Table S1. *Optimised geometry calculated for **3** at DFT level (total charge =1, spin multiplicity = 1) in orthogonal Cartesian coordinate format.*

Atomic	No	X	Y	Z
1	47	-0.283739	-0.831243	-0.432824
2	34	2.040814	-1.643672	-0.958177
3	15	3.129209	-0.305726	0.393121
4	6	4.906284	-0.619683	0.213421
5	6	2.827931	1.450830	0.056428
6	6	2.716338	-0.623790	2.133851
7	1	3.383778	-0.054390	2.794768
8	1	1.668003	-0.362093	2.329372
9	1	2.862268	-1.695774	2.318986
10	6	2.747250	2.387027	1.096189
11	6	2.558859	3.736242	0.800918
12	6	2.454257	4.154859	-0.524344
13	6	2.535124	3.224262	-1.560749
14	6	2.718863	1.874795	-1.275208
15	1	2.832109	2.079495	2.138941
16	1	2.498644	4.463047	1.612374
17	1	2.309321	5.212218	-0.751482
18	1	2.453145	3.550715	-2.598382
19	1	2.769261	1.144466	-2.085511
20	6	5.818073	0.443105	0.197987
21	6	7.183243	0.179514	0.108720
22	6	7.639389	-1.134878	0.034294
23	6	6.731202	-2.193635	0.045744
24	6	5.365674	-1.941658	0.132654
25	1	5.468440	1.475360	0.247615
26	1	7.892504	1.008127	0.092068
27	1	8.709153	-1.336515	-0.039111
28	1	7.087270	-3.222584	-0.017545
29	1	4.658704	-2.773998	0.122828
30	15	-2.549433	-0.140594	0.016593
31	6	-2.662200	0.925731	1.494500
32	6	-3.292105	0.814470	-1.347869
33	6	-3.664170	-1.551797	0.316632
34	6	-3.616295	0.714597	2.495663
35	6	-3.663961	1.562135	3.602495
36	6	-2.767767	2.622682	3.713662
37	6	-1.814174	2.836577	2.717300
38	6	-1.755145	1.988739	1.615514
39	1	-4.323104	-0.112690	2.414588
40	1	-4.409381	1.391242	4.380653
41	1	-2.810285	3.284625	4.580034
42	1	-1.111520	3.667218	2.800910
43	1	-1.003164	2.160190	0.840620
44	6	-4.123938	1.916369	-1.115752
45	6	-4.693028	2.596767	-2.191237
46	6	-4.439492	2.181987	-3.497333
47	6	-3.610187	1.085318	-3.733222
48	6	-3.033327	0.406564	-2.663789
49	1	-4.326195	2.247247	-0.095674
50	1	-5.339200	3.456060	-2.005404

51	1	-4.886692	2.717537	-4.336243
52	1	-3.407162	0.760624	-4.754795
53	1	-2.378895	-0.447760	-2.855422
54	6	-4.993282	-1.549179	-0.123718
55	6	-5.816684	-2.641310	0.144283
56	6	-5.322632	-3.735978	0.851523
57	6	-3.998523	-3.744327	1.289962
58	6	-3.169473	-2.659596	1.018706
59	1	-5.385608	-0.697844	-0.682362
60	1	-6.850293	-2.636438	-0.204939
61	1	-5.969909	-4.590149	1.056338
62	1	-3.607306	-4.603266	1.837113
63	1	-2.129101	-2.677020	1.353844

Table S2. *Optimised geometry calculated for **3a** at DFT level (total charge =2, spin multiplicity = 1) in orthogonal Cartesian coordinate format.*

