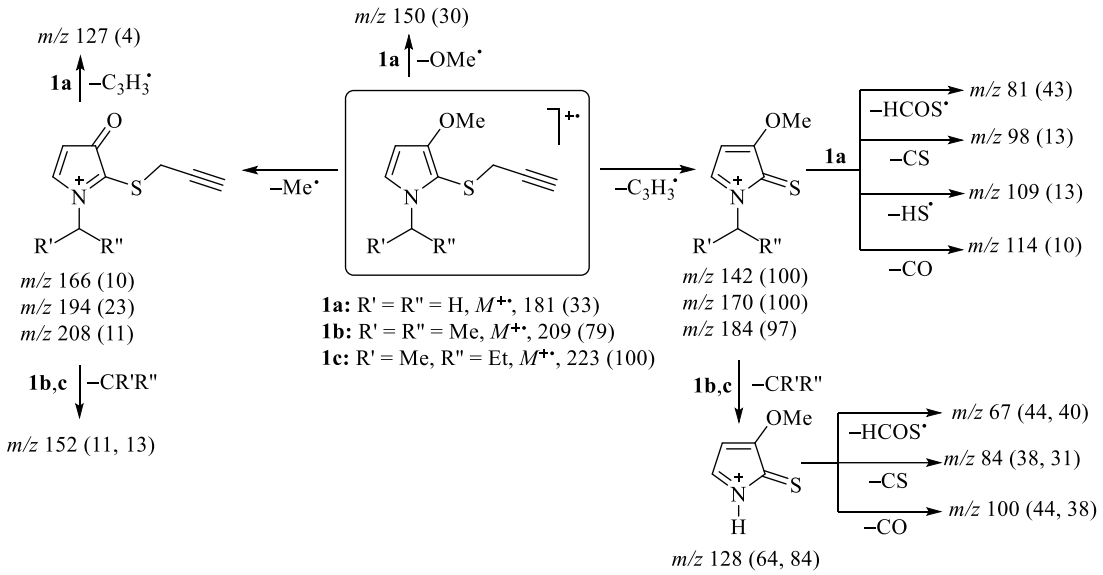
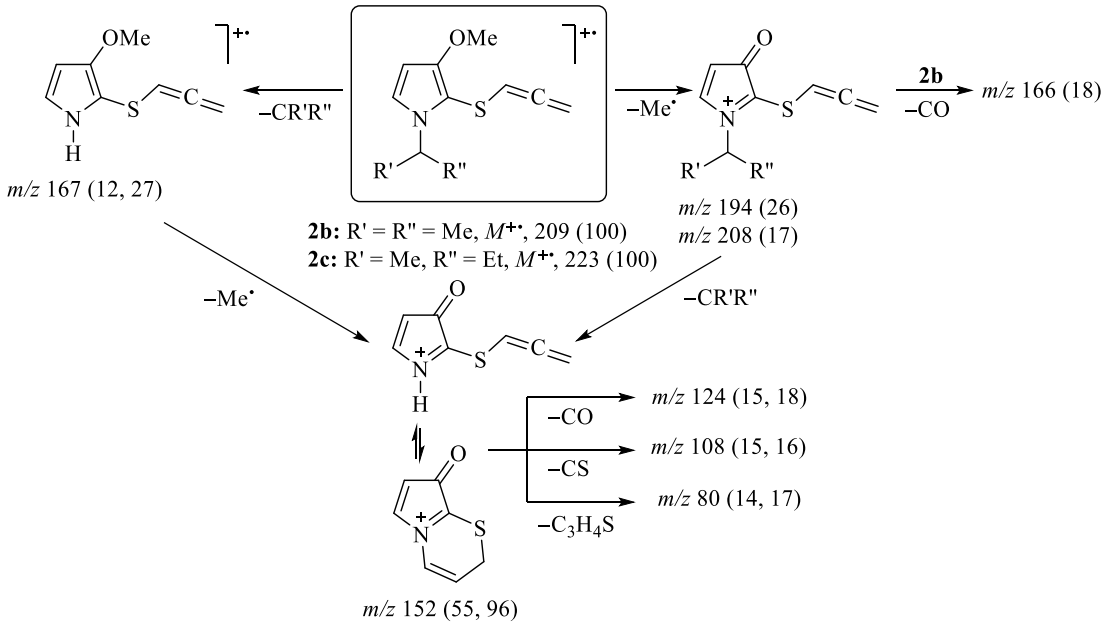
Electronic supplementary materials *Mendeleev Commun.*, 2024, **34**, 142–144

Effect of intramolecular conjugation on the primary fragmentation in EI mass spectrum of 2-allenylthio-1*H*-pyrrole derivative

Vera V. Belyaeva and Lyudmila V. Klyba



Scheme S1[S1]



Scheme S2[S1]

S1 L. V. Klyba, O. A. Tarasova and N. A. Nedolya, *Russ. J. Org.Chem.*, 2016, **52**, 1773 (*Zh. Org. Khim.*, 2016, **52**, 1782).

The atom numbering in Tables S1-S5 may not coincide with those used in the main text since these tables relate to the current non-systematized working results.

