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

H	79	4.7040945	-5.6818254	-5.9691004
N	80	4.1227565	4.0574446	-3.2980471
H	81	5.7557240	3.3646268	-5.8862890
H	82	-4.7378413	-5.6029223	-5.9470099
H	83	4.7567195	-7.0621367	-4.8406766
C	84	-6.3845629	.1178151	-5.2715754
H	85	-7.0954599	-.7205767	-5.2547309
H	86	6.1618138	-5.9736536	-4.9828085
H	87	-5.7664836	.0329915	-6.1763220
C	88	4.5244287	-5.1839388	-3.9410368
C	89	5.3191624	.2599832	-4.2217934
N	90	4.7658413	.0315073	-3.2251932
C	91	6.0081967	.5621990	-5.4502428
H	92	5.9428815	1.6439376	-5.6718898
H	93	5.5649510	.0082182	-6.2895330
H	94	7.0701201	.2872936	-5.3750644
C	95	-5.5592737	.1015979	-4.0915515
N	96	-4.8992052	.0885565	-3.1344190
N	97	4.0926344	-4.5171056	-3.0927896
C	98	-4.4883981	5.3068603	-3.8307425
N	99	-4.0767908	4.6096383	-2.9969690
C	100	-5.0013953	6.1771178	-4.8572669
H	101	-4.6100831	7.1964675	-4.7282878
H	102	-6.0991694	6.2193300	-4.8121972
H	103	-4.7072334	5.8151223	-5.8524385
C	104	-4.5549169	-5.1075920	-3.9185354
N	105	-4.1297745	-4.4356598	-3.0709385
C	106	-5.0850824	-5.9463551	-4.9624173
H	107	-6.1842971	-5.9233766	-4.9529734
H	108	-4.7593435	-6.9870621	-4.8222619
C	109	6.7731300	-.0600137	4.8563521
N	110	5.8398803	-.0456527	4.1650835
C	111	7.9327189	-.0776693	5.7112650
H	112	7.6360760	.0243038	6.7643343
H	113	8.6093352	.7504327	5.4583507
H	114	8.4821100	-1.0220957	5.5943324
C	115	-6.7182039	.0369309	4.9203237
N	116	-5.7889599	.0351890	4.2235607
C	117	-7.8728792	.0391304	5.7820525
H	118	-8.4603628	.9560475	5.6351149
H	119	-7.5666362	-.0128728	6.8360191
H	120	-8.5170819	-.8238903	5.5636722
C	121	4.0077385	-5.0042200	4.9923295
N	122	3.6677825	-4.4487275	4.0299397
C	123	4.4333052	-5.6974879	6.1807811
H	124	4.1649058	-5.1231082	7.0785617
H	125	5.5233350	-5.8408717	6.1720529
H	126	3.9544599	-6.6850736	6.2428608
C	127	-4.0216163	-4.9270622	5.0206206
N	128	-3.6796534	-4.3783465	4.0550667
C	129	-4.4498143	-5.6118617	6.2130336
H	130	-5.5259043	-5.8319850	6.1639169
H	131	-4.2613782	-4.9926050	7.1012755
H	132	-3.9069186	-6.5607435	6.3282739
C	133	4.1372922	4.9540141	5.0123910
N	134	3.7763666	4.3996709	4.0569642
C	135	4.5886794	5.6460053	6.1920014
H	136	4.1995130	5.1587453	7.0970390
H	137	4.2431871	6.6896260	6.1820741
H	138	5.6870232	5.6451976	6.2408732
C	139	-3.9578832	4.9789208	5.0933667
N	140	-3.6261062	4.4347718	4.1216771
C	141	-4.3731595	5.6583335	6.2933989
H	142	-4.0734324	6.7155456	6.2606146
H	143	-3.9147553	5.1934673	7.1775320
H	144	-5.4661250	5.6113886	6.4024397
Cl	145	.0034793	.0420286	-.3478349
C	146	-.0287501	.0659127	-2.0399931
C	147	-.0844217	.1048250	-4.7995002
C	148	-.0489768	1.2899538	-2.7037541
C	149	-.0356907	-1.1389317	-2.7383393
C	150	-.0634326	-1.1179069	-4.1273072

C 151	-.0774985	1.3080197	-4.0927430
H 152	-.0432066	2.2296858	-2.1353285
H 153	-.0199118	-2.0939351	-2.1964956
H 154	-.0695408	-2.0533945	-4.6992518
H 155	-.0963677	2.2593656	-4.6375329
Cl156	-.1192471	.1286261	-6.4752143

Heat of Formation: 1159.599 kcal/mol

HYDROQUINONE/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Tue Sep 26 13:43:12 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 242
158 S shells
84 P shells
Number of basis functions: 410
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 468 degrees of freedom

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

Cycle no: 262 Heat of formation = 1082.696 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	4.8799840	-2.9285842	-.1543592
N	2	3.4611493	-3.4145517	-.1662214
C	3	.7272641	-3.8974872	-.1843757
C	4	2.8101852	-3.5649520	-1.3663730
C	5	2.8093415	-3.6376007	1.0222599
C	6	1.4401633	-3.8830131	1.0219628
C	7	1.4431049	-3.8115851	-1.3851985
H	8	3.3978685	-3.5049330	-2.3470497
H	9	3.4098609	-3.6359706	2.0019616
H	10	.9081226	-4.0541334	1.9777596
H	11	.9044509	-3.9372071	-2.3667532
C	12	-.7412274	-3.8998940	-.1941055
H	13	5.4056661	-3.3335999	.7384780
H	14	5.4167316	-3.3333974	-1.0407319
C	15	4.9095078	-1.4277219	-.1488785
N	16	-3.4672937	-3.3975344	-.1979149
H	17	-4.9184163	1.2762028	-2.3460337
C	18	-1.4576780	-3.8526352	1.0091891
C	19	-2.8234435	-3.5934702	.9994510
H	20	-4.9473226	-1.2002530	-2.3531339
C	21	-1.4509921	-3.8513857	-1.4027229
H	22	-.9304082	-4.0065038	1.9705393
H	23	-3.4264488	-3.5546133	1.9777558
C	24	-4.8707476	-2.8689623	-.1987759
H	25	-5.4157878	-3.2580920	.6896670
C	26	4.9380512	1.3664017	-.1407515
C	27	4.7993982	-.7281287	1.0548449
C	28	5.0696116	-.7247714	-1.3435737
C	29	5.0835099	.6668716	-1.3393165
C	30	4.8136078	.6620431	1.0588616
H	31	4.7070106	-1.2734789	2.0036161

H	32	5.1920224	-1.2656071	-2.2912073
H	33	5.2155320	1.2101739	-2.2840110
H	34	4.7318604	1.2036284	2.0108607
C	35	4.9406734	2.8678961	-.1368036
H	36	5.4715890	3.2552704	.7607526
H	37	5.4903864	3.2661609	-1.0179308
N	38	3.5329748	3.3853181	-.1494810
C	39	.8076459	3.8994263	-.1691351
C	40	2.8953955	3.5922644	-1.3490980
C	41	2.8775993	3.5783253	1.0423720
C	42	1.5127704	3.8410036	1.0408114
C	43	1.5295941	3.8526144	-1.3694017
H	44	3.5101065	3.5695627	-2.3169920
H	45	3.4713030	3.5373011	2.0246925
H	46	.9782560	3.9906168	1.9986279
H	47	.9975045	4.0209167	-2.3507622
C	48	-.6612148	3.9091521	-.1752154
H	49	-5.3432356	3.3250576	.7092821
C	50	-1.3777367	3.8581154	1.0281899
C	51	-1.3736637	3.8733119	-1.3820706
H	52	-3.3495459	3.6208048	-2.3472211
C	53	-2.7460882	3.6131922	1.0180667
H	54	-.8497453	3.9989158	1.9912043
H	55	-.8302143	4.0364472	-2.3589712
C	56	-2.7424327	3.6320657	-1.3739597
H	57	-3.3481886	3.5747900	1.9968124
C	58	-4.8068149	2.9304134	-.1820164
N	59	-3.3939045	3.4329902	-.1796420
H	60	-5.3432406	3.3328091	-1.0695103
C	61	-4.8208951	1.4285641	-.1867989
C	62	-2.8175900	-3.5975547	-1.3930601
H	63	-4.8294453	-1.2135787	1.9679124
H	64	-5.4138520	-3.2554733	-1.0892785
C	65	-4.8532715	-1.3670421	-.1947972
C	66	-4.8122915	.7226847	1.0177962
C	67	-4.8760706	.7302519	-1.3943296
C	68	-4.8922981	-.6608104	-1.3983435
C	69	-4.8284215	-.6684532	1.0138156
H	70	-4.8008701	1.2622445	1.9749962
H	71	-3.4244238	-3.5757524	-2.3667492
H	72	-.9111697	-4.0069413	-2.3836716
H	73	1.1087428	6.4155330	-6.2402031
C	74	4.3701954	-4.9972357	-6.2727698
C	75	-5.9817429	-4.8467029	-5.6629804
C	76	4.2267016	-4.3707956	-4.9837872
H	77	5.0373178	-5.8688833	-6.2099855
H	78	4.7889889	-4.2930764	-7.0052240
H	79	-5.6737832	-4.4196758	-6.6277138
N	80	4.0826994	-3.8766400	-3.9425012
H	81	3.3806214	-5.3347949	-6.6309977
H	82	-5.6228274	4.4603762	-6.6004456
H	83	-7.0388577	-4.5965236	-5.4933888
C	84	.1304574	5.9345663	-6.0989771
H	85	-.6409589	6.7178032	-6.0891362
H	86	-5.8898716	-5.9408142	-5.7208081
H	87	-.0577372	5.2701723	-6.9539531
C	88	-5.1639795	-4.3285251	-4.5966746
C	89	.2712814	-4.9564927	-4.9537507
N	90	.0423209	-4.4596083	-3.9278819
C	91	.5736479	-5.5760713	-6.2185986
H	92	1.6573343	-5.5100059	-6.4303217
H	93	.0295677	-5.0786154	-7.0336513
H	94	.2869818	-6.6374800	-6.2069383
C	95	.1085375	5.1910523	-4.8658810
N	96	.0908628	4.5971305	-3.8663734
N	97	-4.5089402	-3.9136515	-3.7309383
C	98	5.3004473	4.2885423	-4.5256597
N	99	4.6143266	3.9035324	-3.6703214
C	100	6.1571149	4.7693070	-5.5789414
H	101	7.1870456	4.4149873	-5.4289284
H	102	6.1679746	5.8686319	-5.5940233
H	103	5.8050758	4.4108253	-6.5564055

C 104	-5.0982079	4.3765904	-4.5727825
N 105	-4.4350036	3.9669376	-3.7107703
C 106	-5.9262012	4.8879800	-5.6344932
H 107	-5.8407960	5.9824383	-5.6954445
H 108	-6.9807408	4.6325249	-5.4568653
C 109	-.0579531	-7.0148931	4.0340440
N 110	-.0356298	-6.0407893	3.4018626
C 111	-.0855115	-8.2250357	4.8154829
H 112	.3172914	-8.0428149	5.8213923
H 113	.5187742	-9.0068870	4.3347076
H 114	-1.1153833	-8.5948497	4.9151470
C 115	.0609473	6.9618423	4.0931695
N 116	.0646540	5.9924428	3.4534480
C 117	.0563089	8.1661539	4.8840364
H 118	.9321190	8.7856621	4.6460040
H 119	.0825481	7.9232034	5.9553033
H 120	-.8495541	8.7546640	4.6826975
C 121	-5.0147537	-4.1620217	4.3460350
N 122	-4.4466026	-3.8128066	3.3944203
C 123	-5.7242145	-4.5980891	5.5209854
H 124	-5.1392555	-4.3822677	6.4260836
H 125	-5.9112776	-5.6806249	5.4769776
H 126	-6.6916824	-4.0820860	5.6001484
C 127	-4.9221759	4.1909428	4.3726472
N 128	-4.3625209	3.8384504	3.4172196
C 129	-5.6210865	4.6312320	5.5523404
H 130	-5.7437047	5.7237447	5.5407345
H 131	-5.0624651	4.3530655	6.4570419
H 132	-6.6181691	4.1710738	5.6032704
C 133	5.0270913	-4.3789108	4.3144340
N 134	4.4355404	-3.9649425	3.4038278
C 135	5.7655537	-4.8954237	5.4377984
H 136	5.3797462	-4.4769138	6.3779917
H 137	6.8300858	-4.6345921	5.3513018
H 138	5.6796814	-5.9905521	5.4829302
C 139	5.0738665	4.2075437	4.3715139
N 140	4.4875922	3.8188052	3.4465041
C 141	5.8058630	4.6927736	5.5129387
H 142	6.8817098	4.5031572	5.3890984
H 143	5.4671183	4.1906442	6.4300092
H 144	5.6563719	5.7752788	5.6330818
O 145	-1.4242497	-.0165537	4.6694612
C 146	-.7237922	-.0139751	3.4985322
C 147	.5335893	-.0080299	1.0314550
C 148	.6786564	-.0206257	3.4346370
C 149	-1.4959522	-.0041916	2.3282507
C 150	-.8644468	-.0012769	1.0924783
C 151	1.3086556	-.0175594	2.1987285
H 152	1.2811330	-.0279411	4.3518587
H 153	-2.5944136	.0014161	2.3831760
H 154	-1.4670279	.0065730	.1766511
H 155	2.4067643	-.0221925	2.1337122
O 156	1.2260249	-.0072729	-.1562419
H 157	.5894873	.0098457	-.8598717
H 158	-.8070890	-.0220814	5.3910767

Heat of Formation: 1082.696 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Oct 7 13:29:42 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 250
164 S shells

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  86 P shells
Number of basis functions: 422
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 486 degrees of freedom

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

Cycle no: 241 Heat of formation =  1096.081  rmsG =  .0000 rmsD =  .0000
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Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	4.9509129	2.8117450	.2219189
N	2	3.5445476	3.3318212	.2509690
C	3	.8231997	3.8795681	.2958500
C	4	2.9059458	3.4812046	1.4578843
C	5	2.8900117	3.5875524	-.9295162
C	6	1.5272860	3.8659155	-.9157417
C	7	1.5452969	3.7597669	1.4900484
H	8	3.4985860	3.3928302	2.4330688
H	9	3.4833625	3.5853407	-1.9133590
H	10	.9927029	4.0635322	-1.8648826
H	11	1.0160947	3.8805124	2.4771469
C	12	-.6448134	3.9138403	.3160468
H	13	5.4811022	3.2196377	-.6669536
H	14	5.5025086	3.1878307	1.1118229
C	15	4.9451416	1.3108059	.1900094
N	16	-3.3813842	3.4716614	.3290245
H	17	-4.8794819	-1.1997427	2.4141709
C	18	-1.3706863	3.9104036	-.8824222
C	19	-2.7420145	3.6817495	-.8682156
H	20	-4.8538768	1.2767069	2.4591151
C	21	-1.3468677	3.8516856	1.5287291
H	22	-.8467318	4.0734967	-1.8439696
H	23	-3.3530329	3.6802952	-1.8419594
C	24	-4.7969602	2.9764053	.3292778
H	25	-5.3373105	3.3929306	-.5495444
C	26	4.9126018	-1.4831359	.1312773
C	27	4.8124304	.6355439	-1.0253239
C	28	5.0963698	.5827761	1.3707505
C	29	5.0798901	-.8086210	1.3412786
C	30	4.7962149	-.7544016	-1.0545342
H	31	4.7281372	1.2000054	-1.9636396
H	32	5.2360422	1.1034951	2.3272243
H	33	5.2054978	-1.3717968	2.2751679
H	34	4.6987050	-1.2768023	-2.0157135
C	35	4.8839261	-2.9841509	.0994756
H	36	5.3977473	-3.3655121	-.8105322
H	37	5.4341029	-3.4098911	.9673472
N	38	3.4660258	-3.4726738	.1173662
C	39	.7297366	-3.9233791	.1555949
C	40	2.8348593	-3.6816746	1.3201020
C	41	2.7956767	-3.6347677	-1.0707783
C	42	1.4252610	-3.8667719	-1.0599868
C	43	1.4635118	-3.9091282	1.3496208
H	44	3.4587459	-3.6866502	2.2821292
H	45	3.3811527	-3.5930294	-2.0579536
H	46	.8785876	-3.9922253	-2.0143263
H	47	.9359384	-4.0724424	2.3340839
C	48	-.7388523	-3.8950849	.1753421
H	49	-5.4110799	-3.1927343	-.6695923
C	50	-1.4661500	-3.8288265	-1.0206335
C	51	-1.4376100	-3.8369713	1.3896051
H	52	-3.3969710	-3.5373138	2.3739651
C	53	-2.8284335	-3.5513669	-.9969766
H	54	-.9511133	-3.9823786	-1.9886716

