002	.007	.001	-.128	.069	.800	-.014	-.035

Dipole moment: X = .055494 Y = 1.125627 Z = .818674
Total Dipole: 1.392962 Debye

Molecule is non-linear

Zero-point vibrational energy is 59.727 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 62.249 kcal/mol

Translational Entropy: 40.454 cal/mol.K
Rotational Entropy: 28.614 cal/mol.K
Vibrational Entropy: 13.545 cal/mol.K

p-NITROANILINE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b

Calculation started: Sat Feb 24 16:06:07 1996
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 26
16 S shells
10 P shells

Number of basis functions: 46
Number of electrons: 52
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
N	1	.0045393	.0512081	-2.1943249
C	2	.0014653	.0139670	-.7049559
C	3	-.0043830	-.0530720	2.0920827
C	4	-1.2113778	.0016408	-.0015521
C	5	1.2113760	-.0097671	.0032343
C	6	1.2113480	-.0464775	1.3867737
C	7	-1.2171656	-.0348214	1.3820018
H	8	-2.1689150	.0201559	-.5413328
H	9	2.1711831	-.0000070	-.5327204
H	10	2.1681062	-.0659696	1.9235070
H	11	-2.1761846	-.0450389	1.9149443
N	12	-.0067473	.0227619	3.5056483
O	13	-1.0519190	.0606459	-2.7973296
O	14	1.0634692	.0694592	-2.7927456
H	15	-.8358366	-.3442320	3.9141033
H	16	.8171245	-.3523591	3.9173296

Point Group = C1 Order = 1 Nsymop = 1
This system has 42 degrees of freedom

Heat of Formation: 10.685 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	32.86			96.57			220.61		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.001	.000	.000	.000	-.086	-.006	.019	.001	.000
2	.001	.000	.000	.001	.257	.003	.321	-.001	.001
3	.003	.000	.000	.000	-.007	-.002	-.011	-.001	.000
4	.000	-.230	-.004	.002	.344	.005	.251	.010	-.109
5	.003	.230	.005	.002	.344	.006	.251	-.013	.110
6	.004	.238	.005	.000	.215	.002	.073	-.007	.135
7	.002	-.238	-.005	.001	.215	.002	.073	.002	-.135
8	.000	-.116	-.002	.001	.130	.002	.082	.007	-.051
9	.001	.116	.002	.001	.129	.002	.082	-.008	.051
10	.002	.124	.002	.000	.066	.001	.000	-.003	.076
11	.001	-.124	-.002	.000	.066	.001	.000	.001	-.076
12	-.018	.000	.000	-.003	-.552	.030	-.374	.003	-.001
13	-.004	.599	.015	-.001	-.294	-.008	-.239	-.008	.433
14	.001	-.599	-.015	-.001	-.294	-.014	-.238	.012	-.434
15	.015	-.046	-.001	-.001	-.193	-.033	-.125	-.010	-.060
16	.016	.046	.001	-.001	-.193	-.033	-.126	.013	.059

Dipole moment: X = -.018686 Y = -1.246942 Z = 6.516662
Total Dipole: 6.634915 Debye

Molecule is non-linear

Zero-point vibrational energy is 75.533 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 78.977 kcal/mol

Translational Entropy: 40.679 cal/mol.K
Rotational Entropy: 29.408 cal/mol.K
Vibrational Entropy: 21.305 cal/mol.K

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy:	.889	kcal/mol
Rotational Enthalpy:	.889	kcal/mol
Vibrational Enthalpy:	77.941	kcal/mol
Translational Entropy:	40.003	cal/mol.K
Rotational Entropy:	27.965	cal/mol.K
Vibrational Entropy:	16.045	cal/mol.K

p-METHOXYTOLUENE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b

Calculation started: Sat Feb 24 16:23:17 1996
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 28
19 S shells
9 P shells
Number of basis functions: 46
Number of electrons: 48
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
O	1	2.3558211	-.1828791	-.1178670
C	2	.9789733	-.0930102	-.0456655
C	3	-1.8011439	-.1929191	.1210063
C	4	.3322739	-1.3325156	.0859302
C	5	.2392896	1.0920307	-.0920234
C	6	-1.1474301	1.0311225	-.0075487
C	7	-1.0507359	-1.3713739	.1683968
H	8	.9146657	-2.2601880	.1236991
H	9	.7282577	2.0672856	-.1927972
H	10	-1.7307774	1.9582736	-.0419291
H	11	-1.5612166	-2.3355517	.2727046
C	12	-3.2838086	-.2477263	.1939360
H	13	-3.7145974	-.3390290	-.8126447
H	14	-3.7035721	.6576908	.6518963
H	15	-3.6315850	-1.1079531	.7811272
C	16	3.0765822	1.0164353	-.2512293
H	17	4.1109826	.6637745	-.2842124
H	18	2.9351997	1.6852207	.6057638
H	19	2.8318502	1.5490362	-1.1775843

Point Group = C1 Order = 1 Nsymop = 1
This system has 51 degrees of freedom

Heat of Formation: -23.817 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	40.56			51.60			121.70		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.007	-.014	-.081	.023	.030	.408	-.031	-.040	-.522
2	-.003	.003	-.035	.011	.016	.193	.003	.005	.071
3	-.002	.030	.006	-.003	.002	-.044	.003	.005	.066
4	-.016	.000	-.078	-.003	.000	-.015	.015	.021	.282
5	.010	.009	.024	.020	.025	.321	.012	.017	.222
6	.006	.024	.043	.012	.019	.201	.011	.016	.209
7	-.010	.016	-.055	-.009	-.007	-.132	.015	.020	.276

