Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Mechanistic investigation of 1,3-Dipolar Cycloaddition between Bifunctional 2-Pyridylselenyl Reagents and Nitriles Including Reactions with Cyanamides

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Table S1. Crystal data and structure refinement for all compounds studied.

Compound	**1**	**3**	**4**	**5**
Empirical formula	$C_8H_{10}ClN_3Se$	$C_{13}H_{12}ClN_3OSe$	$C_{16}H_{12}ClN_3Se$	$C_{10}H_{14}ClN_3O_2Se$
Formula weight	262.60	340.67	360.70	322.65
Temperature/K	120.00	100.00	300.00	100.00
Crystal system	monoclinic	orthorhombic	tetragonal	monoclinic
Space group	$P2_1/c$	$P2_12_12_1$	$P4_1$	$P2_1/c$
a/Å	7.3227(9)	6.9994(10)	7.811(4)	5.3306(7)
b/Å	8.9950(14)	8.8877(10)	7.811	14.043(4)
c/Å	15.321(2)	20.694(5)	23.699(8)	16.798(2)
β/°	103.442(6)	90	90	93.025(4)
Volume/Å^3	981.5(2)	1287.3(4)	1445.9(14)	1255.7(4)
Z	4	4	4	4
ρ_{calc}g/cm^3	1.777	1.758	1.657	1.707
μ/mm^{-1}	4.053	3.118	2.777	3.197
F(000)	520.0	680.0	720.0	648.0
Crystal size/mm^3	0.4 × 0.2 × 0.01	0.6 × 0.4 × 0.03	0.6 × 0.5 × 0.4	0.6 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range /°	4.528 - 51.988	4.988 - 59.992	5.216 - 54.93	3.782 - 54.974
Index ranges	-9 ≤ h ≤ 8 -11 ≤ k ≤ 10 -15 ≤ l ≤ 18	-9 ≤ h ≤ 9 -12 ≤ k ≤ 9 -29 ≤ l ≤ 16	-10 ≤ h ≤ 9 -10 ≤ k ≤ 10 -30 ≤ l ≤ 30	-6 ≤ h ≤ 6 -14 ≤ k ≤ 18 -21 ≤ l ≤ 21
Reflections collected	5237	6508	12885	6030
Independent reflections	1935 [R_{int} = 0.0245, R_{sigma} = 0.0300]	3641 [R_{int} = 0.0319, R_{sigma} = 0.0628]	3287 [R_{int} = 0.0234, R_{sigma} = 0.0359]	2763 [R_{int} = 0.0242, R_{sigma} = 0.0383]
Goodness-of-fit on F^2	1.241	1.015	1.114	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0265, wR_2 = 0.0648	R_1 = 0.0334, wR_2 = 0.0836	R_1 = 0.0331, wR_2 = 0.0858	R_1 = 0.0286, wR_2 = 0.0576
Final R indexes [all data]	R_1 = 0.0294, wR_2 = 0.0689	R_1 = 0.0383, wR_2 = 0.0858	R_1 = 0.0348, wR_2 = 0.0866	R_1 = 0.0396, wR_2 = 0.0609

Table S1 (continued). Crystal data and structure refinement for all compounds studied.

Compound	6	7	8	9
Empirical formula	$C_7H_{10}ClN_5OSe$	$C_9H_{11}ClN_4Se$	$C_8H_{10}ClN_3O_4Se$	$C_{32}H_{30}BN_3Se$
Formula weight	294.61	289.63	326.60	546.36
Temperature/K	100.00	100.00	100.00	120.00
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_1/c$	P2/c	P-1	$P2_1/c$
a/Å	7.8986(15)	11.922(4)	6.8384(15)	15.3881(6)
b/Å	14.662(4)	6.546(3)	9.403(2)	9.8662(3)
c/Å	9.851(4)	14.620(5)	10.236(2)	18.2499(8)
α/°	90	90	67.561(9)	90
β/°	111.161(15)	108.226(16)	74.848(10)	105.5660(10)
γ/°	90	90	70.534(11)	90
Volume/Å^3	1063.9(6)	1083.7(7)	566.8(2)	2669.11(18)
Z	4	4	2	4
ρ_{calc}g/cm^3	1.839	1.775	1.914	1.360
μ/mm^{-1}	3.762	3.682	3.555	1.433
F(000)	584.0	576.0	324.0	1128.0
Crystal size/mm^3	0.6 × 0.4 × 0.4	0.6 × 0.2 × 0.1	0.5 × 0.4 × 0.2	0.6 × 0.4 × 0.15
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range /°	5.232 - 66.304	5.868 - 60.046	4.856 - 59.998	4.634 - 54.998
Index ranges	-11 ≤ h ≤ 12 -17 ≤ k ≤ 22 -15 ≤ l ≤ 10	-16 ≤ h ≤ 15 -9 ≤ k ≤ 8 -20 ≤ l ≤ 16	-9 ≤ h ≤ 8 -13 ≤ k ≤ 11 -14 ≤ l ≤ 14	-18 ≤ h ≤ 19 -12 ≤ k ≤ 9 -23 ≤ l ≤ 14
Reflections collected	7772	6556	5966	13351
Independent reflections	3987 [R_{int} = 0.0364, R_{sigma} = 0.0517]	3107 [R_{int} = 0.0363, R_{sigma} = 0.0551]	3260 [R_{int} = 0.0189, R_{sigma} = 0.0298]	6074 [R_{int} = 0.0717, R_{sigma} = 0.0618]
Goodness-of-fit on F^2	1.053	1.027	1.053	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0387, wR_2 = 0.1028	R_1 = 0.0338, wR_2 = 0.0786	R_1 = 0.0212, wR_2 = 0.0497	R_1 = 0.0480, wR_2 = 0.1230
Final R indexes [all data]	R_1 = 0.0455, wR_2 = 0.1063	R_1 = 0.0481, wR_2 = 0.0888	R_1 = 0.0232, wR_2 = 0.0504	R_1 = 0.0610, wR_2 = 0.1296

Gaussian 09 program package citation: [Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, R.; Kobayashi, J.; Normand, K.; Raghavachari, A.; Rendell, J. C.; Burant, S. S.; Iyengar, T.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Rev. D.01; Gaussian, Inc.: 2013.]

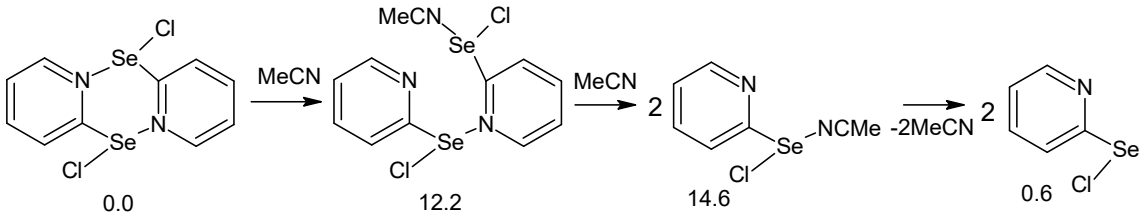


Figure S1. Alternative way of the $(PySeCl)_2$ dimer decomposition (relative Gibbs free energies are indicated in kcal/mol).

