JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1996, 118(42), 10257-10268, DOI:10.1021/ja960700x

	29.26 Au			31.40 Bg			36.71 Au	
	X	Y	Z	X	Y	Z	X	Y	Z
1	.000	.058	.000	.000	.017	.000	.000	.026	.000
2	.000	.058	.000	.000	-.017	.000	.000	.026	.000
3	.000	.056	.000	.000	-.084	.000	.000	.023	.000
4	-.002	.056	-.108	-.029	-.033	-.057	.000	.025	.291
5	.002	.056	.108	.029	-.033	.058	.000	.025	-.291
6	.003	.055	.107	.027	-.067	.063	.001	.024	-.301
7	-.003	.055	-.107	-.027	-.067	-.062	-.001	.024	.301
8	-.001	.016	-.053	-.015	-.006	-.030	.000	.007	.144
9	.001	.016	.053	.015	-.006	.030	.000	.007	-.144
10	-.001	.017	.053	.017	-.025	.035	-.001	.008	-.159
11	.001	.017	-.053	-.017	-.025	-.035	.001	.008	.159
12	.000	-.300	.000	.000	.216	-.001	.000	-.123	.000
13	.000	.056	.000	.000	.084	.000	.000	.023	.000
14	-.002	.056	-.108	.029	.033	.058	.000	.025	.291
15	.002	.056	.108	-.029	.033	-.057	.000	.025	-.291
16	.003	.055	.107	-.027	.067	-.062	.001	.024	-.301
17	-.003	.055	-.107	.027	.067	.063	-.001	.024	.301
18	-.001	.016	-.053	.015	.006	.030	.000	.007	.144
19	.001	.016	.053	-.015	.006	-.030	.000	.007	-.144
20	-.001	.017	.053	-.017	.025	-.035	-.001	.008	-.159
21	.001	.017	-.053	.017	.025	.035	.001	.008	.159
22	.000	-.300	.000	.000	-.216	-.001	.000	-.123	.000
23	-.017	.220	-.342	-.013	.261	-.371	-.010	.072	-.119
24	.017	.220	.342	.012	.261	.371	.010	.072	.119
25	.017	.220	.342	-.013	-.261	-.371	.010	.072	.119
26	-.017	.220	-.342	.012	-.261	.371	-.010	.072	-.119

Dipole moment: X = -.000211 Y = .000000 Z = .000020

Total Dipole: .000212 Debye

Zero-point vibrational energy is 117.911 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:	124.941	kcal/mol
Translational Entropy:	42.041	cal/mol.K
Rotational Entropy:	31.211	cal/mol.K
Vibrational Entropy:	49.295	cal/mol.K

CYCLOBIS(PARAQUAT-*p*-PHENYLENE), 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Mon Sep 25 17:39:38 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 220
144 S shells
76 P shells
Number of basis functions: 372
Number of electrons: 384
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 426 degrees of freedom

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	5.5381971	1.2492639	.5113708
N	2	4.8298563	-.0697422	.4195164
C	3	3.1530168	-2.2733390	.2145076
C	4	4.5755853	-.6123035	-.8165333
C	5	4.3736587	-.6768534	1.5642905
C	6	3.5344727	-1.7819271	1.4702240
C	7	3.7425559	-1.7184305	-.9283544
H	8	5.0655968	-.1640224	-1.7503635
H	9	4.7106399	-.2746021	2.5878334
H	10	3.1618526	-2.2728862	2.3902485
H	11	3.5358415	-2.1703709	-1.9402919
C	12	2.0965600	-3.2854078	.0879999
H	13	6.1326389	1.2889589	1.4508571
H	14	6.2692407	1.3385566	-.3224867
C	15	4.5346951	2.3646267	.4660547
N	16	-.1871414	-4.8363751	-.1643672
H	17	-4.2097127	-2.3729450	-2.6020723
C	18	1.4250105	-3.7539708	1.2253099
C	19	.2784821	-4.5276387	1.0907132
H	20	-2.5244846	-4.1871582	-2.5216474
C	21	1.6842205	-3.7388718	-1.1728461
H	22	1.8064906	-3.5014853	2.2335356
H	23	-.2757860	-4.9313893	2.0134888
C	24	-1.5487577	-5.4483543	-.3105411
H	25	-1.7398501	-6.1390905	.5402675
C	26	2.6319595	4.4066942	.3796657
C	27	3.9654835	2.8426367	1.6477513
C	28	4.1819688	2.9423294	-.7547993
C	29	3.2338239	3.9592406	-.7976886
C	30	3.0180254	3.8596153	1.6047026
H	31	4.2688675	2.4229011	2.6161504
H	32	4.6575761	2.6028820	-1.6844777
H	33	2.9676101	4.4132173	-1.7612260
H	34	2.5802580	4.2347082	2.5395198
C	35	1.5906072	5.4871802	.3328383
H	36	1.6304651	6.1152234	1.2501890
H	37	1.7713581	6.1754394	-.5220911
N	38	.2291144	4.8707060	.2053056
C	39	-2.0602378	3.3233634	-.0364439
C	40	-.2937368	4.6316667	-1.0428619
C	41	-.4384957	4.4779346	1.3399840
C	42	-1.5879262	3.7052972	1.2268262
C	43	-1.4428997	3.8598153	-1.1744012
H	44	.2181950	5.0964637	-1.9590159
H	45	-.0484169	4.8125593	2.3683294
H	46	-2.1293013	3.3861317	2.1383768
H	47	-1.8788507	3.6598894	-2.1972156
C	48	-3.1228018	2.3169121	-.1612166

H	49	-6.2335788	-1.3093559	.3256710
C	50	-3.6783472	1.7244866	.9812319
C	51	-3.5440622	1.8707908	-1.4211104
H	52	-4.7535663	.3939349	-2.5428529
C	53	-4.5133222	.6201765	.8613777
H	54	-3.4478168	2.1347332	1.9834597
H	55	-3.1995099	2.4097741	-2.3522987
C	56	-4.3805141	.7646207	-1.5226770
H	57	-4.9899093	.1348502	1.7880595
C	58	-5.4939528	-1.2069604	-.4989837
N	59	-4.7962167	.1158372	-.3848157
H	60	-6.0779519	-1.2412018	-1.4450704
C	61	-4.4860006	-2.3186878	-.4534703
C	62	.5357401	-4.5145015	-1.2879287
H	63	-2.9272799	-4.3707839	1.7773242
H	64	-1.5818619	-6.0728064	-1.2304842
C	65	-2.5859174	-4.3639757	-.3627833
C	66	-4.1368175	-2.8977070	.7677774
C	67	-3.9112687	-2.7946539	-1.6333301
C	68	-2.9651956	-3.8131534	-1.5882085
C	69	-3.1907661	-3.9162090	.8129215
H	70	-4.6125925	-2.5564015	1.6969304
H	71	.1891881	-4.9142261	-2.3069247
H	72	2.2769956	-3.4670441	-2.0962588
H	73	-3.0630086	5.5518993	-6.1951840
C	74	7.1462267	-.5166311	-5.5062474
C	75	-.4679917	-7.5360915	-5.7303673
C	76	6.4978229	-.1830206	-4.2642096
H	77	8.2188555	-.6996436	-5.3487943
H	78	7.0377309	.2985515	-6.2352922
H	79	-.4805116	-6.9900520	-6.6841034
N	80	5.9611081	.0583726	-3.2627220
H	81	6.6895706	-1.4313030	-5.9263278
H	82	-6.6631673	-.5708256	-6.9520740
H	83	-1.4044885	-8.1055238	-5.6433023
C	84	-3.5560391	4.5804539	-6.0487107
H	85	-4.6437781	4.7399633	-6.0606484
H	86	.3697315	-8.2479548	-5.7471458
H	87	-3.2901243	3.9249174	-6.8898025
C	88	-.3297795	-6.6217871	-4.6261998
C	89	4.0218830	-3.3067953	-4.5122194
N	90	3.4284975	-3.1204025	-3.5299238
C	91	4.7727253	-3.5277313	-5.7215886
H	92	5.5353945	-2.7370343	-5.8510872
H	93	4.1088237	-3.5166351	-6.5973501
H	94	5.2845059	-4.5002228	-5.6861826
C	95	-3.1472690	3.9917896	-4.7996411
N	96	-2.8218334	3.5207809	-3.7875474
N	97	-.2201459	-5.8896880	-3.7302617
C	98	1.1608161	6.9465110	-4.0256106
N	99	.8752610	6.1583900	-3.2205844
C	100	1.5165348	7.9296771	-5.0161323
H	101	2.5029990	8.3609638	-4.7930993
H	102	.7781323	8.7441945	-5.0318798
H	103	1.5542792	7.4741694	-6.0156535
C	104	-6.3779566	-.1621980	-4.9160426
N	105	-5.6833011	-.0340920	-3.9931363
C	106	-7.2461377	-.3229399	-6.0539036
H	107	-7.8046598	.6044329	-6.2455777
H	108	-7.9692681	-1.1315791	-5.8745674
C	109	4.2603519	-5.0616201	4.5932602
N	110	3.6781636	-4.3495973	3.8839164
C	111	4.9841733	-5.9460021	5.4706326
H	112	4.7761773	-5.7008764	6.5213768
H	113	6.0659759	-5.8563182	5.2997150
H	114	4.6905460	-6.9897275	5.2920239
C	115	-4.9421773	4.7737911	4.1725544
N	116	-4.2423016	4.1122923	3.5232219
C	117	-5.8113899	5.5958960	4.9753300
H	118	-5.6142808	6.6606294	4.7881752
H	119	-5.6525493	5.3949746	6.0438651
H	120	-6.8639602	5.3909989	4.7353502

C 121	-1.1764715	-6.5214810	4.2862389
N 122	-.9390383	-5.8471440	3.3700510
C 123	-1.4717265	-7.3630511	5.4169888
H 124	-1.2937691	-6.8217178	6.3568370
H 125	-.8349367	-8.2592701	5.4053270
H 126	-2.5227731	-7.6845057	5.3937277
C 127	-6.7312124	-.5525558	4.0246182
N 128	-6.0042025	-.4043486	3.1301983
C 129	-7.6379593	-.7370847	5.1281515
H 130	-8.5034477	-.0660974	5.0303445
H 131	-7.1346227	-.5194673	6.0806889
H 132	-8.0042623	-1.7732204	5.1564361
C 133	6.1057596	.2494310	5.0930501
N 134	5.5165698	.1616947	4.0951994
C 135	6.8424082	.3595537	6.3256063
H 136	6.1588218	.5298586	7.1692469
H 137	7.5512210	1.1986053	6.2766417
H 138	7.4096930	-.5623754	6.5176032
C 139	.4560779	6.2374491	4.8628535
N 140	.3763452	5.6282394	3.8764340
C 141	.5568908	6.9986281	6.0812475
H 142	1.3703412	7.7347595	6.0088638
H 143	.7617388	6.3359835	6.9338433
H 144	-.3814016	7.5371830	6.2763251

Heat of Formation: 1151.218 kcal/mol

BENZENE/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Mon Sep 25 17:43:08 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 238
156 S shells
82 P shells
Number of basis functions: 402
Number of electrons: 414
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 462 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 223 Heat of formation = 1174.158 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	2.9305256	.0389017	-4.8514342
N 2	3.4515425	.0350767	-3.4455288
C 3	3.9713513	.0160154	-.7192815
C 4	3.6537096	-1.1636640	-2.8053789
C 5	3.6464471	1.2266857	-2.7897743
C 6	3.9102583	1.2257939	-1.4242978
C 7	3.9214544	-1.1826452	-1.4424301
H 8	3.6160965	-2.1432063	-3.3976741
H 9	3.6056518	2.2096999	-3.3841668
H 10	4.0575703	2.1831979	-.8877759
H 11	4.0852192	-2.1627169	-.9104431
C 12	3.9713329	-.0034532	.7488878
H 13	3.3248971	.9279545	-5.3916837
H 14	3.3197374	-.8510484	-5.3940536
C 15	1.4285571	.0440242	-4.8478421

N	16	3.4247213	-.0410982	3.4649313
H	17	-1.2772986	-2.2113416	4.7671962
C	18	3.8791120	1.1935159	1.4722614
C	19	3.5992529	1.1665344	2.8331713
H	20	1.1991396	-2.2210477	4.7956618
C	21	3.9528650	-1.2176250	1.4500128
H	22	4.0135128	2.1620325	.9529967
H	23	3.5274775	2.1378126	3.4427035
C	24	2.8694425	-.0660794	4.8574306
H	25	3.2502631	.8120740	5.4245049
C	26	-1.3679802	.0557919	-4.8754376
C	27	.7308922	1.2535183	-4.8418538
C	28	.7213831	-1.1592690	-4.8853086
C	29	-.6700674	-1.1532513	-4.8984993
C	30	-.6602611	1.2593417	-4.8556707
H	31	1.2778686	2.2059423	-4.8410728
H	32	1.2605145	-2.1153189	-4.9211521
H	33	-1.2161440	-2.1048165	-4.9430838
H	34	-1.1992010	2.2163951	-4.8652805
C	35	-2.8698216	.0639492	-4.9103063
H	36	-3.2444064	.9587887	-5.4550610
H	37	-3.2546993	-.8197878	-5.4656642
N	38	-3.4213381	.0603038	-3.5160800
C	39	-3.9740376	.0400730	-.7993734
C	40	-3.6786691	-1.1361761	-2.8903300
C	41	-3.5875784	1.2541886	-2.8564886
C	42	-3.8694864	1.2522306	-1.4957944
C	43	-3.9615305	-1.1565313	-1.5291560
H	44	-3.6744793	-2.1010124	-3.5108970
H	45	-3.5078016	2.2386175	-3.4434082
H	46	-3.9963603	2.2107456	-.9564104
H	47	-4.1690566	-2.1350717	-1.0046200
C	48	-3.9819039	.0239354	.6691978
H	49	-3.3166312	.8384098	5.3532036
C	50	-3.8841390	1.2203797	1.3932193
C	51	-3.9781794	-1.1884247	1.3725878
H	52	-3.7162317	-2.1764724	3.3360282
C	53	-3.6184124	1.1922711	2.7569056
H	54	-4.0040448	2.1906315	.8735707
H	55	-4.1798820	-2.1551411	.8242757
C	56	-3.7116545	-1.1981054	2.7371534
H	57	-3.5452719	2.1636124	3.3659037
C	58	-2.9316918	-.0433881	4.7945580
N	59	-3.4614271	-.0158887	3.3922574
H	60	-3.3242087	-.9399597	5.3233802
C	61	-1.4294803	-.0498518	4.7857088
C	62	3.6737730	-1.2248877	2.8122175
H	63	1.2150800	2.0996738	4.8912431
H	64	3.2446366	-.9664013	5.3924480
C	65	1.3676354	-.0607914	4.8175059
C	66	-.7222391	1.1532675	4.8277231
C	67	-.7310333	-1.2588623	4.7734529
C	68	.6602792	-1.2643377	4.7894090
C	69	.6690543	1.1478201	4.8436079
H	70	-1.2617461	2.1093756	4.8629604
H	71	3.6665059	-2.2036471	3.4111750
H	72	4.1453444	-2.1894843	.9058950
H	73	-6.5860485	-6.0203285	-1.1635012
C	74	5.1773772	-6.0304023	-4.3939698
C	75	4.9372088	-5.5055441	5.9602147
C	76	4.5207558	-4.7575790	-4.2417046
H	77	6.0350622	-5.9468516	-5.0767612
H	78	4.4848351	-6.7816177	-4.7987463
H	79	4.4767556	-6.4629740	5.6787292
N	80	4.0025074	-3.7290253	-4.0905609
H	81	5.5417154	-6.3777371	-3.4099552
H	82	-4.5118354	-6.4266674	5.6344734
H	83	4.7256161	-5.3167652	7.0224968
C	84	-6.2277929	-5.8118136	-.1454660
H	85	-7.1014816	-5.7109689	.5142738
H	86	6.0259961	-5.5918611	5.8341090
H	87	-5.6300848	-6.6687684	.1954246