p-FLUOROTOLUENE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 4.0.2b

Calculation started: Sat Feb 24 16:46:31 1996
Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  23
  15 S shells
   8 P shells
Number of basis functions:  39
Number of electrons:  42
Use of molecular symmetry disabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
F	1	-.0105832	.0012324	2.7722404
C	2	-.0042052	.0003631	1.4284594
C	3	.0087164	-.0012482	-1.3494758
C	4	.0056638	1.2195835	.7396436
C	5	-.0060540	-1.2193586	.7410291
C	6	.0008739	-1.2082524	-.6477384
C	7	.0125610	1.2067746	-.6487978
H	8	.0084775	2.1670468	1.2891275
H	9	-.0123019	-2.1663168	1.2913620
H	10	.0009944	-2.1571782	-1.1963460
H	11	.0219606	2.1545942	-1.1991392
C	12	-.0000345	-.0000473	-2.8350159
H	13	.4569766	-.9090332	-3.2480739
H	14	.5450272	.8608567	-3.2443735
H	15	-1.0310143	.0520501	-3.2113462

```
Point Group = C1  Order =  1 Nsymop =  1
This system has  39 degrees of freedom

Heat of Formation:       -29.612 kcal/mol
```

Normal Modes and Vibrational Frequencies (cm-1)

	40.80			130.43			322.72		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.005	-.018	.000	-.542	.003	-.004	.336	.003	-.005
2	-.001	.001	.000	.044	.000	-.001	-.330	.001	-.007
3	.005	.031	.000	.098	-.001	.000	.426	-.005	.005
4	.085	.003	.013	.253	-.001	.000	-.350	.002	-.005
5	-.082	.004	-.013	.255	-.001	.000	-.346	-.002	-.003
6	-.076	.021	-.008	.286	-.002	.000	.251	-.007	.000
7	.085	.020	.008	.284	-.001	.000	.254	-.001	-.001
8	.043	.000	.006	.086	.000	.000	-.188	.001	-.001
9	-.043	.000	-.006	.087	.000	.000	-.185	.000	.000
10	-.039	.010	-.009	.104	-.001	.000	.130	-.002	-.001
11	.043	.010	.010	.103	-.001	.000	.132	-.001	-.001
12	-.006	-.039	.000	-.483	.003	.004	-.188	.006	.013
13	.499	.228	.026	-.199	-.002	-.056	-.127	.000	-.071
14	-.479	.277	-.029	-.186	-.002	-.066	-.122	.003	-.081
15	-.032	-.593	.003	-.187	.008	.130	-.118	.006	.173

```
Dipole moment:  X =    -.030021  Y =     .002655  Z =  -1.888948
Total Dipole:   1.889189 Debye

Molecule is non-linear

Zero-point vibrational energy is     75.321 kcal/mol
```

8	-.007	-.002	-.037	-.002	-.002	-.025	.006	.008	.104
9	.005	.002	.016	.009	.011	.148	.004	.006	.081
10	.009	.012	.024	.006	.008	.085	.004	.005	.067
11	-.010	.008	-.024	-.007	-.005	-.088	.006	.008	.104
12	.003	-.041	.040	-.011	-.023	-.219	-.020	-.033	-.449
13	.019	-.589	.056	.035	-.077	-.074	.105	-.008	-.178
14	-.059	.214	-.489	-.031	.018	-.138	-.062	-.015	-.172
15	.045	.289	.478	-.015	.027	-.021	-.063	-.015	-.173
16	.015	-.006	.104	-.031	-.044	-.550	-.004	-.002	-.037
17	.003	-.005	.027	-.011	-.016	-.198	-.011	-.013	-.177
18	-.001	-.032	.053	.070	.121	-.250	.097	-.141	.114
19	.015	.033	.047	-.096	-.158	-.219	-.085	.158	.102

Dipole moment: X = -.127909 Y = 1.056368 Z = -.108476
Total Dipole: 1.069599 Debye

Molecule is non-linear

Zero-point vibrational energy is 99.580 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 103.442 kcal/mol

Translational Entropy: 40.312 cal/mol.K
Rotational Entropy: 28.796 cal/mol.K
Vibrational Entropy: 25.016 cal/mol.K

BIPHENYL

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 34
22 S shells
12 P shells
Number of basis functions: 58
Number of electrons: 58
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	.0000000	.0000000	-4.6298130
C	2	.0000000	.0000000	-3.5352107
C	3	.0000000	.0000000	-.7348729
C	4	-1.2030033	.0000000	-2.8369925
C	5	1.2030033	.0000000	-2.8369925
C	6	1.2040325	.0000000	-1.4481910
C	7	-1.2040325	.0000000	-1.4481910
H	8	-2.1522332	.0000000	-3.3825502
H	9	2.1522332	.0000000	-3.3825502
H	10	2.1552689	.0000000	-.8943709
H	11	-2.1552689	.0000000	-.8943709
C	12	.0000000	.0000000	.7348729
C	13	.0000000	.0000000	3.5352107
C	14	-1.2040325	.0000000	1.4481910
C	15	1.2040325	.0000000	1.4481910
C	16	1.2030033	.0000000	2.8369925
C	17	-1.2030033	.0000000	2.8369925
H	18	-2.1552689	.0000000	.8943709
H	19	2.1552689	.0000000	.8943709

```
    H  20      2.1522332       .0000000      3.3825502
    H  21     -2.1522332       .0000000      3.3825502
    H  22       .0000000       .0000000      4.6298130

Point Group = DNH Order =  2 Nsymop =  8
This system has  11 degrees of freedom

Heat of Formation:       47.578 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

              33.18                    90.98                   215.04
               Au                       B3u                      B2g
        X       Y       Z        X       Y       Z        X       Y       Z
   1    .000    .000    .000     .000    .218    .000     .000   -.234    .000
   2    .000    .000    .000     .000    .397    .000     .000   -.322    .000
   3    .000    .000    .000     .000   -.333    .000     .000    .206    .000
   4    .000    .319    .000     .000    .161    .000     .000    .035    .000
   5    .000   -.319    .000     .000    .161    .000     .000    .035    .000
   6    .000   -.311    .000     .000   -.218    .000     .000    .350    .000
   7    .000    .311    .000     .000   -.218    .000     .000    .350    .000
   8    .000    .167    .000     .000    .085    .000     .000    .001    .000
   9    .000   -.167    .000     .000    .085    .000     .000    .001    .000
  10    .000   -.154    .000     .000   -.108    .000     .000    .160    .000
  11    .000    .154    .000     .000   -.108    .000     .000    .160    .000
  12    .000    .000    .000     .000   -.333    .000     .000   -.206    .000
  13    .000    .000    .000     .000    .397    .000     .000    .322    .000
  14    .000   -.311    .000     .000   -.218    .000     .000   -.350    .000
  15    .000    .311    .000     .000   -.218    .000     .000   -.350    .000
  16    .000    .319    .000     .000    .161    .000     .000   -.035    .000
  17    .000   -.319    .000     .000    .161    .000     .000   -.035    .000
  18    .000   -.154    .000     .000   -.108    .000     .000   -.160    .000
  19    .000    .154    .000     .000   -.108    .000     .000   -.160    .000
  20    .000    .167    .000     .000    .085    .000     .000   -.001    .000
  21    .000   -.167    .000     .000    .085    .000     .000   -.001    .000
  22    .000    .000    .000     .000    .218    .000     .000    .234    .000

Dipole moment:  X =    .000000  Y =    .000000  Z =    .000001

Total Dipole:    .000001 Debye

Zero-point vibrational energy is   113.385 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:         117.231 kcal/mol

Translational Entropy:         41.006  cal/mol.K
Rotational Entropy:            27.662  cal/mol.K
Vibrational Entropy:           23.145  cal/mol.K
```

