Supplementary Materials

Chemical Conversion of Hardly Ionizable Rhenium Aryl Chlorocomplexes with *p*-Substituted Anilines

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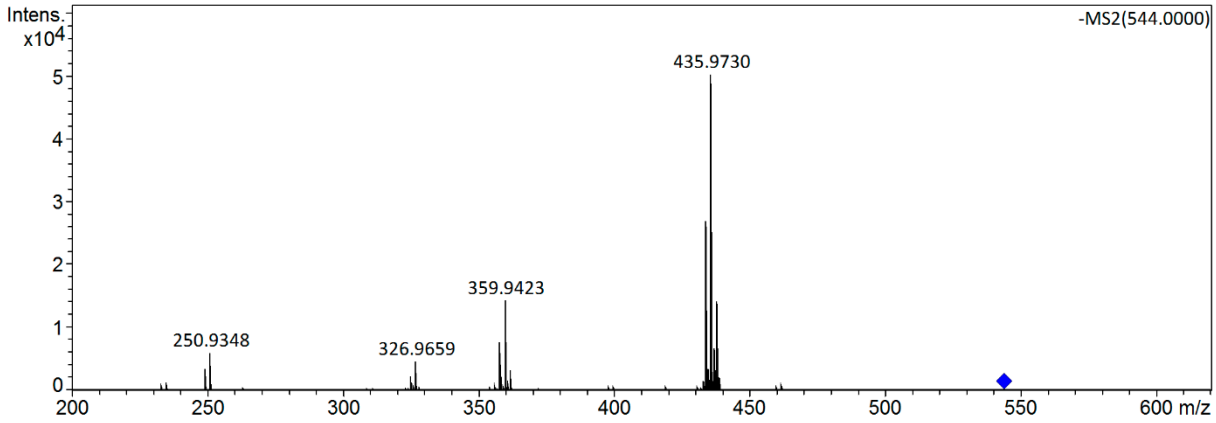
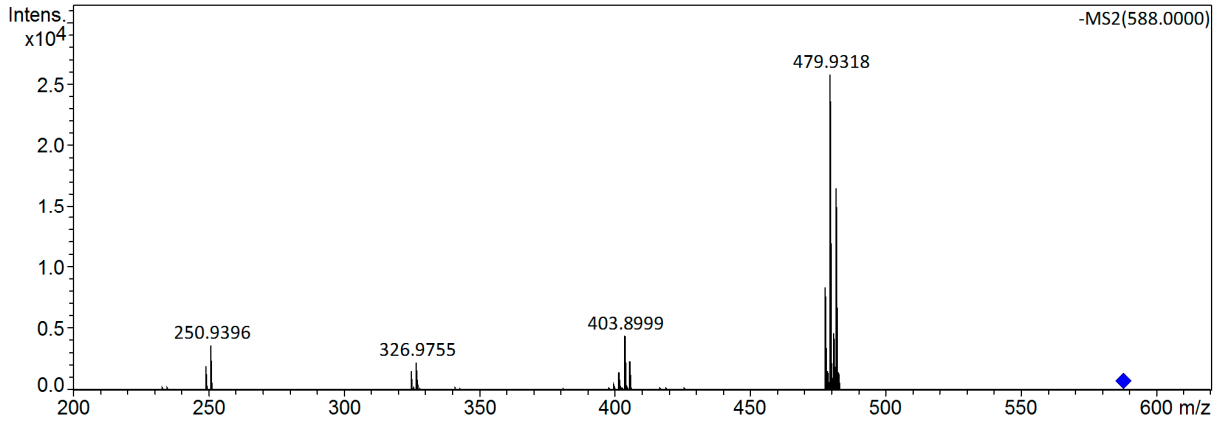


Figure S1. HR ESI– MS/MS spektra of complex 1; collision energy, CE, was 40 eV.



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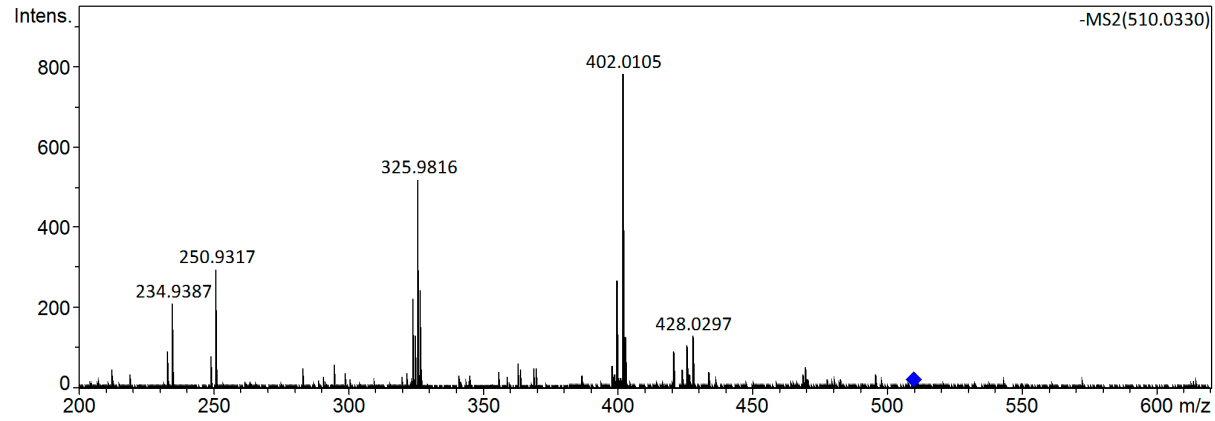

Figure S3. HR ESI– MS/MS spektra of complex 3; collision energy, CE, was 40 eV.