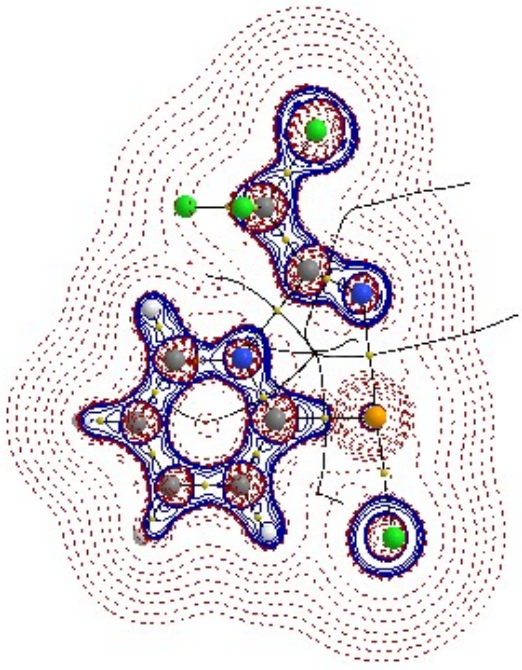


Figure S2. Contour line diagram of the Laplacian distribution, $\nabla^2\rho(r)$, selected zero flux surfaces and bond paths for the N≡C•••N plane in **TSCCl$_3$/Cl**.

Table S2. Atomic Cartesian coordinates (in Å) of the calculated structures (nuclear charge is indicated in the first column).

PySeCl (in DCM)

34	3.097313	0.975548	0.210124
7	0.463938	1.338395	-0.047449
6	1.303856	0.314549	-0.004693
6	0.931708	-1.020576	-0.101265
1	1.658592	-1.820033	-0.060516
6	-0.424771	-1.282907	-0.253448
1	-0.769358	-2.307533	-0.333681
6	-1.328066	-0.226380	-0.301364
1	-2.390193	-0.397920	-0.419056
6	-0.835922	1.068390	-0.194099
1	-1.501635	1.924298	-0.226060
17	4.197754	-0.922243	0.242131

PySeCl (in MeCN)

34	-1.216321	-0.758853	-0.155281
7	1.425235	-1.138811	-0.248496
6	0.596577	-0.121275	-0.061257
6	0.991284	1.192417	0.158616
1	0.273635	1.988170	0.304526
6	2.359244	1.439306	0.180877
1	2.721977	2.447338	0.346777
6	3.250810	0.389541	-0.012604
1	4.321175	0.549776	-0.001951
6	2.736434	-0.883553	-0.224455
1	3.393292	-1.732565	-0.381360
17	-2.296927	1.111484	0.235127

$(PySeCl)_2$

34	3.792184	4.718237	9.126856
17	3.872308	4.742593	11.474606
7	5.708311	2.928912	8.146132
6	5.550222	3.927097	9.015409
6	6.610791	4.396529	9.786082
1	6.455186	5.213393	10.477136
6	7.850103	3.791397	9.646540
1	8.689909	4.138832	10.235974
6	8.007320	2.748610	8.737764
1	8.958854	2.253988	8.598400
6	6.908195	2.350537	7.999969
1	6.960401	1.547240	7.274067
34	4.020393	1.896377	7.036653
17	2.293765	0.946179	5.758077
7	3.885463	4.686661	6.860524

6	3.857411	3.583879	6.112120
6	3.745043	3.647346	4.725601
1	3.733297	2.736456	4.143210
6	3.645053	4.892764	4.125186
1	3.555922	4.967210	3.048185
6	3.673661	6.039956	4.913293
1	3.601577	7.028812	4.481485
6	3.801785	5.892321	6.281752
1	3.832733	6.742332	6.953665

$(PySeCl)_2NCMe$

34	-1.079295	1.541413	-2.614719
17	-1.552601	0.085321	-4.223179
7	0.300806	-0.260730	-0.935623
6	-0.914061	0.203742	-1.228294
6	-2.068295	-0.229273	-0.586644
1	-3.027344	0.189616	-0.859964
6	-1.952016	-1.201916	0.399061
1	-2.830742	-1.561065	0.920685
6	-0.692459	-1.697594	0.700730
1	-0.549201	-2.458143	1.456855
6	0.405462	-1.196801	0.010809
1	1.403072	-1.563562	0.223548
34	2.287624	0.692995	-2.147062
17	4.197819	1.532392	-3.104591
7	3.290189	0.423582	0.447306
6	3.289302	-0.177807	-0.737309
6	3.935161	-1.383693	-0.998231
1	3.891936	-1.824105	-1.985704
6	4.623996	-1.992690	0.044175
1	5.141802	-2.930859	-0.115980
6	4.627284	-1.380840	1.291544
1	5.144442	-1.821576	2.134020
6	3.948058	-0.176305	1.443065
1	3.931076	0.332056	2.401400
7	-0.165348	3.087045	-0.393846
6	0.951251	3.348213	-0.302458
6	2.363335	3.680218	-0.186451
1	2.757986	3.912518	-1.176192
1	2.889878	2.811697	0.214054
1	2.484963	4.541458	0.470316

PySe(Cl)(NCMe)

34	-1.559746	1.635170	-2.775384
17	-2.966718	0.392783	-3.963741
7	-0.527510	-0.873972	-2.086036
6	-1.053949	0.218851	-1.553410
6	-1.251139	0.409531	-0.188657
1	-1.700149	1.322098	0.179625
6	-0.856284	-0.609858	0.669265

1	-0.986766	-0.504664	1.739677
6	-0.312670	-1.768349	0.129165
1	-0.001912	-2.592021	0.758798
6	-0.176508	-1.855572	-1.252631
1	0.240093	-2.745789	-1.711999
7	0.295312	3.066016	-1.229273
6	1.108671	3.730175	-0.764728
6	2.141674	4.571244	-0.176550
1	2.055797	5.582330	-0.572859
1	3.122483	4.166488	-0.423444
1	2.020903	4.594079	0.905789

PySeBr

34	0.647000	-1.089831	-0.012541
7	-2.014121	-1.062479	-0.243042
6	-1.053396	-0.178796	-0.012505
6	-1.263569	1.175578	0.214000
1	-0.447973	1.858579	0.407352
6	-2.580662	1.619911	0.186073
1	-2.798535	2.668331	0.354902
6	-3.606775	0.712968	-0.054701
1	-4.642309	1.027087	-0.082953
6	-3.274534	-0.620296	-0.259810
1	-4.040952	-1.364284	-0.450030
35	2.127905	0.706874	0.133328

PBr/Cl

34	2.847796	-0.512212	-0.330072
7	2.190108	1.242562	-0.344070
7	0.252339	0.055168	0.054521
6	0.954011	1.278797	-0.144777
6	1.075200	-1.034277	-0.004451
6	0.535628	-2.310600	0.172003
1	1.200591	-3.161382	0.122277
6	-0.814271	-2.437999	0.401280
1	-1.244171	-3.422560	0.539626
6	-1.639197	-1.300336	0.457265
1	-2.702335	-1.381274	0.636489
6	-1.092299	-0.066161	0.282527
1	-1.665928	0.847387	0.312978
35	-0.027496	2.894002	-0.096167
17	3.654914	-3.173526	-0.277881

$PCCl_3$/Cl

34	2.817640	-0.491224	-0.326483
7	2.159945	1.232666	-0.338218
7	0.219835	0.060502	0.059569
6	0.914806	1.293345	-0.139101
6	1.051811	-1.024597	-0.001294
6	0.538683	-2.310868	0.171378

1	1.223074	-3.146159	0.117352
6	-0.806897	-2.467001	0.401876
1	-1.218812	-3.459538	0.537723
6	-1.647767	-1.342631	0.461476
1	-2.709408	-1.440107	0.641558
6	-1.125320	-0.097278	0.290111
1	-1.736171	0.788280	0.328656
6	0.170672	2.624471	-0.109582
17	1.301791	3.951964	-0.386029
17	-0.601245	2.857403	1.487300
17	-1.072055	2.658146	-1.395911
17	3.669855	-3.197302	-0.278590