4-PHENYLPHENOL

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  36
  23 S shells
  13 P shells
Number of basis functions:  62
Number of electrons:  64
Use of molecular symmetry disabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	.2331558	-1.4591657	4.8503158
C	2	.1828336	-1.1440299	3.8033343
C	3	.0543309	-.3372506	1.1239701
C	4	.5043057	-2.0388958	2.7882774
C	5	-.2027844	.1531698	3.4821902
C	6	-.2665469	.5541823	2.1541671
C	7	.4405674	-1.6399841	1.4596542
H	8	.8088229	-3.0609362	3.0358597
H	9	-.4569407	.8614353	4.2774047
H	10	-.5704619	1.5810095	1.9001400
H	11	.6942297	-2.3483385	.6565267
C	12	-.0133660	.0857451	-.2811796
C	13	-.1434916	.8911645	-2.9524394
C	14	.2872318	-.8126088	-1.3105403
C	15	-.3805866	1.3959886	-.6147954
C	16	-.4483495	1.8076762	-1.9362655
C	17	.2257819	-.4238011	-2.6408866
H	18	.5774724	-1.8430912	-1.0537837
H	19	-.6184480	2.1055105	.1927775
H	20	-.7360907	2.8353431	-2.1846673
H	21	.4652153	-1.1441614	-3.4314028
O	22	-.2287982	1.3596504	-4.2344535
H	23	-.0061268	.6470535	-4.8204616

Point Group = C1 Order = 1 Nsymop = 1
This system has 63 degrees of freedom

Heat of Formation: 2.415 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	32.41			68.43			166.82		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.000	-.001	.176	.053	.007	.217	.074	.012
2	.001	.001	-.002	.349	.104	.015	.323	.116	.019
3	.000	.000	.000	-.227	-.067	-.009	-.308	-.106	-.017
4	.306	.095	.012	.179	.054	.005	.023	.014	.014
5	-.305	-.093	-.015	.179	.053	.010	.022	.020	-.006
6	-.299	-.091	-.015	-.115	-.035	-.003	-.331	-.103	-.026
7	.299	.092	.012	-.115	-.034	-.007	-.330	-.109	-.006
8	.160	.049	.007	.083	.025	.002	.032	.012	.008
9	-.159	-.049	-.008	.083	.024	.005	.031	.016	-.003
10	-.148	-.045	-.008	-.068	-.021	-.002	-.147	-.046	-.012
11	.148	.046	.005	-.068	-.020	-.004	-.147	-.049	-.003
12	-.001	.000	.000	-.311	-.092	-.013	-.029	-.026	-.007
13	-.002	-.001	.002	.102	.030	.004	.110	.037	.006
14	-.295	-.087	-.010	-.276	-.081	-.012	.176	.041	-.005
15	.293	.085	.013	-.281	-.083	-.011	.183	.038	.011
16	.304	.088	.013	-.071	-.021	-.002	.270	.075	.020
17	-.307	-.090	-.011	-.066	-.019	-.003	.262	.079	.001
18	-.146	-.042	-.004	-.107	-.031	-.005	.058	.014	-.002
19	.145	.042	.007	-.110	-.032	-.004	.062	.013	.004
20	.158	.046	.006	-.002	-.001	.000	.107	.031	.009
21	-.159	-.046	-.006	-.001	.000	.000	.107	.034	.000
22	.021	.005	.003	.532	.155	.021	-.383	-.086	-.006
23	-.059	-.017	-.002	.150	.044	.005	-.073	-.013	-.003

Dipole moment: X = .301699 Y = -1.035541 Z = -.280253
Total Dipole: 1.114410 Debye

Molecule is non-linear

Zero-point vibrational energy is 116.810 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol

```
Rotational Enthalpy:            .889 kcal/mol
Vibrational Enthalpy:        121.431 kcal/mol

Translational Entropy:        41.301  cal/mol.K
Rotational Entropy:           31.041  cal/mol.K
Vibrational Entropy:          28.054  cal/mol.K
```