Table S1 1-Isopropyl-3-methoxy-2-(propa-1,2-dien-1-ylthio)-1*H*-pyrrole (**1**) B3PW91/6-311G**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.370924	0.273908	0.268247
2	6	0	-1.207112	1.347083	-0.022285
3	6	0	-2.425862	0.836582	-0.514800
4	6	0	-2.297599	-0.539911	-0.517591
5	7	0	-1.074094	-0.889422	-0.058213
6	6	0	-0.589048	-2.257256	0.112895
7	16	0	1.208836	0.297928	0.977441
8	8	0	-0.824999	2.628850	0.161203
9	6	0	-1.802889	3.610510	-0.124704
10	6	0	2.272980	0.414627	-0.446914
11	6	0	3.570927	0.297827	-0.391793
12	6	0	4.868739	0.197412	-0.327298
13	6	0	-0.510659	-2.987373	-1.226932
14	6	0	-1.424188	-3.017143	1.142283
15	1	0	-3.294974	1.389006	-0.834267
16	1	0	-3.013182	-1.288032	-0.819653
17	1	0	0.421771	-2.145252	0.506251
18	1	0	-1.340839	4.570416	0.093520
19	1	0	-2.690264	3.484299	0.504728
20	1	0	-2.099361	3.583473	-1.178933
21	1	0	1.774293	0.634934	-1.386210
22	1	0	5.499175	1.065180	-0.148052
23	1	0	5.376832	-0.751597	-0.481738
24	1	0	-0.071857	-3.977806	-1.088923
25	1	0	0.107816	-2.433823	-1.934874
26	1	0	-1.501565	-3.118590	-1.668964
27	1	0	-0.994530	-4.005930	1.316430
28	1	0	-2.453119	-3.154064	0.800449
29	1	0	-1.449110	-2.481506	2.092409

Sum of electronic and zero-point Energies= -955.941276
Sum of electronic and thermal Energies= -955.925229
Sum of electronic and thermal Enthalpies= -955.924285
Sum of electronic and thermal Free Energies= -955.986586

Low frequencies --- -10.6126 -5.9508 -0.0023 -0.0022 0.0003 6.8453
Low frequencies --- 24.9419 29.6176 41.4014

Table S2 2-Ethynylthio-1-isopropyl-3-methoxy-1*H*-pyrrole (**2**)
B3PW91/6-311G**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.792324	-0.748562	0.038450
2	6	0	-0.321265	-1.957627	0.501752
3	6	0	1.086562	-1.944893	0.496046
4	6	0	1.468050	-0.659480	0.003107
5	6	0	0.298872	0.089279	-0.294604
6	8	0	2.722323	-0.152366	-0.185930
7	6	0	3.775968	-1.054221	0.154099
8	6	0	-2.189557	-0.395862	-0.120073
9	16	0	0.156628	1.602600	-0.991278
10	6	0	0.043072	2.631388	0.215482
11	6	0	-0.044394	3.469553	1.077447
12	6	0	-2.945976	-0.370118	1.209574
13	6	0	-2.925311	-1.318168	-1.094363
14	1	0	-0.997924	-2.757338	0.809791
15	1	0	1.743058	-2.749325	0.806887
16	1	0	3.724892	-1.971164	-0.481219
17	1	0	3.721956	-1.327708	1.235469
18	1	0	4.701867	-0.465780	-0.064737
19	1	0	-2.199745	0.654866	-0.553942
20	1	0	-0.113776	4.209165	1.833415
21	1	0	-2.468087	0.337584	1.928278
22	1	0	-2.975089	-1.385409	1.672462
23	1	0	-3.992692	-0.032811	1.018111
24	1	0	-2.958976	-2.364269	-0.706474
25	1	0	-2.428929	-1.322616	-2.094013
26	1	0	-3.971042	-0.947050	-1.216090

Sum of electronic and zero-point Energies= -916.645306
Sum of electronic and thermal Energies= -916.630618
Sum of electronic and thermal Enthalpies= -916.629674
Sum of electronic and thermal Free Energies= -916.687965

Low frequencies --- -11.1036 -8.6876 -0.0028 -0.0012 0.0018 3.0055
Low frequencies --- 30.6622 40.0090 58.2302

