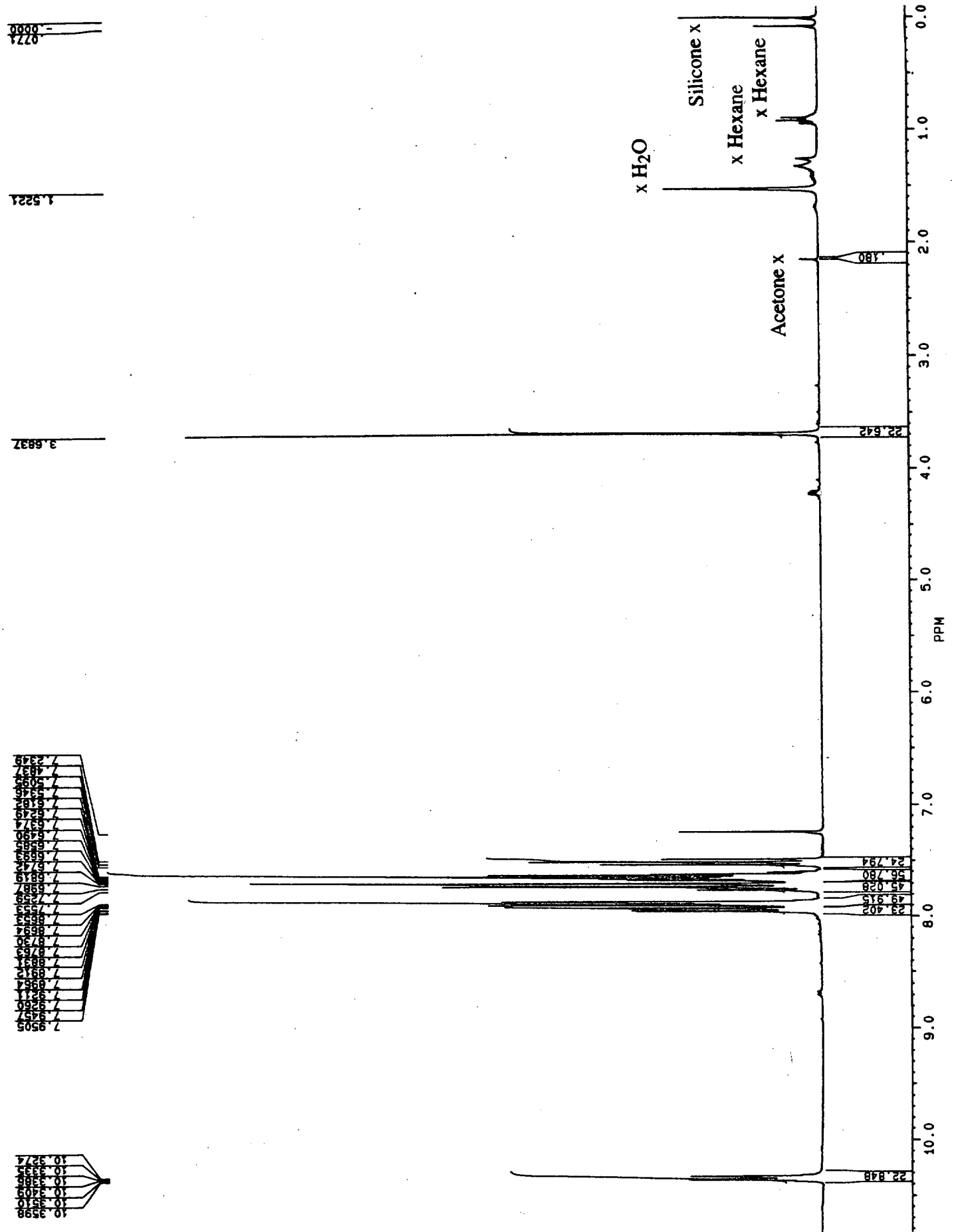
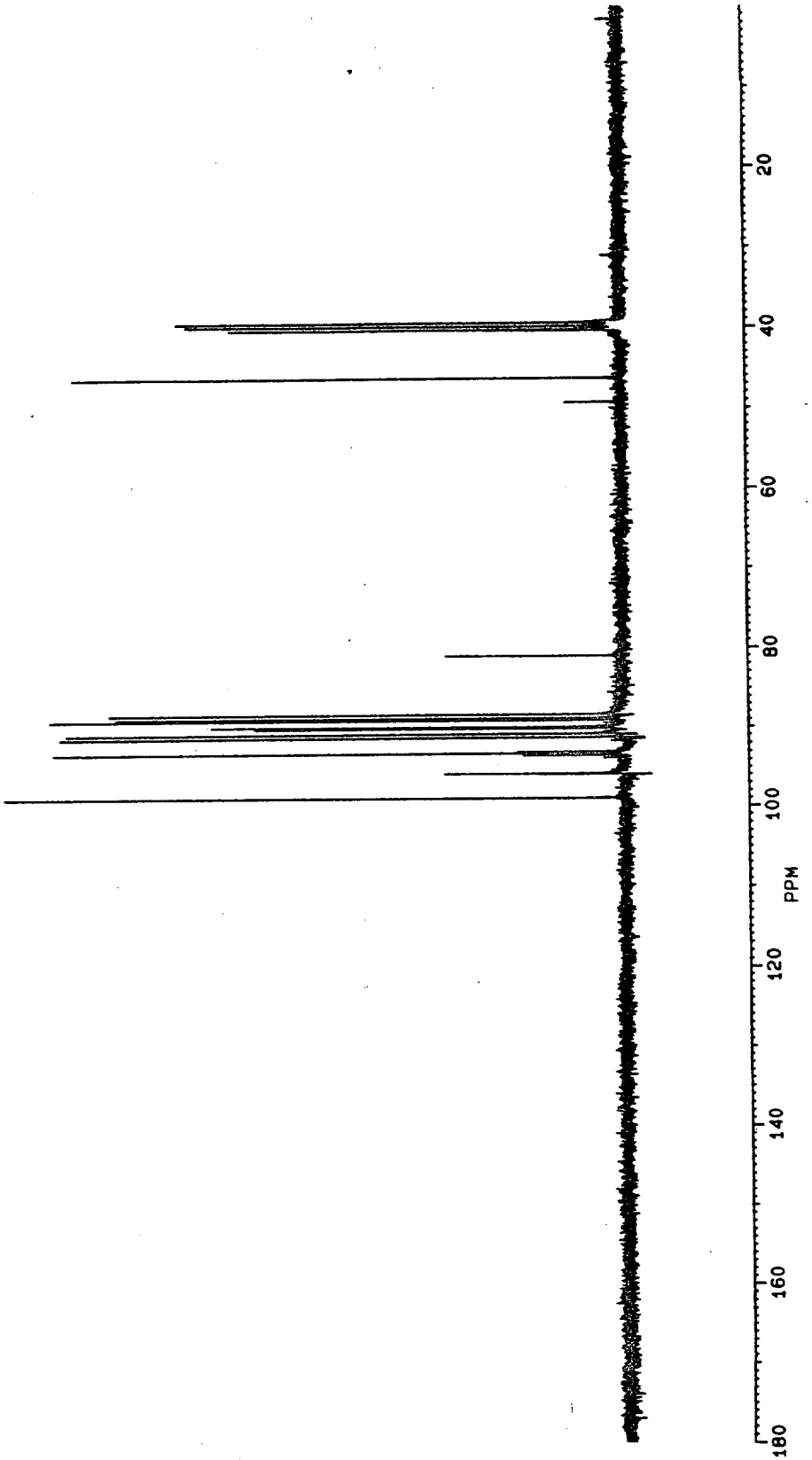
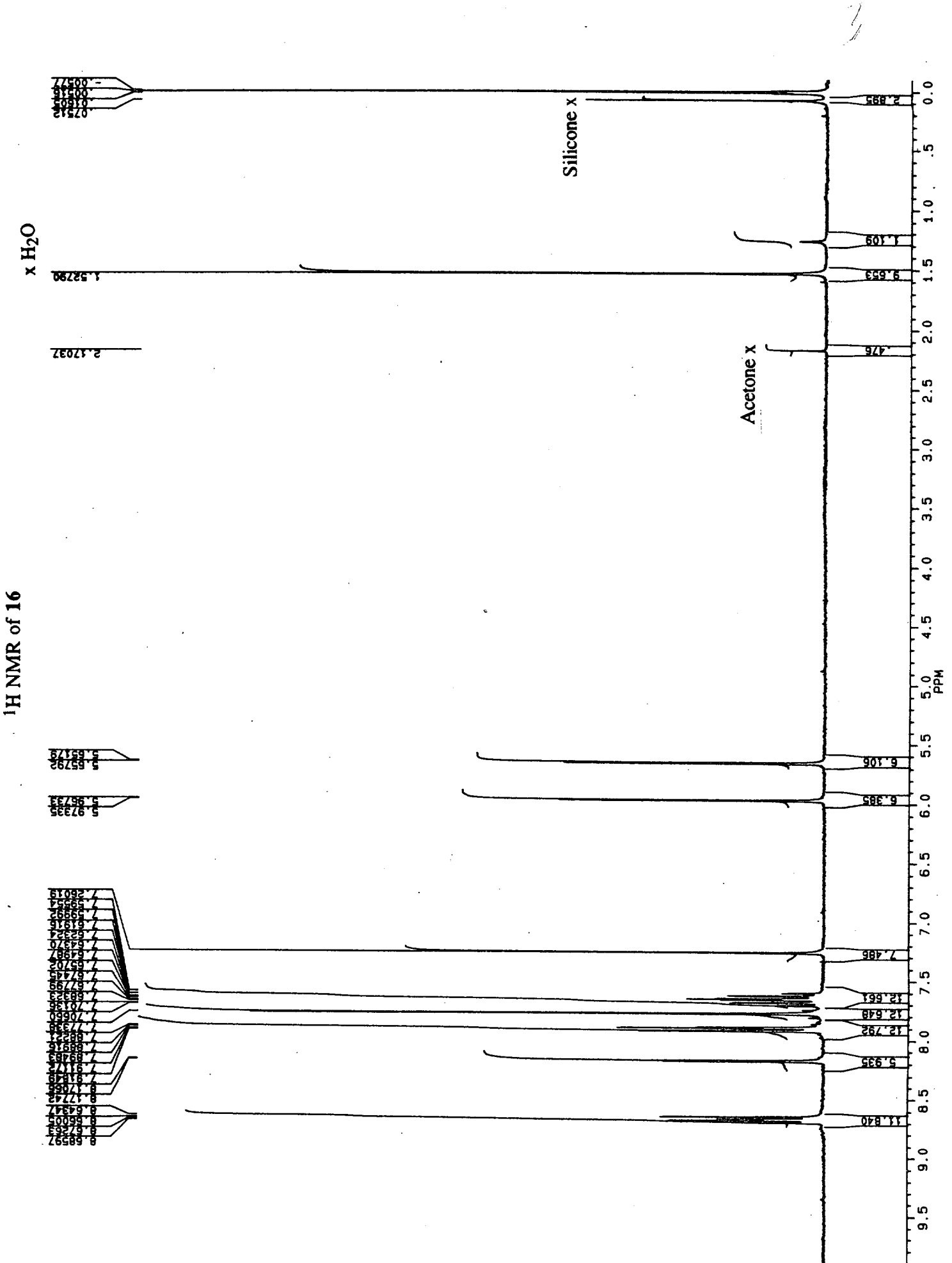
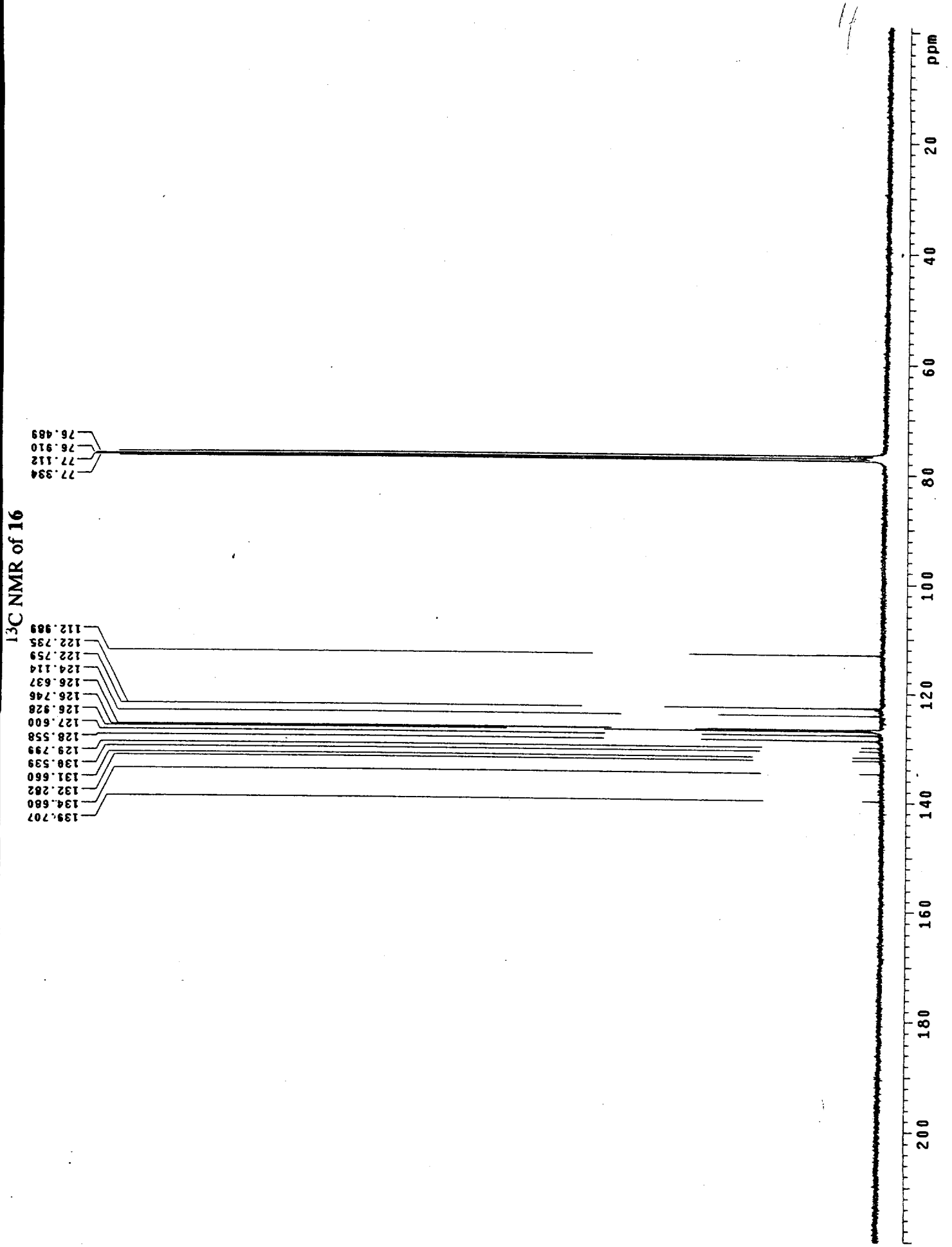
^{1}H NMR of **15**