4-PHENYLANISOLE

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 4.0.2b

Calculation started: Sat Feb 24 17:00:32 1996
Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  40
  26 S shells
  14 P shells
Number of basis functions:  68
Number of electrons:  70
Use of molecular symmetry disabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-.0287126	.0810475	.1680506
C	2	-.0371936	.1230841	1.6364877
C	3	-.0531686	.2026361	4.4363579
C	4	-.0837812	-1.0592523	2.3840799
C	5	.0011120	1.3460082	2.3161315
C	6	-.0066642	1.3843374	3.7042951
C	7	-.0918248	-1.0187536	3.7721703
H	8	-.1139876	-2.0255437	1.8581782
H	9	.0370896	2.2809570	1.7365609
H	10	.0238165	2.3484250	4.2222717
H	11	-.1287441	-1.9518338	4.3437084
H	12	-.1937450	-2.0038326	-4.2645798
C	13	-.0068754	.0027760	-2.6247597
C	14	.0052386	1.2656666	-.5793712
C	15	-.0553982	-1.1421997	-.5098181
C	16	-.0461968	-1.1904546	-1.8960792
C	17	.0173813	1.2398082	-1.9649489
H	18	.0243306	2.2304529	-.0492240
H	19	-.0862793	-2.0768645	.0709549
H	20	-.0772202	-2.1532184	-2.4268356
H	21	.0421074	2.1744826	-2.5364555
O	22	-.0375316	.0742855	-4.0046006
C	23	.2763722	-1.1093100	-4.7000757
H	24	-.0594202	.2337501	5.5304752
H	25	1.3612481	-1.2560861	-4.7364323
H	26	-.1145659	-.9193341	-5.7022863

```
Point Group = C1  Order =  1 Nsymop =  1
This system has  72 degrees of freedom

Heat of Formation:        9.592 kcal/mol
```

Normal Modes and Vibrational Frequencies (cm-1)

	30.72			53.31			83.39		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.039	-.005	-.001	.253	-.005	.008	-.193	.025	-.002
2	-.013	-.001	-.001	.143	-.003	.007	-.171	.011	-.002
3	.055	.006	-.002	-.302	.010	.004	.214	-.031	.001
4	-.320	.012	.000	.011	.001	.005	-.117	.001	-.013

5	.327	-.011	-.004	.086	-.002	.008	-.093	.001	.011
6	.367	-.007	-.004	-.137	.005	.007	.108	-.020	.012
7	-.293	.016	.001	-.217	.007	.003	.080	-.020	-.011
8	-.164	.006	.000	.023	.000	.001	-.058	.003	-.007
9	.158	-.006	-.002	.057	-.001	.003	-.050	.003	.005
10	.186	-.004	-.001	-.055	.002	.002	.055	-.008	.007
11	-.158	.008	.001	-.097	.003	.000	.041	-.008	-.006
12	.138	-.020	.001	-.137	.010	.020	-.261	.046	.007
13	-.061	-.011	.000	.078	.000	.005	.164	.030	-.003
14	-.296	-.001	-.005	.104	-.001	.007	-.291	.032	.003
15	.198	-.014	.005	.415	-.008	.008	-.008	.027	-.008
16	.198	-.017	.005	.325	-.006	.007	.164	.028	-.008
17	-.318	-.004	-.005	.013	.002	.007	-.106	.036	.006
18	-.134	.001	-.002	.009	.000	.002	-.140	.009	.003
19	.108	-.005	.003	.167	-.004	.003	.006	.006	-.005
20	.116	-.007	.002	.117	-.004	.004	.080	.006	.001
21	-.153	.000	-.003	-.037	.002	.002	-.043	.012	.004
22	-.106	-.031	.000	-.123	.028	.016	.595	.077	-.001
23	.242	.056	.008	-.493	-.024	-.076	-.312	-.158	.010
24	.024	.003	.000	-.143	.004	.001	.115	-.014	.001
25	.082	.101	.008	-.152	-.048	-.119	-.119	-.259	-.001
26	.060	-.015	.000	-.225	.007	.012	-.057	.028	.004

Dipole moment: X = .272356 Y = -1.085904 Z = -.183488
Total Dipole: 1.134474 Debye

Molecule is non-linear

Zero-point vibrational energy is 133.496 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 139.028 kcal/mol

Translational Entropy: 41.537 cal/mol.K
Rotational Entropy: 31.617 cal/mol.K
Vibrational Entropy: 35.133 cal/mol.K

4-PHENYLANILINE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 37
24 S shells
13 P shells
Number of basis functions: 63
Number of electrons: 64
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	-.0077912	.0000000	5.0838188
C	2	-.0056306	.0000000	3.9892708
C	3	-.0003295	.0000000	1.1883344
C	4	-.0043968	-1.2028091	3.2908819
C	5	-.0043968	1.2028091	3.2908819
C	6	-.0017855	1.2039212	1.9022166
C	7	-.0017855	-1.2039212	1.9022166
H	8	-.0057476	-2.1523067	3.8359382

H	9	-.0057476	2.1523067	3.8359382
H	10	-.0015511	2.1551617	1.3486636
H	11	-.0015511	-2.1551617	1.3486636
C	12	.0023045	.0000000	-.2802387
C	13	.0064197	.0000000	-3.0875036
C	14	.0042865	-1.2031333	-.9951650
C	15	.0042865	1.2031333	-.9951650
C	16	.0079798	1.2112538	-2.3811538
C	17	.0079798	-1.2112538	-2.3811538
H	18	.0024364	-2.1538973	-.4400500
H	19	.0024364	2.1538973	-.4400500
H	20	.0086642	2.1692810	-2.9144413
H	21	.0086642	-2.1692810	-2.9144413
N	22	-.0982849	.0000000	-4.5120191
H	23	.2992948	-.8214521	-4.9102202
H	24	.2992948	.8214521	-4.9102202

