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SUPPLEMENTARY MATERIAL FOR:

Further, Small-molecule Pyrolysis Products Derived from Chitin

Maryam Nikahd,[A] *Jiri Mikusek,*[A] *Martin G. Banwell,*[A,B,D] *Li-Juan Yu,*[C] *Michelle L. Coote*[C] *and Michael G. Gardiner*[A]

[A]Research School of Chemistry, Institute of Advanced Studies
The Australian National University, Canberra, ACT 2601, Australia
[B]Institute for Advanced and Applied Chemical Synthesis,
Jinan University, Guangzhou 510632, China
[C]ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry,
The Australian National University, Canberra, ACT 2601, Australia
[D]Corresponding author. Email: Martin.Banwell@anu.edu.au

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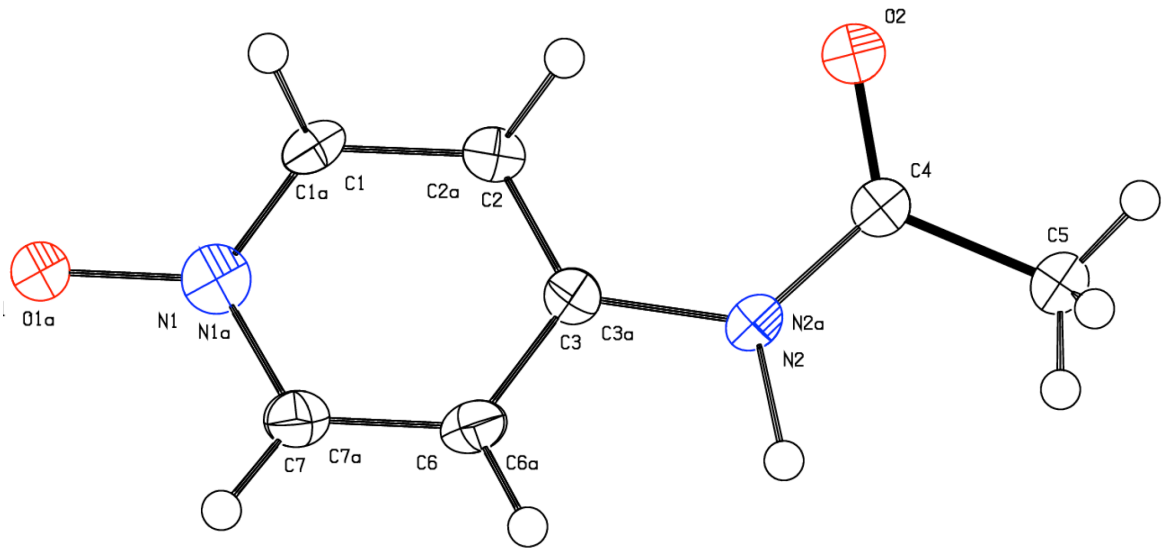

Figure S1: Structure of compound **18** (CCDC 2003422) with labelling of selected atoms. Anisotropic displacement ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii. Disorder has been omitted for clarity.

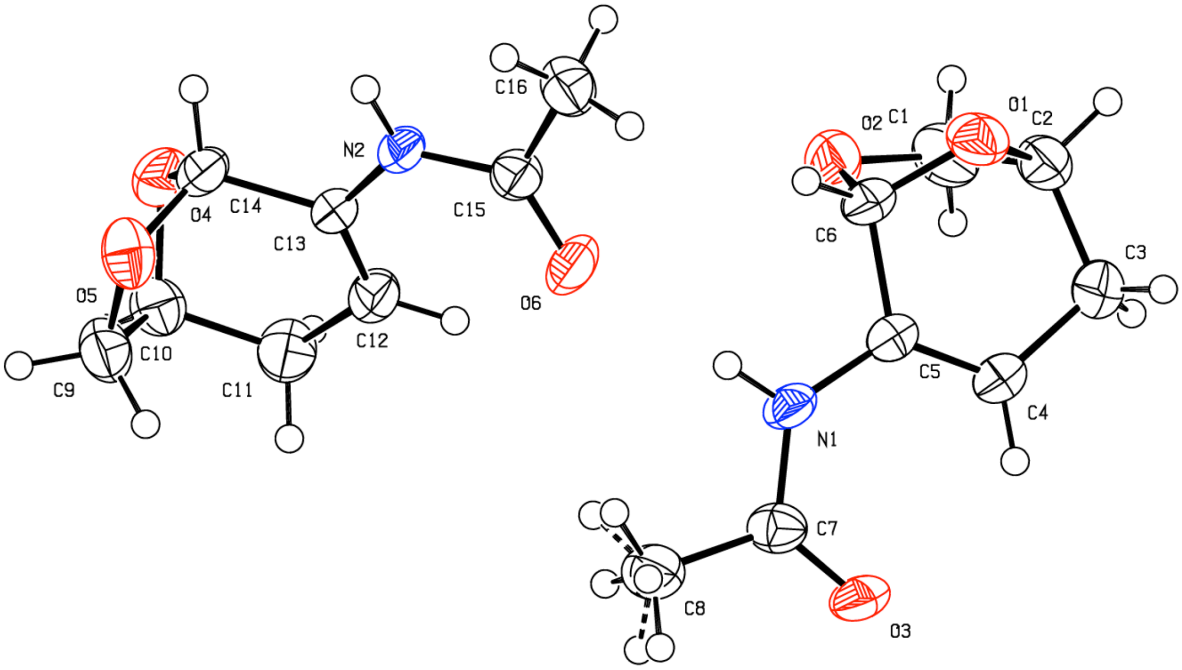

Figure S2: Structure of compound **19** (CCDC 2003423) with labelling of selected atoms showing both molecules in the asymmetric unit. Anisotropic displacement ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii (disorder in one of the methyl groups is shown).

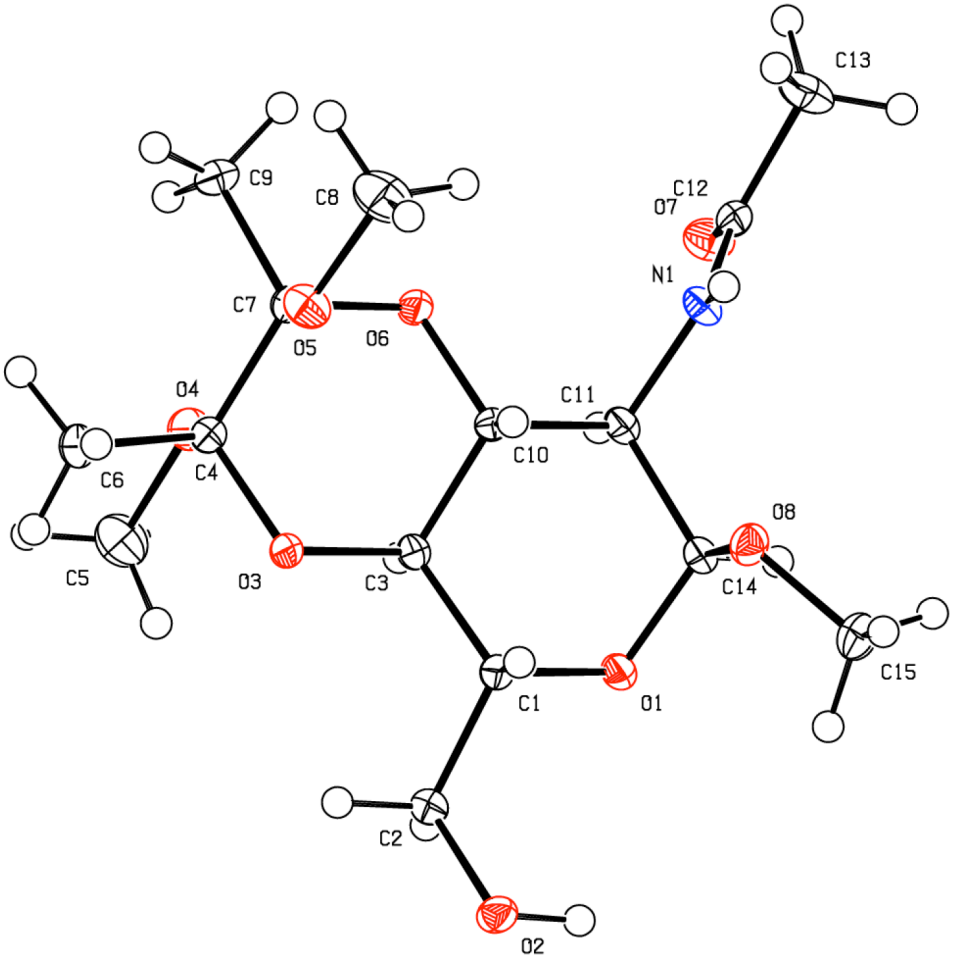

Figure S3: Structure of compound **29** (CCDC 2003424) with labelling of selected atoms. Anisotropic displacement ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

Table S1. Raw data (in Hartree, otherwise indicated) at 648.15 K used in Scheme 6.

Species	ZPVE	TC	S(J mol^{-1} K^{-1})	CCSD(T)/6-31G(d)	UMP2/6-31G(d)	UMP2/G3MP2large	HLC	G3(MP2,CC)
16	0.090422	0.025857	422.7932	-322.5860402	-322.5150527	-322.8666970	-0.174168	-323.0999476
H+	0	0.005131	124.9843	0.0000000	0.0000000	0.0000000	0.0000000	-0.0090620
H2O	0.020821	0.008465	215.7399	-76.20759491	-76.1966592	-76.3148275	-0.038704	-76.3884403
INT1	0.072426	0.021915	385.3193	-246.5771352	-246.5191168	-246.7579449	-0.135464	-246.9008432
CH3COOH	0.060275	0.018152	359.9518	-228.459446	-228.4183641	-228.6892798	-0.116112	-228.8089227
CH3COO–	0.046873	0.016862	361.7318	-227.8761718	-227.8388486	-228.1265800	-0.116112	-228.2573582
20	0.061978	0.020049	370.8459	-246.2466967	-246.1882580	-246.4331202	-0.135464	-246.6365459
9	0.071391	0.020358	389.2561	-208.6153973	-208.5686125	-208.8226756	-0.116112	-208.9899184
TS1	0.134381	0.038821	568.2608	-454.8474977	-454.7415450	-455.2417894	-0.251576	-455.5664011
INT2	0.139696	0.039348	567.3391	-455.0007079	-454.8943155	-455.3871421	-0.251576	-455.7061236
TS2	0.134381	0.038821	568.2608	-454.8474977	-454.7415450	-455.2417894	-0.251576	-455.5664011
21	0.139695	0.039349	567.4019	-455.0007081	-454.8943160	-455.3871427	-0.251576	-455.7061398
INT(H2O2)	0.167903	0.052111	725.024	-606.1672715	-606.04102527	-606.72634949	-0.319308	-607.1308747
TS(H2O2)	0.162723	0.052304	716.7225	-606.0849122	-605.95458264	-606.64570711	-0.319308	-607.0572526
18	0.14348	0.042971	607.4821	-529.9754094	-529.8647099	-530.4430552	-0.280604	-530.7978748
H2O2	0.026218	0.010769	265.0128	-151.1498855	-151.1290711	-151.3226230	-0.067732	-151.4396055
O3	0.00778	0.009702	270.8309	-224.8711951	-224.86173563	-225.10451699	-0.087084	-225.21433347
O2	0.00389	0.007371	228.3757	-149.9602401	-149.9468016	-150.1009031	-0.058056	-150.1870707
INT(O3)	0.148377	0.052334	761.1878	-679.8779579	-679.76356132	-680.49909752	-0.33866	-680.83788314
TS(O3)	0.148047	0.04973	685.693	-679.8413945	-679.69006660	-680.42661984	-0.33866	-680.79669770
CH3CO3H	0.063492	0.021873	407.9884	-303.4032166	-303.3529309	-303.7043134	-0.14514	-303.8607051
INT(CH3CO3H)	0.204559	0.063633	850.492	-758.4202783	-758.2645571	-759.1072576	-0.396716	-759.4880837
TS(CH3CO3H)	0.202386	0.062445	832.4499	-758.3779788	-758.2175066	-759.0592555	-0.396716	-759.4461447
INT(O2)	0.144203	0.049175	723.0782	-604.9629298	-604.8439731	-605.4927063	-0.309632	-605.8100290
TS(O2)	0.144296	0.046196	646.6037	-604.8900027	-604.7631730	-605.4191751	-0.309632	-605.7385728
O	0	0.005131	168.5963	-74.89654824	-74.8800367	-74.9500366	-0.029247	-75.0098101

Table S2. Raw data (in Hartree, otherwise indicated) at 648.15 K used in Scheme 7.

Species	ZPVE	TC	S(J mol^{-1} K^{-1})	CCSD(T)/6-31G(d)	UMP2/6-31G(d)	UMP2/G3MP2large	HLC	G3(MP2,CC)
INT(H2O2)	0.118814	0.038509	576.4687	-473.7528224	-473.66233490	-474.20646042	-0.2419	-474.5238359
TS(H2O2)	0.113629	0.038591	563.6195	-473.6694337	-473.57543849	-474.12502389	-0.2419	-474.4478381
INT(O3)	0.099434	0.038474	590.8698	-547.4620406	-547.38485269	-547.98129531	-0.261252	-548.24892626
TS(O3)	0.099047	0.036084	536.9018	-547.4259717	-547.31417317	-547.90951656	-0.261252	-548.20840611
INT(CH3CO3H)	0.155422	0.050106	701.7988	-626.004907	-625.8850346	-626.5865123	-0.319308	-626.8998606
TS(CH3CO3H)	0.153322	0.048744	686.5793	-625.9615536	-625.8371435	-626.5380996	-0.319308	-626.8577186
INT(O2)	0.095022	0.035622	573.6795	-472.5481421	-472.4646449	-472.9717622	-0.232224	-473.2219864
TS(O2)	0.095371	0.032455	495.9666	-472.476297	-472.3867768	-472.9017614	-0.232224	-473.1520017
22	0.094557	0.029312	456.5816	-397.5628724	-397.4882685	-397.9253478	-0.203196	-398.1919938
23	0.06601	0.023545	406.1735	-321.214846	-321.1509247	-321.4808104	-0.164492	-321.7199396
TS1	0.139238	0.043921	626.5658	-529.8326531	-529.7203516	-530.3026475	-0.280604	-530.6670720
INT2	0.142338	0.043243	606.2087	-529.8440555	-529.7339418	-530.3193306	-0.280604	-530.6741203
TS2	0.13816	0.042302	599.7249	-529.8299565	-529.7205301	-530.3052975	-0.280604	-530.6629179

Table S3. Raw data (in Hartree, otherwise indicated) at 648.15 K used for 3-acetamidopyridine in Scheme 8.