H	55	-.8886305	-4.0112797	2.3612640
C	56	-2.8002429	-3.5643806	1.3949088
H	57	-3.4394827	-3.5006071	-1.9694063
C	58	-4.8616586	-2.8218980	.2240168
N	59	-3.4595704	-3.3538371	.2066677
H	60	-5.4013015	-3.2256770	1.1088760
C	61	-4.8448335	-1.3203800	.2510502
C	62	-2.7186302	3.6284020	1.5236164
H	63	-4.8546875	1.3545023	-1.8626875
H	64	-5.3258996	3.3609399	1.2290704
C	65	-4.8154285	1.4747788	.3017554
C	66	-4.8547925	-.5963608	-.9425315
C	67	-4.8516964	-.6397806	1.4700696
C	68	-4.8372493	.7508251	1.4953456
C	69	-4.8400993	.7948588	-.9172831
H	70	-4.8813329	-1.1209003	-1.9075883
H	71	-3.3187389	3.5966741	2.5008468
H	72	-.7969580	3.9726380	2.5086932
H	73	1.0295611	-6.4413189	6.2361596
C	74	4.5290967	4.8117153	6.3708965
C	75	-5.8262172	4.8582268	5.8400674
C	76	4.3638091	4.2034078	5.0758491
H	77	5.2140832	5.6697682	6.3134634
H	78	4.9377897	4.0904573	7.0923325
H	79	-5.4916409	4.4412453	6.8003078
N	80	4.2024759	3.7244973	4.0299871
H	81	3.5493084	5.1659065	6.7398238
H	82	-5.5435514	-4.5072310	6.6564686
H	83	-6.8837730	4.5944523	5.6958335
C	84	.0393885	-5.9943297	6.0687546
H	85	-.7017179	-6.8049845	6.0209385
H	86	-5.7461434	5.9537079	5.8889349
H	87	-.2017669	-5.3511438	6.9266354
C	88	-5.0263355	4.3427709	4.7589688
C	89	.4210601	4.8715485	5.0836589
N	90	.1745991	4.3906306	4.0542559
C	91	.7452866	5.4710958	6.3527515
H	92	1.8288424	5.3802190	6.5557544
H	93	.1967597	4.9763641	7.1664704
H	94	.4807660	6.5382945	6.3544289
C	95	.0312888	-5.2322305	4.8468810
N	96	.0246319	-4.6233010	3.8563088
N	97	-4.3857173	3.9303203	3.8813784
C	98	5.2525386	-4.4846392	4.4609522
N	99	4.5672284	-4.0667024	3.6205317
C	100	6.1080170	-5.0062473	5.4956015
H	101	7.1456522	-4.6785807	5.3382579
H	102	6.0879817	-6.1055461	5.4931199
H	103	5.7781637	-4.6539190	6.4829942
C	104	-5.1416179	-4.2654487	4.6135608
N	105	-4.4755585	-3.8656916	3.7491112
C	106	-5.9734044	-4.7644319	5.6782173
H	107	-6.0645045	-5.8583205	5.6143327
H	108	-6.9809395	-4.3288806	5.6156541
C	109	.0974879	7.1348642	-3.8100783
N	110	.0977838	6.1421533	-3.2071528
C	111	.0972858	8.3679408	-4.5553127
H	112	.2751061	8.1729829	-5.6219448
H	113	.8858668	9.0392439	-4.1878432
H	114	-.8696384	8.8795229	-4.4516292
C	115	-.1077696	-6.9782886	-4.0777711
N	116	-.0817860	-6.0086828	-3.4389013
C	117	-.1400588	-8.1828164	-4.8676659
H	118	.7507781	-8.7953599	-4.6710486
H	119	-.1659450	-7.9399257	-5.9389537
H	120	-1.0308614	-8.7783309	-4.6241377
C	121	-4.9527448	4.3959885	-4.1730969
N	122	-4.3837878	4.0054207	-3.2382158
C	123	-5.6631623	4.8836555	-5.3270224
H	124	-5.0308921	4.8194027	-6.2236950
H	125	-5.9563660	5.9333721	-5.1821939
H	126	-6.5724075	4.2901720	-5.4986021

C 127	-5.0597038	-4.0891869	-4.3215623
N 128	-4.4801921	-3.7471776	-3.3742239
C 129	-5.7832867	-4.5166255	-5.4910827
H 130	-5.8507982	-5.6135479	-5.5212257
H 131	-5.2765496	-4.1736886	-6.4040416
H 132	-6.8033122	-4.1066945	-5.4837943
C 133	5.0970975	4.3236646	-4.2300292
N 134	4.5057551	3.9099774	-3.3191751
C 135	5.8353659	4.8396492	-5.3537653
H 136	5.2934767	4.6494220	-6.2908482
H 137	6.8226003	4.3603266	-5.4186764
H 138	5.9828048	5.9243226	-5.2508804
C 139	4.9443747	-4.2577193	-4.4324234
N 140	4.3778598	-3.8727553	-3.4936425
C 141	5.6518006	-4.7384936	-5.5910938
H 142	6.7231294	-4.5044571	-5.5124445
H 143	5.2590905	-4.2698474	-6.5043580
H 144	5.5410665	-5.8283630	-5.6836840
O 145	-1.4180214	.1312319	-4.4670508
C 146	-.7086937	.0874369	-3.2880225
C 147	.4662987	.0001997	-.7710601
C 148	.6882790	.0626174	-3.1740087
C 149	-1.5135341	.0684423	-2.1391218
C 150	-.9264525	.0252655	-.8819824
C 151	1.2740445	.0185295	-1.9171372
H 152	1.3286291	.0767938	-4.0649237
H 153	-2.6102829	.0877685	-2.2250219
H 154	-1.5694802	.0114676	.0055951
H 155	2.3705359	-.0015525	-1.8237239
O 156	1.1740176	-.0324284	.4213839
C 157	.4312526	-.1411522	1.6099864
C 158	-.6892523	.1478565	-5.6723109
H 159	-.0851145	-.7569585	-5.8040252
H 160	-.0538632	1.0364572	-5.7601134
H 161	-1.4873101	.1801005	-6.4197567
H 162	-.1628293	-1.0630134	1.6479343
H 163	-.2200895	.7255826	1.7752775
H 164	1.2144313	-.1696930	2.3729932

Heat of Formation: 1096.081 kcal/mol

p-PHENYLENEDIAMINE1/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sun Oct 1 14:15:37 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: 193 Heat of formation = 1168.993 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

C	1	2.9069689	.0535402	-4.8470220
N	2	3.4254953	.0566134	-3.4406380
C	3	3.9465909	.0462899	-.7155155
C	4	3.6432155	-1.1391913	-2.8000425
C	5	3.6055042	1.2514448	-2.7862485
C	6	3.8692782	1.2550490	-1.4209907
C	7	3.9127942	-1.1537964	-1.4374182
H	8	3.6157386	-2.1183398	-3.3916253
H	9	3.5521845	2.2322347	-3.3808662
H	10	4.0003786	2.2143616	-.8842122
H	11	4.0885708	-2.1309732	-.9040439
C	12	3.9470644	.0283401	.7524548
H	13	3.2967514	.9436062	-5.3888923
H	14	3.3024609	-.8352842	-5.3869158
C	15	1.4048380	.0494557	-4.8473012
N	16	3.3995832	-.0144188	3.4673667
H	17	-1.2844303	-2.2234087	4.7692217
C	18	3.8365351	1.2250121	1.4740730
C	19	3.5568409	1.1952956	2.8347484
H	20	1.1922192	-2.2136198	4.7982581
C	21	3.9474734	-1.1853585	1.4547333
H	22	3.9527551	2.1944555	.9527166
H	23	3.4707252	2.1648791	3.4427474
C	24	2.8452731	-.0454266	4.8596600
H	25	3.2190808	.8351793	5.4275432
C	26	-1.3917189	.0440134	-4.8763828
C	27	.6997797	1.2546468	-4.8454042
C	28	.7051222	-1.1582578	-4.8820318
C	29	-.6863204	-1.1607484	-4.8957893
C	30	-.6913724	1.2518710	-4.8603115
H	31	1.2413356	2.2102676	-4.8460341
H	32	1.2504442	-2.1109952	-4.9139263
H	33	-1.2264544	-2.1156356	-4.9388991
H	34	-1.2360244	2.2054466	-4.8741764
C	35	-2.8933568	.0427740	-4.9116033
H	36	-3.2737827	.9353581	-5.4559571
H	37	-3.2727340	-.8432125	-5.4671130
N	38	-3.4450027	.0351048	-3.5171192
C	39	-3.9991631	.0103729	-.8000985
C	40	-3.6927706	-1.1632766	-2.8912463
C	41	-3.6217488	1.2273182	-2.8574602
C	42	-3.9040399	1.2230800	-1.4966899
C	43	-3.9765280	-1.1857968	-1.5303399
H	44	-3.6799228	-2.1286113	-3.5116166
H	45	-3.5504312	2.2122617	-3.4451116
H	46	-4.0389790	2.1806585	-.9574885
H	47	-4.1782977	-2.1656548	-1.0067218
C	48	-4.0069282	-.0064481	.6686049
H	49	-3.3482172	.8096137	5.3539690
C	50	-3.9189126	1.1899233	1.3937896
C	51	-3.9926497	-1.2190296	1.3714680
H	52	-3.7208184	-2.2071256	3.3336961
C	53	-3.6528798	1.1629168	2.7575864
H	54	-4.0472136	2.1596735	.8750839
H	55	-4.1885062	-2.1866394	.8232551
C	56	-3.7251837	-1.2277128	2.7358208
H	57	-3.5887736	2.1342090	3.3681612
C	58	-2.9558383	-.0686430	4.7949664
N	59	-3.4850066	-.0441199	3.3920835
H	60	-3.3418913	-.9686877	5.3225999
C	61	-1.4538349	-.0633358	4.7871076
C	62	3.6667864	-1.1952874	2.8165252
H	63	1.1740665	2.1068495	4.8943948
H	64	3.2277818	-.9431738	5.3938144
C	65	1.3432661	-.0522350	4.8212397
C	66	-.7561014	1.1452549	4.8304384
C	67	-.7458023	-1.2667319	4.7752364
C	68	.6455033	-1.2613110	4.7925757
C	69	.6351505	1.1508296	4.8470495
H	70	-1.3030672	2.0968993	4.8668407
H	71	3.6721918	-2.1724607	3.4160487

H	72	4.1540825	-2.1546168	.9110602
H	73	-6.7556062	-5.9335065	-1.1284411
C	74	5.2337342	-5.9793223	-4.3903693
C	75	5.0172806	-5.4534686	5.9565455
C	76	4.5568863	-4.7163329	-4.2448413
H	77	6.0910517	-5.8851099	-5.0721570
H	78	4.5536724	-6.7429507	-4.7929246
H	79	4.4856640	-6.3958349	5.7637077
N	80	4.0222120	-3.6953342	-4.1002002
H	81	5.6020163	-6.3169820	-3.4044969
H	82	-4.4272428	-6.4604519	5.6632645
H	83	4.9232767	-5.2133768	7.0253518
C	84	-6.2690406	-5.8181681	-.1494410
H	85	-7.0519136	-5.7605842	.6203547
H	86	6.0823468	-5.6006661	5.7271808
H	87	-5.6563584	-6.7102910	.0421846
C	88	4.4711399	-4.3912096	5.1517771
C	89	5.2417493	-4.6686098	-.2900832
N	90	4.7195026	-3.6576969	-.0524046
C	91	5.8927523	-5.9149434	-.6033414
H	92	5.8138258	-6.1284018	-1.6856733
H	93	5.4287468	-6.7439157	-.0509690
H	94	6.9581251	-5.8722064	-.3352160
C	95	-5.4546249	-4.6307448	-.1288716
N	96	-4.8029805	-3.6676093	-.1122405
N	97	4.0336144	-3.5288895	4.5071979
C	98	-4.3594981	-4.3243058	-5.3260732
N	99	-3.9827516	-3.4769953	-4.6253523
C	100	-4.8293214	-5.3677048	-6.2006167
H	101	-4.3673751	-5.2742272	-7.1939497
H	102	-5.9207985	-5.3074361	-6.3192589
H	103	-4.5774595	-6.3563470	-5.7917786
C	104	-4.4387570	-4.4482970	5.0759622
N	105	-4.0452845	-3.5827791	4.4074546
C	106	-4.9295624	-5.5146073	5.9104361
H	107	-6.0117429	-5.6470444	5.7684492
H	108	-4.7447048	-5.2893787	6.9706531
C	109	7.0711078	4.1841604	.0794864
N	110	6.0934869	3.5574304	.0614769
C	111	8.2854598	4.9592391	.1016501
H	112	8.0591900	6.0312919	.0192391
H	113	8.9376983	4.6756858	-.7359841
H	114	8.8323098	4.7900527	1.0395800
C	115	-6.6839456	4.5929755	-.0307045
N	116	-5.7740334	3.8710086	-.0308649
C	117	-7.8148220	5.4856800	-.0306382
H	118	-8.4827747	5.2599076	-.8735336
H	119	-7.4817767	6.5289922	-.1200356
H	120	-8.3866341	5.3815826	.9019459
C	121	4.0642831	4.5425515	5.0255084
N	122	3.6952796	3.5936074	4.4653598
C	123	4.5255711	5.7142615	5.7243517
H	124	4.2983265	6.6213888	5.1469137
H	125	5.6126482	5.6645482	5.8810914
H	126	4.0371980	5.7944139	6.7059410
C	127	-4.1938077	4.4881685	4.9808519
N	128	-3.8291554	3.5548584	4.3921124
C	129	-4.6490041	5.6400635	5.7156600
H	130	-5.7454344	5.6348025	5.7972901
H	131	-4.3420038	6.5660717	5.2094087
H	132	-4.2260981	5.6412132	6.7304609
C	133	4.2011349	4.6136986	-4.9338318
N	134	3.8142218	3.6648548	-4.3857098
C	135	4.6845604	5.7851853	-5.6178943
H	136	4.3911863	6.6956856	-5.0767114
H	137	4.2704645	5.8355054	-6.6350044
H	138	5.7813181	5.7617206	-5.6910024
C	139	-4.1276750	4.5979666	-5.0210001
N	140	-3.7742487	3.6535451	-4.4432271
C	141	-4.5688005	5.7636875	-5.7424553
H	142	-4.1895499	5.7442518	-6.7742147
H	143	-4.2050693	6.6791464	-5.2549474

H 144	-5.6670734	5.8006437	-5.7777392
N 145	.2449189	2.8771956	.0114118
C 146	.0359771	1.4651049	-.0098694
C 147	-.0591911	-1.3354082	-.0519531
C 148	-.0048222	.7764011	-1.2306864
C 149	-.0063325	.7400162	1.1896997
C 150	-.0525512	-.6457391	1.1688308
C 151	-.0513088	-.6093555	-1.2514220
H 152	.0076205	1.3231869	-2.1854685
H 153	.0045225	1.2581311	2.1602781
H 154	-.0748720	-1.1925476	2.1234048
H 155	-.0725079	-1.1274302	-2.2218715
N 156	.0447935	-2.7594494	-.0741606
H 157	-.3537181	-3.1477445	-.8995797
H 158	-.3410605	-3.1728790	.7450303
H 159	-.1136616	3.3195741	-.8049920
H 160	-.1144010	3.2948667	.8404046

Heat of Formation: 1168.993 kcal/mol

p-PHENYLENEDIAMINE2/1^{4+} 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Wed Oct 4 16:40:03 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: 305 Heat of formation = 1167.957 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	-5.5977684	-.8426444	.1351492
N 2	-4.8560577	.4577486	.2055984
C 3	-3.0613287	2.5626673	.3206110
C 4	-4.4676596	1.0737977	-.9599776
C 5	-4.4992361	.9689172	1.4303368
C 6	-3.6015010	2.0277986	1.4981268
C 7	-3.5708090	2.1343417	-.9136338
H 8	-4.9102705	.7141998	-1.9556669
H 9	-4.9708963	.5268072	2.3770188
H 10	-3.3002923	2.4555238	2.4989133
H 11	-3.2430673	2.6368906	-1.8726495
C 12	-1.9180892	3.4826282	.3759453
H 13	-6.3034302	-.9137626	.9919983
H 14	-6.2231086	-.8684439	-.7845314
C 15	-4.6273471	-1.9890103	.1388725
N 16	.5112308	4.8182878	.4529959
H 17	4.3458654	1.9058517	-1.6051558
C 18	-1.3602728	3.8703846	1.6018141
C 19	-.1420197	4.5406443	1.6298533
H 20	2.7739750	3.8188519	-1.6376794