Atomic	No	X	Y	Z
1	6	3.565403	-3.055846	-2.024030
2	6	4.053717	-3.134658	-0.711570
3	6	4.374631	-4.385567	-0.170451
4	6	4.217296	-5.539562	-0.938000
5	6	3.743866	-5.453824	-2.246539
6	6	3.417408	-4.210245	-2.789622
7	15	4.283100	-1.583438	0.226319
8	6	4.422170	-2.063295	1.980429
9	6	5.659189	-2.363705	2.564977
10	6	5.721366	-2.752280	3.902124
11	6	4.555755	-2.842550	4.661339
12	6	3.322247	-2.539627	4.084787
13	6	3.253667	-2.146876	2.750429
14	47	2.543460	0.041310	-0.212909
15	34	1.024301	1.997592	-0.749855
16	15	2.531349	3.594304	-0.832458
17	6	3.777413	3.248133	-2.109251
18	6	1.714582	5.146933	-1.285585
19	6	1.616523	6.201491	-0.369717
20	6	0.977220	7.382824	-0.741542
21	6	0.436399	7.514650	-2.018770
22	6	0.524322	6.460430	-2.929407
23	6	1.156143	5.275671	-2.566204
24	6	3.415165	3.852156	0.730994
25	6	4.584537	4.628686	0.740572
26	6	5.254865	4.855988	1.939152
27	6	4.764629	4.316670	3.129150
28	6	3.600174	3.551154	3.122455
29	6	2.923122	3.317648	1.926742
30	6	5.932225	-0.957267	-0.246411
31	6	6.816300	-1.693340	-1.042570
32	6	8.066924	-1.165992	-1.365667
33	6	8.443077	0.089138	-0.893486
34	6	7.564616	0.826137	-0.097363
35	6	6.311535	0.310750	0.219658
36	1	4.445223	4.110965	-2.234337
37	1	4.358806	2.363968	-1.815627
38	1	3.267527	3.045868	-3.059493
39	1	4.975455	5.069810	-0.177903
40	1	6.162254	5.461617	1.944338
41	1	5.292555	4.499006	4.066484
42	1	3.213257	3.134301	4.053315
43	1	2.009998	2.719113	1.916901
44	1	2.042681	6.108171	0.630046
45	1	0.907880	8.205770	-0.028875
46	1	-0.054843	8.444810	-2.308779
47	1	0.100440	6.562897	-3.929339
48	1	1.205949	4.453577	-3.282992
49	1	6.534082	-2.679940	-1.412998
50	1	8.751739	-1.744637	-1.987345

51	1	9.423904	0.495412	-1.145108
52	1	7.858404	1.807595	0.278261
53	1	5.629280	0.893849	0.844331
54	1	6.577102	-2.288431	1.979268
55	1	6.687603	-2.983130	4.353178
56	1	4.609799	-3.143547	5.708750
57	1	2.410094	-2.599906	4.680649
58	1	2.285480	-1.899851	2.306502
59	1	4.750759	-4.461428	0.851174
60	1	4.475060	-6.510447	-0.511838
61	1	3.631386	-6.358241	-2.846694
62	1	3.048135	-4.138971	-3.813918
63	1	3.305622	-2.084882	-2.454087
64	47	-2.541275	-0.210855	0.404371
65	34	-0.320829	-1.434402	0.407504
66	15	-1.053609	-3.358539	-0.378750
67	6	0.269422	-4.580464	-0.168519
68	6	-2.521156	-3.938025	0.508005
69	6	-1.456831	-3.308020	-2.146860
70	1	-0.079651	-5.563728	-0.511545
71	1	1.131426	-4.265390	-0.772030
72	1	0.572353	-4.636664	0.884364
73	6	-2.017552	-4.450628	-2.739300
74	6	-2.287953	-4.458165	-4.104037
75	6	-2.004345	-3.333150	-4.880090
76	6	-1.449126	-2.198555	-4.292009
77	6	-1.171962	-2.182315	-2.925669
78	1	-2.255019	-5.332766	-2.140558
79	1	-2.724471	-5.345892	-4.563899
80	1	-2.219463	-3.343415	-5.949811
81	1	-1.228585	-1.319132	-4.898745
82	1	-0.733882	-1.296479	-2.461104
83	6	-3.796661	-3.596978	0.035732
84	6	-4.927634	-3.985210	0.749183
85	6	-4.792348	-4.713806	1.930731
86	6	-3.524716	-5.052548	2.403618
87	6	-2.388113	-4.662720	1.700194
88	1	-3.914638	-3.040547	-0.896081
89	1	-5.917230	-3.720792	0.374042
90	1	-5.679779	-5.024379	2.484325
91	1	-3.418961	-5.626295	3.325301
92	1	-1.404446	-4.929100	2.089155
93	15	-4.654247	0.954301	0.463682
94	6	-5.992774	-0.017420	-0.311277
95	6	-5.195779	1.305177	2.168309
96	6	-4.627837	2.551225	-0.414224
97	6	-5.743448	3.024408	-1.116664
98	6	-5.694876	4.269073	-1.742003
99	6	-4.539667	5.045638	-1.668979
100	6	-3.425225	4.576895	-0.973332
101	6	-3.465716	3.331913	-0.351562
102	1	-6.650892	2.421406	-1.179943
103	1	-6.566132	4.633207	-2.288478
104	1	-4.507326	6.019513	-2.160028
105	1	-2.517442	5.179721	-0.919124
106	1	-2.585581	2.966992	0.184137
107	6	-7.206366	-0.263776	0.339295