C	88	4.4192353	-4.4366986	5.1456565
C	89	5.1802181	-4.7216019	-.2959836
N	90	4.6593037	-3.7092623	-.0603547
C	91	5.8288631	-5.9695728	-.6073918
H	92	5.7500593	-6.1843391	-1.6896176
H	93	5.3630782	-6.7970938	-.0541658
H	94	6.8942636	-5.9286749	-.3387660
C	95	-5.4404912	-4.6061644	-.1259653
N	96	-4.8110288	-3.6286104	-.1101245
N	97	4.0043131	-3.5690703	4.4931726
C	98	-4.3918302	-4.2864818	-5.3247031
N	99	-3.9989790	-3.4395605	-4.6325160
C	100	-4.8818339	-5.3293965	-6.1887131
H	101	-4.5197009	-5.1796877	-7.2159852
H	102	-5.9812037	-5.3295976	-6.2057850
H	103	-4.5385510	-6.3131670	-5.8389916
C	104	-4.4733089	-4.4062001	5.0778893
N	105	-4.0632823	-3.5416881	4.4181988
C	106	-4.9848905	-5.4712181	5.9014934
H	107	-6.0717653	-5.5712843	5.7693187
H	108	-4.7826644	-5.2676016	6.9628703
C	109	6.9016787	4.3695941	.0820806
N	110	5.9572279	3.6937846	.0632585
C	111	8.0751022	5.2052608	.1052749
H	112	7.7926572	6.2664721	.0676111
H	113	8.7202565	4.9858879	-.7567979
H	114	8.6528392	5.0311915	1.0236420
C	115	-6.8496672	4.4326682	-.0330152
N	116	-5.9099692	3.7500342	-.0335043
C	117	-8.0172566	5.2768017	-.0324907
H	118	-8.6366976	5.0765343	-.9177558
H	119	-7.7262092	6.3362911	-.0436808
H	120	-8.6246515	5.0921070	.8644242
C	121	4.1154499	4.5048988	5.0407846
N	122	3.7568849	3.5613364	4.4648927
C	123	4.5633098	5.6698095	5.7593993
H	124	4.3529238	6.5820270	5.1835401
H	125	5.6461143	5.6153876	5.9422259
H	126	4.0514178	5.7442912	6.7294248
C	127	-4.1357884	4.5405369	4.9488062
N	128	-3.7761376	3.5918119	4.3821592
C	129	-4.5851464	5.7118927	5.6559262
H	130	-5.6751995	5.6810905	5.7961572
H	131	-4.3320491	6.6218187	5.0938049
H	132	-4.1099888	5.7701996	6.6455524
C	133	4.2458322	4.5829401	-4.9504984
N	134	3.8700046	3.6385343	-4.3871017
C	135	4.7150212	5.7487801	-5.6538045
H	136	4.2672515	6.6595112	-5.2318267
H	137	4.4471668	5.6898027	-6.7184637
H	138	5.8086574	5.8299847	-5.5757338
C	139	-4.0730608	4.6448601	-4.9910221
N	140	-3.7233162	3.6863120	-4.4347890
C	141	-4.5099129	5.8284366	-5.6855121
H	142	-4.3063994	5.7400146	-6.7623238
H	143	-3.9849691	6.7152715	-5.3034450
H	144	-5.5904967	5.9772743	-5.5482265
H	145	.0159961	2.5524825	-.0076675
C	146	.0080245	1.4567210	-.0172296
C	147	-.0135349	-1.3303307	-.0415440
C	148	.0058700	.7693361	-1.2266320
C	149	-.0004810	.7483859	1.1800139
C	150	-.0111780	-.6430470	1.1678438
C	151	-.0049232	-.6221016	-1.2387633
H	152	.0120564	1.3213021	-2.1765126
H	153	.0006168	1.2837727	2.1391612
H	154	-.0182059	-1.1953091	2.1175156
H	155	-.0069034	-1.1577028	-2.1977356
H	156	-.0227774	-2.4258730	-.0510159

Heat of Formation: 1174.158 kcal/mol

TOLUENE/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Sep 28 08:29:45 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 242
159 S shells
83 P shells
Number of basis functions: 408
Number of electrons: 420
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 471 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 212 Heat of formation = 1163.166 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9337441	4.8677960	.3244445
N	2	3.4259944	3.4519687	.3499281
C	3	3.8940322	.7166391	.3645321
C	4	3.6557428	2.8000353	-.8372811
C	5	3.5609854	2.7997269	1.5514847
C	6	3.7957558	1.4290580	1.5673148
C	7	3.8986312	1.4324334	-.8393153
H	8	3.6645724	3.3866260	-1.8217906
H	9	3.5011878	3.4017216	2.5288418
H	10	3.8988904	.8960626	2.5323562
H	11	4.0909291	.8933943	-1.8108424
C	12	3.8960406	-.7513824	.3529426
H	13	3.3445306	5.4186480	1.1993037
H	14	3.3256003	5.3845432	-.5796330
C	15	1.4324886	4.8861378	.3307316
N	16	3.4059337	-3.4777322	.3102347
H	17	-1.2540780	-4.3359918	-1.8292046
C	18	3.7678223	-1.4697204	1.5494019
C	19	3.5198371	-2.8367482	1.5200078
H	20	1.2211484	-4.3645043	-1.8331223
C	21	3.9339866	-1.4577579	-.8575278
H	22	3.8567043	-.9435814	2.5193655
H	23	3.4302939	-3.4441104	2.4911484
C	24	2.8800547	-4.8809401	.2698733
H	25	3.2750082	-5.4488908	1.1410694
C	26	-1.3614282	4.9137235	.3445704
C	27	.7400250	5.1501947	1.5124010
C	28	.7222057	4.6653055	-.8519681
C	29	-.6672965	4.6784826	-.8449045
C	30	-.6520734	5.1640173	1.5192395
H	31	1.2882242	5.3556382	2.4414171
H	32	1.2590661	4.4910939	-1.7943342
H	33	-1.2167141	4.5126861	-1.7814740
H	34	-1.1869505	5.3797399	2.4537332
C	35	-2.8629535	4.9258032	.3536621
H	36	-3.2531096	5.4783204	1.2368812
H	37	-3.2526364	5.4581820	-.5420049
N	38	-3.3844327	3.5204783	.3749189
C	39	-3.8819434	.7935027	.3809354
C	40	-3.6663052	2.8849184	-.8106425
C	41	-3.4916307	2.8613964	1.5756057
C	42	-3.7423155	1.4947201	1.5865937

C	43	-3.9237732	1.5186710	-.8175736
H	44	-3.7035616	3.5014220	-1.7780825
H	45	-3.3949578	3.4541843	2.5549111
H	46	-3.8249802	.9563879	2.5504147
H	47	-4.1584107	.9885802	-1.7874747
C	48	-3.8885591	-.6748825	.3695565
H	49	-3.3210764	-5.3798721	1.1500834
C	50	-3.7552764	-1.3960352	1.5641004
C	51	-3.9372607	-1.3809477	-.8400596
H	52	-3.7385741	-3.3503069	-1.8312235
C	53	-3.5187170	-2.7649387	1.5319917
H	54	-3.8323397	-.8718738	2.5361755
H	55	-4.1667248	-.8336083	-1.8016746
C	56	-3.6938489	-2.7496794	-.8542187
H	57	-3.4287897	-3.3733704	2.5022176
C	58	-2.9177226	-4.8186829	.2783062
N	59	-3.4189338	-3.4066397	.3213370
H	60	-3.3109973	-5.3296551	-.6282197
C	61	-1.4161851	-4.8324135	.2754052
C	62	3.6808650	-2.8248487	-.8676016
H	63	1.2153366	-5.4241455	2.3581408
H	64	3.2611761	-5.3997817	-.6373921
C	65	1.3784204	-4.8640773	.2710804
C	66	-.7166862	-5.1500332	1.4395290
C	67	-.7121628	-4.5567548	-.8996201
C	68	.6771555	-4.5725746	-.9018004
C	69	.6755940	-5.1659038	1.4373710
H	70	-1.2592776	-5.3958800	2.3620321
H	71	3.7169403	-3.4274833	-1.8443210
H	72	4.1551088	-.9163696	-1.8254345
H	73	-6.8361384	1.1001794	-5.5061514
C	74	5.3758636	4.3636091	-5.6507230
C	75	5.0697148	-6.0093642	-5.0883861
C	76	4.6779601	4.2196115	-4.3990970
H	77	6.2394375	5.0350001	-5.5400497
H	78	4.7125054	4.7776747	-6.4228874
H	79	4.6685426	-5.7042632	-6.0650402
N	80	4.1262377	4.0746446	-3.3872752
H	81	5.7377592	3.3748346	-5.9868405
H	82	-4.6754638	-5.6592112	-6.0433715
H	83	4.8073907	-7.0634707	-4.9184859
C	84	-6.3525362	.1202889	-5.3868455
H	85	-7.1377300	-.6463096	-5.3204272
H	86	6.1655553	-5.9259654	-5.1201495
H	87	-5.7446715	-.0792905	-6.2803556
C	88	4.5319727	-5.1811294	-4.0400102
C	89	5.2907201	.2671831	-4.3218960
N	90	4.7445069	.0380931	-3.3216003
C	91	5.9715705	.5698440	-5.5548117
H	92	5.9110284	1.6527228	-5.7721549
H	93	5.5182055	.0215415	-6.3923685
H	94	7.0323879	.2883633	-5.4892585
C	95	-5.5324280	.1046053	-4.2031753
N	96	-4.8769198	.0919375	-3.2430073
N	97	4.1009949	-4.5177075	-3.1887230
C	98	-4.4860901	5.3189404	-3.9381866
N	99	-4.0750221	4.6225391	-3.1035087
C	100	-4.9984827	6.1883397	-4.9657511
H	101	-4.6274914	7.2133703	-4.8225276
H	102	-6.0973902	6.2107229	-4.9376789
H	103	-4.6823188	5.8398120	-5.9589661
C	104	-4.5557200	-5.1128999	-4.0233096
N	105	-4.1297604	-4.4414336	-3.1757946
C	106	-5.0869455	-5.9512495	-5.0669968
H	107	-6.1821068	-5.8642152	-5.1100398
H	108	-4.8303638	-7.0042989	-4.8823364
C	109	6.7204302	-.0591991	4.7740588
N	110	5.7902359	-.0445046	4.0786839
C	111	7.8762524	-.0773263	5.6340528
H	112	7.5705592	-.0999642	6.6892278
H	113	8.4920641	.8177078	5.4691787
H	114	8.4925540	-.9641397	5.4310095

C 115	-6.6585441	.0405981	4.8218563
N 116	-5.7318262	.0388478	4.1217379
C 117	-7.8101219	.0428552	5.6877240
H 118	-8.4435129	.9170583	5.4825972
H 119	-7.4995364	.0774494	6.7411368
H 120	-8.4103251	-.8642161	5.5313923
C 121	4.0004506	-5.0051616	4.8881136
N 122	3.6585336	-4.4485239	3.9270705
C 123	4.4284196	-5.6999180	6.0748329
H 124	4.1968252	-5.1085501	6.9718367
H 125	5.5129939	-5.8778680	6.0454728
H 126	3.9200788	-6.6711559	6.1569704
C 127	-4.0058091	-4.9219526	4.9060700
N 128	-3.6610748	-4.3734059	3.9413977
C 129	-4.4373422	-5.6066422	6.0973444
H 130	-5.5330512	-5.6957859	6.1133227
H 131	-4.1196850	-5.0564611	6.9941964
H 132	-4.0069424	-6.6173902	6.1378989
C 133	4.1274845	4.9552784	4.9153674
N 134	3.7656141	4.4011239	3.9601804
C 135	4.5799835	5.6471275	6.0946361
H 136	4.1274137	5.2095126	6.9955436
H 137	4.3037875	6.7101995	6.0471038
H 138	5.6734336	5.5770918	6.1849837
C 139	-3.9482601	4.9840709	4.9764646
N 140	-3.6121949	4.4395623	4.0064430
C 141	-4.3688068	5.6640175	6.1743574
H 142	-4.0760935	6.7231155	6.1388165
H 143	-3.9078704	5.2046827	7.0600731
H 144	-5.4615125	5.6101209	6.2828649
H 145	.0997983	.0659126	-.7669641
C 146	.0207489	.0706713	-1.8580512
C 147	-.1807531	.0827227	-4.6424448
C 148	-.0331438	1.2773822	-2.5476002
C 149	-.0271483	-1.1301934	-2.5584785
C 150	-.1277566	-1.1261261	-3.9446347
C 151	-.1342279	1.2853281	-3.9339064
H 152	.0031473	2.2287978	-2.0008152
H 153	.0138032	-2.0861310	-2.0202250
H 154	-.1664759	-2.0733414	-4.4955661
H 155	-.1794632	2.2376913	-4.4754354
C 156	-.2740326	.0875302	-6.1246979
H 157	.7298823	.0537427	-6.5706095
H 158	-.7716644	.9907562	-6.5024327
H 159	-.8303004	-.7810786	-6.5019422

Heat of Formation: 1163.166 kcal/mol

PHENOL/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Sep 28 08:28:49 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 240
157 S shells
83 P shells
Number of basis functions: 406
Number of electrons: 420
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 465 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 220 Heat of formation = 1126.533 rmsG = .0000 rmsD = .0001

Atom		Cartesian Coordinates (Angstroms) X	Y	Z
C	1	2.9297951	4.8753342	.2806503
N	2	3.4057783	3.4534576	.3022883
C	3	3.8561176	.7143693	.3150524
C	4	3.6257134	2.7998009	-.8856596
C	5	3.5381920	2.7993863	1.5032332
C	6	3.7638871	1.4273348	1.5181148
C	7	3.8593876	1.4303925	-.8886617
H	8	3.6341001	3.3872045	-1.8691516
H	9	3.4832892	3.4013029	2.4808653
H	10	3.8650838	.8938531	2.4830229
H	11	4.0442234	.8901324	-1.8606445
C	12	3.8569825	-.7538457	.3046884
H	13	3.3426509	5.4186891	1.1591707
H	14	3.3315797	5.3906055	-.6198233
C	15	1.4289627	4.9077681	.2855689
N	16	3.3797478	-3.4832401	.2669108
H	17	-1.2699471	-4.7485433	-1.9197077
C	18	3.7289994	-1.4704120	1.5022459
C	19	3.4878006	-2.8386295	1.4752963
H	20	1.2098506	-4.7781247	-1.9258952
C	21	3.8973122	-1.4624853	-.9044577
H	22	3.8131712	-.9424418	2.4714877
H	23	3.3982734	-3.4439964	2.4474188
C	24	2.8725160	-4.8939606	.2320746
H	25	3.2687375	-5.4523790	1.1088574
C	26	-1.3642005	4.9370482	.3001049
C	27	.7356477	5.0422949	1.4891013
C	28	.7204385	4.8253274	-.9149803
C	29	-.6698814	4.8395886	-.9075801
C	30	-.6556052	5.0568768	1.4963134
H	31	1.2844363	5.1432844	2.4349552
H	32	1.2579443	4.7564256	-1.8706112
H	33	-1.2185279	4.7805604	-1.8574124
H	34	-1.1923533	5.1686716	2.4479258
C	35	-2.8655992	4.9365638	.3112777
H	36	-3.2569011	5.4827829	1.1978477
H	37	-3.2652735	5.4671630	-.5809460
N	38	-3.3722530	3.5252983	.3301427
C	39	-3.8531129	.7943810	.3363927
C	40	-3.6480710	2.8874045	-.8554003
C	41	-3.4742709	2.8649037	1.5306756
C	42	-3.7164905	1.4968192	1.5417991
C	43	-3.8962999	1.5192461	-.8621976
H	44	-3.6890013	3.5036305	-1.8224490
H	45	-3.3801173	3.4581072	2.5099926
H	46	-3.7953807	.9585722	2.5058999
H	47	-4.1254069	.9875352	-1.8320791
C	48	-3.8594187	-.6742246	.3267450
H	49	-3.3271617	-5.3799868	1.1249368
C	50	-3.7260216	-1.3933815	1.5224416
C	51	-3.9120078	-1.3828967	-.8813182
H	52	-3.7257274	-3.3552147	-1.8669949
C	53	-3.4976983	-2.7637431	1.4930650
H	54	-3.7970509	-.8670681	2.4936852
H	55	-4.1382234	-.8360793	-1.8437359
C	56	-3.6768552	-2.7532015	-.8926117
H	57	-3.4075296	-3.3699414	2.4645157
C	58	-2.9242416	-4.8291608	.2463519
N	59	-3.4054720	-3.4095001	.2840260
H	60	-3.3332401	-5.3399568	-.6531704
C	61	-1.4231004	-4.8612552	.2385127
C	62	3.6511479	-2.8310189	-.9119621
H	63	1.2154042	-5.0894143	2.3840625
H	64	3.2669583	-5.4126938	-.6694171
C	65	1.3708862	-4.8943697	.2315679
C	66	-.7200699	-4.9768883	1.4382126