Species	ZPVE	TC	S(J mol^{-1} K^{-1})	CCSD(T)/6-31G(d)	UMP2/6-31G(d)	UMP2/G3MP2large	HLC	G3(MP2,CC)
TS1	0.135575	0.040032	586.6677	-454.8557426	-454.744651232	-455.241523411	-0.251576	-455.5734128
INT2	0.138093	0.039836	573.4577	-454.8627134	-454.754016862	-455.254417217	-0.251576	-455.5783287
TS2	0.13428	0.038804	567.0638	-454.8496645	-454.741799142	-455.241663614	-0.251576	-455.5680100
21(3-sub)	0.139386	0.039576	584.0872	-454.9962979	-454.890769540	-455.383478551	-0.251576	-455.7058129

Table S4. Raw data (in Hartree, otherwise indicated) at 648.15 K used for 3-acetamidopyridine in Scheme 9.

Species	ZPVE	TC	S(J mol^{-1} K^{-1})	CCSD(T)/6-31G(d)	UMP2/6-31G(d)	UMP2/G3MP2large	HLC	G3(MP2,CC)
TS1	0.139415	0.043793	626.2095	-529.8291179	-529.715129264	-530.296915798	-0.280604	-530.6628915
INT2	0.142178	0.043304	610.4465	-529.838438	-529.725459333	-530.311464309	-0.280604	-530.6702640
TS2	0.138296	0.042275	599.4092	-529.8259023	-529.713576373	-530.298927288	-0.280604	-530.6592602
21(3-sub)	0.143496	0.042942	603.0288	-529.9743332	-529.865190633	-530.443308235	-0.280604	-530.7954848

Table S5. Raw data (in Hartree, otherwise indicated) at 648.15 K used for 3-acetamidopyridine in Scheme 10.

Species	Ee	ZPVE	TC	S(J mol^{-1} K^{-1})	TS	H	G
26	-971.073397	0.262728	0.070184	822.282	0.202994	-970.740485	-970.943479
27	-591.66049	0.184294	0.04812	638.2875	0.157572	-591.428075	-591.585647
30	-1128.233685	0.369866	0.094374	1029.6334	0.254183	-1127.769445	-1128.023628
31	-1047.450043	0.287838	0.078586	913.1641	0.22543	-1047.083619	-1047.309049
32	-1204.616397	0.394795	0.102969	1127.0189	0.278224	-1204.118634	-1204.396857
33	-668.048161	0.209096	0.056648	733.9558	0.18119	-667.782418	-667.963607
34	-1049.68214	0.315958	0.082686	919.9887	0.227115	-1049.283495	-1049.51061
35	-1049.630729	0.3164	0.082002	942.8804	0.232766	-1049.232327	-1049.465093
36	-1126.058649	0.340839	0.091387	1027.9947	0.253778	-1125.626422	-1125.8802
37	-1126.012422	0.34107	0.090679	1039.2711	0.256562	-1125.580672	-1125.837234
TS_{26-27}	-970.935946	0.255011	0.07249	851.7106	0.210259	-970.608445	-970.818704
TS_{30-27}	-1128.084774	0.363442	0.096595	1067.1413	0.263442	-1127.624737	-1127.888179
TS_{31-33}	-1047.312513	0.279779	0.081281	955.0744	0.235776	-1046.951453	-1047.18723
TS_{32-33}	-1204.460817	0.387535	0.105696	1171.6689	0.289246	-1203.967586	-1204.256833
TS_{34-27}	-1049.532398	0.308291	0.085505	967.7356	0.238902	-1049.138602	-1049.377504
TS_{35-27}	-1049.48726	0.309487	0.084193	972.0624	0.23997	-1049.09358	-1049.33355
TS_{36-33}	-1125.911499	0.333218	0.093951	1061.0396	0.261936	-1125.484329	-1125.746265
TS_{37-33}	-1125.867133	0.333434	0.093364	1074.2445	0.265196	-1125.440336	-1125.705531
HCOOH	-189.693678	0.033159	0.011993	293.3557	0.07242	-189.648526	-189.720946
$HCOOCH_3$	-228.976241	0.060714	0.017479	352.0699	0.086914	-228.898048	-228.984963
CH_3COOH	-229.001852	0.060275	0.018152	359.9518	0.040876	-228.923425	-228.964301
CH_3COOCH_3	-268.283529	0.087507	0.02391	421.0818	0.103951	-268.172113	-268.276064

Cartesian coordinates for the optimized geometries shown in the manuscript

16.xyz

C	-1.202563	1.134912	0.000014
C	0.182898	1.228664	0.000021
C	0.918910	0.046751	0.000053
C	0.233021	-1.170091	0.000118
C	-1.798389	-0.127254	0.000001
H	-1.817524	2.028462	0.000055
H	0.787678	-2.108782	0.000037
H	-2.879517	-0.231143	-0.000155
N	-1.095459	-1.260484	-0.000081
H	0.700757	2.182025	0.000048
O	2.276167	0.128660	-0.000117
H	2.664223	-0.754344	0.000271

18.xyz

C	0.778851	1.402529	0.002448
C	-0.144443	0.351016	0.003207
C	0.365011	-0.952453	0.001566
C	1.733508	-1.149846	-0.000860
C	2.134148	1.151280	-0.000023
H	0.448855	2.436979	0.003654
H	2.200338	-2.125596	-0.002213
H	2.899359	1.915477	-0.000839
N	2.621105	-0.119695	-0.001727
H	-0.295024	-1.807554	0.002303
N	-1.510691	0.667765	0.005724
H	-1.729724	1.653059	0.005876
C	-2.576994	-0.203784	0.003334
O	-2.447806	-1.413695	0.003455
C	-3.940242	0.453817	-0.007973
H	-3.907286	1.542575	0.065331
H	-4.448494	0.171638	-0.932702
H	-4.519599	0.052457	0.825418
O	3.882761	-0.335165	-0.004080

20.xyz

C	1.427447	-0.190946	-0.000002
C	0.546843	-1.246407	0.000016
C	-0.703112	-1.190712	-0.000002
C	-1.410786	0.005542	-0.000027
C	0.683641	1.017105	-0.000035
H	2.509980	-0.204039	0.000019
H	-2.487056	0.127360	-0.000005
H	1.224733	1.959875	-0.000001
N	-0.644551	1.107045	0.000041

21.xyz

C	1.257122	-1.316474	-0.007837
C	0.301204	-0.292992	-0.012849
C	0.756526	1.028915	-0.003646
C	2.134593	1.239050	0.010663
C	2.603379	-0.979359	0.006448
H	0.957415	-2.360775	-0.014662
H	2.511653	2.258808	0.018197
H	3.356105	-1.763840	0.010628
N	3.058627	0.276657	0.015905
H	0.066145	1.859243	-0.007859
N	-1.050204	-0.661550	-0.027649
H	-1.226857	-1.655930	-0.030603

C	-2.158723	0.160144	-0.015715
O	-2.092611	1.373538	-0.013664
C	-3.481957	-0.575356	0.030790
H	-3.430735	-1.581794	-0.390507
H	-3.805429	-0.647000	1.073231
H	-4.219228	0.013670	-0.514023

22.xyz

C	-0.131741	1.744983	0.000019
C	1.127130	1.158285	0.000058
C	1.184789	-0.234951	0.000025
C	0.016641	-0.983961	-0.000053
C	-1.282780	0.976790	-0.000091
H	-0.235912	2.823998	0.000056
H	-0.024368	-2.065922	0.000101
H	-2.293298	1.359312	-0.000015
N	-1.205762	-0.383182	-0.000082
H	2.042365	1.736898	0.000064
O	2.405210	-0.824813	-0.000003
H	2.323973	-1.785865	-0.000124
O	-2.262292	-1.094314	0.000096

23.xyz

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C	-0.965001	1.331046	0.000000
C	0.403028	1.238532	0.000000
C	-0.027769	-1.134356	-0.000000
H	-2.078476	-1.842692	0.000000
H	1.182554	1.986409	0.000000
H	0.479962	-2.089244	-0.000001
N	0.853749	-0.069135	-0.000001
O	2.106822	-0.294156	0.000000

26.xyz

C	2.370602	-0.459324	-0.536285
C	1.558737	0.608014	0.188509
C	0.329036	0.000466	0.904567
C	-0.239536	-1.317094	0.280414
C	0.878527	-2.085472	-0.424414
H	3.116859	0.015443	-1.175565
H	2.191197	1.085190	0.948995
H	-0.588248	-1.946468	1.101343
H	0.499961	-2.971286	-0.939314
H	0.676593	-0.271988	1.907195
O	1.517174	-1.250996	-1.355427
C	2.934450	-1.515482	0.419604
H	3.812123	-2.011708	-0.004549
H	3.177731	-1.119384	1.410429
O	1.863793	-2.451400	0.530498
N	-1.347531	-1.102756	-0.620847
H	-1.152291	-0.480511	-1.402614
C	-2.642270	-1.012477	-0.186529
O	-3.472432	-0.354719	-0.808762
C	-3.027404	-1.752309	1.074604
H	-2.630416	-2.769902	1.096624
H	-2.648782	-1.209761	1.946835
H	-4.114935	-1.777504	1.120468
O	1.213982	1.579201	-0.783105
O	-0.710004	0.946708	1.127941
C	0.417203	2.610918	-0.253691

C	-0.905011	2.028351	0.228192
H	0.223489	3.285155	-1.092161
H	-1.456406	2.761448	0.825650
O	1.030086	3.261188	0.821577
H	1.782988	3.766411	0.492954
O	-1.574016	1.697209	-0.943480
H	-2.451808	1.313083	-0.774125

27.xyz

C	-2.377962	0.497854	0.504134
C	-1.852327	1.431134	-0.559842
C	-0.621701	1.242587	-1.038711
C	0.248828	0.117183	-0.525654
C	-0.575055	-0.761386	0.435388
H	-3.129216	0.955903	1.147884
H	-2.494836	2.223577	-0.932435
H	0.556020	-0.512481	-1.366494
H	0.056582	-1.442231	1.012957
H	-0.191671	1.900161	-1.789354
O	-1.292354	0.057284	1.322819
C	-2.803530	-0.846474	-0.108121
H	-3.413036	-1.426173	0.592925
H	-3.311744	-0.751174	-1.069870
O	-1.544166	-1.487551	-0.305929
N	1.432711	0.659063	0.112845
H	1.295153	1.416094	0.772990
C	2.685258	0.101299	0.150697
O	3.563065	0.579369	0.848765
C	2.929129	-1.107899	-0.731157
H	2.792048	-0.856057	-1.786971
H	3.955840	-1.430953	-0.568799
H	2.247682	-1.928727	-0.488380

31.xyz

C	-2.232985	-1.500435	-0.593755
C	-0.878565	-1.382753	0.097517
C	-0.826441	-0.162945	1.016467
C	-1.553635	1.074654	0.419355
C	-2.873506	0.575346	-0.193823
H	-2.226444	-2.308152	-1.327882
H	-0.709878	-2.288567	0.696688
H	-1.785200	1.757176	1.241142
H	-3.481049	1.400774	-0.569993
H	-1.384020	-0.411622	1.926409
O	-2.560217	-0.287798	-1.262689
C	-3.367361	-1.575567	0.435612
H	-4.268408	-2.024350	0.007834
H	-3.090446	-2.103729	1.353377
O	-3.613092	-0.200526	0.734451
N	-0.879485	1.810625	-0.620940
H	-0.753692	1.331243	-1.506607
C	-0.066960	2.898118	-0.456884
O	0.546717	3.371467	-1.401935
C	0.020901	3.495581	0.931610
H	-0.951432	3.868242	1.268614
H	0.371686	2.741095	1.642226
H	0.723802	4.326616	0.890426
O	0.128192	-1.281120	-0.892931
O	0.494686	0.076757	1.475819
C	1.433175	-1.314248	-0.336988
C	1.628401	-0.110004	0.641880

```
O        1.603153   -2.474931    0.443963
O        1.763370    1.045829   -0.149159
C        1.473552   -3.708886   -0.239872
H        2.371518   -3.938684   -0.823784
H        1.345261   -4.473230    0.527953
H        0.601425   -3.707630   -0.904470
C        3.010073    1.704490   -0.277627
H        2.811630    2.547295   -0.941615
H        3.374660    2.080222    0.684697
H        3.774691    1.057683   -0.725904
C        2.381811   -1.262817   -1.521908
H        3.418343   -1.349653   -1.184573
H        2.159104   -2.087746   -2.201663
H        2.242482   -0.325645   -2.060110
C        2.778346   -0.331680    1.612408
H        3.725809   -0.481760    1.089480
H        2.859108    0.538807    2.267395
H        2.564132   -1.213310    2.212809

30.xyz
C        0.411723   -1.256421   -0.904317
C       -0.867165   -1.799247   -0.255768
C       -2.021495    0.258826   -0.115162
C       -0.719432    1.052052   -0.317129
C        0.321924    0.292305   -1.139186
H       -1.070838   -2.826523   -0.588060
H       -0.926823    1.985471   -0.858474
H       -2.185670    0.176721    0.966173
H        0.018560    0.415989   -2.184316
H        0.473535   -1.710020   -1.899270
O       -1.968177   -1.040147   -0.696079
O       -0.714716   -1.758172    1.126359
C       -1.775027   -2.394185    1.823161
H       -1.815479   -3.459911    1.564201
H       -1.560910   -2.284136    2.885836
H       -2.739083   -1.930471    1.585598
C       -3.213130    0.960922   -0.730847
H       -3.206031    2.007959   -0.394851
H       -3.114217    0.940480   -1.826102
O       -4.380578    0.295587   -0.299275
H       -5.135661    0.596834   -0.813689
N        1.577497   -1.685075   -0.176831
H        1.594076   -1.434160    0.808421
C        2.785140   -1.736725   -0.789829
H        2.719921   -1.905996   -1.878912
O        3.858460   -1.627522   -0.215644
O       -0.222436    1.395880    0.970105
O        1.595935    0.919880   -1.069827
C        0.916137    2.217462    0.899824
H        1.232904    2.360567    1.936526
C        2.040901    1.515797    0.139859
H        2.781690    2.249118   -0.194040
O        0.653810    3.433321    0.256511
H        0.039598    3.942033    0.799059
O        2.583287    0.615840    1.053213
H        3.329808    0.129512    0.663160

32.xyz
C       -1.119845   -1.001252   -0.945983
C       -2.462569   -0.233361   -1.118262
C       -1.423626    1.456788    0.166123
```