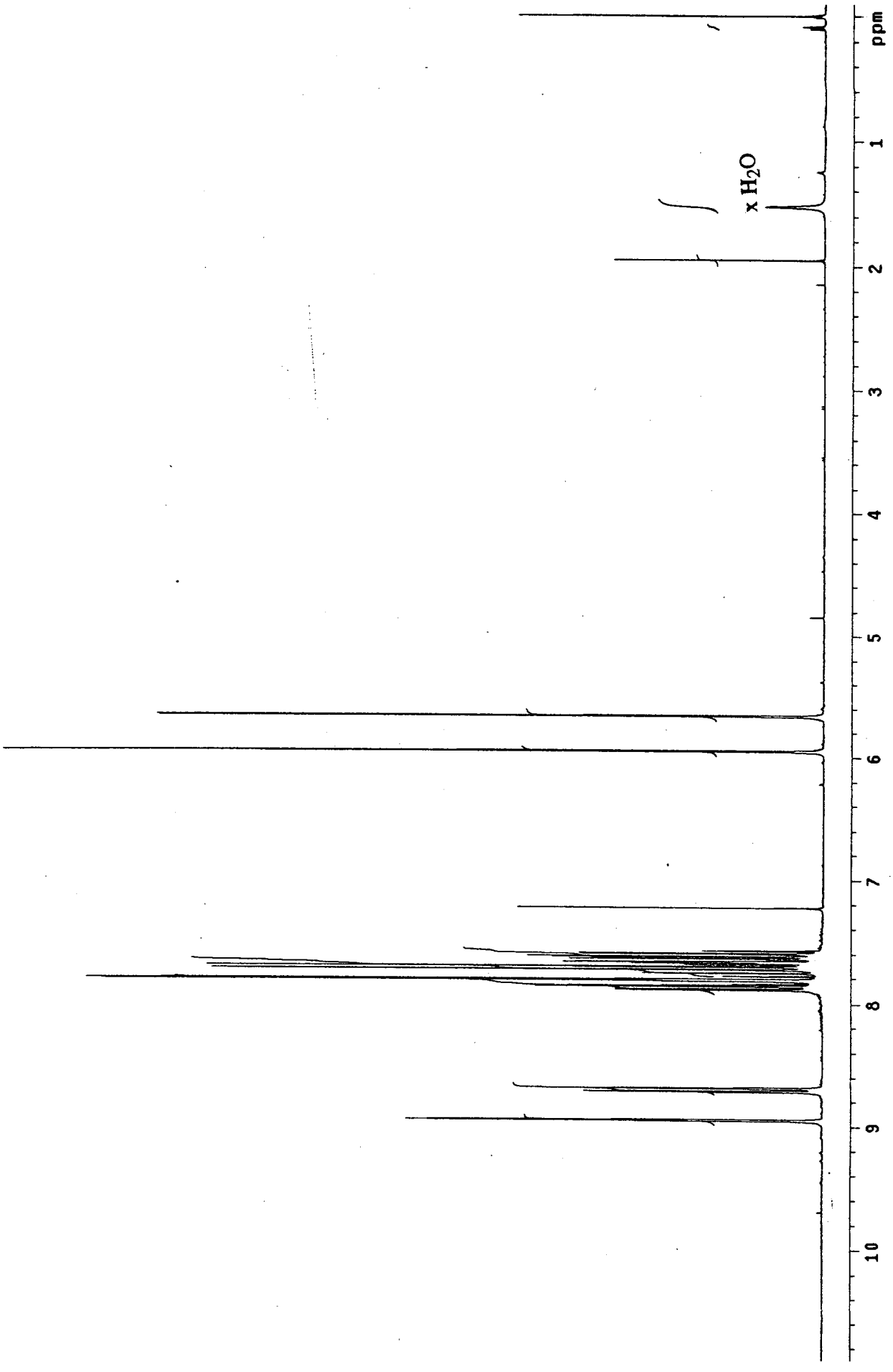


^{13}C NMR of **15**



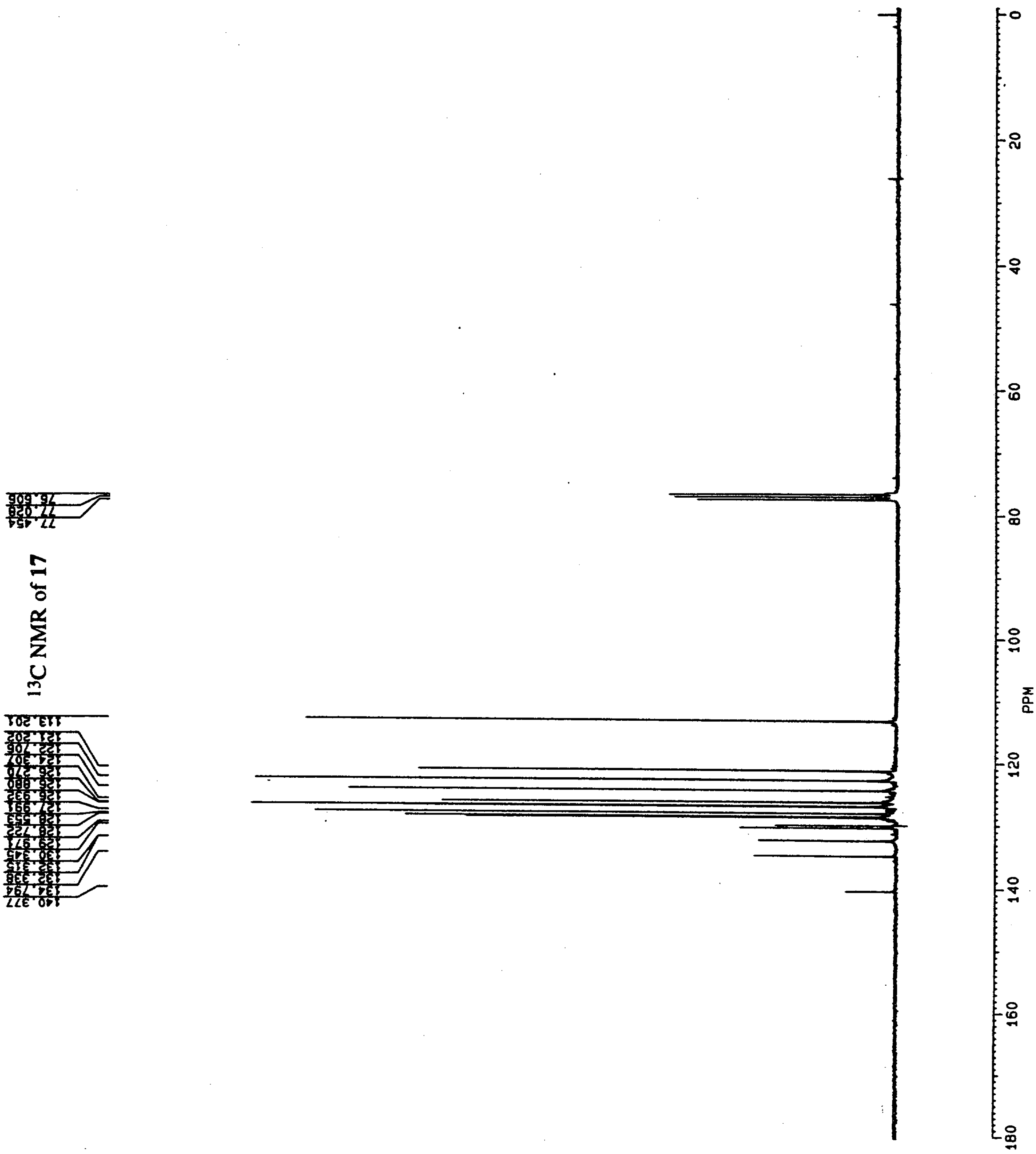

^{1}H NMR of **16**
x H_2O
Silicone x
Acetone x
PPM



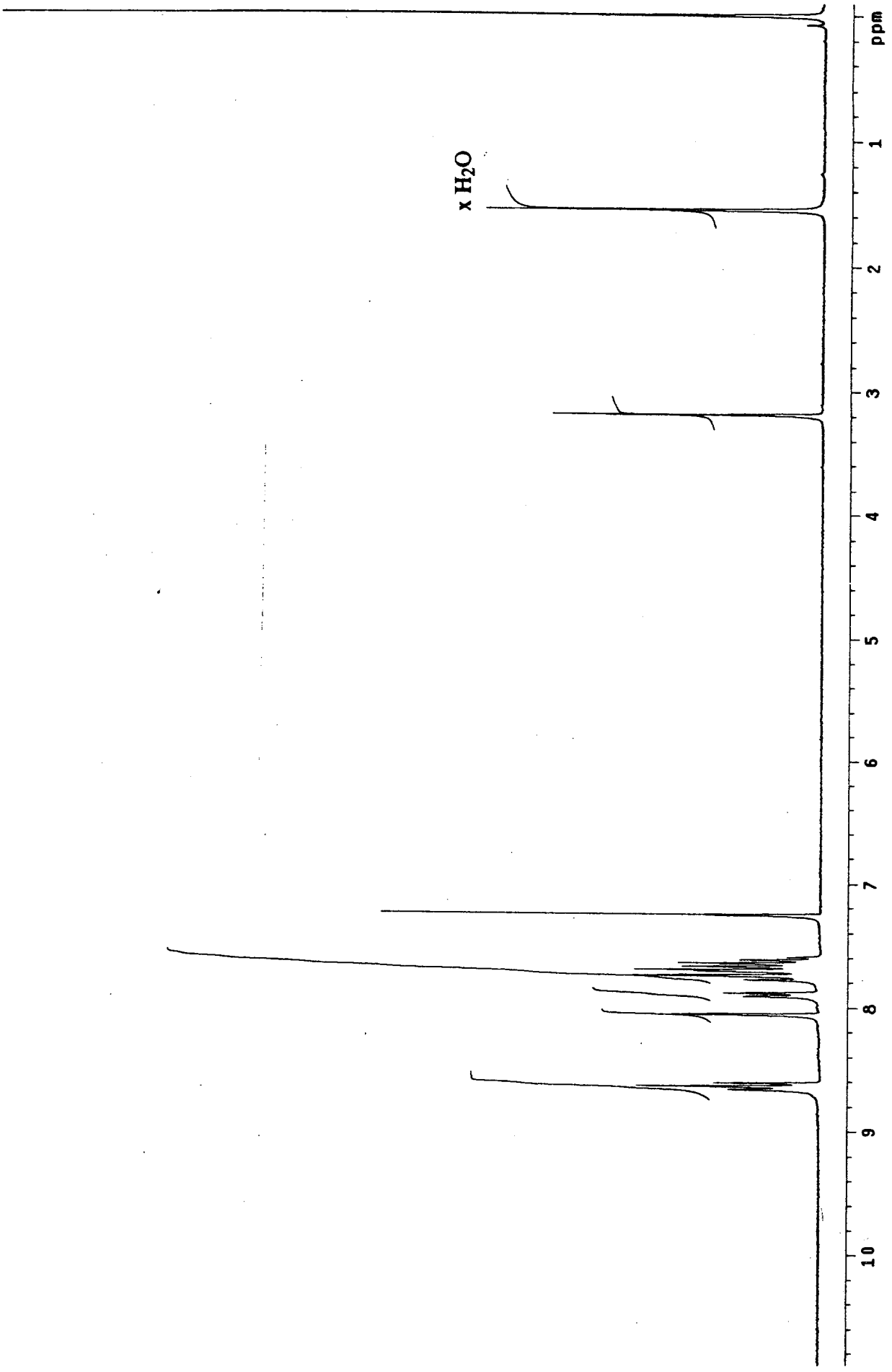


^{1}H NMR of **17**

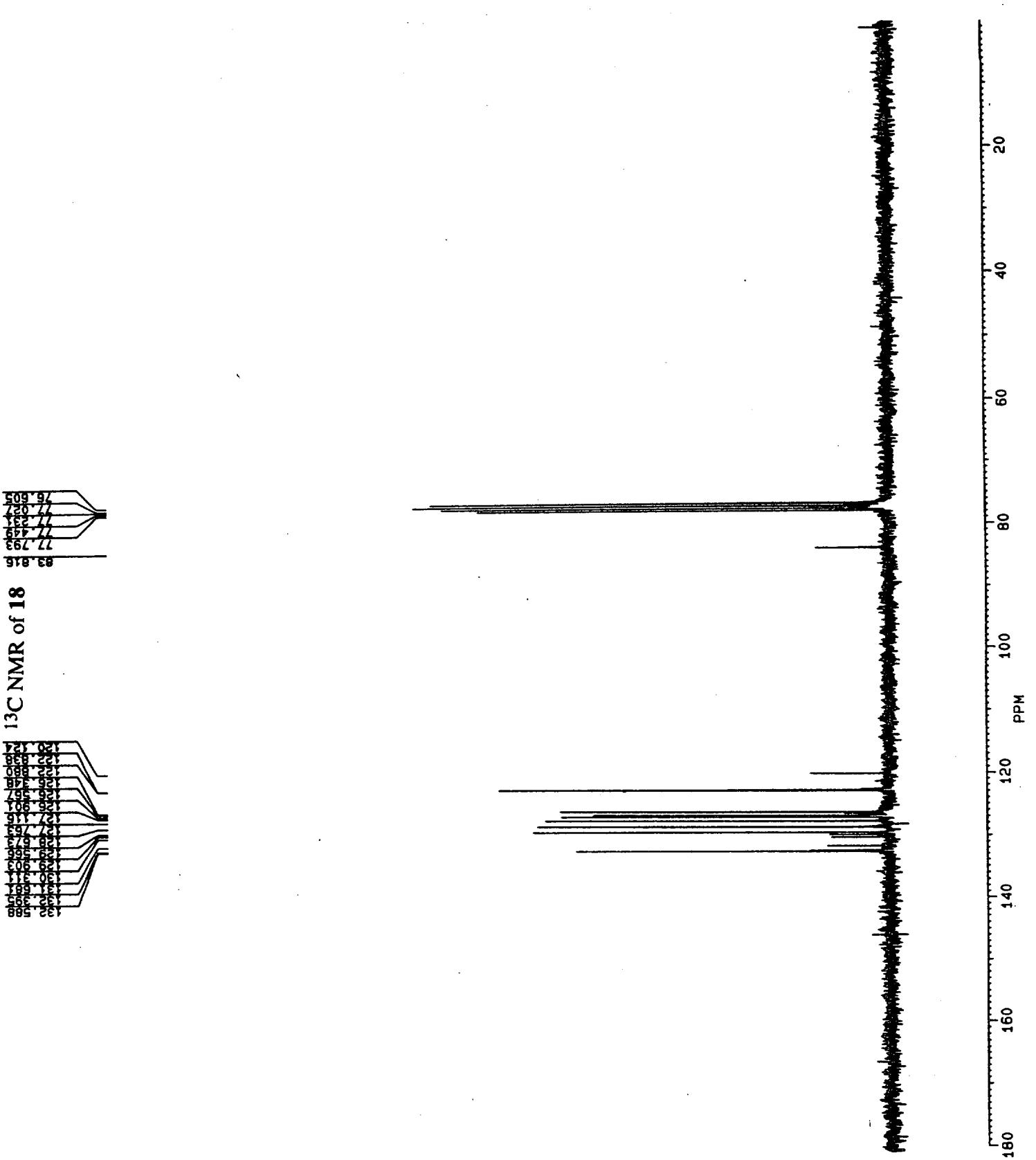
13C NMR of 17

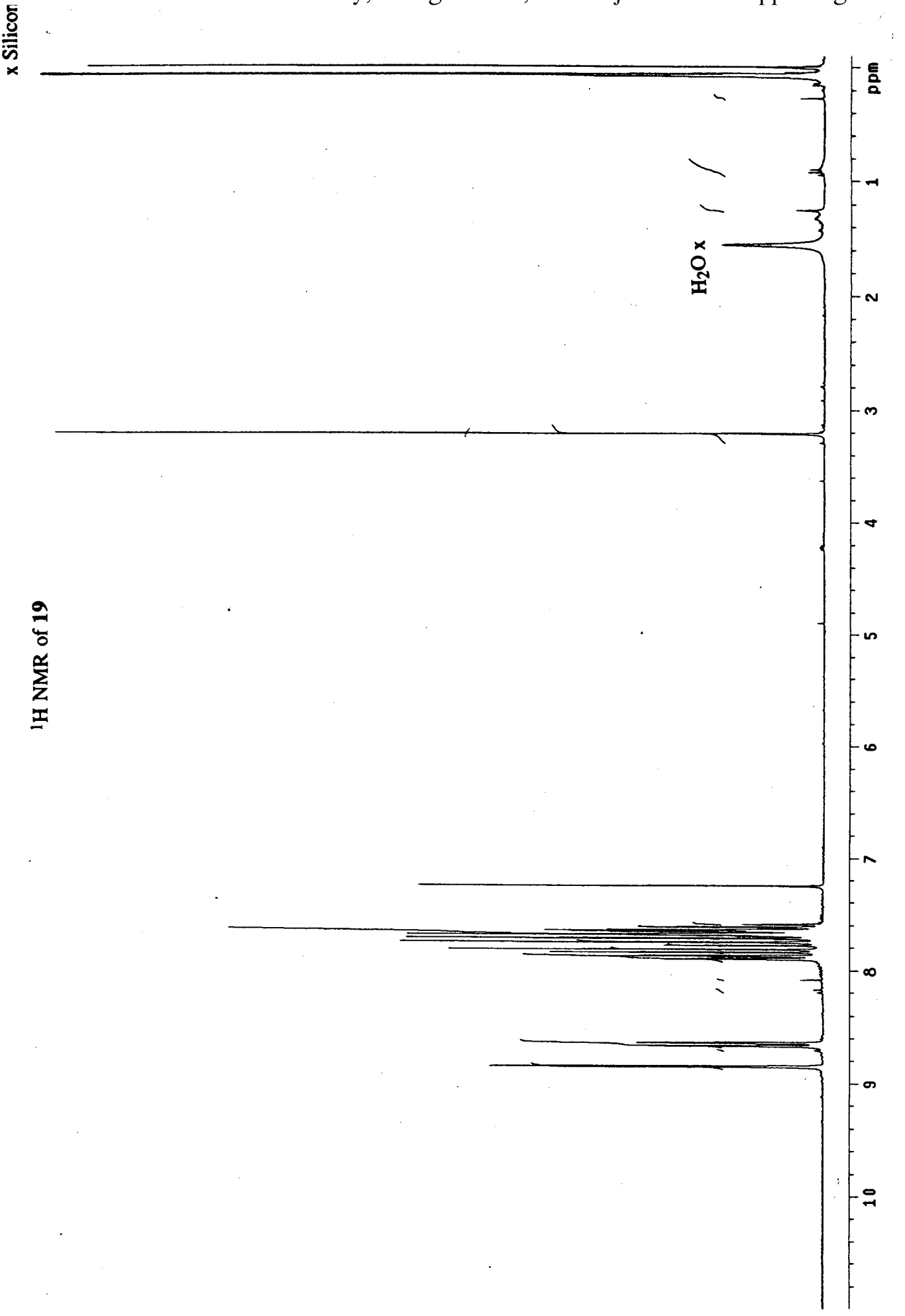


^{1}H NMR of **18**

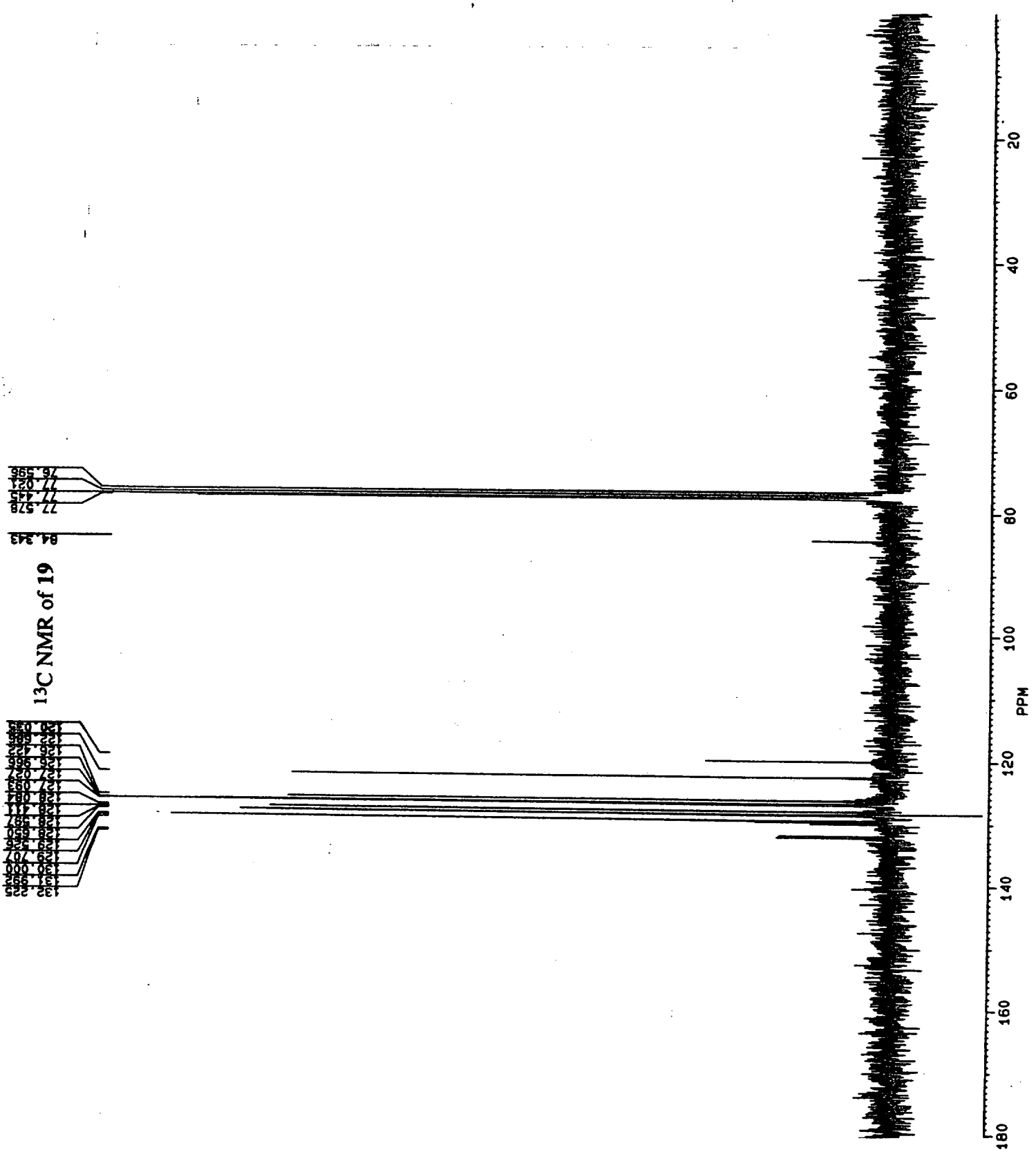


^{13}C NMR of **18**





^{1}H NMR of **19**



SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Mon Jul 20 10:56:35 1998

AM1 PRECISE EF GNORM=0.5
Pyrene (**1**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	67.400954 KCAL
ELECTRONIC ENERGY	=	-13559.781372 EV
CORE-CORE REPULSION	=	11374.528457 EV
GRADIENT NORM	=	35.233166
DIPOLE	=	.00601 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.131498 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	7

COMPUTATION TIME = 1 MINUTES AND 10.080 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
Pyrene (**1**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1279
C	1.3925566	1	.000000	0	.000000	0	1	0	0	-.1132
C	1.4031217	1	119.657666	1	.000000	0	2	1	0	-.0331
C	1.4204238	1	119.415932	1	.000000	1	3	2	1	-.0158
C	1.4396912	1	122.167365	1	-179.928937	1	3	2	1	-.1149
C	1.4189918	1	120.110012	1	.053975	1	4	3	2	-.0331
C	1.4336512	1	120.195193	1	-179.946890	1	4	3	2	-.0152
C	1.3909862	1	121.493846	1	-.097870	1	1	2	3	-.1140
C	1.4389117	1	118.996940	1	179.948309	1	6	4	3	-.1150
C	1.3569747	1	121.407986	1	179.921368	1	5	3	2	-.1143
C	1.4189053	1	120.009586	1	.027441	1	7	4	3	-.0335
C	1.4007508	1	119.257666	1	179.948033	1	11	7	4	-.1136
C	1.4197654	1	120.055927	1	-179.996751	1	7	4	3	-.0336
C	1.3559407	1	121.268348	1	.074382	1	9	6	4	-.1143
C	1.4006201	1	119.312780	1	-179.957843	1	13	7	4	-.1140
C	1.3926996	1	120.361470	1	.000000	1	15	13	7	-.1274
H	1.1014956	1	119.183084	1	179.951414	1	1	2	3	.1312
H	1.0992388	1	120.459746	1	-179.965888	1	2	1	3	.1353
H	1.1001419	1	120.126633	1	-179.927047	1	8	1	2	.1342
H	1.1007544	1	117.575316	1	-.072404	1	5	3	2	.1328
H	1.1009745	1	121.033978	1	-179.995556	1	10	5	3	.1328
H	1.1006391	1	117.589561	1	-179.953271	1	9	6	4	.1331