C	67	-.7234525	-4.7983474	-.9686543
C	68	.6669665	-4.8150021	-.9721523
C	69	.6713187	-4.9934492	1.4347569
H	70	-1.2615372	-5.0600081	2.3902287
H	71	3.6899629	-3.4348002	-1.8861494
H	72	4.1143245	-.9212520	-1.8729566
H	73	-6.9002217	1.0676446	-5.4734100
C	74	5.3464157	4.3712231	-5.6956668
C	75	5.1169509	-5.9975762	-5.1122948
C	76	4.6490953	4.2283210	-4.4435889
H	77	6.2136571	5.0377904	-5.5845610
H	78	4.6844207	4.7903533	-6.4662656
H	79	4.8897680	-5.5813636	-6.1037894
N	80	4.0975878	4.0844675	-3.4314875
H	81	5.7026608	3.3812553	-6.0342090
H	82	-4.8798782	-5.5446146	-6.0837905
H	83	4.7150164	-7.0197520	-5.0636439
C	84	-6.3060199	.1434047	-5.4400449
H	85	-6.9969502	-.7115459	-5.4525740
H	86	6.2093398	-6.0490982	-4.9981203
H	87	-5.6796261	.0989452	-6.3419203
C	88	4.5407299	-5.1794453	-4.0765055
C	89	5.2402908	.2668741	-4.3743501
N	90	4.6945151	.0333665	-3.3748255
C	91	5.9206174	.5743281	-5.6063830
H	92	5.8633306	1.6585364	-5.8178493
H	93	5.4644916	.0321580	-6.4464367
H	94	6.9806146	.2891662	-5.5436415
C	95	-5.4890410	.1130016	-4.2544802
N	96	-4.8359304	.0887110	-3.2928959
N	97	4.0785681	-4.5241090	-3.2352218
C	98	-4.4974233	5.3145702	-3.9803052
N	99	-4.0763499	4.6235382	-3.1461484
C	100	-5.0222145	6.1774789	-5.0071012
H	101	-4.5213390	7.1558264	-4.9805938
H	102	-6.1004610	6.3362811	-4.8616707
H	103	-4.8664141	5.7339215	-6.0005138
C	104	-4.5767185	-5.1053566	-4.0567662
N	105	-4.1201449	-4.4434616	-3.2175494
C	106	-5.1456531	-5.9317148	-5.0900791
H	107	-6.2417547	-5.9522815	-5.0058387
H	108	-4.7727016	-6.9626751	-5.0072621
C	109	6.7041912	-.0591187	4.7121131
N	110	5.7725144	-.0458537	4.0187232
C	111	7.8618269	-.0753926	5.5697110
H	112	7.5591314	-.0432457	6.6255032
H	113	8.5039813	.7925175	5.3650746
H	114	8.4502142	-.9885054	5.4039093
C	115	-6.6508850	.0461193	4.7627827
N	116	-5.7224612	.0421455	4.0649486
C	117	-7.8045545	.0512360	5.6258703
H	118	-8.5185090	.8239812	5.3085938
H	119	-7.5078153	.2562882	6.6637671
H	120	-8.3119173	-.9229493	5.5951181
C	121	3.9796099	-5.0007377	4.8467046
N	122	3.6317391	-4.4466215	3.8862977
C	123	4.4144484	-5.6925974	6.0325922
H	124	4.0763731	-5.1620654	6.9338187
H	125	5.5116077	-5.7584116	6.0581644
H	126	4.0055907	-6.7128478	6.0548574
C	127	-3.9934377	-4.9116726	4.8724691
N	128	-3.6439332	-4.3667164	3.9074315
C	129	-4.4304496	-5.5920963	6.0641619
H	130	-5.5126139	-5.7819568	6.0229665
H	131	-4.2172964	-4.9842297	6.9546920
H	132	-3.9131973	-6.5564704	6.1686130
C	133	4.1204474	4.9554491	4.8653250
N	134	3.7540214	4.4002153	3.9124902
C	135	4.5783301	5.6487297	6.0416550
H	136	4.2864584	5.1017192	6.9491671
H	137	4.1435551	6.6573977	6.0878052
H	138	5.6735957	5.7437926	6.0293682

C 139	-3.9420012	4.9896585	4.9297776
N 140	-3.6025350	4.4431012	3.9620753
C 141	-4.3664513	5.6723072	6.1247358
H 142	-3.9691357	6.6971652	6.1443709
H 143	-4.0083589	5.1426606	7.0187146
H 144	-5.4637672	5.7252751	6.1674358
H 145	.0479067	.9516462	-1.1146838
C 146	.0004294	.7301250	-2.1856423
C 147	-.1215353	.1543537	-4.9184336
C 148	-.0373832	1.7586402	-3.1195350
C 149	-.0236977	-.5954485	-2.6360702
C 150	-.0843275	-.8913831	-4.0039398
C 151	-.0982843	1.4755179	-4.4799690
H 152	-.0194555	2.8012263	-2.7758687
O 153	.0149856	-1.5617239	-1.6632474
H 154	-.1028083	-1.9289632	-4.3579208
H 155	-.1297333	2.2925543	-5.2091395
H 156	-.1701502	-.0646053	-5.9915572
H 157	-.0063978	-2.4126273	-2.0888762

Heat of Formation: 1126.533 kcal/mol

ANISOLE1/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Mon Oct 2 06:45:02 1995
Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 244
160 S shells
84 P shells
Number of basis functions: 412
Number of electrons: 426
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 474 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 125 Heat of formation = 1132.798 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	2.9317699	4.8694740	.3932931
N 2	3.3999067	3.4450223	.4242190
C 3	3.8370940	.7038908	.4584937
C 4	3.6077428	2.7795455	-.7592459
C 5	3.5360309	2.8008145	1.6300635
C 6	3.7555149	1.4279554	1.6556941
C 7	3.8339908	1.4088182	-.7516648
H 8	3.6138571	3.3590819	-1.7477567
H 9	3.4894606	3.4115372	2.6028180
H 10	3.8611666	.9029565	2.6248430
H 11	4.0110025	.8591228	-1.7201582
C 12	3.8378237	-.7644097	.4618267
H 13	3.3454145	5.4162029	1.2693252
H 14	3.3380728	5.3770605	-.5095193
C 15	1.4311552	4.9078443	.3958182
N 16	3.3744666	-3.4967305	.4529968
H 17	-1.2603456	-4.7054617	-1.7266782
C 18	3.7142900	-1.4692529	1.6669350
C 19	3.4785453	-2.8384522	1.6544711

H	20	1.2137210	-4.7356006	-1.7256424
C	21	3.8784396	-1.4849822	-.7399519
H	22	3.7992633	-.9314089	2.6306975
H	23	3.3914513	-3.4338447	2.6331605
C	24	2.8717213	-4.9095344	.4336942
H	25	3.2688823	-5.4566177	1.3170409
C	26	-1.3616038	4.9369575	.4055856
C	27	.7357613	5.0253698	1.6000804
C	28	.7251796	4.8457546	-.8072565
C	29	-.6653096	4.8596856	-.8022352
C	30	-.6553070	5.0399736	1.6048875
H	31	1.2830814	5.1126930	2.5481374
H	32	1.2647693	4.7928930	-1.7629679
H	33	-1.2121323	4.8157695	-1.7541034
H	34	-1.1940982	5.1382001	2.5568537
C	35	-2.8629424	4.9311599	.4142604
H	36	-3.2575204	5.4811319	1.2970268
H	37	-3.2640936	5.4543160	-.4816924
N	38	-3.3627958	3.5174683	.4410622
C	39	-3.8321858	.7844329	.4661785
C	40	-3.6290418	2.8689958	-.7408269
C	41	-3.4672533	2.8657232	1.6461289
C	42	-3.7043793	1.4969206	1.6666882
C	43	-3.8700000	1.4994158	-.7383889
H	44	-3.6709675	3.4784021	-1.7124065
H	45	-3.3796137	3.4667415	2.6214112
H	46	-3.7872872	.9664707	2.6348275
H	47	-4.0912046	.9591738	-1.7056978
C	48	-3.8394820	-.6842564	.4689295
H	49	-3.3327002	-5.3852538	1.3134329
C	50	-3.7128886	-1.3927947	1.6718712
C	51	-3.8911484	-1.4038460	-.7324053
H	52	-3.7241406	-3.3894518	-1.6970238
C	53	-3.4908757	-2.7641923	1.6562336
H	54	-3.7857156	-.8574274	2.6380454
H	55	-4.1097603	-.8651721	-1.7013930
C	56	-3.6666135	-2.7763047	-.7295677
H	57	-3.4058264	-3.3614824	2.6338264
C	58	-2.9240194	-4.8442645	.4315435
N	59	-3.4006549	-3.4225489	.4536830
H	60	-3.3298490	-5.3619875	-.4653845
C	61	-1.4231662	-4.8788747	.4289815
C	62	3.6424018	-2.8555768	-.7325957
H	63	1.2081937	-5.1600648	2.5767594
H	64	3.2678153	-5.4369165	-.4619729
C	65	1.3703577	-4.9121404	.4300191
C	66	-.7240279	-5.0241082	1.6280442
C	67	-.7199025	-4.7880167	-.7738007
C	68	.6703330	-4.8047450	-.7732968
C	69	.6671631	-5.0406822	1.6285855
H	70	-1.2684413	-5.1305830	2.5758440
H	71	3.6911270	-3.4713455	-1.6993505
H	72	4.0897674	-.9527116	-1.7149810
H	73	-6.8941825	.9380155	-5.3399500
C	74	5.2922660	4.3063547	-5.5980292
C	75	5.2389994	-6.0949685	-4.8245440
C	76	4.6136561	4.1796280	-4.3340006
H	77	6.1670974	4.9658499	-5.5060060
H	78	4.6217771	4.7253182	-6.3612930
H	79	4.9321486	-5.7762969	-5.8306071
N	80	4.0769742	4.0489997	-3.3122299
H	81	5.6341225	3.3105890	-5.9343018
H	82	-4.9948940	-5.6835923	-5.8271755
H	83	4.9371678	-7.1428587	-4.6844182
C	84	-6.1911720	.0930024	-5.3546638
H	85	-6.7702798	-.8358529	-5.4554153
H	86	6.3351823	-6.0387223	-4.7604640
H	87	-5.5407805	.1955911	-6.2345120
C	88	4.6325550	-5.2574698	-3.8219763
C	89	5.1790087	.2121411	-4.2410534
N	90	4.6529853	-.0098548	-3.2284600
C	91	5.8350821	.5053802	-5.4895714

H	92	5.7823559	1.5885585	-5.7072626
H	93	5.3561502	-.0384446	-6.3157017
H	94	6.8937285	.2115913	-5.4477681
C	95	-5.4077246	.0692185	-4.1465414
N	96	-4.7817333	.0505665	-3.1670368
N	97	4.1462265	-4.5864282	-3.0072010
C	98	-4.5057165	5.2697494	-3.8765407
N	99	-4.0779934	4.5907902	-3.0359339
C	100	-5.0390429	6.1178419	-4.9112591
H	101	-4.6461109	7.1398273	-4.8115297
H	102	-6.1357620	6.1606315	-4.8459608
H	103	-4.7637787	5.7348360	-5.9039261
C	104	-4.6636302	-5.1822817	-3.8189944
N	105	-4.1842661	-4.5033779	-3.0065901
C	106	-5.2611860	-6.0296876	-4.8186089
H	107	-6.3566771	-6.0207724	-4.7251110
H	108	-4.9122525	-7.0658864	-4.7030824
C	109	6.6854077	-.0331880	4.8695922
N	110	5.7535840	-.0240709	4.1763296
C	111	7.8432854	-.0442163	5.7269499
H	112	7.5666228	.2423205	6.7510136
H	113	8.6001161	.6629060	5.3598314
H	114	8.2910033	-1.0472740	5.7553836
C	115	-6.6277609	.0761299	4.9097338
N	116	-5.6999716	.0675004	4.2111006
C	117	-7.7806587	.0868684	5.7737944
H	118	-8.2976701	1.0545437	5.7128146
H	119	-7.4811207	-.0823832	6.8173246
H	120	-8.4871840	-.7025023	5.4818402
C	121	3.9681841	-4.9632030	5.0510358
N	122	3.6246961	-4.4171927	4.0844580
C	123	4.3976842	-5.6450271	6.2446665
H	124	4.1332194	-5.0615619	7.1377397
H	125	5.4875308	-5.7895474	6.2332302
H	126	3.9181453	-6.6314960	6.3183125
C	127	-4.0010108	-4.8793805	5.0547158
N	128	-3.6500105	-4.3409563	4.0865862
C	129	-4.4399023	-5.5517998	6.2502645
H	130	-5.5377723	-5.6006813	6.2822259
H	131	-4.0890181	-5.0168294	7.1439364
H	132	-4.0464033	-6.5778355	6.2814143
C	133	4.1367765	4.9900323	4.9682879
N	134	3.7668502	4.4237450	4.0233375
C	135	4.5989135	5.6970476	6.1347303
H	136	4.3441603	5.1412277	7.0480483
H	137	4.1343347	6.6918026	6.1912289
H	138	5.6902015	5.8258643	6.0983576
C	139	-3.9493181	5.0172465	5.0271922
N	140	-3.6072225	4.4622561	4.0652254
C	141	-4.3769131	5.7103385	6.2149905
H	142	-3.9031035	6.7005492	6.2745972
H	143	-4.1042253	5.1390220	7.1134469
H	144	-5.4676867	5.8480437	6.2075219
H	145	.0715024	.6647557	-1.9175278
C	146	.0182077	.8375897	-2.9972422
C	147	-.1179815	1.2763583	-5.7501507
C	148	-.0126342	2.1311233	-3.5002986
C	149	-.0204217	-.2448782	-3.8892843
C	150	-.0881361	-.0286360	-5.2696128
C	151	-.0804492	2.3541601	-4.8720796
H	152	.0161234	2.9835336	-2.8097208
O	153	.0135216	-1.4825702	-3.2730620
H	154	-.1189614	-.8634113	-5.9802053
H	155	-.1056847	3.3775470	-5.2614432
H	156	-.1725504	1.4530642	-6.8309289
C	157	-.0146041	-2.6185077	-4.1042090
H	158	.8545516	-2.6690264	-4.7699775
H	159	-.9366391	-2.6805837	-4.6935587
H	160	.0213546	-3.4370837	-3.3770429

Heat of Formation: 1132.798 kcal/mol

ANISOLE2/1^{4+} , 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Fri Oct 6 11:17:51 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 244
160 S shells
84 P shells
Number of basis functions: 412
Number of electrons: 426
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 474 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 154 Heat of formation = 1134.316 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9463102	4.8693545	.4427378
N	2	3.4379978	3.4532367	.4627127
C	3	3.9061248	.7178233	.4649724
C	4	3.6732514	2.8075917	-.7268926
C	5	3.5678471	2.7946303	1.6613709
C	6	3.8028082	1.4239285	1.6710368
C	7	3.9158010	1.4399956	-.7350951
H	8	3.6885913	3.3994045	-1.7079056
H	9	3.5039432	3.3914924	2.6415694
H	10	3.9023530	.8858637	2.6336475
H	11	4.1121044	.9059509	-1.7087181
C	12	3.9083113	-.7501074	.4456994
H	13	3.3575358	5.4166194	1.3196400
H	14	3.3382869	5.3894030	-.4593709
C	15	1.4450617	4.8884038	.4500309
N	16	3.4177237	-3.4760809	.3871846
H	17	-1.2323404	-4.2605878	-1.7613650
C	18	3.7786368	-1.4750952	1.6379905
C	19	3.5308529	-2.8419809	1.6006814
H	20	1.2412968	-4.2917596	-1.7544861
C	21	3.9474619	-1.4497306	-.7685667
H	22	3.8659360	-.9542696	2.6109270
H	23	3.4405027	-3.4547478	2.5683204
C	24	2.8907233	-4.8785253	.3379384
H	25	3.2823369	-5.4512086	1.2075372
C	26	-1.3488677	4.9168571	.4670483
C	27	.7537584	5.1322881	1.6367866
C	28	.7336075	4.6884185	-.7355895
C	29	-.6559727	4.7021823	-.7269570
C	30	-.6382247	5.1464799	1.6452312
H	31	1.3030601	5.3212668	2.5686798
H	32	1.2694625	4.5295664	-1.6812116
H	33	-1.2063537	4.5524462	-1.6656314
H	34	-1.1722033	5.3460108	2.5838537
C	35	-2.8503939	4.9292101	.4785031
H	36	-3.2387502	5.4743612	1.3670773
H	37	-3.2414476	5.4693493	-.4118763
N	38	-3.3725941	3.5240258	.4888455
C	39	-3.8720812	.7974931	.4714963
C	40	-3.6606451	2.8998304	-.7013446

