

Supporting Information

Rhenium(I) and Platinum(II) Complexes with Diimine Ligands Bearing Acidic Phenol Substituents: Hydrogen-Bonding, Acid-Base Chemistry and Optical Properties

Wei Liu and Katja Heinze*

Johannes Gutenberg-University of Mainz, Duesbergweg 10-14, 55128 Mainz, Germany

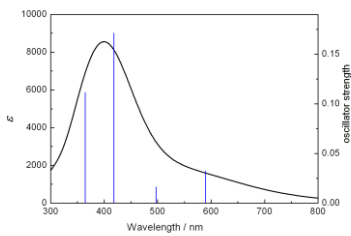
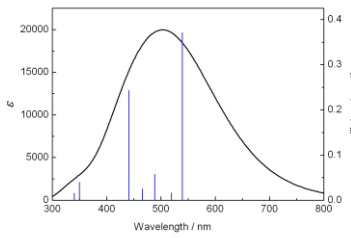
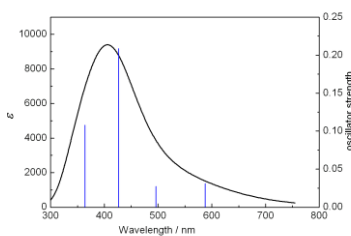
Table S1. Geometrical parameters of H...A contacts for **1** and **4**.

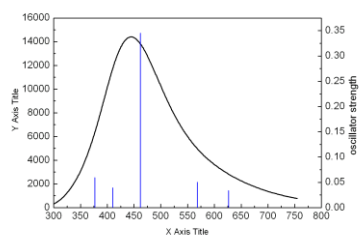
D	A	D–H (Å)	H...A (Å)	D–H...A (°)	D...A (Å)	symmetry operation
1						
O(4)–H(4A)	Cl(1)	0.84	2.85	102	3.129(3)	$\frac{1}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$
O(4)–H(4A)	O(2)	0.84	2.53	142	3.240(5)	$\frac{1}{2}-x, -\frac{1}{2}+y, \frac{3}{2}-z$
C(5)–H(5A)	O(2)	0.95	2.47	130	3.168(5)	$\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$
C(9)–H(9A)	O(3)	0.95	2.38	159	3.291(5)	$-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$
4						
C(10)–H(10A)	O(3)	0.98	2.53	160	3.470(4)	$2-x, 1-y, 1-z$
C(12)–H(12A)	Cl(1)	0.95	2.74	161	3.646(2)	$2-x, 2-y, -z$
C(18)–H(18A)	O(2)	0.95	2.54	162	3.452(3)	$1+x, y, z$

Table S2. Relevant C–O and C–C bond lengths / Å of the catecholato ligand in **7**.

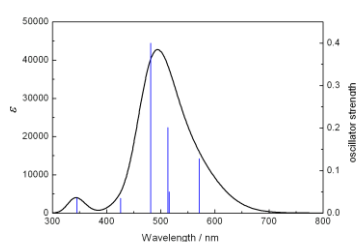
7	
C1–O1	1.359(3)
C6–O2	1.359(3)
C1–C2	1.415(3)
C2–C3	1.396(3)
C3–C4	1.399(4)
C4–C5	1.390(3)
C5–C6	1.415(3)
C6–C1	1.409(3)

Table S3. Main calculated optical transitions for complexes **1**, **1⁻**, **2**, **3**, **3⁻**, **4**, **6**, **6⁻**, **7** (gas phase, CH₂Cl₂, THF, CH₃CN).

