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Ring Scission Of Diastereomeric 4-Butylspiropentylcarbinyl Radicals As A Chemical Model For Identifying Enzyme-Catalyzed FAD Adducts Resulting From Spiropentylacetyl-CoA

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Computed structures and energies

Cyclopropylcarbinyl radical UHF/6-31G(d)

UHF/6-31G(d) = -155.466320
UMP2/6-31G(d)//UHF/6-31G(d) = -155.960393
PMP2/6-31G(d)//UHF/6-31G(d) = -155.962873
UMP2/6-31G(d) = -155.961020; PMP2/6-31G(d) = -155.963663
UMP2/cc-pvdz//UMP2/6-31G(d) = -156.012548
PMP2/cc-pvdz//UMP2/6-31G(d) = -156.015104
UMP3/cc-pvdz//UMP2/6-31G(d) = -156.056295
PMP3/cc-pvdz//UMP2/6-31G(d) = -156.057841
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -156.062171
UCCSD/cc-pvdz//UMP2/6-31G(d) = -156.063403
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -156.081680
UMP2/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.168238
PMP2/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.170948
UMP3/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.206292
PMP3/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.207899
UMP4(SDQ)/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.208881
UCCSD/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.209151
UCCSD(T)/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.237558
ZPE (UHF, unscaled) = 0.101114, ZPE (UMP2, unscaled) = 0.096959
Temp Correction not including ZPE (UHF) = 0.005913, (UMP2) = 0.005933

H	-0.708396	1.206360	-1.128666
C	-0.893849	0.747598	-0.173233
C	-0.909347	-0.742588	-0.098174
C	0.254557	0.013921	0.485150
H	-1.566756	1.300501	0.458772
H	-0.736658	-1.297405	-1.004174
H	-1.597076	-1.214973	0.581213
C	1.581965	-0.040733	-0.153725
H	0.276794	0.073482	1.560130
H	2.463810	0.243869	0.389301
H	1.668323	-0.181020	-1.216682

Cyclopropylcarbinyl radical UMP2/6-31G(d)

H	-0.707835	1.258386	-1.075256
C	-0.901533	0.748576	-0.137154
C	-0.904749	-0.746136	-0.134605
C	0.263576	-0.001086	0.489320
H	-1.581709	1.271230	0.527466
H	-0.714786	-1.260130	-1.071232
H	-1.586976	-1.263484	0.532251
C	1.571944	-0.004885	-0.161183
H	0.280848	0.000349	1.575741
H	2.486100	0.021072	0.415041
H	1.648933	-0.006236	-1.242279

Homoallyl radical UHF/6-31G(d)

UHF/6-31G(d) = -155.473394
UMP2/6-31G(d)//UHF/6-31G(d) = -155.958384
PMP2/6-31G(d)//UHF/6-31G(d) = -155.961760
UQCISD/6-31G(d) = -156.012429
UMP2/cc-pvdz//UQCISD/6-31G(d) = -156.013532
PMP2/cc-pvdz//UQCISD/6-31G(d) = -156.016694
UMP3/cc-pvdz//UQCISD/6-31G(d) = -156.060570
PMP3/cc-pvdz//UQCISD/6-31G(d) = -156.062754
UMP4(SDQ)/cc-pvdz//UQCISD/6-31G(d) = -156.067438
UCCSD/cc-pvdz//UQCISD/6-31G(d) = -156.069546
UCCSD(T)/cc-pvdz//UQCISD/6-31G(d) = -156.088182
UMP2/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.167257
PMP2/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.173714
UMP3/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.208909
PMP3/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.213975
UMP4(SDQ)/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.212506
UCCSD/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.213458
UCCSD(T)/6-311+G(2df,2pd)//UQCISD/6-31G(d) = -156.241965
ZPE (UHF, unscaled) = 0.099488, ZPE (UMP2, unscaled) = 0.094923
Temp Correction not including ZPE (UHF) = 0.006278, (UMP2) = 0.0060872

H	-1.903941	0.999143	-0.765787
C	-1.803254	0.050572	-0.265955
C	-0.665786	-0.329565	0.284932
H	-2.679302	-0.572841	-0.238373
C	0.605509	0.478047	0.300852
H	-0.614777	-1.291757	0.771924
H	0.849542	0.725941	1.337514
H	0.444667	1.427465	-0.202593
C	1.766554	-0.242942	-0.325780
H	1.814920	-1.317187	-0.313044
H	2.670754	0.292567	-0.553929

Homoallyl radical UQCISD/6-31G(d)

C	1.795018	-0.049456	-0.268445
C	0.660676	-0.188086	0.422977
C	-0.618957	0.557335	0.130236
C	-1.752820	-0.361824	-0.215151
H	1.872336	0.638911	-1.109712
H	2.690623	-0.615707	-0.021128
H	0.620279	-0.892980	1.256395
H	-0.433470	1.273096	-0.691535
H	-0.897344	1.168194	1.003051
H	-2.784786	-0.069447	-0.039579
H	-1.571146	-1.249886	-0.815199

Cyclopropylcarbinyl to homoally radical T.S. UHF/6-31G(d)

UHF/6-31G(d) = -155.447903
UMP2/6-31G(d)//UHF/6-31G(d) = -155.958384
PMP2/6-31G(d)//UHF/6-31G(d) = -155.948172
UMP2/6-31G(d) = -156.012429; PMP2/6-31G(d) = -155.947536
UMP2/cc-pvdz//UMP2/6-31G(d) = -156.013532
PMP2/cc-pvdz//UMP2/6-31G(d) = -156.000190
UMP3/cc-pvdz//UMP2/6-31G(d) = -156.060570
PMP3/cc-pvdz//UMP2/6-31G(d) = -156.042213
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -156.067438
UCCSD/cc-pvdz//UMP2/6-31G(d) = -156.069546
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -156.088182
UMP2/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.167257
PMP2/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.156709
UMP3/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.208909
PMP3/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.193402
UMP4(SDQ)/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.212506
UCCSD/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.213458
UCCSD(T)/6-311+G(2df,2pd)//UMP2/6-31G(d) = -156.241965
ZPE (UHF, unscaled) = 0.099488, ZPE (UMP2, unscaled) = 0.094923
Temp Correction not including ZPE (UHF) = 0.006278, (UMP2) = 0.0060872
Imaginary frequency = 741i (UHF), 808i (UMP2)

H	-.659736	1.134751	-1.146039
C	-.812640	.726022	-.158123
C	-1.146224	-.714885	-.098657
C	.400454	.155714	.485440
H	-1.409042	1.385569	.454303
H	-.986109	-1.339031	-.955908
H	-1.738095	-1.106425	.706571
C	1.604960	-.106186	-.179922
H	.383313	.081646	1.557641
H	2.426160	-.574742	.330099
H	1.704206	.054244	-1.239101

Cyclopropylcarbinyl to homoally radical T.S. UMP2/6-31G(d)

H	-.622255	1.133402	-1.148471
C	-.785678	.727084	-.150305
C	-1.202929	-.690616	-.103082
C	.438353	.159676	.480161
H	-1.357914	1.416034	.470634
H	-1.022504	-1.336840	-.950025
H	-1.766301	-1.080713	.733866
C	1.592131	-.130640	-.182572
H	.399443	.031349	1.558105
H	2.423163	-.613014	.317058
H	1.695109	.056753	-1.246381

Vinylcyclopropylcarbinyl radical UHF/6-31G(d)

UHF/6-31G(d) = -232.344890
UMP2/6-31G(d)//UHF/6-31G(d) = -233.090322
PMP2/6-31G(d)//UHF/6-31G(d) = -233.093771
UMP2/6-31G(d) = -233.091210; PMP2/6-31G(d) = -233.0944904
UMP2/cc-pvdz//UMP2/6-31G(d) = -233.159460
PMP2/cc-pvdz//UMP2/6-31G(d) = -233.162313
UMP3/cc-pvdz//UMP2/6-31G(d) = -233.216487
PMP3/cc-pvdz//UMP2/6-31G(d) = -233.218367
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -233.225060
UCCSD/cc-pvdz//UMP2/6-31G(d) = -233.226724
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -233.256936
ZPE (UHF, unscaled) = 0.137021, ZPE (UMP2, unscaled) = 0.134507
Temp Correction not including ZPE (UHF) = 0.007656, (UMP2) = 0.007598

H	-1.294225	-1.388905	-1.256251
C	-1.442939	-.466923	-.721246
C	-1.379146	-.488005	.764970
C	-.240703	.140059	-.007206
H	-2.129604	.211694	-1.194953
H	-1.192437	-1.426685	1.256761
H	-2.027392	.172108	1.314792
C	1.024914	-.647832	-.072903
C	-.128904	1.615897	.002368
C	2.254930	-.183738	.060137
H	.890868	-1.705878	-.237518
H	2.467418	.854672	.240370
H	3.102220	-.843105	-.001254
H	-.970900	2.208872	.312010
H	.625138	2.100480	-.590682

Vinylcyclopropylcarbinyl radical UMP2/6-31G(d)

H	-1.296621	-1.389963	-1.257959
C	-1.451881	-.465431	-.709643
C	-1.361757	-.492983	.778639
C	-.233403	.144163	-.013070
H	-2.148313	.224264	-1.174432
H	-1.153995	-1.438650	1.269127
H	-1.998956	.177237	1.347340
C	1.021736	-.648598	-.098781
C	-.129237	1.610913	-.011097
C	2.240985	-.181631	.074436
H	.887467	-1.708608	-.320924
H	2.430606	.859571	.314174
H	3.107576	-.829464	-.004577
H	-.967217	2.209368	.327180
H	.620798	2.097645	-.622833

Allylcyclopropyl radical UHF/6-31G(d)

UHF/6-31G(d) = -232.334248
UMP2/6-31G(d)//UHF/6-31G(d) = -233.075382
PMP2/6-31G(d)//UHF/6-31G(d) = -233.078047
UMP2/6-31G(d) = -233.076237; PMP2/6-31G(d) = -233.078684
UMP2/cc-pvdz//UMP2/6-31G(d) = -233.143442
PMP2/cc-pvdz//UMP2/6-31G(d) = -233.145582
UMP3/cc-pvdz//UMP2/6-31G(d) = -233.203135
PMP3/cc-pvdz//UMP2/6-31G(d) = -233.204579
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -233.211460
UCCSD/cc-pvdz//UMP2/6-31G(d) = -233.213193
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -233.242758
ZPE (UHF, unscaled) = 0.138714, ZPE (UMP2, unscaled) = 0.135942
Temp Correction not including ZPE (UHF) = 0.007218, (UMP2) =0.00718

H	-2.481160	-1.081340	.748045
C	-2.208557	-.531682	-.139797
C	-1.764480	.912532	.019944
C	-.803031	-.145161	-.329153
H	-2.801589	-.779154	-1.004909
H	-1.743147	1.329351	1.015452
H	-2.066225	1.614910	-.739618
C	.439469	-.606728	.364836
H	3.563629	.759545	-.369605
H	.719677	-1.591458	.003853
H	.215246	-.720114	1.429752
C	1.591368	.350190	.203224
C	2.775864	.032430	-.283339
H	1.404514	1.364778	.518006
H	3.005261	-.966005	-.615264

Allylcyclopropyl radical UMP2/6-31G(d)

H	-2.474541	-1.068094	.780779
C	-2.211377	-.517234	-.121338
C	-1.724749	.926545	.020864
C	-.800985	-.160332	-.346441
H	-2.844536	-.742172	-.976252
H	-1.660865	1.355425	1.020368
H	-2.045046	1.632509	-.741648
C	.434056	-.633565	.338436
H	3.550094	.787159	-.342471
H	.733015	-1.614515	-.050492
H	.200829	-.781192	1.407621
C	1.572502	.342666	.209556
C	2.760200	.046387	-.271332
H	1.361624	1.358408	.543630
H	3.001551	-.954334	-.620010

Spiropenyllcarbinyl radical UHF/6-31G(d)

UHF/6-31G(d) = -232.325788
UMP2/6-31G(d)//UHF/6-31G(d) = -233.077721
PMP2/6-31G(d)//UHF/6-31G(d) = -233.080253
UMP2/6-31G(d) = -233.078641; PMP2/6-31G(d) = -233.081326
UMP2/cc-pvdz//UMP2/6-31G(d) = -233.144036
PMP2/cc-pvdz//UMP2/6-31G(d) = -233.146641
UMP3/cc-pvdz//UMP2/6-31G(d) = -233.198850
PMP3/cc-pvdz//UMP2/6-31G(d) = -233.200438
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -233.206978
UCCSD/cc-pvdz//UMP2/6-31G(d) = -233.208072
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -233.237691
ZPE (UHF, unscaled) = 0.137598, ZPE (UMP2, unscaled) = 0.131735
Temp Correction not including ZPE (UHF) = 0.00744, (UMP2) = 0.007492

C	-1.982004	-.806185	-.069095
C	-1.005677	.217208	-.482815
C	-.470616	1.242823	.529042
C	.394492	.178283	.000602
H	-1.150511	.606238	-1.477637
H	-.824847	1.164673	1.543044
H	-.325236	2.251882	.181313
C	1.308881	-.842850	.545495
C	1.739880	.062734	-.591984
H	1.117401	-1.877222	.315193
H	1.748903	-.677034	1.514257
H	2.463651	.830311	-.375606
H	1.835576	-.375140	-1.571088
H	-1.844665	-1.345696	.850577
H	-2.930008	-.890088	-.567519

Spiropenyllcarbinyl radical UMP2/6-31G(d)