C	21	-1.3070531	3.9158777	-.8078758
H	22	-1.8997385	3.6300640	2.5645661
H	23	.3197236	4.8935757	2.6185253
C	24	1.9271928	5.3090149	.4829662
H	25	2.0757560	5.9599068	1.3726194
C	26	-2.8393913	-4.1383973	.1405936
C	27	-4.4274964	-2.7344949	1.3007053
C	28	-3.9428414	-2.3353381	-1.0288754
C	29	-3.0534776	-3.4030717	-1.0278911
C	30	-3.5372099	-3.8048925	1.3014319
H	31	-4.9774627	-2.4876461	2.2182661
H	32	-4.1136917	-1.7719085	-1.9563939
H	33	-2.5272185	-3.6724303	-1.9537346
H	34	-3.3948394	-4.3895818	2.2198030
C	35	-1.8932146	-5.3046929	.1377744
H	36	-2.1052350	-5.9905882	.9874089
H	37	-2.0281719	-5.9073559	-.7874809
N	38	-.4759219	-4.8270504	.2265549
C	39	1.9581962	-3.5135578	.3726121
C	40	.2309606	-4.5918973	-.9284804
C	41	.0733618	-4.5665388	1.4592671
C	42	1.2940780	-3.9083692	1.5425277
C	43	1.4573337	-3.9414319	-.8649433
H	44	-.1967555	-4.9566497	-1.9268906
H	45	-.4754050	-4.9225331	2.3991687
H	46	1.7490089	-3.6837325	2.5506394
H	47	2.0457040	-3.7453558	-1.8081989
C	48	3.0953528	-2.5864556	.4364038
H	49	6.2613361	.8714216	1.4629816
C	50	3.5333756	-2.0797372	1.6680693
C	51	3.6981923	-2.1172676	-.7391925
H	52	5.0933183	-.6484574	-1.6299499
C	53	4.4235449	-1.0136235	1.7028902
H	54	3.1553133	-2.5338954	2.6295981
H	55	3.4540239	-2.6024373	-1.7288713
C	56	4.5817665	-1.0461425	-.6848039
H	57	4.8150463	-.5974778	2.6954467
C	58	5.6167343	.8363165	.5571794
N	59	4.8712308	-.4630803	.5257626
H	60	6.3049343	.8949801	-.3148256
C	61	4.6524805	1.9876212	.5394038
C	62	-.0864053	4.5761207	-.7598303
H	63	3.2264610	4.2620933	2.6385099
H	64	2.1190330	5.9501135	-.4059151
C	65	2.8746101	4.1442394	.5037390
C	66	4.3416141	2.6603032	1.7213092
C	67	4.0864048	2.4118050	-.6652433
C	68	3.2031687	3.4847492	-.6831829
C	69	3.4561804	3.7343268	1.7036174
H	70	4.7999246	2.3519702	2.6702165
H	71	.4134667	4.9330972	-1.7267130
H	72	-1.8019094	3.7180973	-1.8019269
N	73	-.1886591	.9378782	-5.9500870
C	74	-.0347294	.5645742	-4.5821632
C	75	.1017950	.0486838	-1.8374456
C	76	-.9555981	-.3065029	-3.9800557
C	77	.9675049	1.1585044	-3.8003591
C	78	1.0328274	.9043891	-2.4388336
C	79	-.8877223	-.5611072	-2.6189159
H	80	-1.7359513	-.7921944	-4.5793644
H	81	1.7073880	1.8273570	-4.2576023
H	82	1.8235621	1.3847521	-1.8440671
H	83	-1.6191718	-1.2457869	-2.1654718
N	84	.2220397	-.2804719	-.4419931
H	85	.6776499	1.1996539	-6.3649207
H	86	-.6492162	.2325719	-6.4807052
H	87	.6270001	.4773873	.0637217
H	88	-.6686181	-.5117668	-.0581019
C	89	3.0196981	-3.9777023	5.1643545
N	90	2.7151687	-3.5360382	4.1329614
C	91	3.4022270	-4.5310368	6.4377515
H	92	3.3003138	-5.6255676	6.4272441

H	93	2.7674249	-4.1290512	7.2397063
H	94	4.4489007	-4.2840701	6.6649862
C	95	-3.3628877	3.8228057	5.0757155
N	96	-2.9804555	3.4173672	4.0552969
C	97	-3.8411588	4.3315318	6.3352151
H	98	-4.6705223	3.7147639	6.7089529
H	99	-4.2013738	5.3640333	6.2209449
H	100	-3.0372752	4.3234458	7.0845378
C	101	3.7244024	-4.2041548	-4.1590871
N	102	3.2644124	-3.7058210	-3.2149123
C	103	4.2999119	-4.8285971	-5.3223170
H	104	3.5249082	-5.3473069	-5.9036536
H	105	5.0622877	-5.5635514	-5.0264544
H	106	4.7738639	-4.0765818	-5.9684280
C	107	-2.8675622	4.1441099	-4.4173899
N	108	-2.7843834	3.6443383	-3.3712599
C	109	-2.9582775	4.7763559	-5.7084767
H	110	-3.8752518	5.3784464	-5.7804858
H	111	-2.9730794	4.0221956	-6.5076291
H	112	-2.0902290	5.4417549	-5.8723051
C	113	-1.4636154	-6.6154171	4.5842184
N	114	-1.1738930	-5.8828575	3.7299259
C	115	-1.8242587	-7.5304219	5.6364946
H	116	-2.6776535	-8.1520623	5.3297656
H	117	-2.1034769	-6.9810796	6.5465163
H	118	-.9807742	-8.1940485	5.8747057
C	119	-6.8422006	-.0822138	4.5503522
N	120	-6.0593997	.0545914	3.7024084
C	121	-7.8193305	-.2521500	5.5947748
H	122	-8.2128670	-1.2786403	5.5903911
H	123	-8.6599960	.4418799	5.4513235
H	124	-7.3701139	-.0563477	6.5784815
C	125	6.5194968	-.0662726	5.0252587
N	126	5.8010815	-.1669808	4.1174326
C	127	7.4175198	.0592727	6.1443831
H	128	8.4220245	.3455924	5.8008587
H	129	7.4951507	-.8950297	6.6842622
H	130	7.0573104	.8268773	6.8436963
C	131	1.1437345	6.5567309	4.8864839
N	132	.9093172	5.8352819	4.0060603
C	133	1.4365973	7.4581572	5.9709822
H	134	.6115699	7.4679753	6.6970981
H	135	1.5779757	8.4810042	5.5928440
H	136	2.3546091	7.1501666	6.4911598
C	137	-6.7134437	.2754426	-4.2196538
N	138	-5.9533803	.3355347	-3.3426313
C	139	-7.6628751	.2002881	-5.3000286
H	140	-8.1672121	-.7765818	-5.3018312
H	141	-7.1578254	.3328438	-6.2670375
H	142	-8.4265402	.9844068	-5.1955072
C	143	-1.0125124	-6.6281648	-4.1965019
N	144	-.7819967	-5.9012422	-3.3196818
C	145	-1.3008953	-7.5359519	-5.2769278
H	146	-1.5565697	-6.9800983	-6.1899092
H	147	-2.1484985	-8.1861517	-5.0167496
H	148	-.4291956	-8.1716080	-5.4881773
C	149	7.0638391	-.0547943	-3.7217695
N	150	6.2385110	-.1869985	-2.9144261
C	151	8.0936749	.1104877	-4.7150389
H	152	9.0609822	.3168488	-4.2346747
H	153	7.8526914	.9480311	-5.3847225
H	154	8.1949735	-.8015806	-5.3199918
C	155	.5640867	6.2038368	-4.3194717
N	156	.7503623	5.7052320	-3.2870710
C	157	.2982242	6.8097666	-5.5987246
H	158	1.0949997	6.5715290	-6.3170582
H	159	.2318548	7.9031775	-5.5052012
H	160	-.6612511	6.4301037	-5.9947642

Heat of Formation: 1167.957 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Tue Aug 8 18:42:24 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 134
86 S shells
48 P shells
Number of basis functions: 230
Number of electrons: 234
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 252 degrees of freedom

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

Cycle no: 90 Heat of formation = 1099.043 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	4.8446295	2.8968857	.2450704
N	2	3.4430365	3.4514009	.2251790
C	3	.7039013	4.0185090	.1972738
C	4	2.7727046	3.6670820	1.4085821
C	5	2.7958357	3.6544399	-.9719210
C	6	1.4337867	3.9454224	-.9976470
C	7	1.4116652	3.9574230	1.4069687
H	8	3.3381137	3.5924279	2.3577274
H	9	3.3757033	3.5648229	-1.9110488
H	10	.9197162	4.0906180	-1.9658648
H	11	.8791861	4.1176943	2.3629003
C	12	-.7678637	4.0222795	.1857467
H	13	5.4100251	3.2891947	-.6321554
H	14	5.3840254	3.2778833	1.1433787
C	15	4.8176061	1.3938507	.2430055
N	16	-3.5078610	3.4621876	.1691631
H	17	-5.3159075	-1.2178650	2.2942701
C	18	-1.4753912	3.9391866	-1.0229888
C	19	-2.8369073	3.6528204	-1.0184552
H	20	-5.3110632	1.2481780	2.2899160
C	21	-1.4978053	3.9780790	1.3814054
H	22	-.9421500	4.0763171	-1.9816656
H	23	-3.4026507	3.5592187	-1.9652962
C	24	-4.9126162	2.9151398	.1578561
H	25	-5.4531005	3.2967811	-.7393590
C	26	4.8119190	-1.4104553	.2475109
C	27	5.0637038	.6869081	-.9356659
C	28	4.6259805	.6891998	1.4359523
C	29	4.6231529	-.7012044	1.4381892
C	30	5.0608835	-.7083009	-.9334178
H	31	5.2923168	1.2200159	-1.8700234
H	32	4.5181372	1.2292858	2.3864260
H	33	4.5131129	-1.2377885	2.3903909
H	34	5.2873486	-1.2453214	-1.8660547
C	35	4.8329468	-2.9135720	.2544207
H	36	5.3967177	-3.3109287	-.6215811
H	37	5.3709057	-3.2937964	1.1539158
N	38	3.4291848	-3.4626381	.2363638
C	39	.6878786	-4.0192944	.2105015
C	40	2.7582433	-3.6725017	1.4204681
C	41	2.7809808	-3.6664511	-.9600641

C	42	1.4178241	-3.9522570	-.9847449
C	43	1.3960939	-3.9576520	1.4198992
H	44	3.3241114	-3.5974112	2.3693061
H	45	3.3609894	-3.5816022	-1.8995510
H	46	.9029922	-4.0980885	-1.9524666
H	47	.8632005	-4.1133405	2.3763586
C	48	-.7838910	-4.0173870	.1991358
H	49	-5.4664220	-3.2765624	-.7276574
C	50	-1.4911651	-3.9350963	-1.0098069
C	51	-1.5135849	-3.9668192	1.3946882
H	52	-3.4551423	-3.5957795	2.3140928
C	53	-2.8515264	-3.6433070	-1.0060539
H	54	-.9585194	-4.0771925	-1.9680991
H	55	-1.0001964	-4.1290808	2.3603447
C	56	-2.8759402	-3.6730972	1.3737694
H	57	-3.4169476	-3.5502127	-1.9531380
C	58	-4.9242259	-2.8939297	.1681010
N	59	-3.5216600	-3.4465354	.1810280
H	60	-5.4845649	-3.2865458	1.0482276
C	61	-4.8997603	-1.3912455	.1705420
C	62	-2.8612994	3.6896769	1.3612757
H	63	-4.6466934	1.2399998	-1.9842209
H	64	-5.4715633	3.3130923	1.0364688
C	65	-4.8941474	1.4123906	.1656019
C	66	-4.7367233	-.6869313	-1.0274121
C	67	-5.1163587	-.6844626	1.3540925
C	68	-5.1135975	.7106554	1.3516311
C	69	-4.7339302	.7032170	-1.0298653
H	70	-4.6516370	-1.2274178	-1.9798702
H	71	-3.4408491	3.6173727	2.3017825
H	72	-.9838202	4.1411456	2.3466149
S	73	-1.1786437	.0056563	1.7990259
C	74	-.3713040	.0014140	.2412611
C	75	.7674741	-.0054833	-2.3352080
C	76	1.0154870	-.0022075	.0797258
C	77	-1.1810193	.0016353	-.8989796
C	78	-.6218056	-.0017441	-2.1690888
C	79	1.5731817	-.0056096	-1.1886809
H	80	1.6783035	-.0023960	.9558481
H	81	-2.2785270	.0044454	-.7917313
H	82	-1.2804198	-.0015037	-3.0487666
H	83	2.6705906	-.0084203	-1.3029930
S	84	1.6126817	-.0102556	-3.8569412
H	85	-.1459738	.0048165	2.6126593
H	86	.6118635	-.0080803	-4.7130908

Heat of Formation: 1099.043 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Wed Oct 18 11:46:35 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 242
158 S shells
84 P shells
Number of basis functions: 410
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 468 degrees of freedom

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

Cycle no: 184 Heat of formation = 1165.233 rmsG = .0000 rmsD = .0001

Atom		Cartesian Coordinates (Angstroms) X	Y	Z
C	1	2.9177011	4.8542476	.3967616
N	2	3.4213297	3.4426641	.4170938
C	3	3.9164467	.7125794	.4295598
C	4	3.6469520	2.7923060	-.7718606
C	5	3.5759223	2.7933936	1.6181418
C	6	3.8243828	1.4254689	1.6328112
C	7	3.9046500	1.4273644	-.7750002
H	8	3.6363791	3.3772383	-1.7565261
H	9	3.5196241	3.3956962	2.5946609
H	10	3.9401671	.8940267	2.5970694
H	11	4.0889756	.8879634	-1.7475631
C	12	3.9175467	-.7553957	.4196051
H	13	3.3286680	5.4068781	1.2704855
H	14	3.3018370	5.3754877	-.5080984
C	15	1.4160900	4.8655014	.4113822
N	16	3.3992948	-3.4763334	.3844553
H	17	-1.2784214	-4.3982169	-1.7542055
C	18	3.7949176	-1.4716184	1.6181732
C	19	3.5321919	-2.8356845	1.5926765
H	20	1.1978233	-4.4250644	-1.7619735
C	21	3.9383030	-1.4634314	-.7904504
H	22	3.8968437	-.9450844	2.5864684
H	23	3.4450819	-3.4410118	2.5645056
C	24	2.8611262	-4.8747668	.3515606
H	25	3.2539649	-5.4427227	1.2237696
C	26	-1.3786890	4.8965241	.4366340
C	27	.7278312	5.0857150	1.6046261
C	28	.7008695	4.6863846	-.7752782
C	29	-.6889049	4.7013929	-.7625319
C	30	-.6642180	5.1014092	1.6171751
H	31	1.2800235	5.2568251	2.5383790
H	32	1.2344898	4.5468930	-1.7253356
H	33	-1.2420251	4.5732329	-1.7027658
H	34	-1.1952963	5.2853926	2.5606029
C	35	-2.8802278	4.9202773	.4495960
H	36	-3.2630203	5.4706739	1.3374363
H	37	-3.2689170	5.4610149	-.4415378
N	38	-3.4132874	3.5188861	.4632957
C	39	-3.9219823	.7934458	.4608681
C	40	-3.6802091	2.8846351	-.7264281
C	41	-3.5425135	2.8598585	1.6618067
C	42	-3.8003880	1.4942456	1.6687008
C	43	-3.9420648	1.5191341	-.7378650
H	44	-3.7016441	3.5017395	-1.6950093
H	45	-3.4573367	3.4520874	2.6437251
H	46	-3.9033686	.9564387	2.6312421
H	47	-4.1619811	.9900782	-1.7123653
C	48	-3.9289880	-.6751737	.4486787
H	49	-3.3366404	-5.3749763	1.2444876
C	50	-3.8153091	-1.3971734	1.6447179
C	51	-3.9551333	-1.3805803	-.7619993
H	52	-3.7356711	-3.3489706	-1.7519081
C	53	-3.5725049	-2.7652829	1.6153994
H	54	-3.9131678	-.8743151	2.6160135
H	55	-4.1690725	-.8332093	-1.7277778
C	56	-3.7078724	-2.7487801	-.7729728
H	57	-3.4958101	-3.3743123	2.5876049
C	58	-2.9380346	-4.8146646	.3698774
N	59	-3.4496849	-3.4058630	.4062913
H	60	-3.3287583	-5.3323039	-.5340203
C	61	-1.4362590	-4.8180041	.3669522
C	62	3.6708807	-2.8277809	-.7966705
H	63	1.2005086	-5.3318747	2.4644093
H	64	3.2357562	-5.4003971	-.5545635