PMe_2N/Cl

34	3.049139	-0.084762	-0.038473
7	2.187539	1.548681	-0.023771
7	0.399209	0.098990	0.103122
6	0.921780	1.437894	0.061116
6	1.356206	-0.867464	0.107123
6	0.982967	-2.212915	0.168311
1	1.762670	-2.962797	0.184280
6	-0.356423	-2.524720	0.188621
1	-0.664793	-3.562179	0.236575
6	-1.328464	-1.508626	0.119000
1	-2.384263	-1.741142	0.092187
6	-0.934095	-0.205185	0.070727
1	-1.610511	0.632329	-0.015992
7	0.002743	2.468757	0.081949
17	4.262302	-2.808271	0.003758
6	0.525421	3.731003	-0.442962
6	-0.671197	2.672007	1.376862
1	-0.311465	4.423793	-0.535897
1	0.967724	3.571238	-1.425234
1	1.278654	4.165593	0.224119
1	-1.552069	3.293542	1.214569
1	0.002189	3.175285	2.080920
1	-0.985654	1.725838	1.816219

PMe/Br

34	3.042879	0.917555	-0.526794
7	2.385543	2.648388	-0.538875
7	0.467454	1.452933	-0.143228
6	1.131230	2.706612	-0.338308
6	1.286306	0.366576	-0.201809
6	0.756284	-0.912946	-0.026808
1	1.426976	-1.760599	-0.077810
6	-0.594545	-1.042174	0.202777
1	-1.023505	-2.027298	0.340928
6	-1.421576	0.094245	0.259267
1	-2.484398	0.008266	0.438796

6	-0.875152	1.331164	0.084472
1	-1.445898	2.248006	0.114265
6	0.327979	3.960010	-0.293735
1	0.998855	4.799550	-0.461193
1	-0.156881	4.074054	0.678590
1	-0.442049	3.953411	-1.068669
35	4.016908	-2.046044	-0.481093

PMe/Cl

34	0.645887	4.144715	5.170787
7	-0.163348	5.711670	5.701005
7	1.808803	6.503856	4.833518
6	0.544026	6.741716	5.458611
6	2.076815	5.192203	4.584846
6	3.279453	4.828819	3.977793
1	3.468764	3.780235	3.790884
6	4.173108	5.820849	3.642990
1	5.112479	5.559494	3.170894
6	3.876045	7.170160	3.908991
1	4.569098	7.959314	3.651168
6	2.692461	7.493293	4.503241
1	2.394648	8.504603	4.738453
6	0.149002	8.141936	5.776009
1	-0.833349	8.120382	6.242471
1	0.103549	8.745795	4.866733
1	0.864900	8.598651	6.463322
17	2.149965	1.644952	4.222888

PPh/Cl

34	-1.093194	-0.438010	0.857592
7	-1.802454	1.264096	0.809817
7	-3.664866	0.003812	0.328803
6	-3.043113	1.279755	0.528614
6	-2.808671	-1.050947	0.441172
6	-3.282645	-2.354252	0.269669
1	-2.580339	-3.172472	0.355555
6	-4.619473	-2.542240	0.009412
1	-5.003111	-3.546291	-0.125602
6	-5.492736	-1.441292	-0.067359
1	-6.550349	-1.573286	-0.250121
6	-5.001748	-0.181120	0.095836
1	-5.611886	0.709305	0.063072
17	-0.123611	-3.230478	0.850986
6	-5.188803	4.945588	0.191545
6	-4.500647	4.637579	1.361624
6	-5.190995	4.049585	-0.874676
6	-3.817297	3.431792	1.471652
6	-4.514378	2.840342	-0.769945
6	-3.831793	2.528616	0.408362
1	-5.719059	5.887118	0.107127

1	-4.494007	5.336410	2.189685
1	-3.273231	3.185108	2.376222
1	-4.499428	2.152406	-1.608777
1	-5.711746	4.295115	-1.792674

PPhNH/Cl

34	1.429111	-1.265291	-0.258502
7	-0.367839	-0.847727	-0.284816
7	0.569876	1.240360	0.009365
6	-0.583673	0.397623	-0.143629
6	1.750859	0.564310	-0.060216
6	2.956521	1.264124	0.036081
1	3.880800	0.705980	-0.030453
6	2.918691	2.626236	0.219440
1	3.844848	3.183467	0.292438
6	1.686501	3.297506	0.328006
1	1.639335	4.363857	0.500461
6	0.526212	2.590794	0.226929
1	-0.449885	3.040405	0.331272
7	-1.803545	1.019885	-0.072519
17	4.360551	-1.750131	-0.169470
1	-1.876563	1.907999	-0.556287
6	-3.163744	-0.851784	0.759358
6	-4.405985	-1.469780	0.846530
6	-3.028183	0.311285	0.000149
6	-5.516305	-0.938763	0.195391
6	-4.136570	0.848530	-0.655315
6	-5.375111	0.225902	-0.552547
1	-2.310308	-1.269605	1.276275
1	-4.502975	-2.374480	1.435799
1	-6.480191	-1.427766	0.271364
1	-6.228945	0.653754	-1.065240
1	-4.024717	1.753938	-1.242999

TSBr/Cl

34	2.898006	-0.526617	0.034541
7	2.034744	1.688678	-0.479059
7	0.104487	-0.090777	0.127473
6	0.927242	1.817220	-0.131750
6	1.012536	-1.052418	0.004615
6	0.632691	-2.387295	-0.141057
1	1.369960	-3.165844	-0.264058
6	-0.719061	-2.696619	-0.134831
1	-1.030835	-3.727588	-0.255122
6	-1.660449	-1.685361	0.017593
1	-2.722979	-1.888503	0.030695
6	-1.197238	-0.387538	0.136046
1	-1.882694	0.446174	0.239237
35	-0.470860	2.903619	0.322001
17	3.668331	-2.574910	0.629027

$TSCCl_3/Cl$

34	2.881434	-0.533268	-0.266579
7	2.101378	1.657028	-0.413937
7	0.048815	-0.097548	-0.241493
6	0.951445	1.822998	-0.335202
6	0.982032	-1.047735	-0.308398
6	0.629116	-2.396961	-0.403627
1	1.381517	-3.164832	-0.475729
6	-0.710122	-2.745485	-0.408832
1	-0.989613	-3.789718	-0.489072
6	-1.677395	-1.753292	-0.313989
1	-2.735627	-1.977790	-0.307443
6	-1.247567	-0.443546	-0.236258
1	-1.967158	0.361740	-0.169873
6	-0.201386	2.758859	-0.279689
17	0.463811	4.406791	-0.339898
17	-1.095295	2.538700	1.237021
17	-1.256547	2.505785	-1.685486
17	3.715012	-2.657586	-0.081186

$TSMe_2N/Cl$

34	2.883508	-0.006791	0.025596
7	2.326281	1.847490	0.232472
7	0.165281	0.507027	-0.186754
6	1.220805	2.297265	0.167704
6	1.011992	-0.506108	-0.236183
6	0.577934	-1.816496	-0.454127
1	1.283354	-2.632670	-0.492355
6	-0.782080	-2.026729	-0.616880
1	-1.148546	-3.032766	-0.786469
6	-1.670841	-0.954045	-0.561693
1	-2.737087	-1.091585	-0.684462
6	-1.148540	0.306696	-0.342811
1	-1.777773	1.188252	-0.286801
7	0.333653	3.250153	0.185509
17	3.725303	-2.497673	-0.249606
6	-0.186624	3.764407	-1.085929
6	-0.508401	3.434166	1.372675
1	-0.025035	2.984598	2.237827
1	-1.488231	2.977075	1.216638
1	-0.628034	4.505080	1.539901
1	-1.064857	3.194569	-1.399950
1	0.586049	3.703300	-1.849816
1	-0.462542	4.808054	-0.934047

TSMe/Br

34	2.806578	-0.386909	-0.023811
7	1.990323	1.631769	-0.173629
7	-0.000869	-0.059659	0.003197