C	-0.003952	1.202637	-0.351060
C	-0.008128	-0.003390	-1.303331
H	-2.796696	-0.299676	-2.165580
H	0.367744	2.081893	-0.890764
H	-1.625673	0.816127	1.035142
H	-0.251935	0.370623	-2.302755
H	-1.105876	-1.810526	-1.686770
O	-2.323325	1.150778	-0.890700
O	-3.400483	-0.812183	-0.275414
C	-4.682752	-0.207376	-0.356329
H	-5.055344	-0.228559	-1.389677
H	-5.341948	-0.797152	0.280298
H	-4.643978	0.826685	-0.003204
C	-1.632559	2.898610	0.561509
H	-0.800590	3.198506	1.213800
H	-1.616949	3.515809	-0.348221
O	-2.876769	2.991325	1.226815
H	-3.059542	3.911892	1.438922
N	-0.936249	-1.563627	0.373947
H	-0.190432	-1.203745	0.963945
C	-1.497085	-2.735815	0.760518
H	-2.217433	-3.136939	0.026030
O	-1.237859	-3.307530	1.804816
O	0.826671	0.962565	0.773806
O	1.275782	-0.593683	-1.449838
C	2.174578	0.697627	0.434267
C	2.204766	-0.629368	-0.377344
O	2.612687	1.738704	-0.414091
O	1.875332	-1.617789	0.565767
C	3.880588	2.327615	-0.203061
H	4.692412	1.592965	-0.266022
H	4.005038	3.056038	-1.005460
H	3.938192	2.846748	0.758916
C	1.798411	-2.954172	0.090481
H	1.239172	-3.512289	0.842990
H	1.265544	-2.999594	-0.865672
H	2.798822	-3.386479	-0.022551
C	2.910717	0.603246	1.758081
H	3.963491	0.346774	1.622429
H	2.830687	1.560579	2.277519
H	2.437714	-0.170518	2.360076
C	3.545603	-0.894367	-1.044370
H	3.800543	-0.061143	-1.700011
H	4.326341	-1.037846	-0.292462
H	3.473258	-1.796800	-1.655282

38.xyz

C	1.052188	0.573147	-0.327124
C	0.144260	-0.642920	-0.544675
C	-1.791791	0.413511	0.326719
C	-0.899126	1.460311	0.932180
C	0.395986	1.537359	0.634192
H	0.443307	-1.201922	-1.442399
H	-1.346597	2.139265	1.654464
H	-2.038135	-0.338775	1.093885
H	1.038440	2.289995	1.084470
H	1.183317	1.063271	-1.300421
O	-1.175110	-0.233165	-0.782041
O	0.248751	-1.451972	0.589859
C	-0.429798	-2.691301	0.452741
H	0.000473	-3.274490	-0.371360

```
H       -0.291897   -3.230093    1.389941
H       -1.497604   -2.535711    0.264741
C       -3.099211    0.995314   -0.177175
H       -3.519019    1.648411    0.601131
H       -2.890956    1.596651   -1.071582
O       -3.971190   -0.080908   -0.457465
H       -4.691742    0.222219   -1.017958
N        2.362461    0.152500    0.118019
H        2.411732   -0.466354    0.919872
C        3.529443    0.496475   -0.484788
H        3.377309    1.146853   -1.367715
O        4.631603    0.143771   -0.117306

33.xyz
C        1.893689   -1.768392    0.450227
C        0.589055   -1.544117   -0.309432
C        0.511532   -0.114313   -0.916482
C        1.409955    0.982066   -0.247368
C        2.609392    0.325089    0.433379
H        1.811954   -2.673157    1.054411
H        0.548048   -2.268574   -1.136314
H        1.800048    1.622866   -1.041269
H        3.208056    1.051653    0.987959
H        0.887994   -0.207108   -1.941898
O        2.160588   -0.669459    1.316850
C        3.118484   -1.723457   -0.465768
H        3.969938   -2.246390   -0.020345
H        2.929117   -2.113881   -1.469816
O        3.400944   -0.326902   -0.547846
N        0.710361    1.815366    0.701491
H        0.343581    1.310705    1.505360
C       -0.098236    2.847315    0.311421
O       -1.063488    3.185668    0.994229
C        0.234279    3.565261   -0.975388
H        1.300414    3.788500   -1.059804
H       -0.061911    2.940232   -1.824052
H       -0.341452    4.489190   -0.997609
O       -0.460198   -1.832648    0.581909
O       -0.830690    0.343608   -1.070792
C       -1.753201   -1.578172    0.048022
C       -1.855955   -0.050226   -0.125511
O       -1.932569   -2.216505   -1.188557
H       -1.613295   -1.635374   -1.893024
O       -1.681392    0.477021    1.144877
H       -1.840825    1.439257    1.147162
C       -2.739209   -2.161650    1.032951
H       -3.761095   -1.984886    0.692683
H       -2.565686   -3.238373    1.085863
H       -2.588417   -1.712774    2.014329
C       -3.146663    0.440782   -0.758999
H       -3.068949    1.522354   -0.907312
H       -3.329959   -0.034199   -1.723959
H       -3.984373    0.235019   -0.090463

35.xyz
C       -0.001444    2.553611   -0.641409
C       -0.847865    1.462046    0.003673
C       -0.021376    0.624395    0.982408
C        1.420272    0.351315    0.480529
C        1.951036    1.652058   -0.150523
H       -0.573796    3.082013   -1.405121
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H       -1.691342    1.922622    0.533466
H        2.030697    0.105724    1.352626
H        2.986585    1.548959   -0.483795
H        0.088444    1.207828    1.902198
O        1.146900    1.980687   -1.253756
C        0.649494    3.454966    0.415129
H        0.924342    4.427394   -0.002767
H        0.032549    3.597787    1.307945
O        1.832614    2.732876    0.763029
N        1.523863   -0.717675   -0.480101
H        0.829440   -0.757288   -1.219762
C        2.371256   -1.785010   -0.443218
O        2.300396   -2.676566   -1.277037
C        3.401633   -1.827950    0.670860
H        3.997540   -0.911797    0.713995
H        2.917989   -1.963812    1.643794
H        4.054906   -2.677028    0.477257
O       -1.350277    0.631496   -1.035276
O       -0.719833   -0.547318    1.385296
C       -2.247285   -0.317105   -0.539208
C       -1.551273   -1.237531    0.473312
O       -3.337522    0.345452    0.046664
O       -0.880733   -2.188450   -0.287208
C       -4.550881   -0.375322   -0.028680
H       -5.315547    0.243103    0.441156
H       -4.826996   -0.565703   -1.073695
H       -4.491462   -1.332258    0.505795
C       -0.289697   -3.224040    0.479063
H        0.220033   -3.881267   -0.223621
H        0.437091   -2.815895    1.190175
H       -1.062779   -3.774813    1.032384
H       -2.566056   -0.919558   -1.398065
H       -2.294260   -1.726296    1.121431

34.xyz
C        0.624422    1.468760   -0.897476
C        2.140717    1.176594   -0.716293
C        1.693805   -1.038040   -0.092030
C        0.267271   -1.160354   -0.614784
C       -0.193388    0.175604   -1.248283
H        2.740582    1.714040   -1.463195
H        0.228146   -1.918804   -1.409297
H        1.664802   -0.613646    0.920612
H       -0.049667    0.039642   -2.325129
H        0.518572    2.111618   -1.777725
O        2.424780   -0.180998   -0.960478
O        2.516524    1.561401    0.566591
C        3.893182    1.329090    0.837890
H        4.517605    1.816377    0.077192
H        4.092141    1.775899    1.811856
H        4.114608    0.257440    0.858633
C        2.404996   -2.369218   -0.036472
H        1.738254   -3.096033    0.446814
H        2.615719   -2.696948   -1.064177
O        3.599620   -2.191500    0.702438
H        4.125810   -2.996196    0.663800
N        0.063138    2.218546    0.196075
H        0.126666    1.811135    1.123472
C       -0.984893    3.045236   -0.015411
H       -1.041097    3.425854   -1.049480
O       -1.801403    3.367874    0.838012
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O       -0.522187   -1.607108    0.469956
O       -1.576639    0.439857   -1.099131
C       -1.916115   -1.561001    0.230363
C       -2.305183   -0.084905    0.012084
O       -2.244250   -2.242428   -0.953750
O       -1.980115    0.539864    1.218123
C       -2.569395   -2.186644    1.447261
H       -3.653238   -2.219005    1.320466
H       -2.190991   -3.207646    1.561494
H       -2.319633   -1.614695    2.340230
C       -3.761498    0.126832   -0.361544
H       -4.007074   -0.433497   -1.263952
H       -4.409411   -0.184548    0.460140
H       -3.917029    1.193957   -0.547012
H       -2.158575   -3.190141   -0.792756
H       -2.272309    1.467975    1.209574

36.xyz
C       -0.782403    0.979192    0.948080
C       -2.145290    0.242972    1.105138
C       -1.160369   -1.451501   -0.212918
C        0.273980   -1.233994    0.280453
C        0.305854   -0.054811    1.266686
H       -2.481701    0.301713    2.152047
H        0.651878   -2.133197    0.783299
H       -1.359532   -0.791465   -1.068563
H        0.065842   -0.454117    2.256644
H       -0.742570    1.763069    1.714552
O       -2.037634   -1.142012    0.860197
O       -3.063061    0.856529    0.266578
C       -4.363060    0.288994    0.339741
H       -4.737487    0.313356    1.372283
H       -5.002674    0.902845   -0.293994
H       -4.353745   -0.742988   -0.021459
C       -1.405690   -2.881405   -0.630591
H       -0.591004   -3.186317   -1.301972
H       -1.387993   -3.515495    0.267460
O       -2.662292   -2.934547   -1.275719
H       -2.862110   -3.844878   -1.515085
N       -0.587893    1.585395   -0.349553
H        0.105879    1.201773   -0.985093
C       -1.083280    2.806917   -0.670731
H       -1.750099    3.221332    0.107050
O       -0.825793    3.404025   -1.699405
O        1.079122   -0.975921   -0.865050
O        1.604201    0.509513    1.413970
C        2.413763   -0.724378   -0.535459
C        2.487976    0.545928    0.317394
O        2.938897   -1.830637    0.144280
O        2.241026    1.589762   -0.571596
C        4.334050   -1.993423   -0.015073
H        4.895011   -1.146357    0.399566
H        4.609702   -2.897002    0.528355
H        4.594357   -2.112181   -1.074730
C        2.285826    2.883321    0.008694
H        2.039549    3.587102   -0.785933
H        1.552790    2.974239    0.816743
H        3.289467    3.090622    0.402672
H        3.477773    0.662343    0.782108
H        2.938041   -0.552711   -1.483601
```

9.xyz
C -0.073863 0.144806 0.007330
O -0.352286 1.330517 -0.000516
N -1.034889 -0.823771 0.001987
H -0.815439 -1.805142 0.002644
H -2.001063 -0.534947 -0.023852
C 1.359552 -0.346345 0.000370
H 1.455159 -1.407585 0.238855
H 1.780263 -0.165285 -0.991992
H 1.929454 0.244460 0.718357

CH3CO3H.xyz
C 1.788434 -0.428632 0.000028
H 2.317901 -0.071401 0.885241
H 2.319283 -0.068592 -0.883198
H 1.751144 -1.517093 -0.001631
C 0.413250 0.167407 -0.000067
O 0.132757 1.343553 -0.000014
O -0.535756 -0.789457 -0.000086
O -1.839669 -0.241480 0.000072
H -1.657082 0.723502 0.000051

CH3COO-.xyz
C -1.347079 0.049655 -0.000693
H -1.731958 -0.530738 -0.846428
H -1.714517 1.078048 -0.056984
H -1.721091 -0.425556 0.913387
C 0.209621 -0.001390 -0.002177
O 0.699353 -1.157052 0.000382
O 0.799686 1.105634 0.000523

CH3COOCH3.xyz
C 0.458499 0.173055 -0.000054
O -0.546599 -0.721909 -0.000076
O 0.275980 1.366616 -0.000008
C -1.861747 -0.162583 0.000049
H -2.011016 0.453821 -0.888826
H -2.543027 -1.011348 0.000007
H -2.010918 0.453656 0.889056
C 1.798744 -0.510143 0.000019
H 1.886169 -1.147762 0.882708
H 1.885388 -1.149842 -0.881224
H 2.585383 0.241846 -0.001127

CH3COOH.xyz
C -1.392813 -0.119199 0.000006
H -1.666938 -0.701421 -0.882790
H -1.915012 0.835265 0.001078
H -1.667064 -0.703705 0.881206
C 0.089584 0.124039 0.000128
O 0.785558 -1.033154 0.000017
H 1.727299 -0.802491 -0.000289
O 0.632079 1.201067 -0.000019

H+.xyz
H 0.000000 0.000000 0.000000

H2O.xyz
O 0.000000 -0.000000 0.115587
H 0.000000 0.768653 -0.462347
H -0.000000 -0.768653 -0.462347

H2O2.xyz
O 0.000000 -0.713471 -0.054457
H -0.812754 -0.900615 0.435653
O 0.000000 0.713471 -0.054457
H 0.812754 0.900615 0.435653