C	-1.960700	-.809464	-.062856
C	-1.013442	.216582	-.491056
C	-.474270	1.252956	.528556
C	.393630	.189047	-.000074
H	-1.160230	.613804	-1.493975
H	-.842888	1.169774	1.547604
H	-.339177	2.270445	.170135
C	1.294719	-.847462	.549694
C	1.743815	.060463	-.590835
H	1.086069	-1.887009	.311746
H	1.738151	-.685697	1.528407
H	2.480747	.826827	-.365607
H	1.837146	-.381823	-1.578848
H	-1.818801	-1.320207	.881897
H	-2.883525	-.978854	-.601930

Methylspiropentane HF/6-31G(d)

HF/6-31G(d) = -232.955004
MP2/6-31G(d)//UHF/6-31G(d) = -233.733996
MP2/6-31G(d) = -233.734817

C	-1.986197	-.738272	-.035011
C	-.945311	.258981	-.492776
C	-.398912	1.292655	.473965
C	.446934	.181928	-.008386
H	-1.072350	.603114	-1.507542
H	-.754724	1.261792	1.490860
H	-.208704	2.285333	.101609
C	1.333496	-.837898	.584270
C	1.795885	.016848	-.580278
H	1.126200	-1.876929	.390048
H	1.767402	-.646565	1.551130
H	2.535140	.774831	-.383195
H	1.894110	-.458693	-1.541675
H	-1.808087	-1.042621	.991272
H	-2.984545	-.313895	-.090231
H	-1.969816	-1.631823	-.652988

Methylspiropentane MP2/6-31G(d)

C	-1.970556	-.746563	-.037230
C	-.949854	.262810	-.502005
C	-.406665	1.297410	.479817
C	.445200	.189026	-.011478
H	-1.080159	.618659	-1.523745
H	-.774644	1.252469	1.502562
H	-.217697	2.302385	.110963
C	1.320780	-.846544	.582463
C	1.802844	.023230	-.574498
H	1.105962	-1.890724	.369881
H	1.751609	-.665375	1.563484
H	2.550572	.781299	-.356985
H	1.907286	-.447939	-1.548232
H	-1.763571	-1.043883	.995146
H	-2.984145	-.334430	-.077731
H	-1.945707	-1.648677	-.657760

Spiropentaylcarbinyl to vinylcyclopropylcarbinyl radical TS UHF/6-31G(d)

UHF/6-31G(d) = -232.312527
UMP2/6-31G(d)//UHF/6-31G(d) = -233.058409
PMP2/6-31G(d)//UHF/6-31G(d) = -233.071448
UMP2/6-31G(d) = -233.056737; PMP2/6-31G(d) = -233.071587
UMP2/cc-pvdz//UMP2/6-31G(d) = -233.124455
PMP2/cc-pvdz//UMP2/6-31G(d) = -233.136985
UMP3/cc-pvdz//UMP2/6-31G(d) = -233.180567
PMP3/cc-pvdz//UMP2/6-31G(d) = -233.189502
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -233.190620
UCCSD/cc-pvdz//UMP2/6-31G(d) = -233.195120
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -233.226112
ZPE (UHF, unscaled) = 0.135574, ZPE (UMP2, unscaled) = 0.130787
Temp Correction not including ZPE (UHF) = 0.007164, (UMP2) = 0.006739
Imaginary frequency = 736i (UHF), 812i (UMP2)

C	-2.017817	-0.730390	0.033472
C	-1.009193	0.062349	-0.548512
C	-0.255612	1.418246	0.459810
C	0.357988	0.183768	-0.024003
H	-1.186362	0.474216	-1.526646
H	-0.637244	1.473737	1.461960
H	-0.137923	2.336604	-0.085784
C	1.241758	-0.808070	0.633027
C	1.678417	-0.105828	-0.631184
H	0.976542	-1.848657	0.561516
H	1.721320	-0.530599	1.555686
H	2.447421	0.643115	-0.551369
H	1.706185	-0.681443	-1.540268
H	-1.849498	-1.251232	0.958855
H	-3.013681	-0.736190	-0.369609

Spiropentaylcarbinyl to vinylcyclopropylcarbinyl radical TS UMP2/6-31G(d)

C	-1.993092	-0.714783	0.051559
C	-1.019620	0.034926	-0.552375
C	-0.194664	1.462939	0.445213
C	0.345104	0.195356	-0.030685
H	-1.220462	0.491323	-1.519443
H	-0.609741	1.539586	1.442423
H	-0.115222	2.364201	-0.151956
C	1.207840	-0.807866	0.650618
C	1.658764	-0.149543	-0.641022
H	0.902553	-1.848924	0.604577
H	1.704831	-0.514882	1.570306
H	2.452001	0.589848	-0.582292
H	1.660314	-0.755117	-1.542340
H	-1.796247	-1.247584	0.975474
H	-3.004020	-0.744621	-0.336599

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Spiropentaylcarbinyl to allylcyclopropyl radical TS UHF/6-31G(d)

UHF/6-31G(d) = -232.302631
UMP2/6-31G(d)//UHF/6-31G(d) = -233.046373
PMP2/6-31G(d)//UHF/6-31G(d) = -233.060692
UMP2/6-31G(d) = -233.045630
PMP2/6-31G(d) = -233.059811
UMP2/cc-pvdz//UMP2/6-31G(d) = -233.112571
PMP2/cc-pvdz//UMP2/6-31G(d) = -233.126207
UMP3/cc-pvdz//UMP2/6-31G(d) = -233.170008
PMP3/cc-pvdz//UMP2/6-31G(d) = -233.180011
UMP4(SDQ)/cc-pvdz//UMP2/6-31G(d) = -233.180672
UCCSD/cc-pvdz//UMP2/6-31G(d) = -233.186127
UCCSD(T)/cc-pvdz//UMP2/6-31G(d) = -233.217324
ZPE (UHF, unscaled) = 0.136218, ZPE (UMP2, unscaled) =0.130886
Temp Correction not including ZPE (UHF) = 0.007070, (UMP2) = 0.006686
Imaginary frequency = 654i (UHF), 706i (UMP2)

C	-2.149269	-0.737179	-0.066602
C	-1.286648	0.298604	-0.426879
C	-0.467589	1.099116	0.542681
C	0.518438	0.152710	0.020478
H	-1.298454	0.653028	-1.441659
H	-0.744271	0.976488	1.580724
H	-0.329812	2.140387	0.286884
C	1.470858	-0.847622	0.501499
C	1.837822	0.125580	-0.615373
H	1.326561	-1.881203	0.231601
H	1.933898	-0.707288	1.466184
H	2.540503	0.913131	-0.388842
H	1.938206	-0.275382	-1.610865
H	-2.241046	-1.057918	0.955813
H	-2.667253	-1.308499	-0.814660

Spiropentaylcarbinyl to allylcyclopropyl radical TS UMP2/6-31G(d)

H	-.622255	1.133402	-1.148471
C	-.785678	.727084	-.150305
C	-1.202929	-.690616	-.103082
C	.438353	.159676	.480161
H	-1.357914	1.416034	.470634
H	-1.022504	-1.336840	-.950025
H	-1.766301	-1.080713	.733866
C	1.592131	-.130640	-.182572
H	.399443	.031349	1.558105
H	2.423163	-.613014	.317058
H	1.695109	.056753	-1.246381

Figure S1. Computed MP2/6-31G(d) geometries for **39-41**.

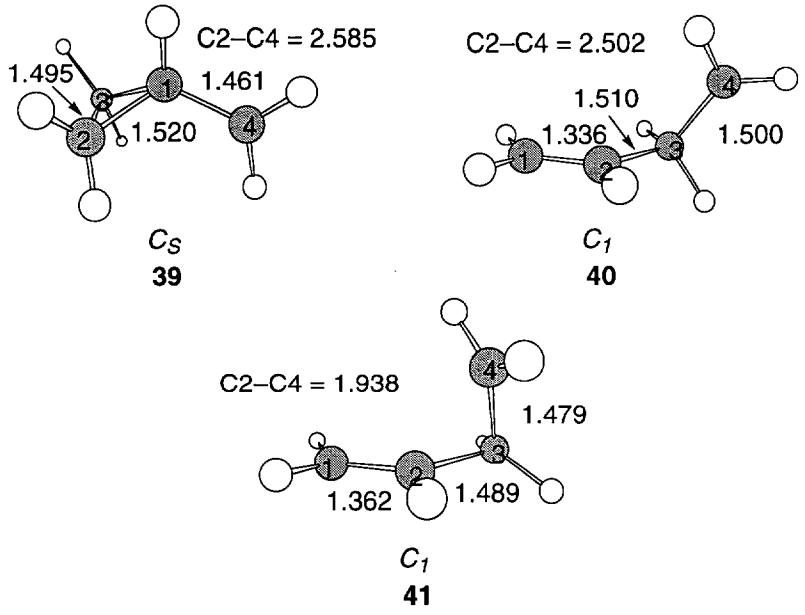
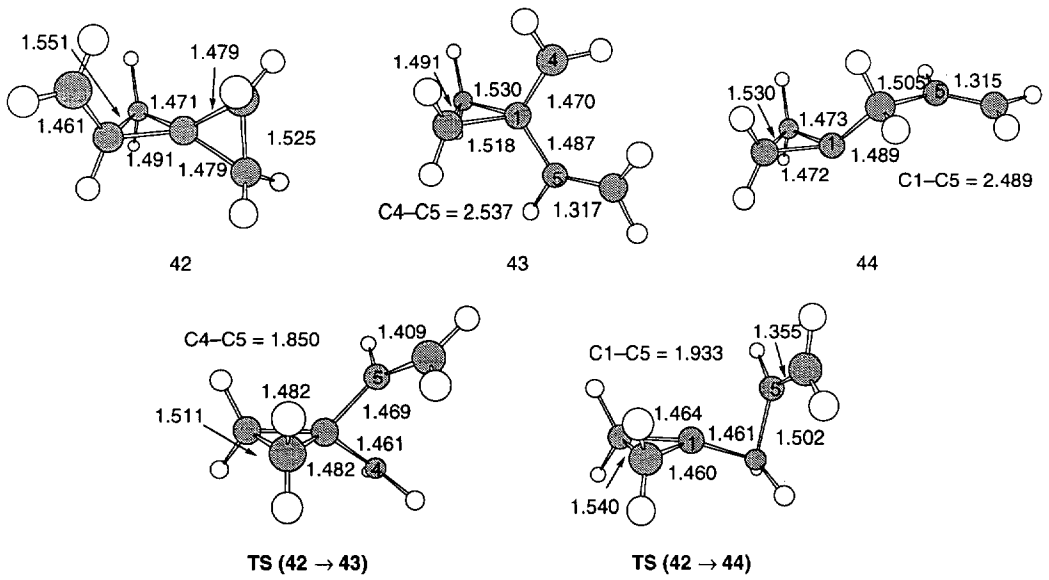


Figure S2. Computed MP2/6-31G(d) geometries for **42-44**.



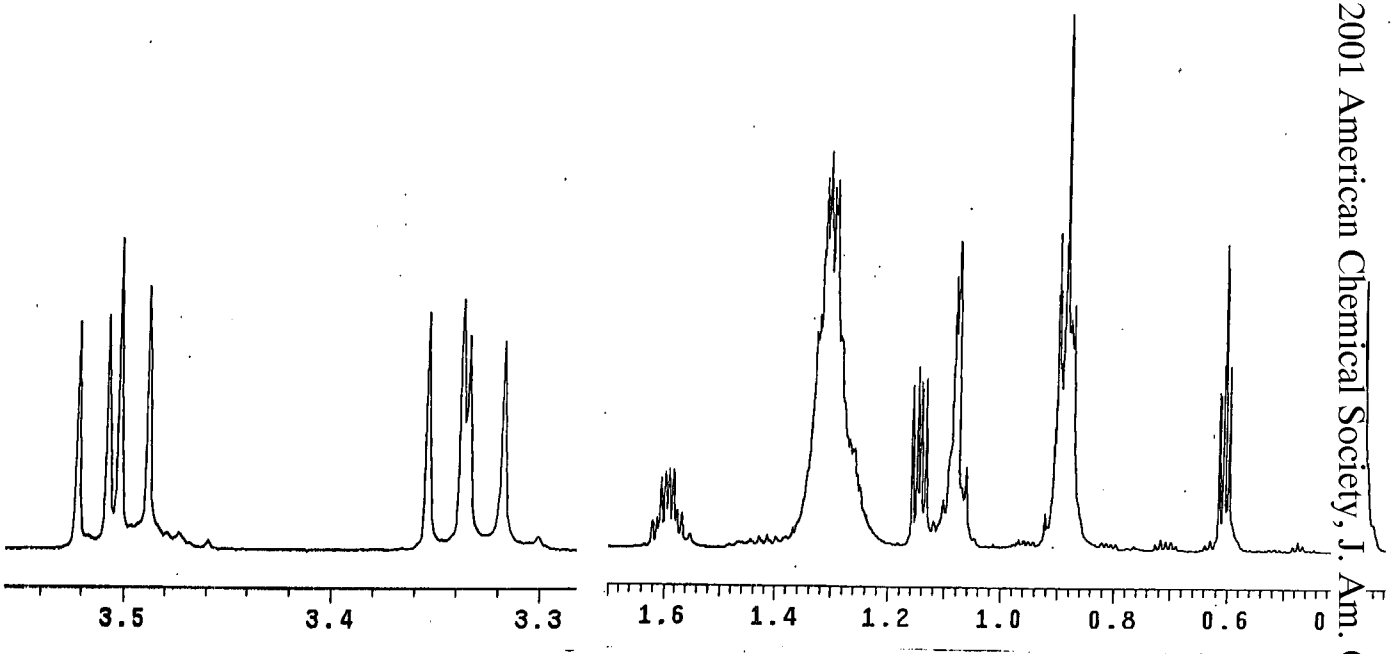
Univ of Minnesota, VI-500

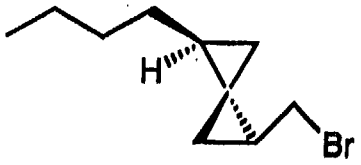
Pulse Sequence: s2pul

Date: Aug. 8, 2001
Solvent: CDCl3
File: spbr-h
Starting Time: 11:56:26
Completion Time: 11:56:51
Total acq. time 1 minute