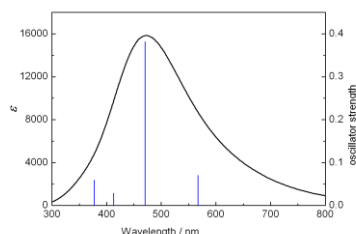
complex / simulated spectrum ^d	Orbital Excitations ^b	Composition	λ / nm	f
1 ($f > 0.016$) 	84 (H-5)→90 (L)	0.52679	364	0.1115
	85 (H-4)→90 (L)	-0.11268		
	88 (H-1)→91 (L+1)	0.27482		
	89 (H)→91 (L+1)	0.28022		
	86 (H-3)→90 (L)	0.60113	418	0.1712
	87 (H-2)→90 (L)	-0.28949		
	86 (H-3)→90 (L)	0.32459	497	0.0162
	87 (H-2)→90 (L)	0.62019		
	88 (H-1)→90 (L)	0.67189	589	0.0323
	1⁻ ($f > 0.016$) 	89 (H)→93 (L+3)	0.69438	350
86 (H-3)→90 (L)		0.21825	441	0.2430
89 (H)→90 (L)		0.18168		
89 (H)→91 (L+1)		0.56897		
86 (H-3)→90 (L)		0.65745	465	0.0250
89 (H)→91 (L+1)		-0.21801		
87 (H-2)→90 (L)		0.64598	488	0.0578
89 (H)→90 (L)		0.13633		
89 (H)→91 (L+1)		-0.20353		
87 (H-2)→90 (L)		-0.11816	519	0.0168
88 (H-1)→90 (L)		0.66230		
87 (H-2)→90 (L)		-0.21997	539	0.3710
88 (H-1)→90 (L)		-0.16156		
89 (H)→90 (L)	0.48449			
89 (H)→91 (L+1)	-0.22744			
2 ($f > 0.016$) 	104 (H-5)→110 (L)	0.54633	364	0.1079
	108 (H-1)→110 (L)	0.26665		
	109 (H)→111 (L+1)	0.26355		
	106 (H-3)→110 (L)	0.57564	427	0.2087
	107 (H-2)→110 (L)	-0.34521		
	106 (H-3)→110 (L)	0.38123	496	0.0273
	107 (H-2)→110 (L)	0.58559		
	108 (H-1)→110 (L)	0.67141	588	0.0312

3^- ($f > 0.016$)

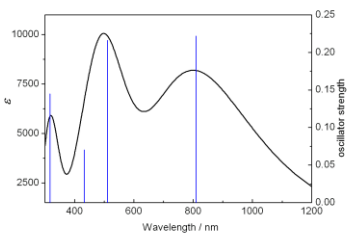
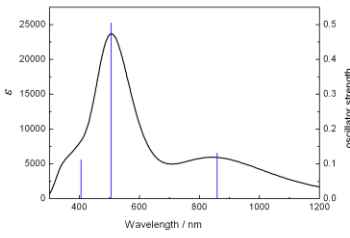
94 (H-6)→101 (L)	0.61718	377	0.0596
95 (H-5)→101 (L)	-0.13006		
96 (H-4)→101 (L)	0.18526		
94 (H-6)→101 (L)	0.21390	410	0.0392
95 (H-5)→101 (L)	0.60321		
96 (H-4)→101 (L)	-0.25050		
97 (H-3)→101 (L)	0.55491	462	0.3450
98 (H-2)→101 (L)	-0.35869		
97 (H-3)→101 (L)	0.40589	568	0.0502
98 (H-2)→101 (L)	0.56199		
94 (H-6)→101 (L)	0.11987	627	0.0338
99 (H-1)→101 (L)	0.65491		

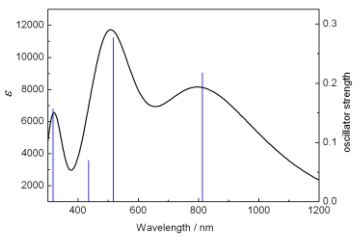
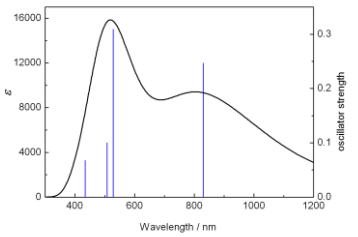
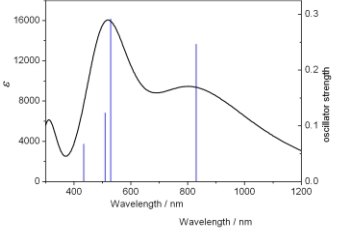
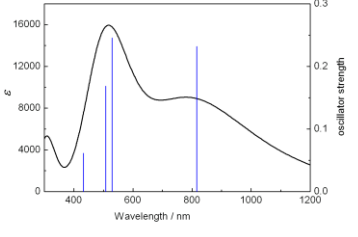
 3^- ($f > 0.016$)