HCOOCH3.xyz
C -0.826534 0.436256 -0.000034
O 0.476138 0.729296 -0.000052
O -1.286986 -0.674672 0.000046
C 1.355188 -0.400915 0.000032
H 1.184267 -1.010437 -0.889525
H 2.362776 0.009289 0.000011
H 1.184255 -1.010315 0.889670
H -1.416439 1.362421 -0.000103

HCOOH.xyz
C -0.000000 0.423191 -0.000000
O -1.028072 -0.435455 -0.000000
H -0.664976 -1.336001 0.000000
O 1.157226 0.102947 0.000000
H -0.368255 1.456922 -0.000000

O.xyz
O 0.000000 0.000000 0.000000

O2.xyz
O 0.000000 0.000000 0.599016
O 0.000000 0.000000 -0.599016

O3.xyz
O -0.000000 0.000000 0.424485
O -0.000000 -1.062634 -0.212242
O 0.000000 1.062634 -0.212242

Scheme6_INT1.xyz
C -1.462048 0.085594 -0.000154
C -0.780812 -1.133369 0.000032
C 0.565758 -0.851309 -0.000020
C 1.690343 -0.162899 -0.000097
C -0.542896 1.164454 0.000145
H -2.540829 0.197443 -0.000163
H 2.771948 -0.088357 -0.000086
H -0.755360 2.226419 0.000303
N 0.701675 0.739482 0.000054
H -1.209557 -2.126713 0.000125

Scheme6_INT2.xyz
C -0.972488 -1.178866 -0.648883
C -0.314270 0.023029 -0.536231
C -0.769363 1.225568 0.002413
C -2.076112 1.172525 0.475145
C -2.282453 -1.038295 -0.117995
H -2.541007 2.052419 0.912335
H -2.956858 -1.894432 -0.127282
N -2.823996 0.062147 0.421113
C 2.137080 -0.012098 0.071957
O 3.004770 0.803454 -0.008762
N 1.118050 -0.040871 -1.032226
H 1.095144 -0.970163 -1.492382

```
H        1.364460    0.693428   -1.704074
C        1.892213   -1.007625    1.156934
H        2.816588   -1.145982    1.715506
H        1.113478   -0.611319    1.816500
H        1.506700   -1.945947    0.750006
H       -0.182685    2.140010    0.057234

Scheme6_INT_CH3CO3H.xyz
C       -1.143260   -0.511235   -0.452790
C       -1.920349    0.520337    0.086300
C       -1.283111    1.724645    0.419161
C        0.078199    1.847221    0.200105
C        0.217947   -0.281351   -0.629203
H       -1.582580   -1.459220   -0.724593
H        0.595876    2.770476    0.446203
H        0.862928   -1.054864   -1.036090
N        0.827564    0.866173   -0.314400
C        4.694798   -1.452533    1.188081
H        4.886433   -0.801806    2.041305
H        5.651718   -1.727850    0.736635
H        4.180384   -2.361081    1.499251
C        3.864156   -0.757381    0.140901
O        3.147543   -1.296980   -0.662786
O        4.044255    0.578303    0.231474
O        3.438109    1.285113   -0.832925
H        2.456785    1.113932   -0.673200
H       -1.841811    2.554913    0.840792
N       -3.295150    0.429467    0.316538
H       -3.726212    1.257600    0.702834
C       -4.138116   -0.636839    0.055651
C       -5.594290   -0.361773    0.364801
H       -5.724141    0.269943    1.246886
H       -6.053064    0.139055   -0.493084
H       -6.096821   -1.315647    0.518086
O       -3.753937   -1.691620   -0.405516

Scheme6_INT_H2O2.xyz
C        0.200556    1.737004   -0.080932
C        0.886102    0.515569   -0.019182
C        0.132136   -0.658612    0.083469
C       -1.254729   -0.542303    0.117264
C       -1.183997    1.734584   -0.037766
H        0.739192    2.676733   -0.160401
H       -1.878361   -1.429253    0.190928
H       -1.733708    2.670813   -0.082658
N       -1.914331    0.619218    0.058634
H        0.607402   -1.626659    0.133578
N        2.282575    0.551533   -0.064830
H        2.690843    1.473384   -0.128982
C        3.167528   -0.510285   -0.012300
O        2.813833   -1.669328    0.059450
C        4.625389   -0.102098   -0.016232
H        4.810683    0.800736   -0.602956
H        4.945630    0.079139    1.014135
H        5.210125   -0.928482   -0.418066
O       -4.598518   -0.020070    0.286762
O       -4.327073   -1.316554   -0.252503
H       -4.817935   -1.286708   -1.084226
H       -3.695432    0.379524    0.226427

Scheme6_INT_O2.xyz
```

```
C         0.999917    0.495608    1.381724
C         0.045925    0.556974    0.358257
C         0.491715    0.832947   -0.937728
C         1.861190    1.013562   -1.126625
C         2.336967    0.694098    1.067484
H         0.706752    0.284283    2.406408
H         2.231581    1.222673   -2.127283
H         3.088981    0.642616    1.851003
N         2.784560    0.947883   -0.165776
H        -0.198100    0.893443   -1.766427
N        -1.292155    0.324499    0.698437
H        -1.463122    0.134398    1.675741
C        -2.384798    0.252329   -0.141959
O        -2.321159    0.444945   -1.339997
C        -3.678511   -0.122890    0.550252
H        -3.720362    0.215873    1.588038
H        -4.504897    0.310619   -0.011775
H        -3.784313   -1.211671    0.533059
O         1.663942   -2.174500   -0.413880
O         0.552493   -2.487280   -0.094351

Scheme6_INT_O3.xyz
C        -0.242671   -1.474855   -0.192605
C        -1.116701   -0.380585   -0.162316
C        -0.579963    0.894578   -0.366418
C         0.792429    0.991699   -0.586100
C         1.107059   -1.251694   -0.421691
H        -0.608330   -2.486022   -0.037501
H         1.235199    1.972618   -0.742067
H         1.800431   -2.089062   -0.443269
N         1.637315   -0.040986   -0.621135
H        -1.205464    1.774577   -0.352662
N        -2.473229   -0.635798    0.071779
H        -2.712474   -1.607105    0.211525
C        -3.510280    0.271430    0.158261
O        -3.366171    1.468430    0.008299
C        -4.852143   -0.345485    0.493627
H        -4.945476   -1.379546    0.154116
H        -4.989156   -0.319094    1.578622
H        -5.631494    0.263299    0.036452
O         4.187568   -0.885752    0.494967
O         4.414690    0.252306    0.062363
O         3.929136    1.212179    0.672338

Scheme6_TS1.xyz
C        -1.161322    1.278363    0.414837
C        -0.518983    0.160128    0.448884
C        -0.798549   -1.141796    0.124771
C        -2.127886   -1.208551   -0.330612
C        -2.478460    1.053158   -0.062509
H        -2.538250   -2.167953   -0.634062
H        -3.190052    1.869175   -0.165951
N        -2.939493   -0.151004   -0.421518
C         2.218315   -0.083848   -0.005717
O         2.604945   -1.226239   -0.085807
N         1.415225    0.306392    1.087208
H         1.364635    1.296184    1.307904
H         1.505963   -0.299517    1.898037
C         2.430461    0.987105   -1.039710
H         2.875658    0.540315   -1.926787
H         1.474457    1.460114   -1.286819
```

```
H        3.098817    1.758876   -0.645520
H       -0.142371   -2.002367    0.180167

Scheme6_TS2.xyz
C        0.955112   -1.321483   -0.129370
C        0.379368   -0.147445    0.318759
C        0.983063    1.087830    0.498399
C        2.340636    1.091106    0.183171
C        2.328965   -1.138800   -0.399457
H        2.921843    2.004628    0.279280
H        2.935711   -1.967856   -0.760523
N        3.002647    0.010458   -0.249618
C       -2.124944    0.198912   -0.165201
O       -1.850791    1.086610   -0.910953
N       -1.046500   -0.474189    0.604769
H       -1.269232   -0.503107    1.604561
H       -0.796404   -1.510585    0.252292
C       -3.481242   -0.400694    0.066513
H       -4.224487    0.183896   -0.472813
H       -3.484933   -1.432424   -0.299495
H       -3.724559   -0.422889    1.132639
H        0.469612    1.985012    0.828739

Scheme6_TS_CH3CO3H.xyz
C       -1.503002   -0.868573   -0.115330
C       -2.110865    0.389578    0.004842
C       -1.293479    1.531812    0.013144
C        0.077505    1.382632   -0.092992
C       -0.118288   -0.915747   -0.217727
H       -2.089575   -1.774683   -0.132660
H        0.758867    2.227523   -0.104073
H        0.414995   -1.855199   -0.325449
N        0.634975    0.178500   -0.191674
C        6.163821   -0.281455    0.277224
H        6.635098   -0.005115   -0.665406
H        6.396557   -1.325022    0.505550
H        6.539490    0.335221    1.095279
C        4.660485   -0.138328    0.195067
O        3.963737   -0.146040    1.231126
O        4.153342   -0.032748   -0.976547
O        2.374102    0.074099   -0.655277
H        2.676883   -0.006588    0.311992
H       -1.722774    2.525354    0.096865
N       -3.486864    0.579899    0.113156
H       -3.789561    1.540940    0.192035
C       -4.487900   -0.381108    0.102441
C       -5.886089    0.190135    0.183218
H       -5.956890    1.002606    0.910847
H       -6.178414    0.576141   -0.798100
H       -6.567118   -0.612408    0.461239
O       -4.262113   -1.569215    0.013470

Scheme6_TS_H2O2.xyz
C       -0.023608    1.501583    0.021290
C       -0.874113    0.383565    0.018192
C       -0.299780   -0.895884    0.001126
C        1.086926   -0.987229   -0.009320
C        1.346418    1.307967    0.011251
H       -0.426581    2.509715    0.027317
H        1.600531   -1.943620   -0.035297
H        2.053081    2.132156    0.003531
```

```
N        1.869247    0.085510    0.006507
H       -0.912557   -1.784682   -0.007533
N       -2.247702    0.617975    0.028243
H       -2.524722    1.589928    0.030316
C       -3.275971   -0.313952    0.015601
O       -3.082697   -1.511019    0.015782
C       -4.657829    0.299633   -0.026894
H       -4.747498    1.157763    0.644069
H       -4.877177    0.631379   -1.046335
H       -5.379508   -0.464804    0.255925
O        3.627605   -0.148632   -0.215792
O        5.471717   -0.427197    0.119864
H        5.798128    0.364751   -0.323740
H        4.120221   -0.196289    0.662187

Scheme6_TS_O2.xyz
C        0.390949    1.309743   -0.014088
C       -0.575487    0.292624   -0.015814
C       -0.152483   -1.050650   -0.008555
C        1.208371   -1.305456    0.000859
C        1.732493    0.969313   -0.004674
H        0.099633    2.355327   -0.019735
H        1.627206   -2.307082    0.007023
H        2.593850    1.646393   -0.001966
N        2.078230   -0.302148    0.002430
H       -0.865926   -1.860784   -0.010709
N       -1.915725    0.675256   -0.026169
H       -2.083380    1.671876   -0.028461
C       -3.039792   -0.137021   -0.010812
O       -2.979918   -1.348765   -0.008988
C       -4.346608    0.622677    0.035873
H       -5.139652   -0.041186   -0.304493
H       -4.555413    0.916160    1.069140
H       -4.326934    1.522447   -0.583893
O        3.698384   -0.570606    0.013732
O        4.307587    0.579086    0.013073

Scheme6_TS_O3.xyz
C       -0.140183    1.192813   -0.722076
C        0.796092    0.230253   -0.339671
C        0.365809   -1.102783   -0.145252
C       -0.966904   -1.386431   -0.335345
C       -1.467326    0.827485   -0.903639
H        0.143111    2.232610   -0.846112
H       -1.383811   -2.373532   -0.164581
H       -2.244483    1.519357   -1.200267
N       -1.829336   -0.452927   -0.767486
H        1.058848   -1.876098    0.149778
N        2.109974    0.642490   -0.146269
H        2.274752    1.633495   -0.259606
C        3.210908   -0.125524    0.210977
O        3.155841   -1.326305    0.369757
C        4.476971    0.678264    0.404413
H        4.628516    1.399309   -0.403129
H        4.422609    1.224678    1.350939
H        5.317594   -0.012211    0.442631
O       -3.412546   -0.564864   -0.211580
O       -3.353152   -0.146644    1.035254
O       -3.119369    1.167937    1.095343

Scheme7_INT1.xyz
```

```
C        1.240130    1.006138   -0.109813
C        1.895955   -0.283806    0.046601
C        0.916722   -1.164778   -0.012205
C       -0.401150   -1.262540   -0.048512
C       -0.115482    1.153406   -0.043378
H        1.866698    1.892788   -0.042517
H       -1.071703   -2.044244   -0.384637
H       -0.636740    2.102254   -0.020566
N       -0.973182    0.047747    0.082442
H        2.895124   -0.377269    0.459147
O       -2.182269    0.175214    0.051915

Scheme7_INT2.xyz
C       -0.494491   -1.231327   -0.660751
C        0.129751   -0.002241   -0.610554
C       -0.402486    1.211004   -0.184542
C       -1.723312    1.181734    0.211666
C       -1.820253   -1.146107   -0.236018
H       -2.289024    2.033893    0.560660
H       -2.509606   -1.982958   -0.193432
N       -2.431946    0.010770    0.185518
C        2.489276    0.075162    0.166610
O        3.039098    1.121804    0.327419
N        1.585991   -0.040224   -1.029946
H        1.638090   -0.972185   -1.470037
H        1.837535    0.699633   -1.693160
C        2.538925   -1.156051    1.007764
H        2.971348   -0.904775    1.974643
H        1.538360   -1.586213    1.106846
H        3.171620   -1.897385    0.506804
H        0.147754    2.148315   -0.149367
O       -3.650204    0.012547    0.560453

Scheme7_INT_CH3CO3H.xyz
C       -1.937351    1.785888   -0.201099
C       -3.017694    1.005434    0.185745
C       -2.845612   -0.375779    0.264014
C       -1.597740   -0.911653   -0.051066
C       -0.720150    1.171895   -0.497661
H       -2.031885    2.863555   -0.273747
H       -1.421994   -1.985745   -0.004899
H        0.159010    1.734141   -0.795178
N       -0.565354   -0.151463   -0.420536
H       -3.984537    1.434559    0.427143
O       -3.903801   -1.136593    0.643863
H       -3.665144   -2.071207    0.652743
C        3.854650    0.350019    1.277195
H        3.691447    1.312882    1.759982
H        4.854671    0.343509    0.835343
H        3.787627   -0.463867    1.999145
C        2.849830    0.185504    0.167243
O        2.382696    1.072601   -0.499926
O        2.543583   -1.122880    0.022114
O        1.747338   -1.373888   -1.119320
H        0.894156   -0.889358   -0.896859

Scheme7_INT_H2O2.xyz
C       -1.859954    1.531894   -0.110051
C       -2.328886    0.225511   -0.066544
C       -1.399740   -0.807273    0.037698
C       -0.042062   -0.487847    0.091844
```

```
C       -0.486604    1.763318   -0.047417
H       -2.549338    2.365107   -0.189700
H        0.721161   -1.262063    0.162710
H       -0.084230    2.771148   -0.075694
N        0.399161    0.770591    0.050056
H       -3.386802   -0.011033   -0.110665
O       -1.855738   -2.084613    0.080065
H       -1.119190   -2.702570    0.162333
O        3.130561    0.401391    0.397064
O        3.041167   -0.819272   -0.341588
H        3.593502   -0.623393   -1.109905
H        2.206333    0.735008    0.293025

Scheme7_INT_O2.xyz
C       -0.152404    1.359521   -1.033508
C        0.870116    0.431314   -1.177654
C        1.330726   -0.217523   -0.034972
C        0.746474    0.095029    1.195201
C       -0.674838    1.603898    0.237720
H       -0.545683    1.887891   -1.895399
H        1.089474   -0.401319    2.103503
H       -1.477985    2.321255    0.379541
N       -0.235128    0.983702    1.333652
H        1.311878    0.198213   -2.140791
O        2.329042   -1.130391   -0.166203
H        2.544362   -1.515653    0.691535
O       -2.521046   -0.891677   -0.147837
O       -1.557569   -1.604148   -0.135293

Scheme7_INT_O3.xyz
C        1.365513    1.404452   -0.739986
C        1.665396    0.053340   -0.822708
C        1.159762   -0.792671    0.165165
C        0.395099   -0.239299    1.197615
C        0.576519    1.862170    0.318666
H        1.727919    2.099064   -1.490039
H       -0.004546   -0.878118    1.985150
H        0.321500    2.914385    0.406533
N        0.105339    1.058384    1.272969
H        2.260896   -0.362619   -1.628458
O        1.436616   -2.116556    0.083439
H        0.965499   -2.600837    0.772410
O       -2.556529   -0.380551    0.496258
O       -2.124308    0.182307   -0.521523
O       -1.378577   -0.473765   -1.266785

Scheme7_TS1.xyz
C       -0.839619   -1.403164   -0.381151
C       -0.135928   -0.351926   -0.479129
C       -0.371407    0.989221   -0.313781
C       -1.708144    1.165376    0.026807
C       -2.163969   -1.189555   -0.038747
H       -2.166972    2.126389    0.213918
H       -2.957109   -1.912455    0.105303
N       -2.583897    0.110184    0.160808
C        2.681078    0.137570    0.040011
O        2.923263    1.320775   -0.069073
N        2.056023   -0.549292   -0.998848
H        2.073186   -1.561487   -1.002182
H        2.117746   -0.107353   -1.909193
C        2.925977   -0.675763    1.285003
```

```
H        3.258771   -0.011400    2.080290
H        2.007924   -1.190437    1.585065
H        3.694912   -1.430882    1.095925
H        0.328849    1.811078   -0.409108
O       -3.797028    0.344195    0.478097

Scheme7_TS2.xyz
C        0.530220   -1.318286   -0.060194
C       -0.067990   -0.145942    0.379385
C        0.550554    1.077749    0.576703
C        1.907870    1.103277    0.318485
C        1.895048   -1.195027   -0.291821
H        2.540381    1.974225    0.416062
H        2.552259   -1.984359   -0.637468
N        2.574942   -0.016312   -0.102851
C       -2.538132    0.195033   -0.216106
O       -2.223386    1.049470   -0.984812
N       -1.493464   -0.479840    0.594586
H       -1.770461   -0.542126    1.579204
H       -1.186190   -1.515621    0.224473
C       -3.916901   -0.350685    0.016129
H       -4.624094    0.201389   -0.600290
H       -3.940093   -1.411831   -0.250480
H       -4.197292   -0.262945    1.070062
H        0.043204    1.984051    0.890637
O        3.829377    0.054726   -0.323917

Scheme7_TS_CH3CO3H.xyz
C        2.580082   -1.714857   -0.025986
C        3.420985   -0.616400   -0.138436
C        2.872054    0.666651   -0.090979
C        1.492542    0.797724    0.066123
C        1.209569   -1.510962    0.131540
H        2.977741   -2.722836   -0.055265
H        0.986494    1.758572    0.124231
H        0.491866   -2.317036    0.238246
N        0.721383   -0.278112    0.161433
H        4.493563   -0.725303   -0.257898
O        3.708018    1.725020   -0.196989
H        3.222641    2.557468   -0.145838
C       -4.801012    0.239066   -0.199614
H       -5.226751   -0.767016   -0.243485
H       -5.082287    0.765390   -1.113033
H       -5.185444    0.754181    0.680046
C       -3.295778    0.113840   -0.139390
O       -2.641516   -0.190016   -1.160170
O       -2.740912    0.310827    0.997252
O       -0.982669    0.021278    0.649467
H       -1.341530   -0.143889   -0.293047

Scheme7_TS_H2O2.xyz
C        1.343677    1.752820    0.027269
C        2.226882    0.681689    0.033866
C        1.717421   -0.618215    0.007818
C        0.333599   -0.793075   -0.020492
C       -0.028582    1.503743   -0.004254
H        1.709921    2.773116    0.042441
H       -0.147357   -1.768520   -0.050228
H       -0.778159    2.287696   -0.021819
N       -0.476699    0.256459   -0.020177
H        3.301858    0.825096    0.054855
```

```
O        2.593236   -1.649416    0.009626
H        2.131274   -2.496236   -0.018909
O       -2.221603   -0.143567   -0.210577
O       -4.030548   -0.535818    0.152303
H       -4.418241    0.156307   -0.396919
H       -2.749071   -0.104024    0.655758

Scheme7_TS_O2.xyz
C       -1.305942   -0.648916   -0.000000
C       -1.934404    0.596932   -0.000001
C       -1.158867    1.754732   -0.000000
C        0.226876    1.649752    0.000001
C        0.088386   -0.695211    0.000001
H        0.916741    2.486370    0.000001
H        0.743321   -1.578487    0.000002
N        0.759115    0.433891    0.000001
H       -1.625260    2.733028   -0.000001
O        2.392345    0.222136   -0.000001
O        2.646353   -1.051025   -0.000001
H       -3.017885    0.638891   -0.000002
O       -2.075803   -1.759264    0.000001
H       -1.530177   -2.555546   -0.000004

Scheme7_TS_O3.xyz
C       -1.226780    1.755730    0.435000
C       -1.986649    0.576674    0.436321
C       -1.460092   -0.570792   -0.131023
C       -0.189131   -0.515804   -0.727103
C        0.036884    1.749200   -0.113471
H       -1.620772    2.667085    0.869315
H        0.271741   -1.350785   -1.240739
H        0.709373    2.598801   -0.115662
N        0.483912    0.634082   -0.720731
H       -2.968090    0.535152    0.895451
O       -2.175338   -1.717205   -0.092922
H       -1.611177   -2.477611   -0.281939
O        2.117878    0.294850   -0.575113
O        2.223578   -0.205093    0.641628
O        1.682151   -1.420209    0.716450

Scheme8_INT2_3-sub.xyz
C       -0.940495    1.239243    0.556835
C       -0.329117    0.002188    0.513474
C       -0.833341   -1.202933    0.033347
C       -2.248042    1.120039    0.029376
H       -2.901328    1.989982   -0.020386
C        2.099116   -0.066497   -0.075617
O        2.687384   -1.096308   -0.208678
N        1.100926    0.010145    1.041410
H        1.118176    0.927890    1.515089
H        1.293872   -0.753495    1.696645
C        2.194449    1.181067   -0.889158
H        2.709659    0.954875   -1.821131
H        1.197896    1.596690   -1.061620
H        2.769460    1.923559   -0.324675
H       -0.262533   -2.133264    0.032694
C       -2.753745   -0.091433   -0.442504
H       -3.764740   -0.149561   -0.842164
N       -2.071281   -1.249610   -0.449917

Scheme8_RC_3-sub.xyz
```

```
C        1.508170   -1.291498    0.016004
C        0.647766   -0.383889   -0.022385
C        0.939568    0.977789   -0.065778
C        2.874989   -1.118387    0.019483
H        3.655901   -1.867833    0.049828
C       -2.425502    0.159512    0.054723
O       -2.098163    1.331531   -0.045146
N       -2.488497   -0.469091    1.263503
H       -2.593916   -1.468561    1.327616
H       -2.122238    0.024504    2.064282
C       -2.773478   -0.690652   -1.147354
H       -3.179342   -0.045025   -1.925491
H       -1.852552   -1.148721   -1.522147
H       -3.487163   -1.482017   -0.907787
H        0.219821    1.786402   -0.102086
C        3.159808    0.269326   -0.022616
H        4.199845    0.585906   -0.022964
N        2.253785    1.244789   -0.062438

Scheme8_TS1_3-sub.xyz
C        1.147528   -1.250135    0.433569
C        0.535993   -0.119007    0.451035
C        0.877652    1.164639    0.098258
C        2.468658   -1.120746   -0.038749
H        3.154332   -1.959754   -0.130065
C       -2.242268    0.088589   -0.027523
O       -2.644091    1.204723   -0.260944
N       -1.452306   -0.149687    1.113865
H       -1.402175   -1.100707    1.463386
H       -1.546048    0.560150    1.834314
C       -2.437292   -1.111348   -0.914135
H       -2.867250   -0.786557   -1.859906
H       -1.478505   -1.613022   -1.080268
H       -3.114624   -1.823440   -0.432390
H        0.250473    2.049743    0.139570
C        2.893755    0.163618   -0.408519
H        3.904053    0.314846   -0.781364
N        2.136352    1.267873   -0.346629

Scheme8_TS2_3-sub.xyz
C        0.973490   -1.330956   -0.146097
C        0.381460   -0.162750    0.315373
C        0.984091    1.070882    0.507044
C        2.343284   -1.137424   -0.404320
H        2.970102   -1.945588   -0.774783
C       -2.115541    0.170307   -0.196529
O       -1.828278    0.977511   -1.023844
N       -1.040712   -0.495108    0.583788
H       -1.279614   -0.545303    1.578577
H       -0.776177   -1.527855    0.216221
C       -3.491536   -0.324067    0.145146
H       -4.216379    0.181847   -0.490178
H       -3.546583   -1.405434   -0.012686
H       -3.721423   -0.124829    1.196330
H        0.449774    1.956317    0.848369
C        2.932175    0.111191   -0.191057
H        3.992883    0.256132   -0.388548
N        2.284869    1.202469    0.250511

Scheme9_INT2_3-sub.xyz
C        0.391386    1.682317   -0.406099
```

```
C       -0.009917    0.374864   -0.556849
C        0.679460   -0.808370   -0.315042
C        1.736606    1.692090    0.050302
H        2.245503    2.637494    0.227525
C       -2.344159   -0.280514    0.082659
O       -2.771054   -1.386727   -0.040154
N       -1.445754    0.227486   -1.015080
H       -1.652997    1.209086   -1.267077
H       -1.552429   -0.393539   -1.824092
C       -2.551951    0.693785    1.193027
H       -3.007139    0.174785    2.034590
H       -1.602857    1.161614    1.467306
H       -3.220085    1.488944    0.844408
H        0.322823   -1.825732   -0.433510
N        1.956376   -0.703019    0.117307
C        2.478404    0.551734    0.296311
H        3.504337    0.531727    0.642492
O        2.659744   -1.749660    0.356019
```