UNITYplus-500 "v300"
Ambient temperature

PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.882 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.8671199 MHz
DATA PROCESSING
FT size 32768





14a

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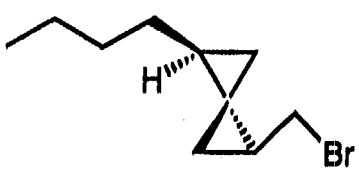
Univ of Minnesota, VI-500

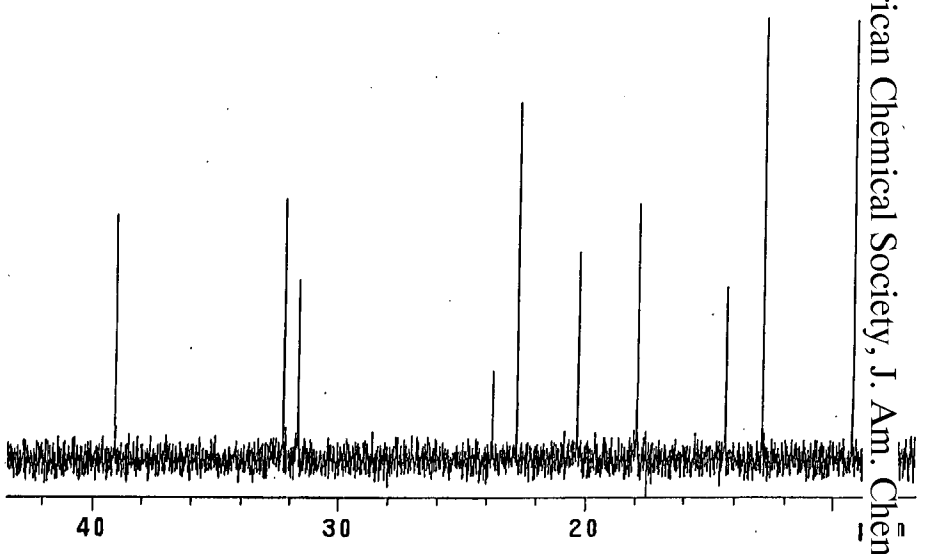
Pulse Sequence: s2pul

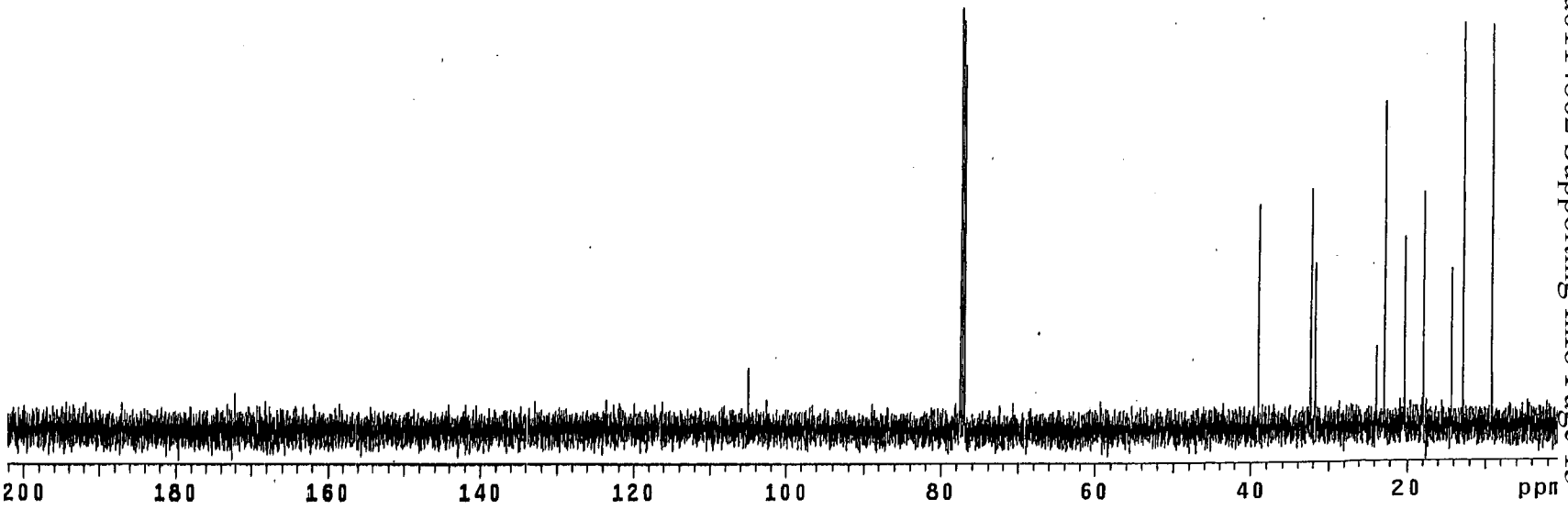
Date: Aug. 8, 2001
Solvent: CDCl3
File: spbr-h-c13
Starting Time: 12:00:38
Completion Time: 12:10:13
Total acq. time 9 minutes

UNITYplus-500 "v500"
Ambient temperature

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 67.5 degrees
Acq. time 0.860 sec
Width 32888.7 Hz
96 repetitions
OBSERVE C13, 125.6816608 MHz
DECOUPLE H1, 499.8698213 MHz
Power 36 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536







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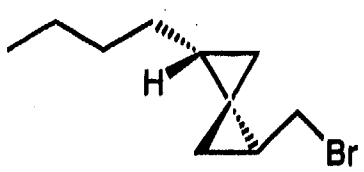
Univ of Minnesota, VI-500

Pulse Sequence: s2pul

Date: Aug. 8, 2001
Solvent: CDCl3
File: spbr-b
Starting Time: 11:35:10
Completion Time: 11:35:38
Total acq. time 1 minute

UNITYplus-500 "v300"
Ambient temperature

PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.882 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.8671188 MHz
DATA PROCESSING
FT size 32768



14b

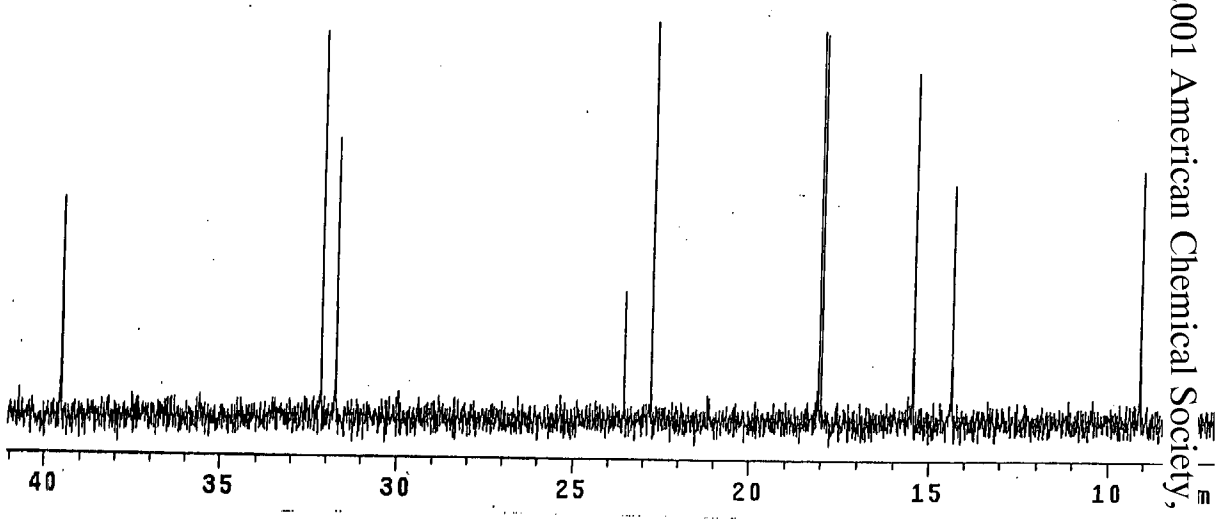
Univ of Minnesota, VI-500

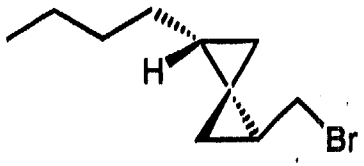
Pulse Sequence: s2pul

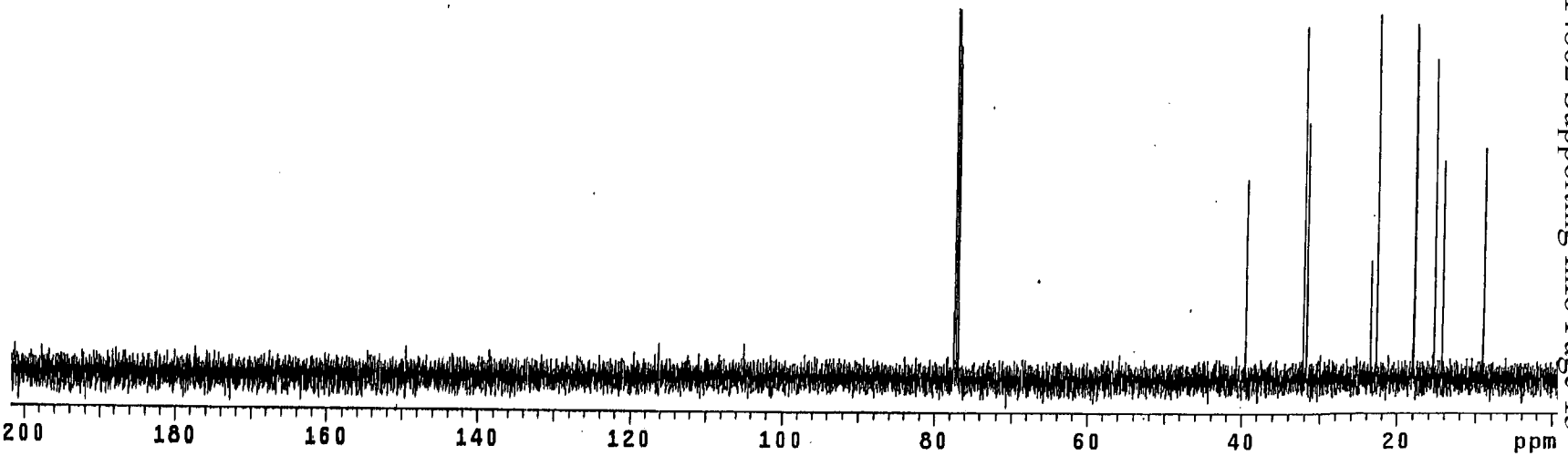
Date: Aug. 8, 2001
Solvent: CDCl3
File: spbr-b-c13
Starting Time: 11:41:50
Completion Time: 11:51:22
Total acq. time 9 minutes

UNITYplus-500 "v300"
Ambient temperature

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 67.5 degrees
Acq. time 0.860 sec
Width 32989.7 Hz
96 repetitions
OBSERVE C13, 125.6816608 MHz
DECOUPLE H1, 499.8686213 MHz
Power 36 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536







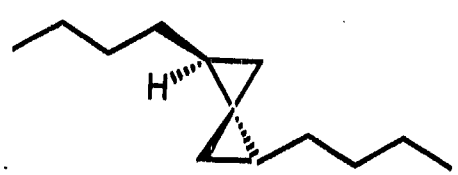
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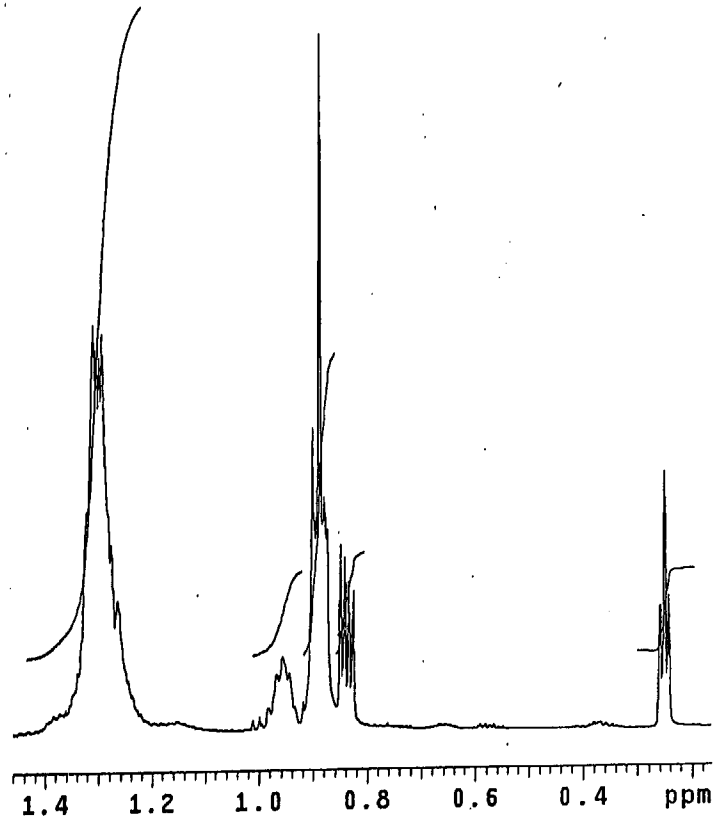
Pulse Sequence: s2pul
User: skalgl
Date: Apr. 21, 1998
Solvent: CDCl3
File: red-H4
Starting Time: 17:26:47
Completion Time: 17:27:20
Total acq. time 1 minute