H	1.1012516	1	121.059550	1	179.973209	1	14	9	6	.1332
H	1.1004732	1	119.558683	1	-179.951481	1	12	11	7	.1336
H	1.0999415	1	119.604607	1	179.979298	1	16	15	13	.1330
H	1.1007110	1	119.516329	1	-179.977984	1	15	13	7	.1337

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Mon Jul 20 11:16:34 1998

AM1 PRECISE EF GNORM=0.05
Fluoranthene (**3**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	87.933023 KCAL
ELECTRONIC ENERGY	=	-13402.844700 EV
CORE-CORE REPULSION	=	11218.482122 EV
GRADIENT NORM	=	81.872298
DIPOLE	=	.23964 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.628851 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	7

COMPUTATION TIME = 1 MINUTES AND 8.600 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.05
Fluoranthene (**3**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.0837
C	1.4251663	1	.000000	0	.000000	0	1	0	0	-.1367
C	1.3780743	1	122.983436	1	.000000	0	2	1	0	-.0993
C	1.4247557	1	120.183748	1	.000000	1	3	2	1	-.0328
C	1.3934039	1	116.011387	1	.000000	1	4	3	2	-.0648
C	1.4245216	1	127.974986	1	179.950406	1	4	3	2	-.0992
C	1.3778321	1	120.139508	1	179.988478	1	6	4	3	-.1366
C	1.4253364	1	122.942474	1	.034888	1	7	6	4	-.0836
C	1.3709040	1	118.631489	1	.031778	1	8	7	6	-.0339
C	1.3700321	1	118.379667	1	.000000	1	1	2	3	-.0349
C	1.4690890	1	136.364909	1	179.964182	1	9	8	7	-.0323
C	1.4469940	1	108.458086	1	179.970838	1	11	9	8	-.0335
C	1.3806053	1	131.486462	1	.000000	1	11	9	8	-.1047
C	1.4056332	1	118.795737	1	179.954224	1	13	11	9	-.1288
C	1.3886449	1	121.086858	1	.088071	1	14	13	11	-.1284
C	1.3804050	1	120.381228	1	-179.994240	1	12	11	9	-.1051
H	1.1003195	1	119.925244	1	179.993668	1	15	14	13	.1319
H	1.0992695	1	120.963356	1	-179.975139	1	16	12	11	.1356
H	1.0993584	1	121.013254	1	.000000	1	13	11	9	.1355
H	1.1003699	1	119.047787	1	179.957363	1	14	13	11	.1317
H	1.0987840	1	119.463753	1	-179.999607	1	1	2	3	.1367
H	1.1012979	1	117.570023	1	-179.998670	1	2	1	3	.1313
H	1.0996725	1	120.775796	1	-179.998820	1	3	2	1	.1340
H	1.0996249	1	119.061043	1	.119507	1	6	4	3	.1340
H	1.1010549	1	119.411513	1	-179.938487	1	7	6	4	.1315
H	1.0989864	1	119.296870	1	179.930706	1	8	7	6	.1362