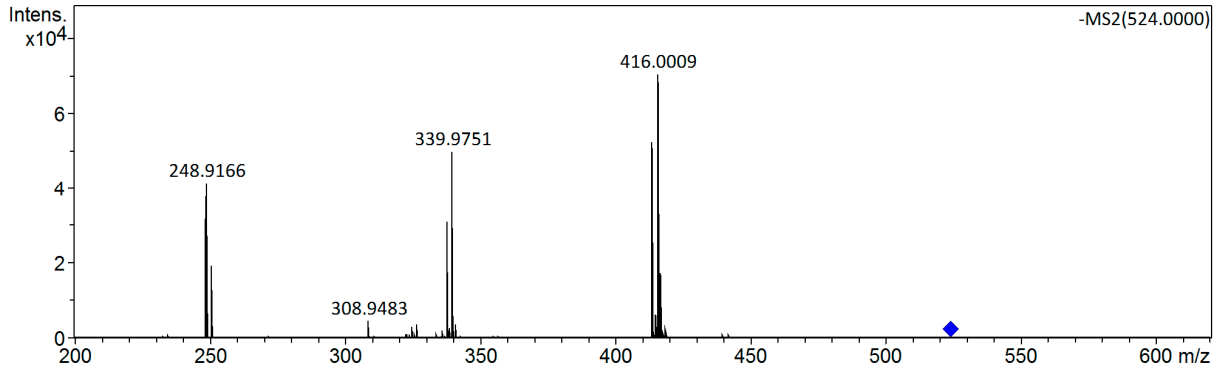

Figure S4. HR ESI– MS/MS spektra of complex 4; collision energy, CE, was 40 eV.

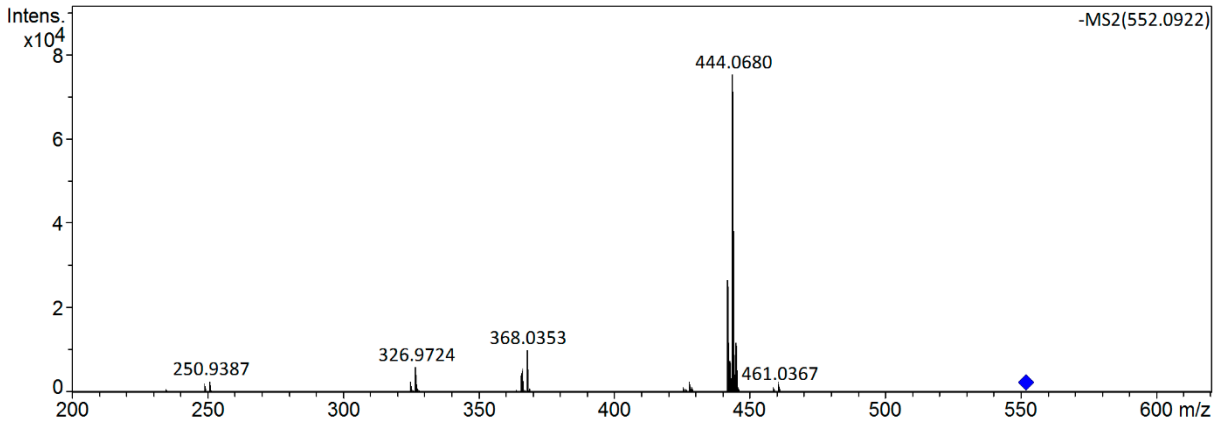

Figure S5. HR ESI– MS/MS spektra of complex 5; collision energy, CE, was 40 eV.

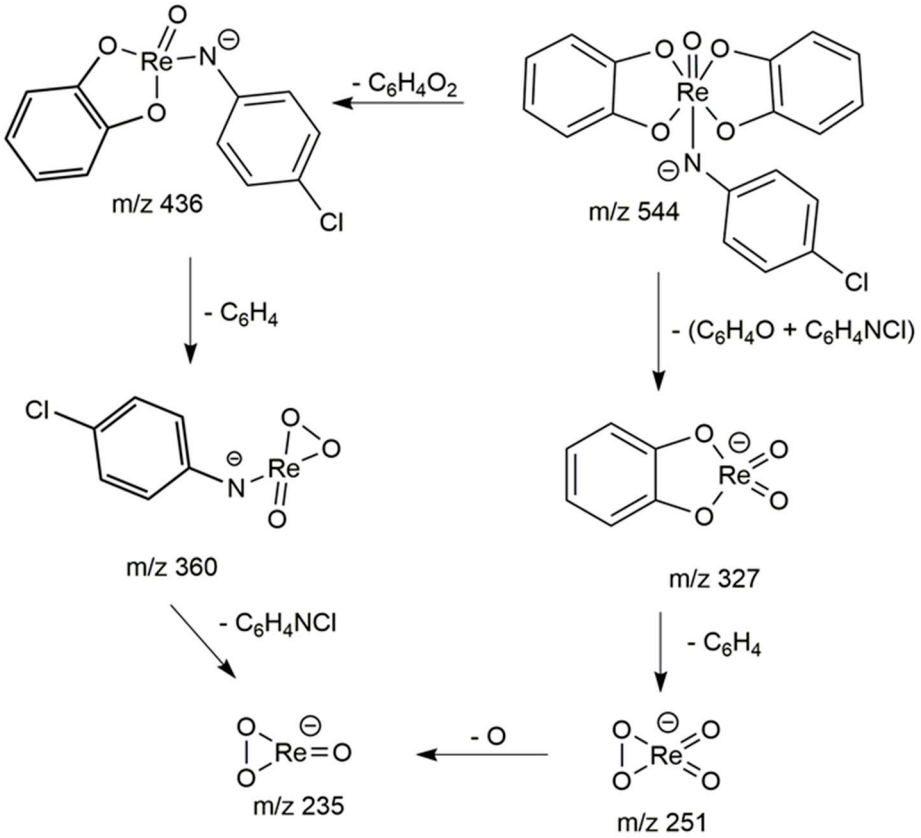

Figure S6. Proposed fragmentation scheme of complex 1.