108	6	-8.199906	-1.008648	-0.297593
109	6	-7.990375	-1.506097	-1.581923
110	6	-6.780449	-1.262129	-2.235076
111	6	-5.783079	-0.526619	-1.601800
112	1	-7.381189	0.127344	1.342766
113	1	-9.146221	-1.193090	0.213290
114	1	-8.772604	-2.082007	-2.078977
115	1	-6.616179	-1.644975	-3.243637
116	1	-4.839783	-0.336518	-2.121135
117	6	-5.873075	2.485272	2.498714
118	6	-6.292774	2.702174	3.810045
119	6	-6.043124	1.747208	4.794072
120	6	-5.366041	0.571330	4.470283
121	6	-4.937541	0.352345	3.163986
122	1	-6.070112	3.239366	1.735067
123	1	-6.817997	3.624319	4.063087
124	1	-6.373127	1.921746	5.819316
125	1	-5.164981	-0.174707	5.240531
126	1	-4.400121	-0.567535	2.917892

Table S3. *Optimised geometry calculated for* ***6*** *at DFT level (total charge =0, spin multiplicity = 1) in orthogonal Cartesian coordinate format.*

Atomic	No	X	Y	Z
1	79	8.616195	1.220477	1.051245
2	34	6.933772	1.214526	-0.803641
3	15	5.774513	2.878372	0.000324
4	9	9.164506	-0.662380	3.583760
5	9	11.015626	-0.549488	5.522704
6	9	12.860103	1.441743	5.537323
7	9	12.839054	3.329492	3.585863
8	9	11.000929	3.236182	1.634983
9	6	10.008704	1.277964	2.525775
10	6	10.052824	0.333196	3.545377
11	6	11.002371	0.369413	4.564824
12	6	11.949911	1.389547	4.576069
13	6	11.936310	2.355503	3.573394
14	6	10.970460	2.281505	2.572356
15	6	5.243467	2.584091	1.712302
16	1	4.737499	1.612867	1.779792
17	1	4.585548	3.393135	2.057971
18	1	6.151196	2.547658	2.329605
19	6	6.628099	4.487154	0.004766
20	6	8.007514	4.576089	-0.195649
21	1	8.589069	3.674115	-0.395820
22	6	8.638629	5.817215	-0.124253
23	1	9.718233	5.877351	-0.267354
24	6	7.896071	6.966122	0.135498
25	1	8.393283	7.936067	0.190294
26	6	6.515796	6.880699	0.325370
27	1	5.932165	7.781018	0.523801
28	6	5.879286	5.645416	0.261759
29	1	4.797568	5.588380	0.403042
30	6	4.286524	3.100520	-1.016066
31	6	4.422156	3.682161	-2.284109
32	1	5.399017	4.031043	-2.625036
33	6	3.311000	3.816121	-3.110262
34	1	3.421948	4.270037	-4.096115
35	6	2.060931	3.371062	-2.679742
36	1	1.190755	3.477387	-3.329535
37	6	1.923024	2.788921	-1.421756
38	1	0.947169	2.437377	-1.083547
39	6	3.032427	2.649219	-0.589855
40	1	2.909350	2.183996	0.388743

Table S4. *Optimised geometry calculated for* ***6'*** *at DFT level (total charge =0, spin multiplicity = 1) in orthogonal Cartesian coordinate format.*