93 (H-7)→101 (L)	0.14726	345	0.0358
94 (H-6)→101 (L)	0.63408		
95 (H-5)→101 (L)	0.20837		
95 (H-5)→101 (L)	0.19357	426	0.0348
96 (H-4)→101 (L)	0.66462		
96 (H-4)→101 (L)	0.10670	481	0.3996
98 (H-2)→101 (L)	0.49089		
99 (H-1)→101 (L)	0.19725		
100 (H)→101 (L)	0.30573		
97 (H-3)→101 (L)	0.24688	513	0.2014
98 (H-2)→101 (L)	0.46215		
99 (H-1)→101 (L)	-0.29753		
100 (H)→101 (L)	-0.26690		
97 (H-3)→101 (L)	0.63223	515	0.0498
98 (H-2)→101 (L)	-0.10503		
99 (H-1)→101 (L)	0.17154		
100 (H)→101 (L)	0.13538		
99 (H-1)→101 (L)	0.57573	571	0.1280
100 (H)→101 (L)	-0.32455		

 4^- ($f > 0.016$)

102 (H-6)→109 (L)	0.63184	377	0.0592
104 (H-4)→109 (L)	-0.12728		
105 (H-3)→109 (L)	0.10127		
102 (H-6)→109 (L)	0.14935	413	0.0284
103 (H-5)→109 (L)	0.64435		
104 (H-4)→109 (L)	0.16729		
105 (H-3)→109 (L)	-0.10890		
104 (H-4)→109 (L)	0.33836	470	0.3819
105 (H-3)→109 (L)	0.43126		
106 (H-2)→109 (L)	-0.37846		
104 (H-4)→109 (L)	0.29646	567	0.0699
105 (H-3)→109 (L)	0.30475		
106 (H-2)→109 (L)	0.54719		
102 (H-6)→109 (L)	0.11754	625	0.0361
107 (H-1)→109 (L)	0.65515		

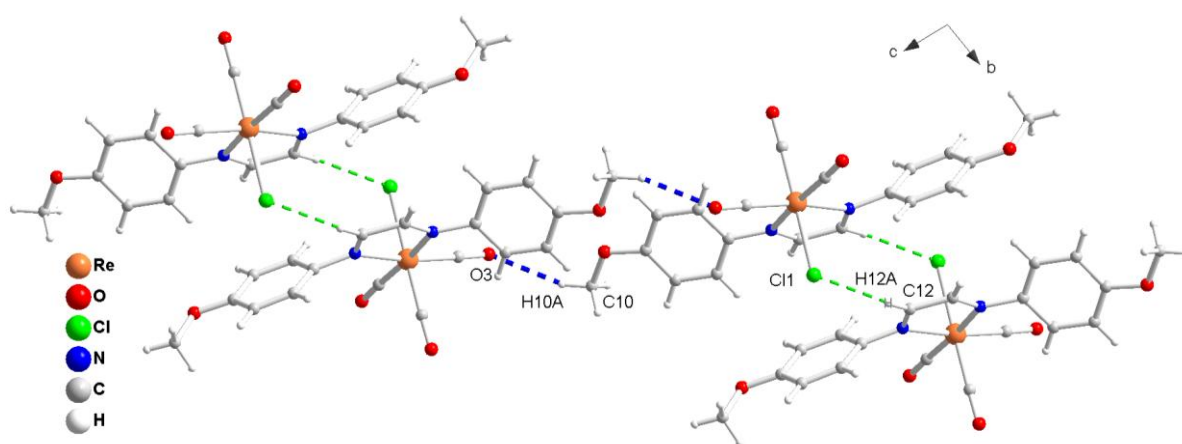
6⁺ ($f > 0.06$) 	132 (H)→137 (L+4)	0.68958	317	0.1449
	126 (H-6)→133 (L)	-0.11524	432	0.0702
	127 (H-5)→133 (L)	0.64908		
	130 (H-2)→133 (L)	-0.17122		
	126 (H-6)→133 (L)	0.10564	511	0.2159
	127 (H-5)→133 (L)	0.16839		
	128 (H-4)→133 (L)	0.20652		
	130 (H-2)→133 (L)	0.59525		
	132 (H)→133 (L)	0.53556	809	0.2216
	6⁻ ($f > 0.06$) 	125 (H-7)→133(L)	-0.14634	405
126 (H-6)→133(L)		0.19985		
127 (H-5)→133(L)		0.53725		
131 (H-1)→133(L)		-0.13373		
132 (H)→133(L)		-0.26301		
127(H-5)→133(L)		0.16568	506	0.5048
130 (H-2)→133(L)		-0.40734		
131 (H-1)→133(L)		0.39158		
131 (H-1)→133(L)		-0.19734	859	0.1311
132 (H)→133(L)		0.59328		