Point Group = CS Order = 1 Nsymop = 2
This system has 36 degrees of freedom

Heat of Formation: 45.272 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	33.91			71.18			164.00		
	A"			A'			A'		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	-.001	.000	-.180	.000	-.001	.233	.000	.000
2	.000	-.002	.000	-.358	.000	-.002	.351	.000	-.002
3	.000	.001	.000	.225	.000	-.001	-.335	.000	-.003
4	-.321	-.001	-.002	-.185	.000	-.002	.033	.000	-.003
5	.321	-.001	.002	-.185	.000	-.002	.033	.000	-.003
6	.313	.000	.002	.113	.000	-.002	-.349	.000	-.004
7	-.313	.000	-.002	.113	.000	-.002	-.349	.000	-.004
8	-.167	.000	-.001	-.085	.000	-.001	.037	.000	-.001
9	.167	.000	.001	-.085	.000	-.001	.037	.000	-.001
10	.155	.000	.001	.068	.000	.000	-.155	.000	-.001
11	-.155	.000	-.001	.068	.000	.000	-.155	.000	-.001
12	.000	.002	.000	.313	.000	-.001	-.053	.000	-.002
13	.000	.003	.000	-.095	.000	-.001	.126	.000	.000
14	.304	.002	.000	.288	.000	-.001	.166	.000	-.001
15	-.304	.002	.000	.288	.000	-.001	.166	.000	-.001
16	-.315	.004	.000	.083	.000	-.002	.277	.001	-.001
17	.315	.004	.000	.083	.000	-.002	.277	-.001	-.001
18	.150	.001	.000	.112	.000	.000	.054	.000	.000
19	-.150	.001	.000	.112	.000	.000	.054	.000	.000
20	-.165	.001	.000	.008	.000	.000	.116	.000	.000
21	.165	.001	.000	.008	.000	.000	.116	.000	.000
22	.000	-.026	.000	-.541	.000	.032	-.340	.000	.040
23	.063	.023	.000	-.180	.000	-.025	-.132	.000	-.029
24	-.063	.023	.000	-.180	.000	-.025	-.132	.000	-.029

Dipole moment: X = 1.190682 Y = .000000 Z = -.723725

Total Dipole: 1.393378 Debye

Zero-point vibrational energy is 124.407 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy:	.889	kcal/mol
Rotational Enthalpy:	.889	kcal/mol
Vibrational Enthalpy:	129.122	kcal/mol
Translational Entropy:	41.284	cal/mol.K
Rotational Entropy:	31.038	cal/mol.K
Vibrational Entropy:	28.510	cal/mol.K

4,4'-BIPHENOL

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Tue Dec 27 17:42:38 1994
Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 38
    24 S shells
    14 P shells
Number of basis functions: 66
Number of electrons: 70
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
H	1	-1.9265041	1.2530428	.3989492
C	2	-1.7267776	.2182049	.7168917
C	3	-1.2005503	-2.4059133	1.5127688
C	4	-.5038095	-.3731182	.3822092
C	5	-2.6852946	-.4777518	1.4392830
C	6	-2.4192823	-1.7940547	1.8375623
C	7	-.2584849	-1.6907904	.7906163
C	8	.5036554	.3729868	-.3825392
H	9	-3.6362938	.0057312	1.6903108
O	10	-3.3056230	-2.5530091	2.5513899
H	11	.7023049	-2.1608126	.5300994
H	12	-.9965678	-3.4358443	1.8262104
C	13	2.4193681	1.7941263	-1.8373805
C	14	.2555879	1.6882949	-.7968694
C	15	1.7293983	-.2159442	-.7112296
C	16	2.6881402	.4802032	-1.4331414
C	17	1.1976804	2.4034395	-1.5189646
H	18	-.7072013	2.1565969	-.5406656
H	19	1.9309618	-1.2491962	-.3893162
H	20	3.6414497	-.0012899	-1.6791814
H	21	.9914631	3.4314430	-1.8372338
O	22	3.3055822	2.5529709	-2.5514826
H	23	4.0841830	2.0303570	-2.6979171
H	24	-4.0812561	-2.0278207	2.7042455

Point Group = C1 Order = 1 Nsymop = 1
This system has 66 degrees of freedom

Heat of Formation: -42.700 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	31.23			54.71			128.37		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.061	-.052	-.131	.035	.030	.076	.039	.032	.080
2	-.123	-.105	-.264	.086	.074	.186	.109	.090	.228
3	.126	.107	.272	.005	.004	.009	.090	.078	.199
4	-.001	-.001	-.002	.111	.095	.238	.059	.046	.123
5	-.127	-.109	-.273	.002	.001	.005	.091	.078	.191
6	-.001	-.001	-.001	-.056	-.048	-.120	.020	.020	.046
7	.121	.104	.262	.089	.076	.190	.109	.090	.235
8	-.001	-.001	-.002	.110	.095	.238	-.055	-.052	-.123
9	-.066	-.056	-.142	-.008	-.007	-.016	.031	.027	.065
10	.009	.008	.020	-.204	-.175	-.440	-.174	-.140	-.365
11	.060	.051	.130	.037	.031	.079	.039	.032	.084
12	.065	.056	.141	-.007	-.006	-.015	.029	.026	.065
13	.000	.000	-.001	-.056	-.048	-.120	-.022	-.017	-.046
14	.121	.105	.262	.088	.076	.191	-.108	-.097	-.233
15	-.122	-.106	-.265	.086	.075	.185	-.103	-.093	-.230
16	-.126	-.109	-.273	.002	.002	.004	-.088	-.076	-.194