Atomic	No	X	Y	Z
1	79	-0.730650	1.325829	0.728516
2	34	-2.470245	1.387652	-1.069884
3	15	-3.556371	3.075739	-0.217626
4	9	-0.570404	-0.203787	3.531063
5	9	1.383369	-0.392307	5.354846
6	9	3.711062	0.962651	5.011607
7	9	4.061683	2.528132	2.823307
8	9	2.121123	2.737900	0.986713
9	6	0.687963	1.280189	2.181712
10	6	0.545424	0.501774	3.326376
11	6	1.541729	0.390478	4.293225
12	6	2.736831	1.081528	4.119878
13	6	2.911452	1.885069	2.997423
14	6	1.889786	1.970379	2.054763
15	6	-4.077318	2.761454	1.496777
16	1	-4.639371	1.819457	1.523471
17	1	-4.705627	3.580008	1.872307
18	1	-3.173920	2.652286	2.112213
19	6	-2.627998	4.640056	-0.200947
20	6	-1.414186	4.738855	-0.886995
21	1	-1.024175	3.869545	-1.420526
22	6	-0.701620	5.936454	-0.867179
23	1	0.250028	6.003990	-1.395982
24	6	-1.195897	7.033931	-0.166534
25	1	-0.632487	7.968416	-0.147912
26	6	-2.408098	6.939249	0.518018
27	1	-2.795448	7.797065	1.070011
28	6	-3.124660	5.746337	0.504100
29	1	-4.072510	5.687251	1.042436
30	6	-5.074955	3.342732	-1.184842
31	6	-5.307892	4.531855	-1.883875
32	1	-4.579619	5.342916	-1.846776
33	6	-6.471798	4.678928	-2.637039
34	1	-6.646737	5.607472	-3.182662
35	6	-7.402247	3.644589	-2.698651
36	1	-8.310904	3.762150	-3.291430
37	6	-7.167553	2.453135	-2.011894
38	1	-7.887358	1.635301	-2.069101
39	6	-6.006737	2.297388	-1.261372
40	1	-5.816135	1.350092	-0.752422
41	79	0.730650	-1.325829	-0.728516
42	34	2.470245	-1.387652	1.069884
43	15	3.556371	-3.075739	0.217626
44	9	0.570404	0.203787	-3.531063
45	9	-1.383369	0.392307	-5.354846
46	9	-3.711062	-0.962651	-5.011607
47	9	-4.061683	-2.528132	-2.823307
48	9	-2.121123	-2.737900	-0.986713
49	6	-0.687963	-1.280189	-2.181712
50	6	-0.545424	-0.501774	-3.326376

51	6	-1.541729	-0.390478	-4.293225
52	6	-2.736831	-1.081528	-4.119878
53	6	-2.911452	-1.885069	-2.997423
54	6	-1.889786	-1.970379	-2.054763
55	6	4.077318	-2.761454	-1.496777
56	1	4.639371	-1.819457	-1.523471
57	1	4.705627	-3.580008	-1.872307
58	1	3.173920	-2.652286	-2.112213
59	6	2.627998	-4.640056	0.200947
60	6	1.414186	-4.738855	0.886995
61	1	1.024175	-3.869545	1.420526
62	6	0.701620	-5.936454	0.867179
63	1	-0.250028	-6.003990	1.395982
64	6	1.195897	-7.033931	0.166534
65	1	0.632487	-7.968416	0.147912
66	6	2.408098	-6.939249	-0.518018
67	1	2.795448	-7.797065	-1.070011
68	6	3.124660	-5.746337	-0.504100
69	1	4.072510	-5.687251	-1.042436
70	6	5.074955	-3.342732	1.184842
71	6	5.307892	-4.531855	1.883875
72	1	4.579619	-5.342916	1.846776
73	6	6.471798	-4.678928	2.637039
74	1	6.646737	-5.607472	3.182662
75	6	7.402247	-3.644589	2.698651
76	1	8.310904	-3.762150	3.291430
77	6	7.167553	-2.453135	2.011894
78	1	7.887358	-1.635301	2.069101
79	6	6.006737	-2.297388	1.261372
80	1	5.816135	-1.350092	0.752422

Table S5. *Optimised geometry calculated for **7** at DFT level (total charge =0, spin multiplicity = 1) in orthogonal Cartesian coordinate format.*