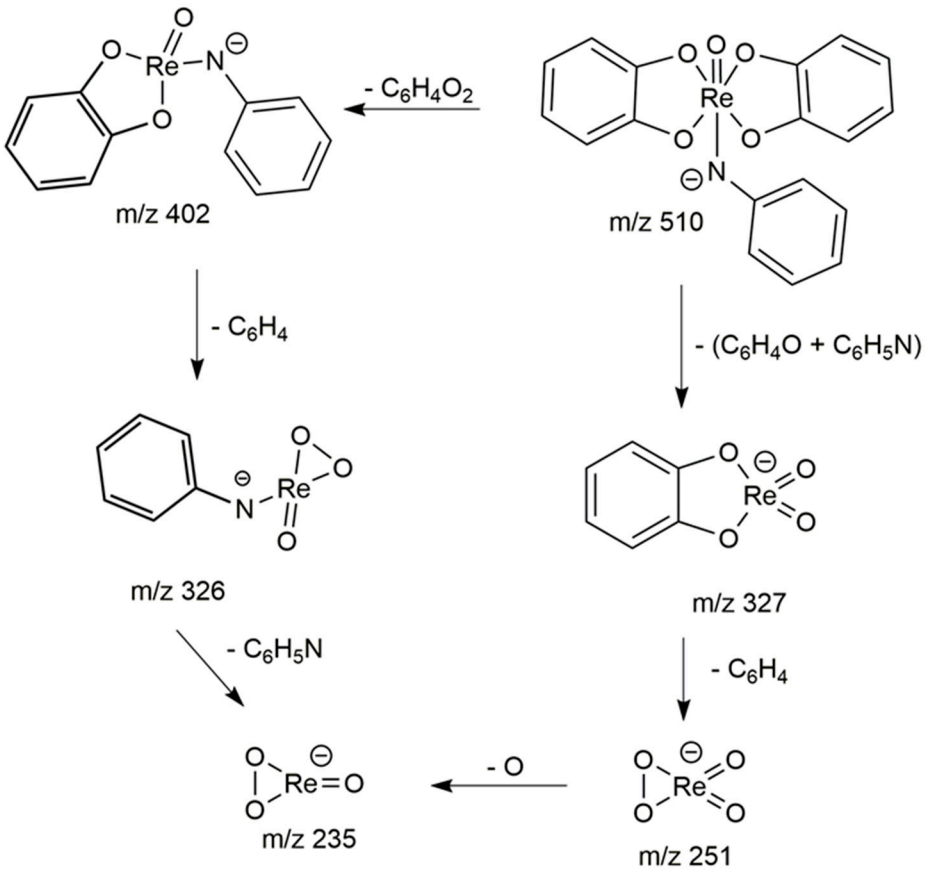

Figure S7. Proposed fragmentation scheme of complex 3

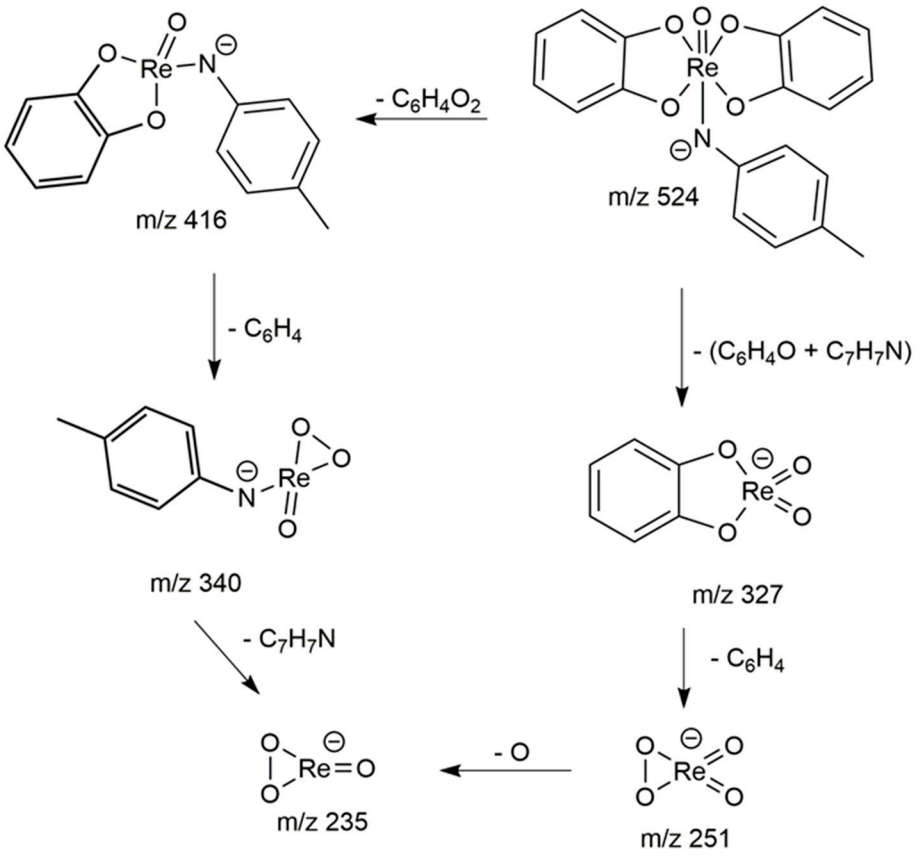

Figure S8. Proposed fragmentation scheme of complex 4

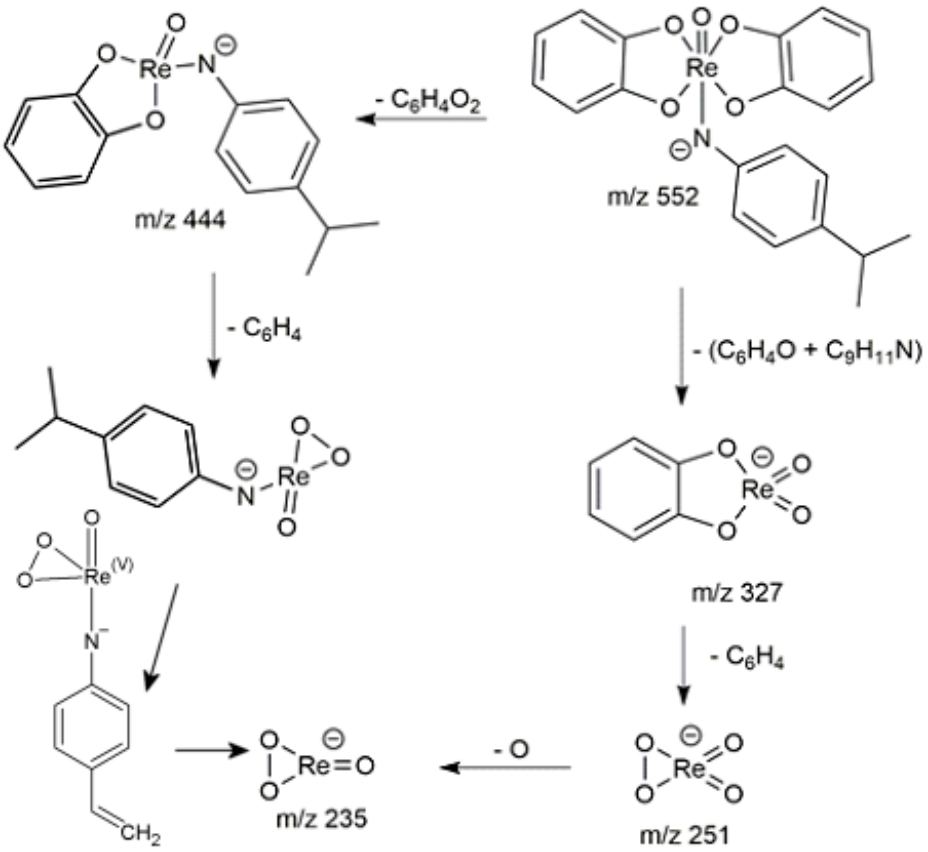

Figure S9. Proposed fragmentation scheme of complex 5

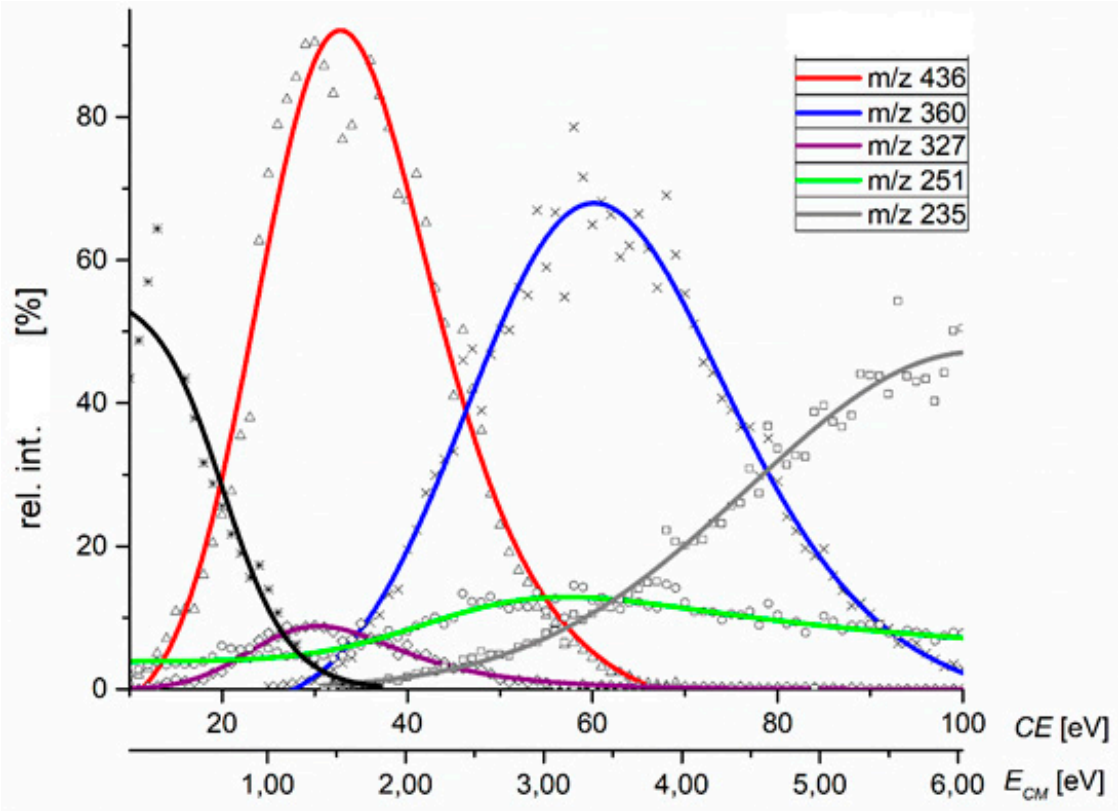

Figure S10. CID diagram of complex 1

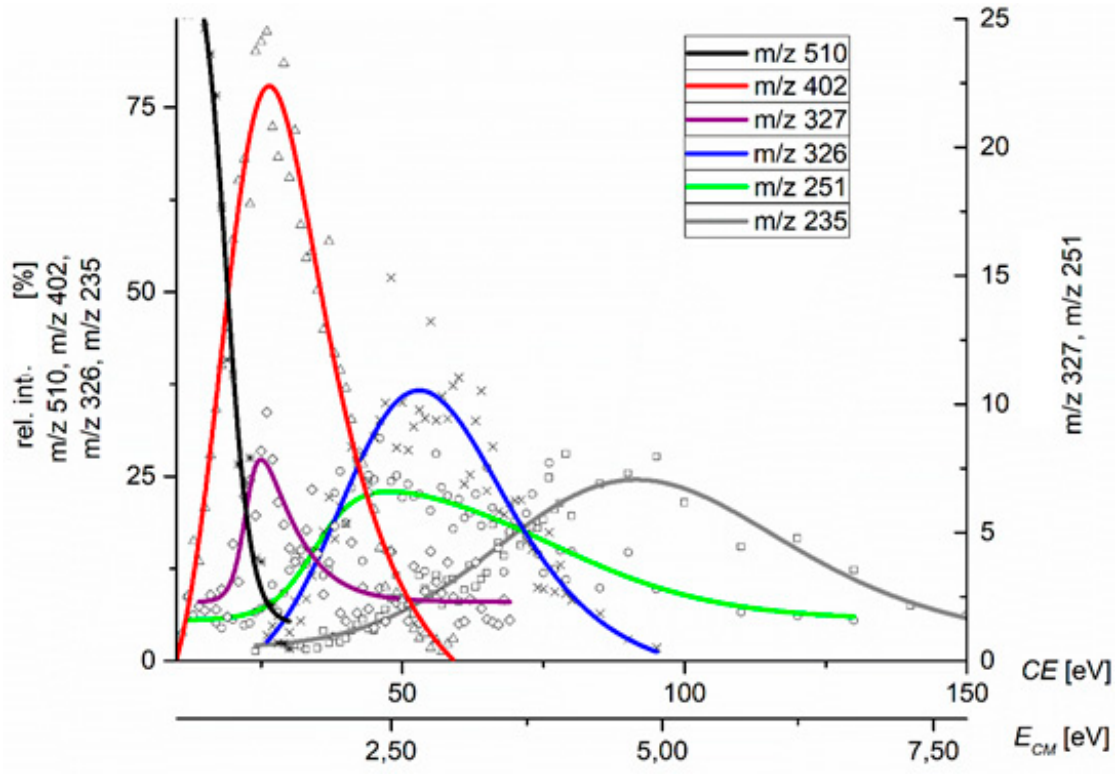

Figure S11. CID diagram of complex 3

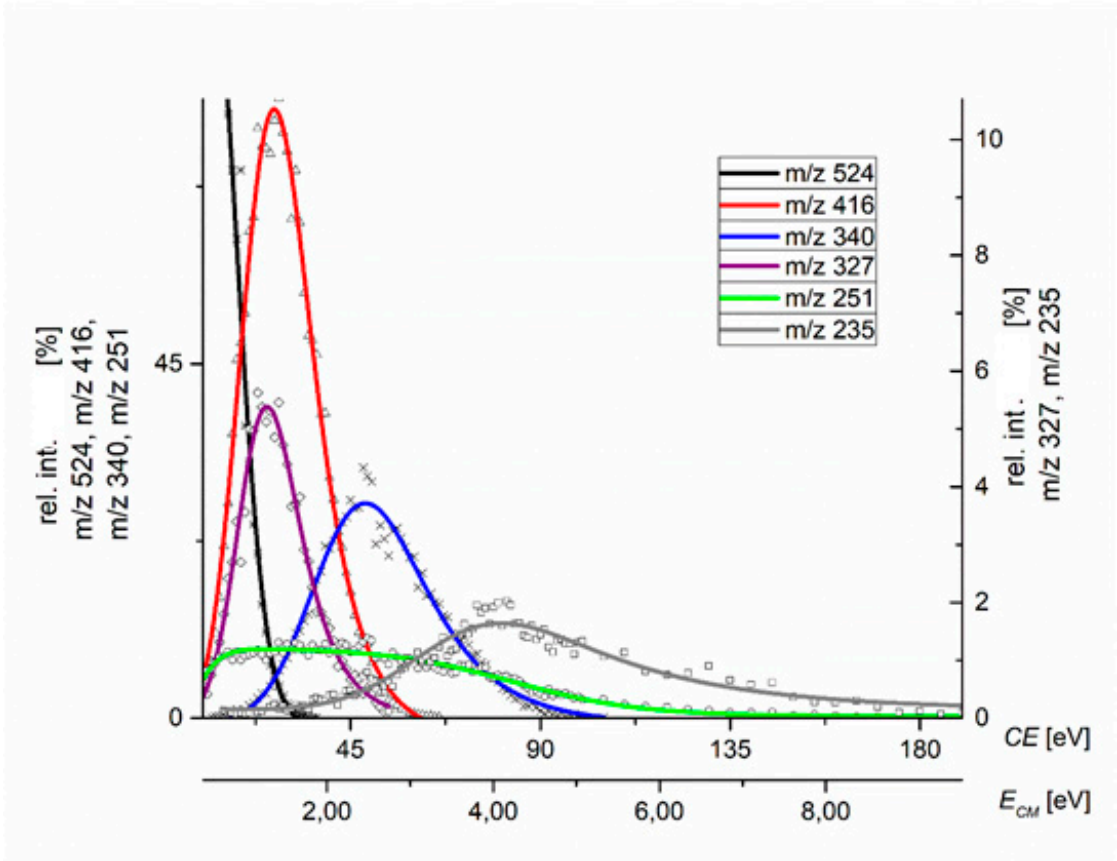

Figure S12. CID diagram of complex 4