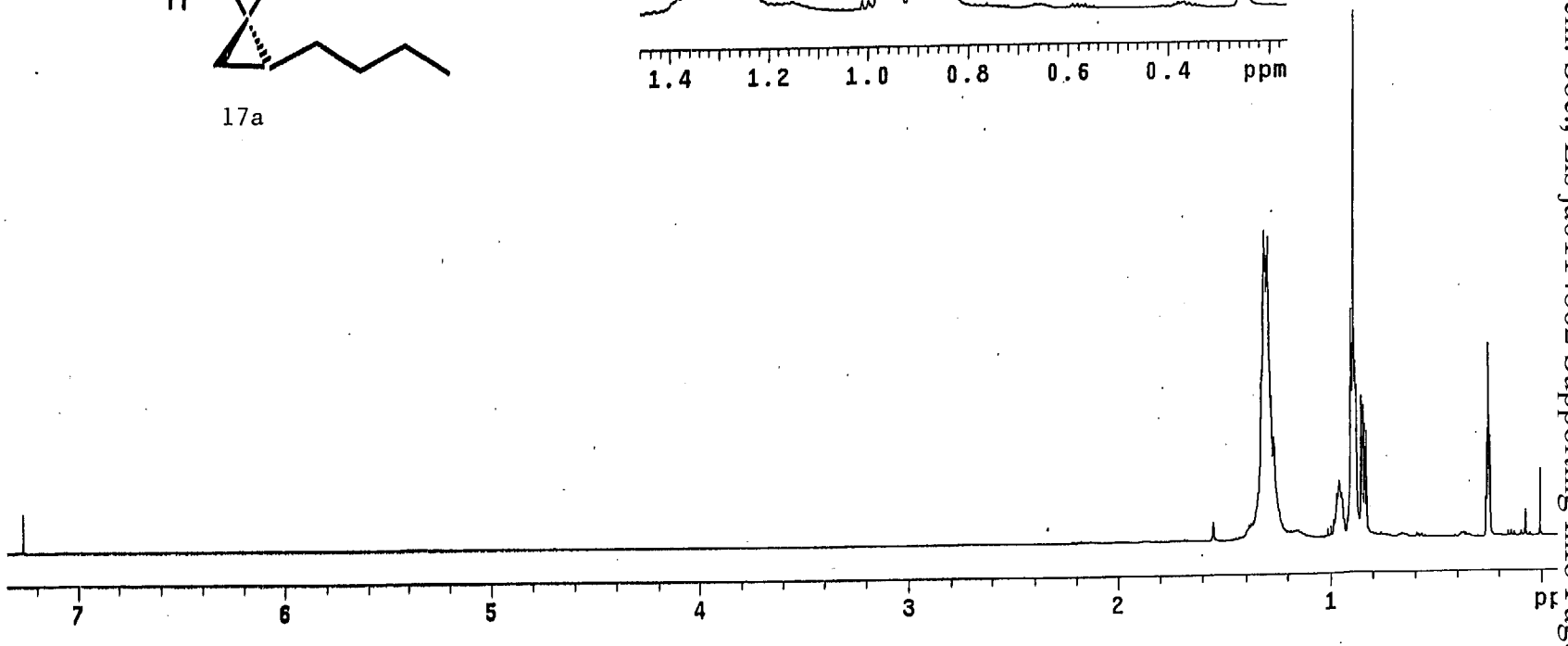
UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.882 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.8671218 MHz
DATA PROCESSING
FT size 32768



17a





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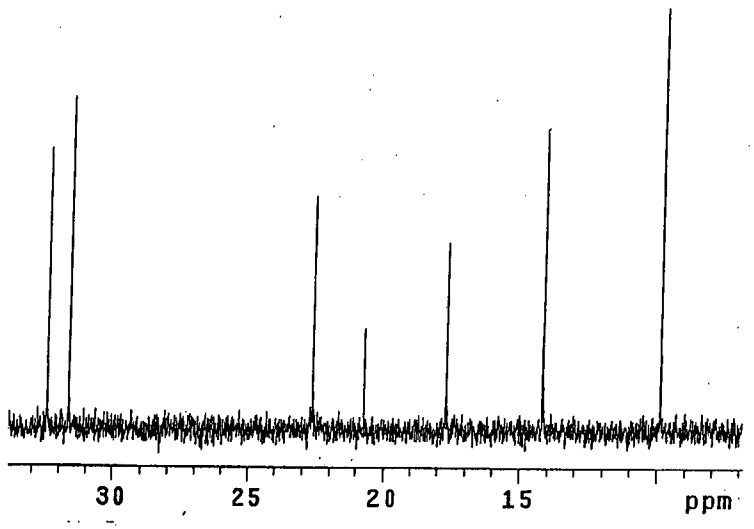
Univ of Minnesota, VI-500

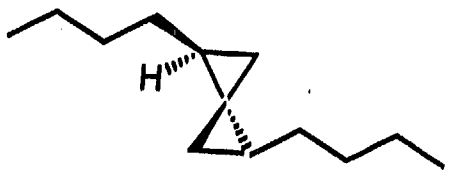
Pulse Sequence: s2pul

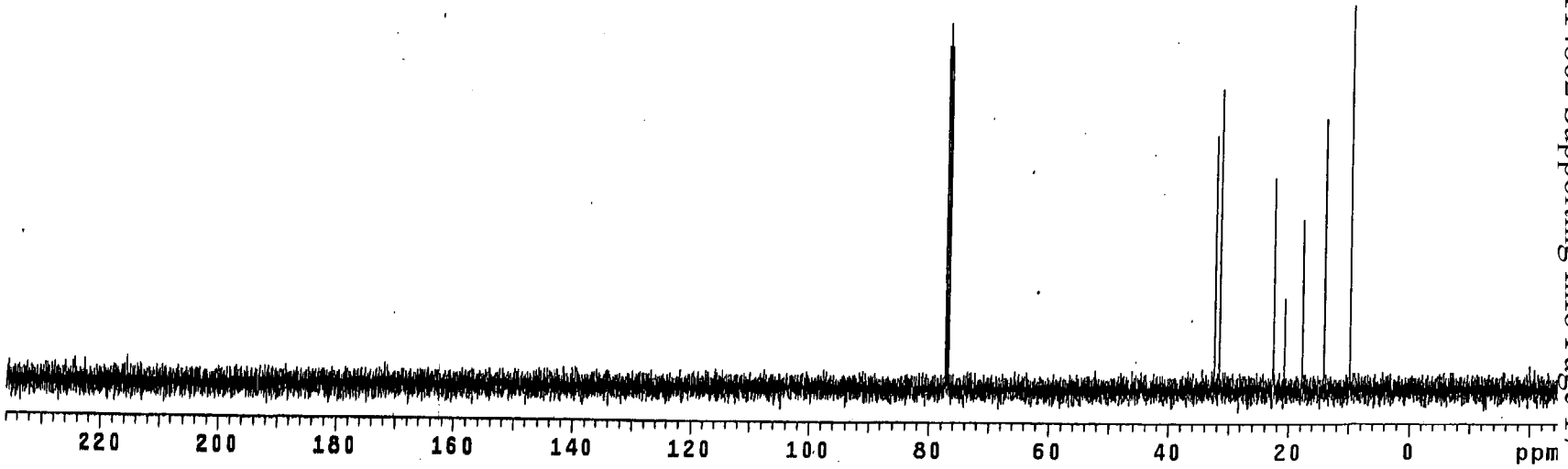
User: 1-14-87
Date: Apr. 21, 1999
Solvent: CDCl3
File: red-H4-c13
Starting Time: 17:36:05
Completion Time: 17:49:11
Total acq. time 6 minutes

UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 10.000 sec
Pulse 67.5 degrees
Acq. time 0.860 sec
Width 32888.7 Hz
32 repetitions
OBSERVE C13, 125.6816844 MHz
DECOUPLE H1, 498.8696212 MHz
Power 36 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536







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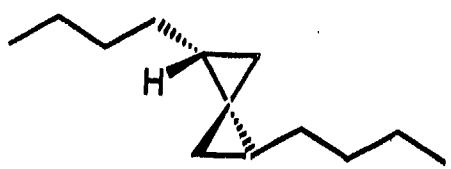
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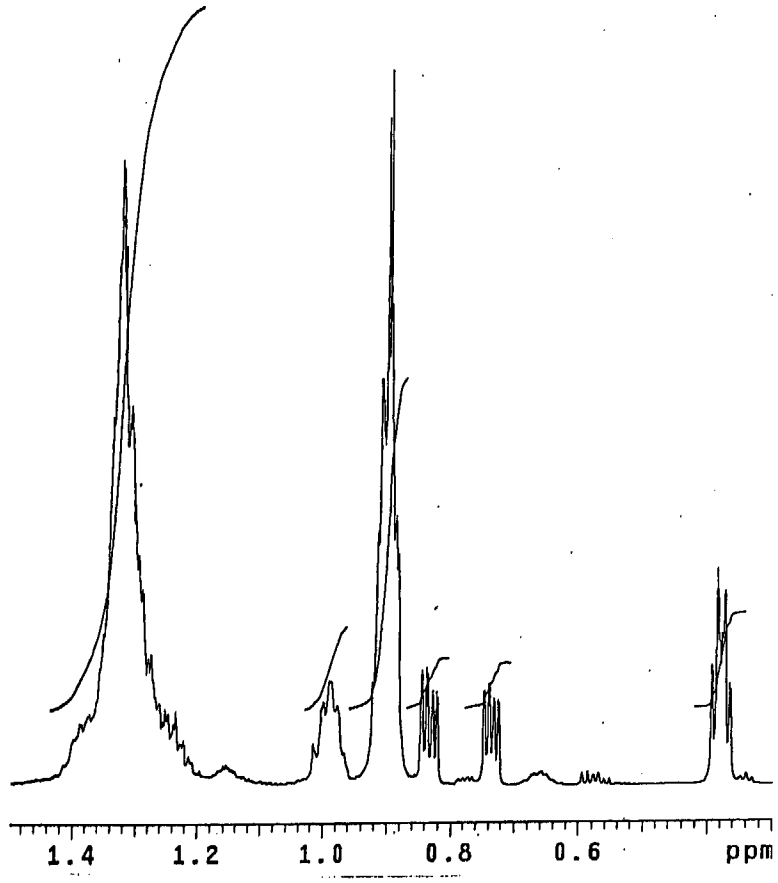
Pulse Sequence: s2pul
User: skalgl
Date: Apr. 21, 1999
Solvent: CDCl3
File: red-B-4
Starting Time: 15:00:14
Completion Time: 15:00:47
Total acq. time 1 minute

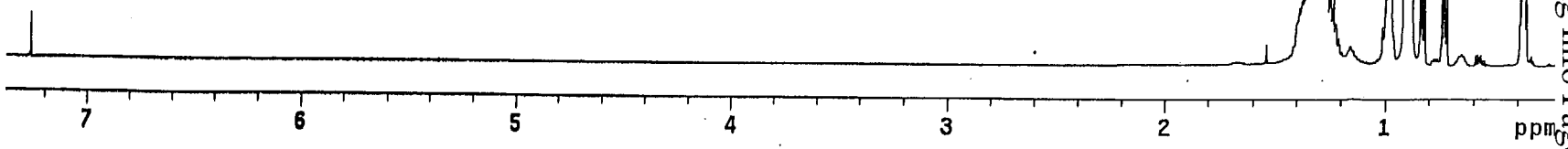
UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.882 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.8671218 MHz
DATA PROCESSING
FT size 32768



17b





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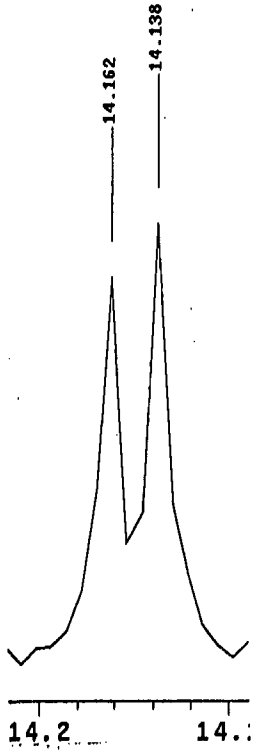
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Univ of Minnesota, VI-500