Atomic	No	X	Y	Z
1	79	0.720078	0.039991	-0.231785
2	6	1.955403	1.695139	-0.351024
3	6	1.903928	2.696699	0.608359
4	6	2.729069	3.817185	0.559934
5	6	3.642717	3.944071	-0.483724
6	6	3.719423	2.955333	-1.461423
7	6	2.876248	1.848394	-1.377721
8	9	1.040700	2.615562	1.625704
9	9	2.653951	4.760414	1.488623
10	9	4.433338	5.002397	-0.546855
11	9	4.586451	3.078841	-2.454920
12	9	2.978067	0.922585	-2.330630
13	6	2.344709	-1.094912	0.227129
14	6	3.008294	-0.942128	1.435835
15	6	4.126448	-1.708767	1.757797
16	6	4.594138	-2.651210	0.845586
17	6	3.943234	-2.820654	-0.373716
18	6	2.826124	-2.040690	-0.666970
19	9	2.589748	-0.049760	2.328507
20	9	4.744866	-1.549868	2.917533
21	9	5.653982	-3.385172	1.137497
22	9	4.388161	-3.717770	-1.239192
23	9	2.224943	-2.232142	-1.836338
24	6	-0.450017	-1.667052	-0.084389
25	6	-1.050273	-2.229897	-1.203030
26	6	-1.826780	-3.384022	-1.130587
27	6	-2.005301	-4.013265	0.097784
28	6	-1.403869	-3.486784	1.236838
29	6	-0.635749	-2.331172	1.119525
30	9	-0.922416	-1.657995	-2.397549
31	9	-2.419905	-3.875188	-2.209712
32	9	-2.769981	-5.089932	0.186670
33	9	-1.586328	-4.073437	2.412145
34	9	-0.099955	-1.841694	2.246466
35	34	-1.181935	1.617370	-0.933600
36	15	-2.781765	1.072103	0.461603
37	6	-2.169186	0.850145	2.153479
38	1	-3.014283	0.775119	2.850821
39	1	-1.568565	1.735296	2.399324
40	1	-1.528884	-0.037576	2.222811
41	6	-3.930665	2.482290	0.517274
42	6	-3.413720	3.773713	0.693701
43	1	-2.334356	3.931690	0.743353
44	6	-4.279320	4.859054	0.787139
45	1	-3.873143	5.862443	0.922670
46	6	-5.657961	4.665240	0.700241
47	1	-6.333553	5.519434	0.769014
48	6	-6.172895	3.383469	0.519970
49	1	-7.250561	3.230246	0.446137
50	6	-5.314171	2.289668	0.428235

51	1	-5.723452	1.289041	0.282786
52	6	-3.747390	-0.381890	-0.030267
53	6	-4.247852	-1.282571	0.917724
54	1	-4.031665	-1.158845	1.979470
55	6	-5.026494	-2.362249	0.503158
56	1	-5.402238	-3.071474	1.241912
57	6	-5.309112	-2.542991	-0.848969
58	1	-5.908802	-3.395956	-1.169932
59	6	-4.809711	-1.647002	-1.794522
60	1	-5.014076	-1.798020	-2.855053
61	6	-4.026323	-0.570989	-1.390549
62	1	-3.608595	0.112681	-2.132371

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Table S6. *Optimised geometry calculated for **8** at DFT level (total charge =1, spin multiplicity = 1) in orthogonal Cartesian coordinate format.*

Atomic	No	X	Y	Z
1	29	-0.296338	-0.878541	-0.519774
2	34	1.815578	-1.698244	-1.034173
3	15	2.895871	-0.380130	0.346979
4	6	4.679115	-0.650321	0.161989
5	6	2.565578	1.375961	0.041727
6	6	2.487859	-0.743979	2.078575
7	1	3.120004	-0.148715	2.751668
8	1	1.425351	-0.546937	2.273447
9	1	2.691957	-1.809711	2.244460
10	6	2.193168	2.247871	1.072496
11	6	1.975642	3.597001	0.794160
12	6	2.133687	4.077640	-0.503895
13	6	2.501930	3.208987	-1.533236
14	6	2.714201	1.860863	-1.266024
15	1	2.070654	1.891634	2.095730
16	1	1.687066	4.274075	1.599324
17	1	1.971332	5.135739	-0.715797
18	1	2.625564	3.584217	-2.550098
19	1	2.991177	1.181062	-2.074633
20	6	5.570066	0.398894	0.425735
21	6	6.942095	0.174096	0.349138
22	6	7.426609	-1.088393	0.010243
23	6	6.540224	-2.131462	-0.254916
24	6	5.166563	-1.917604	-0.181022
25	1	5.198659	1.393077	0.680796
26	1	7.635329	0.992139	0.549576
27	1	8.502382	-1.259098	-0.053229
28	1	6.918832	-3.117695	-0.526543
29	1	4.476327	-2.734568	-0.401310
30	15	-2.362514	-0.190337	-0.030039
31	6	-2.834304	1.356825	-0.868925
32	6	-3.624498	-1.426979	-0.475303
33	6	-2.558074	0.109881	1.760436
34	6	-4.146803	1.596889	-1.293321
35	6	-4.467295	2.801927	-1.915561
36	6	-3.485090	3.770550	-2.115876
37	6	-2.175747	3.533907	-1.697976
38	6	-1.847720	2.329279	-1.081911
39	1	-4.918790	0.839734	-1.145698
40	1	-5.490432	2.982674	-2.248465
41	1	-3.739589	4.711296	-2.606627
42	1	-1.403648	4.287057	-1.861613
43	1	-0.817088	2.144831	-0.767985
44	6	-4.738672	-1.680860	0.333348
45	6	-5.686587	-2.621698	-0.065792
46	6	-5.529830	-3.309018	-1.268132
47	6	-4.420056	-3.060447	-2.075842
48	6	-3.466755	-2.127019	-1.679579
49	1	-4.865491	-1.149249	1.278041
50	1	-6.552177	-2.818850	0.568461