6	0.838537	1.841695	-0.093770
6	0.932938	-0.997755	-0.057132
6	0.584823	-2.347974	-0.143344
1	1.338340	-3.116746	-0.206365
6	-0.760142	-2.685808	-0.150315
1	-1.044990	-3.729258	-0.221487
6	-1.730190	-1.691944	-0.070018
1	-2.787584	-1.921813	-0.069681
6	-1.298417	-0.380286	0.000901
1	-1.997143	0.447945	0.054538
6	-0.363293	2.667820	-0.024016
1	-0.055398	3.713936	-0.049057
1	-0.898550	2.462499	0.903857
1	-1.010962	2.454423	-0.874996
35	3.822139	-2.694493	0.213530

TSMe/Cl

34	3.196653	1.010717	0.148318
7	2.453994	3.008152	-0.027723
7	0.400686	1.370699	-0.072624
6	1.318739	3.292049	-0.060920
6	1.321491	0.421175	-0.039462
6	0.969620	-0.927511	-0.136896
1	1.715756	-1.705706	-0.122947
6	-0.374653	-1.247998	-0.257439
1	-0.666467	-2.288996	-0.336669
6	-1.335097	-0.241788	-0.279158
1	-2.391092	-0.460645	-0.369847
6	-0.895049	1.066071	-0.187291
1	-1.584408	1.904026	-0.206637
6	0.132560	4.136615	-0.096676
1	0.457819	5.178111	-0.082406
1	-0.488022	3.930735	0.776302
1	-0.434639	3.938549	-1.006705
17	4.057750	-1.230366	0.397563

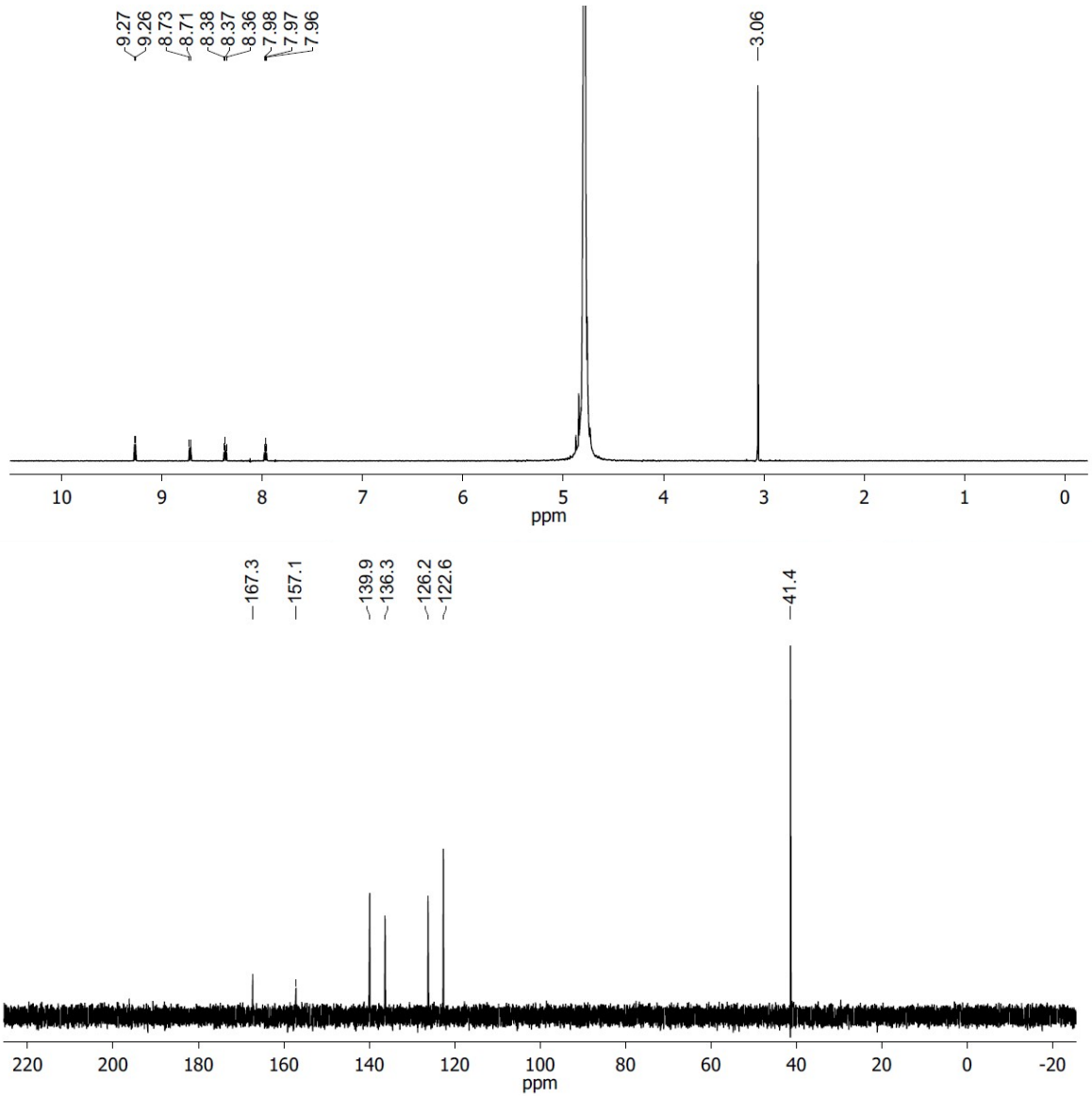
TSPh/Cl

34	-0.708274	0.148431	1.159091
7	-1.403266	2.177038	0.861853
7	-3.383453	0.544580	0.343034
6	-2.496420	2.433377	0.519901
6	-2.525765	-0.415941	0.646962
6	-2.914342	-1.758646	0.600743
1	-2.225411	-2.550170	0.847732
6	-4.216851	-2.053733	0.227931
1	-4.534341	-3.089476	0.188596
6	-5.105632	-1.031325	-0.092123
1	-6.126825	-1.232179	-0.387855
6	-4.637810	0.267638	-0.019490
1	-5.266514	1.122467	-0.252658