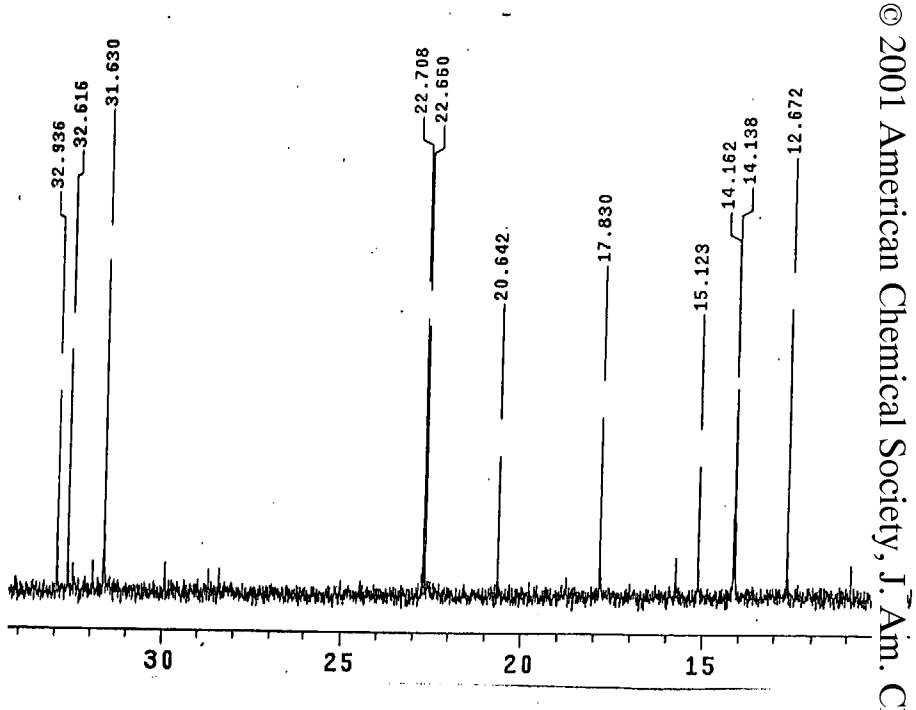
Pulse Sequence: s2pul

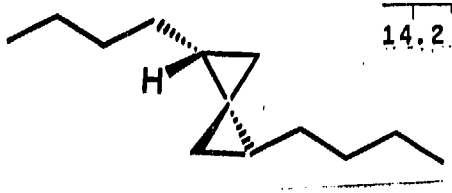
User:      1-14-87
Date:      Apr. 21, 1988
Solvent: CDCl3
File:      red-B-4-c13
Starting Time:   15:06:54
Completion Time: 15:14:00
Total acq. time 6 minutes

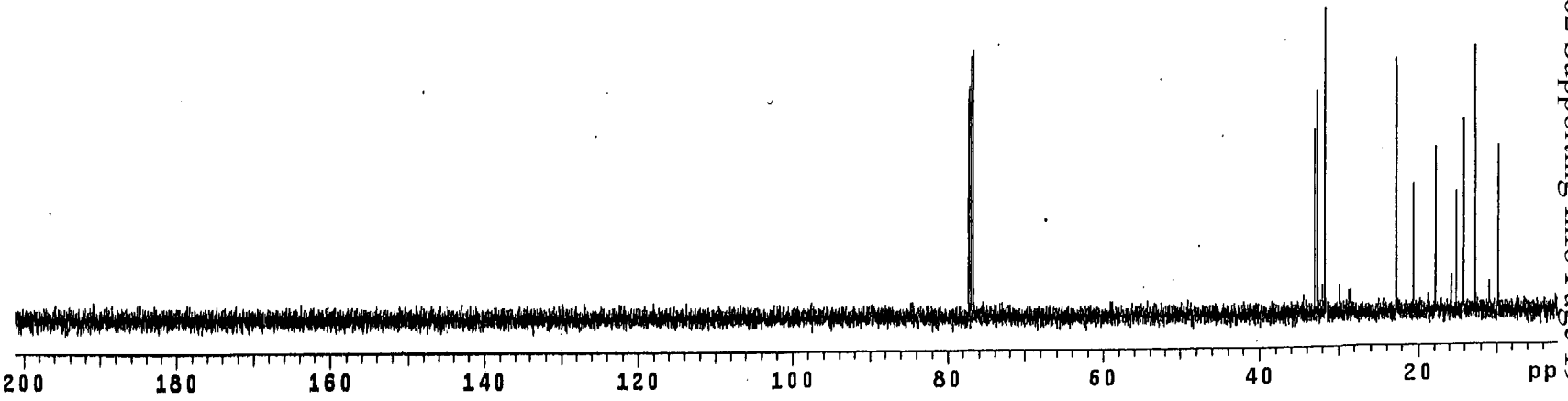
UNITYplus-500  "spectrum"
Ambient temperature

PULSE SEQUENCE
 Relax. delay 10.000 sec
 Pulse 67.5 degrees
 Acq. time 0.880 sec
 Width 32888.7 Hz
 32 repetitions
OBSERVE  C13, 125.6818844 MHz
DECOUPLE  H1, 499.8888212 MHz
 Power 36 dB
 on during acquisition
 off during delay
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
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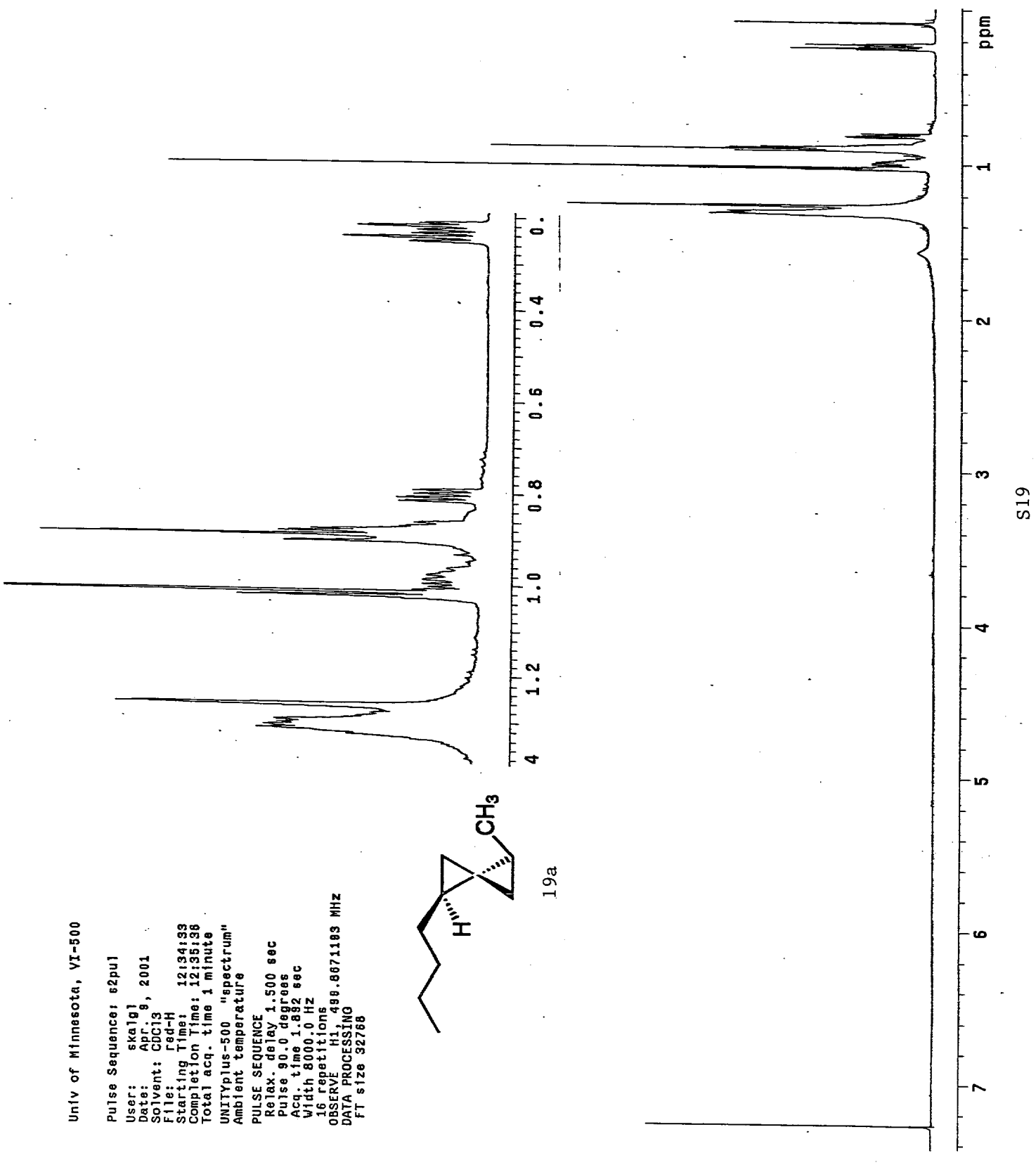








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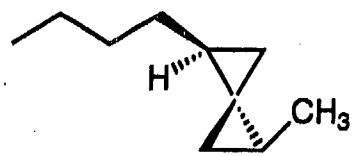
13C OBSERVE

Pulse Sequence: s2pul

User: skalgl
Date: Apr. 6, 2001
Solvent: CDCl3
File: red-H300-c13
Starting Time: 11:13:30
Completion Time: 11:39:49
Total acq. time 26 minutes

UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 0.100 sec
Pulse 67.5 degrees
Acq. time 0.800 sec
Width 17361.1 Hz
560 repetitions
OBSERVE C13, 75.4773716 MHz
DECOUPLE H1, 300.1685405 MHz
Power 36 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Line broadening 0.4 Hz
FT size 131072

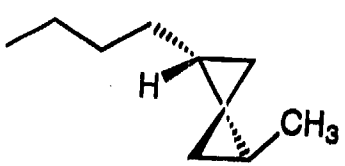


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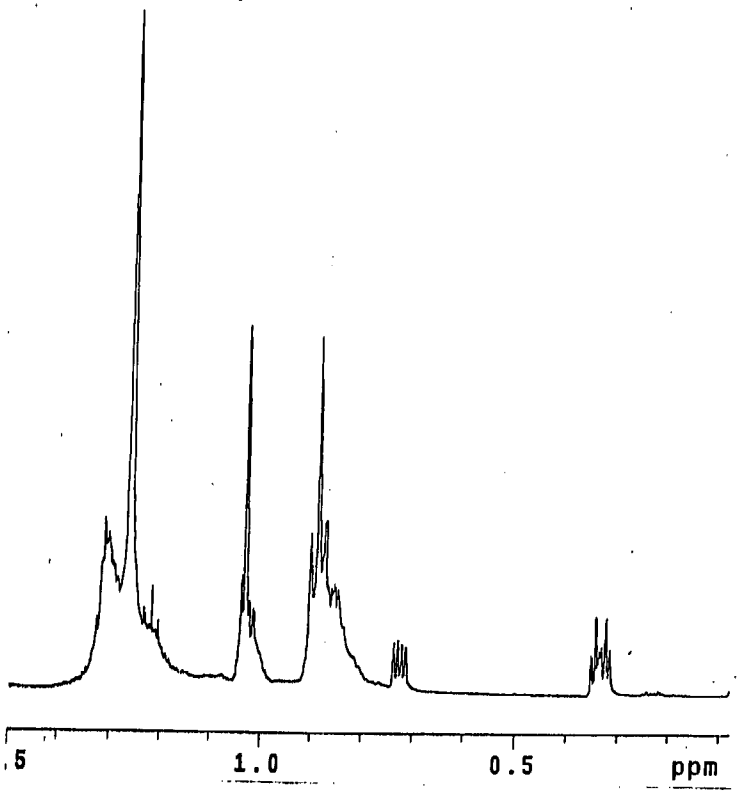
Univ of Minnesota, VI-500

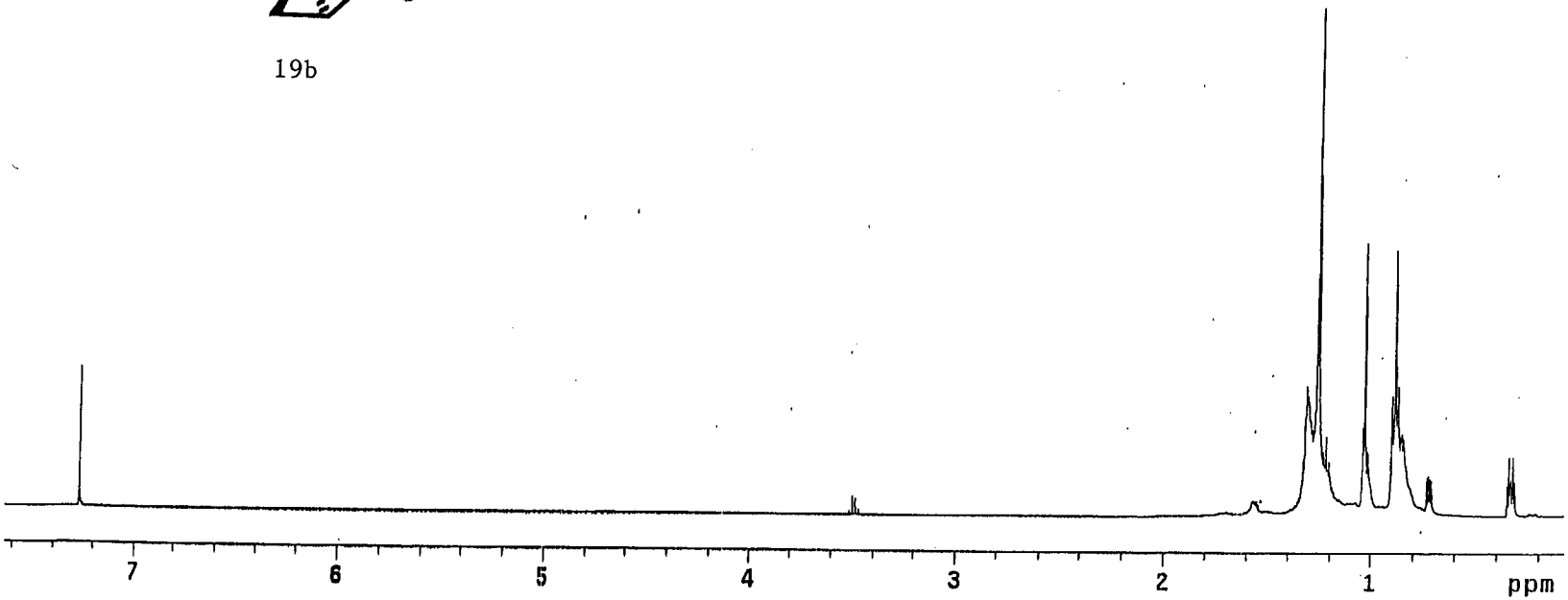
Pulse Sequence: s2pul

Date: Aug. 13, 2001
Solvent: CDCl3
File: spme-b2
Starting Time: 16:41:04
Completion Time: 16:41:30
Total acq. time 1 minute
UNITYplus-500 "v300"
Ambient temperature
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.882 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.8671188 MHz
DATA PROCESSING
FT size 32768