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Mon Jul 20 11:33:22 1998

AM1 PRECISE EF GNORM=0.5
Acephenanthrylene (**9**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	95.601048 KCAL
ELECTRONIC ENERGY	=	-13405.413892 EV
CORE-CORE REPULSION	=	11221.396833 EV
GRADIENT NORM	=	42.210725
DIPOLE	=	.42108 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.671977 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	5
COMPUTATION TIME =	49.590 SECONDS	

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
Acephenanthrylene (**9**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.0812
C	1.4167976	1	.000000	0	.000000	0	1	0	0	-.1401
C	1.3865491	1	122.600723	1	.000000	0	2	1	0	-.0980
C	1.4187393	1	120.509008	1	.000000	1	3	2	1	-.0192
C	1.3867961	1	115.661839	1	.000000	1	4	3	2	-.0745
C	1.4467130	1	128.403823	1	-179.992566	1	4	3	2	-.0016
C	1.3759501	1	118.401368	1	.000000	1	1	2	3	-.0588
C	1.4517605	1	125.404317	1	-179.999218	1	5	4	3	-.0586
C	1.3554700	1	118.256702	1	.000000	1	8	5	4	-.0571
C	1.4748248	1	105.208200	1	-179.990582	1	8	5	4	-.1221
C	1.4236216	1	119.163084	1	179.986059	1	6	4	3	-.0479
C	1.4133808	1	118.908173	1	179.995380	1	11	6	4	-.1132
C	1.4100890	1	121.764847	1	.000000	1	6	4	3	-.1232
C	1.3821938	1	120.856908	1	-179.999239	1	13	6	4	-.1196
C	1.3814067	1	120.910463	1	.000000	1	12	11	6	-.1322
C	1.3699505	1	109.569204	1	.000000	1	10	8	5	-.1143
H	1.0988036	1	119.695921	1	179.999731	1	1	2	3	.1356
H	1.1006672	1	118.189220	1	179.988141	1	2	1	3	.1316
H	1.0994647	1	119.815065	1	179.977290	1	3	2	1	.1318
H	1.0996959	1	122.638481	1	179.998403	1	9	8	5	.1370
H	1.1003061	1	119.175054	1	.000000	1	13	6	4	.1339
H	1.0999841	1	120.233523	1	-179.988967	1	14	13	6	.1333
H	1.0998656	1	120.351763	1	-179.990606	1	15	12	11	.1337
H	1.1008148	1	118.896583	1	-179.998258	1	12	11	6	.1326
H	1.0890385	1	127.280798	1	-179.998770	1	16	10	8	.1461
H	1.0888260	1	122.986579	1	179.999231	1	10	8	5	.1462

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Thu Jul 23 11:52:47 1998

AM1 PRECISE EF GNORM=0.5
9-Ethynylphenanthrene (**14**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	113.277966	KCAL
ELECTRONIC ENERGY	=	-13188.590532	EV
CORE-CORE REPULSION	=	11005.326993	EV
DIPOLE	=	.25770	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.538422	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	39	

COMPUTATION TIME = 6 MINUTES AND 26.520 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
9-Ethynylphenanthrene (**14**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1140
C	1.3795749	1	.000000	0	.000000	0	1	0	0	-.1282
C	1.4062589	1	119.788636	1	.000000	0	2	1	0	-.1237
C	1.3812407	1	120.425384	1	.001510	1	3	2	1	-.1202
C	1.4143498	1	121.011101	1	.002969	1	4	3	2	-.0136
C	1.4148806	1	118.282130	1	-.001009	1	5	4	3	-.0407
C	1.4456265	1	122.565369	1	-179.998331	1	5	4	3	-.0206
C	1.4313319	1	120.033247	1	179.996218	1	6	5	4	-.0905
C	1.3682837	1	121.210534	1	.003331	1	8	6	5	.0389
C	1.4456707	1	120.169586	1	.008391	1	9	8	6	-.0204
C	1.4136951	1	120.622823	1	-179.995548	1	10	9	8	-.1130
C	1.4147117	1	121.934851	1	.004562	1	7	5	4	-.1200
C	1.3809139	1	121.148268	1	179.996201	1	12	7	5	-.1264
C	1.4053507	1	120.254206	1	-.001140	1	13	12	7	-.1270
H	1.1005951	1	120.547462	1	-179.999219	1	1	2	3	.1343
H	1.0997667	1	119.649493	1	-179.999371	1	2	3	1	.1342
H	1.1002204	1	119.418024	1	179.998594	1	3	2	1	.1332
H	1.0998191	1	118.941699	1	-179.999337	1	4	3	2	.1334
H	1.1014992	1	118.040316	1	179.998800	1	8	6	5	.1405
H	1.1001034	1	120.204367	1	179.999893	1	13	12	7	.1329
H	1.0998026	1	119.942578	1	.000363	1	12	7	5	.1325
H	1.0997796	1	119.701827	1	-179.999330	1	14	13	12	.1341
H	1.1015792	1	120.346088	1	-179.998348	1	11	14	13	.1422
C	1.4103095	1	119.458527	1	-179.998796	1	9	10	7	-.1267
XX	1.0000000	0	90.000000	0	180.000000	0	24	9	10	
C	1.1978654	1	89.303125	1	179.999480	1	24	25	9	-.1963
H	2.2578204	1	89.328341	1	-179.999719	1	24	25	9	.2253

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Mon Jul 20 11:49:42 1998

AM1 PRECISE EF GNORM=0.5
4-Ethynylphenanthrene (**15**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	119.811498 KCAL
ELECTRONIC ENERGY	=	-13279.363064 EV
CORE-CORE REPULSION	=	11096.300450 EV
DIPOLE	=	.16296 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.563437 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	37

COMPUTATION TIME = 9 MINUTES AND 41.160 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
4-Ethynylphenanthrene (**15**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1322
C	1.4035508	1	.000000	0	.000000	0	1	0	0	-.1229
C	1.3790865	1	119.138464	1	.000000	0	2	1	0	-.1235
C	1.4133451	1	120.798226	1	.005344	1	3	2	1	-.0356
C	1.3820649	1	120.603427	1	-.010922	1	1	2	3	-.1173
C	1.4143690	1	121.986379	1	-.007834	1	5	1	2	-.0162
C	1.4535688	1	123.831553	1	-179.979969	1	6	5	1	.0139
C	1.4338551	1	118.717800	1	-179.977031	1	4	3	2	-.1150
C	1.3533531	1	120.329159	1	179.998004	1	8	4	3	-.1203
C	1.4361439	1	120.950875	1	.016941	1	9	8	4	-.0421
C	1.4117573	1	117.649362	1	179.989816	1	10	9	8	-.1097
C	1.4265210	1	125.374642	1	.057313	1	7	6	5	.0345
C	1.3996326	1	120.480684	1	-179.989597	1	12	7	6	-.1072
C	1.4120518	1	125.350263	1	.025788	1	12	7	6	-.1196
C	1.3979088	1	121.553663	1	-.001797	1	13	12	7	-.1325
XX	1.0000000	0	90.000000	0	180.000000	0	14	12	7	
C	1.1992735	1	84.035005	1	179.992489	1	14	16	12	-.2045
H	1.1007084	1	120.445272	1	-179.992961	1	3	2	1	.1321
H	1.0994146	1	120.821902	1	179.997656	1	2	3	1	.1331
H	1.1002951	1	119.515088	1	179.989338	1	1	2	3	.1321
H	1.0980510	1	117.264684	1	179.983199	1	5	1	2	.1474
H	1.1007881	1	118.203278	1	.003623	1	8	4	3	.1345
H	1.1011435	1	121.238448	1	-179.991351	1	9	8	4	.1336
H	1.1017575	1	119.265798	1	-179.998556	1	13	12	7	.1392
H	1.0997223	1	119.898654	1	179.993402	1	15	13	12	.1374
H	1.1009788	1	118.977139	1	.019800	1	11	10	9	.1348
H	2.2590570	1	84.719706	1	179.993317	1	14	16	12	.2260

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Wed Jul 22 13:45:19 1998

AM1 PRECISE EF GNORM=0.5
2-Ethynylphenanthrene (**18**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	112.105877	KCAL
ELECTRONIC ENERGY	=	-13007.306094	EV
CORE-CORE REPULSION	=	10823.987394	EV
DIPOLE	=	.35950	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.697363	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	31	

COMPUTATION TIME = 6 MINUTES AND 12.500 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
2-Ethynylphenanthrene (**18**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1184
C	1.3799664	1	.000000	0	.000000	0	1	0	0	-.1252
C	1.4060077	1	119.818258	1	.000000	0	2	1	0	-.1276
C	1.3812382	1	120.398490	1	.001806	1	3	2	1	-.1171
C	1.4142866	1	120.990494	1	.001540	1	4	3	2	-.0218
C	1.4157815	1	118.334642	1	-.003252	1	5	4	3	-.0338
C	1.4456041	1	122.421093	1	179.997680	1	5	4	3	-.0119
C	1.4351967	1	119.857270	1	-179.995277	1	6	5	4	-.1157
C	1.3569441	1	120.896288	1	.001089	1	8	6	5	-.1148
C	1.4357191	1	120.853649	1	-.005296	1	9	8	6	-.0393
C	1.4112557	1	120.019584	1	-179.995141	1	10	9	8	-.0938
C	1.4142087	1	122.471041	1	-.008534	1	7	5	4	-.1223
C	1.3791110	1	121.290726	1	-179.996542	1	12	7	5	-.1066
C	1.4155336	1	120.455394	1	-.001703	1	13	12	7	.0276
H	1.1005242	1	120.524791	1	179.997477	1	1	2	3	.1335
H	1.0997920	1	119.633642	1	179.998454	1	2	3	1	.1336
H	1.1001578	1	119.442824	1	-179.996872	1	3	2	1	.1330
H	1.0998599	1	119.038282	1	-179.999180	1	4	3	2	.1326
H	1.1008905	1	117.921157	1	-179.999459	1	8	6	5	.1343
H	1.1008911	1	121.198507	1	179.997314	1	9	8	6	.1348
H	1.1001803	1	119.920712	1	.003359	1	12	7	5	.1352
H	1.1004289	1	120.365428	1	179.998552	1	13	12	7	.1403
H	1.1008699	1	120.228719	1	179.999902	1	11	14	13	.1407
C	1.4085060	1	119.900769	1	-179.999924	1	14	13	12	-.1291
XX	1.0000000	0	90.000000	0	180.000000	0	24	14	13	
C	1.1974978	1	90.181672	1	-179.998918	1	24	25	14	-.1931
H	2.2575002	1	90.182295	1	-179.999312	1	24	25	14	.2250

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Thu Jul 23 11:39:14 1998

AM1 PRECISE EF GNORM=0.5
3-Ethynylphenanthrene (**19**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	112.060690	KCAL
ELECTRONIC ENERGY	=	-13050.289137	EV
CORE-CORE REPULSION	=	10866.971512	EV
DIPOLE	=	.33791	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.576642	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	34	

COMPUTATION TIME = 5 MINUTES AND 30.870 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
3-Ethynylphenanthrene (**19**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1172
C	1.3799594	1	.000000	0	.000000	0	1	0	0	-.1267
C	1.4059604	1	119.799480	1	.000000	0	2	1	0	-.1260
C	1.3813525	1	120.411741	1	.001572	1	3	2	1	-.1190
C	1.4141693	1	120.995659	1	.000912	1	4	3	2	-.0178
C	1.4157148	1	118.318051	1	-.002824	1	5	4	3	-.0374
C	1.4466947	1	122.457653	1	179.999989	1	5	4	3	-.0226
C	1.4350420	1	119.881196	1	-179.998216	1	6	5	4	-.1112
C	1.3571846	1	120.891431	1	-.000653	1	8	6	5	-.1193
C	1.4346329	1	120.839922	1	-.002417	1	9	8	6	-.0285
C	1.4132776	1	120.279601	1	-179.996900	1	10	9	8	-.1219
C	1.4120918	1	122.198891	1	-.004453	1	7	5	4	-.0947
C	1.3911500	1	121.114743	1	-179.999468	1	12	7	5	.0268
C	1.4156202	1	119.781765	1	-.000424	1	13	12	7	-.1057
H	1.1005267	1	120.517256	1	179.998897	1	1	2	3	.1332
H	1.0997689	1	119.640688	1	179.999330	1	2	3	1	.1336
H	1.1001909	1	119.438333	1	-179.998622	1	3	2	1	.1332
H	1.0999149	1	118.986283	1	-179.999601	1	4	3	2	.1336
H	1.1009258	1	117.934527	1	179.999396	1	8	6	5	.1341
H	1.1008239	1	121.212041	1	179.998580	1	9	8	6	.1345
H	1.1002232	1	120.142634	1	.000667	1	12	7	5	.1402
H	1.1000450	1	119.369764	1	-179.999720	1	14	13	12	.1409
H	1.1008378	1	120.259140	1	179.999790	1	11	14	13	.1359
C	1.4090319	1	120.516717	1	179.999681	1	13	12	7	-.1295
XX	1.0000000	0	90.000000	0	180.000000	0	24	13	12	
C	1.1975088	1	90.008266	1	-179.999873	1	24	25	13	-.1936
H	2.2575189	1	89.987758	1	-179.999802	1	24	25	13	.2250

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Thu Jul 23 11:58:35 1998

AM1 PRECISE EF GNORM=0.5
4-Ethylidenecarbenephenanthrene (**24**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	178.586793 KCAL
ELECTRONIC ENERGY	=	-13341.790562 EV
CORE-CORE REPULSION	=	11161.359026 EV
GRADIENT NORM	=	161.011497
DIPOLE	=	1.68405 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.649247 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	7