Table S3 1-Isopropyl-3-methoxy-2-(buta-2,3-dien-1-ylthio)-1*H*-pyrrole (**3**) B3PW91/6-311G**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.741726	0.852410	-0.584666
2	6	0	1.531869	1.332976	-0.036426
3	6	0	2.636232	-0.525826	-0.611105
4	6	0	0.719716	0.241750	0.254328
5	8	0	1.131072	2.607610	0.173361
6	7	0	1.426883	-0.899691	-0.123931
7	6	0	0.988510	-2.279176	0.096092
8	6	0	1.724787	-2.906193	1.278759
9	6	0	1.114260	-3.108260	-1.178628
10	6	0	2.089327	3.606938	-0.105804
11	16	0	-0.863867	0.230927	0.972527
12	6	0	-1.960405	0.564852	-0.488753
13	6	0	-3.329344	0.926208	-0.004572
14	6	0	-4.389851	0.187016	-0.189364
15	6	0	-5.448396	-0.545914	-0.385658
16	1	0	3.590632	1.423497	-0.926054
17	1	0	3.356540	-1.257882	-0.941598
18	1	0	-0.069424	-2.192451	0.357595
19	1	0	1.603566	-2.294269	2.175333
20	1	0	2.794719	-3.002941	1.071419
21	1	0	1.327612	-3.903747	1.487173
22	1	0	0.685402	-4.101246	-1.019333
23	1	0	2.159343	-3.243870	-1.472486
24	1	0	0.585076	-2.633367	-2.007984
25	1	0	2.369865	3.609655	-1.166556
26	1	0	2.991444	3.477982	0.504582
27	1	0	1.620534	4.558626	0.142956
28	1	0	-1.989258	-0.312813	-1.135062
29	1	0	-1.507189	1.401274	-1.024651
30	1	0	-3.428318	1.858731	0.549062
31	1	0	-6.070636	-0.415741	-1.267079
32	1	0	-5.745372	-1.310008	0.327659

Low frequencies --- -0.0025 -0.0025 -0.0011 1.6465 4.5905 7.9699
Low frequencies --- 20.4468 27.3715 31.9775
Sum of electronic and zero-point Energies= -995.223298
Sum of electronic and thermal Energies= -995.205904
Sum of electronic and thermal Enthalpies= -995.204960
Sum of electronic and thermal Free Energies= -995.271008

Table S4 1-Isopropyl-3-methoxy-2-(prop-2-yn-1-ylthio)-1*H*-pyrrole (**4**) B3PW91/6-311G**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.737411	-0.836139	-0.043485
2	6	0	-0.222207	-1.975818	0.479410
3	6	0	1.156552	-1.886351	0.528736
4	6	0	1.493889	-0.613987	0.015540
5	6	0	0.312701	0.030619	-0.330557
6	8	0	2.706365	-0.047952	-0.150337
7	6	0	3.814774	-0.837171	0.231842
8	6	0	-2.162718	-0.520697	-0.173414
9	16	0	0.131170	1.587657	-1.096378
10	6	0	-0.161048	2.641646	0.207118
11	6	0	-0.386012	3.452375	1.073075
12	6	0	-2.770456	-0.173879	1.184472
13	6	0	-2.912688	-1.641555	-0.886090
14	1	0	-0.862448	-2.787026	0.788577
15	1	0	1.823181	-2.654756	0.886885
16	1	0	3.869810	-1.761332	-0.356253
17	1	0	3.777644	-1.088632	1.298683
18	1	0	4.700079	-0.233293	0.036125
19	1	0	-2.194367	0.370776	-0.805090
20	1	0	-0.561651	4.159587	1.847650
21	1	0	-2.218562	0.642458	1.654702
22	1	0	-2.750278	-1.038473	1.854888
23	1	0	-3.811453	0.138966	1.063689
24	1	0	-2.943942	-2.555706	-0.286077
25	1	0	-2.446939	-1.875336	-1.846076
26	1	0	-3.945565	-1.334259	-1.069363

Low frequencies ---	-11.1036	-8.6876	-0.0028	-0.0012	0.0018	3.0055
Low frequencies ---	30.6622	40.0090	58.2302			

Sum of electronic and zero-point Energies= -916.645306
Sum of electronic and thermal Energies= -916.630618
Sum of electronic and thermal Enthalpies= -916.629674
Sum of electronic and thermal Free Energies= -916.687965

Table S5 1-Methyl-3-methoxy-2-methylthio-1*H*-pyrrole (**5**)
B3PW91/6-311G**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.820301	1.349965	0.011721
2	6	0	-0.207452	2.194829	0.273476
3	6	0	-1.396785	1.490572	0.254736
4	6	0	-1.060118	0.150372	-0.044725
5	6	0	0.320332	0.069262	-0.194424
6	8	0	-1.864612	-0.929518	-0.161025
7	6	0	-3.249622	-0.680406	-0.042038
8	6	0	2.210217	1.733753	-0.094226
9	16	0	1.306904	-1.298544	-0.623866
10	6	0	1.548687	-2.134035	0.984836
11	1	0	-0.029279	3.244418	0.452086
12	1	0	-2.375572	1.905515	0.435902
13	1	0	-3.597204	0.022832	-0.808683
14	1	0	-3.502710	-0.285637	0.949938
15	1	0	-3.746412	-1.639870	-0.183263
16	1	0	2.294801	2.791480	0.156468
17	1	0	2.585349	1.575611	-1.108098
18	1	0	2.828315	1.155903	0.596370
19	1	0	0.586639	-2.439630	1.395516
20	1	0	2.075673	-1.492277	1.691967
21	1	0	2.153177	-3.021331	0.784010

Low frequencies --- -14.2178 -3.6451 0.0016 0.0020 0.0024 4.1773
Low frequencies --- 42.0063 69.4383 82.2524
Sum of electronic and zero-point Energies= -801.253180
Sum of electronic and thermal Energies= -801.241559
Sum of electronic and thermal Enthalpies= -801.240615
Sum of electronic and thermal Free Energies= -801.291574