C	41	-3.4752616	2.8538705	1.6837628
C	42	-3.7275132	1.4874384	1.6830509
C	43	-3.9182235	1.5337592	-.7201635
H	44	-3.7045924	3.5261643	-1.6617630
H	45	-3.3737682	3.4373263	2.6680924
H	46	-3.8077663	.9403091	2.6420938
H	47	-4.1558137	1.0125131	-1.6943868
C	48	-3.8791242	-.6707169	.4469927
H	49	-3.3152488	-5.3828735	1.1852467
C	50	-3.7519910	-1.4031857	1.6353202
C	51	-3.9212737	-1.3652883	-.7693957
H	52	-3.7102430	-3.3234081	-1.7800424
C	53	-3.5159400	-2.7718561	1.5914020
H	54	-3.8330506	-.8880576	2.6118746
H	55	-4.1467871	-.8092578	-1.7265896
C	56	-3.6761238	-2.7335439	-.7956150
H	57	-3.4321244	-3.3896630	2.5561970
C	58	-2.9071675	-4.8133051	.3211397
N	59	-3.4088283	-3.4018626	.3751859
H	60	-3.2954317	-5.3154788	-.5924717
C	61	-1.4056464	-4.8274071	.3252571
C	62	3.6932210	-2.8165343	-.7867468
H	63	1.2155882	-5.4893572	2.3997483
H	64	3.2742870	-5.3930884	-.5707635
C	65	1.3891022	-4.8606653	.3331585
C	66	-.7117995	-5.1839580	1.4813681
C	67	-.6957803	-4.5131628	-.8365968
C	68	.6933467	-4.5300494	-.8327091
C	69	.6806194	-5.2004739	1.4853721
H	70	-1.2586581	-5.4600735	2.3926815
H	71	3.7267441	-3.4126633	-1.7679754
H	72	4.1702600	-.9033615	-1.7331116
H	73	-6.7914105	1.1069366	-5.4632121
C	74	5.4704065	4.3846746	-5.5019058
C	75	4.9985619	-5.9574736	-5.0734509
C	76	4.7468927	4.2387443	-4.2651111
H	77	6.3422970	5.0408830	-5.3677566
H	78	4.8284393	4.8177133	-6.2816841
H	79	4.6146872	-5.6036005	-6.0405631
N	80	4.1743506	4.0923206	-3.2651227
H	81	5.8229338	3.3939231	-5.8422346
H	82	-4.5089914	-5.5285542	-6.0681107
H	83	4.6903540	-7.0042016	-4.9387689
C	84	-6.3438015	.1161488	-5.3013786
H	85	-7.1563581	-.6176348	-5.2015093
H	86	6.0970853	-5.9204852	-5.0996716
H	87	-5.7451406	-.1443744	-6.1853542
C	88	4.4928514	-5.1413451	-3.9999631
C	89	5.3234452	.2831090	-4.2180835
N	90	4.7697368	.0579589	-3.2210425
C	91	6.0137343	.5811770	-5.4468411
H	92	5.9744561	1.6665556	-5.6563152
H	93	5.5525203	.0474899	-6.2895544
H	94	7.0687808	.2790388	-5.3802032
C	95	-5.5226864	.1217721	-4.1183232
N	96	-4.8663035	.1254948	-3.1586905
N	97	4.0874777	-4.4877405	-3.1287909
C	98	-4.5352044	5.3759412	-3.7767370
N	99	-4.1003651	4.6667204	-2.9652012
C	100	-5.0772620	6.2611813	-4.7751663
H	101	-4.8998469	7.3098457	-4.4962744
H	102	-6.1613207	6.1086332	-4.8765951
H	103	-4.6064576	6.0766968	-5.7509811
C	104	-4.4491353	-5.0469856	-4.0291672
N	105	-4.0614643	-4.3918978	-3.1510718
C	106	-4.9325453	-5.8651020	-5.1114132
H	107	-6.0286260	-5.8086949	-5.1761153
H	108	-4.6485678	-6.9157654	-4.9556574
C	109	6.7247384	-.0801064	4.8740072
N	110	5.7955554	-.0586229	4.1774621
C	111	7.8793187	-.1066681	5.7354489
H	112	7.5729295	-.0858443	6.7904618

H 113	8.5228491	.7629196	5.5425796
H 114	8.4675933	-1.0183873	5.5617228
C 115	-6.6545144	.0151435	4.9014764
N 116	-5.7267993	.0196428	4.2026979
C 117	-7.8073241	.0096121	5.7656882
H 118	-8.4231901	.9026651	5.5906561
H 119	-7.4979458	.0012594	6.8199871
H 120	-8.4248277	-.8795273	5.5770421
C 121	4.0023357	-5.0314363	4.9570380
N 122	3.6648183	-4.4677279	3.9985854
C 123	4.4249567	-5.7349242	6.1405319
H 124	4.2850543	-5.1073917	7.0319385
H 125	5.4884188	-6.0044321	6.0678391
H 126	3.8415948	-6.6577181	6.2690664
C 127	-4.0211636	-4.9631883	4.9409390
N 128	-3.6723798	-4.4041319	3.9838017
C 129	-4.4578099	-5.6608347	6.1228023
H 130	-5.5464738	-5.8126371	6.0988189
H 131	-4.2063491	-5.0852148	7.0246753
H 132	-3.9722321	-6.6447267	6.1907496
C 133	4.1271519	4.9292381	5.0391952
N 134	3.7657113	4.3822280	4.0797321
C 135	4.5791244	5.6122509	6.2238017
H 136	4.1150995	5.1771699	7.1201016
H 137	4.3155386	6.6785845	6.1775927
H 138	5.6710193	5.5293218	6.3217300
C 139	-3.9199356	4.9409227	5.1077171
N 140	-3.5858614	4.4078497	4.1306810
C 141	-4.3380260	5.6067082	6.3143916
H 142	-4.0169799	6.6581090	6.3050441
H 143	-3.9010589	5.1168071	7.1958540
H 144	-5.4330998	5.5797571	6.4080053
H 145	.1453143	.3855302	-.6636330
C 146	.0340821	.2356068	-1.7412720
C 147	-.2482613	-.1465233	-4.4824497
C 148	-.0418910	1.3304826	-2.5931423
C 149	-.0306473	-1.0554789	-2.2609638
C 150	-.1716794	-1.2587470	-3.6244055
C 151	-.1826657	1.1527167	-3.9654322
H 152	.0088930	2.3482421	-2.1839383
H 153	.0305073	-1.9244884	-1.5930634
H 154	-.2221825	-2.2758512	-4.0318939
H 155	-.2411020	2.0286358	-4.6224654
O 156	-.3900838	-.4756922	-5.8095331
C 157	-.4495379	.5726408	-6.7478403
H 158	.4641054	1.1777012	-6.7526106
H 159	-1.3211228	1.2184191	-6.5920614
H 160	-.5467045	.0285744	-7.6920010

Heat of Formation: 1134.316 kcal/mol

ANILINE1/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Tue Oct 3 06:40:10 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 241
158 S shells
83 P shells
Number of basis functions: 407
Number of electrons: 420
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 468 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 216 Heat of formation = 1169.210 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.8853563	4.8620098	.2798777
N	2	3.3754886	3.4456167	.3088794
C	3	3.8422232	.7103901	.3331870
C	4	3.6009454	2.7888022	-.8763213
C	5	3.5141982	2.7983299	1.5128400
C	6	3.7478700	1.4277396	1.5334669
C	7	3.8434722	1.4209837	-.8736790
H	8	3.6069490	3.3717129	-1.8628123
H	9	3.4591038	3.4045081	2.4874171
H	10	3.8535328	.8985699	2.5002318
H	11	4.0327219	.8778117	-1.8439755
C	12	3.8447341	-.7576266	.3280230
H	13	3.3106200	5.4185981	1.1440901
H	14	3.2641054	5.3712031	-.6340348
C	15	1.3844102	4.8836500	.3089459
N	16	3.3574235	-3.4844843	.2972592
H	17	-1.3139638	-4.2952001	-1.8003016
C	18	3.7174182	-1.4709149	1.5276699
C	19	3.4705633	-2.8381714	1.5043253
H	20	1.1601531	-4.3249505	-1.8198746
C	21	3.8832379	-1.4691146	-.8793564
H	22	3.8062294	-.9405288	2.4952166
H	23	3.3818431	-3.4413460	2.4777159
C	24	2.8319842	-4.8878180	.2624697
H	25	3.2325242	-5.4538591	1.1323310
C	26	-1.4088188	4.9137308	.3669496
C	27	.7109930	5.1629127	1.4980917
C	28	.6552957	4.6496499	-.8596776
C	29	-.7338124	4.6641122	-.8306172
C	30	-.6808168	5.1779121	1.5270092
H	31	1.2740896	5.3786476	2.4158238
H	32	1.1764567	4.4613210	-1.8080929
H	33	-1.2983101	4.4878370	-1.7563325
H	34	-1.2004356	5.4052947	2.4672643
C	35	-2.9099414	4.9252893	.4003274
H	36	-3.2864764	5.4743773	1.2915605
H	37	-3.3140512	5.4604584	-.4872143
N	38	-3.4297679	3.5193563	.4248195
C	39	-3.9222625	.7913368	.4299017
C	40	-3.7210532	2.8854493	-.7594693
C	41	-3.5242790	2.8576255	1.6249357
C	42	-3.7728282	1.4903500	1.6355175
C	43	-3.9754296	1.5188002	-.7668505
H	44	-3.7694361	3.5040907	-1.7252082
H	45	-3.4185607	3.4483420	2.6047756
H	46	-3.8460413	.9499740	2.5989879
H	47	-4.2176497	.9904719	-1.7358232
C	48	-3.9287421	-.6770426	.4154701
H	49	-3.3641257	-5.3852757	1.1801458
C	50	-3.7887779	-1.4011371	1.6073327
C	51	-3.9855367	-1.3801900	-.7955616
H	52	-3.7968482	-3.3474684	-1.7927805
C	53	-3.5548189	-2.7705492	1.5704443
H	54	-3.8585009	-.8790510	2.5811254
H	55	-4.2211540	-.8306763	-1.7544006
C	56	-3.7446415	-2.7491618	-.8145323
H	57	-3.4595639	-3.3813037	2.5389062
C	58	-2.9654799	-4.8223272	.3073319
N	59	-3.4640440	-3.4095883	.3578091
H	60	-3.3654100	-5.3300505	-.5980906
C	61	-1.4640991	-4.8382983	.2939697

C	62	3.6321885	-2.8365759	-.8833502
H	63	1.1793349	-5.4777371	2.3471103
H	64	3.2075865	-5.4083300	-.6461407
C	65	1.3303400	-4.8719622	.2719136
C	66	-.7578945	-5.1825563	1.4463179
C	67	-.7669561	-4.5376128	-.8791102
C	68	.6221276	-4.5547025	-.8901459
C	69	.6343843	-5.1992803	1.4353533
H	70	-1.2948772	-5.4483840	2.3665162
H	71	3.6711114	-3.4437642	-1.8567139
H	72	4.1025557	-.9313152	-1.8503260
H	73	-6.9028841	1.1182519	-5.4464450
C	74	5.3096783	4.3316292	-5.6973387
C	75	5.0840365	-6.0467554	-5.0580087
C	76	4.6167833	4.1996025	-4.4416413
H	77	6.1959353	4.9728468	-5.5873373
H	78	4.6546884	4.7746340	-6.4604571
H	79	4.7980069	-5.6747834	-6.0518072
N	80	4.0682656	4.0645246	-3.4267392
H	81	5.6358294	3.3345576	-6.0452783
H	82	-4.6672772	-5.7281559	-5.9849274
H	83	4.7239889	-7.0805866	-4.9565737
C	84	-6.4523354	.1249678	-5.3098758
H	85	-7.2629059	-.6113292	-5.2124195
H	86	6.1814844	-6.0539197	-4.9912566
H	87	-5.8662650	-.1179691	-6.2071899
C	88	4.5225012	-5.2139933	-4.0258013
C	89	5.1712374	.2313187	-4.3794555
N	90	4.6746076	.0124383	-3.3515408
C	91	5.7889671	.5205109	-5.6481826
H	92	5.7617310	1.6075575	-5.8502003
H	93	5.2612764	.0031477	-6.4614998
H	94	6.8385619	.1935045	-5.6505584
C	95	-5.6144850	.1090790	-4.1387015
N	96	-4.9447801	.0961791	-3.1883619
N	97	4.0725505	-4.5468813	-3.1873327
C	98	-4.5772319	5.3286736	-3.8697631
N	99	-4.1577158	4.6273102	-3.0434924
C	100	-5.1000689	6.2042775	-4.8867420
H	101	-4.7888887	7.2417834	-4.6979884
H	102	-6.1989229	6.1688099	-4.8968806
H	103	-4.7325635	5.9061451	-5.8786860
C	104	-4.6236663	-5.1066774	-3.9836085
N	105	-4.1961961	-4.4342858	-3.1376061
C	106	-5.1567464	-5.9462562	-5.0253623
H	107	-6.2373629	-5.7787408	-5.1390621
H	108	-4.9942896	-7.0068417	-4.7852139
C	109	6.6959029	-.0505795	4.7255373
N	110	5.7585553	-.0380539	4.0398287
C	111	7.8606185	-.0660217	5.5735083
H	112	7.5661670	-.1147541	6.6309861
H	113	8.4595179	.8424748	5.4204599
H	114	8.4896670	-.9379952	5.3466720
C	115	-6.6628209	.0334882	4.8909287
N	116	-5.7433582	.0316975	4.1812994
C	117	-7.8054111	.0357441	5.7686218
H	118	-8.3749172	.9686896	5.6557656
H	119	-7.4861343	-.0525227	6.8162930
H	120	-8.4709992	-.8068974	5.5352650
C	121	3.9628656	-4.9888038	4.8816408
N	122	3.6157013	-4.4390664	3.9185404
C	123	4.3974375	-5.6750003	6.0709512
H	124	4.0273003	-5.1610290	6.9691476
H	125	5.4954601	-5.7074565	6.1158501
H	126	4.0197549	-6.7073778	6.0796030
C	127	-4.0177588	-4.9330678	4.9448239
N	128	-3.6826612	-4.3828873	3.9776994
C	129	-4.4374857	-5.6197354	6.1391774
H	130	-5.5058367	-5.8729653	6.0811616
H	131	-4.2772746	-4.9869612	7.0234284
H	132	-3.8672572	-6.5505349	6.2689309
C	133	4.1127889	4.9630692	4.8644205

N 134	3.7384891	4.4083481	3.9143880
C 135	4.5807662	5.6555796	6.0372531
H 136	4.2297890	5.1508449	6.9482979
H 137	4.2096728	6.6903581	6.0471436
H 138	5.6797505	5.6815339	6.0548076
C 139	-3.9381313	4.9726885	5.0368461
N 140	-3.6177641	4.4297891	4.0606423
C 141	-4.3393030	5.6506127	6.2425060
H 142	-3.9824437	6.6904228	6.2365089
H 143	-3.9237729	5.1447405	7.1253272
H 144	-5.4351322	5.6609842	6.3306213
H 145	-.5610541	.0196081	-1.0443903
C 146	-.2138743	.0614107	-2.0806333
C 147	.6664559	.1681512	-4.7274928
C 148	-.0403541	1.2904914	-2.7088130
C 149	.0454321	-1.1147462	-2.7773078
C 150	.4820586	-1.0712568	-4.0938840
C 151	.3937454	1.3530452	-4.0254849
H 152	-.2483425	2.2209807	-2.1647783
H 153	-.0976366	-2.0863504	-2.2870126
H 154	.6771006	-2.0071716	-4.6319866
H 155	.5162788	2.3295789	-4.5099961
N 156	1.2330729	.2276237	-6.0328760
H 157	1.0495223	-.5959945	-6.5610913
H 158	.9579571	1.0482403	-6.5247389

Heat of Formation: 1169.210 kcal/mol

ANILINE2/1^{4+} , 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Sep 28 08:31:54 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 241
158 S shells
83 P shells
Number of basis functions: 407
Number of electrons: 420
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 468 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 214 Heat of formation = 1171.148 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	2.9132264	4.8572215	.2220247
N 2	3.4158018	3.4453657	.2467001
C 3	3.9093783	.7151205	.2629138
C 4	3.6543316	2.7957301	-.9400685
C 5	3.5572140	2.7953610	1.4490263
C 6	3.8045072	1.4273271	1.4655578
C 7	3.9113132	1.4306121	-.9412249
H 8	3.6562570	3.3816336	-1.9240823
H 9	3.4916161	3.3972994	2.4249746
H 10	3.9096338	.8952879	2.4306404
H 11	4.1065977	.8916592	-1.9117694
C 12	3.9109005	-.7528017	.2522010