C	65	1.3592796	-4.8491792	.3578755
C	66	-.7337786	-5.0915393	1.5406090
C	67	-.7343802	-4.5824675	-.8180061
C	68	.6552410	-4.5979810	-.8225597
C	69	.6585267	-5.1069497	1.5360912
H	70	-1.2743679	-5.3055120	2.4722207
H	71	3.6906469	-3.4312459	-1.7724922
H	72	4.1514105	-.9238770	-1.7609208
H	73	-6.7922626	1.0375518	-5.4664838
C	74	5.2612334	4.3465543	-5.6231735
C	75	5.0172597	-5.9976055	-5.0387068
C	76	4.5861871	4.2067817	-4.3586034
H	77	6.1242894	5.0214151	-5.5312459
H	78	4.5827242	4.7543613	-6.3854479
H	79	4.6370889	-5.6654036	-6.0149245
N	80	4.0526150	4.0658677	-3.3364850
H	81	5.6205794	3.3574376	-5.9610362
H	82	-4.5787447	-5.6416691	-5.9904450
H	83	4.7311778	-7.0491932	-4.8934597
C	84	-6.1840053	.1238185	-5.4063758
H	85	-6.8586234	-.7431068	-5.4496001
H	86	6.1149199	-5.9360527	-5.0527965
H	87	-5.5171508	.0907903	-6.2793523
C	88	4.4807645	-5.1789470	-3.9822062
C	89	5.2320102	.2550763	-4.2853805
N	90	4.7125720	.0280437	-3.2704929
C	91	5.8791384	.5550480	-5.5369528
H	92	5.8107739	1.6371282	-5.7556068
H	93	5.4042844	.0036027	-6.3604379
H	94	6.9417886	.2755354	-5.4989896
C	95	-5.4204860	.1069699	-4.1855457
N	96	-4.8099261	.0934525	-3.1960411
N	97	4.0508385	-4.5230914	-3.1245268
C	98	-4.4442144	5.3075634	-3.8745912
N	99	-4.0461281	4.6145941	-3.0307054
C	100	-4.9403628	6.1725129	-4.9137597
H	101	-4.5885181	7.2024313	-4.7575650
H	102	-6.0398655	6.1789002	-4.9163399
H	103	-4.5915545	5.8316312	-5.8987235
C	104	-4.5072215	-5.0973200	-3.9675490
N	105	-4.0967064	-4.4304919	-3.1087211
C	106	-5.0191188	-5.9297254	-5.0255006
H	107	-6.1118129	-5.8313214	-5.0976582
H	108	-4.7785330	-6.9854937	-4.8347312
C	109	6.8025381	-.0606756	4.7979169
N	110	5.8594309	-.0467391	4.1201737
C	111	7.9743577	-.0778184	5.6360095
H	112	7.6910426	-.0062397	6.6952288
H	113	8.6325712	.7680880	5.3937129
H	114	8.5385966	-1.0091658	5.4887905
C	115	-6.6968946	.0399747	4.9137270
N	116	-5.7730276	.0380258	4.2097556
C	117	-7.8449372	.0424356	5.7842401
H	118	-8.4317133	.9608777	5.6439556
H	119	-7.5308159	-.0127012	6.8357487
H	120	-8.4925934	-.8187474	5.5687070
C	121	4.0302828	-5.0034044	4.9574713
N	122	3.6748559	-4.4489165	4.0000751
C	123	4.4749417	-5.6954254	6.1396388
H	124	4.2567309	-5.1016258	7.0383938
H	125	5.5588754	-5.8741132	6.0950183
H	126	3.9672685	-6.6661327	6.2315902
C	127	-4.0787434	-4.9352783	4.9787256
N	128	-3.7317994	-4.3778658	4.0198684
C	129	-4.5127407	-5.6309926	6.1626555
H	130	-5.5854948	-5.8637321	6.0997732
H	131	-4.3422111	-5.0139689	7.0560946
H	132	-3.9598954	-6.5739257	6.2798066
C	133	4.1649157	4.9555873	4.9727331
N	134	3.7881590	4.4017304	4.0231300
C	135	4.6358453	5.6469819	6.1450278
H	136	4.2534088	5.1653788	7.0559475

H 137	4.2988517	6.6933949	6.1362650
H 138	5.7346512	5.6372342	6.1809464
C 139	-4.0100224	4.9923023	5.0556025
N 140	-3.6745838	4.4395566	4.0899597
C 141	-4.4294913	5.6824819	6.2479680
H 142	-4.0463702	6.7129499	6.2513736
H 143	-4.0532784	5.1680080	7.1434016
H 144	-5.5268775	5.7207585	6.3034999
N 145	.2056004	.0505258	-.1094794
C 146	.0450773	.0623423	-1.5356387
C 147	-.0607711	.0879978	-4.3135948
C 148	.0062834	1.2825519	-2.2241491
C 149	.0245646	-1.1450101	-2.2472891
C 150	-.0265144	-1.1285767	-3.6342910
C 151	-.0457353	1.2916957	-3.6111792
H 152	.0179977	2.2401600	-1.6827073
H 153	.0498693	-2.1122276	-1.7239095
H 154	-.0399627	-2.0672121	-4.2007592
H 155	-.0758874	2.2407761	-4.1592501
Cl156	-.1235442	.1036672	-5.9915332
H 157	-.1816186	-.7774025	.2879120
H 158	-.2036839	.8599122	.3037004

Heat of Formation: 1165.233 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sun Oct 8 15:04:39 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 241
157 S shells
84 P shells
Number of basis functions: 409
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 465 degrees of freedom

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

Cycle no: 212 Heat of formation = 1120.026 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	2.9220120	4.8501400	.3395745
N 2	3.4249346	3.4383210	.3669307
C 3	3.9150237	.7072206	.3839468
C 4	3.6614806	2.7876189	-.8197387
C 5	3.5659981	2.7885831	1.5690532
C 6	3.8112316	1.4196614	1.5861668
C 7	3.9169953	1.4225268	-.8203404
H 8	3.6628172	3.3729474	-1.8047897
H 9	3.5011393	3.3907176	2.5457459
H 10	3.9156777	.8875412	2.5514711
H 11	4.1153703	.8842917	-1.7905908
C 12	3.9168829	-.7607464	.3722223
H 13	3.3301648	5.4051761	1.2130477
H 14	3.3092505	5.3681888	-.5657452
C 15	1.4206457	4.8604510	.3471248

N	16	3.4034508	-3.4823778	.3249611
H	17	-1.2754872	-4.3129837	-1.7979514
C	18	3.7771629	-1.4786996	1.5675262
C	19	3.5171268	-2.8435485	1.5357533
H	20	1.1988810	-4.3406007	-1.8116992
C	21	3.9583128	-1.4671046	-.8384007
H	22	3.8640516	-.9534085	2.5380504
H	23	3.4167091	-3.4504184	2.5058244
C	24	2.8668283	-4.8811951	.2803556
H	25	3.2616549	-5.4552806	1.1476056
C	26	-1.3736377	4.8869757	.3619083
C	27	.7284478	5.1375511	1.5258803
C	28	.7096539	4.6217447	-.8317319
C	29	-.6797576	4.6342696	-.8241874
C	30	-.6637102	5.1509281	1.5331640
H	31	1.2767521	5.3542004	2.4522644
H	32	1.2460739	4.4348752	-1.7718941
H	33	-1.2294025	4.4551405	-1.7580838
H	34	-1.1980418	5.3776298	2.4653503
C	35	-2.8751086	4.9063057	.3706941
H	36	-3.2622418	5.4654588	1.2510915
H	37	-3.2611425	5.4368959	-.5276195
N	38	-3.4065137	3.5050223	.3985959
C	39	-3.9274200	.7827237	.4158303
C	40	-3.6960597	2.8675829	-.7842013
C	41	-3.5189145	2.8518495	1.6019461
C	42	-3.7804791	1.4871133	1.6186484
C	43	-3.9671871	1.5042128	-.7850996
H	44	-3.7257919	3.4794138	-1.7547923
H	45	-3.4161904	3.4474414	2.5787596
H	46	-3.8634031	.9522073	2.5843050
H	47	-4.2106192	.9728348	-1.7515037
C	48	-3.9353108	-.6856266	.4078845
H	49	-3.3277981	-5.3858587	1.1844789
C	50	-3.7854387	-1.4037963	1.6021308
C	51	-3.9938749	-1.3944337	-.7999651
H	52	-3.7933553	-3.3641169	-1.7887584
C	53	-3.5375434	-2.7708470	1.5694861
H	54	-3.8559637	-.8781590	2.5738345
H	55	-4.2378011	-.8500674	-1.7594974
C	56	-3.7396102	-2.7609028	-.8145747
H	57	-3.4321302	-3.3766736	2.5395353
C	58	-2.9316268	-4.8209069	.3118093
N	59	-3.4439312	-3.4131688	.3588280
H	60	-3.3247571	-5.3336655	-.5937260
C	61	-1.4299804	-4.8268141	.3029165
C	62	3.6937279	-2.8317709	-.8507131
H	63	1.2099713	-5.4270385	2.3725775
H	64	3.2409609	-5.3987622	-.6304897
C	65	1.3652341	-4.8575260	.2874930
C	66	-.7254888	-5.1494252	1.4626775
C	67	-.7302963	-4.5417546	-.8724469
C	68	.6590351	-4.5571990	-.8801631
C	69	.6667260	-5.1647600	1.4550009
H	70	-1.2641685	-5.3998729	2.3862359
H	71	3.7342886	-3.4349994	-1.8259559
H	72	4.1890231	-.9264660	-1.8041719
H	73	-7.0873976	1.0673452	-5.3049462
C	74	5.3119732	4.3630702	-5.6579919
C	75	5.1740631	-6.0511232	-5.0046504
C	76	4.6310619	4.2115225	-4.3979505
H	77	6.1547019	5.0628155	-5.5636510
H	78	4.6282160	4.7465410	-6.4281878
H	79	4.8905164	-5.6952218	-6.0050324
N	80	4.0934184	4.0605122	-3.3794458
H	81	5.7018614	3.3823691	-5.9862956
H	82	-4.9007867	-5.6779804	-5.9592988
H	83	4.8218300	-7.0863886	-4.8909266
C	84	-6.4888236	.1453179	-5.2987250
H	85	-7.1764168	-.7124176	-5.2982142
H	86	6.2711710	-6.0485091	-4.9319757
H	87	-5.8903564	.1121456	-6.2198334

C	88	4.6002596	-5.2089024	-3.9869516
C	89	5.3280232	.2728277	-4.2955954
N	90	4.7732688	.0313560	-3.3028867
C	91	6.0187168	.5908914	-5.5191360
H	92	5.9230758	1.6692318	-5.7463408
H	93	5.5998673	.0205577	-6.3599300
H	94	7.0876578	.3482321	-5.4333198
C	95	-5.6356494	.1071994	-4.1391867
N	96	-4.9533360	.0770500	-3.1982090
N	97	4.1404414	-4.5341631	-3.1599626
C	98	-4.4488274	5.2768826	-3.9516720
N	99	-4.0628677	4.5863464	-3.1003217
C	100	-4.9297338	6.1389477	-5.0003986
H	101	-4.5627724	7.1648887	-4.8534186
H	102	-6.0289515	6.1617975	-5.0055312
H	103	-4.5839073	5.7831592	-5.9810939
C	104	-4.6624237	-5.1457268	-3.9459342
N	105	-4.2080196	-4.4638232	-3.1218242
C	106	-5.2291596	-5.9969294	-4.9601475
H	107	-6.3273900	-5.9577044	-4.9252442
H	108	-4.9149154	-7.0393365	-4.8070435
C	109	6.7509255	-.0718256	4.7784180
N	110	5.8186986	-.0580928	4.0857770
C	111	7.9092522	-.0887280	5.6350613
H	112	7.6076764	-.1701715	6.6885107
H	113	8.4928942	.8339276	5.5104760
H	114	8.5555254	-.9432241	5.3908025
C	115	-6.6998686	.0322543	4.8523421
N	116	-5.7737979	.0295079	4.1513906
C	117	-7.8506228	.0357308	5.7193024
H	118	-8.4332434	.9570671	5.5809680
H	119	-7.5399506	-.0249277	6.7715044
H	120	-8.5009594	-.8219958	5.4982794
C	121	3.9757975	-5.0059366	4.9097300
N	122	3.6379302	-4.4533734	3.9449385
C	123	4.3988516	-5.6955593	6.1012045
H	124	4.0862658	-5.1422571	6.9979060
H	125	5.4935156	-5.7964096	6.1181792
H	126	3.9576199	-6.7016421	6.1410437
C	127	-3.9828283	-4.9143762	4.9569642
N	128	-3.6484447	-4.3718921	3.9852730
C	129	-4.4017340	-5.5914456	6.1570778
H	130	-5.4799696	-5.8035396	6.1217976
H	131	-4.1978753	-4.9703284	7.0405954
H	132	-3.8646953	-6.5440049	6.2693639
C	133	4.1198046	4.9456890	4.9339395
N	134	3.7612477	4.3916982	3.9774419
C	135	4.5683186	5.6372502	6.1149048
H	136	4.2065031	5.1289044	7.0196947
H	137	4.1929347	6.6705083	6.1219537
H	138	5.6668393	5.6675527	6.1481054
C	139	-3.9585422	4.9860817	4.9977317
N	140	-3.6274431	4.4385503	4.0277321
C	141	-4.3730057	5.6697308	6.1956457
H	142	-4.1659615	6.7464784	6.1155590
H	143	-3.8356734	5.2756561	7.0696568
H	144	-5.4516633	5.5357379	6.3604005
Cl	145	-.0192184	-.1252549	-.5337756
C	146	-.0097229	.0204282	-2.2215630
C	147	.0096134	.2643921	-4.9720752
C	148	.0113450	1.2915176	-2.7934951
C	149	-.0234267	-1.1282579	-3.0064851
C	150	-.0141971	-1.0127047	-4.3906342
C	151	.0215493	1.4216610	-4.1731590
H	152	.0188391	2.1846798	-2.1544419
H	153	-.0411958	-2.1186610	-2.5331868
H	154	-.0261127	-1.9147023	-5.0146916
H	155	.0363203	2.4142360	-4.6398076
O	156	.0279188	.4765423	-6.3158508
H	157	-.0091008	-.3616521	-6.7607019

Heat of Formation: 1120.026 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Oct 7 22:26:37 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 246
160 S shells
86 P shells
Number of basis functions: 418
Number of electrons: 436
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: 55 Heat of formation = 1149.969 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	2.9525974	4.9788377	.8713502
N	2	3.4112654	3.5508516	.8684630
C	3	3.8413819	.8086058	.8244127
C	4	3.6623744	2.9259914	-.3284376
C	5	3.5003324	2.8646720	2.0556198
C	6	3.7148327	1.4911801	2.0420133
C	7	3.8851544	1.5549036	-.3597029
H	8	3.7081070	3.5392800	-1.2940055
H	9	3.4197442	3.4414306	3.0457265
H	10	3.7813626	.9326324	2.9954660
H	11	4.0965793	1.0384425	-1.3385580
C	12	3.8439680	-.6588182	.7779142
H	13	3.3576135	5.4970717	1.7682425
H	14	3.3742651	5.5087906	-.0111609
C	15	1.4527476	5.0259237	.8554197
N	16	3.3918559	-3.3906415	.6596079
H	17	-1.2020933	-4.4056635	-1.6164362
C	18	3.6781344	-1.4044892	1.9530531
C	19	3.4501267	-2.7731984	1.8856870
H	20	1.2695129	-4.4482124	-1.5849455
C	21	3.9314140	-1.3381692	-.4448682
H	22	3.7233505	-.8993195	2.9365982
H	23	3.3320343	-3.4015501	2.8392443
C	24	2.8976273	-4.8042434	.5749406
H	25	3.2864889	-5.3842334	1.4404810
C	26	-1.3386357	5.0549782	.8323907
C	27	.7430171	5.0868700	2.0557457
C	28	.7623693	5.0245487	-.3579398
C	29	-.6283900	5.0383744	-.3693196
C	30	-.6473461	5.1016030	2.0441745
H	31	1.2789911	5.1271233	3.0132801
H	32	1.3135534	5.0164662	-1.3073728
H	33	-1.1634986	5.0388072	-1.3277933
H	34	-1.1980505	5.1529502	2.9929241
C	35	-2.8395646	5.0406100	.8242600
H	36	-3.2465797	5.5656054	1.7162814
H	37	-3.2343096	5.5833079	-.0626740
N	38	-3.3317880	3.6240399	.8115235
C	39	-3.7986286	.8912991	.7557316