17	.126	.109	.271	.004	.004	.010	-.093	-.080	-.196
18	.060	.053	.130	.036	.031	.079	-.038	-.034	-.083
19	-.060	-.052	-.131	.035	.031	.076	-.036	-.033	-.081
20	-.065	-.057	-.142	-.007	-.006	-.016	-.030	-.025	-.066
21	.065	.057	.141	-.007	-.006	-.014	-.031	-.026	-.064
22	.010	.008	.019	-.204	-.176	-.440	.165	.151	.365
23	-.024	-.021	-.052	-.057	-.050	-.124	.041	.038	.089
24	-.024	-.021	-.052	-.058	-.050	-.124	-.042	-.034	-.090

Dipole moment: X = .003954 Y = .003431 Z = .008562
Total Dipole: .010036 Debye

Mulliken Population Analysis

Atom	Occupancy	Charge
H 1	.890512	.109488
C 2	4.062235	-.062235
C 3	4.138376	-.138376
C 4	4.059995	-.059995
C 5	4.190187	-.190187
C 6	3.902724	.097276
C 7	4.068131	-.068131
C 8	4.059994	-.059994
H 9	.889375	.110625
O 10	6.225834	-.225834
H 11	.890958	.109042
H 12	.878399	.121601
C 13	3.902724	.097276
C 14	4.068131	-.068131
C 15	4.062235	-.062235
C 16	4.190187	-.190187
C 17	4.138375	-.138375
H 18	.890958	.109042
H 19	.890512	.109488
H 20	.889375	.110625
H 21	.878399	.121601
O 22	6.225835	-.225835
H 23	.803274	.196726
H 24	.803274	.196726

Total Charge = .000000

Molecule is non-linear

Zero-point vibrational energy is 120.217 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 125.623 kcal/mol

Translational Entropy: 41.569 cal/mol.K
Rotational Entropy: 31.603 cal/mol.K
Vibrational Entropy: 33.118 cal/mol.K

BENZIDINE

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 40
26 S shells
14 P shells
Number of basis functions: 68

Number of electrons: 70
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-.6900472	.0320655	-.2475702
C	2	.6900260	-.0328799	.2475057
C	3	3.3302784	-.1558252	1.1946486
C	4	.9570811	-.0505433	1.6213209
C	5	1.7684193	-.0760782	-.6436707
C	6	3.0745531	-.1356456	-.1836574
C	7	2.2578299	-.1095599	2.0964274
H	8	.1147501	-.0167384	2.3293003
H	9	1.5673949	-.0614357	-1.7259342
H	10	3.8990936	-.1691923	-.9055637
H	11	2.4363103	-.1222474	3.1781486
N	12	4.6657276	-.3240043	1.6750063
C	13	-3.3302642	.1562393	-1.1946307
C	14	-.9565718	.0624024	-1.6212606
C	15	-1.7689634	.0629031	.6435137
C	16	-3.0750923	.1225953	.1835105
C	17	-2.2573043	.1225216	-2.0963351
H	18	-.1138585	.0371127	-2.3291312
H	19	-1.5682863	.0390960	1.7256716
H	20	-3.9000462	.1458418	.9053497
H	21	-2.4353179	.1458859	-3.1779653
N	22	-4.6661036	.3253578	-1.6735692
H	23	-5.3332664	-.0588920	-1.0419831
H	24	-4.7785016	-.0532971	-2.5877059
H	25	4.7804968	.0673337	2.5834523
H	26	5.3341966	.0478888	1.0374891

Point Group = C1 Order = 1 Nsymop = 1
This system has 72 degrees of freedom

Heat of Formation: 43.032 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	34.78			53.75			123.72		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.001	.001	.003	-.014	-.273	-.004	-.004	-.139	-.007
2	-.001	.001	.003	-.014	-.273	-.003	.008	.139	-.005
3	.000	.000	.002	.004	.140	.000	.000	.060	.003
4	-.013	-.306	.001	-.012	-.217	-.003	.009	.265	-.003
5	.013	.307	.005	-.011	-.215	-.002	.016	.264	-.001
6	.014	.317	.005	-.002	-.008	.000	.013	.229	.002
7	-.014	-.317	.002	-.004	-.010	-.001	.006	.229	.001
8	-.006	-.151	.001	-.005	-.089	-.001	.003	.092	-.001
9	.007	.152	.002	-.004	-.088	-.001	.006	.092	.000
10	.007	.165	.002	.000	.017	.000	.005	.079	.001
11	-.007	-.165	.000	.000	.016	.000	.001	.079	.001
12	.011	-.002	-.027	.044	.492	.012	-.058	-.394	-.006
13	-.002	.000	.002	.004	.140	.001	-.002	-.060	.003
14	-.014	-.306	-.002	-.011	-.217	-.003	-.012	-.265	-.008
15	.011	.307	.007	-.012	-.215	-.003	-.006	-.265	-.006
16	.011	.317	.007	-.003	-.008	-.001	-.006	-.229	-.001
17	-.015	-.317	-.002	-.002	-.010	-.001	-.012	-.229	-.004
18	-.007	-.151	-.002	-.004	-.089	-.001	-.005	-.092	-.003
19	.005	.152	.003	-.005	-.088	-.001	-.002	-.092	-.002
20	.006	.165	.003	.000	.017	.000	-.001	-.079	.000
21	-.007	-.165	-.002	.001	.016	.000	-.005	-.079	-.001
22	.008	-.001	-.028	.044	.492	.014	.050	.394	.028
23	-.006	.062	.022	-.012	.159	-.005	-.020	.145	-.004
24	-.010	-.063	.020	-.012	.159	-.005	-.021	.145	-.005
25	-.010	-.063	.021	-.012	.160	-.006	.017	-.146	.011
26	-.005	.063	.022	-.012	.159	-.006	.019	-.145	.012

```
Dipole moment:  X =    .005298  Y =    .000356  Z =   -.015932
Total Dipole:    .016793 Debye

Molecule is non-linear

Zero-point vibrational energy is   135.392 kcal/mol

Standard Thermodynamic quantities at   298.15 K  and     1.00 atm

Translational Enthalpy:          .889 kcal/mol
Rotational Enthalpy:             .889 kcal/mol
Vibrational Enthalpy:         141.003 kcal/mol

Translational Entropy:         41.537  cal/mol.K
Rotational Entropy:            31.594  cal/mol.K
Vibrational Entropy:           34.281  cal/mol.K
```