COMPUTATION TIME = 1 MINUTES AND 21.400 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
4-Ethylidenecarbenephenanthrene (**24**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1290
C	1.4049192	1	.000000	0	.000000	0	1	0	0	-.1253
C	1.3788166	1	119.977958	1	.000000	0	2	1	0	-.1196
C	1.4120469	1	120.529480	1	-.547223	1	3	2	1	-.0364
C	1.3835144	1	119.991853	1	-.441016	1	1	2	3	-.1243
C	1.4152664	1	121.550079	1	-1.510935	1	5	1	2	-.0187
C	1.4501537	1	123.374614	1	-178.631042	1	6	5	1	-.0087
C	1.4348506	1	119.482023	1	-173.322736	1	4	3	2	-.1144
C	1.3548115	1	120.432808	1	174.286936	1	8	4	3	-.1181
C	1.4193435	1	118.239121	1	-165.571081	1	7	6	5	-.0347
C	1.4116070	1	120.712301	1	172.489113	1	10	7	6	-.1176
C	1.4233169	1	124.392797	1	14.932741	1	7	6	5	.0131
C	1.3793645	1	120.434137	1	2.403982	1	11	10	7	-.1233
C	1.3931402	1	120.331342	1	-172.202731	1	12	7	6	-.1275
C	1.4543926	1	122.446164	1	11.898075	1	12	7	6	-.4454
H	1.1007008	1	118.135990	1	-3.881622	1	8	4	3	.1351
H	1.1003237	1	121.362493	1	-176.367537	1	9	8	4	.1348
H	1.1006155	1	120.600748	1	-179.023245	1	3	2	1	.1338
H	1.1002036	1	119.576749	1	-179.803802	1	2	1	3	.1330
H	1.0987704	1	119.678508	1	178.205832	1	1	2	3	.1348
H	1.1002136	1	118.244610	1	175.404802	1	5	1	2	.1423
H	1.1012336	1	118.997753	1	-177.601987	1	11	10	7	.1356
H	1.0995421	1	120.794381	1	-178.577514	1	13	11	10	.1371
H	1.1010457	1	119.586625	1	178.222467	1	14	12	7	.1386
C	1.3168917	1	127.873826	1	-137.189338	1	15	12	7	.2002
H	1.1154294	1	114.344047	1	45.221533	1	15	12	7	.2047

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Wed Jul 22 13:58:31 1998

AM1 PRECISE EF GNORM=0.5
1-Ethynylphenanthrene (**25**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	113.141770	KCAL
ELECTRONIC ENERGY	=	-13149.008175	EV
CORE-CORE REPULSION	=	10965.738730	EV
DIPOLE	=	.24488	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.567225	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	36	

COMPUTATION TIME = 6 MINUTES AND 27.670 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
1-Ethynylphenanthrene (**25**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1173
C	1.3798523	1	.000000	0	.000000	0	1	0	0	-.1265
C	1.4060145	1	119.779342	1	.000000	0	2	1	0	-.1273
C	1.3812955	1	120.419951	1	-.003407	1	3	2	1	-.1188
C	1.4144413	1	121.024865	1	-.003615	1	4	3	2	-.0200
C	1.4153417	1	118.245186	1	.003039	1	5	4	3	-.0357
C	1.4469565	1	122.415284	1	-179.998710	1	5	4	3	-.0220
C	1.4343779	1	119.733784	1	-179.995245	1	6	5	4	-.1146
C	1.3571088	1	120.927970	1	.000256	1	8	6	5	-.1147
C	1.4353830	1	121.033362	1	-.003094	1	9	8	6	-.0138
C	1.4236482	1	120.610336	1	179.999648	1	10	9	8	.0354
C	1.4132588	1	121.973115	1	-.005886	1	7	5	4	-.1101
C	1.3812952	1	120.987032	1	179.997779	1	12	7	5	-.1327
C	1.4021206	1	120.546694	1	-.001600	1	13	12	7	-.1031
H	1.1005100	1	120.540118	1	-179.998184	1	1	2	3	.1335
H	1.0997510	1	119.633607	1	-179.998481	1	2	3	1	.1334
H	1.1001533	1	119.413867	1	179.998928	1	3	2	1	.1326
H	1.0997637	1	118.897649	1	179.998851	1	4	3	2	.1317
H	1.1009421	1	117.967971	1	179.999531	1	8	6	5	.1344
H	1.1018620	1	121.073288	1	179.998933	1	9	8	6	.1431
H	1.0999435	1	120.092492	1	-.001519	1	12	7	5	.1343
H	1.1004499	1	120.177933	1	179.999370	1	13	12	7	.1356
H	1.1002863	1	119.796993	1	-179.999906	1	14	13	12	.1406
C	1.4098857	1	120.409351	1	-.002226	1	11	10	9	-.1264
XX	1.0000000	0	90.000000	0	180.000000	0	24	11	14	
C	1.1978344	1	90.787240	1	179.999736	1	24	25	11	-.1968
H	2.2578187	1	90.778852	1	-179.999543	1	24	25	11	.2252

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Thu Jul 23 13:11:34 1998

AM1 PRECISE EF GNORM=0.5
2-ethylidenecarbenephenanthrene (**26**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	173.074130	KCAL
ELECTRONIC ENERGY	=	-13059.138205	EV
CORE-CORE REPULSION	=	10878.463286	EV
DIPOLE	=	1.65796	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.715211	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	34	

COMPUTATION TIME = 6 MINUTES AND 23.540 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
2-ethylidenecarbenephenanthrene (**26**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1172
C	1.3799858	1	.000000	0	.000000	0	1	0	0	-.1262
C	1.4060566	1	119.816632	1	.000000	0	2	1	0	-.1261
C	1.3812478	1	120.405597	1	.000551	1	3	2	1	-.1186
C	1.4143061	1	120.983595	1	.001527	1	4	3	2	-.0186
C	1.4158070	1	118.333780	1	-.000682	1	5	4	3	-.0366
C	1.4453850	1	122.437222	1	-179.998304	1	5	4	3	-.0208
C	1.4351566	1	119.841502	1	-179.999620	1	6	5	4	-.1120
C	1.3570017	1	120.923352	1	-.000890	1	8	6	5	-.1187
C	1.4358004	1	120.840741	1	.002322	1	9	8	6	-.0291
C	1.4113579	1	120.064256	1	-179.999462	1	10	9	8	-.1165
C	1.4142424	1	122.497603	1	-.006499	1	7	5	4	-.1097
C	1.3789627	1	121.240914	1	179.999753	1	12	7	5	-.1309
C	1.4145654	1	120.608935	1	-.015657	1	13	12	7	.0107
C	1.4492794	1	120.252063	1	179.996345	1	14	13	12	-.4393
H	1.1005278	1	120.517601	1	179.998787	1	1	2	3	.1334
H	1.0997930	1	119.626484	1	179.999211	1	2	3	1	.1338
H	1.1001920	1	119.426053	1	-179.998634	1	3	2	1	.1333
H	1.0998568	1	119.038257	1	-179.998464	1	4	3	2	.1326
H	1.1009651	1	117.912526	1	179.999612	1	8	6	5	.1342
H	1.1007694	1	121.210753	1	179.996692	1	9	8	6	.1338
H	1.1003001	1	119.941275	1	-.012525	1	12	7	5	.1358
H	1.1010223	1	120.163285	1	179.966161	1	13	12	7	.1363
H	1.1006626	1	118.832598	1	-.005488	1	11	10	9	.1335
C	1.3181607	1	127.901417	1	2.388968	1	15	14	13	.2091
H	1.1132085	1	115.483128	1	-177.680738	1	15	14	13	.1936

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 13:45:49 1998

AM1 PRECISE EF GNORM=0.5
3-Ethylidenecarbenephenanthrene (**27**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	173.066986 KCAL
ELECTRONIC ENERGY	=	-13116.949924 EV
CORE-CORE REPULSION	=	10936.279031 EV
GRADIENT NORM	=	197.416096
DIPOLE	=	1.51491 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.543460 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	7
COMPUTATION TIME =	1 MINUTES AND	17.010 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
3-Ethylidenecarbenephenanthrene (**27**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1189
C	1.3792783	1	.000000	0	.000000	0	1	0	0	-.1249
C	1.4073873	1	119.198026	1	.000000	0	2	1	0	-.1262
C	1.3825951	1	120.641735	1	.000000	1	3	2	1	-.1174
C	1.4146361	1	121.113974	1	.000000	1	4	3	2	-.0199
C	1.4116679	1	121.062993	1	.000000	1	1	2	3	-.0357
C	1.4474120	1	123.061701	1	179.983769	1	5	4	3	-.0107
C	1.4348248	1	119.805066	1	-179.995796	1	6	1	2	-.1135
C	1.3564630	1	120.819708	1	-179.994448	1	8	6	1	-.1174
C	1.4161657	1	119.224126	1	-179.999704	1	7	5	4	-.0370
C	1.4126982	1	119.826311	1	-179.992186	1	10	7	5	-.1119
C	1.4120270	1	122.383826	1	.037954	1	7	5	4	-.1218
C	1.3907346	1	121.310061	1	179.990823	1	12	7	5	.0103
C	1.3773225	1	120.836075	1	.000000	1	11	10	7	-.1247
C	1.4494808	1	121.007943	1	179.994378	1	13	12	7	-.4386
H	1.1010169	1	120.282724	1	-179.996529	1	1	2	3	.1322
H	1.0995489	1	120.781382	1	179.998979	1	2	1	3	.1352
H	1.1002529	1	119.364958	1	179.976280	1	3	2	1	.1334
H	1.1000102	1	119.029156	1	-179.994066	1	4	3	2	.1335
H	1.1009959	1	117.952514	1	.000000	1	8	6	1	.1343
H	1.1009189	1	121.301797	1	179.988113	1	9	8	6	.1342
H	1.1007206	1	119.803517	1	-.029448	1	12	7	5	.1358
H	1.1000079	1	120.446665	1	-179.996455	1	14	11	10	.1333
H	1.1009565	1	118.882686	1	-179.992657	1	11	10	7	.1354
C	1.3179474	1	128.217610	1	.104569	1	15	13	12	.2069
H	1.1133854	1	115.380996	1	-179.887666	1	15	13	12	.1940

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 13:59:52 1998

AM1 PRECISE EF GNORM=0.5
Cyclobuta[a]phenanthrene (**28**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	152.791315	KCAL
ELECTRONIC ENERGY	=	-13231.888916	EV
CORE-CORE REPULSION	=	11050.338804	EV
DIPOLE	=	.30648	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.063176	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	37	

COMPUTATION TIME = 9 MINUTES AND 53.520 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
Cyclobuta[a]phenanthrene (**28**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1181
C	1.3847360	1	.000000	0	.000000	0	1	0	0	-.1275
C	1.4004946	1	119.662941	1	.000000	0	2	1	0	-.1278
C	1.3862064	1	120.335013	1	.001856	1	3	2	1	-.1204
C	1.4096108	1	121.130234	1	.000825	1	4	3	2	-.0181
C	1.4150726	1	118.196716	1	.004802	1	5	4	3	-.0358
C	1.4556177	1	122.002345	1	-179.996927	1	5	4	3	-.0189
C	1.4426837	1	120.214696	1	179.996528	1	6	5	4	-.1157
C	1.3503996	1	121.090863	1	-.006374	1	8	6	5	-.1102
C	1.4399569	1	120.955911	1	-.003067	1	9	8	6	-.0047
C	1.3634973	1	123.820656	1	179.992155	1	10	9	8	-.0824
C	1.3900941	1	122.078956	1	.008646	1	7	5	4	-.1211
C	1.4227946	1	123.208587	1	-179.996740	1	12	7	5	-.0968
C	1.3562903	1	116.225765	1	.002413	1	13	12	7	-.0863
C	1.5073805	1	149.853561	1	179.996502	1	14	13	12	-.1078
C	1.5070574	1	148.878280	1	.001696	1	11	10	9	-.1068
H	1.1005561	1	120.263741	1	-179.998375	1	1	2	3	.1326
H	1.0996470	1	119.930698	1	-179.999171	1	2	3	1	.1329
H	1.1000925	1	119.699276	1	179.998596	1	3	2	1	.1321
H	1.0998235	1	118.569585	1	179.997884	1	4	3	2	.1318
H	1.1009689	1	117.536011	1	179.999415	1	8	6	5	.1330
H	1.1006662	1	121.643777	1	-179.997599	1	9	8	6	.1350
H	1.1003152	1	120.412290	1	.001415	1	12	7	5	.1322
H	1.0975087	1	119.933365	1	-179.999138	1	13	12	7	.1407
H	1.0788356	1	131.176032	1	.002810	1	16	11	10	.1637
H	1.0787970	1	131.192578	1	.002584	1	15	14	13	.1645

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 14:09:48 1998

AM1 PRECISE EF GNORM=0.5
Cyclobuta[b]phenanthrene (**29**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	146.767722	KCAL
ELECTRONIC ENERGY	=	-13199.576391	EV
CORE-CORE REPULSION	=	11017.765076	EV
DIPOLE	=	.35063	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.226990	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	35	

COMPUTATION TIME = 6 MINUTES AND 19.540 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
Cyclobuta[b]phenanthrene (**29**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1178
C	1.3751726	1	.000000	0	.000000	0	1	0	0	-.1274
C	1.4107085	1	119.757223	1	.000000	0	2	1	0	-.1280
C	1.3766292	1	120.501910	1	.001987	1	3	2	1	-.1187
C	1.4202169	1	121.183413	1	-.000848	1	4	3	2	-.0190
C	1.4180431	1	117.949486	1	.000962	1	5	4	3	-.0367
C	1.4383737	1	122.681898	1	-179.998346	1	5	4	3	-.0167
C	1.4266218	1	119.782042	1	-179.995431	1	6	5	4	-.1174
C	1.3635079	1	120.595591	1	.001688	1	8	6	5	-.1173
C	1.4263563	1	120.950395	1	-.004222	1	9	8	6	-.0338
C	1.4496792	1	118.035895	1	-179.997536	1	10	9	8	-.0905
C	1.4500981	1	120.632452	1	-.008521	1	7	5	4	-.0910
C	1.3428299	1	117.033283	1	-179.997572	1	12	7	5	-.0914
C	1.4729669	1	122.597889	1	-.001278	1	13	12	7	-.0895
C	1.4979971	1	149.418564	1	179.999890	1	13	12	7	-.1050
C	1.4974959	1	88.046055	1	-179.998120	1	14	13	12	-.1043
H	1.1005325	1	120.719710	1	179.999848	1	1	2	3	.1325
H	1.0996752	1	119.455204	1	179.999687	1	2	3	1	.1329
H	1.1001928	1	119.197497	1	-179.998712	1	3	2	1	.1320
H	1.0996232	1	118.895116	1	179.998902	1	4	3	2	.1318
H	1.1006716	1	118.392907	1	-179.999109	1	8	6	5	.1336
H	1.1010363	1	120.771862	1	179.997672	1	9	8	6	.1333
H	1.0968173	1	120.369320	1	.001473	1	12	7	5	.1406
H	1.0977433	1	118.926056	1	-.007297	1	11	10	9	.1409
H	1.0793458	1	131.227151	1	-179.999974	1	16	14	13	.1634
H	1.0793411	1	131.241228	1	-.001784	1	15	13	12	.1632