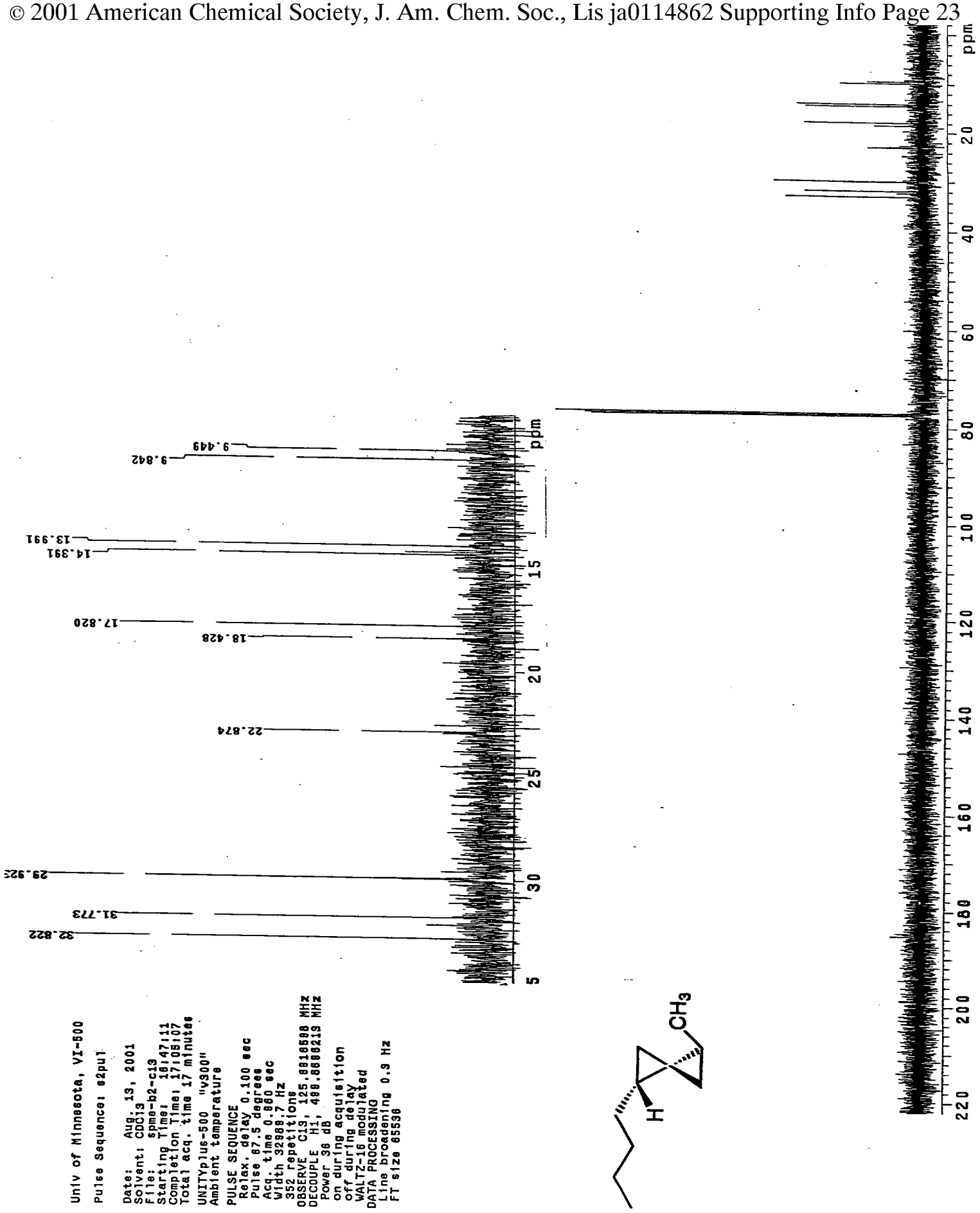
19b

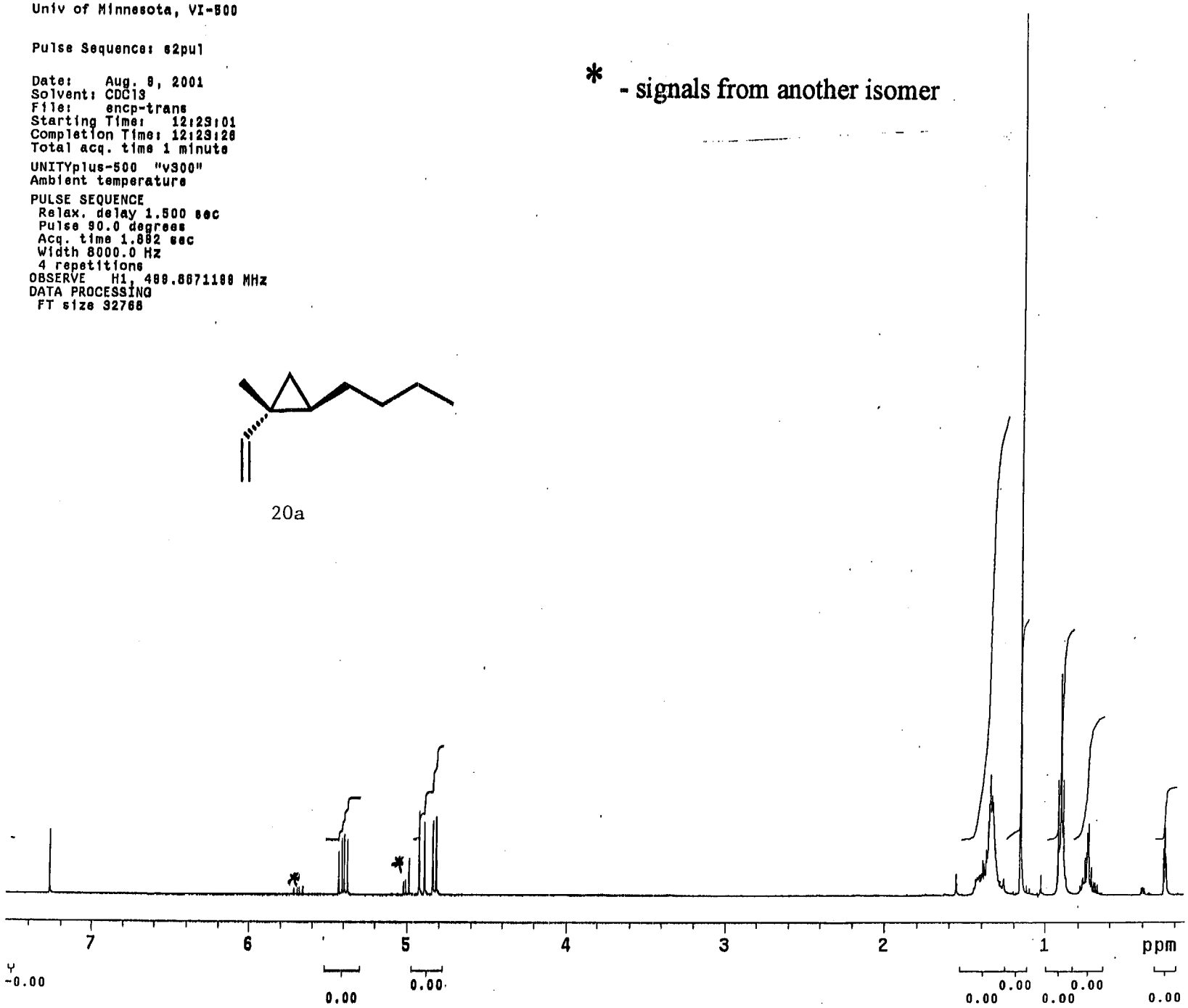




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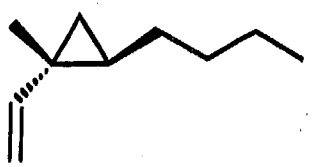
Pulse Sequence: s2pul

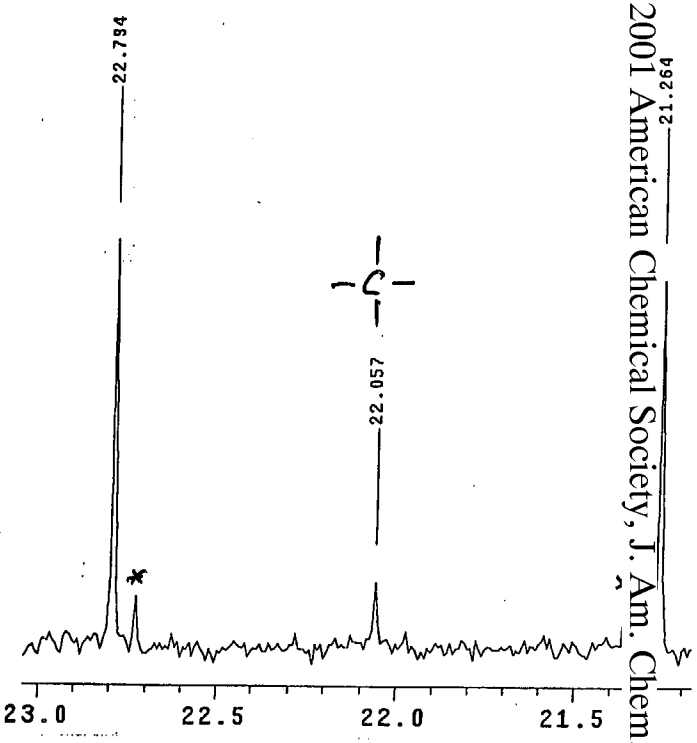
Date: Aug. 8, 2001
Solvent: CDCl3
File: encp-trans-c13
Starting Time: 12:28:45
Completion Time: 13:08:00
Total acq. time 39 minutes

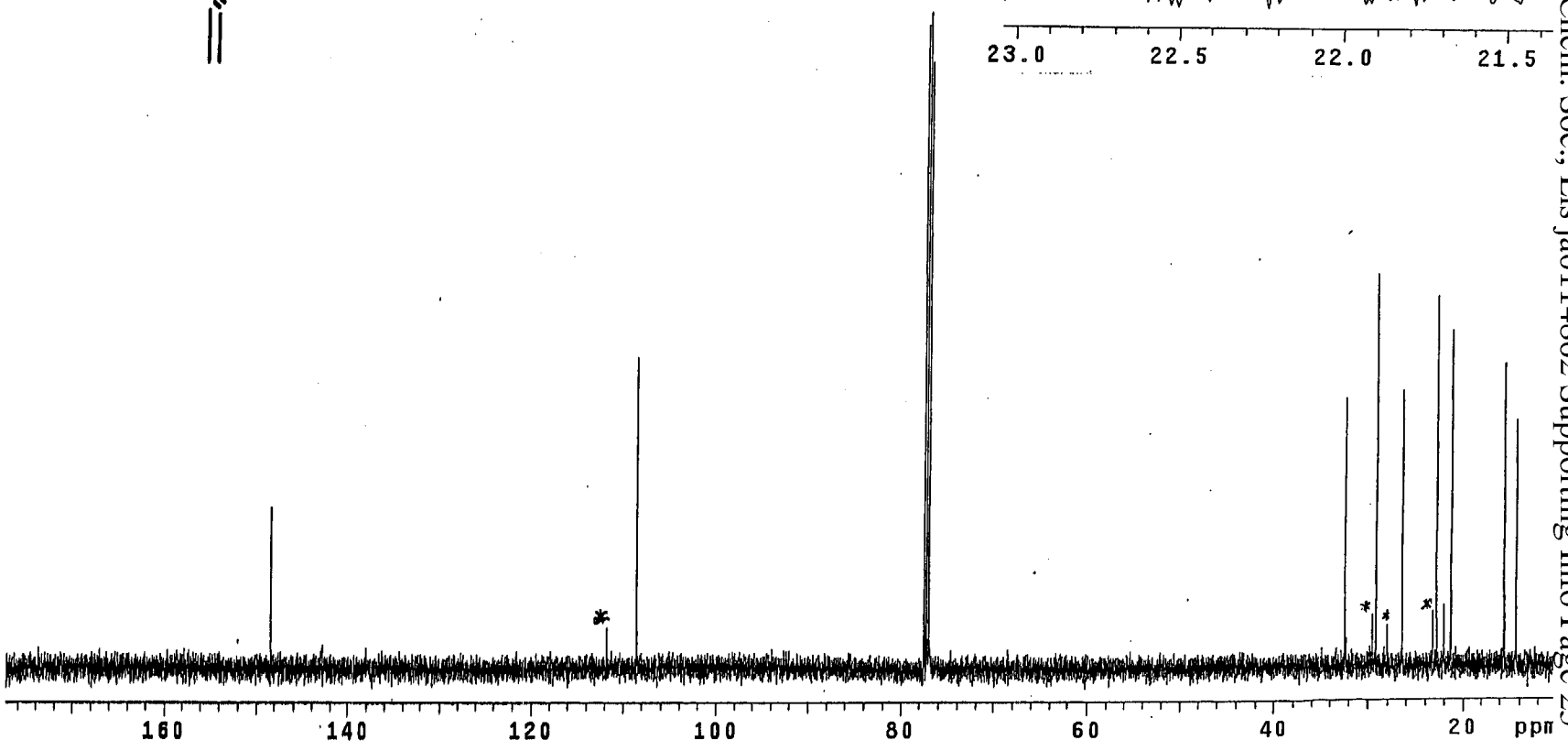
UNITYplus-500 "v300"
Ambient temperature