Scheme9_TS1_3-sub.xyz

```
C       -0.779210   -1.726127   -0.260028
C       -0.236128   -0.592829   -0.432218
C       -0.648726    0.704642   -0.311314
C       -2.130141   -1.647999    0.136053
H       -2.753196   -2.516422    0.327954
C        2.506697    0.237541   -0.008142
O        2.656898    1.432245   -0.131544
N        1.885650   -0.500011   -1.023584
H        2.013976   -1.504847   -1.041742
H        1.884042   -0.049746   -1.933020
C        2.858246   -0.554214    1.224185
H        3.168745    0.133633    2.008466
H        1.993142   -1.137770    1.554528
H        3.674587   -1.249015    1.004578
H       -0.133924    1.645334   -0.452902
N       -1.965424    0.774316    0.072509
C       -2.680711   -0.386084    0.289203
H       -3.701611   -0.191036    0.589066
O       -2.522837    1.910274    0.228314
```

Scheme9_TS2_3-sub.xyz

```
C        0.431089    1.657957    0.052317
C        0.037027    0.380240   -0.306374
C        0.793247   -0.773674   -0.393801
C        1.811816    1.692876    0.345272
H        2.301210    2.614678    0.649152
C       -2.386369   -0.283242    0.212942
O       -1.995857   -0.932888    1.130699
N       -1.405878    0.463542   -0.622505
H       -1.621856    0.380565   -1.620716
H       -1.301715    1.557534   -0.348908
C       -3.810347   -0.065472   -0.207401
H       -4.465539   -0.596543    0.480810
H       -4.043102    1.003545   -0.195930
H       -3.969801   -0.435344   -1.224975
H        0.467443   -1.773459   -0.650473
N        2.112354   -0.660673   -0.102642
C        2.608538    0.563868    0.262116
H        3.670067    0.533744    0.473381
O        2.884351   -1.684628   -0.165292
```