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 14:30:51 1998

AM1 PRECISE EF GNORM=0.5
Cyclobuta[c]phenanthrene (**30**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	151.707221 KCAL
ELECTRONIC ENERGY	=	-13328.560153 EV
CORE-CORE REPULSION	=	11146.963032 EV
DIPOLE	=	.34632 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.037773 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	37
COMPUTATION TIME =	6 MINUTES AND 30.960 SECONDS	

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
Cyclobuta[c]phenanthrene (**30**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1187
C	1.3855802	1	.000000	0	.000000	0	1	0	0	-.1264
C	1.4013953	1	119.976932	1	.000000	0	2	1	0	-.1288
C	1.3860894	1	120.209484	1	.001938	1	3	2	1	-.1149
C	1.4079085	1	120.726317	1	.002985	1	4	3	2	-.0176
C	1.4131424	1	118.919385	1	.002371	1	5	4	3	-.0341
C	1.4489126	1	121.466085	1	-179.999911	1	5	4	3	.0105
C	1.4421423	1	119.624602	1	179.996188	1	6	5	4	-.1159
C	1.3516187	1	121.356350	1	.000786	1	8	6	5	-.1160
C	1.4440059	1	121.736174	1	.000056	1	9	8	6	-.0357
C	1.3892068	1	120.239122	1	-179.999822	1	10	9	8	-.1191
C	1.3654943	1	125.465110	1	.003951	1	7	5	4	-.0799
C	1.4508623	1	122.538803	1	-179.998834	1	12	7	5	-.0857
C	1.5093196	1	149.285805	1	.001676	1	12	7	5	-.1095
C	1.3571806	1	122.436881	1	-.000096	1	13	12	7	-.0973
C	1.5061106	1	88.585256	1	179.999969	1	13	12	7	-.1077
H	1.1003488	1	120.323961	1	179.999875	1	1	2	3	.1328
H	1.0998064	1	119.776568	1	179.999693	1	2	3	1	.1324
H	1.0998943	1	119.712012	1	179.999702	1	3	2	1	.1319
H	1.1005573	1	120.072055	1	-179.999673	1	4	3	2	.1341
H	1.1011033	1	117.443794	1	-179.998070	1	8	6	5	.1326
H	1.1014932	1	120.988792	1	-179.999474	1	9	8	6	.1317
H	1.0972784	1	123.865162	1	179.999836	1	15	13	12	.1413
H	1.1009629	1	119.365355	1	.000171	1	11	10	9	.1330
H	1.0791231	1	131.499225	1	.000311	1	14	12	7	.1625
H	1.0788664	1	131.224391	1	-179.999814	1	16	13	12	.1646

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Thu Jul 23 12:32:33 1998

AM1 PRECISE EF GNORM=0.5
9-Ethylidenecarbenephenanthrene (**32**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	174.180770	KCAL
ELECTRONIC ENERGY	=	-13274.772204	EV
CORE-CORE REPULSION	=	11094.149609	EV
DIPOLE	=	1.60337	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.537409	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	62	

COMPUTATION TIME = 11 MINUTES AND 43.270 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE EF GNORM=0.5
9-Ethylidenecarbenephenanthrene (**32**)

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1173
C	1.3794811	1	.000000	0	.000000	0	1	0	0	-.1253
C	1.4062466	1	119.788851	1	.000000	0	2	1	0	-.1263
C	1.3812263	1	120.431707	1	-.013368	1	3	2	1	-.1175
C	1.4144727	1	120.997262	1	.002064	1	4	3	2	-.0203
C	1.4458107	1	122.645126	1	-179.989578	1	5	4	3	-.0130
C	1.4142591	1	118.278252	1	.020753	1	5	4	3	-.0329
C	1.4306075	1	119.881189	1	179.948250	1	7	5	4	-.1132
C	1.3668699	1	121.531735	1	-.005100	1	8	7	5	.0189
C	1.4453207	1	120.071739	1	.044176	1	9	8	7	-.0327
C	1.4522310	1	119.628161	1	-179.949104	1	9	8	7	-.4294
C	1.4136115	1	121.290759	1	179.950027	1	10	9	8	-.1256
C	1.4147145	1	121.544265	1	.064274	1	6	5	4	-.1169
C	1.3805823	1	121.253481	1	-179.949733	1	13	6	5	-.1271
C	1.4046603	1	120.081046	1	-.075099	1	14	13	6	-.1179
H	1.1014721	1	117.676971	1	179.996712	1	8	7	5	.1337
H	1.1004651	1	120.566094	1	-179.994137	1	1	2	3	.1336
H	1.0998100	1	119.643120	1	-179.995530	1	2	3	1	.1343
H	1.1002111	1	119.415679	1	179.986469	1	3	2	1	.1335
H	1.0997413	1	118.870227	1	179.990290	1	4	3	2	.1330
H	1.0999603	1	119.931058	1	.032558	1	13	6	5	.1341
H	1.1001078	1	120.317140	1	179.942139	1	14	13	6	.1352
H	1.1000926	1	119.757277	1	-179.935492	1	15	14	13	.1379
H	1.1096335	1	120.972220	1	-.024264	1	12	10	9	.1482
C	1.3184755	1	127.734478	1	-179.973129	1	11	9	8	.1828
H	1.1123168	1	115.361513	1	.057521	1	11	9	8	.1903

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Thu Jul 23 12:14:25 1998

AM1 PRECISE EF GNORM=0.5
1-Ethylidenecarbenephenanthrene (**33**)

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	175.056741	KCAL
ELECTRONIC ENERGY	=	-13240.882780	EV
CORE-CORE REPULSION	=	11060.254806	EV
DIPOLE	=	1.54827	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.586604	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	57	

COMPUTATION TIME = 11 MINUTES AND 41.400 SECONDS

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE EF GNORM=0.5
1-Ethylidenecarbenephenanthrene (**33**)

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1155
C	1.3797982	1	.000000	0	.000000	0	1	0	0	-.1261
C	1.4059965	1	119.750810	1	.000000	0	2	1	0	-.1255
C	1.3813330	1	120.459075	1	-.017218	1	3	2	1	-.1189
C	1.4146975	1	121.031463	1	-.038160	1	4	3	2	-.0186
C	1.4147721	1	118.159060	1	.077222	1	5	4	3	-.0384
C	1.4474193	1	122.461948	1	-179.973872	1	5	4	3	-.0112
C	1.4335968	1	119.580063	1	179.912781	1	6	5	4	-.1039
C	1.3574035	1	120.943993	1	.030439	1	8	6	5	-.1252
C	1.4352933	1	121.392668	1	-.051592	1	9	8	6	-.0346
C	1.4231190	1	121.297465	1	-179.905337	1	10	9	8	.0188
C	1.4129935	1	121.538169	1	.106598	1	7	5	4	-.1202
C	1.3809243	1	120.934843	1	-179.892050	1	12	7	5	-.1232
C	1.4012493	1	120.384494	1	-.039404	1	13	12	7	-.1248
C	1.4516583	1	121.324499	1	.007738	1	11	10	9	-.4295
H	1.1005482	1	120.569801	1	-179.964269	1	1	2	3	.1346
H	1.0997838	1	119.654258	1	-179.983444	1	2	3	1	.1344
H	1.1002541	1	119.416238	1	179.958869	1	3	2	1	.1333
H	1.0997206	1	118.817456	1	179.956142	1	4	3	2	.1327
H	1.1013044	1	118.025657	1	-179.998095	1	8	6	5	.1377
H	1.1090494	1	118.620625	1	179.936651	1	9	8	6	.1466
H	1.0997123	1	120.174227	1	.109720	1	12	7	5	.1347
H	1.1004080	1	120.230672	1	179.959216	1	13	12	7	.1351
H	1.1002932	1	119.425471	1	179.970532	1	14	13	12	.1334
C	1.3185546	1	127.907375	1	-.007261	1	15	11	10	.1839
H	1.1125099	1	115.280300	1	179.944940	1	15	11	10	.1905

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 15:19:12 1998

AM1 PRECISE TS
TS 33->9

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	188.947309 KCAL
ELECTRONIC ENERGY	=	-13326.045788 EV
CORE-CORE REPULSION	=	11146.063518 EV
DIPOLE	=	1.12335 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.680506 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	14.500 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 33 -> 9

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1170
C	1.3804096	1	.000000	0	.000000	0	1	0	0	-.1264
C	1.4058461	1	119.914935	1	.000000	0	2	1	0	-.1253
C	1.3813599	1	120.323575	1	.004170	1	3	2	1	-.1184
C	1.4132275	1	120.955720	1	.019782	1	4	3	2	-.0172
C	1.4188212	1	118.550161	1	-.004684	1	5	4	3	-.0392
C	1.4459793	1	122.006139	1	179.999756	1	5	4	3	-.0103
C	1.4425834	1	120.598540	1	-179.999345	1	6	5	4	-.0888
C	1.3493738	1	119.033312	1	.000659	1	8	6	5	-.2441
C	1.4234233	1	121.871367	1	.000129	1	9	8	6	-.0453
C	1.4226597	1	117.408717	1	179.999897	1	10	9	8	-.0282
C	1.4153982	1	124.705245	1	-.000088	1	7	5	4	-.1133
C	1.3829914	1	120.809388	1	-179.999934	1	12	7	5	-.1270
C	1.4095699	1	121.509119	1	-.000498	1	13	12	7	-.1071
C	1.4625611	1	112.715303	1	-.002305	1	11	10	9	-.2270
H	1.1006460	1	120.420411	1	179.997897	1	1	2	3	.1336
H	1.0998728	1	119.605286	1	179.989889	1	2	3	1	.1340
H	1.1001395	1	119.466766	1	-179.999798	1	3	2	1	.1334
H	1.1001336	1	119.427597	1	-179.999923	1	4	3	2	.1330
H	1.0996622	1	118.212248	1	-179.999876	1	8	6	5	.1383
H	1.4504232	1	111.721556	1	-179.998998	1	9	8	6	.3235
H	1.0999030	1	119.791868	1	.000035	1	12	7	5	.1343
H	1.1007385	1	119.753006	1	179.978954	1	13	12	7	.1340
H	1.0990785	1	119.977253	1	-179.985900	1	14	13	12	.1376
C	1.3228961	1	117.931794	1	.015000	1	15	11	10	-.0454
H	1.0989478	1	119.269897	1	179.989765	1	15	11	10	.1783

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 11:13:06 1998

AM1 PRECISE TS
TS 14->32

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	191.892211 KCAL
ELECTRONIC ENERGY	=	-13194.323114 EV
CORE-CORE REPULSION	=	11014.511908 EV
DIPOLE	=	2.43077 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.619883 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	16

COMPUTATION TIME = 2 MINUTES AND 8.800 SECONDS

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 14->32

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1177
C	1.3794811	1	.000000	0	.000000	0	1	0	0	-.1248
C	1.4062466	1	119.788851	1	.000000	0	2	1	0	-.1255
C	1.3812263	1	120.431707	1	-.013368	1	3	2	1	-.1172
C	1.4144727	1	120.997262	1	.002064	1	4	3	2	-.0183
C	1.4458107	1	122.645126	1	-179.989578	1	5	4	3	-.0145
C	1.4142591	1	118.278252	1	.020753	1	5	4	3	-.0321
C	1.4306075	1	119.881189	1	179.948250	1	7	5	4	-.1207
C	1.3668699	1	121.531735	1	-.005100	1	8	7	5	.0204
C	1.4453207	1	120.071739	1	.044176	1	9	8	7	-.0180
C	1.4522310	1	119.628161	1	-179.949104	1	9	8	7	-.2819
C	1.4136115	1	121.290759	1	179.950027	1	10	9	8	-.1118
C	1.4147145	1	121.544265	1	.064274	1	6	5	4	-.1222
C	1.3805823	1	121.253481	1	-179.949733	1	13	6	5	-.1226
C	1.4046603	1	120.081046	1	-.075099	1	14	13	6	-.1277
H	1.1014721	1	117.676971	1	179.996712	1	8	7	5	.1292
H	1.1004651	1	120.566094	1	-179.994137	1	1	2	3	.1329
H	1.0998100	1	119.643120	1	-179.995530	1	2	3	1	.1347
H	1.1002111	1	119.415679	1	179.986469	1	3	2	1	.1341
H	1.0997413	1	118.870227	1	179.990290	1	4	3	2	.1340
H	1.0999603	1	119.931058	1	.032558	1	13	6	5	.1335
H	1.1001078	1	120.317140	1	179.942139	1	14	13	6	.1342
H	1.1000926	1	119.757277	1	-179.935492	1	15	14	13	.1369
H	1.0996335	1	120.972220	1	-.024264	1	12	10	9	.1440
C	1.2702253	1	167.804214	1	-179.973129	1	11	9	8	.0016
H	1.3839856	1	60.995578	1	-179.942479	1	11	25	9	.2195

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 10:38:51 1998

AM1 PRECISE TS
TS 24->1

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	189.103396 KCAL
ELECTRONIC ENERGY	=	-13424.790472 EV
CORE-CORE REPULSION	=	11244.814971 EV
DIPOLE	=	.98825 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.526055 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	16.370 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 24->1

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1215
C	1.4015478	1	.000000	0	.000000	0	1	0	0	-.1251
C	1.3806278	1	119.009630	1	.000000	0	2	1	0	-.1200
C	1.4107946	1	120.808017	1	.000055	1	3	2	1	-.0363
C	1.3833839	1	120.317090	1	-.000006	1	1	2	3	-.2381
C	1.4043577	1	122.818035	1	-.000005	1	5	1	2	.0008
C	1.4520985	1	125.342721	1	179.999700	1	6	5	1	-.0053
C	1.4348886	1	118.297288	1	-179.999940	1	4	3	2	-.1163
C	1.3526682	1	120.588819	1	179.999786	1	8	4	3	-.1177
C	1.4358401	1	120.700033	1	.000025	1	9	8	4	-.0340
C	1.4100862	1	118.044640	1	-179.999863	1	10	9	8	-.1168
C	1.4214704	1	124.270653	1	.000016	1	7	6	5	-.0153
C	1.3804608	1	120.522547	1	-179.999900	1	11	10	9	-.1257
C	1.3970785	1	119.236423	1	.000009	1	13	11	10	-.1193
C	1.4486506	1	123.504737	1	.000003	1	12	7	6	-.2489
H	1.1010534	1	118.028235	1	-.000005	1	8	4	3	.1346
H	1.1010408	1	121.354230	1	-179.999973	1	9	8	4	.1346
H	1.1009518	1	120.316889	1	-179.999100	1	3	2	1	.1338
H	1.0994604	1	120.907759	1	179.999900	1	2	3	1	.1360
H	1.1012213	1	119.111802	1	179.997632	1	1	2	3	.1356
H	1.3540053	1	99.573644	1	179.999963	1	5	1	2	.3202
H	1.1007657	1	119.038831	1	.000077	1	11	10	9	.1347
H	1.0997610	1	120.802044	1	-179.999986	1	13	11	10	.1362
H	1.1014440	1	119.003196	1	179.999743	1	14	13	11	.1324
C	1.3102090	1	129.777807	1	.000904	1	15	12	7	-.0352
H	1.1128576	1	115.298793	1	179.999963	1	15	12	7	.1767