7 gas phase ($f > 0.06$) 	140 (H)→145 (L+4)	0.69086	317	0.1573
	135 (H-5)→141 (L)	0.65872	435	0.0700
	138 (H-2)→141 (L)	-0.15645		
	135 (H-5)→141 (L)	0.15214	517	0.2772
	136 (H-4)→141 (L)	0.12744		
	138 (H-2)→141 (L)	0.62278		
	140 (H)→141 (L)	0.53761	813	0.2177
7 in THF ($f > 0.06$) 	135 (H-5)→141 (L)	0.65556	434	0.0674
	137 (H-3)→141 (L)	0.11778		
	138 (H-2)→141 (L)	-0.10609		
	139 (H-1)→141 (L)	0.11514		
	134 (H-6)→141 (L)	0.10381	508	0.1001
	136 (H-4)→141 (L)	0.60497		
	138 (H-2)→141 (L)	-0.30545		
	134 (H-6)→141 (L)	0.10057	528	0.3094
	136 (H-4)→141 (L)	0.31351		
	138 (H-2)→141 (L)	0.57809		
	140 (H)→141 (L)	0.57766	830	0.2465
7 in CH₂Cl₂ ($f > 0.06$) 	135 (H-5)→141 (L)	0.65618	434	0.0673
	137 (H-3)→141 (L)	0.11817		
	138 (H-2)→141 (L)	-0.10293		
	139 (H-1)→141 (L)	0.11918		
	136 (H-4)→141 (L)	0.58703	509	0.1233
	138 (H-2)→141 (L)	-0.33723		
	134 (H-6)→141 (L)	0.10371	529	0.2918
	136 (H-4)→141 (L)	0.34697		
	138 (H-2)→141 (L)	0.56129		
	140 (H)→141 (L)	0.58041	829	0.2465
7 in CH₃CN ($f > 0.06$) 	135 (H-5)→141 (L)	0.64991	432	0.0615
	137 (H-3)→141 (L)	0.14767		
	139 (H-1)→141 (L)	-0.12832		
	136 (H-4)→141 (L)	0.54727	508	0.1684
	138 (H-2)→141 (L)	-0.39584		
	134 (H-6)→141 (L)	0.10770	529	0.2456
	136 (H-4)→141 (L)	0.40883		
	138 (H-2)→141 (L)	0.52336		
	140 (H)→141 (L)	0.58546	815	0.2317

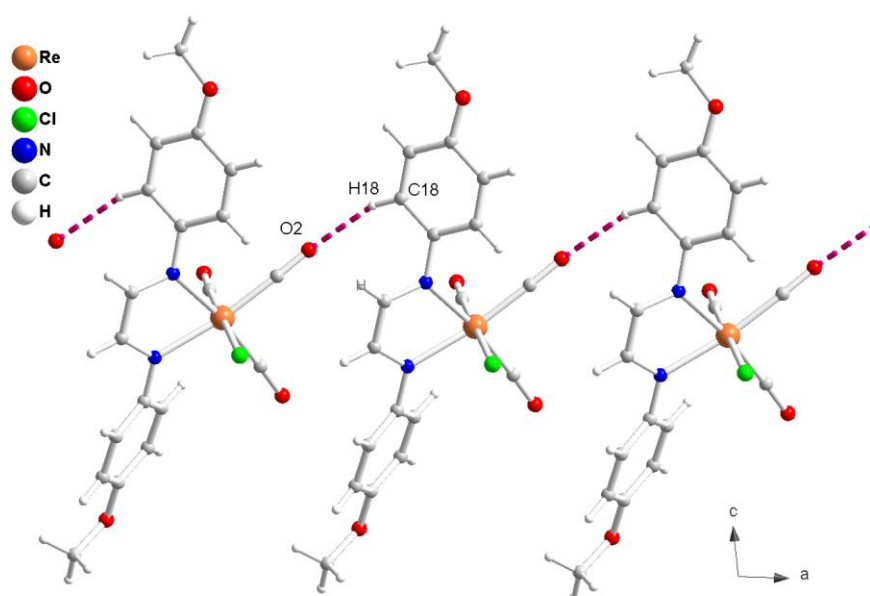
^a The simulated UV/Vis spectra were obtained with the GaussSum program V 2.2; N. M. O'Boyle, J. G. Vos, GaussSum; Dublin City University; Dublin, Ireland, 2005; available at <http://gausssum.sourceforge.net>.