TS26-27.xyz

C	2.391596	-0.445028	0.425644
C	1.360042	-0.883252	-0.589119
C	0.443851	0.079051	-1.048263
C	0.375036	1.434557	-0.328942
C	1.652824	1.631095	0.497009
H	2.777390	-1.286571	1.002782
H	1.720648	-1.598635	-1.324555
H	0.331126	2.230132	-1.076149
H	1.594678	2.525532	1.121984
H	0.239560	0.085634	-2.110359
O	1.819509	0.502522	1.320505
C	3.453035	0.427048	-0.253728
H	4.346448	0.521850	0.372054
H	3.728995	0.091853	-1.256361
O	2.787305	1.686769	-0.348905
N	-0.747040	1.586158	0.581187
H	-0.722074	0.946569	1.373337
C	-2.011153	1.895686	0.175749
O	-2.986330	1.553457	0.843660
C	-2.172397	2.673955	-1.105956
H	-1.497805	3.532001	-1.154769
H	-1.963349	2.011342	-1.952322
H	-3.206251	3.009554	-1.166466
O	0.617904	-2.137055	0.566941
O	-1.414734	-0.574868	-0.985264
C	-0.477087	-2.724159	0.303114
C	-1.844928	-1.454959	-0.176972
H	-1.096560	-2.984785	1.162035
H	-2.417030	-2.268470	-0.635685
O	-0.495502	-3.651127	-0.713852
H	0.410208	-3.777405	-1.024403
O	-2.252686	-1.098185	1.083292
H	-2.645338	-0.197779	1.078337