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 11:40:02 1998

AM1 PRECISE TS
TS 26->18

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	190.699318 KCAL
ELECTRONIC ENERGY	=	-13013.640587 EV
CORE-CORE REPULSION	=	10833.764644 EV
DIPOLE	=	2.72156 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.804942 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	8
COMPUTATION TIME =	55.970 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 26->18

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1171
C	1.3799858	1	.000000	0	.000000	0	1	0	0	-.1253
C	1.4060566	1	119.816632	1	.000000	0	2	1	0	-.1255
C	1.3812478	1	120.405597	1	.000551	1	3	2	1	-.1181
C	1.4143061	1	120.983595	1	.001527	1	4	3	2	-.0194
C	1.4158070	1	118.333780	1	-.000682	1	5	4	3	-.0364
C	1.4453850	1	122.437222	1	-179.998304	1	5	4	3	-.0186
C	1.4351566	1	119.841502	1	-179.999620	1	6	5	4	-.1103
C	1.3570017	1	120.923352	1	-.000890	1	8	6	5	-.1198
C	1.4358004	1	120.840741	1	.002322	1	9	8	6	-.0280
C	1.4113579	1	120.064256	1	-179.999462	1	10	9	8	-.1202
C	1.4142424	1	122.497603	1	-.006499	1	7	5	4	-.1116
C	1.3789627	1	121.240914	1	179.999753	1	12	7	5	-.1099
C	1.4145654	1	120.608935	1	-.015657	1	13	12	7	.0050
C	1.4492794	1	120.252063	1	179.996345	1	14	13	12	-.2837
H	1.1005278	1	120.517601	1	179.998787	1	1	2	3	.1339
H	1.0997930	1	119.626484	1	179.999211	1	2	3	1	.1344
H	1.1001920	1	119.426053	1	-179.998634	1	3	2	1	.1339
H	1.0998568	1	119.038257	1	-179.998464	1	4	3	2	.1329
H	1.1009651	1	117.912526	1	179.999612	1	8	6	5	.1349
H	1.1007694	1	121.210753	1	179.996692	1	9	8	6	.1337
H	1.1003001	1	119.941275	1	-.012525	1	12	7	5	.1377
H	1.1010223	1	120.163285	1	179.966161	1	13	12	7	.1435
H	1.1006626	1	118.832598	1	-.005488	1	11	10	9	.1303
C	1.2700476	1	167.340711	1	2.388968	1	15	14	13	.0038
H	1.3851735	1	60.878185	1	179.680738	1	15	25	14	.2198

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 15:38:51 1998

AM1 PRECISE TS
TS 26->28

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	222.348196 KCAL
ELECTRONIC ENERGY	=	-13157.331279 EV
CORE-CORE REPULSION	=	10978.797380 EV
DIPOLE	=	.84263 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.538050 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	16.200 SECONDS	

FINAL GEOMETRY OBTAINED

AM1 PRECISE TS
TS 26->28

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1175
C	1.3816764	1	.000000	0	.000000	0	1	0	0	-.1265
C	1.4039274	1	119.741147	1	.000000	0	2	1	0	-.1267
C	1.3830132	1	120.375794	1	.000342	1	3	2	1	-.1192
C	1.4126728	1	121.071209	1	.000185	1	4	3	2	-.0189
C	1.4156927	1	118.252100	1	.016425	1	5	4	3	-.0363
C	1.4494996	1	122.251493	1	-179.999345	1	5	4	3	-.0186
C	1.4384104	1	120.152754	1	-179.984532	1	6	5	4	-.1129
C	1.3543602	1	120.981679	1	.006532	1	8	6	5	-.1117
C	1.4356309	1	120.670100	1	.000345	1	9	8	6	-.0081
C	1.3767976	1	123.246493	1	179.998532	1	10	9	8	-.2418
C	1.4074371	1	122.296801	1	.000234	1	7	5	4	-.1198
C	1.3974888	1	122.759731	1	-179.999964	1	12	7	5	-.1114
C	1.3864303	1	117.666919	1	.000021	1	13	12	7	-.0544
C	1.4794535	1	138.040060	1	-179.496532	1	14	13	12	-.1936
H	1.1005897	1	120.403197	1	-179.996432	1	1	2	3	.1333
H	1.0997390	1	119.751655	1	179.999986	1	2	3	1	.1337
H	1.1001660	1	119.534364	1	-179.999991	1	3	2	1	.1329
H	1.0998295	1	118.809178	1	-179.998432	1	4	3	2	.1324
H	1.1009723	1	117.764667	1	179.996422	1	8	6	5	.1343
H	1.1004577	1	121.605345	1	179.896433	1	9	8	6	.1341
H	1.1006177	1	119.665171	1	.034453	1	12	7	5	.1326
H	1.0984003	1	120.555280	1	179.998743	1	13	12	7	.1403
H	1.6155583	1	125.911956	1	.000332	1	11	10	9	.3086
C	1.3386400	1	102.839467	1	179.995422	1	15	14	13	-.0427
H	1.0867236	1	126.151439	1	.000223	1	15	14	13	.1778

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 15:45:46 1998

AM1 PRECISE TS
TS 26->29

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	219.819602 KCAL
ELECTRONIC ENERGY	=	-13136.671666 EV
CORE-CORE REPULSION	=	10958.028119 EV
DIPOLE	=	.83373 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.604609 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	16.200 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 26->29

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1176
C	1.3777833	1	.000000	0	.000000	0	1	0	0	-.1262
C	1.4081553	1	119.777656	1	.000000	0	2	1	0	-.1270
C	1.3791131	1	120.449292	1	.000123	1	3	2	1	-.1186
C	1.4170922	1	121.089379	1	.000423	1	4	3	2	-.0201
C	1.4165246	1	118.133218	1	.002638	1	5	4	3	-.0355
C	1.4423592	1	122.515384	1	-179.998532	1	5	4	3	-.0180
C	1.4312721	1	119.789786	1	-179.989642	1	6	5	4	-.1156
C	1.3594863	1	120.751991	1	.002347	1	8	6	5	-.1176
C	1.4323311	1	121.031199	1	.006322	1	9	8	6	-.0335
C	1.4308703	1	118.700191	1	179.996722	1	10	9	8	-.1033
C	1.4360799	1	121.289827	1	.000334	1	7	5	4	-.0926
C	1.3493252	1	117.365154	1	-179.989532	1	12	7	5	-.2538
C	1.4345192	1	123.814135	1	.000726	1	13	12	7	-.0537
C	1.4769602	1	101.276717	1	-179.993839	1	14	13	12	-.1958
H	1.1005442	1	120.611118	1	-179.993839	1	1	2	3	.1333
H	1.0997461	1	119.556417	1	179.999934	1	2	3	1	.1336
H	1.1001989	1	119.324596	1	-179.993730	1	3	2	1	.1328
H	1.0996995	1	118.933444	1	-179.999938	1	4	3	2	.1317
H	1.1008333	1	118.136826	1	179.993389	1	8	6	5	.1342
H	1.1010324	1	120.953369	1	179.994849	1	9	8	6	.1338
H	1.0973978	1	120.651025	1	.011937	1	12	7	5	.1414
H	1.5957720	1	125.840992	1	179.993394	1	13	12	7	.3108
H	1.0986409	1	119.320438	1	.000009	1	11	10	9	.1411
C	1.3388931	1	103.027568	1	.000067	1	15	14	13	-.0410
H	1.0869599	1	126.163194	1	179.993967	1	15	14	13	.1774

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 11:46:32 1998

AM1 PRECISE TS
TS 27->19

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	190.670341 KCAL
ELECTRONIC ENERGY	=	-13054.154415 EV
CORE-CORE REPULSION	=	10874.281552 EV
DIPOLE	=	2.53269 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.629311 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	8
COMPUTATION TIME =	54.920 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 27->19

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1188
C	1.3792783	1	.000000	0	.000000	0	1	0	0	-.1242
C	1.4073873	1	119.198026	1	.000000	0	2	1	0	-.1255
C	1.3825951	1	120.641735	1	.000000	1	3	2	1	-.1172
C	1.4146361	1	121.113974	1	.000000	1	4	3	2	-.0195
C	1.4116679	1	121.062993	1	.000000	1	1	2	3	-.0361
C	1.4474120	1	123.061701	1	179.983769	1	5	4	3	-.0121
C	1.4348248	1	119.805066	1	-179.995796	1	6	1	2	-.1111
C	1.3564630	1	120.819708	1	-179.994448	1	8	6	1	-.1189
C	1.4161657	1	119.224126	1	-179.999704	1	7	5	4	-.0355
C	1.4126982	1	119.826311	1	-179.992186	1	10	7	5	-.1094
C	1.4120270	1	122.383826	1	.037954	1	7	5	4	-.0991
C	1.3907346	1	121.310061	1	179.990823	1	12	7	5	.0006
C	1.3773225	1	120.836075	1	.000000	1	11	10	7	-.1284
C	1.4494808	1	121.007943	1	179.994378	1	13	12	7	-.2828
H	1.1010169	1	120.282724	1	-179.996529	1	1	2	3	.1326
H	1.0995489	1	120.781382	1	179.998979	1	2	1	3	.1357
H	1.1002529	1	119.364958	1	179.976280	1	3	2	1	.1340
H	1.1000102	1	119.029156	1	-179.994066	1	4	3	2	.1347
H	1.1009959	1	117.952514	1	.000000	1	8	6	1	.1350
H	1.1009189	1	121.301797	1	179.988113	1	9	8	6	.1347
H	1.1007206	1	119.803517	1	-.029448	1	12	7	5	.1429
H	1.1000079	1	120.446665	1	-179.996455	1	14	11	10	.1298
H	1.1009565	1	118.882686	1	-179.992657	1	11	10	7	.1367
C	1.2699963	1	167.541324	1	.104569	1	15	13	12	.0019
H	1.3851639	1	60.879094	1	-179.887666	1	15	25	13	.2200

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 16:06:05 1998

AM1 PRECISE TS
TS 27->30

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	221.463073 KCAL
ELECTRONIC ENERGY	=	-13236.326632 EV
CORE-CORE REPULSION	=	11057.754351 EV
DIPOLE	=	.75307 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.432439 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	14.720 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 27->30

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1169
C	1.3822055	1	.000000	0	.000000	0	1	0	0	-.1262
C	1.4046321	1	119.978722	1	.000000	0	2	1	0	-.1257
C	1.3830145	1	120.264681	1	.000105	1	3	2	1	-.1152
C	1.4110770	1	120.779721	1	.003503	1	4	3	2	-.0161
C	1.4141787	1	118.808473	1	.000044	1	5	4	3	-.0349
C	1.4446344	1	121.889929	1	179.993033	1	5	4	3	.0057
C	1.4378033	1	119.697599	1	179.993273	1	6	5	4	-.1142
C	1.3556663	1	121.203174	1	.000036	1	8	6	5	-.1165
C	1.4380266	1	121.279630	1	-.019782	1	9	8	6	-.0349
C	1.4066513	1	120.393485	1	-179.987826	1	10	9	8	-.1189
C	1.3788152	1	124.977488	1	.019782	1	7	5	4	-.2373
C	1.4090653	1	123.966516	1	-179.993830	1	12	7	5	-.0545
C	1.3876400	1	120.460151	1	.000302	1	13	12	7	-.1115
C	1.4788220	1	102.454625	1	179.990378	1	13	12	7	-.1934
H	1.1004482	1	120.453370	1	-179.998882	1	1	2	3	.1336
H	1.0998768	1	119.621933	1	-179.992178	1	2	3	1	.1337
H	1.1000734	1	119.552088	1	-179.992799	1	3	2	1	.1338
H	1.0996758	1	119.684427	1	-179.928299	1	4	3	2	.1281
H	1.1010572	1	117.696851	1	179.999279	1	8	6	5	.1338
H	1.1012324	1	121.055816	1	179.992783	1	9	8	6	.1336
H	1.6219875	1	126.563060	1	.000949	1	12	7	5	.3061
H	1.0981751	1	121.779429	1	-179.992739	1	14	13	12	.1408
H	1.1012676	1	118.619334	1	.000063	1	11	10	9	.1335
C	1.3376295	1	102.940384	1	.000300	1	15	13	12	-.0445
H	1.0868689	1	126.031695	1	179.984983	1	15	13	12	.1779

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 15:32:42 1998

AM1 PRECISE TS
TS 28->33

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	222.605398 KCAL
ELECTRONIC ENERGY	=	-13196.031790 EV
CORE-CORE REPULSION	=	11017.630462 EV
DIPOLE	=	.65639 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.491790 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	21

COMPUTATION TIME = 2 MINUTES AND 51.920 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE TS
TS 28->33

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1172
C	1.3798105	1	.000000	0	.000000	0	1	0	0	-.1272
C	1.4046820	1	119.803535	1	.000000	0	2	1	0	-.1264
C	1.3803403	1	120.409824	1	.004170	1	3	2	1	-.1191
C	1.4141115	1	121.232399	1	.019782	1	4	3	2	-.0177
C	1.4161570	1	118.027913	1	-.004684	1	5	4	3	-.0380
C	1.4462062	1	122.710075	1	180.000000	1	5	4	3	-.0198
C	1.4338625	1	119.927626	1	-179.999000	1	6	5	4	-.1153
C	1.3576116	1	120.615169	1	.000659	1	8	6	5	-.1171
C	1.4354642	1	121.351470	1	.000129	1	9	8	6	-.0164
C	1.4198370	1	121.051724	1	180.000000	1	10	9	8	-.0637
C	1.4137291	1	121.732126	1	-.000088	1	7	5	4	-.1133
C	1.3798044	1	120.989664	1	-179.999900	1	12	7	5	-.1072
C	1.4032954	1	120.331322	1	-.000498	1	13	12	7	-.2454
C	1.4842865	1	137.346729	1	-.000005	1	11	10	9	-.1866
H	1.0995206	1	120.608236	1	179.999900	1	1	2	3	.1332
H	1.0998770	1	119.674049	1	179.999900	1	2	3	1	.1332
H	1.1002520	1	119.447100	1	-179.999900	1	3	2	1	.1327
H	1.0999755	1	118.800693	1	-179.999900	1	4	3	2	.1314
H	1.1010288	1	118.273019	1	-179.999900	1	8	6	5	.1343
H	1.0992676	1	119.069915	1	-179.999900	1	9	8	6	.1310
H	1.0998787	1	120.030889	1	.000035	1	12	7	5	.1363
H	1.1003543	1	120.359716	1	179.999900	1	13	12	7	.1336
H	1.6415291	1	130.088765	1	-179.999900	1	14	13	12	.3122
C	1.3337342	1	103.072388	1	180.000000	1	15	11	10	-.0272
H	1.0872297	1	119.724300	1	.000000	1	15	11	10	.1796