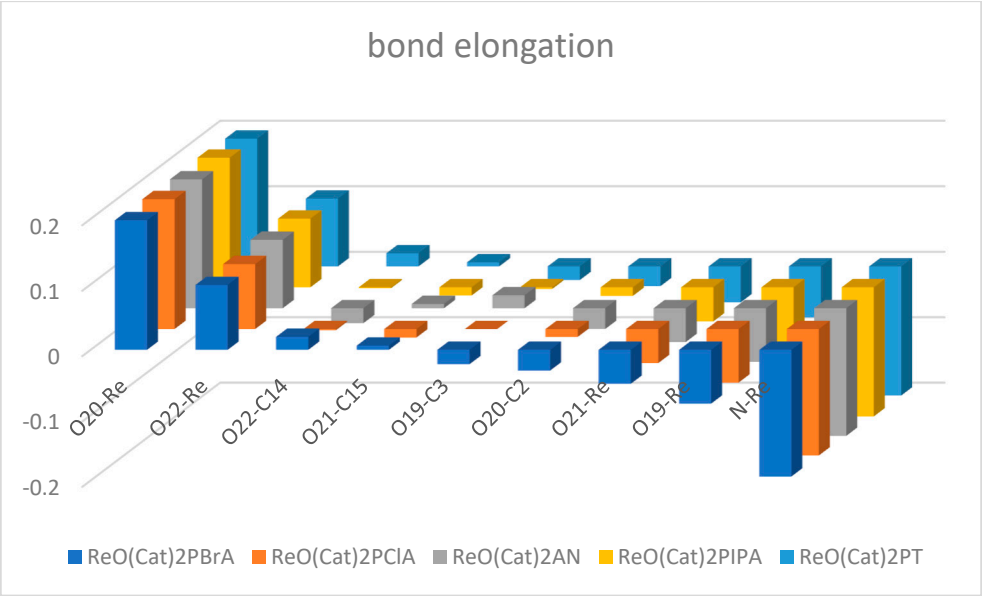

Figure S13. Graph of calculated bond elongation of prepared complexes.

Table S1. Cartesian coordinates calculated for the optimized neutral structure of complex 1.

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.542844	0.634768	0.330638
2	6	0	5.333374	-0.228210	1.433435
3	6	0	4.068715	-0.802056	1.671272
4	6	0	3.042556	-0.483579	0.776820
5	6	0	3.243373	0.370372	-0.333618
6	6	0	4.501732	0.950356	-0.563964
7	6	0	-2.461768	-1.075022	-0.484426
8	6	0	-1.908257	-1.884622	0.538139
9	6	0	-2.663186	-2.839711	1.229027