H	13	3.3247921	5.4119434	1.0940939
H	14	3.2974401	5.3755965	-.6844357
C	15	1.4116849	4.8693984	.2365641
N	16	3.3948053	-3.4739177	.2107201
H	17	-1.2845327	-4.3730845	-1.9217505
C	18	3.7767559	-1.4695985	1.4492208
C	19	3.5158996	-2.8338628	1.4205593
H	20	1.1913443	-4.3999761	-1.9338685
C	21	3.9446691	-1.4602785	-.9578546
H	22	3.8684531	-.9433890	2.4186532
H	23	3.4210890	-3.4399794	2.3909735
C	24	2.8580629	-4.8727374	.1725165
H	25	3.2527650	-5.4437020	1.0418734
C	26	-1.3828842	4.8997669	.2629346
C	27	.7240585	5.1031565	1.4275666
C	28	.6959921	4.6766409	-.9476693
C	29	-.6937446	4.6912725	-.9343555
C	30	-.6679396	5.1185470	1.4406669
H	31	1.2766559	5.2846036	2.3591081
H	32	1.2290743	4.5254189	-1.8962287
H	33	-1.2471653	4.5510460	-1.8726702
H	34	-1.1985575	5.3126815	2.3822966
C	35	-2.8843604	4.9222252	.2771702
H	36	-3.2670846	5.4751894	1.1634095
H	37	-3.2740595	5.4595743	-.6155523
N	38	-3.4161989	3.5204667	.2963634
C	39	-3.9238613	.7949266	.3001218
C	40	-3.6944162	2.8856397	-.8904378
C	41	-3.5338960	2.8620208	1.4964127
C	42	-3.7905407	1.4962341	1.5064217
C	43	-3.9565076	1.5201563	-.8986071
H	44	-3.7248934	3.5022954	-1.8589579
H	45	-3.4405589	3.4549247	2.4770006
H	46	-3.8833587	.9586767	2.4700726
H	47	-4.1878816	.9907595	-1.8701423
C	48	-3.9306022	-.6736639	.2885262
H	49	-3.3380570	-5.3751955	1.0750535
C	50	-3.8042059	-1.3952115	1.4835605
C	51	-3.9697902	-1.3795175	-.9215303
H	52	-3.7595070	-3.3481317	-1.9130309
C	53	-3.5621136	-2.7633644	1.4521534
H	54	-3.8915716	-.8719572	2.4555745
H	55	-4.1956831	-.8325936	-1.8847110
C	56	-3.7219989	-2.7476047	-.9347345
H	57	-3.4762401	-3.3722005	2.4235233
C	58	-2.9407401	-4.8132022	.2009688
N	59	-3.4514899	-3.4042346	.2419983
H	60	-3.3334490	-5.3284767	-.7034024
C	61	-1.4390478	-4.8175182	.1947804
C	62	3.6775086	-2.8247262	-.9673833
H	63	1.2009992	-5.3545037	2.2821371
H	64	3.2318508	-5.3942849	-.7362944
C	65	1.3562746	-4.8485800	.1807928
C	66	-.7347356	-5.1043668	1.3641321
C	67	-.7391735	-4.5689012	-.9886881
C	68	.6504093	-4.5844078	-.9957024
C	69	.6575092	-5.1196976	1.3571715
H	70	-1.2737668	-5.3283439	2.2942668
H	71	3.7065969	-3.4277432	-1.9431355
H	72	4.1687254	-.9202192	-1.9254863
H	73	-6.8760158	1.0668672	-5.5793075
C	74	5.3585960	4.3600837	-5.7553461
C	75	5.0580213	-6.0036743	-5.1930168
C	76	4.6593163	4.2184176	-4.5042108
H	77	6.2179179	5.0371778	-5.6465241
H	78	4.6941035	4.7662238	-6.5307227
H	79	4.6309813	-5.7190633	-6.1648718
N	80	4.1064788	4.0759631	-3.4926335
H	81	5.7270828	3.3719331	-6.0860896
H	82	-4.6382120	-5.6537896	-6.1376073
H	83	4.8290533	-7.0632090	-5.0092835
C	84	-6.3178469	.1228697	-5.5034325

H	85	-7.0406456	-.7054164	-5.4931672
H	86	6.1502630	-5.8894082	-5.2452289
H	87	-5.6829126	.0208077	-6.3946422
C	88	4.5155292	-5.1815047	-4.1423024
C	89	5.3093680	.2647702	-4.4228477
N	90	4.7663306	.0335731	-3.4213754
C	91	5.9860856	.5699554	-5.6574324
H	92	5.9176111	1.6519748	-5.8763593
H	93	5.5350642	.0171686	-6.4932917
H	94	7.0488985	.2959223	-5.5931773
C	95	-5.5168030	.1066694	-4.3068435
N	96	-4.8763402	.0936325	-3.3364455
N	97	4.0807618	-4.5228872	-3.2892286
C	98	-4.4828849	5.3140886	-4.0293187
N	99	-4.0816608	4.6179142	-3.1896035
C	100	-4.9829206	6.1831223	-5.0632224
H	101	-4.5674227	7.1947239	-4.9497186
H	102	-6.0791210	6.2511681	-5.0113953
H	103	-4.7040532	5.8021239	-6.0557176
C	104	-4.5501826	-5.1043047	-4.1167536
N	105	-4.1348437	-4.4335743	-3.2633352
C	106	-5.0680760	-5.9416392	-5.1678922
H	107	-6.1618479	-5.8486018	-5.2299543
H	108	-4.8206494	-6.9957833	-4.9769490
C	109	6.7622133	-.0592825	4.6516990
N	110	5.8239350	-.0450085	3.9673156
C	111	7.9280689	-.0768740	5.4980658
H	112	7.6356205	-.0447638	6.5567264
H	113	8.5690013	.7904971	5.2874717
H	114	8.5139487	-.9904845	5.3263123
C	115	-6.6689741	.0413225	4.7685053
N	116	-5.7493355	.0397196	4.0590354
C	117	-7.8117924	.0433677	5.6458776
H	118	-8.4188233	.9449873	5.4842658
H	119	-7.4905258	.0237310	6.6964877
H	120	-8.4421479	-.8369195	5.4580563
C	121	3.9994542	-5.0014554	4.7870824
N	122	3.6472173	-4.4475669	3.8281810
C	123	4.4402469	-5.6927717	5.9711189
H	124	4.1617394	-5.1288683	6.8724431
H	125	5.5328828	-5.8144614	5.9602193
H	126	3.9811696	-6.6900001	6.0282166
C	127	-4.0457273	-4.9301716	4.8206198
N	128	-3.7048258	-4.3741375	3.8588207
C	129	-4.4723419	-5.6241968	6.0082290
H	130	-5.5520524	-5.8277326	5.9670819
H	131	-4.2659051	-5.0196415	6.9026060
H	132	-3.9425856	-6.5825095	6.1056035
C	133	4.1259576	4.9535526	4.8092920
N	134	3.7540340	4.4013340	3.8568534
C	135	4.5909678	5.6429643	5.9851263
H	136	4.1110574	5.2352375	6.8858913
H	137	4.3569350	6.7152148	5.9205045
H	138	5.6796939	5.5317887	6.0898833
C	139	-3.9834246	4.9941763	4.8924808
N	140	-3.6525229	4.4421160	3.9249027
C	141	-4.3973599	5.6835321	6.0872658
H	142	-4.1042552	6.7421811	6.0420753
H	143	-3.9320595	5.2307853	6.9741141
H	144	-5.4895304	5.6311420	6.2018902
N	145	.2001037	.0651607	-.3757753
C	146	.0469905	.0692131	-1.8038445
C	147	-.0504712	.0796355	-4.5897133
C	148	.0110358	1.2844461	-2.4996174
C	149	.0279794	-1.1408076	-2.5092994
C	150	-.0187350	-1.1268952	-3.8979045
C	151	-.0364677	1.2808852	-3.8882578
H	152	.0211977	2.2445590	-1.9633068
H	153	.0508971	-2.1048431	-1.9807169
H	154	-.0308063	-2.0730110	-4.4506099
H	155	-.0640690	2.2312010	-4.4331146
H	156	-.0884102	.0835841	-5.6849240

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    H 157      -.1921286      -.7601205       .0225992
    H 158      -.2142230       .8762741       .0292987

Heat of Formation:      1171.148 kcal/mol
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t-BUTYLBENZENE1/1^{4+}, 12 ACETONITRILES

```
SPARTAN SEMIEMPIRICAL PROGRAM:  IBM  Release 3.1.7

Calculation started: Mon Sep 25 18:59:21 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 254
 168 S shells
  86 P shells
Number of basis functions: 426
Number of electrons: 438
Use of molecular symmetry disabled
Molecular charge:   4
Spin multiplicity:  1

Point Group = C1  Order =  1 Nsymop =  1
This system has 498 degrees of freedom

Convergence on Energy - difference below    .5000D-03 kcal/mol

Cycle no: 268 Heat of formation =  1149.033  rmsG =  .0000 rmsD =  .0000

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

    C   1      1.0361136     4.7514387     2.9090982
    N   2      1.1972544     3.3334916     3.3688517
    C   3      1.3544162      .5953916     3.7944764
    C   4      2.3855644     2.6823187     3.1415155
    C   5       .1344298     2.6803055     3.9450137
    C   6       .2053716     1.3084322     4.1625981
    C   7      2.4763408     1.3137329     3.3611085
    H   8      3.3043890     3.2681465     2.7878702
    H   9      -.7935542     3.2818183     4.2568720
    H  10      -.6528162      .7729869     4.6128497
    H  11      3.4493544      .7727316     3.1812178
    C  12      1.3510939     -.8720779     3.7468583
    H  13       .3740320     5.2968927     3.6175099
    H  14      2.0206999     5.2684967     2.9445941
    C  15       .4723356     4.7877925     1.5173519
    N  16      1.1556555    -3.5651517     3.1258070
    H  17      1.3841049    -4.4885125    -2.0787190
    C  18       .1842962    -1.5879834     4.0473601
    C  19       .0932782    -2.9382322     3.7311434
    H  20      2.3242735    -4.5963913      .2080190
    C  21      2.4751746    -1.5764397     3.2917626
    H  22      -.6713188    -1.0701779     4.5220560
    H  23      -.8495873    -3.5435567     3.9835647
    C  24       .9668549    -4.9369466     2.5509974
    H  25       .2987287    -5.5269212     3.2167638
    C  26      -.5765663     4.8968167    -1.0738208
    C  27      -.9027836     4.9249238     1.3209992
    C  28      1.3224798     4.7192381      .4113071
    C  29       .8005389     4.7705325     -.8772407
    C  30     -1.4244289     4.9805404      .0318769
    H  31     -1.5786633     5.0031007     2.1831619
    H  32      2.4083832     4.6382250      .5538253
    H  33      1.4798676     4.7224885    -1.7390766
    H  34     -2.5066890     5.1026735     -.1102109
    C  35     -1.1398014     4.9818596    -2.4639822
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H	36	-2.0921596	5.5569971	-2.4684759
H	37	-.4425429	5.5329050	-3.1331741
N	38	-1.3854976	3.6089393	-3.0138829
C	39	-1.6451204	.9149064	-3.6140632
C	40	-.4019519	2.9837101	-3.7427320
C	41	-2.5634563	2.9663610	-2.7178226
C	42	-2.7019301	1.6163113	-3.0172344
C	43	-.5269457	1.6351052	-4.0569275
H	44	.5048882	3.5925658	-4.0945641
H	45	-3.4246573	3.5589980	-2.2422854
H	46	-3.6427429	1.0881300	-2.7693040
H	47	.2736436	1.1120905	-4.6593326
C	48	-1.6593736	-.5526773	-3.6650710
H	49	-2.2021064	-5.2540591	-2.8548925
C	50	-2.7293230	-1.2732488	-3.1164973
C	51	-.5556929	-1.2619114	-4.1590796
H	52	.4356409	-3.2318497	-4.3390072
C	53	-2.6178829	-2.6436282	-2.9133835
H	54	-3.6592723	-.7452677	-2.8300878
H	55	.2555417	-.7136730	-4.7237842
C	56	-.4580869	-2.6316674	-3.9418078
H	57	-3.4907141	-3.2505210	-2.4789757
C	58	-1.2370775	-4.7021245	-2.8112573
N	59	-1.4537967	-3.2874004	-3.2574808
H	60	-.5537416	-5.2171264	-3.5222149
C	61	-.6675470	-4.7345194	-1.4214670
C	62	2.3628815	-2.9254823	2.9740407
H	63	-1.6507345	-5.1355930	1.8181994
H	64	1.9413913	-5.4733928	2.5362863
C	65	.3953091	-4.8492840	1.1644035
C	66	-1.5085187	-4.9209351	-.3233251
C	67	.7098697	-4.6168627	-1.2209582
C	68	1.2384141	-4.6753247	.0643878
C	69	-.9798413	-4.9773014	.9631085
H	70	-2.5909109	-5.0359257	-.4697590
H	71	3.2689086	-3.5233269	2.6010538
H	72	3.4657872	-1.0443803	3.1714363
H	73	2.4660036	1.2890563	-8.6814672
C	74	7.5014632	4.1909011	3.0545395
C	75	6.7707943	-6.1168578	2.4555140
C	76	6.0844924	4.0643735	2.8295509
H	77	7.7044769	4.9009382	3.8690416
H	78	8.0106073	4.5487272	2.1486973
H	79	7.5169101	-5.7776454	1.7232605
N	80	4.9426740	3.9338905	2.6604829
H	81	7.9208013	3.2063915	3.3314938
H	82	4.0352993	-5.4963221	-6.7610957
H	83	6.5098866	-7.1604917	2.2284156
C	84	2.5824793	.3056406	-8.2042225
H	85	2.1955996	-.4598384	-8.8920005
H	86	7.2243609	-6.0832686	3.4564996
H	87	3.6539857	.1210335	-8.0438626
C	88	5.5981803	-5.2821612	2.4059250
C	89	6.2044282	.1240091	3.5524014
N	90	5.0864081	-.1019398	3.3271168
C	91	7.5847920	.4249446	3.8337012
H	92	7.7875036	1.4979091	3.6569565
H	93	8.2496074	-.1653093	3.1875166
H	94	7.8249766	.1941921	4.8815399
C	95	1.8694477	.2654140	-6.9537404
N	96	1.2876133	.2331638	-5.9474410
N	97	4.6483472	-4.6134648	2.3701374
C	98	2.3083764	5.4083492	-5.5195655
N	99	1.6511379	4.7098033	-4.8632117
C	100	3.1162624	6.2801566	-6.3328922
H	101	3.2224338	7.2640951	-5.8539613
H	102	2.6532713	6.4235113	-7.3198151
H	103	4.1189036	5.8536439	-6.4770726
C	104	2.1917966	-4.9658356	-5.9164829
N	105	1.5539243	-4.3099814	-5.1997777
C	106	2.9755546	-5.7843693	-6.8052876
H	107	2.6261791	-5.6702400	-7.8414748

H 108	2.8913103	-6.8445303	-6.5263865
C 109	-1.7027912	-.2724082	8.0315110
N 110	-1.4042989	-.2282287	6.9099139
C 111	-2.0699453	-.3271652	9.4236433
H 112	-3.1631451	-.3181412	9.5340082
H 113	-1.6583781	.5366615	9.9639237
H 114	-1.6807229	-1.2438651	9.8880245
C 115	-6.8004387	.2627316	-4.6016529
N 116	-5.8111434	.2311056	-3.9939709
C 117	-8.0259602	.3020468	-5.3582230
H 118	-8.0706034	1.2134543	-5.9704599
H 119	-8.8943326	.2920092	-4.6850390
H 120	-8.0932975	-.5678248	-6.0262626
C 121	-2.8663319	-5.1473833	5.3507555
N 122	-2.1081726	-4.5680098	4.6874244
C 123	-3.8004089	-5.8704681	6.1745934
H 124	-4.7278756	-5.2945925	6.3017011
H 125	-3.3693020	-6.0600724	7.1680851
H 126	-4.0507692	-6.8373607	5.7152952
C 127	-5.9435450	-4.7954156	-2.1551450
N 128	-4.9169130	-4.2511895	-2.1723480
C 129	-7.2134104	-5.4745861	-2.1393420
H 130	-7.5880249	-5.6120507	-3.1638433
H 131	-7.9541999	-4.8928439	-1.5729619
H 132	-7.1151293	-6.4641092	-1.6706656
C 133	-2.7615085	4.8329166	5.7480764
N 134	-2.0208979	4.2819609	5.0420507
C 135	-3.6736528	5.5206914	6.6249925
H 136	-4.6986863	5.1509444	6.4816251
H 137	-3.6613887	6.6012210	6.4224330
H 138	-3.3898453	5.3619149	7.6751937
C 139	-5.8398169	5.1374317	-1.8120155
N 140	-4.8279408	4.5685560	-1.8664919
C 141	-7.0911054	5.8476762	-1.7494774
H 142	-6.9205771	6.9327106	-1.7990523
H 143	-7.6169565	5.6202354	-.8115530
H 144	-7.7383202	5.5598789	-2.5901795
H 145	-2.5911869	.0547754	1.2044224
C 146	-1.5989670	.0501186	.7397881
C 147	.9310952	.0388363	-.4679092
C 148	-.9431997	1.2476364	.4757496
C 149	-.9848811	-1.1534982	.4107452
C 150	.2710329	-1.1585781	-.1845305
C 151	.3126846	1.2413189	-.1196493
H 152	-1.4141388	2.2050988	.7346931
H 153	-1.4896264	-2.1054717	.6184919
H 154	.7613631	-2.1142136	-.4437043
H 155	.8355844	2.1922707	-.3272140
C 156	2.3098596	.0323133	-1.0989809
C 157	3.3415247	-.0131305	.0298412
C 158	2.5355937	1.2912523	-1.9377896
C 159	2.4957021	-1.1886934	-2.0010631
H 160	3.5261336	-1.2521427	-2.3736773
H 161	1.8258266	-1.1514041	-2.8730226
H 162	2.2727226	-2.1253053	-1.4609752
H 163	3.5683195	1.3414261	-2.3060117
H 164	2.3405699	2.2055837	-1.3510965
H 165	1.8668427	1.3189046	-2.8108202
H 166	4.3652566	-.0253290	-.3673491
H 167	3.2152328	-.9098885	.6535390
H 168	3.2503770	.8610821	.6904355

Heat of Formation: 1149.033 kcal/mol

t-BUTYLBENZENE/1^{4+} , 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

```
Calculation started: Tue Oct  3 06:49:08 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 254
168 S shells
 86 P shells
Number of basis functions: 426
Number of electrons: 438
Use of molecular symmetry disabled
Molecular charge:   4
Spin multiplicity:  1