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 15:57:31 1998

AM1 PRECISE TS
TS 29->27

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	219.832012 KCAL
ELECTRONIC ENERGY	=	-13150.678340 EV
CORE-CORE REPULSION	=	10972.037066 EV
DIPOLE	=	.84853 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.510674 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	14.940 SECONDS	

FINAL GEOMETRY OBTAINED

AM1 PRECISE TS
TS 29->27

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1174
C	1.3777155	1	.000000	0	.000000	0	1	0	0	-.1266
C	1.4080585	1	119.756198	1	.000000	0	2	1	0	-.1267
C	1.3791974	1	120.451865	1	.000234	1	3	2	1	-.1191
C	1.4169971	1	121.118155	1	.034605	1	4	3	2	-.0194
C	1.4164499	1	118.095712	1	.006084	1	5	4	3	-.0366
C	1.4439885	1	122.505235	1	179.993022	1	5	4	3	-.0163
C	1.4311901	1	119.846243	1	179.993073	1	6	5	4	-.1142
C	1.3597969	1	120.713273	1	.003940	1	8	6	5	-.1184
C	1.4307651	1	120.947109	1	-.019782	1	9	8	6	-.0350
C	1.4354964	1	118.850314	1	-179.983738	1	10	9	8	-.0922
C	1.4312705	1	121.133745	1	.019782	1	7	5	4	-.1041
C	1.3640933	1	118.376803	1	-179.993037	1	12	7	5	-.0554
C	1.4345745	1	120.725091	1	.000730	1	13	12	7	-.2526
C	1.4774865	1	138.101804	1	179.999373	1	13	12	7	-.1965
H	1.1005486	1	120.607741	1	-179.993083	1	1	2	3	.1332
H	1.0997319	1	119.568792	1	-179.993722	1	2	3	1	.1336
H	1.1002026	1	119.329538	1	-179.993729	1	3	2	1	.1327
H	1.0997066	1	118.865142	1	-179.993722	1	4	3	2	.1319
H	1.1008121	1	118.163214	1	179.999942	1	8	6	5	.1343
H	1.1009858	1	120.989415	1	179.999927	1	9	8	6	.1340
H	1.0978556	1	120.621392	1	.003902	1	12	7	5	.1406
H	1.5944311	1	110.484142	1	-179.993727	1	14	13	12	.3118
H	1.0981310	1	119.381399	1	.000333	1	11	10	9	.1420
C	1.3389216	1	103.025010	1	179.903938	1	15	13	12	-.0407
H	1.0869239	1	126.162206	1	.000050	1	15	13	12	.1772

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Fri Jul 24 16:11:22 1998

AM1 PRECISE TS
TS 30->24

GRADIENTS WERE INITIALLY ACCEPTABLY SMALL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	223.857112 KCAL
ELECTRONIC ENERGY	=	-13306.771728 EV
CORE-CORE REPULSION	=	11128.302827 EV
DIPOLE	=	.98713 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.438288 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	1
COMPUTATION TIME =	14.890 SECONDS	

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 30->24

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1286
C	1.4031808	1	.000000	0	.000000	0	1	0	0	-.1246
C	1.3815527	1	119.529219	1	.000000	0	2	1	0	-.1191
C	1.4112352	1	120.662637	1	-.000223	1	3	2	1	-.0352
C	1.3832654	1	120.380256	1	-.000016	1	1	2	3	-.1170
C	1.4114297	1	121.477041	1	-.000935	1	5	1	2	-.0150
C	1.4494967	1	122.699981	1	179.999958	1	6	5	1	-.0005
C	1.4368433	1	119.681826	1	179.999954	1	4	3	2	-.1144
C	1.3529401	1	120.765657	1	-179.999954	1	8	4	3	-.1195
C	1.4337122	1	118.665705	1	179.999959	1	7	6	5	-.0344
C	1.4052639	1	122.115743	1	-179.999957	1	10	7	6	-.1201
C	1.3993948	1	125.704544	1	.000041	1	7	6	5	-.0332
C	1.3987185	1	121.549140	1	.000082	1	11	10	7	-.0996
C	1.4145192	1	120.089078	1	179.999959	1	12	7	6	-.2487
C	1.4853053	1	139.795592	1	.000075	1	12	7	6	-.2023
H	1.1009648	1	117.901159	1	-.000022	1	8	4	3	.1343
H	1.1013942	1	121.056001	1	179.999953	1	9	8	4	.1333
H	1.1006144	1	120.408070	1	179.999955	1	3	2	1	.1333
H	1.0996345	1	119.875126	1	179.999958	1	2	1	3	.1339
H	1.1001587	1	119.583128	1	-179.999958	1	1	2	3	.1330
H	1.0968354	1	118.604804	1	-179.999998	1	5	1	2	.1330
H	1.1009044	1	119.036079	1	179.999953	1	11	10	7	.1354
H	1.0975426	1	121.308415	1	179.999956	1	13	11	10	.1434
H	1.5733835	1	112.277586	1	-179.999953	1	14	12	7	.3081
C	1.3398821	1	103.512949	1	179.999952	1	15	12	7	-.0506
H	1.0863357	1	128.268741	1	.000003	1	15	12	7	.1750

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 10:55:30 1998

AM1 PRECISE TS
TS 32->9

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	188.809856 KCAL
ELECTRONIC ENERGY	=	-13315.009596 EV
CORE-CORE REPULSION	=	11135.643629 EV
DIPOLE	=	1.11067 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.481833 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	22

COMPUTATION TIME = 3 MINUTES AND 2.520 SECONDS

FINAL GEOMETRY OBTAINED

AM1 PRECISE TS
TS 32->9

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1150
C	1.3794811	1	.000000	0	.000000	0	1	0	0	-.1295
C	1.4062466	1	119.788851	1	.000000	0	2	1	0	-.1239
C	1.3812263	1	120.431707	1	-.013368	1	3	2	1	-.1200
C	1.4144727	1	120.997262	1	.002064	1	4	3	2	-.0107
C	1.4458107	1	122.645126	1	-179.989578	1	5	4	3	-.0122
C	1.4142591	1	118.278252	1	.020753	1	5	4	3	-.0428
C	1.4306075	1	119.881189	1	179.948250	1	7	5	4	-.1000
C	1.3668699	1	121.531735	1	-.005100	1	8	7	5	-.0488
C	1.4354509	1	119.987522	1	.044176	1	9	8	7	-.0549
C	1.4522310	1	119.628161	1	-179.949104	1	9	8	7	-.1723
C	1.4136115	1	121.290759	1	179.950027	1	10	9	8	-.2555
C	1.4147145	1	121.544265	1	.064274	1	6	5	4	-.1355
C	1.3805823	1	121.253481	1	-179.949733	1	13	6	5	-.1189
C	1.4046603	1	120.081046	1	-.075099	1	14	13	6	-.1115
H	1.1014721	1	117.676971	1	179.996712	1	8	7	5	.1306
H	1.1004651	1	120.566094	1	-179.994137	1	1	2	3	.1318
H	1.0998100	1	119.643120	1	-179.995530	1	2	3	1	.1335
H	1.1002111	1	119.415679	1	179.986469	1	3	2	1	.1329
H	1.0997413	1	118.870227	1	179.990290	1	4	3	2	.1344
H	1.0999603	1	119.931058	1	.032558	1	13	6	5	.1305
H	1.1001078	1	120.317140	1	179.942139	1	14	13	6	.1327
H	1.1000926	1	119.757277	1	-179.935492	1	15	14	13	.1316
H	1.7392617	1	114.230173	1	-.024264	1	12	10	9	.3140
C	1.3272797	1	109.059614	1	-179.973129	1	11	9	8	-.0199
H	1.1123168	1	115.361513	1	.057521	1	11	9	8	.1996

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 11:21:47 1998

AM1 PRECISE TS
TS 33->25

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	191.740040 KCAL
ELECTRONIC ENERGY	=	-13152.464911 EV
CORE-CORE REPULSION	=	10972.647973 EV
DIPOLE	=	2.39388 DEBYE
NO. OF FILLED LEVELS	=	37
IONIZATION POTENTIAL	=	8.617344 EV
MOLECULAR WEIGHT	=	202.255
SCF CALCULATIONS	=	8
COMPUTATION TIME =	55.360 SECONDS	

FINAL GEOMETRY OBTAINED

AM1 PRECISE TS
TS 33->25

										CHARGE
C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1172
C	1.3797982	1	.000000	0	.000000	0	1	0	0	-.1247
C	1.4059965	1	119.750810	1	.000000	0	2	1	0	-.1274
C	1.3813330	1	120.459075	1	-.017218	1	3	2	1	-.1179
C	1.4146975	1	121.031463	1	-.038160	1	4	3	2	-.0228
C	1.4147721	1	118.159060	1	.077222	1	5	4	3	-.0343
C	1.4474193	1	122.461948	1	-179.973872	1	5	4	3	-.0132
C	1.4335968	1	119.580063	1	179.912781	1	6	5	4	-.1142
C	1.3574035	1	120.943993	1	.030439	1	8	6	5	-.1166
C	1.4352933	1	121.392668	1	-.051592	1	9	8	6	-.0116
C	1.4231190	1	121.297465	1	-179.905337	1	10	9	8	.0139
C	1.4129935	1	121.538169	1	.106598	1	7	5	4	-.1171
C	1.3809243	1	120.934843	1	-179.892050	1	12	7	5	-.1226
C	1.4012493	1	120.384494	1	-.039404	1	13	12	7	-.1306
C	1.4516583	1	121.324499	1	.007738	1	11	10	9	-.2807
H	1.1005482	1	120.569801	1	-179.964269	1	1	2	3	.1347
H	1.0997838	1	119.654258	1	-179.983444	1	2	3	1	.1342
H	1.1002541	1	119.416238	1	179.958869	1	3	2	1	.1332
H	1.0997206	1	118.817456	1	179.956142	1	4	3	2	.1318
H	1.1013044	1	118.025657	1	-179.998095	1	8	6	5	.1368
H	1.1090494	1	118.620625	1	179.936651	1	9	8	6	.1453
H	1.0997123	1	120.174227	1	.109720	1	12	7	5	.1358
H	1.1004080	1	120.230672	1	179.959216	1	13	12	7	.1362
H	1.1002932	1	119.425471	1	179.970532	1	14	13	12	.1290
C	1.2702260	1	167.902909	1	-.007261	1	15	11	10	.0005
H	1.3837715	1	61.008723	1	179.944940	1	15	25	11	.2193

SUMMARY OF AM1 CALCULATION

VERSION 7.00

C16 H10

Tue Jul 28 11:32:38 1998

AM1 PRECISE TS
TS 24->15

GEOMETRY OPTIMISED USING EIGENVECTOR FOLLOWING (EF).
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	197.723601	KCAL
ELECTRONIC ENERGY	=	-13320.226438	EV
CORE-CORE REPULSION	=	11140.568364	EV
DIPOLE	=	2.84194	DEBYE
NO. OF FILLED LEVELS	=	37	
IONIZATION POTENTIAL	=	8.753375	EV
MOLECULAR WEIGHT	=	202.255	
SCF CALCULATIONS	=	18	

COMPUTATION TIME = 2 MINUTES AND 24.510 SECONDS

FINAL GEOMETRY OBTAINED CHARGE

AM1 PRECISE TS
TS 24->15

C	.0000000	0	.000000	0	.000000	0	0	0	0	-.1262
C	1.4049192	1	.000000	0	.000000	0	1	0	0	-.1239
C	1.3788166	1	119.977958	1	.000000	0	2	1	0	-.1193
C	1.4120469	1	120.529480	1	-.547223	1	3	2	1	-.0344
C	1.3835144	1	119.991853	1	-.441016	1	1	2	3	-.1324
C	1.4152664	1	121.550079	1	-1.510935	1	5	1	2	-.0247
C	1.4501537	1	123.374614	1	-178.631042	1	6	5	1	.0005
C	1.4348506	1	119.482023	1	-173.322736	1	4	3	2	-.1148
C	1.3548115	1	120.432808	1	174.286936	1	8	4	3	-.1170
C	1.4193435	1	118.239121	1	-165.614104	1	7	6	5	-.0407
C	1.4116070	1	120.712301	1	172.489113	1	10	7	6	-.1064
C	1.4233169	1	124.392797	1	14.932741	1	7	6	5	-.0018
C	1.3793645	1	120.434137	1	2.403982	1	11	10	7	-.1316
C	1.3931402	1	120.331342	1	-172.202731	1	12	7	6	-.0969
C	1.4543926	1	122.446164	1	11.898075	1	12	7	6	-.2907
H	1.1007008	1	118.135990	1	-3.881622	1	8	4	3	.1361
H	1.1003237	1	121.362493	1	-176.367537	1	9	8	4	.1356
H	1.1006155	1	120.600748	1	-179.023245	1	3	2	1	.1347
H	1.1002036	1	119.576749	1	-179.803802	1	2	1	3	.1343
H	1.0987704	1	119.678508	1	178.205832	1	1	2	3	.1374
H	1.1002136	1	118.244610	1	175.404802	1	5	1	2	.1462
H	1.1012336	1	118.997753	1	-177.601987	1	11	10	7	.1369
H	1.0995421	1	120.794381	1	-178.577514	1	13	11	10	.1394
H	1.1010457	1	119.586625	1	178.222467	1	14	12	7	.1438
C	1.2703642	1	166.837046	1	-155.221379	1	15	12	7	-.0076
H	1.3799806	1	61.573893	1	162.359785	1	15	25	12	.2237