10	6	0	-4.018191	-2.965728	0.871484
11	6	0	-4.585946	-2.146348	-0.138025
12	6	0	-3.822829	-1.180954	-0.818852
13	8	0	2.121291	0.538634	-1.094926
14	8	0	1.735225	-0.933728	0.860682
15	8	0	-1.558712	-0.209201	-1.019813
16	8	0	-0.587901	-1.559890	0.789217
17	75	0	0.395234	-0.416098	-0.446351
18	8	0	0.591228	-1.358134	-1.898465
19	6	0	-1.989149	1.820752	1.119712
20	6	0	-3.080841	2.623249	1.478496
21	6	0	-3.268120	3.886376	0.879111
22	6	0	-2.345833	4.346562	-0.083010
23	6	0	-1.250757	3.549753	-0.448826

24	6	0	-1.063389	2.275499	0.147368
25	7	0	0.080100	1.520576	-0.179237
26	1	0	6.529739	1.059717	0.165941
27	1	0	6.157328	-0.451868	2.105412
28	1	0	3.882026	-1.464161	2.510523
29	1	0	4.657131	1.602218	-1.417691
30	1	0	-2.208609	-3.447442	2.004576
31	1	0	-4.638699	-3.700286	1.377320
32	1	0	-5.634495	-2.271092	-0.395977
33	1	0	-4.247332	-0.550414	-1.592927
34	1	0	-1.829047	0.864330	1.608095
35	1	0	-3.781765	2.269159	2.229936
36	1	0	-2.482727	5.319903	-0.547289
37	1	0	-0.545739	3.898279	-1.201026
38	17	0	-4.641158	4.887768	1.336911
39	1	0	0.619836	1.765067	0.954570