Point Group = C1  Order =  1 Nsymop =  1
This system has 498 degrees of freedom

Convergence on Energy - difference below    .5000D-03 kcal/mol

Cycle no: 210 Heat of formation =  1148.400  rmsG =  .0000 rmsD =  .0001
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Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9664331	4.8639084	.6450553
N	2	3.4547618	3.4467030	.6694175
C	3	3.9159255	.7100577	.6831897
C	4	3.6743923	2.7929559	-.5187915
C	5	3.5952895	2.7949940	1.8704967
C	6	3.8269073	1.4236398	1.8859037
C	7	3.9131496	1.4247561	-.5213591
H	8	3.6791904	3.3789636	-1.5037419
H	9	3.5426885	3.3976577	2.8480160
H	10	3.9350514	.8912205	2.8507528
H	11	4.0973821	.8847684	-1.4939631
C	12	3.9179177	-.7579859	.6726451
H	13	3.3835106	5.4143757	1.5171854
H	14	3.3547605	5.3786974	-.2616521
C	15	1.4653321	4.8863448	.6583960
N	16	3.4344430	-3.4857228	.6344918
H	17	-1.2283999	-4.2904130	-1.4743552
C	18	3.7975580	-1.4757388	1.8701717
C	19	3.5523576	-2.8434602	1.8430687
H	20	1.2448741	-4.3175211	-1.4869917
C	21	3.9498888	-1.4650412	-.5376400
H	22	3.8905649	-.9487851	2.8393348
H	23	3.4682921	-3.4499648	2.8153926
C	24	2.9116308	-4.8901214	.5968522
H	25	3.3109469	-5.4564880	1.4671023
C	26	-1.3284167	4.9166227	.6869790
C	27	.7796639	5.1830295	1.8361438
C	28	.7482871	4.6357616	-.5143858
C	29	-.6407935	4.6505536	-.4999704
C	30	-.6125386	5.1981306	1.8503916
H	31	1.3329005	5.4126745	2.7564389
H	32	1.2790458	4.4348088	-1.4549167
H	33	-1.1948991	4.4592434	-1.4290273
H	34	-1.1416945	5.4392084	2.7818718
C	35	-2.8299826	4.9258541	.7050641
H	36	-3.2168478	5.4707796	1.5944453
H	37	-3.2252269	5.4641149	-.1845795
N	38	-3.3472416	3.5189504	.7176656
C	39	-3.8275311	.7885194	.7107706
C	40	-3.5994457	2.8823901	-.4741987
C	41	-3.4738002	2.8577565	1.9150318
C	42	-3.7196392	1.4899064	1.9194951
C	43	-3.8415701	1.5137058	-.4883583
H	44	-3.6297922	3.5015348	-1.4398486
H	45	-3.3966764	3.4490909	2.8970450
H	46	-3.8225837	.9508669	2.8809898
H	47	-4.0333808	.9824800	-1.4670168
C	48	-3.8343381	-.6799137	.6987981

H	49	-3.2877008	-5.3836788	1.5028939
C	50	-3.7337482	-1.4020019	1.8958820
C	51	-3.8546956	-1.3852390	-.5120499
H	52	-3.6643122	-3.3589241	-1.4958609
C	53	-3.5025305	-2.7721895	1.8692542
H	54	-3.8314394	-.8776705	2.8660428
H	55	-4.0408129	-.8362119	-1.4820587
C	56	-3.6269459	-2.7564073	-.5200500
H	57	-3.4331251	-3.3799054	2.8417187
C	58	-2.8861627	-4.8290312	.6260818
N	59	-3.3827415	-3.4152426	.6613964
H	60	-3.2838742	-5.3447400	-.2757684
C	61	-1.3845787	-4.8461086	.6165456
C	62	3.7011378	-2.8328077	-.5453225
H	63	1.2535859	-5.4961012	2.6730240
H	64	3.2905722	-5.4088147	-.3114008
C	65	1.4100165	-4.8765397	.6022928
C	66	-.6813593	-5.1968831	1.7686831
C	67	-.6841912	-4.5383371	-.5528550
C	68	.7047803	-4.5533387	-.5599885
C	69	.7110717	-5.2121600	1.7615277
H	70	-1.2205322	-5.4690606	2.6857263
H	71	3.7353233	-3.4364251	-1.5215930
H	72	4.1633935	-.9240284	-1.5074946
H	73	-5.8659563	1.0219745	-5.7062066
C	74	5.3696870	4.3553587	-5.3422134
C	75	5.0912005	-6.0303833	-4.7547537
C	76	4.6795896	4.2114660	-4.0862641
H	77	6.2418323	5.0159733	-5.2338870
H	78	4.7054189	4.7819990	-6.1066894
H	79	4.7083243	-5.7156930	-5.7356829
N	80	4.1340233	4.0663888	-3.0711499
H	81	5.7174653	3.3645727	-5.6871544
H	82	-4.8006369	-5.6757347	-5.6570525
H	83	4.8095707	-7.0806263	-4.5920095
C	84	-5.2763827	.1179187	-5.4987004
H	85	-5.9013593	-.7594330	-5.7169808
H	86	6.1885864	-5.9646576	-4.7714322
H	87	-4.4048991	.1048038	-6.1719898
C	88	4.5527703	-5.1968617	-3.7109293
C	89	5.2561045	.2549886	-4.0236921
N	90	4.7286028	.0285166	-3.0128467
C	91	5.9136424	.5541157	-5.2700280
H	92	5.8682365	1.6394812	-5.4785048
H	93	5.4304533	.0204210	-6.1003153
H	94	6.9702777	.2526562	-5.2313563
C	95	-4.8433301	.1011085	-4.1256273
N	96	-4.4881220	.0875828	-3.0189938
N	97	4.1213864	-4.5292151	-2.8631699
C	98	-4.4879115	5.3377563	-3.5554097
N	99	-4.0379092	4.6330470	-2.7481990
C	100	-5.0493447	6.2173589	-4.5480796
H	101	-4.5813659	7.2105851	-4.4909418
H	102	-6.1312018	6.3343310	-4.3900692
H	103	-4.8866502	5.8139124	-5.5573253
C	104	-4.5546300	-5.1380877	-3.6460766
N	105	-4.0907762	-4.4592209	-2.8247147
C	106	-5.1336408	-5.9854486	-4.6565449
H	107	-6.2312245	-5.9300941	-4.6218732
H	108	-4.8344558	-7.0316088	-4.4988691
C	109	6.7625187	-.0642298	5.0821958
N	110	5.8305797	-.0494726	4.3891590
C	111	7.9204955	-.0823768	5.9392796
H	112	7.6199314	-.0121843	6.9938388
H	113	8.5825281	.7638770	5.7088500
H	114	8.4871610	-1.0134964	5.8000906
C	115	-6.7119705	.0357444	5.0800327
N	116	-5.7674126	.0337209	4.4041682
C	117	-7.8856298	.0383032	5.9157195
H	118	-8.4772072	.9483959	5.7447167
H	119	-7.6026564	.0013264	6.9768033
H	120	-8.5176632	-.8326628	5.6933670

C 121	4.0396114	-5.0054089	5.2153593
N 122	3.6993640	-4.4508935	4.2525086
C 123	4.4654912	-5.6975016	6.4043863
H 124	4.2727508	-5.0848864	7.2963120
H 125	5.5422318	-5.9148913	6.3572663
H 126	3.9243737	-6.6483970	6.5112606
C 127	-4.0339298	-4.9251060	5.2407136
N 128	-3.6807170	-4.3790436	4.2777160
C 129	-4.4760343	-5.6065435	6.4299753
H 130	-5.5582491	-5.7951576	6.3845301
H 131	-4.2655656	-4.9999308	7.3219901
H 132	-3.9602236	-6.5715685	6.5352354
C 133	4.1765951	4.9490888	5.2335205
N 134	3.8135560	4.3958430	4.2782574
C 135	4.6305304	5.6397584	6.4129275
H 136	4.2833497	5.1236961	7.3190868
H 137	4.2448791	6.6691332	6.4287523
H 138	5.7289847	5.6810132	6.4348015
C 139	-3.9697818	4.9737259	5.3161146
N 140	-3.6268622	4.4324589	4.3466953
C 141	-4.3988561	5.6494974	6.5133462
H 142	-4.0915769	6.7048112	6.4909549
H 143	-3.9571845	5.1767847	7.4018371
H 144	-5.4936656	5.6093716	6.6053893
H 145	.2039893	.0649286	-.8199646
C 146	.0335358	.0732946	-1.9004203
C 147	-.4072731	.0947059	-4.6646716
C 148	-.0751038	1.2814946	-2.5805471
C 149	-.0714098	-1.1242467	-2.5997699
C 150	-.2873838	-1.1131488	-3.9723659
C 151	-.2914341	1.2916533	-3.9531292
H 152	.0110111	2.2310623	-2.0373385
H 153	.0179204	-2.0819356	-2.0718310
H 154	-.3663702	-2.0569296	-4.5356452
H 155	-.3747047	2.2441954	-4.5007867
C 156	-.6001698	.1059692	-6.1694449
C 157	.7893613	.1094224	-6.8127574
C 158	-1.3683621	1.3492149	-6.6211309
C 159	-1.3698487	-1.1297914	-6.6388831
H 160	-.9091028	2.2701281	-6.2262593
H 161	-2.4102913	1.3280045	-6.2727205
H 162	-1.3862516	1.4260716	-7.7163042
H 163	1.3641080	-.7797368	-6.5229070
H 164	1.3649927	.9938845	-6.5107056
H 165	.7197464	.1170668	-7.9090991
H 166	-.9105748	-2.0567473	-6.2583938
H 167	-1.3889425	-1.1902146	-7.7350623
H 168	-2.4113507	-1.1130497	-6.2889934

Heat of Formation: 1148.400 kcal/mol

THIOPHENOL/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Oct 7 13:31:05 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 240
157 S shells
83 P shells
Number of basis functions: 406
Number of electrons: 420
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 465 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 309 Heat of formation = 1176.451 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9304080	4.8849409	.4901986
N	2	3.4211039	3.4683001	.4930944
C	3	3.8882191	.7327838	.4602804
C	4	3.6634583	2.8391439	-.7038905
C	5	3.5430342	2.7928776	1.6832783
C	6	3.7766196	1.4219615	1.6753774
C	7	3.9065874	1.4718917	-.7293429
H	8	3.6843672	3.4443687	-1.6767283
H	9	3.4741913	3.3763309	2.6712402
H	10	3.8689589	.8702276	2.6310258
H	11	4.1132353	.9516622	-1.7084486
C	12	3.8907596	-.7347116	.4199390
H	13	3.3410797	5.4209967	1.3742643
H	14	3.3236902	5.4159746	-.4049297
C	15	1.4291580	4.9045378	.4969792
N	16	3.4009066	-3.4593188	.3152126
H	17	-1.2567807	-4.2187879	-1.8407596
C	18	3.7413833	-1.4762113	1.5999212
C	19	3.4935052	-2.8420183	1.5393206
H	20	1.2079668	-4.2486005	-1.8451003
C	21	3.9515345	-1.4174943	-.8026444
H	22	3.8140022	-.9691712	2.5811679
H	23	3.3878451	-3.4686083	2.4963521
C	24	2.8714721	-4.8597107	.2379196
H	25	3.2657097	-5.4509307	1.0936709
C	26	-1.3647207	4.9328251	.5139488
C	27	.7374860	5.1142550	1.6901289
C	28	.7181420	4.7394103	-.6941686
C	29	-.6715884	4.7530756	-.6855759
C	30	-.6543771	5.1283698	1.6985450
H	31	1.2867312	5.2763351	2.6271644
H	32	1.2542825	4.6088611	-1.6439778
H	33	-1.2217701	4.6319110	-1.6285197
H	34	-1.1888800	5.3009158	2.6422776
C	35	-2.8662382	4.9443748	.5258270
H	36	-3.2542525	5.4821944	1.4190147
H	37	-3.2586171	5.4912394	-.3598830
N	38	-3.3872459	3.5386347	.5256254
C	39	-3.8870438	.8121859	.4851634
C	40	-3.6847049	2.9262802	-.6683351
C	41	-3.4797605	2.8563200	1.7145750
C	42	-3.7304970	1.4896987	1.7022439
C	43	-3.9447136	1.5608606	-.6982464
H	44	-3.7334101	3.5613539	-1.6230641
H	45	-3.3716516	3.4302568	2.7039013
H	46	-3.8005587	.9324942	2.6563837
H	47	-4.1975272	1.0503376	-1.6744391
C	48	-3.8957593	-.6556851	.4449929
H	49	-3.3285640	-5.3809751	1.1054881
C	50	-3.7352548	-1.4001528	1.6220236
C	51	-3.9753607	-1.3382234	-.7759427
H	52	-3.8151726	-3.2921444	-1.8084231
C	53	-3.5001581	-2.7679250	1.5575037
H	54	-3.7903512	-.8951649	2.6054797
H	55	-4.2260486	-.7725089	-1.7209253
C	56	-3.7361231	-2.7073551	-.8224339
H	57	-3.3887902	-3.3955847	2.5129765
C	58	-2.9261343	-4.7955648	.2495188
N	59	-3.4299260	-3.3861359	.3323251
H	60	-3.3180210	-5.2818005	-.6712077
C	61	-1.4246696	-4.8064541	.2451966

C	62	3.6997783	-2.7846122	-.8438822
H	63	1.2063037	-5.4875052	2.3010265
H	64	3.2502622	-5.3553279	-.6832940
C	65	1.3699848	-4.8391425	.2396020
C	66	-.7251043	-5.1735272	1.3948966
C	67	-.7207409	-4.4805118	-.9167245
C	68	.6689504	-4.4969479	-.9193920
C	69	.6668792	-5.1898420	1.3921754
H	70	-1.2676730	-5.4584854	2.3059780
H	71	3.7600260	-3.3705846	-1.8310364
H	72	4.1900453	-.8579986	-1.7555845
H	73	-6.5868886	1.2398666	-5.6250145
C	74	5.4740400	4.4843843	-5.4518402
C	75	5.1199941	-5.9272463	-5.0963495
C	76	4.7464661	4.3192552	-4.2198635
H	77	6.3324337	5.1565685	-5.3099428
H	78	4.8282628	4.9083989	-6.2334679
H	79	4.6776028	-5.6306830	-6.0576217
N	80	4.1708866	4.1573724	-3.2239807
H	81	5.8474126	3.5020457	-5.7943692
H	82	-5.2241709	-5.3433921	-5.9901034
H	83	4.8809074	-6.9849160	-4.9149573
C	84	-6.5035785	.2205629	-5.2225167
H	85	-7.5111433	-.1305964	-4.9570857
H	86	6.2123433	-5.8265586	-5.1691531
H	87	-6.1032505	-.4325698	-6.0104620
C	88	4.6083938	-5.1053996	-4.0299842
C	89	5.3745455	.3731992	-4.2038655
N	90	4.8010964	.1323983	-3.2217303
C	91	6.0889746	.6912840	-5.4136696
H	92	6.0320137	1.7765779	-5.6195799
H	93	5.6605017	.1519758	-6.2699575
H	94	7.1481498	.4109507	-5.3217573
C	95	-5.6439834	.2036498	-4.0672125
N	96	-4.9567310	.1894410	-3.1294871
N	97	4.1987395	-4.4477002	-3.1641494
C	98	-4.5386680	5.4192820	-3.7391116
N	99	-4.1147224	4.7074359	-2.9240991
C	100	-5.0668901	6.3077829	-4.7420335
H	101	-4.3843187	7.1540458	-4.9047644
H	102	-6.0429628	6.7049447	-4.4279010
H	103	-5.1978492	5.7780429	-5.6960322
C	104	-4.7051948	-5.0443964	-3.9817216
N	105	-4.2889661	-4.3744192	-3.1285196
C	106	-5.2247193	-5.8818106	-5.0320803
H	107	-6.2561809	-6.1876088	-4.8051443
H	108	-4.6106812	-6.7870618	-5.1413813
C	109	6.6650626	-.1306846	4.8806974
N	110	5.7405516	-.0934078	4.1786310
C	111	7.8138953	-.1767124	5.7489764
H	112	7.5004338	-.1819583	6.8020911
H	113	8.4574311	.6981365	5.5816539
H	114	8.4046510	-1.0831609	5.5570825
C	115	-6.6067098	-.0304206	4.9377790
N	116	-5.6858703	-.0096321	4.2302517
C	117	-7.7510389	-.0560397	5.8128425
H	118	-8.3692112	.8400920	5.6635192
H	119	-7.4313979	-.0872942	6.8636457
H	120	-8.3697285	-.9413802	5.6106884
C	121	3.9388981	-5.0801917	4.8657721
N	122	3.6060797	-4.4992763	3.9160155
C	123	4.3557543	-5.8050555	6.0383755
H	124	3.9711517	-5.3213251	6.9472111
H	125	5.4529784	-5.8383343	6.0992395
H	126	3.9791520	-6.8373884	6.0069810
C	127	-3.9383227	-4.9908263	4.8943677
N	128	-3.6059858	-4.4196152	3.9385822
C	129	-4.3547390	-5.7035785	6.0745345
H	130	-5.4512167	-5.7738953	6.1136544
H	131	-4.0065130	-5.1864993	6.9796709
H	132	-3.9420882	-6.7224978	6.0746734
C	133	4.0950377	4.8792628	5.0911675