51	1	-6.273184	-4.046184	-1.575571
52	1	-4.292627	-3.601179	-3.014753
53	1	-2.595376	-1.941087	-2.312807
54	6	-3.149705	1.271751	2.266710
55	6	-3.274540	1.445859	3.645262
56	6	-2.815990	0.464761	4.521489
57	6	-2.224850	-0.696381	4.020891
58	6	-2.089060	-0.871400	2.646882
59	1	-3.514965	2.042598	1.586188
60	1	-3.738254	2.353656	4.034375
61	1	-2.919694	0.603097	5.598847
62	1	-1.868784	-1.468660	4.704673
63	1	-1.627701	-1.784227	2.260126

Table S7. ***Principal computed electronic transitions (f > 0.02) calculated for** 6**. For each transition, the excitation energy E (eV), the oscillator strength f and molecular orbital composition of the excited-state function are reported.***

Exc. State	*E*	*f*	Composition	%
S3	4.234	0.031	104→107	31
			105→107	64
S11	4.858	0.043	102→107	77
S12	4.881	0.043	102→107	14
			104→109	53
			105→109	18
S22	5.374	0.155	104→111	22
			105→111	54
S23	5.464	0.021	103→110	75
S24	5.486	0.030	101→107	76
S25	5.520	0.021	100→107	88
S27	5.581	0.020	106→111	41
			106→112	39
S29	5.673	0.027	99→107	29
			103→111	56
S30	5.691	0.033	98→107	24
			102→109	46
S32	5.760	0.054	104→112	34
			105→112	14
			105→113	25
S33	5.780	0.058	100→108	35
			101→108	26
			105→113	15
S34	5.807	0.031	104→112	18
			105→112	20
			105→113	31
S36	5.884	0.048	96→107	39
			99→108	23
			102→110	14
S38	5.895	0.057	96→107	34
			99→108	33
			102→110	12
S41	6.002	0.022	103→112	11

			104→113	65
S43	6.048	0.028	102→111	63

Table S8. ***Principal computed electronic transitions (f > 0.02) calculated for** 6'**. For each transition, the excitation energy E (eV), the oscillator strength f and molecular orbital composition of the excited-state function are reported.***

Exc. State	*E*	*f*	Composition	%
S3	4.026	0.103	212→213	91
S11	4.327	0.031	208→213	89
S17	4.413	0.027	209→214	73
S19	4.477	0.038	208→216	17
			209→214	15
			209→190	58
S38	4.850	0.084	212→219	70
S39	4.889	0.134	203→213	21
			205→214	49

Table S9. ***Principal computed electronic transitions (f > 0.02) calculated for 7. For each transition, the excitation energy E (eV), the oscillator strength f and molecular orbital composition of the excited-state function are reported.***

Exc. State	*E*	*f*	Composition	%
S3	4.053	0.021	181→188	15
			195→188	30
			186→188	13
			187→188	15
S6	4.128	0.040	181→189	33
			184→189	27
S7	4.241	0.030	181→188	19
			183→188	51
S9	4.326	0.080	182→188	68
S31	5.338	0.042	180→188	22
			180→189	16
			181→191	19
			184→191	16
S35	5.379	0.021	183→194	12
			178→188	6
			179→189	8
			181→191	9
S40	5.494	0.497	180→188	16
			180→189	40
			195→192	14
S41	5.499	0.031	195→192	54
S42	5.515	0.218	178→188	42
			179→188	16
S43	5.553	0.059	179→188	17
			182→192	38
			183→192	10
S44	5.578	0.049	177→188	36
			179→188	29
S46	5.628	0.033	178→189	10
			187→193	34
S47	5.633	0.138	178→189	15
			179→189	14
			176→188	9