TS30-27.xyz

C	-1.543323	-2.103712	-0.591444
C	-0.740107	-1.642666	0.594761
C	-0.921916	-0.323712	1.054235
C	-1.986292	0.571865	0.373582
C	-2.764552	-0.267880	-0.647851
H	-1.014888	-2.859035	-1.175326
H	-0.521193	-2.402112	1.337655
H	-2.695380	0.887280	1.145002
H	-3.371664	0.365764	-1.299198
H	-0.850323	-0.199876	2.129552
O	-1.849296	-0.993487	-1.431831
C	-2.955946	-2.497368	-0.145478
H	-3.469545	-3.075020	-0.921700
H	-2.989184	-3.031847	0.806718
O	-3.579139	-1.223531	0.012760
N	-1.499858	1.748079	-0.321233
H	-0.964848	1.518239	-1.155955
C	-0.937017	2.823467	0.321996
O	-0.156829	3.564620	-0.258743
C	-1.358356	3.068436	1.754107
H	-2.446822	3.065757	1.858154
H	-0.944334	2.286088	2.398050
H	-0.961416	4.033493	2.065018
O	0.968027	-2.015182	-0.237807
O	0.617475	0.696641	0.934095

```
C        2.042837   -1.345161   -0.190681
C        1.508739    0.622869    0.020742
O        2.899750   -1.540023    0.883578
O        1.045219    0.900350   -1.252318
C        2.290939   -1.963053    2.091956
H        1.753653   -2.906511    1.951317
H        3.102189   -2.105780    2.806153
H        1.601633   -1.198390    2.468574
C        1.774115    1.802009   -2.080638
H        1.247580    1.813205   -3.035828
H        1.758608    2.807508   -1.651399
H        2.800705    1.460169   -2.245869
C        2.824269   -1.289309   -1.490638
H        3.695504   -0.637764   -1.424223
H        3.178082   -2.304839   -1.691109
H        2.161903   -0.973834   -2.294592
C        2.837799    1.210666    0.468029
H        3.673940    0.951232   -0.179374
H        2.718777    2.298937    0.488349
H        3.047246    0.856975    1.474716

TS31-33.xyz
C        0.250577    1.410698    0.934260
C       -0.982972    1.812065    0.099233
C       -2.050968   -0.272983    0.262347
C       -0.795252   -0.891462    0.852379
C        0.202276   -0.052961    1.368262
H       -1.209651    2.877261    0.246088
H       -0.944761   -1.826518    1.389574
H       -2.067454   -0.435130   -0.822124
H        0.552689   -0.259312    2.370146
H        0.223917    2.015864    1.848563
O       -2.117849    1.122536    0.542615
O       -0.705957    1.557262   -1.243551
C       -1.725585    2.010636   -2.120595
H       -1.859284    3.095615   -2.020976
H       -1.394921    1.773832   -3.131382
H       -2.677222    1.510728   -1.910312
C       -3.296890   -0.899105    0.857236
H       -3.204687   -1.992633    0.781579
H       -3.367650   -0.619822    1.917654
O       -4.404832   -0.432973    0.117564
H       -5.216476   -0.601796    0.605454
N        1.440913    1.783610    0.194244
H        1.439536    1.483785   -0.778176
C        2.652497    1.868021    0.785990
H        2.611325    2.092137    1.865855
O        3.713316    1.734517    0.190714
O       -0.241211   -1.618338   -0.781051
O        1.986454   -0.836052    1.010447
C        0.834004   -2.282764   -0.907621
H        1.355700   -2.169504   -1.859917
C        2.324696   -1.395023   -0.076048
H        2.814859   -2.368918    0.026363
O        0.876535   -3.558072   -0.385371
H       -0.013600   -3.787394   -0.088458
O        2.783678   -0.626413   -1.121554
H        3.275930    0.144077   -0.770793

TS32-33.xyz
C       -1.285861   -0.953614   -1.080067
```

```
C       -2.681683   -0.248909   -1.056543
C       -1.501096    1.482850    0.076076
C       -0.244323    1.241351   -0.751520
C       -0.268995    0.069908   -1.521391
H       -3.116928   -0.273318   -2.067673
H        0.231928    2.117238   -1.185108
H       -1.483296    0.883522    0.994433
H        0.018920    0.108671   -2.560982
H       -1.344768   -1.772731   -1.804669
O       -2.616041    1.117986   -0.729186
O       -3.496286   -0.952538   -0.174695
C       -4.820706   -0.449457   -0.106295
H       -5.287257   -0.452346   -1.101229
H       -5.372253   -1.117634    0.555174
H       -4.827498    0.567257    0.295746
C       -1.643819    2.940743    0.441896
H       -0.691880    3.271107    0.881502
H       -1.835214    3.513385   -0.477235
O       -2.710496    3.064830    1.360066
H       -2.876462    3.996333    1.534503
N       -0.919125   -1.492723    0.221455
H       -0.113438   -1.097236    0.700373
C       -1.422570   -2.643608    0.729709
H       -2.217069   -3.086774    0.106470
O       -1.036926   -3.157560    1.766520
O        0.846785    1.065544    0.675730
O        1.454992   -0.986102   -1.416089
C        2.104933    0.974737    0.501897
C        2.330873   -0.912568   -0.516788
O        2.600303    1.899509   -0.382986
O        2.157719   -1.697532    0.620090
C        3.917691    2.406399   -0.217206
H        4.671324    1.615980   -0.237625
H        4.083647    3.079207   -1.058437
H        4.002539    2.970438    0.717122
C        1.872006   -3.073734    0.351845
H        1.505170   -3.502629    1.283461
H        1.098311   -3.163252   -0.414366
H        2.784576   -3.587023    0.024795
C        2.887452    0.641103    1.752883
H        3.904735    0.304258    1.557257
H        2.925457    1.554635    2.357444
H        2.352895   -0.128742    2.301942
C        3.768195   -0.783678   -0.992082
H        3.842292    0.022223   -1.723223
H        4.468529   -0.633357   -0.169995
H        4.036627   -1.722400   -1.489956

TS34-27.xyz
C        1.793913   -1.909856    0.310420
C        0.752117   -1.456746   -0.687823
C        0.758907   -0.101720   -1.066339
C        1.630162    0.881214   -0.273761
C        2.678225    0.097479    0.527205
H        1.489803   -2.823485    0.823759
H        0.560443   -2.177848   -1.480616
H        2.162202    1.527656   -0.975486
H        3.235362    0.748596    1.205115
H        0.621807    0.112912   -2.117360
O        2.012928   -0.889304    1.277857
C        3.173108   -1.958828   -0.355883
```

```
H        3.877526   -2.551665    0.236588
H        3.154708   -2.317495   -1.387969
O        3.562006   -0.585262   -0.343974
N        0.908695    1.716559    0.671708
H        0.458604    1.190403    1.418461
C        0.215892    2.833554    0.310343
O       -0.738012    3.226357    0.981072
C        0.663320    3.574890   -0.924938
H        1.744199    3.733529   -0.940975
H        0.378305    2.996342   -1.809771
H        0.146703    4.532926   -0.946458
O       -0.642353   -1.924836    0.387647
O       -1.047924    0.709081   -0.959913
C       -1.865050   -1.659758    0.129604
C       -2.020995    0.343546   -0.224634
O       -2.397926   -2.226135   -1.012699
H       -1.676056   -2.591332   -1.538682