N 134	3.7329937	4.3467384	4.1238005
C 135	4.5478559	5.5444069	6.2855783
H 136	4.6995911	4.8180516	7.0963829
H 137	3.8082361	6.2868894	6.6171220
H 138	5.4998707	6.0621413	6.0995350
C 139	-3.9132203	4.9075720	5.1602582
N 140	-3.5796398	4.3854615	4.1771308
C 141	-4.3308114	5.5598318	6.3744697
H 142	-3.5542337	6.2538601	6.7258195
H 143	-4.5186300	4.8187797	7.1641260
H 144	-5.2554900	6.1303126	6.2056659
H 145	-.0279201	2.4984582	-2.3124808
C 146	-.0442984	1.4950675	-2.7574118
C 147	-.0860082	-1.0577773	-3.8917830
C 148	-.1129056	1.3457508	-4.1381613
C 149	.0030161	.3678837	-1.9424373
C 150	-.0176727	-.9017629	-2.5033016
C 151	-.1336241	.0759770	-4.7053085
H 152	-.1520741	2.2293813	-4.7853268
H 153	.0567185	.4806097	-.8552122
H 154	.0194881	-1.7950838	-1.8639905
H 155	-.1883866	-.0261819	-5.7968139
S 156	-.1061386	-2.7075064	-4.4889616
H 157	-.1674020	-2.5006655	-5.7860867

Heat of Formation: 1176.451 kcal/mol

THIOANISOLE/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Oct 7 21:12:19 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 244
160 S shells
84 P shells
Number of basis functions: 412
Number of electrons: 426
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 474 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 293 Heat of formation = 1170.972 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	2.9486523	4.9430074	.7008346
N 2	3.4358402	3.5255356	.6708168
C 3	3.8959538	.7905250	.5721684
C 4	3.6814173	2.9255547	-.5403878
C 5	3.5511730	2.8206116	1.8444411
C 6	3.7810466	1.4496927	1.8035116
C 7	3.9212141	1.5587228	-.5987156
H 8	3.7075439	3.5546646	-1.4978053
H 9	3.4800696	3.3796141	2.8461345
H 10	3.8677097	.8741853	2.7455307
H 11	4.1304979	1.0622959	-1.5895062
C 12	3.8951532	-.6754863	.4954941
H 13	3.3600295	5.4569304	1.5976012

H	14	3.3437826	5.4940753	-.1812742
C	15	1.4474807	4.9662966	.7062494
N	16	3.3997888	-3.3954119	.3212395
H	17	-1.2618219	-4.1019018	-1.8537361
C	18	3.7381767	-1.4454539	1.6561401
C	19	3.4876235	-2.8087034	1.5606971
H	20	1.2045342	-4.1365283	-1.8617599
C	21	3.9606858	-1.3280148	-.7432326
H	22	3.8070208	-.9628711	2.6498797
H	23	3.3760212	-3.4584393	2.5013084
C	24	2.8680604	-4.7923895	.2070852
H	25	3.2615582	-5.4065715	1.0468330
C	26	-1.3462623	5.0006908	.7206132
C	27	.7551742	5.1718441	1.8996546
C	28	.7372425	4.8084315	-.4864357
C	29	-.6523292	4.8250517	-.4791480
C	30	-.6367395	5.1890468	1.9067624
H	31	1.3036802	5.3278879	2.8381069
H	32	1.2739345	4.6807485	-1.4363201
H	33	-1.2017433	4.7089303	-1.4231774
H	34	-1.1716372	5.3580090	2.8508772
C	35	-2.8477303	5.0150716	.7310942
H	36	-3.2361428	5.5335374	1.6354618
H	37	-3.2374044	5.5824260	-.1428383
N	38	-3.3716048	3.6108414	.6987804
C	39	-3.8764084	.8870989	.5951999
C	40	-3.6709731	3.0270409	-.5089015
C	41	-3.4645229	2.9012355	1.8716232
C	42	-3.7175055	1.5357023	1.8276314
C	43	-3.9338103	1.6632332	-.5703643
H	44	-3.7183871	3.6840812	-1.4487201
H	45	-3.3549185	3.4518095	2.8738349
H	46	-3.7872936	.9564375	2.7685362
H	47	-4.1885952	1.1761614	-1.5579265
C	48	-3.8880195	-.5793725	.5206124
H	49	-3.3318459	-5.3201967	1.0686889
C	50	-3.7264577	-1.3514986	1.6795540
C	51	-3.9717201	-1.2328704	-.7158355
H	52	-3.8181995	-3.1624734	-1.7938387
C	53	-3.4946674	-2.7178772	1.5825349
H	54	-3.7780764	-.8695092	2.6746568
H	55	-4.2228707	-.6446320	-1.6468922
C	56	-3.7357261	-2.6010689	-.7948201
H	57	-3.3825352	-3.3679227	2.5226772
C	58	-2.9290424	-4.7158528	.2261758
N	59	-3.4286896	-3.3073889	.3430423
H	60	-3.3236415	-5.1790972	-.7051704
C	61	-1.4276486	-4.7306413	.2194807
C	62	3.7062394	-2.6931691	-.8193201
H	63	1.2039476	-5.4584107	2.2582737
H	64	3.2457442	-5.2641797	-.7269948
C	65	1.3666431	-4.7692515	.2100731
C	66	-.7277862	-5.1223117	1.3608353
C	67	-.7243696	-4.3830673	-.9365678
C	68	.6653202	-4.4023833	-.9412008
C	69	.6640797	-5.1416045	1.3561745
H	70	-1.2700715	-5.4241318	2.2666323
H	71	3.7710655	-3.2551291	-1.8198361
H	72	4.2049782	-.7457222	-1.6809753
H	73	-6.9224822	1.4518085	-5.2446002
C	74	5.5102403	4.6882139	-5.2398836
C	75	5.1691144	-5.7422936	-5.1230267
C	76	4.7801078	4.4932906	-4.0137870
H	77	6.3685481	5.3564069	-5.0798637
H	78	4.8661614	5.1313993	-6.0122031
H	79	4.9741495	-5.2592316	-6.0906170
N	80	4.2025056	4.3073307	-3.0233258
H	81	5.8839606	3.7143764	-5.6054772
H	82	-5.0043219	-5.2367511	-6.0440396
H	83	4.6994102	-6.7362111	-5.1293065
C	84	-6.5056627	.4424606	-5.1193162
H	85	-7.3402156	-.2643654	-5.0070506

H	86	6.2550785	-5.8727121	-5.0111973
H	87	-5.9469761	.1810621	-6.0287882
C	88	4.6443160	-4.9439487	-4.0452650
C	89	5.4042748	.5456215	-4.0916107
N	90	4.8282622	.2795470	-3.1175843
C	91	6.1221420	.8948011	-5.2907642
H	92	6.0651733	1.9849309	-5.4692594
H	93	5.6965467	.3771950	-6.1617048
H	94	7.1811902	.6127866	-5.2027767
C	95	-5.6454513	.3926823	-3.9654282
N	96	-4.9578352	.3520412	-3.0288032
N	97	4.2243368	-4.3055455	-3.1700409
C	98	-4.5123590	5.5922576	-3.5243030
N	99	-4.0951878	4.8610060	-2.7231371
C	100	-5.0322224	6.5046090	-4.5100221
H	101	-4.6002911	7.5062962	-4.3727081
H	102	-6.1253347	6.5837312	-4.4218992
H	103	-4.7887038	6.1569768	-5.5238018
C	104	-4.7256326	-4.8631648	-4.0007918
N	105	-4.3015188	-4.2153315	-3.1345345
C	106	-5.2553789	-5.6733056	-5.0673093
H	107	-6.3496451	-5.7451343	-4.9884432
H	108	-4.8373436	-6.6891061	-5.0224193
C	109	6.6560872	-.1892160	4.9789129
N	110	5.7334911	-.1332535	4.2755839
C	111	7.8025500	-.2583601	5.8487964
H	112	7.4864467	-.2841281	6.9008209
H	113	8.4502950	.6169436	5.7012564
H	114	8.3898190	-1.1632167	5.6394884
C	115	-6.5822617	-.0569953	5.0412141
N	116	-5.6646527	-.0216566	4.3300964
C	117	-7.7226028	-.1006019	5.9207587
H	118	-8.3376897	.8016001	5.7976073
H	119	-7.3982011	-.1603345	6.9688597
H	120	-8.3459311	-.9778799	5.6987143
C	121	3.9193887	-5.1260949	4.8339862
N	122	3.5892641	-4.5229808	3.8972273
C	123	4.3329668	-5.8783570	5.9903852
H	124	4.0911651	-5.3311733	6.9123601
H	125	5.4176959	-6.0558824	5.9650843
H	126	3.8231701	-6.8518639	6.0190398
C	127	-3.9324618	-5.0162839	4.8679520
N	128	-3.6000121	-4.4243884	3.9248899
C	129	-4.3490812	-5.7545679	6.0322477
H	130	-5.4393210	-5.8964524	6.0270299
H	131	-4.0725274	-5.2155811	6.9492663
H	132	-3.8710218	-6.7442647	6.0521017
C	133	4.0972200	4.8190993	5.3056603
N	134	3.7374926	4.3123458	4.3237181
C	135	4.5472592	5.4523515	6.5183172
H	136	4.3948601	4.7868269	7.3796134
H	137	3.9915556	6.3841522	6.6953981
H	138	5.6175818	5.6946648	6.4505937
C	139	-3.8943781	4.8730962	5.3639017
N	140	-3.5620409	4.3731547	4.3689219
C	141	-4.3104272	5.4979851	6.5929454
H	142	-3.7711382	6.4435922	6.7460342
H	143	-4.1069369	4.8384894	7.4482914
H	144	-5.3882267	5.7137890	6.5682800
H	145	-.0085892	2.5608156	-2.1047363
C	146	-.0230632	1.5869892	-2.6107482
C	147	-.0601687	-.8923639	-3.9043066
C	148	-.0728693	1.5230978	-3.9982055
C	149	.0075562	.4103359	-1.8673446
C	150	-.0109222	-.8210077	-2.5067508
C	151	-.0912278	.2907042	-4.6434401
H	152	-.0992247	2.4448945	-4.5902177
H	153	.0461349	.4549476	-.7746163
H	154	.0128699	-1.7519484	-1.9222052
H	155	-.1314214	.2578495	-5.7404090
S	156	-.0779831	-2.5144783	-4.5817034
C	157	-.1355268	-2.3146322	-6.3734124

H 158	.7352561	-1.7877814	-6.7798616
H 159	-1.0349122	-1.7957866	-6.7240449
H 160	-.1440990	-3.3275641	-6.7983728

Heat of Formation: 1170.972 kcal/mol

p-XYLENE/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Sep 30 09:58:32 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 246
162 S shells
84 P shells
Number of basis functions: 414
Number of electrons: 426
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 480 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 208 Heat of formation = 1154.457 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9308113	.0062481	-4.8559162
N	2	3.4473777	.0170184	-3.4483080
C	3	3.9554076	.0159045	-.7194276
C	4	3.6837144	-1.1741443	-2.8064008
C	5	3.6005453	1.2147366	-2.7920159
C	6	3.8536829	1.2229302	-1.4249004
C	7	3.9477993	-1.1837203	-1.4423051
H	8	3.6771680	-2.1553505	-3.3972557
H	9	3.5351648	2.1949760	-3.3881282
H	10	3.9546503	2.1859457	-.8868902
H	11	4.1406094	-2.1579636	-.9093276
C	12	3.9550205	-.0026961	.7488656
H	13	3.3312701	.8870060	-5.4050266
H	14	3.3169035	-.8919045	-5.3871346
C	15	1.4288748	.0199380	-4.8558918
N	16	3.4190714	-.0552813	3.4672001
H	17	-1.2900827	-2.2166786	4.7832359
C	18	3.8234153	1.1913938	1.4712709
C	19	3.5540956	1.1568469	2.8338036
H	20	1.1859790	-2.2405628	4.8154848
C	21	3.9765109	-1.2160837	1.4509532
H	22	3.9125257	2.1642177	.9493652
H	23	3.4596703	2.1253108	3.4441101
C	24	2.8688429	-.0935666	4.8615243
H	25	3.2551377	.7771359	5.4361709
C	26	-1.3674457	.0501804	-4.8814588
C	27	.7389320	1.2339446	-4.8434649
C	28	.7140506	-1.1783938	-4.9008819
C	29	-.6775223	-1.1631698	-4.9118529
C	30	-.6518947	1.2490389	-4.8573445
H	31	1.2922281	2.1827970	-4.8372818
H	32	1.2465789	-2.1377508	-4.9428513
H	33	-1.2297476	-2.1109536	-4.9600872
H	34	-1.1846333	2.2095882	-4.8620375

C	35	-2.8692075	.0694111	-4.9117795
H	36	-3.2385430	.9652144	-5.4584716
H	37	-3.2627169	-.8132509	-5.4627535
N	38	-3.4162650	.0752898	-3.5157991
C	39	-3.9649192	.0648881	-.7981291
C	40	-3.6924090	-1.1165515	-2.8893360
C	41	-3.5606880	1.2719200	-2.8559887
C	42	-3.8390196	1.2749787	-1.4945791
C	43	-3.9746408	-1.1317234	-1.5279850
H	44	-3.7033267	-2.0818602	-3.5088530
H	45	-3.4667485	2.2543999	-3.4435223
H	46	-3.9466210	2.2354764	-.9547216
H	47	-4.1988988	-2.1063562	-1.0032789
C	48	-3.9728988	.0486554	.6704295
H	49	-3.3125814	.8442672	5.3589624
C	50	-3.8544647	1.2429643	1.3948486
C	51	-3.9909169	-1.1638181	1.3734712
H	52	-3.7445338	-2.1575790	3.3356397
C	53	-3.5926126	1.2097921	2.7591599
H	54	-3.9553322	2.2152129	.8750796
H	55	-4.2088464	-2.1266728	.8247404
C	56	-3.7253004	-1.1787096	2.7381359
H	57	-3.5058760	2.1791265	3.3690449
C	58	-2.9319944	-.0380080	4.7981504
N	59	-3.4570444	-.0010924	3.3942929
H	60	-3.3323345	-.9338728	5.3222534
C	61	-1.4299198	-.0543435	4.7936604
C	62	3.6999204	-1.2312595	2.8139246
H	63	1.2265997	2.0804496	4.8912818
H	64	3.2422293	-1.0009407	5.3857894
C	65	1.3669638	-.0812101	4.8261548
C	66	-.7159044	1.1448761	4.8327685
C	67	-.7384717	-1.2673197	4.7869166
C	68	.6529263	-1.2807870	4.8045138
C	69	.6751008	1.1314666	4.8479050
H	70	-1.2500235	2.1041188	4.8646650
H	71	3.7197446	-2.2103779	3.4121260
H	72	4.1975349	-2.1820482	.9071487
H	73	-6.8016875	-5.8694232	-1.1479429
C	74	5.3261277	-6.0080575	-4.3874638
C	75	5.0351793	-5.4947237	5.9615366
C	76	4.6437951	-4.7485306	-4.2377026
H	77	6.1796436	-5.9093801	-5.0734375
H	78	4.6479580	-6.7749895	-4.7870737
H	79	4.6522366	-6.4677426	5.6231385
N	80	4.1048201	-3.7304321	-4.0884194
H	81	5.7007821	-6.3439488	-3.4033539
H	82	-4.6777948	-6.4223210	5.5401239
H	83	4.7463491	-5.3537953	7.0129757
C	84	-6.3784996	-5.7143709	-.1453692
H	85	-7.2088805	-5.6120949	.5678815
H	86	6.1329767	-5.5127950	5.9034286
H	87	-5.7924998	-6.6035070	.1264493
C	88	4.5053915	-4.4319234	5.1466634
C	89	5.3057813	-4.6854323	-.2925309
N	90	4.7588446	-3.6867536	-.0575577
C	91	5.9862688	-5.9165564	-.6030711
H	92	5.9087527	-6.1367107	-1.6843178
H	93	5.5450739	-6.7545433	-.0454415
H	94	7.0512947	-5.8463951	-.3390515
C	95	-5.5498862	-4.5367375	-.1253980
N	96	-4.8868671	-3.5816154	-.1092005
N	97	4.0807941	-3.5692024	4.4939276
C	98	-4.4387782	-4.2660032	-5.3174835
N	99	-4.0396556	-3.4209826	-4.6265674
C	100	-4.9362850	-5.3066961	-6.1798859
H	101	-4.6446842	-5.1143995	-7.2224195
H	102	-6.0335893	-5.3549709	-6.1306951
H	103	-4.5306161	-6.2831277	-5.8798950
C	104	-4.5191893	-4.3851464	5.0730299
N	105	-4.1027392	-3.5232414	4.4139547
C	106	-5.0385319	-5.4470001	5.8958626