			177→189	9
S49	5.664	0.043	181→192	35
			184→192	14
			195→193	10
S51	5.677	0.021	177→189	44
			178→189	24
S56	5.836	0.075	180→190	11
			181→193	14
			184→194	16
			187→194	18
S58	5.861	0.026	186→194	39
			187→194	16
S59	5.871	0.172	174→188	13
			175→188	14
			180→190	18
S60	5.895	0.048	175→189	21
			176→189	21
			180→190	24
S62	5.945	0.056	175→189	31
			195→194	16
S64	5.970	0.020	179→190	29
			195→194	10
			175→189	9
S67	6.022	0.034	184→195	51
S68	6.033	0.030	178→190	38
			175→188	8
			195→194	9
S70	6.052	0.037	177→190	28
			179→190	7
			181→194	6
			186→196	9
S72	6.067	0.030	182→194	17
			184→196	17
			187→196	14

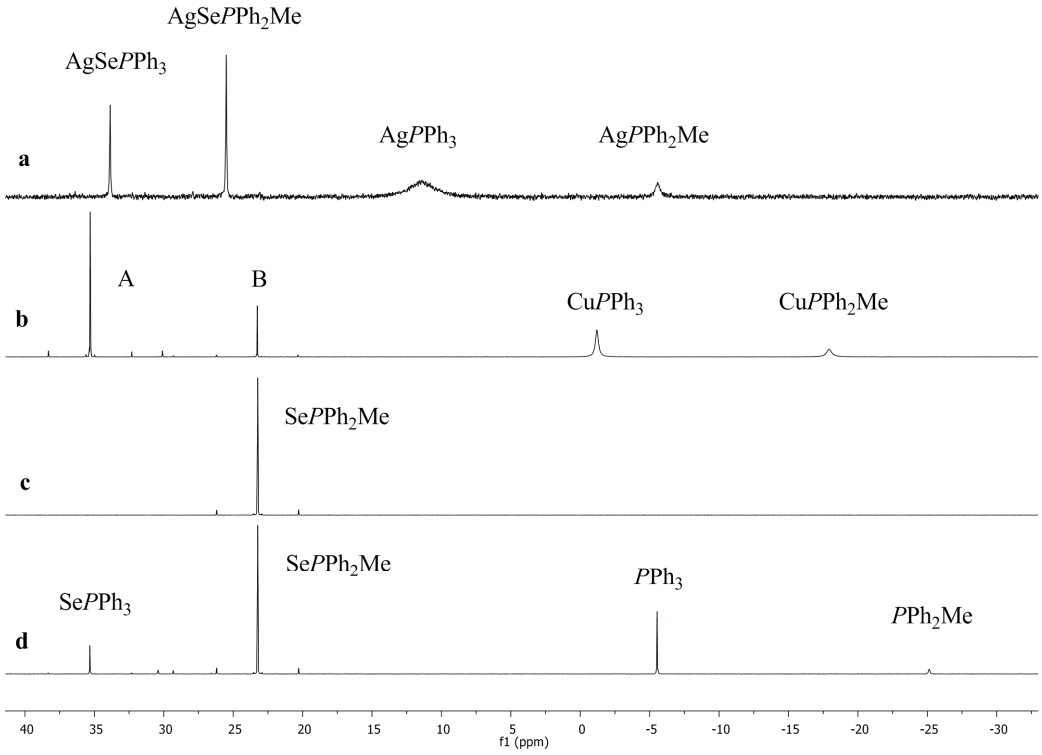

Figure S1 RT ^{31}P NMR spectra of (**a**) the solid isolated from reaction *(iii)*, (**b**) the solid isolated from reaction *(vii)*, (**c**) the free ligand $SePPh_2Me$ and (**d**) a 1:1 mixture of PPh_3 and $SePPh_2Me$ in $CDCl_3$. (-25 ÷ +45 ppm region).