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 67.5 degrees
Acq. time 0.860 sec
Width 32989.7 Hz
400 repetitions
OBSERVE C13, 125.6816598 MHz
DECOUPLE H1, 499.8698213 MHz
Power 36 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536

* - signals from another isomer







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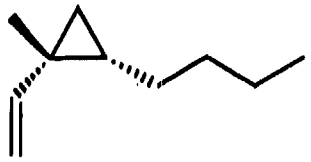
STANDARD 1H OBSERVE

Pulse Sequence: s2pul

User: skalgl
Date: May. 25, 2001
Solvent: CDCl3
File: encp-min
Starting Time: 17:47:15
Completion Time: 17:47:28
Total acq. time 1 minute

UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.888 sec
Width 6003.3 Hz
Single scan
OBSERVE H1, 300.1683375 MHz
DATA PROCESSING
FT size 131072



20b

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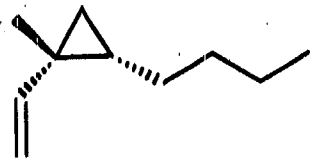
13C OBSERVE

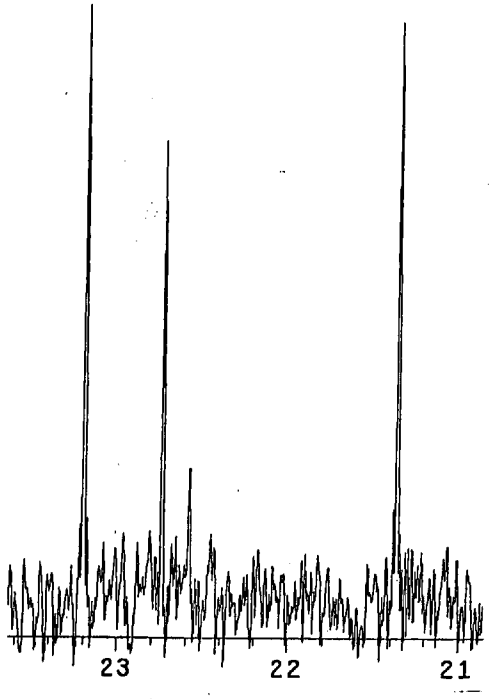
Pulse Sequence: s2pul

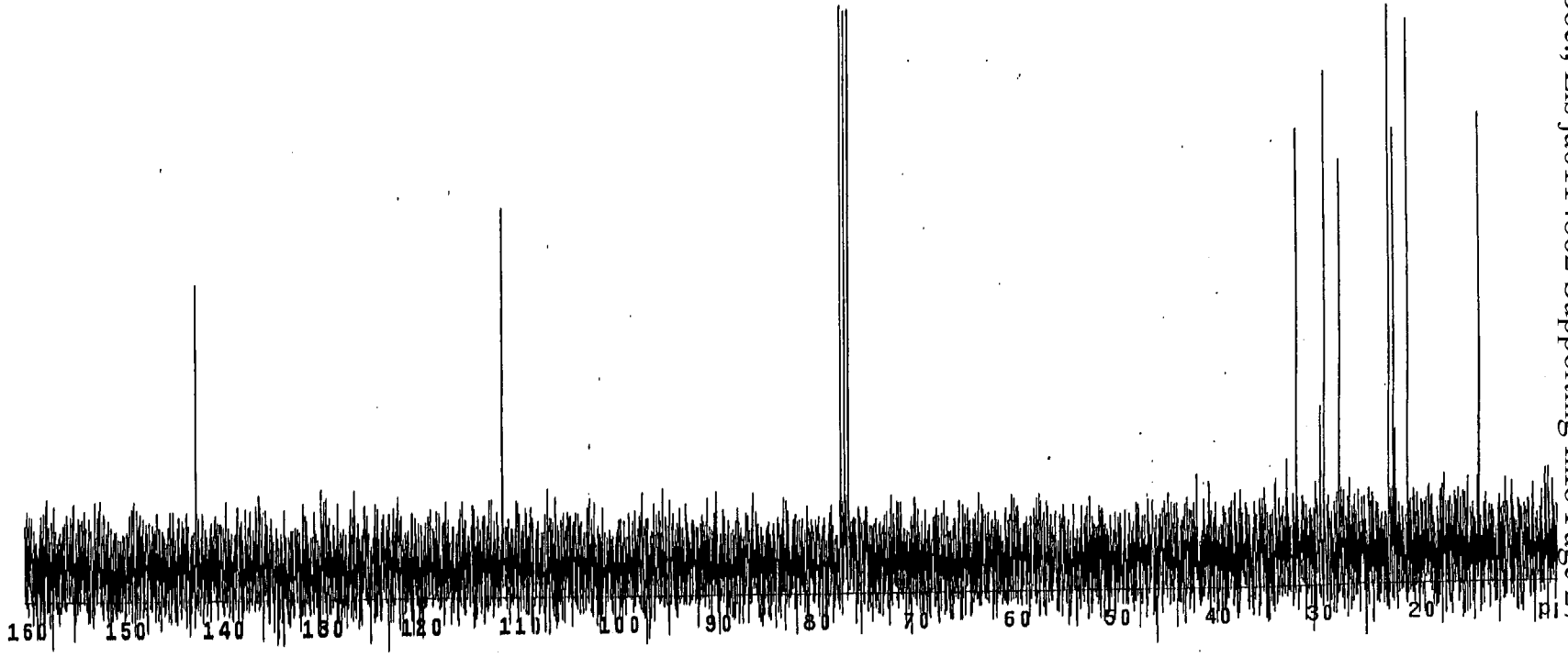
User: skalgl
Date: May. 25, 2001
Solvent: CDCl3
File: encp-min-c13
Starting Time: 17:56:23
Completion Time: 18:07:49
Total acq. time 11 minutes

UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 0.100 sec
Pulse 67.5 degrees
Acq. time 0.800 sec
Width 17361.1 Hz
240 repetitions
OBSERVE C13, 75.4779713 MHz
DECOUPLE H1, 300.1885405 MHz
Power 36 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Line broadening 0.4 Hz
FT size 131072







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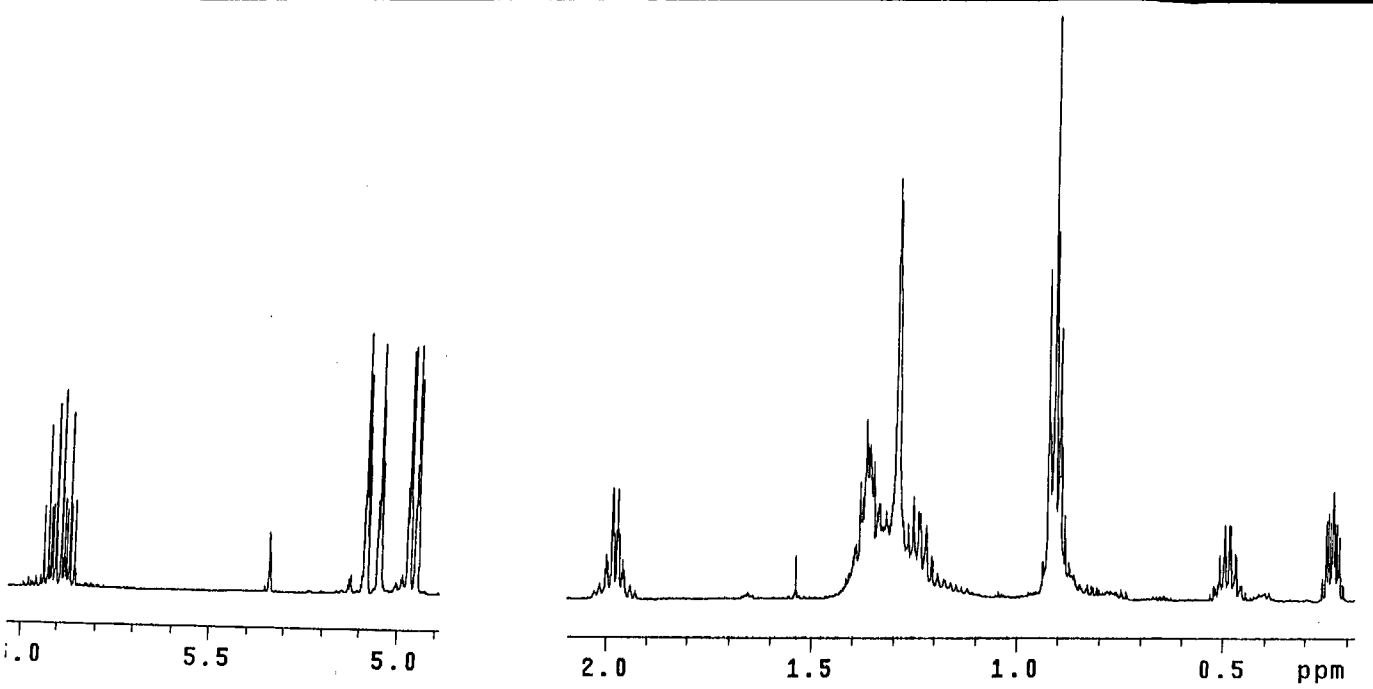
Univ of Minnesota, VI-500

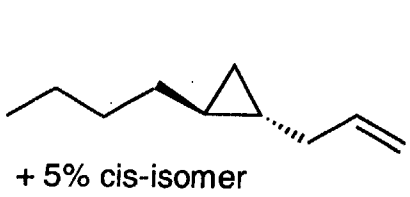
Pulse Sequence: s2pul

User: skalgl
Date: May. 5, 2000
Solvent: cd2cl2
File: allylbuthylcyclopr
Starting Time: 15:35:58
Completion Time: 15:36:27
Total acq. time 1 minute

UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
4 repetitions
OBSERVE H1, 499.8680816 MHz
DATA PROCESSING
FT size 32768