4,4′-DIMETHOXYBIPHENYL

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 4.0.2b

Calculation started: Sat Feb 24 17:04:32 1996
Run type: Single point energy
          Numerical Frequency
Model: RHF/PM3
Number of shells:  46
  30 S shells
  16 P shells
Number of basis functions:  78
Number of electrons:  82
Use of molecular symmetry disabled
Molecular charge:   0
Spin multiplicity:  1
```

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-.0606440	-.0345903	-.7339402
C	2	-.0704146	.0350048	.7328689
C	3	-.0825799	.1651736	3.5244068
C	4	-.0612439	-1.1355443	1.5030104
C	5	-.0900443	1.2708334	1.3880730
C	6	-.0979591	1.3447704	2.7732115
C	7	-.0657736	-1.0839746	2.8879570
H	8	-.0490176	-2.1106145	.9921004
H	9	-.1011522	2.1953095	.7907023
H	10	-.1237327	2.3176008	3.2855941
H	11	-.0600804	-2.0080514	3.4768723
O	12	-.1315007	.1201003	4.9052167
C	13	-.0360493	-.1645164	-3.5254054
C	14	-.0643485	1.1360445	-1.5039995
C	15	-.0484724	-1.2704724	-1.3892409
C	16	-.0378834	-1.3443096	-2.7743688
C	17	-.0509185	1.0846169	-2.8888871
H	18	-.0769969	2.1111014	-.9930832
H	19	-.0491982	-2.1950561	-.7919262
H	20	-.0385233	-2.3173386	-3.2870382
H	21	-.0557301	2.0087348	-3.4777409
O	22	-.0695041	-.1201766	-4.9067030
C	23	.2879380	-1.3045493	-5.5793133
C	24	.1928472	1.3117592	5.5817029
H	25	1.3774839	-1.4121337	-5.6133072
H	26	-.1094329	-1.1485767	-6.5848408
H	27	-.1490956	-2.2072061	-5.1264063
H	28	1.2793624	1.4432849	5.6272767
H	29	-.2115957	1.1467603	6.5829628
H	30	-.2590781	2.2047207	5.1242451

Point Group = C1 Order = 1 Nsymop = 1
This system has 84 degrees of freedom

Heat of Formation: -28.350 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	26.94			41.09			66.69		
		A			A			A	
	X	Y	Z	X	Y	Z	X	Y	Z
1	-.093	-.004	-.001	-.226	.000	-.001	.054	.016	.007
2	-.093	.002	-.001	-.226	-.004	-.001	-.056	.015	.006
3	-.030	.013	-.001	.037	-.007	-.001	-.156	.009	.003
4	-.323	.003	.003	-.029	-.003	-.003	.015	.015	.004
5	.154	.008	-.004	-.350	-.006	.000	-.227	.014	.006
6	.195	.014	-.004	-.221	-.008	.001	-.270	.010	.005
7	-.300	.008	.003	.108	-.004	-.003	-.038	.013	.005
8	-.147	.000	.002	.008	.000	-.002	.038	.005	.001
9	.090	.002	-.002	-.151	-.002	.000	-.090	.004	.001
10	.117	.006	-.002	-.086	-.004	.002	-.103	.001	.005
11	-.141	.003	.002	.082	-.001	-.001	.007	.004	.001
12	-.013	.037	.001	.275	-.005	.008	-.215	.042	.009
13	-.030	-.014	.000	.036	.007	.002	.157	.012	.004
14	-.323	-.009	-.007	-.029	.003	.003	-.018	.015	.003
15	.154	-.005	.006	-.351	.000	-.005	.226	.019	.008
16	.194	-.010	.007	-.222	.004	-.004	.271	.015	.008
17	-.300	-.014	-.007	.108	.006	.004	.037	.014	.006
18	-.147	-.002	-.004	.008	.001	.002	-.039	.004	.001
19	.090	-.001	.003	-.151	-.001	-.002	.089	.005	.002
20	.117	-.004	.003	-.087	.002	-.003	.103	.003	.006
21	-.141	-.005	-.003	.082	.003	.002	-.007	.004	.001
22	-.012	-.037	-.002	.274	.010	-.005	.218	.047	.012
23	.331	.059	.020	.322	-.002	.058	-.400	-.109	-.037
24	.331	-.052	-.015	.322	.008	-.054	.403	-.100	-.032
25	.104	.099	.021	.094	-.017	.082	-.129	-.146	-.075
26	.098	-.014	.000	.156	.008	-.007	-.159	.005	.012
27	.157	-.015	.001	.053	.005	-.011	-.182	.016	.019
28	.107	-.096	-.019	.094	.019	-.080	.133	-.143	-.073
29	.097	.016	.001	.156	-.005	.008	.158	.008	.013
30	.156	.019	.001	.052	-.004	.012	.181	.019	.021

Dipole moment: X = .598426 Y = .006273 Z = .006673
Total Dipole: .598496 Debye

Molecule is non-linear

Zero-point vibrational energy is 153.597 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy: .889 kcal/mol
Rotational Enthalpy: .889 kcal/mol
Vibrational Enthalpy: 160.825 kcal/mol

Translational Entropy: 41.987 cal/mol.K
Rotational Entropy: 32.617 cal/mol.K
Vibrational Entropy: 47.472 cal/mol.K

4,4'-DIMERCAPTOBIPHENYL

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 38
24 S shells
14 P shells

Number of basis functions: 66
Number of electrons: 70
Use of molecular symmetry disabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	.0008334	.0042127	-.7339512
C	2	-.0011590	-.0046478	.7339512
C	3	-.0047308	-.0220113	3.5437228