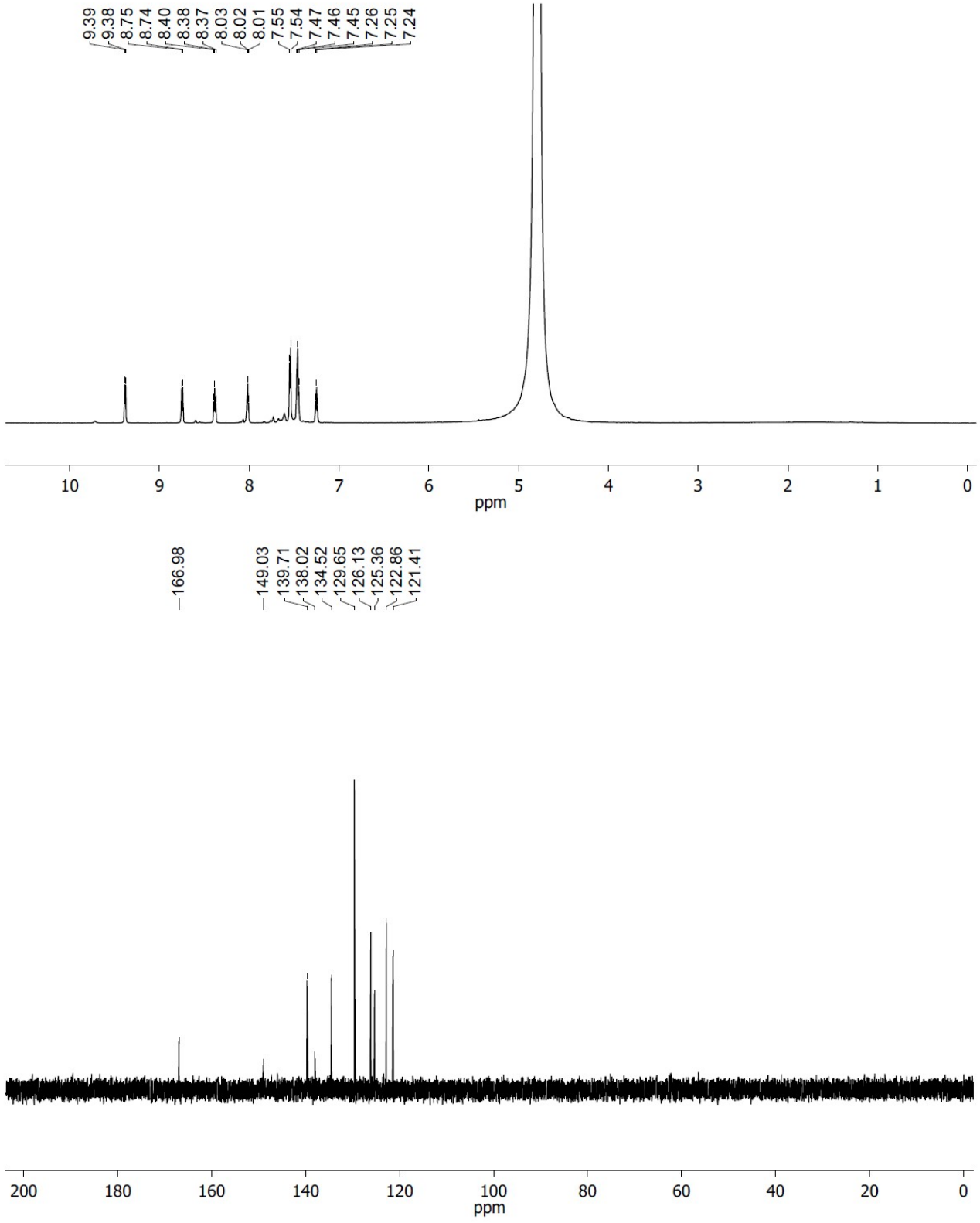
17	0.076990	-2.085316	1.492055
6	-5.740010	4.869187	-0.607077
6	-5.615383	4.454795	0.717361
6	-4.799795	4.483116	-1.559646
6	-4.548657	3.650860	1.097876
6	-3.727142	3.680017	-1.193093
6	-3.606098	3.275624	0.137814
1	-6.574982	5.496358	-0.898079
1	-6.349303	4.758496	1.454208
1	-4.440330	3.314303	2.122371
1	-2.988543	3.367032	-1.921692
1	-4.901340	4.807079	-2.588482

TSPhNH/Cl

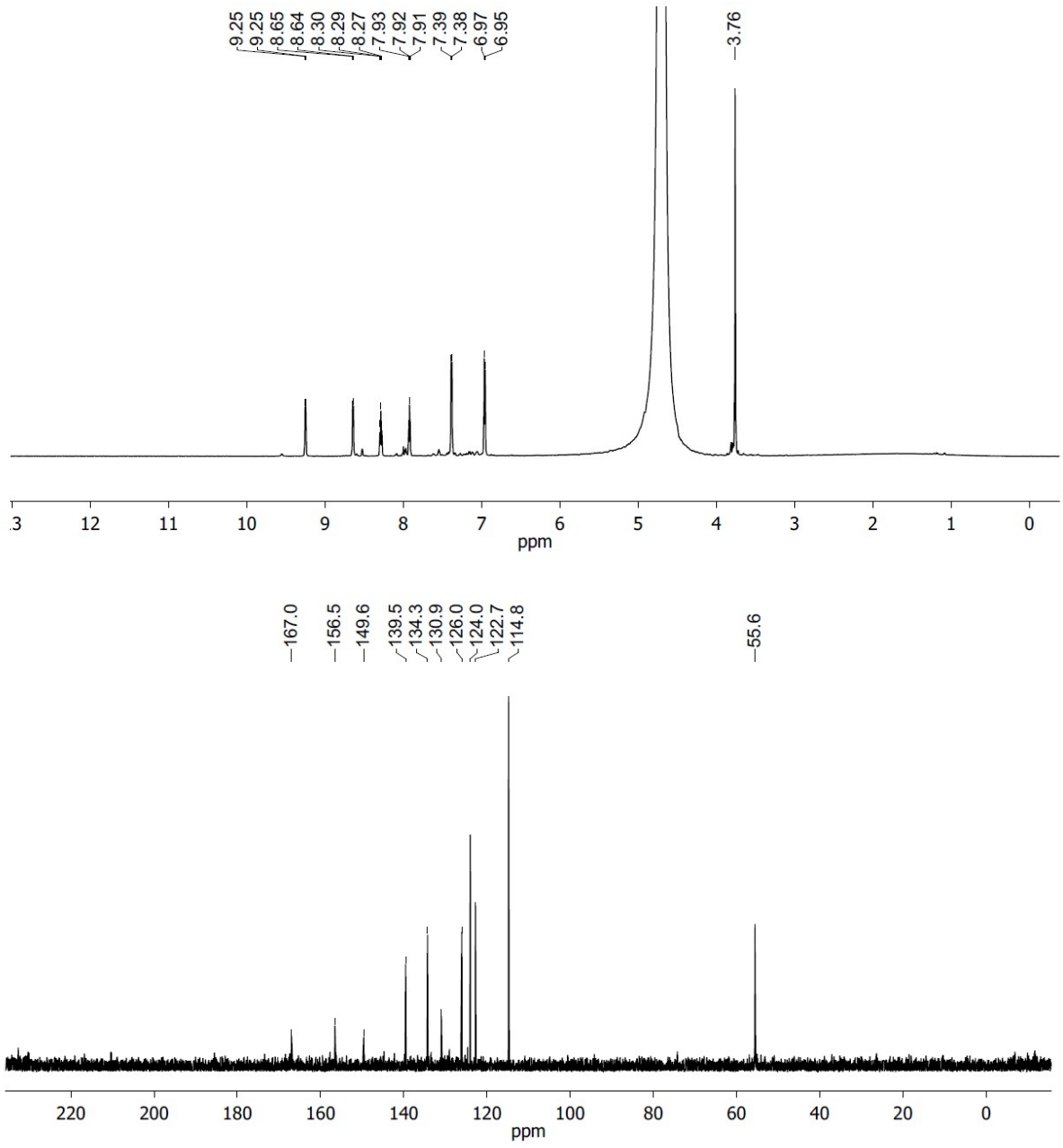
34	1.807743	-2.097901	0.435785
7	1.913189	-0.285409	1.445843
7	-0.598201	-0.922593	1.250724
6	0.992163	0.343768	1.839493
6	-0.143641	-2.001382	0.638078
6	-1.014693	-2.997811	0.187483
1	-0.645582	-3.879114	-0.312598
6	-2.372465	-2.823347	0.407570
1	-3.066406	-3.583671	0.067402
6	-2.839032	-1.686235	1.063101
1	-3.892817	-1.529245	1.252133
6	-1.904596	-0.752982	1.471679
1	-2.187881	0.159847	1.987611
7	0.362068	1.374934	2.367171
17	1.728856	-4.217032	-0.823858
1	0.223867	1.375616	3.373830
6	-0.422999	2.167482	0.192083
6	-1.184627	3.069244	-0.544073
6	-0.404628	2.273321	1.580923
6	-1.920962	4.062827	0.093314
6	-1.138116	3.262064	2.233340
6	-1.893079	4.154838	1.483007
1	0.143850	1.391718	-0.311332
1	-1.199748	2.988082	-1.624670
1	-2.513378	4.759665	-0.487276
1	-2.462483	4.925391	1.989762
1	-1.111113	3.327503	3.315927