H 107	-6.1376852	-5.4511296	5.8696477
H 108	-4.7176797	-5.3170012	6.9393815
C 109	6.6710458	4.5293616	.0785692
N 110	5.7533127	3.8176750	.0606258
C 111	7.8115284	5.4094941	.1007079
H 112	7.4874537	6.4584015	.1469184
H 113	8.4201451	5.2727494	-.8039414
H 114	8.4412323	5.2006837	.9767169
C 115	-6.7950321	4.4788626	-.0331359
N 116	-5.8604050	3.7893236	-.0327898
C 117	-7.9563514	5.3316167	-.0336451
H 118	-8.5781148	5.1336916	-.9178003
H 119	-7.6574836	6.3888854	-.0478333
H 120	-8.5642071	5.1537193	.8643183
C 121	4.0370709	4.4931121	5.0490503
N 122	3.6818391	3.5514167	4.4680415
C 123	4.4808493	5.6555023	5.7742689
H 124	4.2625455	6.5705932	5.2059902
H 125	5.5647047	5.6063471	5.9523019
H 126	3.9725400	5.7198035	6.7469141
C 127	-4.0870401	4.5582207	4.9541267
N 128	-3.7304244	3.6085625	4.3871451
C 129	-4.5328194	5.7306953	5.6616808
H 130	-5.6114397	5.6690663	5.8657012
H 131	-4.3421977	6.6350697	5.0669098
H 132	-4.0036901	5.8262832	6.6205096
C 133	4.1604473	4.5691940	-4.9630769
N 134	3.7893330	3.6264219	-4.3938290
C 135	4.6238708	5.7328100	-5.6738678
H 136	4.2065255	6.6473571	-5.2295323
H 137	4.3175981	5.6867965	-6.7287678
H 138	5.7208064	5.7954319	-5.6340749
C 139	-4.0209813	4.6628435	-4.9937714
N 140	-3.6749151	3.7034100	-4.4367860
C 141	-4.4534760	5.8474734	-5.6892095
H 142	-4.1084434	5.8287547	-6.7328793
H 143	-4.0496285	6.7476177	-5.2048442
H 144	-5.5508797	5.9140796	-5.6882559
C 145	.4699158	2.7620033	-.0023319
C 146	.2170970	1.2985703	-.0167465
C 147	-.1690668	-1.4782791	-.0428099
C 148	.1133476	.6103628	-1.2264707
C 149	.1072797	.5885569	1.1800798
C 150	-.0817868	-.7875880	1.1671919
C 151	-.0757603	-.7661022	-1.2394886
H 152	.1816245	1.1580687	-2.1774402
H 153	.1709924	1.1192302	2.1407542
H 154	-.1601620	-1.3335525	2.1182077
H 155	-.1492143	-1.2941718	-2.2007648
C 156	-.3499971	-2.9521586	-.0544462
H 157	.6246941	-3.4574001	-.0066146
H 158	-.8560148	-3.2961075	-.9664525
H 159	-.9426448	-3.2962578	.8038343
H 160	1.5536814	2.9557509	.0124980
H 161	.0355286	3.2455596	.8826354
H 162	.0570895	3.2599128	-.8896447

Heat of Formation: 1154.457 kcal/mol

1,4-DICHLOROBENZENE/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Sep 30 10:01:13 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 240

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 156 S shells
   84 P shells
Number of basis functions: 408
Number of electrons: 426
Use of molecular symmetry disabled
Molecular charge:   4
Spin multiplicity:  1

Point Group = C1  Order =  1 Nsymop =  1
This system has 462 degrees of freedom

Convergence on Energy - difference below    .5000D-03 kcal/mol

Cycle no: 183 Heat of formation =  1161.754  rmsG =  .0000 rmsD =  .0001
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Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	3.4909649	-4.4578782	-.0108460
N	2	3.8490841	-3.0020547	-.0036984
C	3	4.0497558	-.2342919	.0173118
C	4	3.9664470	-2.3431248	1.1961837
C	5	3.9783726	-2.3282288	-1.1942137
C	6	4.0828806	-.9414396	-1.1923346
C	7	4.0749136	-.9583619	1.2161822
H	8	3.9894296	-2.9358224	2.1762807
H	9	4.0158263	-2.9233120	-2.1773165
H	10	4.1773065	-.3912225	-2.1487951
H	11	4.1688374	-.4107048	2.1971117
C	12	3.8735537	1.2232459	.0354888
H	13	3.9523477	-4.9498916	-.8957122
H	14	3.9311778	-4.9528200	.8831813
C	15	1.9983924	-4.6263311	-.0299903
N	16	2.9940881	3.8501780	.0661356
H	17	-1.8604287	4.5812990	2.1906889
C	18	3.7045311	1.9302415	-1.1629211
C	19	3.2573210	3.2457348	-1.1394717
H	20	.5942863	4.9061862	2.2243024
C	21	3.7590624	1.9165706	1.2488675
H	22	3.9127365	1.4322269	-2.1296888
H	23	3.1196527	3.8421414	-2.1121623
C	24	2.2673659	5.1613658	.0850397
H	25	2.5817723	5.7724228	-.7899631
C	26	-.7750333	-4.9886437	-.0687537
C	27	1.3154430	-4.6953012	-1.2460288
C	28	1.2895557	-4.7531294	1.1662211
C	29	-.0903357	-4.9328474	1.1467769
C	30	-.0639636	-4.8755817	-1.2652771
H	31	1.8669690	-4.6244871	-2.1933021
H	32	1.8203087	-4.7298581	2.1274337
H	33	-.6354367	-5.0481668	2.0930435
H	34	-.5890605	-4.9450705	-2.2276587
C	35	-2.2607620	-5.2110078	-.0918777
H	36	-2.5545285	-5.7988091	-.9897208
H	37	-2.5817804	-5.8103523	.7886921
N	38	-2.9837147	-3.8975917	-.0958634
C	39	-3.8692886	-1.2707888	-.0846897
C	40	-3.3310030	-3.3094637	1.0969796
C	41	-3.2183163	-3.2638206	-1.2923271
C	42	-3.6672851	-1.9487785	-1.2950040
C	43	-3.7812109	-1.9940248	1.1126983
H	44	-3.2609149	-3.9251646	2.0627249
H	45	-3.0561102	-3.8362509	-2.2755195
H	46	-3.8513087	-1.4292764	-2.2553873
H	47	-4.0647737	-1.4995931	2.0881808
C	48	-4.0533134	.1862002	-.0698915
H	49	-3.9215815	4.9161024	-.8795492
C	50	-4.0285075	.9173155	-1.2657940
C	51	-4.1458296	.8844093	1.1419241
H	52	-4.1233782	2.8644044	2.1318240
C	53	-3.9220666	2.3025014	-1.2355876

H	54	-4.0788346	.3876940	-2.2369105
H	55	-4.2950296	.3154268	2.1065758
C	56	-4.0384927	2.2706318	1.1537013
H	57	-3.9099426	2.9165697	-2.2067878
C	58	-3.4846003	4.4039940	.0063079
N	59	-3.8515791	2.9507898	-.0260801
H	60	-3.9437793	4.8841074	.8986825
C	61	-1.9912074	4.5672358	.0276357
C	62	3.3128083	3.2335728	1.2525817
H	63	.6449573	4.9719153	-2.0969480
H	64	2.5639193	5.7389952	.9884305
C	65	.7822763	4.9338982	.0655925
C	66	-1.2807260	4.6830092	-1.1688485
C	67	-1.3088489	4.6456468	1.2433400
C	68	.0705842	4.8281725	1.2622510
C	69	.0985544	4.8654088	-1.1499663
H	70	-1.8103598	4.6472290	-2.1305651
H	71	3.2233045	3.8269978	2.2309540
H	72	4.0103576	1.4002391	2.2228554
H	73	-6.5838263	-1.9358846	5.8846157
C	74	5.6074363	-3.7393605	6.0831704
C	75	4.1392940	6.5060384	5.5457276
C	76	4.9540988	-3.6669955	4.8016471
H	77	6.5391574	-4.3188306	6.0130214
H	78	4.9565580	-4.2195047	6.8272120
H	79	3.6672767	6.1971783	6.4889883
N	80	4.4351480	-3.5792711	3.7661065
H	81	5.8513473	-2.7190562	6.4312535
H	82	-5.2985578	4.9535861	6.3919074
H	83	3.8456032	7.5440680	5.3333117
C	84	-6.2598563	-.8960230	5.7361581
H	85	-7.1553745	-.2620666	5.6665386
H	86	5.2306294	6.4746663	5.6752795
H	87	-5.6784993	-.5835726	6.6149219
C	88	3.7348478	5.6379086	4.4700963
C	89	5.1583712	.3305323	4.7640508
N	90	4.6274486	.5031871	3.7442554
C	91	5.8216489	.0975223	6.0213836
H	92	5.8646057	-.9862791	6.2383034
H	93	5.2843631	.5948701	6.8410001
H	94	6.8496533	.4865660	5.9937135
C	95	-5.4679355	-.7816772	4.5388418
N	96	-4.8346564	-.6900347	3.5679543
N	97	3.4109825	4.9425321	3.5970327
C	98	-3.7680923	-5.8098288	4.2455712
N	99	-3.4554500	-5.0782102	3.3983902
C	100	-4.1578667	-6.7230485	5.2888202
H	101	-3.6129857	-7.6730510	5.1919243
H	102	-5.2353542	-6.9345112	5.2317810
H	103	-3.9385254	-6.2957019	6.2773567
C	104	-5.0963002	4.5024725	4.3550056
N	105	-4.6050919	3.8988525	3.4918432
C	106	-5.7091325	5.2561537	5.4183396
H	107	-6.7957869	5.0891241	5.4311079
H	108	-5.5258558	6.3317003	5.2826126
C	109	6.9271096	.9156050	-4.2782422
N	110	5.9819141	.7833553	-3.6162933
C	111	8.1014017	1.0797377	-5.0967027
H	112	7.8344026	1.0546997	-6.1622814
H	113	8.8228486	.2746410	-4.8995840
H	114	8.5880510	2.0413380	-4.8822219
C	115	-6.7921155	-.8569567	-4.4795308
N	116	-5.8633621	-.7442467	-3.7912491
C	117	-7.9461005	-.9971055	-5.3306944
H	118	-8.4776647	-1.9323735	-5.1065703
H	119	-7.6453431	-1.0122006	-6.3874203
H	120	-8.6401594	-.1589383	-5.1782699
C	121	3.5243260	5.4957702	-4.4778160
N	122	3.2313847	4.8838935	-3.5342419
C	123	3.8902347	6.2593120	-5.6427570
H	124	3.7232899	5.6716656	-6.5564407
H	125	4.9520797	6.5411287	-5.5991233

H 126	3.2901090	7.1782923	-5.7049743
C 127	-4.6513171	4.4169207	-4.5932496
N 128	-4.2395854	3.8993100	-3.6376957
C 129	-5.1658120	5.0627379	-5.7731644
H 130	-6.2651612	5.0470025	-5.7709731
H 131	-4.8121074	4.5494498	-6.6783925
H 132	-4.8343564	6.1101080	-5.8144211
C 133	4.8509269	-4.3992264	-4.5462329
N 134	4.4050841	-3.8876102	-3.6028114
C 135	5.4074487	-5.0378219	-5.7108803
H 136	4.9881124	-4.6000056	-6.6276730
H 137	5.1827616	-6.1139959	-5.7042175
H 138	6.4994661	-4.9120205	-5.7327395
C 139	-3.3978079	-5.4355988	-4.6883684
N 140	-3.1298109	-4.8449301	-3.7240923
C 141	-3.7327971	-6.1730651	-5.8791226
H 142	-3.2826371	-7.1756657	-5.8504152
H 143	-3.3630937	-5.6506089	-6.7726357
H 144	-4.8229391	-6.2851378	-5.9673023
Cl145	-.0529465	-.0610235	3.0777848
C 146	.0234644	-.0143126	-1.3710260
C 147	-.0232977	-.0434034	1.3993952
C 148	.1601848	-1.2233003	-.6903065
C 149	-.1364917	1.1802086	-.6700861
C 150	-.1598682	1.1657114	.7189640
C 151	.1367373	-1.2380078	.6987524
H 152	.2854105	-2.1613128	-1.2505721
H 153	-.2443089	2.1294934	-1.2144717
H 154	-.2860158	2.1036173	1.2789198
H 155	.2435745	-2.1873802	1.2428046
Cl156	.0513100	.0031647	-3.0492974

Heat of Formation: 1161.754 kcal/mol

1,4-DICHLOROBENZENE2/1^{4+} , 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sun Oct 8 15:08:42 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 240
156 S shells
84 P shells
Number of basis functions: 408
Number of electrons: 426
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 462 degrees of freedom

Convergence on Energy - difference below .5000D-03 kcal/mol

Cycle no: 199 Heat of formation = 1159.599 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9300884	4.8544755	.4203815
N	2	3.4355641	3.4435605	.4478399
C	3	3.9287736	.7129866	.4660000
C	4	3.6723029	2.7925141	-.7386813
C	5	3.5793794	2.7947967	1.6501539
C	6	3.8267789	1.4262211	1.6678871

C	7	3.9286300	1.4276003	-.7387702
H	8	3.6749132	3.3772358	-1.7239267
H	9	3.5150988	3.3975571	2.6266521
H	10	3.9343271	.8949652	2.6333831
H	11	4.1256939	.8887625	-1.7091679
C	12	3.9299733	-.7550192	.4553369
H	13	3.3395541	5.4110594	1.2922875
H	14	3.3143431	5.3722536	-.4863632
C	15	1.4286486	4.8629686	.4321788
N	16	3.4135880	-3.4762431	.4126854
H	17	-1.2631637	-4.3146021	-1.7163724
C	18	3.7986374	-1.4724953	1.6518568
C	19	3.5373319	-2.8372220	1.6223863
H	20	1.2120585	-4.3421729	-1.7247071
C	21	3.9611552	-1.4617931	-.7553176
H	22	3.8929059	-.9468959	2.6215902
H	23	3.4436209	-3.4438058	2.5935336
C	24	2.8751425	-4.8744750	.3722327
H	25	3.2679745	-5.4464353	1.2418248
C	26	-1.3658829	4.8902916	.4545978
C	27	.7394628	5.1271512	1.6157108
C	28	.7143908	4.6367739	-.7471565
C	29	-.6750625	4.6498357	-.7358236
C	30	-.6526716	5.1408268	1.6268392
H	31	1.2903107	5.3336905	2.5429446
H	32	1.2483456	4.4598678	-1.6905251
H	33	-1.2275098	4.4817532	-1.6701110
H	34	-1.1844605	5.3576472	2.5628515
C	35	-2.8674041	4.9119642	.4672900
H	36	-3.2510647	5.4680183	1.3512008
H	37	-3.2549358	5.4472684	-.4275706
N	38	-3.4014428	3.5115897	.4903158
C	39	-3.9236386	.7895098	.4982840
C	40	-3.6891865	2.8778016	-.6950197
C	41	-3.5175491	2.8551078	1.6914214
C	42	-3.7810170	1.4906084	1.7035113
C	43	-3.9593586	1.5143220	-.7008762
H	44	-3.7202059	3.4934458	-1.6629277
H	45	-3.4161761	3.4476581	2.6703752
H	46	-3.8686972	.9532905	2.6674583
H	47	-4.1973953	.9853198	-1.6702663
C	48	-3.9305342	-.6788486	.4866643
H	49	-3.3215484	-5.3786919	1.2626280
C	50	-3.7951178	-1.4003404	1.6806138
C	51	-3.9728211	-1.3841871	-.7238521
H	52	-3.7549290	-3.3498174	-1.7170842
C	53	-3.5463056	-2.7672669	1.6470989
H	54	-3.8774128	-.8774239	2.6529367
H	55	-4.2052728	-.8375535	-1.6848734
C	56	-3.7170058	-2.7503360	-.7393851
H	57	-3.4525565	-3.3759255	2.6168001
C	58	-2.9234292	-4.8134002	.3910308
N	59	-3.4370560	-3.4060667	.4358939
H	60	-3.3135254	-5.3267287	-.5155383
C	61	-1.4217163	-4.8175848	.3866455
C	62	3.6943079	-2.8260054	-.7654631
H	63	1.2138133	-5.4087737	2.4645531
H	64	3.2498191	-5.3955437	-.5364411
C	65	1.3735332	-4.8485038	.3773116
C	66	-.7197584	-5.1346606	1.5494189
C	67	-.7194842	-4.5372828	-.7883943
C	68	.6698232	-4.5527434	-.7930710
C	69	.6725603	-5.1501154	1.5447655
H	70	-1.2604332	-5.3813482	2.4728370
H	71	3.7232939	-3.4284631	-1.7421316
H	72	4.1861734	-.9221024	-1.7229287
H	73	-6.9571181	1.0545820	-5.3270387
C	74	5.3841323	4.3512552	-5.5543997
C	75	5.0631520	-6.0162492	-4.9856699
C	76	4.6796687	4.2045504	-4.3067638
H	77	6.2418233	5.0295236	-5.4398398
H	78	4.7224075	4.7586172	-6.3315436