Table S2. Cartesian coordinates calculated for the optimized neutral structure of complex 2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.063120	-0.822081	1.673164
2	6	0	-3.037877	-0.499696	0.779060
3	6	0	-3.240724	0.356227	-0.329489
4	6	0	-4.500288	0.934244	-0.558189
5	6	0	-5.540488	0.614719	0.336074
6	6	0	-5.328973	-0.250198	1.436961
7	1	0	-3.874864	-1.485608	2.510940
8	1	0	-6.528264	1.038091	0.172604
9	1	0	-6.152269	-0.476894	2.108726
10	6	0	2.672592	-2.845660	1.224387
11	6	0	4.027724	-2.968270	0.866138
12	6	0	4.593551	-2.145630	-0.141799
13	6	0	3.828331	-1.180272	-0.820315
14	6	0	2.467176	-1.077710	-0.485224
15	6	0	1.915578	-1.890572	0.535785
16	1	0	4.649828	-3.702695	1.370204
17	1	0	5.642256	-2.267776	-0.400355
18	1	0	4.251352	-0.547253	-1.593178
19	8	0	-2.119222	0.528300	-1.090799
20	8	0	-1.729643	-0.947471	0.861538
21	8	0	0.594673	-1.568952	0.787982
22	8	0	1.562258	-0.212510	-1.018468
23	8	0	-0.585724	-1.363758	-1.898880
24	75	0	-0.391093	-0.424443	-0.444822

25	1	0	-4.657237	1.587620	-1.410474
26	1	0	2.219455	-3.455932	1.998783
27	6	0	1.062471	2.268726	0.154158
28	6	0	1.247158	3.544608	-0.439383
29	6	0	2.340798	4.342772	-0.072227
30	6	0	3.264297	3.882339	0.888614
31	6	0	3.079678	2.617577	1.485368
32	6	0	1.989435	1.813717	1.125231
33	1	0	0.541215	3.893358	-1.190610
34	1	0	2.475643	5.317364	-0.534477
35	1	0	3.781538	2.263256	2.235826
36	1	0	1.831359	0.855947	1.611629
37	7	0	-0.079651	1.512270	-0.173683
38	1	0	-0.844224	2.072103	-0.555460
39	35	0	4.752397	4.970922	1.387259

Table S3. Cartesian coordinates calculated for the optimized neutral structure of complex 3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.503665	0.619118	-0.417995
2	6	0	-5.272530	-0.298844	-1.444051
3	6	0	-3.997197	-0.850686	-1.657932
4	6	0	-2.976104	-0.446975	-0.808412
5	6	0	-3.208607	0.490725	0.246751
6	6	0	-4.475102	1.032016	0.445606
7	6	0	2.338411	-1.066907	0.554059
8	6	0	1.760862	-1.818623	-0.515814
9	6	0	2.493059	-2.770799	-1.213134
10	6	0	3.830048	-2.962088	-0.826945
11	6	0	4.401333	-2.222613	0.212784
12	6	0	3.667625	-1.257821	0.920882
13	8	0	-2.124800	0.781686	0.975455
14	8	0	-1.695355	-0.868402	-0.899448
15	8	0	1.490780	-0.193647	1.111506
16	8	0	0.478405	-1.479462	-0.776911
17	75	0	-0.438529	-0.297584	0.513150
18	8	0	-0.769616	-1.167986	1.923151
19	6	0	1.899900	1.555041	-1.300597
20	6	0	3.115252	2.107022	-1.711273
21	6	0	3.641995	3.231804	-1.068705
22	6	0	2.947427	3.811388	-0.001369
23	6	0	1.735144	3.272554	0.429766
24	6	0	1.210461	2.133798	-0.216401

25	7	0	-0.049292	1.595891	0.190364
26	1	0	-6.503627	1.027578	-0.275784
27	1	0	-6.091643	-0.599636	-2.095002
28	1	0	-3.808137	-1.566384	-2.453663
29	1	0	-4.653843	1.740756	1.248666
30	1	0	2.040587	-3.339781	-2.021147
31	1	0	4.428820	-3.704614	-1.352055
32	1	0	5.441691	-2.396537	0.486735
33	1	0	4.107113	-0.679774	1.729108
34	1	0	1.496985	0.690452	-1.829894
35	1	0	3.654636	1.655570	-2.544246
36	1	0	4.588421	3.654564	-1.397319
37	1	0	3.356465	4.687976	0.500511
38	1	0	1.207488	3.719859	1.268892
39	1	0	-0.715466	2.331344	0.483086

Table S4. Cartesian coordinates calculated for the optimized neutral structure of complex 4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.594446	-1.223763	1.885324
2	6	0	3.630113	-0.921844	0.919151
3	6	0	3.489533	-1.672997	-0.271846
4	6	0	4.319007	-2.779940	-0.515151
5	6	0	5.295221	-3.091341	0.451031
6	6	0	5.433892	-2.327128	1.635131
7	1	0	4.678620	-0.624627	2.786118
8	1	0	5.959985	-3.934111	0.279652
9	1	0	6.197178	-2.593954	2.360776
10	6	0	-0.190822	3.920480	1.390666
11	6	0	-1.257372	4.742570	0.983292
12	6	0	-2.044858	4.409672	-0.149147
13	6	0	-1.793482	3.251991	-0.906876
14	6	0	-0.708778	2.446186	-0.519939
15	6	0	0.059833	2.776485	0.623803
16	1	0	-1.482321	5.644543	1.545588
17	1	0	-2.858862	5.067754	-0.441889
18	1	0	-2.389025	2.990015	-1.774996
19	8	0	2.500038	-1.204566	-1.089878
20	8	0	2.703890	0.104927	1.000890
21	8	0	1.007771	1.808180	0.899741
22	8	0	-0.303024	1.290037	-1.112612
23	8	0	2.210597	1.267547	-1.730836
24	75	0	1.422590	0.434686	-0.419687