C	4	-.0026610	-1.2113540	1.4414258
C	5	-.0015129	1.1945384	1.4566962
C	6	-.0033002	1.1879799	2.8429535
C	7	-.0043923	-1.2211502	2.8289769
H	8	-.0023811	-2.1603559	.8831457
H	9	-.0003483	2.1499328	.9094120
H	10	-.0035253	2.1356720	3.3960680
H	11	-.0054998	-2.1814262	3.3582169
S	12	-.0073140	.0785775	5.2961242
C	13	.0049673	.0220264	-3.5437228
C	14	.0031924	1.2110341	-1.4412538
C	15	.0005296	-1.1948510	-1.4568639
C	16	.0026075	-1.1880579	-2.8431402
C	17	.0052915	1.2210655	-2.8287822
H	18	.0033840	2.1599135	-.8827281
H	19	-.0013532	-2.1503614	-.9098265
H	20	.0024780	-2.1356720	-3.3963948
H	21	.0071054	2.1814262	-3.3578683
S	22	.0064042	-.0781016	-5.2961593
H	23	.0190620	1.1957267	-5.6030533
H	24	-.0023564	-1.1951830	5.6034831

Point Group = C1 Order = 1 Nsymop = 1
This system has 66 degrees of freedom

Heat of Formation: 55.948 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)

	36.28			39.41			97.80		
	A			A			A		
	X	Y	Z	X	Y	Z	X	Y	Z
1	.047	.000	.000	-.261	.000	.000	.128	-.001	.000
2	.047	.000	.000	-.261	.000	.000	-.129	-.001	.000
3	.002	.000	.000	.028	.000	.000	-.183	.000	.000
4	.342	.000	.000	-.164	.000	.000	-.238	.000	.000
5	-.261	.000	.000	-.281	.000	.000	-.257	.000	-.001
6	-.293	.000	.000	-.139	.000	.000	-.290	.000	-.001
7	.329	.000	.000	-.018	.000	.000	-.269	.000	.000
8	.163	.000	.000	-.054	.000	.000	-.071	.000	.000
9	-.134	.000	.000	-.112	.000	.000	-.081	.000	.000
10	-.159	.000	.000	-.041	.000	.000	-.100	.000	.000
11	.166	.000	.000	.022	.000	.000	-.090	.000	.000
12	-.122	.000	.000	.524	.000	.001	.375	.001	.000
13	.002	.000	.000	.028	.000	.000	.183	.000	.000
14	.343	.000	.000	-.164	.000	.000	.238	-.001	.001
15	-.260	.000	.000	-.281	.000	.000	.258	-.001	.000
16	-.293	.000	.000	-.139	.000	.000	.291	.000	.000
17	.330	.000	.000	-.018	.000	.000	.268	.000	.001
18	.164	.000	.000	-.054	.000	.000	.071	.000	.000
19	-.134	.000	.000	-.112	.000	.000	.081	.000	.000
20	-.159	.000	.000	-.040	.000	.000	.100	.000	.000
21	.166	.000	.000	.022	.000	.000	.090	.000	.000
22	-.123	.000	.000	.524	-.001	.001	-.375	.002	.000
23	.075	-.001	.000	.114	.000	.001	-.016	.000	-.001
24	.075	.000	.000	.114	.000	.000	.016	.000	.000

Dipole moment: X = .017946 Y = -.000117 Z = .001022
Total Dipole: .017975 Debye

Molecule is non-linear

Zero-point vibrational energy is 109.957 kcal/mol

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Translational Enthalpy:	.889	kcal/mol
Rotational Enthalpy:	.889	kcal/mol
Vibrational Enthalpy:	116.191	kcal/mol
Translational Entropy:	42.041	cal/mol.K
Rotational Entropy:	32.526	cal/mol.K
Vibrational Entropy:	39.571	cal/mol.K

4,4'-DIPHOSPHINOBIPHENYL

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Run type: Single point energy
Numerical Frequency
Model: RHF/PM3
Number of shells: 40
26 S shells
14 P shells
Number of basis functions: 68
Number of electrons: 70
Use of molecular symmetry enabled
Molecular charge: 0
Spin multiplicity: 1

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	-.7344663	.0000000	.0027452
C	2	.7344663	.0000000	-.0027452
C	3	3.5403539	.0000000	-.0172858
C	4	1.4490252	-1.2035921	-.0056701
C	5	1.4490252	1.2035921	-.0056701
C	6	2.8378791	1.1998899	-.0124149
C	7	2.8378791	-1.1998899	-.0124149
H	8	.8956721	-2.1551157	-.0028448
H	9	.8956721	2.1551157	-.0028448
H	10	3.3829879	2.1509417	-.0153231
H	11	3.3829879	-2.1509417	-.0153231
P	12	5.3748549	.0000000	.1337330
C	13	-3.5403539	.0000000	.0172858
C	14	-1.4490252	1.2035921	.0056701
C	15	-1.4490252	-1.2035921	.0056701
C	16	-2.8378791	-1.1998899	.0124149
C	17	-2.8378791	1.1998899	.0124149
H	18	-.8956721	2.1551157	.0028448
H	19	-.8956721	-2.1551157	.0028448
H	20	-3.3829879	-2.1509417	.0153231
H	21	-3.3829879	2.1509417	.0153231
P	22	-5.3748549	.0000000	-.1337330
H	23	-5.6808992	1.0048745	.6859992
H	24	-5.6808992	-1.0048745	.6859992
H	25	5.6808992	1.0048745	-.6859992
H	26	5.6808992	-1.0048745	-.6859992

Point Group = CNH Order = 2 Nsymop = 4
This system has 20 degrees of freedom

Heat of Formation: 58.629 kcal/mol

Normal Modes and Vibrational Frequencies (cm-1)