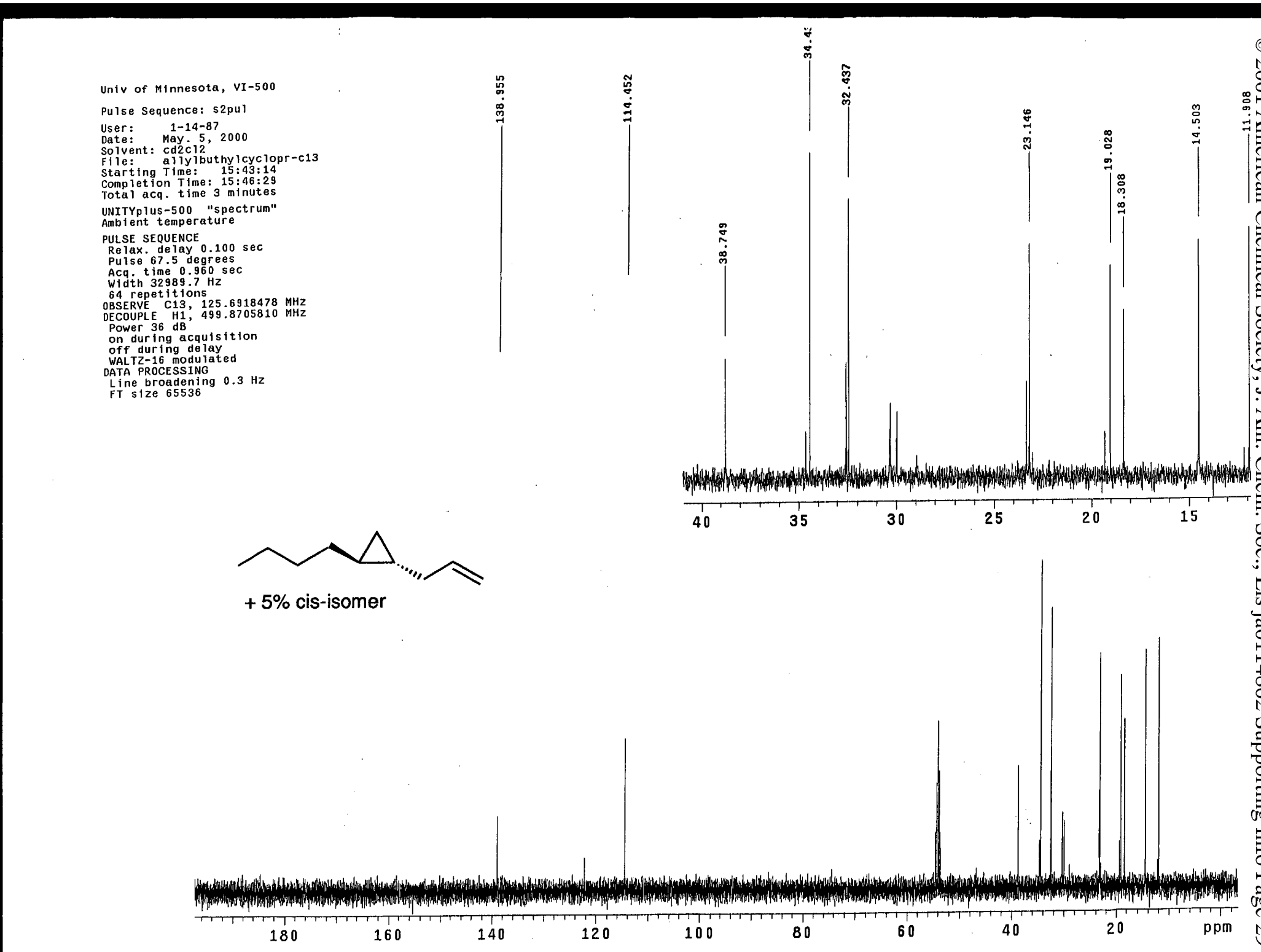




+ 5% cis-isomer

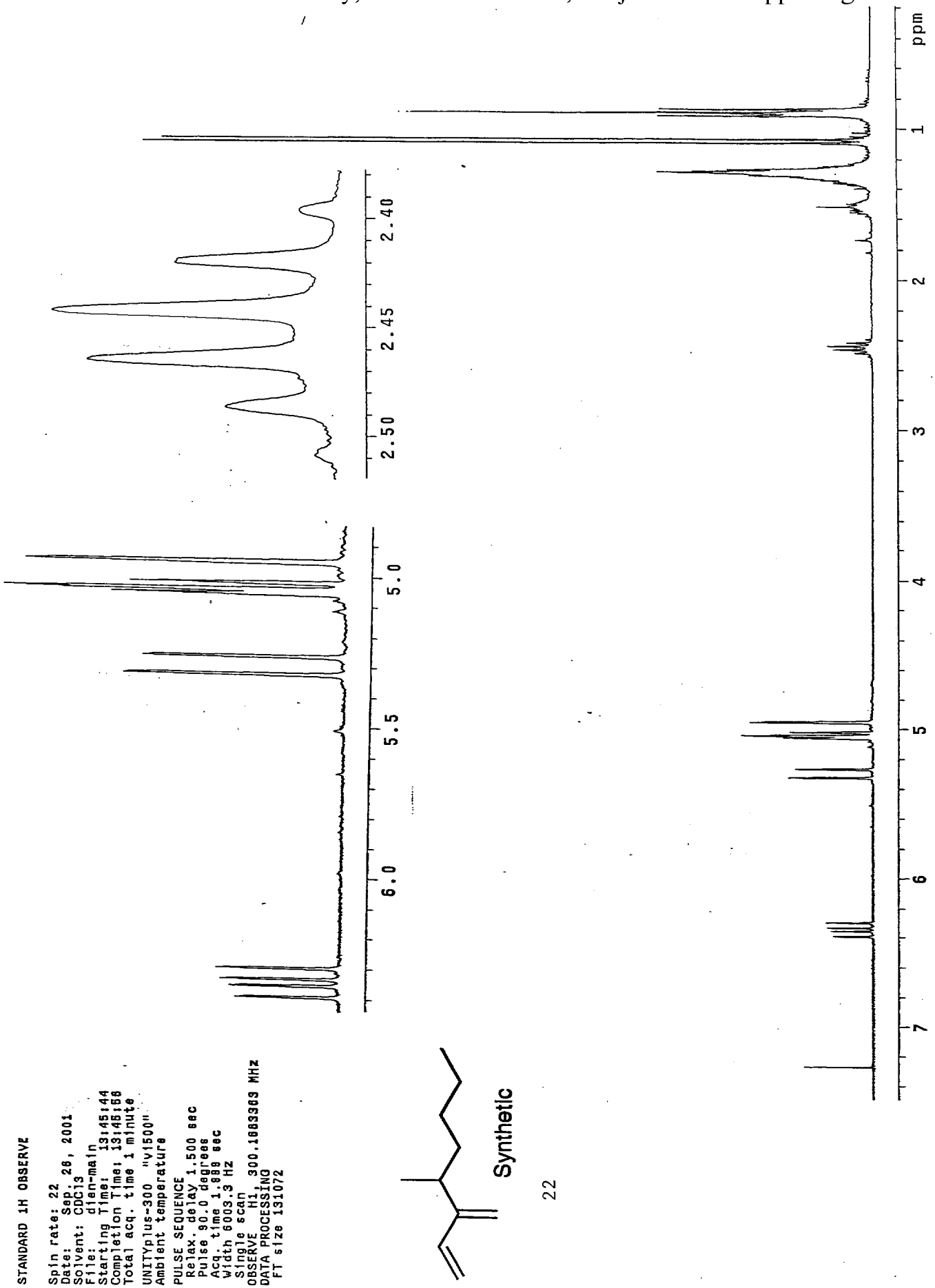
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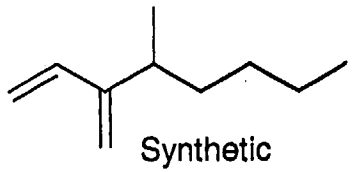
13C OBSERVE

Pulse Sequence: s2pul

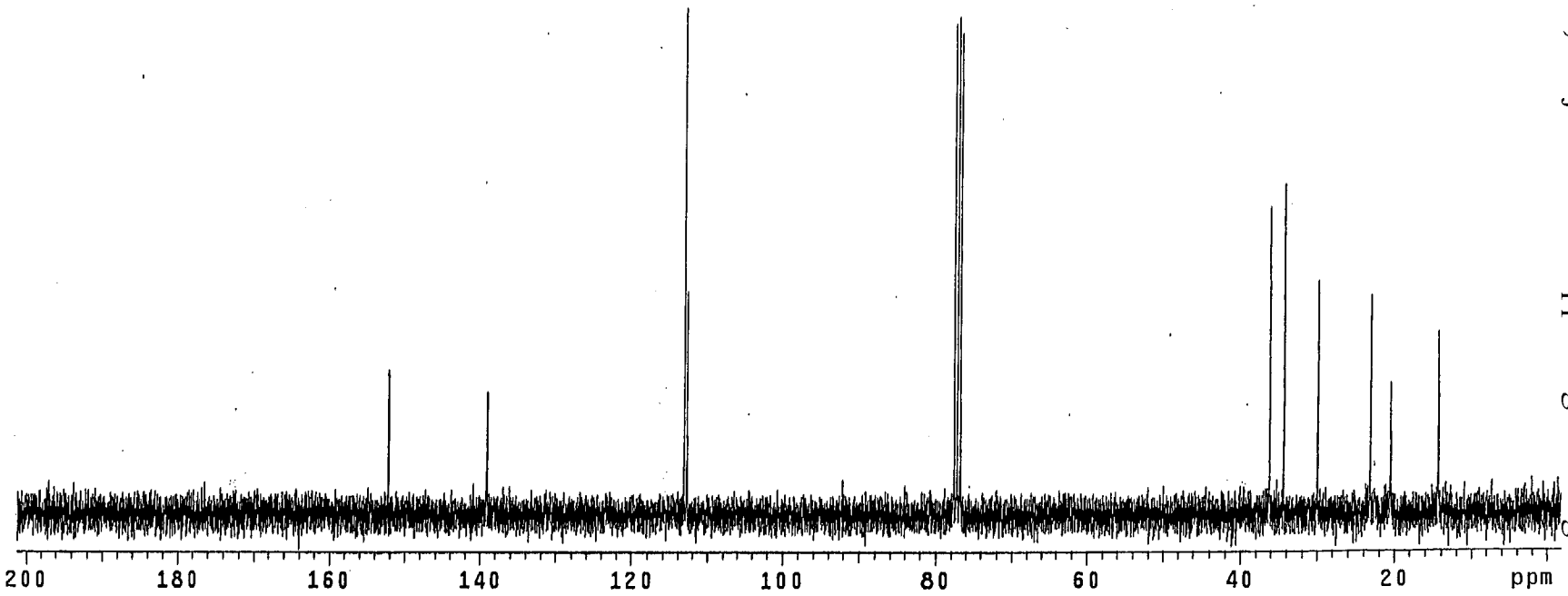
User: skalgl
Date: Sep. 26, 2001
Solvent: CDCl3
File: dien-main-c13
Starting Time: 13:54:12
Completion Time: 14:09:51
Total acq. time 15 minutes

UNITYplus-500 "spectrum"
Ambient temperature

PULSE SEQUENCE
Relax. delay 3.000 sec
Pulse 67.5 degrees
Acq. time 0.800 sec
Width 17361.1 Hz
160 repetitions
OBSERVE C13, 75.4773714 MHz
DECOUPLE H1, 300.1695405 MHz
Power 36 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Line broadening 0.4 Hz
FT size 131072



Synthetic



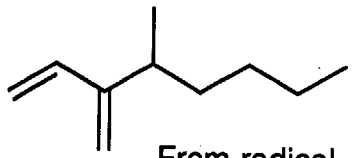
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STANDARD 1H OBSERVE

User: skaesk
Date: Mar. 31, 191999
Solvent: CDCl3
File: lev-secpr-prGCH1
Starting Time: 17:24:03
Completion Time: 17:25:04
Total acq. time 1 minute

UNITYplus-500 "fid"
Ambient temperature

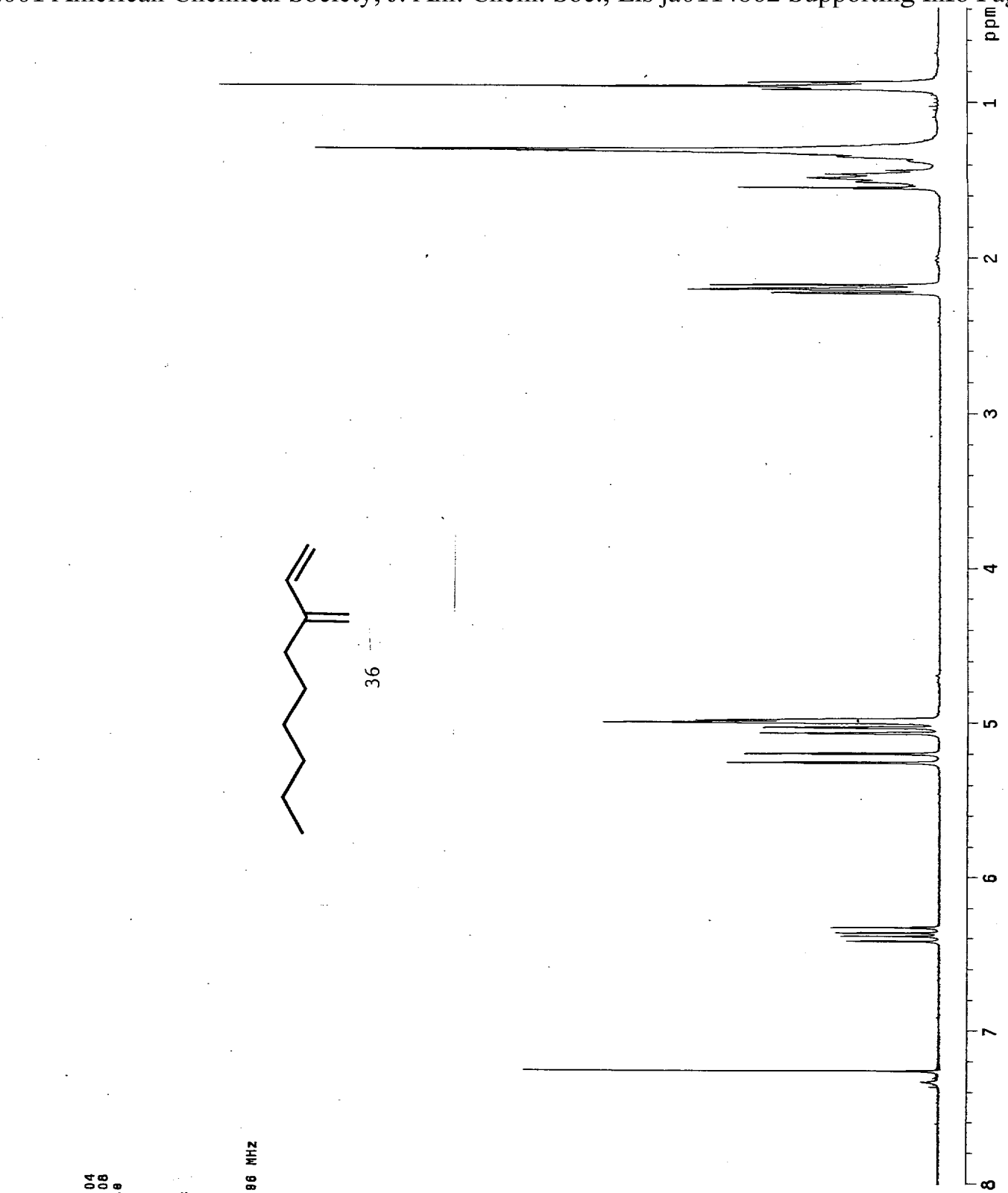
PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.999 sec
Width 6003.3 Hz
16 repetitions
OBSERVE H1, 300.1683396 MHz
DATA PROCESSING
FT size 131072



From radical degradation

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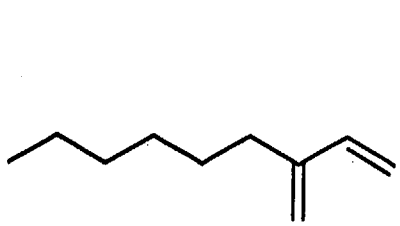


13C OBSERVE

Spin rate: 12
Date: Mar. 18, 1999
Solvent: CDCl3
Starting Time: 13:57:17
Completion Time: 14:09:23
Total acq. time 11 minutes

UNITYplus-300 "v1300"
Ambient temperature

PULSE SEQUENCE
Relax. delay 0.100 sec
Pulse 67.5 degrees
Acq. time 0.800 sec
Width 17361.1 Hz
256 repetitions
OBSERVE C13, 75.4773713 MHz
DECOUPLE H1, 300.1685405 MHz
Power 36 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072



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