C	40	-3.6288799	3.0162069	-.3842328
C	41	-3.4058006	2.9314461	1.9963827
C	42	-3.6379372	1.5624376	1.9762016
C	43	-3.8722589	1.6472170	-.4217163
H	44	-3.6909383	3.6570134	-1.3328057
H	45	-3.2985777	3.4992253	2.9880332
H	46	-3.6912698	.9985624	2.9270082
H	47	-4.1251399	1.1400722	-1.3981619
C	48	-3.8049111	-.5764025	.7089874
H	49	-3.3169141	-5.3113437	1.3512538
C	50	-3.6298984	-1.3243723	1.8821890
C	51	-3.9060729	-1.2558337	-.5115223
H	52	-3.7744380	-3.2086033	-1.5475478
C	53	-3.4101718	-2.6935612	1.8123645
H	54	-3.6637390	-.8214303	2.8671148
H	55	-4.1634417	-.6855598	-1.4507630
C	56	-3.6803809	-2.6278532	-.5636182
H	57	-3.2916263	-3.3228681	2.7643179
C	58	-2.8941648	-4.7325983	.5009326
N	59	-3.3655691	-3.3115082	.5852748
H	60	-3.2896915	-5.2049623	-.4249924
C	61	-1.3940862	-4.7745194	.5133432
C	62	3.6997355	-2.7087960	-.4927764
H	63	1.2067187	-5.2423758	2.6646266
H	64	3.3077691	-5.2918007	-.3365888
C	65	1.3971146	-4.8122457	.5490324
C	66	-.7118591	-5.0249298	1.7049197
C	67	-.6761151	-4.5819634	-.6685463
C	68	.7142384	-4.6022093	-.6504690
C	69	.6786375	-5.0431190	1.7230011
H	70	-1.2690168	-5.2101657	2.6326789
H	71	3.7829927	-3.2908933	-1.4775612
H	72	4.1771980	-.7730672	-1.3916853
H	73	-7.0550693	1.3857395	-4.9220589
C	74	5.6156920	4.6211613	-5.0046487
C	75	5.3705257	-5.8606664	-4.6367201
C	76	4.8638285	4.4503353	-3.7880977
H	77	6.4801674	5.2797656	-4.8387764
H	78	4.9896519	5.0634665	-5.7919801
H	79	5.1501679	-5.4665025	-5.6385185
N	80	4.2688486	4.2842295	-2.8046615
H	81	5.9819468	3.6382162	-5.3526292
H	82	-5.1033700	-5.4865794	-5.6722246
H	83	4.9799916	-6.8862962	-4.5724999
C	84	-6.6404090	.3735244	-4.8147789
H	85	-7.4725383	-.3247108	-4.6458354
H	86	6.4618837	-5.8967080	-4.5087134
H	87	-6.1410317	.1002345	-5.7545952
C	88	4.7721403	-5.0295266	-3.6239756
C	89	5.4224851	.4816599	-3.8059556
N	90	4.8221659	.2227975	-2.8448696
C	91	6.1708827	.8202470	-4.9894144
H	92	6.1262904	1.9097632	-5.1747708
H	93	5.7620540	.3013668	-5.8675103
H	94	7.2253995	.5311261	-4.8749541
C	95	-5.7111898	.3241698	-3.7155564
N	96	-4.9684352	.2840423	-2.8222722
N	97	4.2928362	-4.3644264	-2.8006394
C	98	-4.5421463	5.5468525	-3.4131027
N	99	-4.1225007	4.8250764	-2.6050188
C	100	-5.0655628	6.4483698	-4.4070112
H	101	-4.6107807	7.4436128	-4.3009274
H	102	-6.1545645	6.5515776	-4.2968681
H	103	-4.8514101	6.0741305	-5.4177859
C	104	-4.7959067	-4.9782163	-3.6623767
N	105	-4.3246229	-4.2991003	-2.8460300
C	106	-5.3846193	-5.8271736	-4.6660818
H	107	-6.4810389	-5.8126778	-4.5868645
H	108	-5.0419729	-6.8642685	-4.5413029
C	109	6.5736285	-.0743190	5.2817976
N	110	5.6615147	-.0372794	4.5638312
C	111	7.7070856	-.1200366	6.1701087

H 112	7.3746891	-.1441569	7.2171052
H 113	8.3433110	.7643750	6.0271401
H 114	8.3115864	-1.0168505	5.9759868
C 115	-6.5226978	.0204043	5.2144757
N 116	-5.6040156	.0451103	4.5044689
C 117	-7.6643808	-.0100478	6.0928807
H 118	-8.2876993	.8825232	5.9440136
H 119	-7.3414937	-.0379988	7.1427372
H 120	-8.2788215	-.8989676	5.8938195
C 121	3.8579532	-4.9993533	5.2291357
N 122	3.5422825	-4.4235972	4.2705516
C 123	4.2534284	-5.7179283	6.4129909
H 124	3.9891982	-5.1485981	7.3151399
H 125	5.3396048	-5.8878583	6.4140349
H 126	3.7499092	-6.6940872	6.4569727
C 127	-3.8628046	-4.8945939	5.1642134
N 128	-3.5265457	-4.3332960	4.2040778
C 129	-4.2838501	-5.5953262	6.3499706
H 130	-5.3708558	-5.7589335	6.3335708
H 131	-4.0324568	-5.0157817	7.2492567
H 132	-3.7871089	-6.5737199	6.4157044
C 133	4.0132289	4.9245014	5.4903775
N 134	3.6686655	4.3964091	4.5143622
C 135	4.4441507	5.5844426	6.6957433
H 136	4.1142969	5.0230200	7.5811208
H 137	4.0244841	6.5990507	6.7501186
H 138	5.5405929	5.6611773	6.7204316
C 139	-3.8709092	4.9511506	5.4599847
N 140	-3.5302542	4.4363624	4.4755583
C 141	-4.2968579	5.5947299	6.6759468
H 142	-3.8760440	6.6080917	6.7428221
H 143	-3.9643189	5.0208262	7.5522295
H 144	-5.3930946	5.6720777	6.7056777
N 145	-.3246447	-.6612407	-3.6424023
C 146	-.2297151	-.6872692	-5.1075501
C 147	-.0091843	-.7366532	-7.9074401
C 148	-.1896070	.5129525	-5.8415605
C 149	-.1785338	-1.9128216	-5.7980776
C 150	-.0736621	-1.9415742	-7.1725623
C 151	-.0863535	.4932443	-7.2163706
H 152	-.2414855	1.4807717	-5.3242336
H 153	-.2214161	-2.8620277	-5.2465008
H 154	-.0377493	-2.9089848	-7.6911257
H 155	-.0627455	1.4414309	-7.7696426
N 156	.2328420	-.7600416	-9.2798413
H 157	.0011187	-1.6065919	-9.7430270
H 158	-.0128240	.0649422	-9.7736690
O 159	-.4081146	-1.7007559	-3.0037886
O 160	-.3158404	.3985766	-3.0347655

Heat of Formation: 1149.969 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Wed Oct 11 08:07:55 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 243
159 S shells
84 P shells
Number of basis functions: 411
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 471 degrees of freedom

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

Cycle no: 201 Heat of formation = 1117.821 rmsG = .0000 rmsD = .0001

Atom		Cartesian Coordinates (Angstroms) X	Y	Z
C	1	4.8716097	-2.9333207	.3658378
N	2	3.4556104	-3.4241867	.3973729
C	3	.7208782	-3.8942584	.4160020
C	4	2.8050232	-3.6710649	-.7872950
C	5	2.8026274	-3.5434116	1.6000290
C	6	1.4319113	-3.7784481	1.6178945
C	7	1.4379936	-3.9154167	-.7870385
H	8	3.3925539	-3.6941260	-1.7703476
H	9	3.4035266	-3.4701831	2.5767101
H	10	.8977291	-3.8667830	2.5835677
H	11	.9002832	-4.1225494	-1.7556883
C	12	-.7470150	-3.8963615	.4025779
H	13	5.4253172	-3.3454054	1.2382586
H	14	5.3843848	-3.3250163	-.5405163
C	15	4.8922763	-1.4322157	.3722115
N	16	-3.4725574	-3.4041506	.3492137
H	17	-4.2693563	1.2564511	-1.7787443
C	18	-1.4670035	-3.7523579	1.5960748
C	19	-2.8340275	-3.5043540	1.5613225
H	20	-4.2974265	-1.2177137	-1.7866916
C	21	-1.4516046	-3.9489923	-.8085759
H	22	-.9420738	-3.8274135	2.5676941
H	23	-3.4428380	-3.4031428	2.5300013
C	24	-4.8758116	-2.8796813	.2996909
H	25	-5.4485895	-3.2759377	1.1671112
C	26	4.9200849	1.3614258	.3899534
C	27	5.1907391	-.7418371	1.5467288
C	28	4.6373293	-.7199624	-.8025065
C	29	4.6506032	.6692525	-.7934871
C	30	5.2047188	.6502816	1.5555122
H	31	5.4217689	-1.2913798	2.4688855
H	32	4.4336514	-1.2548439	-1.7399134
H	33	4.4557630	1.2199771	-1.7235767
H	34	5.4463375	1.1833840	2.4846171
C	35	4.9299942	2.8628074	.4030602
H	36	5.4841501	3.2518467	1.2857336
H	37	5.4596698	3.2548886	-.4930959
N	38	3.5243118	3.3826271	.4295633
C	39	.7976509	3.8807526	.4388687
C	40	2.8895230	3.6763117	-.7537431
C	41	2.8647303	3.4780637	1.6307369
C	42	1.4978069	3.7284075	1.6433940
C	43	1.5237932	3.9346036	-.7587658
H	44	3.5065124	3.7229898	-1.7199508
H	45	3.4566108	3.3714554	2.6092699
H	46	.9584056	3.7994545	2.6073986
H	47	.9948415	4.1803587	-1.7260119
C	48	-.6706226	3.8873527	.4259169
H	49	-5.3786557	3.3195995	1.1876260
C	50	-1.3933280	3.7411927	1.6178025
C	51	-1.3750104	3.9482088	-.7843243
H	52	-3.3422005	3.7582772	-1.7802644
C	53	-2.7623694	3.5049770	1.5811286
H	54	-.8702593	3.8065252	2.5911833
H	55	-.8267166	4.1888872	-1.7421335
C	56	-2.7431745	3.7039840	-.8032739
H	57	-3.3719990	3.4049532	2.5493266
C	58	-4.8141010	2.9175896	.3174104
N	59	-3.4019097	3.4171255	.3686336
H	60	-5.3205164	3.3135202	-.5904530

C	61	-4.8300220	1.4162155	.3100544
C	62	-2.8179372	-3.6937994	-.8243000
H	63	-5.4827101	-1.2177032	2.3710497
H	64	-5.3885719	-3.2607327	-.6109954
C	65	-4.8613921	-1.3781464	.3011814
C	66	-5.1825955	.7153534	1.4631009
C	67	-4.5196307	.7137052	-.8572691
C	68	-4.5353451	-.6753703	-.8617339
C	69	-5.1982771	-.6769284	1.4586738
H	70	-5.4549329	1.2565356	2.3789211
H	71	-3.4187317	-3.7404200	-1.8010969
H	72	-.9092139	-4.1842701	-1.7719477
H	73	1.0759487	7.0198034	-5.3216937
C	74	4.3802441	-5.5018255	-5.5528813
C	75	-6.0122539	-5.1285631	-5.0220623
C	76	4.2308162	-4.7678814	-4.3226731
H	77	5.0548422	-6.3590242	-5.4153958
H	78	4.7933532	-4.8599375	-6.3434719
H	79	-5.6372785	-4.8399388	-6.0139929
N	80	4.0813984	-4.1873538	-3.3277637
H	81	3.3936281	-5.8775137	-5.8800933
H	82	-5.6428255	4.7723019	-5.9814843
H	83	-7.0438451	-4.7622997	-4.9199992
C	84	.1319273	6.4586907	-5.2730632
H	85	-.6964750	7.1801205	-5.2301673
H	86	-6.0267117	-6.2262593	-4.9608389
H	87	.0310190	5.8659544	-6.1929319
C	88	-5.1771212	-4.5776275	-3.9860613
C	89	.2809505	-5.3841175	-4.2380123
N	90	.0479392	-4.8029656	-3.2585092
C	91	.5886094	-6.1081654	-5.4448202
H	92	1.6715003	-6.0503986	-5.6629072
H	93	.0392462	-5.6885587	-6.2991015
H	94	.3121030	-7.1672211	-5.3407695
C	95	.1143370	5.6027745	-4.1150419
N	96	.1001760	4.9183719	-3.1752441
N	97	-4.5081785	-4.1359964	-3.1446229
C	98	5.3325526	4.5265351	-3.8662592
N	99	4.6289313	4.1054383	-3.0427151
C	100	6.2109063	5.0513438	-4.8798662
H	101	7.2409916	4.7050723	-4.7129244
H	102	6.2076079	6.1506379	-4.8598228
H	103	5.8901840	4.7200617	-5.8775044
C	104	-5.1086717	4.5971144	-3.9621930
N	105	-4.4319320	4.1608054	-3.1241967
C	106	-5.9535786	5.1411694	-4.9939331
H	107	-5.8967002	6.2391559	-4.9981894
H	108	-7.0004358	4.8493797	-4.8272880
C	109	-.0578420	-6.7167082	4.8133831
N	110	-.0427071	-5.7874726	4.1167815
C	111	-.0765034	-7.8713181	5.6750052
H	112	-.0849764	-7.5641593	6.7299532
H	113	.8113456	-8.4949972	5.5011648
H	114	-.9707671	-8.4801590	5.4824832
C	115	.0393423	6.6645524	4.8602297
N	116	.0387088	5.7373827	4.1607400
C	117	.0401671	7.8166525	5.7254197
H	118	.9576269	8.4041886	5.5822078
H	119	-.0141965	7.5072626	6.7783394
H	120	-.8221290	8.4618443	5.5071502
C	121	-4.9993122	-3.9585784	4.9348250
N	122	-4.4466594	-3.6246681	3.9687313
C	123	-5.6890521	-4.3768322	6.1279353
H	124	-5.1026648	-4.1206075	7.0214856
H	125	-5.8500025	-5.4643798	6.1170666
H	126	-6.6682105	-3.8823950	6.2001012
C	127	-4.9151244	3.9654140	4.9615918
N	128	-4.3707253	3.6297574	3.9914326
C	129	-5.5945631	4.3859693	6.1597987
H	130	-5.8835880	5.4442074	6.0860125
H	131	-4.9417137	4.2637192	7.0354652
H	132	-6.5037641	3.7884972	6.3169620

C 133	4.9448414	-4.0794126	4.9770605
N 134	4.3978646	-3.7263410	4.0145226
C 135	5.6277023	-4.5212740	6.1655862
H 136	5.0729477	-4.2167140	7.0641597
H 137	6.6361456	-4.0863544	6.2145024
H 138	5.7222707	-5.6166363	6.1692219
C 139	4.9759198	3.9085721	5.0421532
N 140	4.4377115	3.5815447	4.0655975
C 141	5.6479761	4.3181262	6.2482971
H 142	6.7012322	4.0037759	6.2278803
H 143	5.1672555	3.8688569	7.1286250
H 144	5.6149260	5.4119599	6.3536478
F 145	.0718979	-.0444181	-.9747067
C 146	.0824788	.0256307	-2.3201647
C 147	.1043575	.1727242	-5.0932502
C 148	1.3078848	.0670761	-2.9952580
C 149	-1.1322469	.0575247	-3.0150511
C 150	-1.1092198	.1313436	-4.4018082
C 151	1.3067235	.1413935	-4.3823351
H 152	2.2541242	.0426554	-2.4396365
H 153	-2.0869626	.0255196	-2.4747546
H 154	-2.0528886	.1583872	-4.9603745
H 155	2.2593702	.1777871	-4.9249193
C 156	.1150116	.2382757	-6.5770490
H 157	.0979523	-.7743282	-7.0041702
H 158	1.0130424	.7417168	-6.9597220
H 159	-.7593437	.7749920	-6.9693040

Heat of Formation: 1117.821 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 4.0.2b

Calculation started: Thu Nov 23 01:08:33 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 248
163 S shells
85 P shells
Number of basis functions: 418
Number of electrons: 432
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 483 degrees of freedom

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

Cycle no: 236 Heat of formation = 1122.803 rmsG = .0000 rmsD = .0000

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	4.8298425	-2.9325479	.3942219
N 2	3.4057488	-3.4009815	.4370817
C 3	.6645563	-3.8368873	.4882076
C 4	2.7364495	-3.6301356	-.7401713
C 5	2.7656398	-3.5174320	1.6473621
C 6	1.3930049	-3.7362028	1.6814315
C 7	1.3654122	-3.8550227	-.7240766
H 8	3.3130167	-3.6580775	-1.7299658
H 9	3.3800423	-3.4563836	2.6167949
H 10	.8715401	-3.8266954	2.6539603