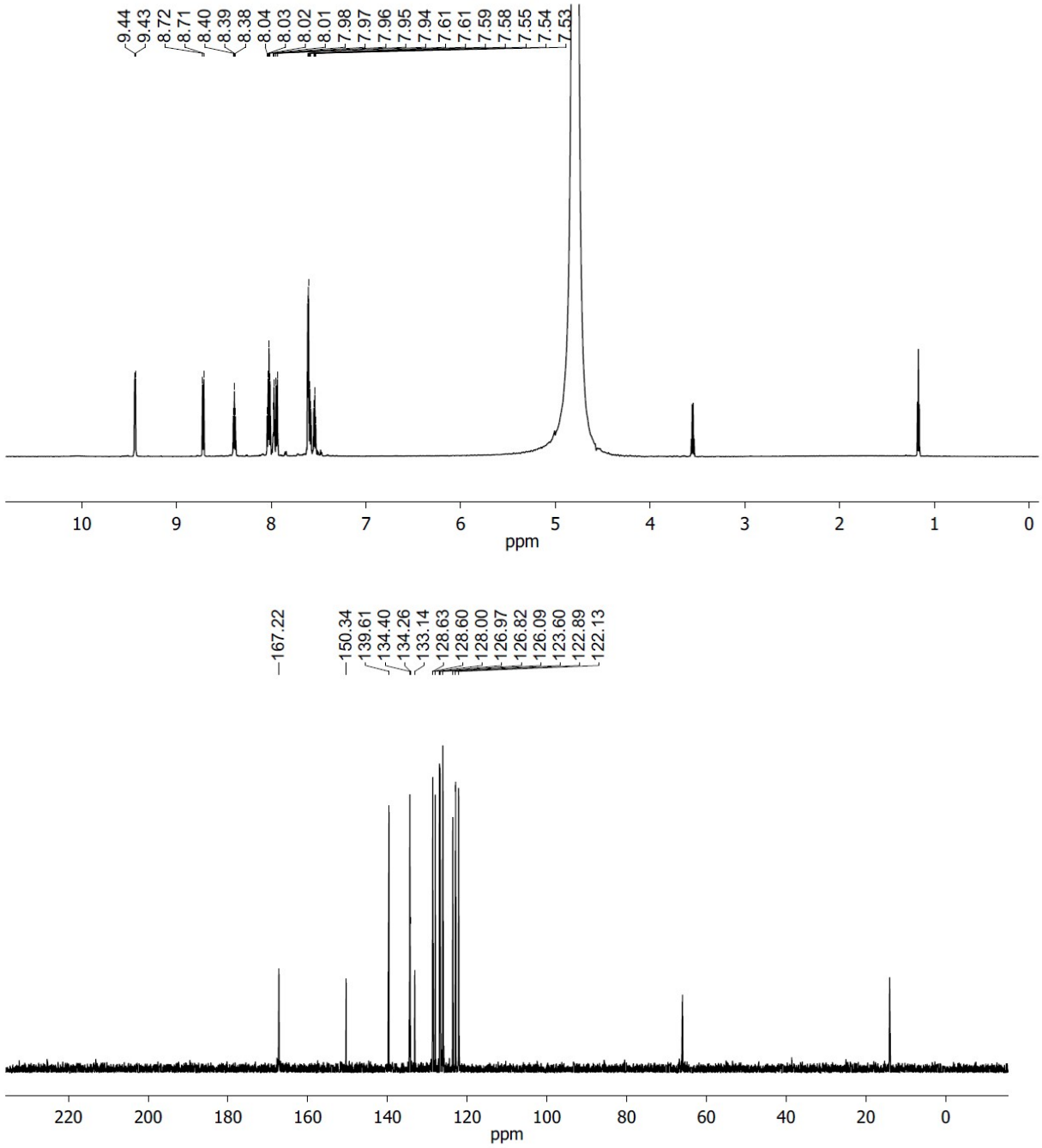
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **1** (D_2O).



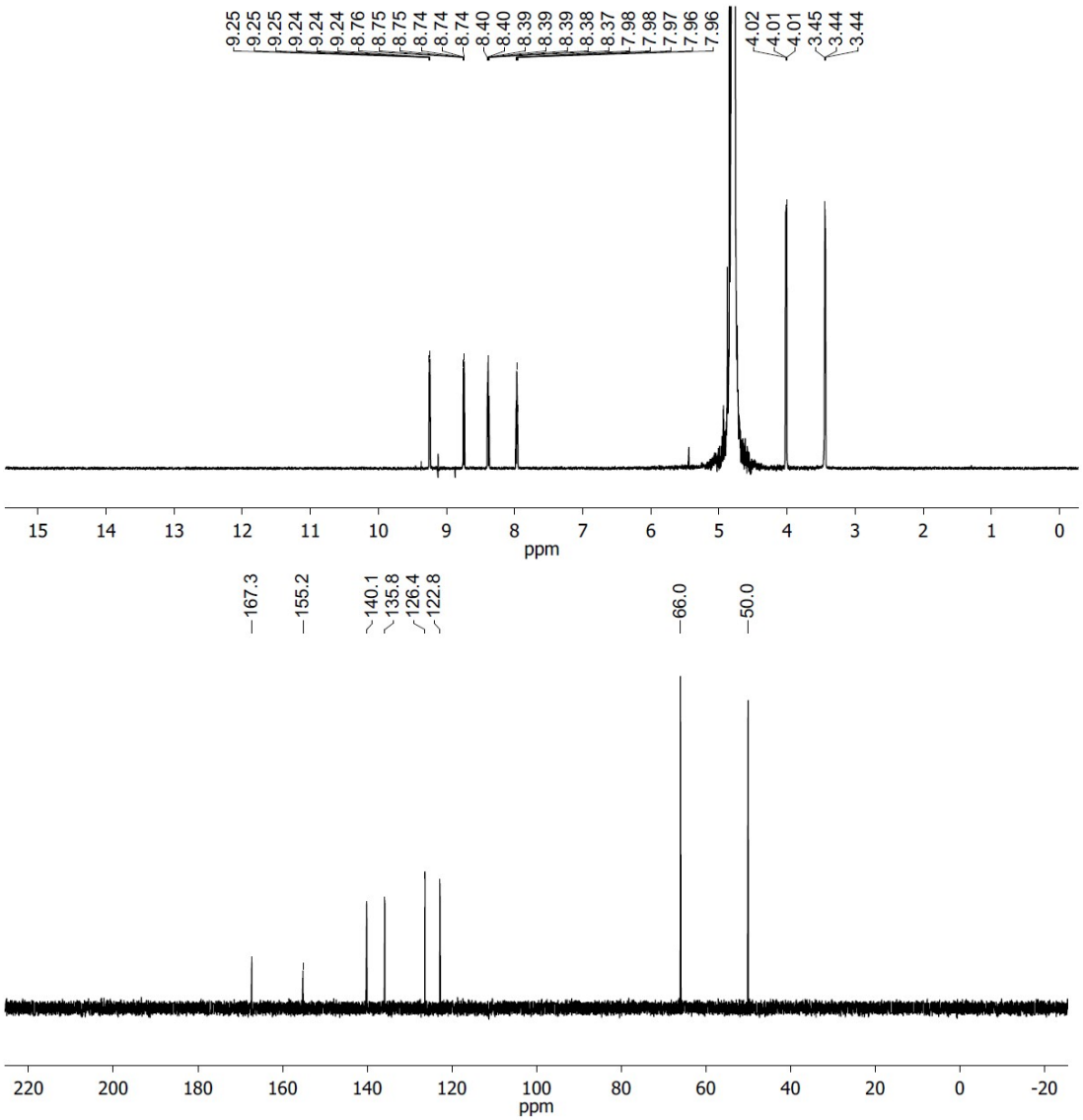
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **2** (D_2O).