O       -2.049774    0.787946    1.082274
H       -1.686191    1.698479    1.131594
C       -2.790606   -1.783736    1.325424
H       -3.792886   -1.420751    1.106107
H       -2.848090   -2.852742    1.551777
H       -2.374181   -1.242447    2.169473
C       -3.374697    0.374661   -0.927992
H       -3.629422    1.431381   -1.057149
H       -3.301484   -0.106251   -1.900725
H       -4.159564   -0.095119   -0.337497

TS35-27.xyz
C        1.478189   -1.930044    0.712387
C        0.555261   -1.628816   -0.439502
C        0.607525   -0.346287   -1.018621
C        1.612812    0.693750   -0.466216
C        2.539338   -0.003378    0.538279
H        1.060637   -2.676492    1.389568
H        0.343519   -2.464261   -1.098712
H        2.229791    1.034034   -1.303275
H        3.138900    0.722339    1.093125
H        0.463563   -0.317387   -2.093033
O        1.749311   -0.737452    1.442905
C        2.881783   -2.242959    0.182358
H        3.500221   -2.711897    0.955319
H        2.890658   -2.848621   -0.726760
O        3.376437   -0.939609   -0.121278
N        1.058757    1.852499    0.205451
H        0.620293    1.634267    1.097111
C        0.371030    2.854200   -0.437480
O       -0.413098    3.565877    0.171330
C        0.665172    3.055965   -1.908024
H        1.739227    3.149595   -2.091532
H        0.285501    2.205016   -2.482145
H        0.157229    3.962145   -2.234095
O       -1.052906   -2.028166    0.565884
O       -1.037205    0.559898   -0.905122
C       -2.157409   -1.423546    0.451684
C       -1.817636    0.444702    0.088921
O       -3.057864   -1.781197   -0.530625
O       -1.377170    0.920520    1.298525
C       -2.513203   -2.446601   -1.660513
H       -1.966903   -3.346074   -1.360090
H       -3.362505   -2.721673   -2.285121
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H       -1.850869   -1.778431   -2.221554
C       -2.358529    1.622665    2.048710
H       -1.948769    1.764337    3.047978
H       -2.551932    2.595469    1.586376
H       -3.288292    1.041461    2.121224
H       -2.679128   -1.174603    1.378687
H       -2.878478    0.586412   -0.136076

TS36-33.xyz
C       -0.521937   -1.645821   -0.898155
C       -1.820380   -1.637549   -0.056744
C       -2.205818    0.677119   -0.274136
C       -0.775059    0.860785   -0.788547
C       -0.181576   -0.267162   -1.412892
H       -2.368003   -2.581305   -0.185481
H       -0.618937    1.803639   -1.311789
H       -2.222085    0.889862    0.803519
H        0.218037   -0.177924   -2.409980
H       -0.702954   -2.298209   -1.760930
O       -2.690267   -0.639443   -0.515257
O       -1.486789   -1.458430    1.287487
C       -2.603155   -1.568362    2.154932
H       -3.061969   -2.561624    2.063646
H       -2.226595   -1.432763    3.168679
H       -3.355715   -0.805032    1.929280
C       -3.159782    1.626887   -0.970220
H       -2.750019    2.644600   -0.898937
H       -3.232461    1.344495   -2.029761
O       -4.409882    1.538211   -0.318508
H       -5.090146    1.939238   -0.867734
N        0.539520   -2.264987   -0.112075
H        0.646130   -1.890877    0.827402
C        1.649712   -2.768100   -0.686701
H        1.509974   -3.071790   -1.738231
O        2.720531   -2.911121   -0.107585
O       -0.001686    1.112472    0.644731
O        1.959997   -0.015904   -1.225003
C        1.108490    1.757695    0.690334
C        2.575970    0.538472   -0.282193
O        1.074835    2.931568   -0.024894
O        2.996084   -0.222365    0.786914
C        1.731349    1.801767    2.064747
H        2.769919    2.136491    2.039201
H        1.140870    2.507467    2.659596
H        1.695738    0.814069    2.516024
C        3.566456    1.637043   -0.639115
H        3.153745    2.267863   -1.427026
H        3.875219    2.228305    0.227645
H        4.463236    1.143171   -1.025132
H        1.932459    3.370001    0.028155
H        2.958703   -1.171329    0.545426

TS37-33.xyz
C       -0.924592    0.889884    1.105546
C       -2.332047    0.206458    1.081152
C       -1.200932   -1.479820   -0.165402
C        0.069186   -1.303783    0.654862
C        0.090175   -0.166850    1.471188
H       -2.742183    0.183155    2.102813
H        0.546049   -2.206805    1.028535
H       -1.191429   -0.834035   -1.051695
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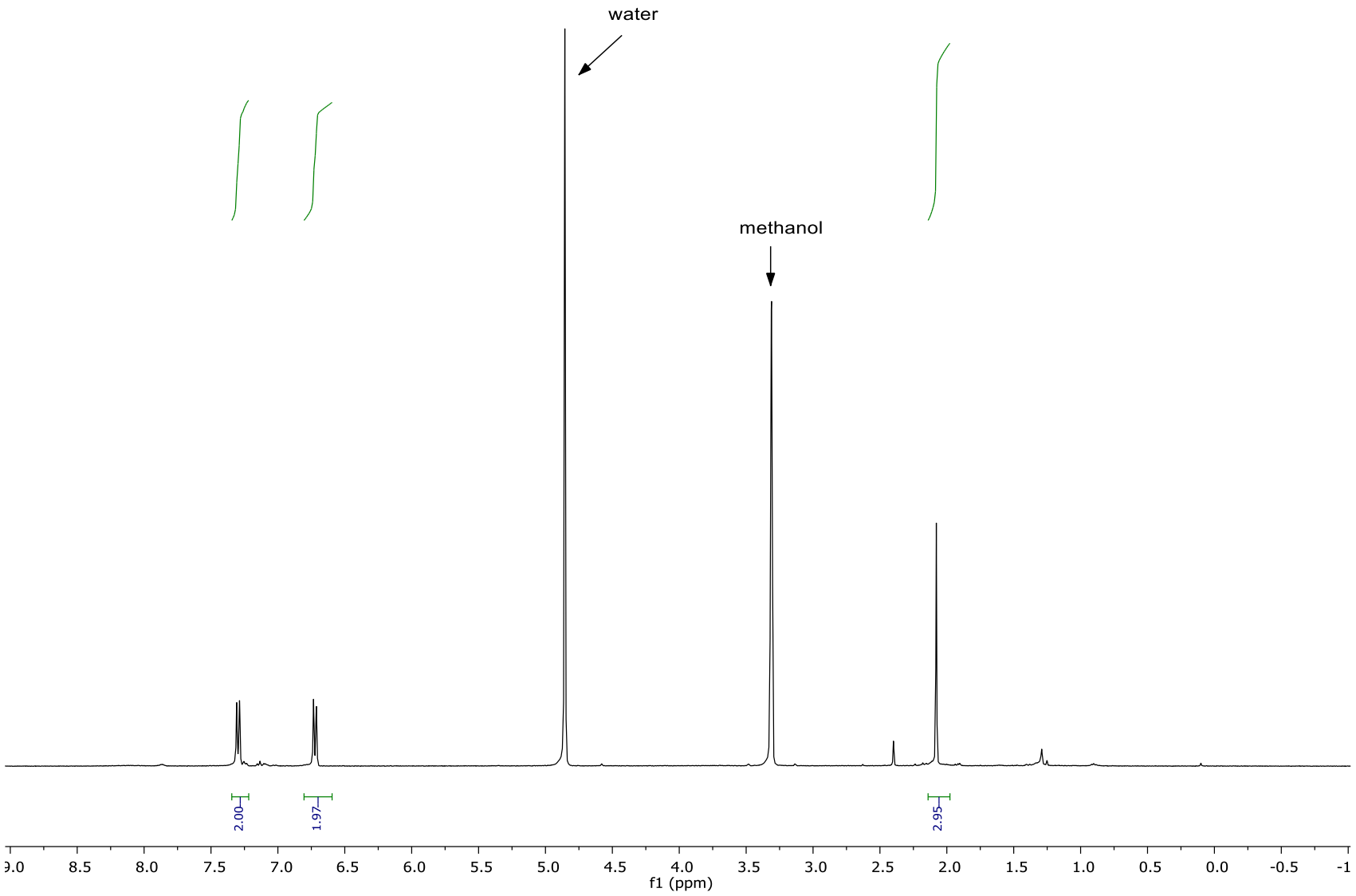
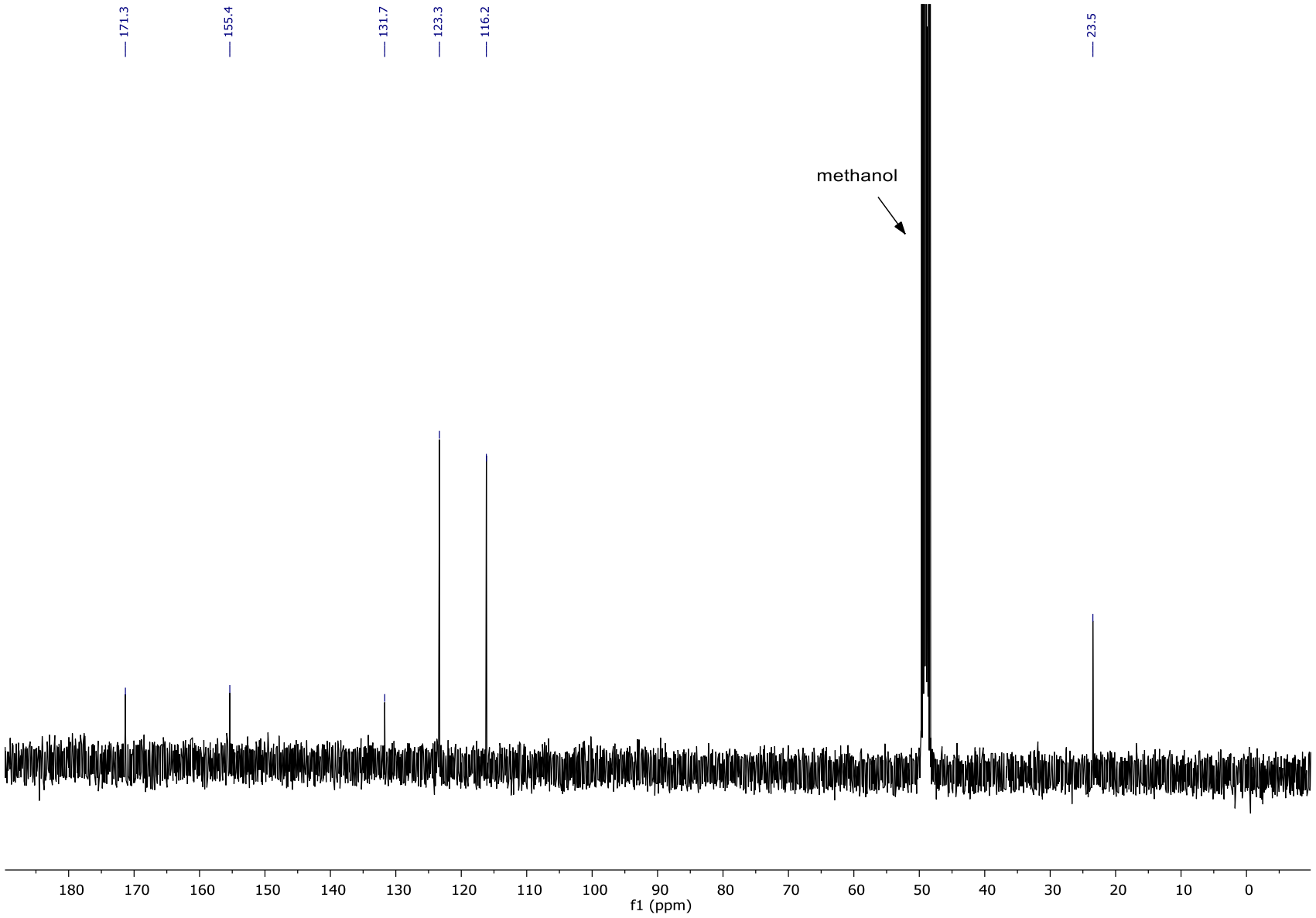
H	0.396841	-0.260079	2.502528
H	-0.954958	1.672708	1.870365
O	-2.296428	-1.140576	0.678454
O	-3.152871	0.971828	0.259681
C	-4.488359	0.496847	0.196198
H	-4.932503	0.457293	1.200454
H	-5.040926	1.208111	-0.417622
H	-4.523071	-0.497461	-0.256994
C	-1.373767	-2.913438	-0.607361
H	-0.439191	-3.228918	-1.091794
H	-1.548142	-3.534965	0.283063
O	-2.468027	-2.969599	-1.498887
H	-2.620224	-3.882655	-1.761463
N	-0.582533	1.494176	-0.172167
H	0.156697	1.078195	-0.733637
C	-1.072868	2.685882	-0.592608
H	-1.812256	3.121751	0.100262
O	-0.728322	3.241697	-1.621342
O	1.159716	-1.083686	-0.820684
O	1.828790	0.850034	1.375275
C	2.398249	-0.947723	-0.614096
C	2.631348	0.771387	0.411761
O	2.999750	-1.962812	0.066181
O	2.466594	1.580888	-0.696951
C	4.408186	-1.879417	0.217565
H	4.663868	-1.372193	1.153169
H	4.786188	-2.901302	0.247916
H	4.867079	-1.352280	-0.626702
C	2.254447	2.967258	-0.407334
H	1.859280	3.416566	-1.317134
H	1.524385	3.082212	0.396528
H	3.204364	3.433813	-0.122470
H	3.676178	0.536407	0.648893
H	2.973925	-0.441066	-1.392480

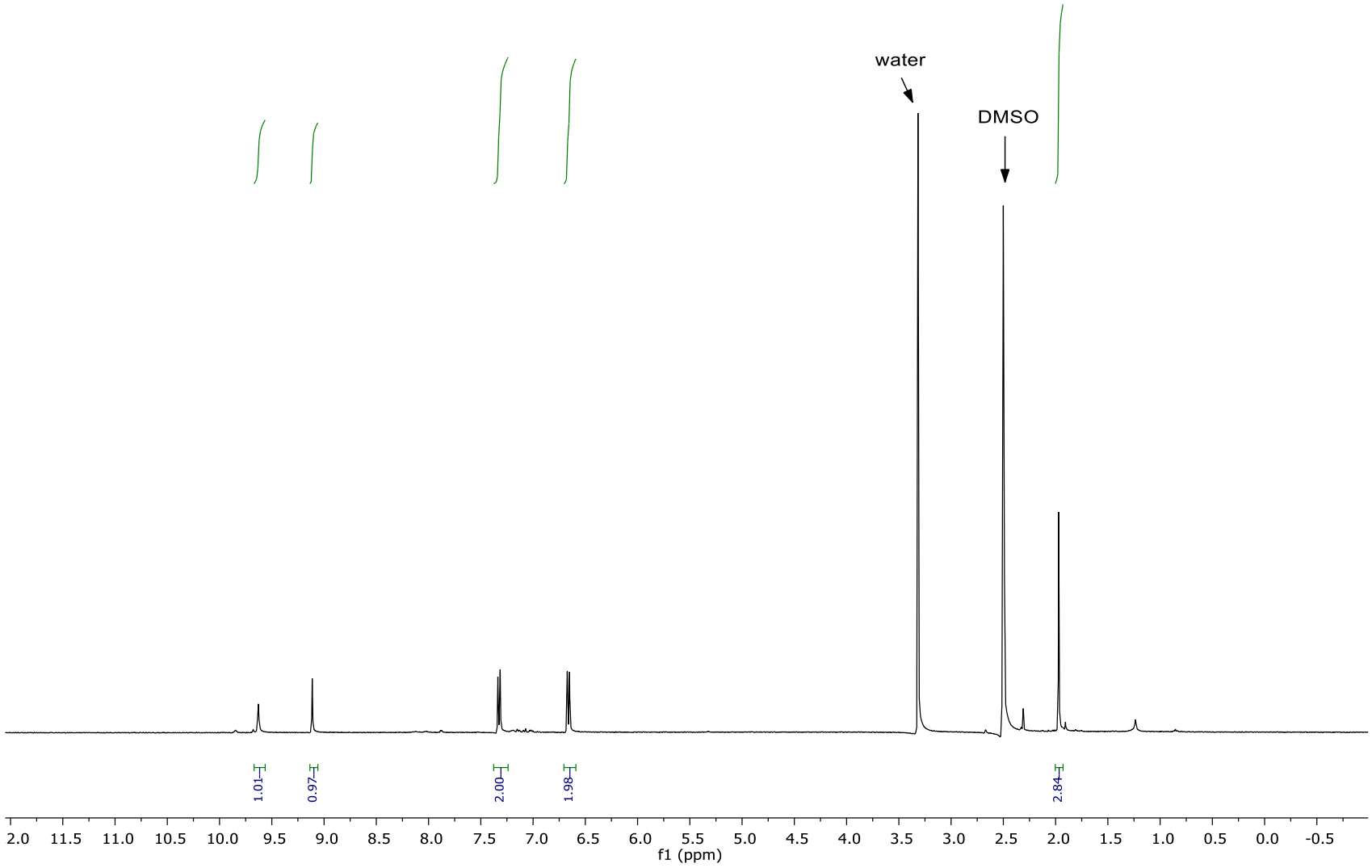
400 MHz ^{1}H NMR spectrum (recorded in CD_3OD) of the bulk material from which a crystal of compound **18** was obtained



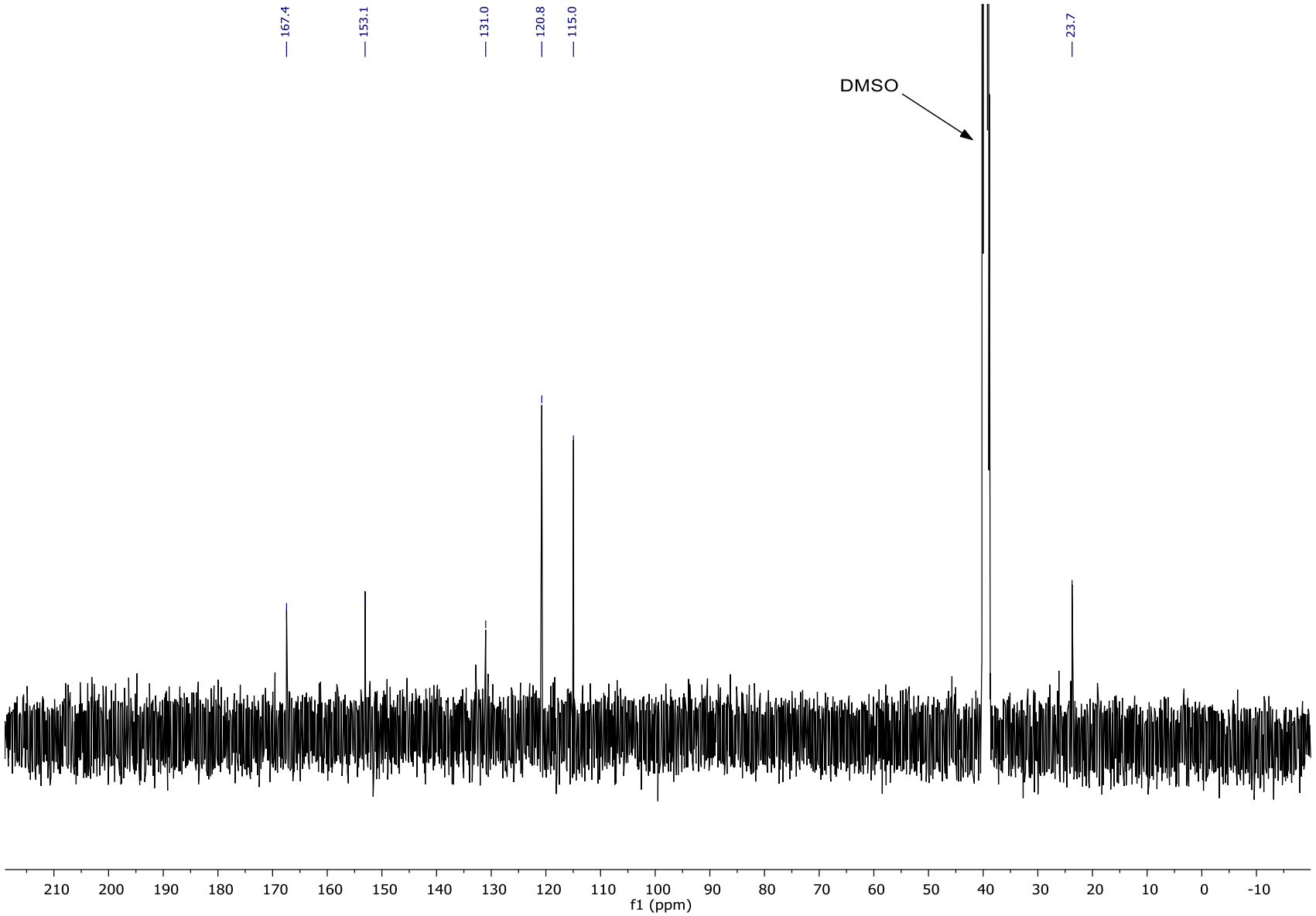
100 MHz ^{13}C NMR spectrum (recorded in CD_3OD) of the bulk material from which a crystal of compound **18** was obtained



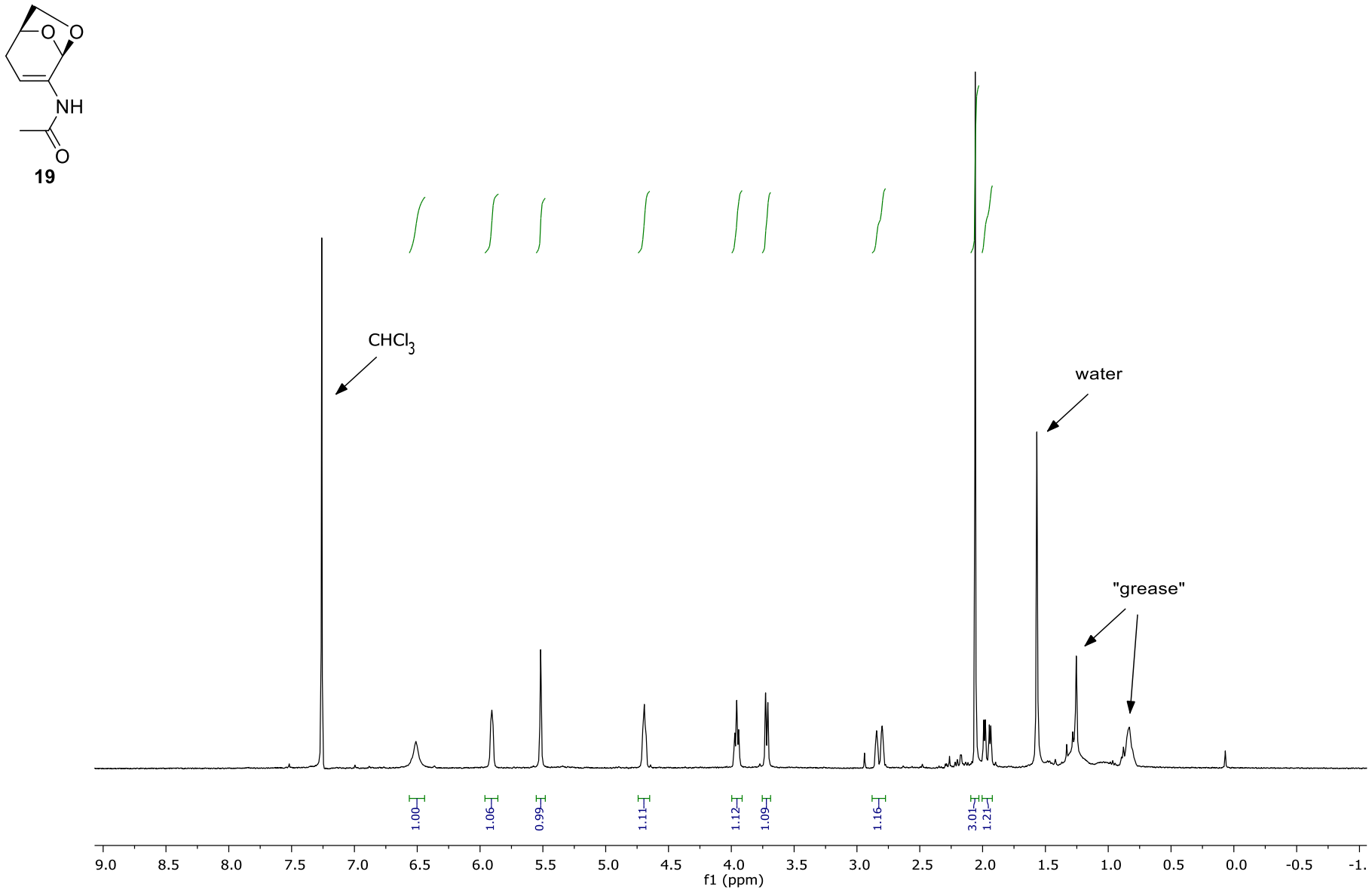
400 MHz ^{1}H NMR spectrum (recorded in DMSO-d_6) of the bulk material from which a crystal of compound **18** was obtained



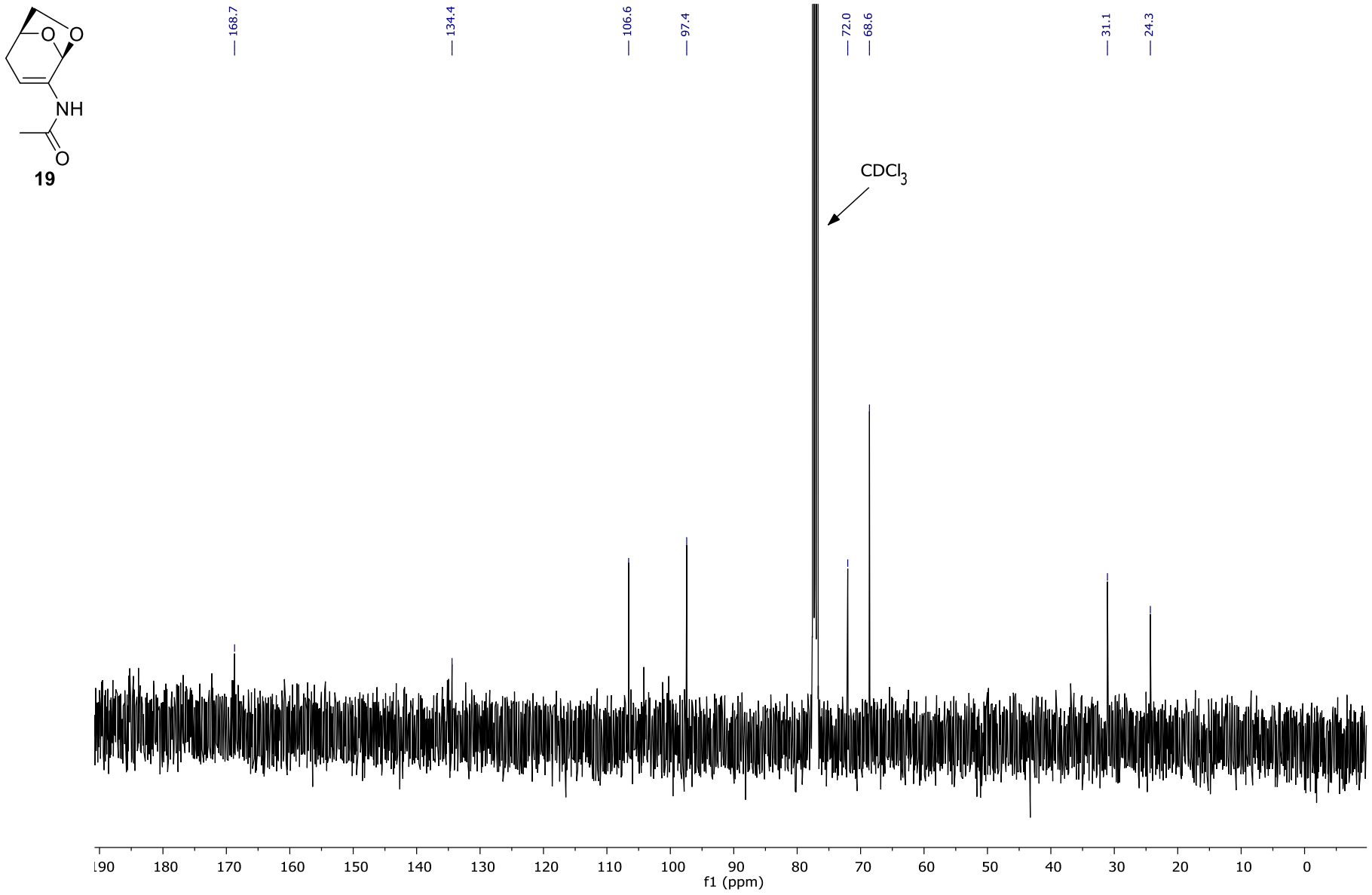
100 MHz ^{13}C NMR spectrum (recorded in DMSO-d_6) of the bulk material from which a crystal of compound **18** was obtained



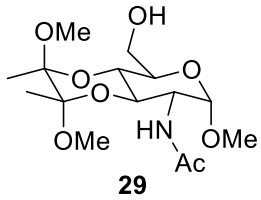
400 MHz ^{1}H NMR spectrum of compound **19** recorded in $CDCl_3$



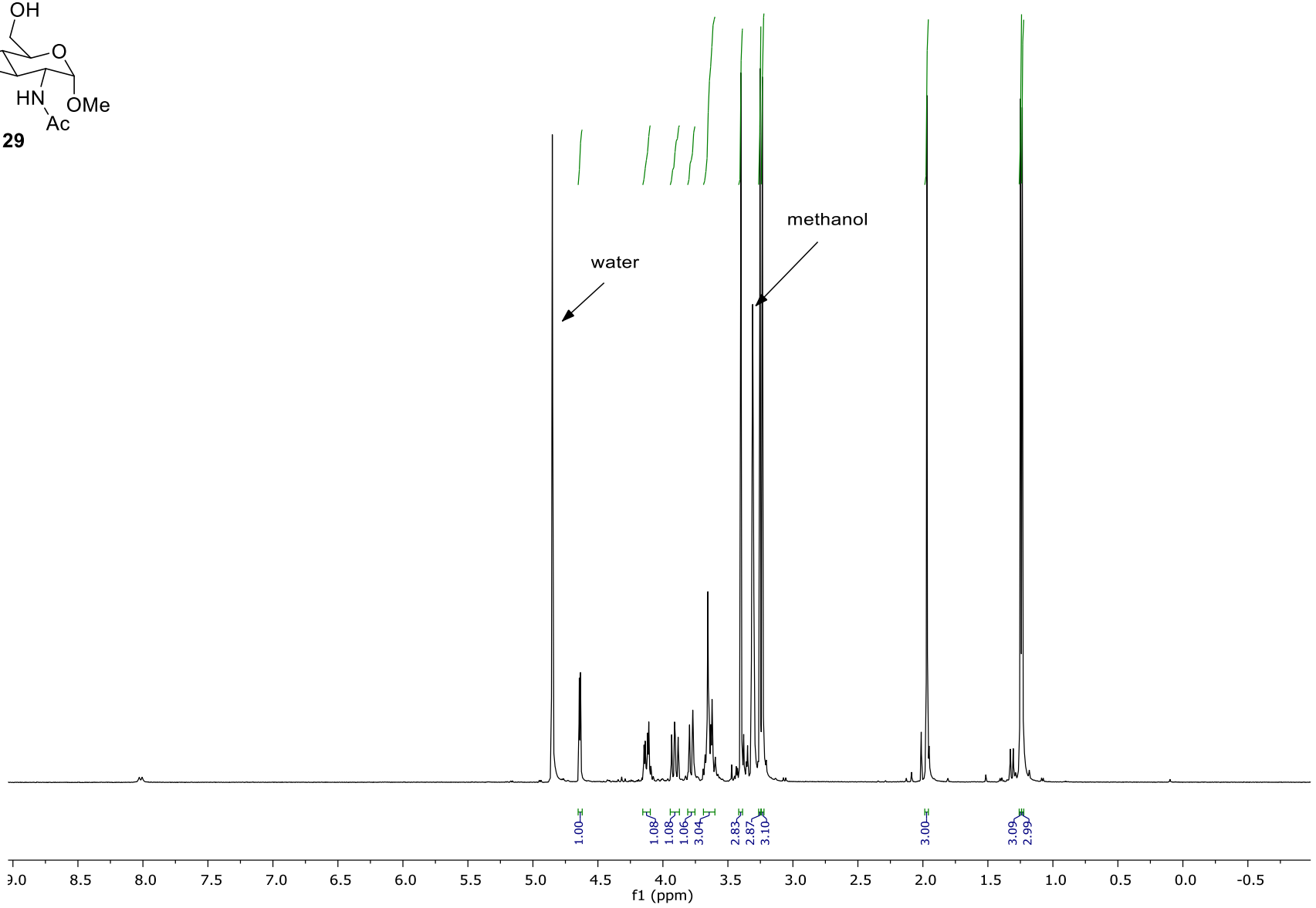
100 MHz ^{13}C NMR spectrum of compound **19** recorded in $CDCl_3$



400 MHz ^{1}H NMR spectrum of compound **29** recorded in CD_3OD



29



100 MHz ^{13}C NMR spectrum of compound **29** recorded in CD_3OD