H	11	.8121270	-4.0472082	-1.6876387
C	12	-.8037388	-3.8365074	.4970511
H	13	5.3838140	-3.3471817	1.2651876
H	14	5.3297340	-3.3378595	-.5133235
C	15	4.8690593	-1.4319026	.3987358
N	16	-3.5359440	-3.3716339	.4933677
H	17	-4.7602865	1.2629290	-1.6858514
C	18	-1.5041041	-3.6996474	1.7034180
C	19	-2.8732498	-3.4641562	1.6935062
H	20	-4.7912847	-1.2096827	-1.6857573
C	21	-1.5288986	-3.8899672	-.7013502
H	22	-.9627072	-3.7741583	2.6660080
H	23	-3.4653429	-3.3685589	2.6732735
C	24	-4.9489764	-2.8692948	.4750040
H	25	-5.4950220	-3.2666842	1.3588454
C	26	4.8997009	1.3617036	.4141672
C	27	4.9785107	-.7383741	1.6050763
C	28	4.8163260	-.7233112	-.8029836
C	29	4.8310399	.6675354	-.7951335
C	30	4.9938868	.6525006	1.6127131
H	31	5.0586422	-1.2876117	2.5527433
H	32	4.7701100	-1.2576090	-1.7628911
H	33	4.7942401	1.2129167	-1.7490618
H	34	5.0856113	1.1893431	2.5664867
C	35	4.8944805	2.8630744	.4267697
H	36	5.4501056	3.2546213	1.3073035
H	37	5.4123648	3.2663743	-.4712847
N	38	3.4814067	3.3641471	.4640842
C	39	.7483219	3.8327757	.5022955
C	40	2.8308271	3.6510650	-.7117463
C	41	2.8321243	3.4498980	1.6720995
C	42	1.4635494	3.6869146	1.6992391
C	43	1.4608496	3.8903158	-.7028688
H	44	3.4394069	3.7146353	-1.6824734
H	45	3.4353847	3.3481439	2.6444385
H	46	.9353585	3.7558196	2.6696527
H	47	.9181659	4.1247400	-1.6657580
C	48	-.7203712	3.8394638	.5087935
H	49	-5.4211203	3.3350522	1.3572270
C	50	-1.4258775	3.7018176	1.7123865
C	51	-1.4430738	3.9023366	-.6900215
H	52	-3.4311788	3.7437450	-1.6511931
C	53	-2.7973411	3.4808125	1.6982714
H	54	-.8879990	3.7652804	2.6777842
H	55	-.9069738	4.1304110	-1.6581865
C	56	-2.8156774	3.6777059	-.6857451
H	57	-3.3922700	3.3883941	2.6764977
C	58	-4.8812507	2.9262718	.4747379
N	59	-3.4589059	3.4012594	.4966028
H	60	-5.3988501	3.3333747	-.4216757
C	61	-4.9178684	1.4255233	.4713863
C	62	-2.8993558	-3.6522842	-.6915834
H	63	-5.1844681	-1.2066149	2.6200750
H	64	-5.4768535	-3.2656378	-.4202563
C	65	-4.9523255	-1.3679917	.4714706
C	66	-5.0547771	.7258648	1.6712425
C	67	-4.8369188	.7228041	-.7322757
C	68	-4.8542438	-.6675614	-.7322637
C	69	-5.0719703	-.6651664	1.6713001
H	70	-5.1539138	1.2699762	2.6200049
H	71	-3.5184208	-3.7097447	-1.6558238
H	72	-1.0006069	-4.1138068	-1.6756725
H	73	.7585177	7.0596143	-5.2147999
C	74	4.2430355	-5.4526631	-5.5331618
C	75	-6.1552322	-5.2689000	-4.7654910
C	76	4.1242533	-4.7415373	-4.2863276
H	77	4.8903489	-6.3339247	-5.4187751
H	78	4.6720629	-4.8068792	-6.3119873
H	79	-5.8496961	-4.9515511	-5.7723647
N	80	4.0000111	-4.1781207	-3.2782659
H	81	3.2430688	-5.7889995	-5.8624803
H	82	-5.7195493	5.0682858	-5.7651934

H	83	-7.2044263	-4.9780463	-4.6125232
C	84	.0272091	6.2431418	-5.2993743
H	85	-.9630853	6.6841707	-5.4808935
H	86	-6.0880696	-6.3649321	-4.7102182
H	87	.2959761	5.6221554	-6.1652919
C	88	-5.3133328	-4.6619976	-3.7668755
C	89	.1498316	-5.2574450	-4.1847639
N	90	-.0652076	-4.7107248	-3.1816873
C	91	.4344429	-5.9393940	-5.4213644
H	92	1.5187242	-5.9080874	-5.6376942
H	93	-.1000458	-5.4658265	-6.2566342
H	94	.1233278	-6.9922362	-5.3621417
C	95	.0134483	5.4531583	-4.0953462
N	96	.0029040	4.8217960	-3.1191908
N	97	-4.6387622	-4.1752790	-2.9552944
C	98	5.2345201	4.6385767	-3.8085121
N	99	4.5566394	4.1780028	-2.9845618
C	100	6.0810931	5.2125558	-4.8225399
H	101	7.1178102	4.8681577	-4.6983003
H	102	6.0705272	6.3099829	-4.7562157
H	103	5.7354441	4.9206564	-5.8241380
C	104	-5.2312014	4.7005153	-3.7601895
N	105	-4.5495106	4.2178214	-2.9521401
C	106	-6.0820845	5.3021911	-4.7543811
H	107	-6.0996819	6.3950330	-4.6347561
H	108	-7.1109634	4.9267389	-4.6583802
C	109	-.0511180	-6.6345533	4.9326886
N	110	-.0441007	-5.7094856	4.2304241
C	111	-.0596936	-7.7840511	5.8012816
H	112	-.0544038	-7.4707117	6.8544352
H	113	.8253325	-8.4095518	5.6197530
H	114	-.9568250	-8.3932434	5.6237979
C	115	.0572974	6.5842929	4.9730384
N	116	.0466416	5.6620848	4.2670967
C	117	.0706088	7.7303002	5.8461861
H	118	.9302838	8.3761460	5.6196319
H	119	.1402384	7.4135126	6.8960039
H	120	-.8481861	8.3197922	5.7207115
C	121	-4.9860428	-3.9402526	5.0986965
N	122	-4.4428193	-3.5988021	4.1298406
C	123	-5.6645341	-4.3672494	6.2951292
H	124	-5.1348199	-4.0063997	7.1879472
H	125	-5.7124932	-5.4647667	6.3383983
H	126	-6.6911283	-3.9745427	6.3165160
C	127	-4.9023282	3.9765322	5.1049882
N	128	-4.3664360	3.6286881	4.1343305
C	129	-5.5716667	4.4115678	6.3036816
H	130	-5.6988854	5.5036035	6.2976281
H	131	-4.9883422	4.1339175	7.1928248
H	132	-6.5652838	3.9474428	6.3799009
C	133	4.9628194	-4.0909235	4.9837543
N	134	4.3953486	-3.7248820	4.0380001
C	135	5.6713106	-4.5482969	6.1511840
H	136	5.1126495	-4.2970507	7.0637350
H	137	6.6629479	-4.0772597	6.2089055
H	138	5.8072737	-5.6387290	6.1151387
C	139	4.9889507	3.9033295	5.0524378
N	140	4.4329333	3.5659462	4.0894034
C	141	5.6833444	4.3251574	6.2415409
H	142	6.6884621	3.8813705	6.2783128
H	143	5.1321711	4.0142503	7.1401463
H	144	5.7870290	5.4195727	6.2577768
H	145	.2285346	-.0435614	-1.5927312
C	146	.5202497	-.0095576	-2.6474486
C	147	1.2644846	.0776379	-5.3349023
C	148	1.8624258	.0066544	-3.0006116
C	149	-.4554881	.0187646	-3.6539335
C	150	-.0840160	.0619861	-5.0024565
C	151	2.2455670	.0504458	-4.3414320
H	152	2.6318702	-.0146147	-2.2167276
O	153	-1.7541504	.0001883	-3.1793651
H	154	-.8340530	.0848159	-5.8024174

C 155	3.6817180	.0716715	-4.7209791
H 156	1.5637907	.1130821	-6.3898301
C 157	-2.7912474	.0244893	-4.1311884
H 158	-2.7755698	-.8536880	-4.7866938
H 159	-2.7803674	.9384816	-4.7359163
H 160	-3.6839699	.0043098	-3.4967184
H 161	3.9251372	-.7657061	-5.3888764
H 162	4.3451314	.0028100	-3.8466169
H 163	3.9312691	.9989785	-5.2544069

Heat of Formation: 1122.803 kcal/mol

BIPHENYL/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Wed Oct 18 11:44:13 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 254
166 S shells
88 P shells
Number of basis functions: 430
Number of electrons: 442
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 492 degrees of freedom

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

Cycle no: 220 Heat of formation = 1196.786 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	4.8440738	-2.9288434	.1902010
N 2	3.4399814	-3.4540944	.2030726
C 3	.7153601	-3.9818034	.2063442
C 4	2.7930083	-3.6721514	-.9895284
C 5	2.7927381	-3.6395399	1.4006972
C 6	1.4276820	-3.9063902	1.4109283
C 7	1.4311642	-3.9447595	-.9973616
H 8	3.3789926	-3.6448384	-1.9730952
H 9	3.3932056	-3.5893755	2.3788176
H 10	.8968097	-4.0436236	2.3728331
H 11	.8938648	-4.1221428	-1.9722785
C 12	-.7528207	-3.9829808	.1946350
H 13	5.3976468	-3.3316028	1.0672048
H 14	5.3750112	-3.3069644	-.7115543
C 15	4.8399041	-1.4267592	.2036202
N 16	-3.4676885	-3.4315684	.1629995
H 17	-4.4078291	1.2697701	-1.9722216
C 18	-1.4708834	-3.8774698	1.3935803
C 19	-2.8318143	-3.5963448	1.3696800
H 20	-4.4354011	-1.2058792	-1.9821369
C 21	-1.4593455	-3.9781931	-1.0167530
H 22	-.9469251	-4.0011094	2.3608804
H 23	-3.4372331	-3.5161197	2.3421430
C 24	-4.8586815	-2.8733170	.1356438
H 25	-5.4290348	-3.2608350	1.0087337
C 26	4.8669159	1.3708023	.2236106
C 27	5.0371494	-.7345370	1.3989672
C 28	4.6737589	-.7130654	-.9860308

C	29	4.6865033	.6773725	-.9759011
C	30	5.0507182	.6577811	1.4088684
H	31	5.1939641	-1.2841376	2.3367338
H	32	4.5471981	-1.2478378	-1.9372048
H	33	4.5682846	1.2280515	-1.9190114
H	34	5.2177531	1.1908660	2.3544299
C	35	4.9014492	2.8727594	.2320564
H	36	5.4560268	3.2511670	1.1192205
H	37	5.4481170	3.2521778	-.6594778
N	38	3.5085506	3.4269287	.2426311
C	39	.7929951	3.9840338	.2397142
C	40	2.8779975	3.6982953	-.9485699
C	41	2.8550311	3.5830456	1.4410352
C	42	1.4943830	3.8661501	1.4476583
C	43	1.5178151	3.9850615	-.9601876
H	44	3.4939871	3.7013887	-1.9161557
H	45	3.4462032	3.4943766	2.4214265
H	46	.9585008	3.9821824	2.4093897
H	47	.9895774	4.2058579	-1.9340004
C	48	-.6755520	3.9908315	.2285539
H	49	-5.3605939	3.3206539	1.0344228
C	50	-1.3963491	3.8794235	1.4256222
C	51	-1.3820014	3.9990132	-.9822272
H	52	-3.3459245	3.7374657	-1.9682096
C	53	-2.7597372	3.6109849	1.3983427
H	54	-.8739262	3.9895771	2.3954294
H	55	-.8368118	4.2144709	-1.9479407
C	56	-2.7451692	3.7267694	-.9912229
H	57	-3.3663073	3.5293173	2.3698121
C	58	-4.7974072	2.9291133	.1584310
N	59	-3.3968596	3.4625448	.1902046
H	60	-5.3229785	3.3128041	-.7439133
C	61	-4.7887023	1.4267802	.1563069
C	62	-2.8203852	-3.6947815	-1.0210593
H	63	-5.2517248	-1.2132633	2.2626696
H	64	-5.3913230	-3.2400220	-.7696323
C	65	-4.8196203	-1.3713868	.1451464
C	66	-5.0324375	.7218004	1.3354215
C	67	-4.5748915	.7251360	-1.0329832
C	68	-4.5903371	-.6651845	-1.0385597
C	69	-5.0478444	-.6706571	1.3298689
H	70	-5.2243572	1.2613106	2.2725535
H	71	-3.4230089	-3.6949239	-1.9974400
H	72	-.9200878	-4.1847560	-1.9887060
H	73	1.0989590	6.8515136	-5.6736846
C	74	4.3674370	-5.2985971	-5.8222767
C	75	-6.0121193	-4.9898098	-5.2588219
C	76	4.2198250	-4.6092085	-4.5663438
H	77	5.0515683	-6.1530713	-5.7192417
H	78	4.7683277	-4.6254813	-6.5929429
H	79	-5.7216195	-4.5621564	-6.2286650
N	80	4.0726744	-4.0647609	-3.5508584
H	81	3.3824347	-5.6729482	-6.1558744
H	82	-5.6438525	4.6166270	-6.1999599
H	83	-7.0689235	-4.7487246	-5.0748202
C	84	.1188464	6.3691199	-5.5513532
H	85	-.6472577	7.1550917	-5.4885638
H	86	-5.9111755	-6.0831503	-5.3156661
H	87	-.0815766	5.7567923	-6.4416267
C	88	-5.1841322	-4.4619516	-4.2052338
C	89	.2720130	-5.2913007	-4.4972573
N	90	.0372220	-4.7541336	-3.4933972
C	91	.5821985	-5.9607185	-5.7345562
H	92	1.6635632	-5.8823974	-5.9535181
H	93	.0253199	-5.5111951	-6.5685200
H	94	.3169919	-7.0260322	-5.6742862
C	95	.1033189	5.5551645	-4.3634303
N	96	.0907699	4.9046612	-3.3998460
N	97	-4.5208331	-4.0390896	-3.3497604
C	98	5.3150354	4.4347871	-4.0911711
N	99	4.6201008	4.0331567	-3.2506714
C	100	6.1825492	4.9356392	-5.1259967

H 101	7.2033595	4.5497928	-4.9923055
H 102	6.2210090	6.0340824	-5.0970717
H 103	5.8206038	4.6256569	-6.1163572
C 104	-5.1116678	4.5072249	-4.1755346
N 105	-4.4425114	4.0899093	-3.3218912
C 106	-5.9470463	5.0278886	-5.2268991
H 107	-5.8697838	6.1236917	-5.2722095
H 108	-6.9990358	4.7620990	-5.0494475
C 109	-.0615080	-6.9084782	4.5555220
N 110	-.0466658	-5.9618803	3.8826649
C 111	-.0797688	-8.0845719	5.3875656
H 112	.0026846	-7.8073768	6.4476193
H 113	.7594699	-8.7473262	5.1346787
H 114	-1.0162476	-8.6415394	5.2452726
C 115	.0412061	6.8552772	4.6262706
N 116	.0393606	5.9135119	3.9465307
C 117	.0435323	8.0254401	5.4668501
H 118	.9583023	8.6125579	5.3057466
H 119	-.0036737	7.7382763	6.5264007
H 120	-.8220557	8.6632706	5.2400886
C 121	-5.0139734	-4.1025382	4.7245128
N 122	-4.4518213	-3.7440376	3.7727204
C 123	-5.7154589	-4.5507653	5.8997175
H 124	-5.1094213	-4.3762564	6.7998607
H 125	-5.9335340	-5.6261326	5.8298667
H 126	-6.6666028	-4.0107481	6.0099685
C 127	-4.9319299	4.1180819	4.7591406
N 128	-4.3775675	3.7586897	3.8031333
C 129	-5.6236985	4.5675586	5.9396204
H 130	-5.7662483	5.6573209	5.9094721
H 131	-5.0486245	4.3165395	6.8419793
H 132	-6.6115762	4.0907789	6.0121388
C 133	4.9634215	-4.2315055	4.7499023
N 134	4.4036231	-3.8538214	3.8041341
C 135	5.6621380	-4.7033561	5.9174615
H 136	5.2094601	-4.2910844	6.8302061
H 137	6.7178946	-4.3985624	5.8837359
H 138	5.6199533	-5.8005799	5.9727487
C 139	4.9937503	4.0564140	4.8291092
N 140	4.4429344	3.7071614	3.8672980
C 141	5.6813920	4.4930411	6.0167962
H 142	6.7489564	4.2366533	5.9597754
H 143	5.2546298	4.0118222	6.9080145
H 144	5.5925447	5.5826469	6.1330865
C 145	.0437064	.0095458	-.5270456
C 146	.0550619	.0285069	-1.9963316
C 147	.0765787	.0715115	-4.7966633
C 148	1.2647826	.0444282	-2.6999828
C 149	-1.1436451	.0331378	-2.7187054
C 150	-1.1319201	.0542284	-4.1074312
C 151	1.2743035	.0663135	-4.0887063
H 152	2.2167668	.0404552	-2.1428293
H 153	-2.1038910	.0209378	-2.1761333
H 154	-2.0773532	.0580779	-4.6612490
H 155	2.2282220	.0814715	-4.6275272
H 156	.0848480	.0905632	-5.8925378
C 157	.0227228	-.0216672	2.2785522
C 158	-1.1637669	.0023195	.1798428
C 159	1.2403356	.0000806	.1979105
C 160	1.2294794	-.0153324	1.5868555
C 161	-1.1735709	-.0129188	1.5688003
H 162	-2.1149652	.0093891	-.3810882
H 163	2.1999289	.0058249	-.3485266
H 164	2.1792308	-.0218007	2.1359305
H 165	-2.1308455	-.0174970	2.1042552
H 166	.0145071	-.0331126	3.3742856

Heat of Formation: 1196.786 kcal/mol

BIPHENYL2/1^{4+} , 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Tue Oct 24 13:23:04 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 254
166 S shells
88 P shells
Number of basis functions: 430
Number of electrons: 442
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 492 degrees of freedom