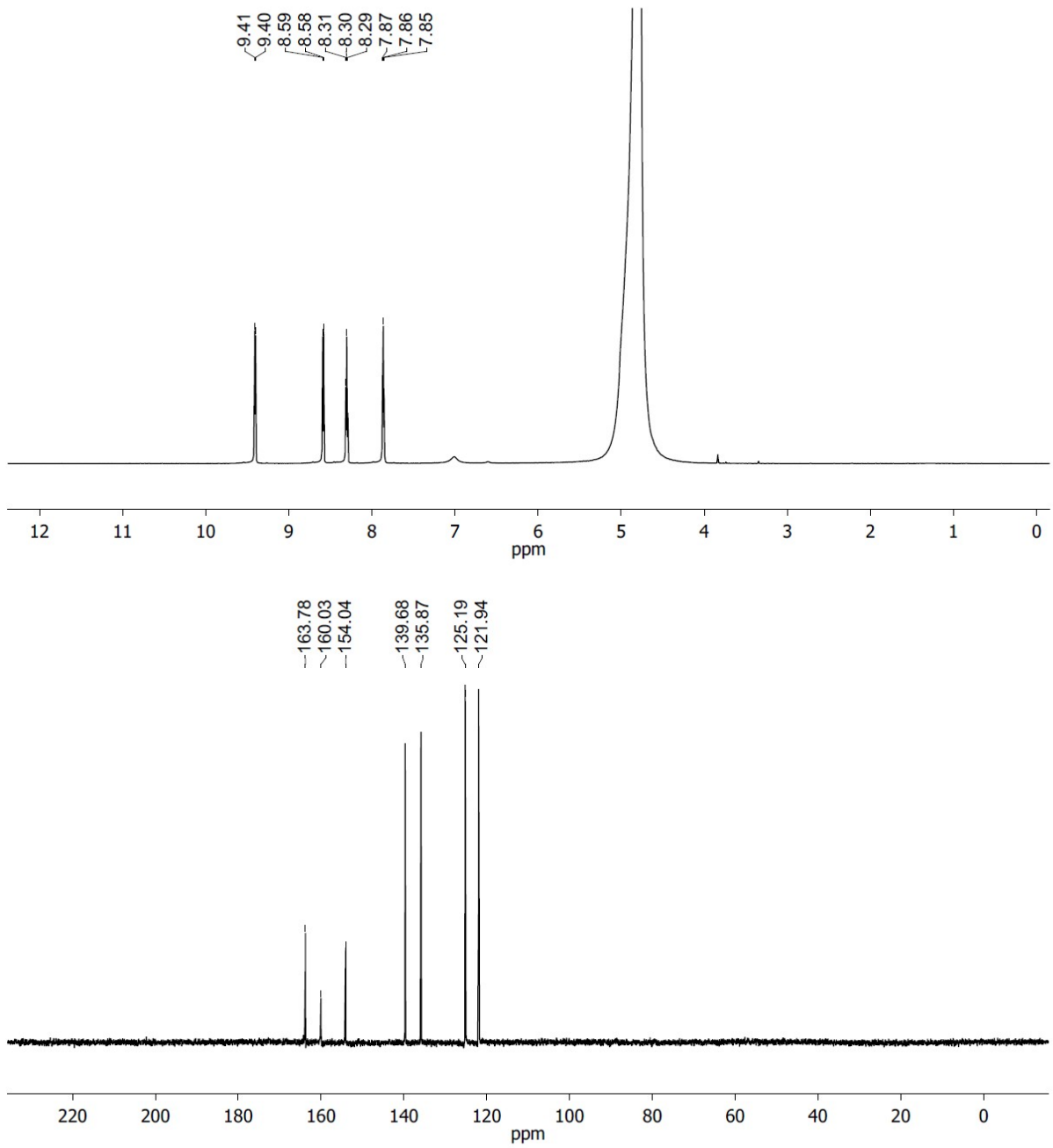
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **3** (D_2O).



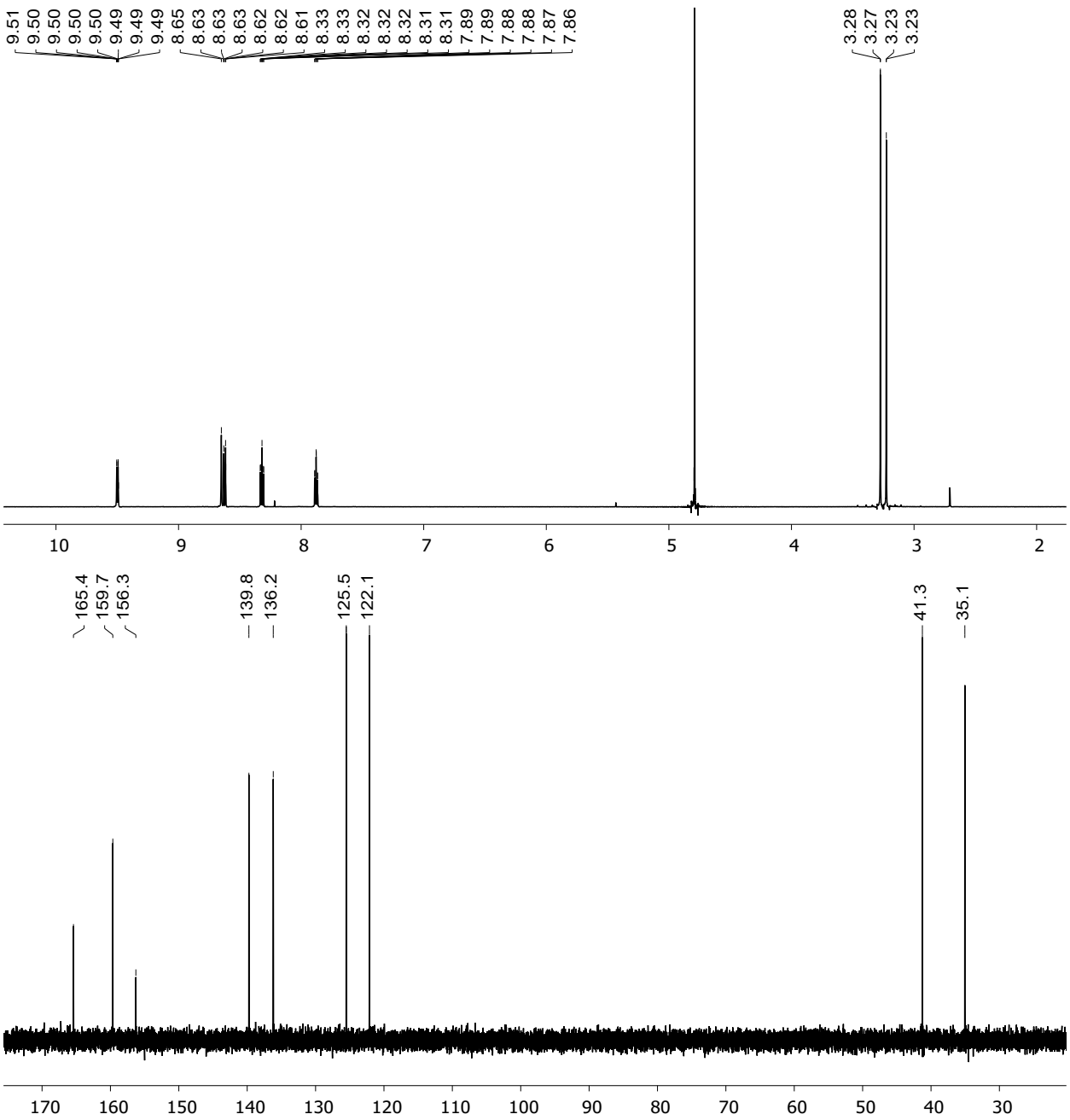
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **4** (D_2O).