25	1	0	4.213630	-3.354396	-1.429866
26	1	0	0.418832	4.148234	2.258897
27	6	0	-1.237000	-1.184782	-0.247753
28	6	0	-1.970365	-2.131927	-1.007792
29	6	0	-3.350573	-2.290487	-0.815126
30	6	0	-4.004846	-1.496724	0.143386
31	6	0	-3.296985	-0.556464	0.914067
32	6	0	-1.918212	-0.402748	0.718128
33	1	0	-1.460772	-2.732557	-1.757943
34	1	0	-3.903990	-3.014793	-1.404362
35	1	0	-3.808929	0.041698	1.661021
36	1	0	-1.364080	0.297628	1.334869
37	7	0	0.157412	-1.092274	-0.409949
38	1	0	0.579656	-1.930680	-0.812784
39	6	0	-5.520446	-1.664908	0.358496
40	1	0	-6.049234	-1.183892	-0.437686
41	1	0	-5.765459	-2.706399	0.371333
42	1	0	-5.799689	-1.221288	1.291300

Table S5. Cartesian coordinates calculated for the optimized neutral structure of complex 5.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.274891	-2.854316	0.507536
2	6	0	-5.383488	-2.043586	1.663255
3	6	0	-4.490584	-0.975945	1.882863
4	6	0	-3.504375	-0.756903	0.916527
5	6	0	-3.392647	-1.555305	-0.246554
6	6	0	-4.276615	-2.625928	-0.459497
7	6	0	1.045716	2.299609	-0.564375
8	6	0	0.273443	2.724611	0.544894
9	6	0	0.578110	3.881971	1.270800
10	6	0	1.703083	4.619266	0.857807
11	6	0	2.493522	4.191300	-0.239914
12	6	0	2.186851	3.020511	-0.956194
13	8	0	-2.376898	-1.165626	-1.073211
14	8	0	-2.530688	0.226937	0.970894
15	8	0	0.581594	1.147917	-1.121169
16	8	0	-0.740871	1.830637	0.834462
17	75	0	-1.208700	0.428836	-0.437375
18	8	0	-1.917159	1.252253	-1.799292
19	6	0	2.036768	-0.574681	0.827798
20	6	0	3.395963	-0.818981	1.067922
21	6	0	4.076234	-1.833377	0.362270
22	6	0	3.381000	-2.611025	-0.586394
23	6	0	2.020841	-2.372938	-0.833787
24	6	0	1.335235	-1.348439	-0.130408
25	7	0	-0.046401	-1.171431	-0.339694
26	1	0	-5.980157	-3.668079	0.358743

27	1	0	-6.164835	-2.245867	2.390563
28	1	0	-4.551302	-0.341977	2.761379
29	1	0	-4.193656	-3.236068	-1.353260
30	1	0	-0.035813	4.183113	2.113340
31	1	0	1.970972	5.528550	1.388756
32	1	0	3.353487	4.785232	-0.538716
33	1	0	2.784167	2.685510	-1.797609
34	1	0	1.508107	0.183630	1.397370
35	1	0	3.923980	-0.225164	1.809361
36	1	0	3.898388	-3.395971	-1.132202
37	1	0	1.486565	-2.963701	-1.575371
38	6	0	5.773882	-2.091804	0.476317
39	6	0	6.330231	-3.239527	-0.525877
40	1	0	5.879747	-4.178003	-0.278587
41	1	0	7.392697	-3.316355	-0.425367
42	1	0	6.085211	-2.981196	-1.534947
43	6	0	6.752344	-1.196838	1.562949
44	1	0	6.260473	-1.107345	-0.650792
45	1	0	6.141948	-0.506280	2.106527
46	1	0	7.496276	-0.659147	1.013069
47	1	0	7.229475	-1.866561	2.247606
48	1	0	-0.542404	-2.030712	-0.464664

Table S6. Chemical names, labels, and formulas of prepared rhenium complexes.

Entry	Name	Label	Formula
1	N-(bis(1,2-dihydroxybenzene)oxorhenium)-parachloroaniline	$[Re^{VII}(O)(Cat)_2PClA]^{-a}$	$C_{18}H_{12}ClNO_5Re$
2	N-(bis(1,2-dihydroxybenzene)oxorhenium)-parabromoaniline	$[Re^{VII}(O)(Cat)_2PBrA]^{-a}$	$C_{18}H_{12}BrNO_5Re$
3	N-(bis(1,2-dihydroxybenzene)oxorhenium)-aniline	$[Re^{VII}(O)(Cat)_2An]^{-a}$	$C_{18}H_{13}NO_5Re$
4	N-(bis(1,2-dihydroxybenzene)oxorhenium)-paratoluidine	$[Re^{VII}(O)(Cat)_2PT]^{-a}$	$C_{19}H_{15}NO_5Re$
5	N-(bis(1,2-dihydroxybenzene)oxorhenium)-paracumidine	$[Re^{VII}(O)(Cat)_2PIPA]^{-a}$	$C_{21}H_{19}NO_5Re$

Table S7. Calculated bond elongation of prepared complexes.

	ReO(Cat)2PBrA	ReO(Cat)2PClA	ReO(Cat)2AN	ReO(Cat)2PIPA	ReO(Cat)2PT
O20-Re	0.1979	0.1983	0.1967	0.1978	0.19499
O22-Re	0.0992	0.0992	0.1043	0.1048	0.10348
O22-C14	0.0199	-0.0019	-0.0229	-0.0014	0.02013
O21-C15	0.0064	-0.013	0.0066	-0.0125	0.00623
O19-C3	-0.022	-0.0002	0.0197	-0.0025	-0.02089
O20-C2	-0.0317	-0.0121	-0.0318	-0.0131	-0.03019
O21-Re	-0.052	-0.0521	-0.0518	-0.0522	-0.05489
O19-Re	-0.0823	-0.082	-0.082	-0.0836	-0.07794
N-Re	-0.1938	-0.1935	-0.1953	-0.1975	-0.19741