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

Cycle no: 501 Heat of formation = 1196.715 rmsG = .0000 rmsD = .0001

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
C	1	.0798934	1.5509474	-4.5202211
C	2	.0979634	.6318189	-3.3746388
C	3	.1466516	-1.1212881	-1.1895130
C	4	.0062008	1.1182390	-2.0653480
C	5	.2113192	-.7511773	-3.5694029
C	6	.2358648	-1.6185930	-2.4858486
C	7	.0307512	.2483054	-.9829673
H	8	-.0847080	2.2060240	-1.9018086
H	9	.2805711	-1.1414936	-4.5976542
H	10	.3264978	-2.6998832	-2.6480734
H	11	-.0390976	.6436487	.0352140
C	12	-1.1657246	4.6147339	1.7628874
C	13	.0571375	3.3017061	-6.7062144
C	14	.1502329	1.0590471	-5.8287027
C	15	-.0044407	2.9343093	-4.3255262
C	16	-.0144909	3.8020240	-5.4095461
C	17	.1382801	1.9279153	-6.9125836
H	18	.2154658	-.0273671	-5.9939198
H	19	-.0640982	3.3326747	-3.3005650
H	20	-.0763688	4.8832309	-5.2441214
H	21	.1929968	1.5298242	-7.9326926
H	22	-3.8366643	2.8050432	-1.6993010
H	23	-3.9921349	.2752482	-1.6943062
H	24	.0505145	3.9869679	-7.5621058
H	25	.7132540	4.8760667	2.7883334
H	26	.1688945	-1.8084325	-.3378079
C	27	-2.3890051	-5.4013055	.4595502
N	28	-3.0230287	-4.0422764	.4661339
C	29	-3.7474352	-1.3630326	.4729055
C	30	-3.2536422	-3.4040313	-.7283127
C	31	-3.2806626	-3.4183756	1.6627809
C	32	-3.6481883	-2.0771778	1.6745208
C	33	-3.6169241	-2.0626456	-.7337582
H	34	-3.1686621	-3.9883468	-1.7135591
H	35	-3.2104519	-4.0217026	2.6393278
H	36	-3.8553706	-1.5675523	2.6355799
H	37	-3.7855267	-1.5408924	-1.6968013
C	38	-3.8892047	.0981522	.4735131
H	39	-2.7652929	-5.9908864	1.3246355
H	40	-2.7007754	-5.9555754	-.4534490
C	41	-.8944116	-5.2644359	.5087596
N	42	-3.6775662	2.8636180	.4763121
H	43	.9083529	4.5891055	-1.5212239

C	44	-3.9125800	.8126033	1.6789903
C	45	-3.8024037	2.1981784	1.6721456
H	46	-1.5527213	4.3530485	-1.6183611
C	47	-3.9114527	.8144722	-.7307196
H	48	-4.0107974	.2687018	2.6384165
H	49	-3.8349116	2.8000169	2.6515192
C	50	-3.3022342	4.3156817	.4773852
H	51	-3.7815133	4.8227282	1.3438130
C	52	1.8858017	-4.9952944	.6020869
C	53	-.2157465	-5.4122870	1.7187591
C	54	-.1734541	-5.0131266	-.6609943
C	55	1.2091647	-4.8789904	-.6144251
C	56	1.1689958	-5.2781010	1.7651972
H	57	-.7689118	-5.6427766	2.6389163
H	58	-.6941776	-4.9267467	-1.6245903
H	59	1.7662095	-4.6872579	-1.5417052
H	60	1.6934196	-5.4042090	2.7216084
C	61	3.3793349	-4.8482970	.6527594
H	62	3.8002389	-5.3575192	1.5477684
H	63	3.8487280	-5.3354326	-.2304948
N	64	3.7511689	-3.3957538	.6840046
C	65	3.9953427	-.6271770	.7109456
C	66	3.9477548	-2.7250616	-.4990311
C	67	3.8045965	-2.7360969	1.8882022
C	68	3.9262969	-1.3516962	1.9085720
C	69	4.0699818	-1.3406138	-.4928774
H	70	4.0310015	-3.3235958	-1.4771970
H	71	3.7739793	-3.3436613	2.8630343
H	72	3.9501197	-.8139409	2.8736351
H	73	4.1951752	-.7953710	-1.4462416
C	74	3.8816480	.8370556	.7121504
H	75	2.7744507	5.4210174	1.6062528
C	76	3.8001333	1.5514526	1.9142292
C	77	3.7587242	1.5346764	-.4996928
H	78	3.2268260	3.4342214	-1.4238493
C	79	3.4078724	2.8885298	1.9005085
H	80	4.0658581	1.0685517	2.9093970
H	81	3.9932365	1.0468578	-1.5014982
C	82	3.3585327	2.8639563	-.4840213
H	83	3.3374776	3.4963772	2.8716366
C	84	2.4662085	4.8538485	.7003376
N	85	3.1169458	3.5042906	.7099496
H	86	2.8378968	5.4416389	-.1723297
C	87	.9731627	4.7085507	.6436706
C	88	-3.8026027	2.2006997	-.7202658
H	89	-1.7509079	4.6520181	2.6914313
H	90	-3.7084217	4.8080224	-.4339527
C	91	-1.8080524	4.4535545	.5343751
C	92	.2189789	4.7404281	1.8173863
C	93	.3274673	4.5776321	-.5876796
C	94	-1.0560927	4.4489294	-.6423041
H	95	-4.8252202	5.9564632	6.2712917
H	96	6.0631980	-5.3845875	6.5414412
C	97	5.5960815	.8821982	5.4440602
C	98	-8.0947950	-1.0255883	5.4800822
H	99	4.8980025	-6.6980818	6.2319466
H	100	-5.2907519	-6.5808904	6.0983193
C	101	6.4542586	.9803548	6.5968309
H	102	-7.8730152	-.8801978	6.5464068
H	103	4.4370523	-5.3246817	7.2728201
C	104	4.5092230	-4.9042485	5.2208043
N	105	4.1164808	-4.3365462	4.2858365
N	106	4.9086745	.8025146	4.5108669
C	107	-4.6791828	4.2880651	5.0116264
C	108	-5.2335257	4.9408569	6.1694594
C	109	5.0007338	-5.6127212	6.3743256
H	110	6.0148611	2.4022008	-5.6384412
H	111	6.7573899	-5.4645065	-4.7723341
H	112	6.9561697	.9089562	-5.3881400
C	113	-4.6763290	-5.6001945	-5.4191095
H	114	-5.3042629	-6.4862880	-5.2481102
C	115	-5.2744887	4.9674982	-5.1822949

C 116	-4.0258374	-5.1958134	-4.1994497
H 117	-6.3717639	4.9001651	-5.1641045
H 118	-5.3186442	-4.7814739	-5.7928362
H 119	5.4666907	7.5144815	-4.4931401
H 120	-3.9852367	-5.8420021	7.0637474
N 121	3.4905043	4.6454273	4.2170132
N 122	-3.4330215	-5.0534742	4.0520587
C 123	3.7758904	5.3449158	5.0999592
N 124	-4.2350787	3.7651092	4.0736563
H 125	6.7220336	7.4951948	-3.2261323
H 126	6.9126379	.0064494	6.8188084
H 127	5.8817319	1.3039024	7.4772260
H 128	7.2582920	1.7079075	6.4165166
H 129	-3.6931704	-7.3677014	6.1865203
H 130	5.3365505	8.6095039	-3.0920255
C 131	4.1317408	6.2186828	6.1882527
H 132	-4.9941160	4.3761066	7.0814723
H 133	5.2211478	6.3619159	6.2257101
C 134	-4.2076091	-6.3971673	6.1415994
H 135	-6.3270913	5.0141548	6.0821917
H 136	3.8027413	5.7940893	7.1470956
C 137	-6.8909594	-.9213557	4.6954209
N 138	-5.9219234	-.8373979	4.0605643
H 139	3.6574180	7.2024823	6.0624855
C 140	-3.7775085	-5.6511709	4.9872506
H 141	5.4021860	.8481767	-6.2623710
N 142	4.3068432	5.7907247	-2.1106901
H 143	-3.9350042	-5.8448567	-6.1926126
C 144	5.6444430	7.6042103	-3.4125023
C 145	-4.7116453	4.3163212	-4.0277539
N 146	4.6974375	.9194160	-3.1813774
H 147	5.2869678	-5.2755977	-5.7647063
C 148	4.9043089	6.5986160	-2.6941938
C 149	-5.7418643	-1.6617597	-4.6692320
N 150	-5.1581011	-1.2273571	-3.7644721
N 151	-4.2616129	3.7944201	-3.0921293
C 152	5.0368866	-4.9012434	-3.7178269
N 153	4.5303088	-4.3249321	-2.8448829
H 154	-4.9925610	6.0299097	-5.2007387
H 155	-6.1378398	-3.2620671	-5.9604740
H 156	-8.5526233	-2.0162583	5.3518034
C 157	5.6691451	-5.6202651	-4.7935644
C 158	-6.4595670	-2.2192442	-5.7874890
H 159	5.4715643	-6.6981544	-4.7044255
H 160	-6.2675995	-1.6386940	-6.7002588
H 161	-4.9118200	4.4945804	-6.1056920
N 162	-3.5148522	-4.8546954	-3.2134038
H 163	-7.5414371	-2.2150482	-5.5947208
C 164	5.2496292	1.0996068	-4.1874972
H 165	-8.8235058	-.2642072	5.1689407
C 166	5.9398207	1.3254786	-5.4313622

Heat of Formation: 1196.715 kcal/mol

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

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Sat Oct 21 14:50:38 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 256
167 S shells
89 P shells
Number of basis functions: 434
Number of electrons: 448
Use of molecular symmetry disabled

Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 495 degrees of freedom

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

Cycle no: 189 Heat of formation = 1151.542 rmsG = .0000 rmsD = .0001

Atom		Cartesian Coordinates (Angstroms) X	Y	Z
C	1	4.8486097	-2.9332028	.2835978
N	2	3.4437549	-3.4565277	.2988459
C	3	.7184603	-3.9810565	.3047623
C	4	2.7971622	-3.6829727	-.8924203
C	5	2.7957027	-3.6326338	1.4974593
C	6	1.4304205	-3.8981669	1.5090621
C	7	1.4348697	-3.9533355	-.8988949
H	8	3.3839374	-3.6669303	-1.8752759
H	9	3.3958081	-3.5757760	2.4753938
H	10	.8991408	-4.0285631	2.4716747
H	11	.8974971	-4.1368919	-1.8727199
C	12	-.7497239	-3.9812667	.2928122
H	13	5.4028153	-3.3354175	1.1604409
H	14	5.3778827	-3.3132960	-.6182627
C	15	4.8458576	-1.4311195	.2970754
N	16	-3.4648322	-3.4307254	.2588267
H	17	-4.4161066	1.2660914	-1.8839330
C	18	-1.4681820	-3.8724326	1.4912542
C	19	-2.8293046	-3.5925554	1.4661421
H	20	-4.4447643	-1.2095786	-1.8914591
C	21	-1.4558115	-3.9791573	-.9187388
H	22	-.9444435	-3.9927890	2.4590490
H	23	-3.4353223	-3.5110933	2.4381256
C	24	-4.8567018	-2.8746758	.2300472
H	25	-5.4269761	-3.2618544	1.1033210
C	26	4.8729678	1.3663941	.3205395
C	27	4.9949139	-.7398772	1.5002411
C	28	4.7268706	-.7165472	-.8974389
C	29	4.7392425	.6741952	-.8855605
C	30	5.0086540	.6521794	1.5118562
H	31	5.1136291	-1.2907726	2.4429320
H	32	4.6368356	-1.2505342	-1.8529263
H	33	4.6565355	1.2256153	-1.8317416
H	34	5.1379129	1.1848109	2.4636676
C	35	4.9073780	2.8683446	.3327894
H	36	5.4610519	3.2434154	1.2219289
H	37	5.4548530	3.2512845	-.5566901
N	38	3.5143224	3.4222548	.3439845
C	39	.7986140	3.9785379	.3391471
C	40	2.8864899	3.7031882	-.8465201
C	41	2.8581053	3.5693511	1.5420154
C	42	1.4974580	3.8525267	1.5477184
C	43	1.5260953	3.9887304	-.8592266
H	44	3.5056941	3.7173592	-1.8113763
H	45	3.4470200	3.4729615	2.5230059
H	46	.9596128	3.9621609	2.5090868
H	47	.9995249	4.2158010	-1.8326976
C	48	-.6699243	3.9846845	.3254486
H	49	-5.3573579	3.3205424	1.1217778
C	50	-1.3930934	3.8725470	1.5210468
C	51	-1.3739434	3.9929140	-.8866362
H	52	-3.3345762	3.7268420	-1.8779631
C	53	-2.7566772	3.6055975	1.4909064
H	54	-.8724437	3.9811761	2.4919486
H	55	-.8270239	4.2091676	-1.8508210
C	56	-2.7370570	3.7201697	-.8986761
H	57	-3.3654333	3.5248770	2.4610957
C	58	-4.7931981	2.9272953	.2471927

N	59	-3.3915229	3.4576989	.2814509
H	60	-5.3160588	3.3115929	-.6564743
C	61	-4.7870396	1.4250440	.2463141
C	62	-2.8167494	-3.6949668	-.9244199
H	63	-5.2433391	-1.2127756	2.3567905
H	64	-5.3882929	-3.2433460	-.6750573
C	65	-4.8190659	-1.3727908	.2378660
C	66	-5.0268843	.7213818	1.4270007
C	67	-4.5790620	.7223912	-.9433390
C	68	-4.5950385	-.6679288	-.9475695
C	69	-5.0428324	-.6710005	1.4227983
H	70	-5.2149933	1.2619513	2.3642760
H	71	-3.4177717	-3.6933379	-1.9020752
H	72	-.9165531	-4.1891211	-1.8897418
H	73	1.0463534	6.9085742	-5.5582840
C	74	4.3608669	-5.4327343	-5.6765955
C	75	-5.9800070	-4.9189891	-5.2112419
C	76	4.2183471	-4.7031540	-4.4429393
H	77	5.0247210	-6.2987636	-5.5420107
H	78	4.7835465	-4.7920983	-6.4631196
H	79	-5.6285702	-4.5301440	-6.1772562
N	80	4.0754366	-4.1260903	-3.4449904
H	81	3.3706603	-5.7950399	-6.0081994
H	82	-5.5380404	4.5606404	-6.1603054
H	83	-7.0266445	-4.6122338	-5.0726689
C	84	.0795779	6.4001846	-5.4350953
H	85	-.7059665	7.1657405	-5.3611964
H	86	-5.9423286	-6.0173434	-5.2430060
H	87	-.1102901	5.7908242	-6.3297155
C	88	-5.1617630	-4.4181360	-4.1370780
C	89	.2637764	-5.3323731	-4.3857408
N	90	.0393394	-4.7797828	-3.3879255
C	91	.5614800	-6.0211698	-5.6154323
H	92	1.6454712	-5.9728886	-5.8298854
H	93	.0199242	-5.5651846	-6.4559804
H	94	.2684741	-7.0786457	-5.5465305
C	95	.0912117	5.5756712	-4.2544277
N	96	.0999451	4.9166358	-3.2966159
N	97	-4.5063411	-4.0167848	-3.2653600
C	98	5.3455820	4.5176330	-3.9473701
N	99	4.6430591	4.0830663	-3.1298380
C	100	6.2224972	5.0595840	-4.9531832
H	101	7.2293405	4.6281313	-4.8588006
H	102	6.3019726	6.1510043	-4.8461085
H	103	5.8409900	4.8353043	-5.9591777
C	104	-5.0794793	4.4463804	-4.1183154
N	105	-4.4194053	4.0547997	-3.2456558
C	106	-5.9036370	4.9347868	-5.1937247
H	107	-5.8919744	6.0339076	-5.2182894
H	108	-6.9434341	4.6024763	-5.0628052
C	109	-.0561016	-6.8937126	4.6613369
N	110	-.0393827	-5.9492283	3.9855650
C	111	-.0767287	-8.0671839	5.4970249
H	112	.0055948	-7.7868197	6.5562542
H	113	.7615721	-8.7320865	5.2466712
H	114	-1.0140378	-8.6230630	5.3559487
C	115	.0462974	6.8399782	4.7289451
N	116	.0463316	5.8999215	4.0468531
C	117	.0462833	8.0080084	5.5724843
H	118	.9517432	8.6063387	5.4004401
H	119	.0169761	7.7176990	6.6318169
H	120	-.8298181	8.6360591	5.3592510
C	121	-5.0140387	-4.0936538	4.8205266
N	122	-4.4503952	-3.7378272	3.8686253
C	123	-5.7174018	-4.5385673	5.9958704
H	124	-5.1031014	-4.3834363	6.8939556
H	125	-5.9563966	-5.6089363	5.9180959
H	126	-6.6573925	-3.9814566	6.1162019
C	127	-4.9366058	4.1151719	4.8468177
N	128	-4.3794097	3.7564254	3.8922282
C	129	-5.6319178	4.5638224	6.0255299
H	130	-5.7602945	5.6555256	6.0032912