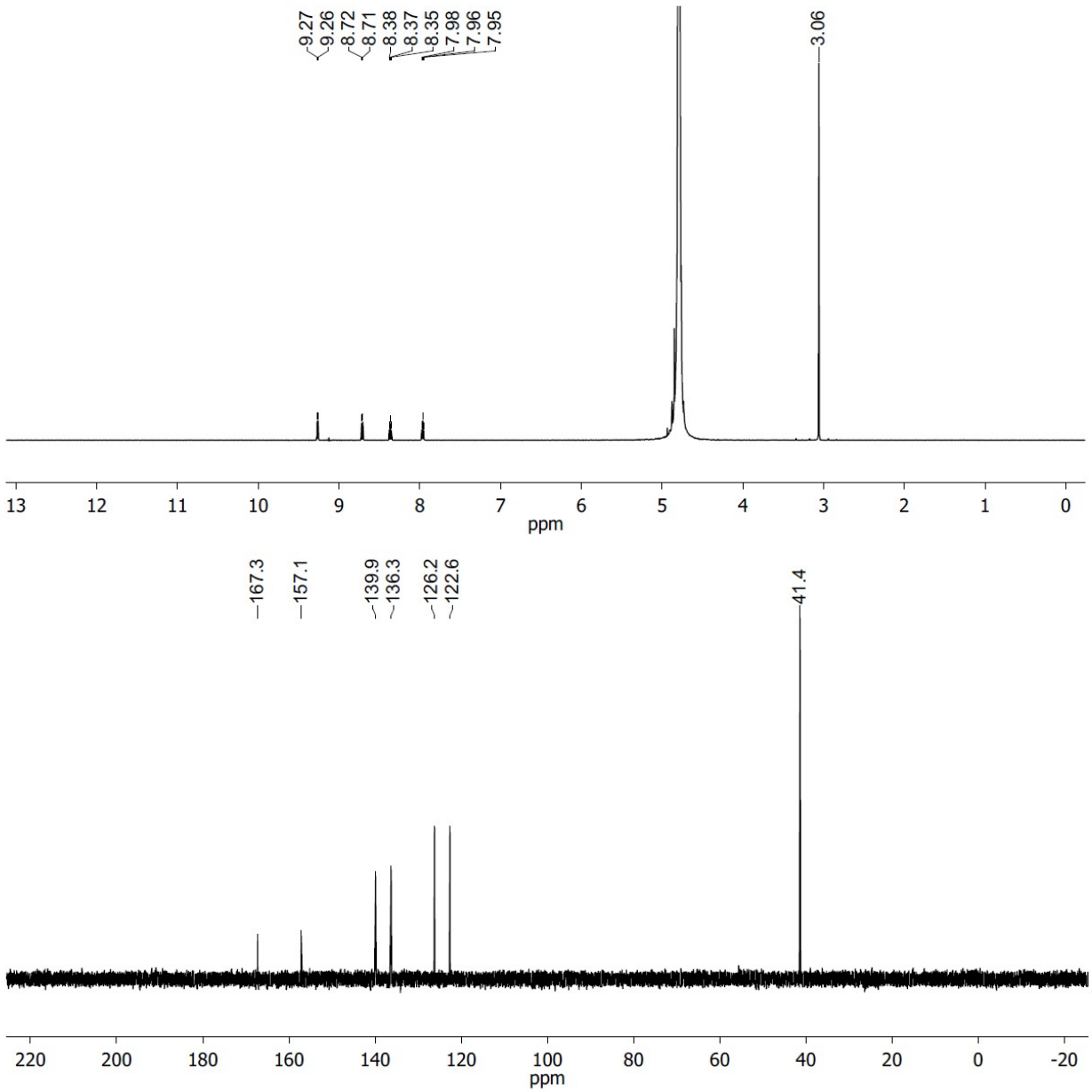
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **5** (D_2O).



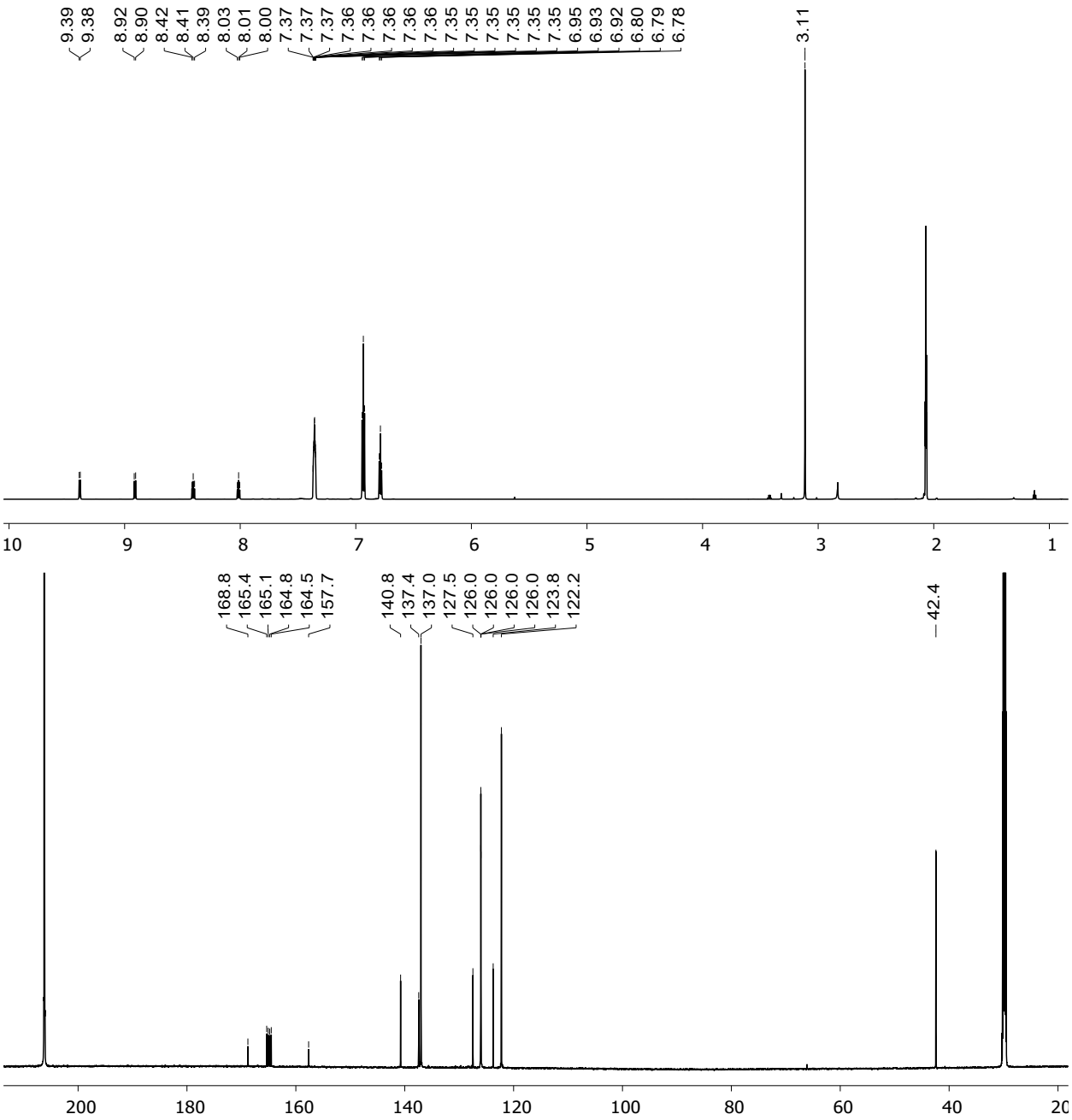
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **6** (D_2O).



^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **7** (D_2O).



^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **8** (D_2O).



^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **9** (Me_2CO).