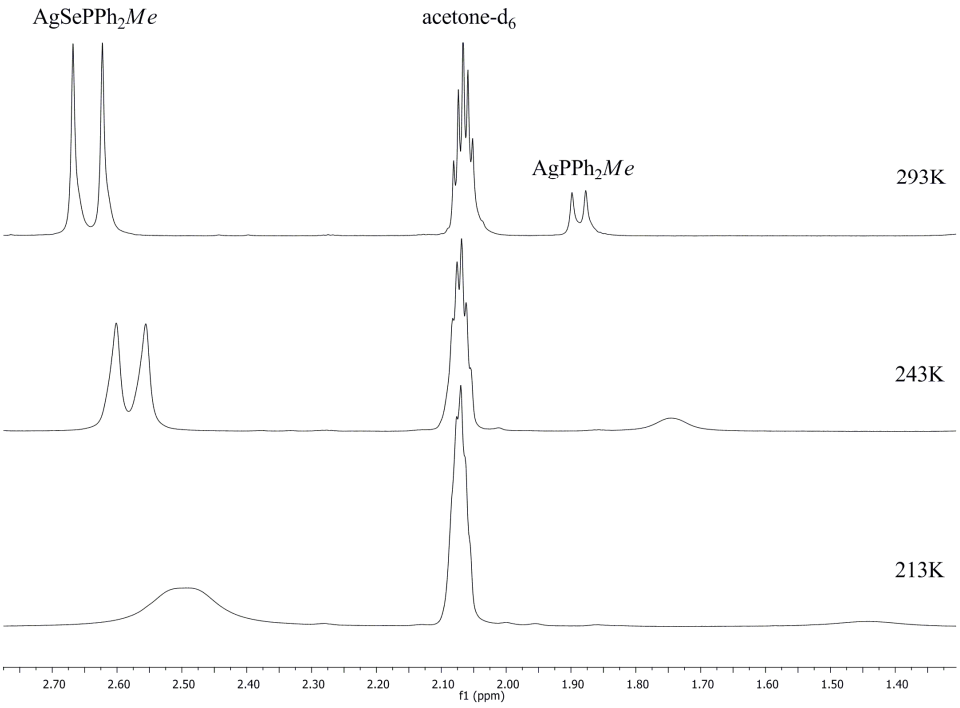

Figure S2 VT ^{1}H NMR spectra (aliphatic region) of the solid isolated from reaction *(iii)*.

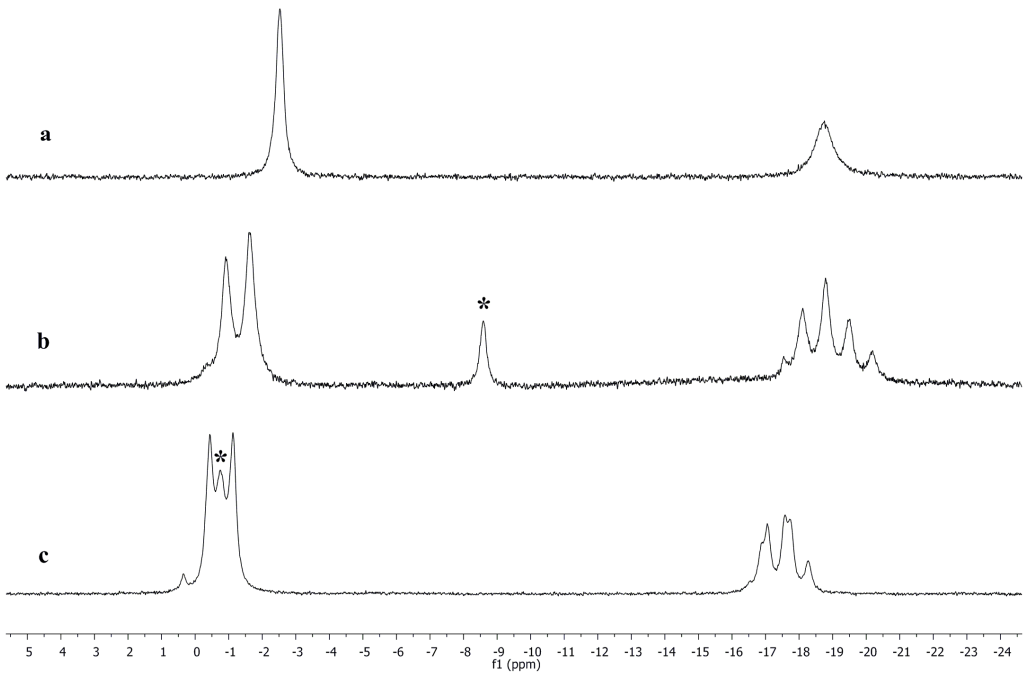

Figure S3 Room temperature (**a**) and low temperature (213K, **b** and **c**) ^{31}P NMR spectra of the solid isolated from reaction *(vii)*. (-25 ÷ +5 ppm region).