H 131	-5.0672933	4.2980476	6.9302525
H 132	-6.6263542	4.0991921	6.0863277
C 133	4.9616634	-4.2098999	4.8518184
N 134	4.4043865	-3.8347777	3.9035383
C 135	5.6572482	-4.6785740	6.0225164
H 136	5.1268838	-4.3708531	6.9346620
H 137	6.6759249	-4.2665498	6.0559123
H 138	5.7274153	-5.7757502	6.0138087
C 139	4.9857171	4.0224470	4.9394554
N 140	4.4392955	3.6776251	3.9735433
C 141	5.6678970	4.4535775	6.1322805
H 142	6.7020680	4.0807376	6.1404739
H 143	5.1542845	4.0759461	7.0275800
H 144	5.6950147	5.5514757	6.1833978
C 145	.0534717	.0166705	-.5862543
C 146	.0079766	.0454054	-2.0529316
C 147	-.0841827	.1095289	-4.8464022
C 148	1.1881208	.0868709	-2.8036440
C 149	-1.2208977	.0347942	-2.7276143
C 150	-1.2798303	.0654512	-4.1099442
C 151	1.1549999	.1196868	-4.1899740
H 152	2.1592731	.0939888	-2.2816513
H 153	-2.1566088	.0032190	-2.1438616
H 154	-2.2465671	.0564781	-4.6278904
H 155	2.0920172	.1554158	-4.7587018
O 156	-.2201716	.1380866	-6.1997418
C 157	.1434952	-.0304581	2.2190873
C 158	-1.1251662	.0025237	.1688423
C 159	1.2774176	.0052587	.0918760
C 160	1.3214511	-.0180807	1.4799966
C 161	-1.0797999	-.0203088	1.5567989
H 162	-2.0981695	.0098599	-.3529839
H 163	2.2156407	.0163211	-.4904507
H 164	2.2942307	-.0258809	1.9893468
H 165	-2.0142782	-.0297303	2.1304388
H 166	.1785388	-.0476829	3.3140741
H 167	.6426214	.1829849	-6.5937249

Heat of Formation: 1151.542 kcal/mol

4-PHENYLPHENOL2/1^{4+}, 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Oct 26 18:52:09 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 256
167 S shells
89 P shells
Number of basis functions: 434
Number of electrons: 448
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 495 degrees of freedom

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

Cycle no: 289 Heat of formation = 1151.851 rmsG = .0000 rmsD = .0000

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

C	1	-1.3948202	.1568100	4.2606843
C	2	-.6996355	.1230794	2.9675120
C	3	.6185947	.0565256	.5046970
C	4	-1.4141604	-.0623468	1.7802931
C	5	.6927636	.2746577	2.8972305
C	6	1.3571582	.2428741	1.6808602
C	7	-.7706640	-.0968925	.5505988
H	8	-2.5110355	-.1836054	1.8261260
H	9	1.2585290	.4195195	3.8322399
H	10	2.4502124	.3583933	1.6380630
H	11	-1.3531514	-.2449091	-.3660313
C	12	-4.8471267	.0388511	-1.7387502
C	13	-2.7175629	.2202785	6.7283333
C	14	-.6788208	.3409091	5.4491115
C	15	-2.7846748	.0049493	4.3287838
C	16	-3.4394886	.0365487	5.5529153
C	17	-1.3354144	.3723968	6.6728646
H	18	.4145094	.4606761	5.4078344
H	19	-3.3602305	-.1413207	3.4011605
H	20	-4.5275032	-.0839383	5.5938956
H	21	-.7630855	.5170964	7.5967083
H	22	-3.6592908	3.3569581	1.4034318
H	23	-1.2155654	4.0327209	1.3297367
H	24	-3.2349115	.2447272	7.6946970
H	25	-4.6862560	-1.9483232	-2.5610007
O	26	1.3310396	.0421809	-.6682645
C	27	4.6820250	3.2735549	-.6097214
N	28	3.2247404	3.6180298	-.7025432
C	29	.4538719	3.8427997	-.8058385
C	30	2.5371755	4.0023625	.4201595
C	31	2.5730682	3.4669789	-1.9061230
C	32	1.1919421	3.5833973	-1.9704331
C	33	1.1495523	4.1199622	.3766598
H	34	3.1182598	4.2337531	1.3872016
H	35	3.1807915	3.2508968	-2.8071949
H	36	.6651505	3.4558326	-2.9336503
H	37	.5909412	4.4134789	1.2873894
C	38	-1.0087019	3.7109577	-.8116692
H	39	5.2130306	3.6730679	-1.5052996
H	40	5.1309446	3.7843902	.2706328
C	41	4.8506226	1.7862841	-.5034925
N	42	-3.6768235	2.9561562	-.7410083
H	43	-4.6320272	-1.6510211	1.7522024
C	44	-1.7073112	3.4723948	-2.0029105
C	45	-3.0427537	3.0876231	-1.9527357
H	46	-4.8821636	.8037513	1.5871322
C	47	-1.7219005	3.7243321	.3949765
H	48	-1.2078358	3.5941708	-3.0161609
H	49	-3.6331409	2.8972444	-2.9158102
C	50	-5.0301018	2.3118057	-.6843107
H	51	-5.6122630	2.5902924	-1.5907286
C	52	5.1294092	-.9872658	-.3136968
C	53	5.0879486	1.0254985	-1.6493257
C	54	4.7947515	1.1593685	.7430903
C	55	4.9333766	-.2210236	.8374118
C	56	5.2259775	-.3559946	-1.5544850
H	57	5.1755827	1.5149556	-2.6288959
H	58	4.6503185	1.7540274	1.6546021
H	59	4.8936843	-.7053032	1.8224307
H	60	5.4167695	-.9449080	-2.4611085
C	61	5.2609830	-2.4796267	-.2129821
H	62	5.8545847	-2.8840207	-1.0622992
H	63	5.8111579	-2.7621031	.7117741
N	64	3.9033249	-3.1172137	-.2037466
C	65	1.2351920	-3.8763770	-.2089766
C	66	3.2546854	-3.2995737	.9933666
C	67	3.2988095	-3.4458863	-1.3933258
C	68	1.9621305	-3.8288946	-1.4061855
C	69	1.9192819	-3.6852293	.9993421
H	70	3.8301705	-3.1466141	1.9758245
H	71	3.9178754	-3.4193841	-2.3585073
H	72	1.4571996	-4.0960170	-2.3798036

H	73	1.3906027	-3.8295497	1.9611615
C	74	-.2262963	-4.0243250	-.2218567
H	75	-4.9366377	-3.9520494	-1.1569326
C	76	-.9275128	-4.1126971	-1.4326911
C	77	-.9559635	-3.9859212	.9741251
H	78	-2.9540688	-3.8545593	1.9174450
C	79	-2.3129266	-4.0019706	-1.4431191
H	80	-.3620458	-4.2704530	-2.3979908
H	81	-.4261084	-4.0306281	1.9453359
C	82	-2.3413684	-3.8742195	.9452386
H	83	-2.9091587	-4.0940525	-2.4186689
C	84	-4.4462178	-3.4459123	-.2963231
N	85	-2.9919139	-3.8108509	-.2628495
H	86	-4.9482448	-3.8334644	.6178598
C	87	-4.6031408	-1.9553947	-.3957570
C	88	-3.0581355	3.3400298	.4234108
H	89	-4.9390703	.5104508	-2.7264463
H	90	-5.5980293	2.7129501	.1842518
C	91	-4.8857620	.8203842	-.5824457
C	92	-4.7059367	-1.3419590	-1.6456822
C	93	-4.6780043	-1.1775140	.7611202
C	94	-4.8185758	.2038100	.6682480
H	95	.7230283	-.1429269	-1.3733443
H	96	6.3213543	5.8077684	4.7294137
H	97	-5.0464125	-6.1920698	5.5182829
C	98	.7812710	-6.8833943	4.0824613
C	99	-.8860625	8.8005764	3.4186213
H	100	-6.1648034	-4.8034504	5.5049311
H	101	-6.3024942	5.7052433	4.6254758
C	102	.9026857	-8.0535517	4.9142131
H	103	-1.0070393	8.7080127	4.5068118
H	104	-4.6164084	-4.6930120	6.3842856
C	105	-4.4655252	-4.5923890	4.2968388
N	106	-3.9530140	-4.1908229	3.3343614
N	107	.6837104	-5.9415011	3.4099707
C	108	4.6030137	5.4025442	3.6005444
C	109	5.2649497	6.1060697	4.6686238
C	110	-5.1049528	-5.0946861	5.4854499
H	111	1.7837720	-6.7497346	-6.0796389
H	112	-5.3512597	-6.8579970	-5.4838286
H	113	.0180767	-6.9900949	-6.0814182
C	114	-5.2402334	3.9297102	-6.7721232
H	115	-6.0347016	4.6848843	-6.6870727
C	116	6.6158272	5.8153644	-5.5823794
C	117	-4.8752576	3.4252145	-5.4733732
H	118	6.4114887	6.8930528	-5.5127408
H	119	-4.3591473	4.3967347	-7.2492282
H	120	6.3081276	-4.1722614	-6.5624812
H	121	-5.4662831	4.5706957	5.7190705
N	122	4.8386211	-3.2344245	3.4261347
N	123	-4.7144080	3.6996428	2.7746456
C	124	5.4309396	-3.4976189	4.3906639
N	125	4.0726532	4.8372252	2.7347870
H	126	6.7429379	-5.5978134	-5.5815461
H	127	.0721583	-8.7475940	4.7247065
H	128	.8870355	-7.7738082	5.9766535
H	129	1.8461940	-8.5769319	4.7059441
H	130	-6.9917393	4.0891216	4.9291380
H	131	7.6723936	-4.0852738	-5.4169539
C	132	6.1704607	-3.8268139	5.5817770
H	133	4.7844084	5.8842948	5.6319202
H	134	6.6015829	-4.8349374	5.4997642
C	135	-6.0544757	4.6474242	4.7938140
H	136	5.2204260	7.1914466	4.4989881
H	137	5.5134769	-3.8000710	6.4624580
C	138	-.7139301	7.5024120	2.8178758
N	139	-.5748888	6.4568762	2.3314602
H	140	6.9900128	-3.1106620	5.7364427
C	141	-5.3105598	4.1215972	3.6784477
H	142	.7283971	-5.5953680	-6.9377506
N	143	5.0504035	-3.7100804	-3.6974828
H	144	-5.6017699	3.1181028	-7.4189062

C 145	6.6672252	-4.5009694	-5.5770983
C 146	5.7991891	5.0862026	-4.6463786
N 147	.6187783	-4.8116469	-3.8746852
H 148	-4.8765980	-5.5778933	-6.6321603
C 149	5.7695225	-4.0622662	-4.5397621
C 150	-1.2506929	4.5238071	-5.8063282
N 151	-.9737609	4.0809483	-4.7685723
N 152	5.1430343	4.4991596	-3.8878639
C 153	-4.5565790	-5.1270968	-4.6103373
N 154	-3.9435686	-4.6106028	-3.7687820
H 155	7.6819277	5.6497236	-5.3723074
H 156	-2.6846801	4.8776444	-7.2933137
H 157	-1.7766866	9.2981240	3.0102644
C 158	-5.3224583	-5.7709139	-5.6463165
C 159	-1.6155872	5.0714989	-7.0879592
H 160	-6.3552982	-5.3941202	-5.6518749
H 161	-1.0179646	4.6154245	-7.8895340
H 162	6.4088876	5.4873513	-6.6105604
N 163	-4.5562969	3.0327655	-4.4274085
H 164	-1.4489149	6.1578963	-7.1063487
C 165	.7056018	-5.4432001	-4.8471543
H 166	-.0117770	9.4354628	3.2184900
C 167	.8141900	-6.2327802	-6.0465796

Heat of Formation: 1151.851 kcal/mol

4-PHENYLPHENOL3/1^{4+} , 12 ACETONITRILES

SPARTAN SEMIEMPIRICAL PROGRAM: IBM Release 3.1.7

Calculation started: Thu Oct 26 18:52:09 1995

Run type: Geometry optimization
Model: RHF/PM3
Number of shells: 256
167 S shells
89 P shells
Number of basis functions: 434
Number of electrons: 448
Use of molecular symmetry disabled
Molecular charge: 4
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1
This system has 495 degrees of freedom

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

Cycle no: 289 Heat of formation = 1151.851 rmsG = .0000 rmsD = .0000

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
C 1	-1.3948202	.1568100	4.2606843
C 2	-.6996355	.1230794	2.9675120
C 3	.6185947	.0565256	.5046970
C 4	-1.4141604	-.0623468	1.7802931
C 5	.6927636	.2746577	2.8972305
C 6	1.3571582	.2428741	1.6808602
C 7	-.7706640	-.0968925	.5505988
H 8	-2.5110355	-.1836054	1.8261260
H 9	1.2585290	.4195195	3.8322399
H 10	2.4502124	.3583933	1.6380630
H 11	-1.3531514	-.2449091	-.3660313
C 12	-4.8471267	.0388511	-1.7387502
C 13	-2.7175629	.2202785	6.7283333
C 14	-.6788208	.3409091	5.4491115

C	15	-2.7846748	.0049493	4.3287838
C	16	-3.4394886	.0365487	5.5529153
C	17	-1.3354144	.3723968	6.6728646
H	18	.4145094	.4606761	5.4078344
H	19	-3.3602305	-.1413207	3.4011605
H	20	-4.5275032	-.0839383	5.5938956
H	21	-.7630855	.5170964	7.5967083
H	22	-3.6592908	3.3569581	1.4034318
H	23	-1.2155654	4.0327209	1.3297367
H	24	-3.2349115	.2447272	7.6946970
H	25	-4.6862560	-1.9483232	-2.5610007
O	26	1.3310396	.0421809	-.6682645
C	27	4.6820250	3.2735549	-.6097214
N	28	3.2247404	3.6180298	-.7025432
C	29	.4538719	3.8427997	-.8058385
C	30	2.5371755	4.0023625	.4201595
C	31	2.5730682	3.4669789	-1.9061230
C	32	1.1919421	3.5833973	-1.9704331
C	33	1.1495523	4.1199622	.3766598
H	34	3.1182598	4.2337531	1.3872016
H	35	3.1807915	3.2508968	-2.8071949
H	36	.6651505	3.4558326	-2.9336503
H	37	.5909412	4.4134789	1.2873894
C	38	-1.0087019	3.7109577	-.8116692
H	39	5.2130306	3.6730679	-1.5052996
H	40	5.1309446	3.7843902	.2706328
C	41	4.8506226	1.7862841	-.5034925
N	42	-3.6768235	2.9561562	-.7410083
H	43	-4.6320272	-1.6510211	1.7522024
C	44	-1.7073112	3.4723948	-2.0029105
C	45	-3.0427537	3.0876231	-1.9527357
H	46	-4.8821636	.8037513	1.5871322
C	47	-1.7219005	3.7243321	.3949765
H	48	-1.2078358	3.5941708	-3.0161609
H	49	-3.6331409	2.8972444	-2.9158102
C	50	-5.0301018	2.3118057	-.6843107
H	51	-5.6122630	2.5902924	-1.5907286
C	52	5.1294092	-.9872658	-.3136968
C	53	5.0879486	1.0254985	-1.6493257
C	54	4.7947515	1.1593685	.7430903
C	55	4.9333766	-.2210236	.8374118
C	56	5.2259775	-.3559946	-1.5544850
H	57	5.1755827	1.5149556	-2.6288959
H	58	4.6503185	1.7540274	1.6546021
H	59	4.8936843	-.7053032	1.8224307
H	60	5.4167695	-.9449080	-2.4611085
C	61	5.2609830	-2.4796267	-.2129821
H	62	5.8545847	-2.8840207	-1.0622992
H	63	5.8111579	-2.7621031	.7117741
N	64	3.9033249	-3.1172137	-.2037466
C	65	1.2351920	-3.8763770	-.2089766
C	66	3.2546854	-3.2995737	.9933666
C	67	3.2988095	-3.4458863	-1.3933258
C	68	1.9621305	-3.8288946	-1.4061855
C	69	1.9192819	-3.6852293	.9993421
H	70	3.8301705	-3.1466141	1.9758245
H	71	3.9178754	-3.4193841	-2.3585073
H	72	1.4571996	-4.0960170	-2.3798036
H	73	1.3906027	-3.8295497	1.9611615
C	74	-.2262963	-4.0243250	-.2218567
H	75	-4.9366377	-3.9520494	-1.1569326
C	76	-.9275128	-4.1126971	-1.4326911
C	77	-.9559635	-3.9859212	.9741251
H	78	-2.9540688	-3.8545593	1.9174450
C	79	-2.3129266	-4.0019706	-1.4431191
H	80	-.3620458	-4.2704530	-2.3979908
H	81	-.4261084	-4.0306281	1.9453359
C	82	-2.3413684	-3.8742195	.9452386
H	83	-2.9091587	-4.0940525	-2.4186689
C	84	-4.4462178	-3.4459123	-.2963231
N	85	-2.9919139	-3.8108509	-.2628495
H	86	-4.9482448	-3.8334644	.6178598