^b The molecular orbital # involved in each transition.

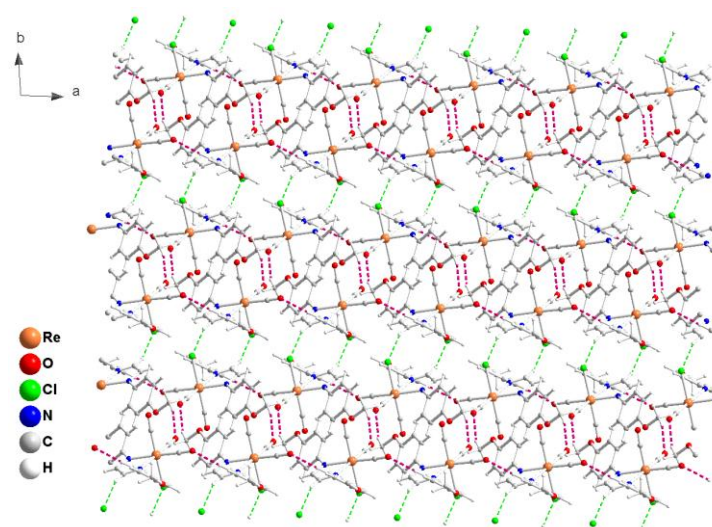
Fig. S1. Crystal packing of complex **4** along the *a*-axis (a), *b*-axis (b), and resulting three-dimensional network (c). Hydrogen contacts are indicated by dashed lines.



(a)



(b)



(c)

Fig. S2. UV/Vis absorption spectrum of **1** in THF and band deconvolution (linear correlation coefficient $R^2 = 0.9998$), with Gaussian line shapes (328, 370, 424 and 430 nm).

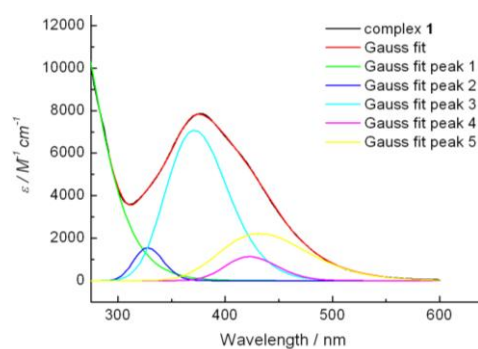


Fig. S3. UV/Vis absorption spectrum of **2** in THF and band deconvolution (linear correlation coefficient $R^2 = 0.9999$), with Gaussian line shapes (338, 368 and 412 nm).

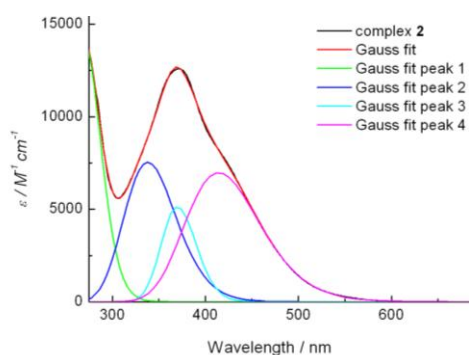


Fig. S4. UV/Vis absorption spectrum of **3** in THF and band deconvolution (linear correlation coefficient $R^2 = 0.9999$), with Gaussian line shapes (413, 435 and 448 nm).

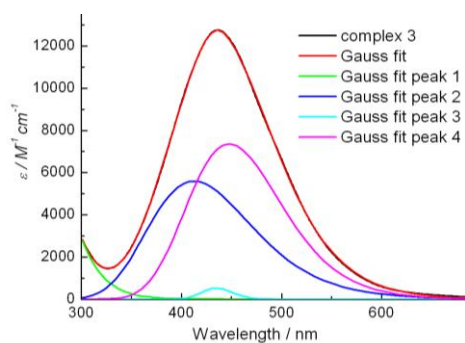


Fig. S5. UV/Vis absorption spectrum of **4** in THF and band deconvolution (linear correlation coefficient $R^2 = 0.9995$), with Gaussian line shapes (419, 442 and 461 nm).

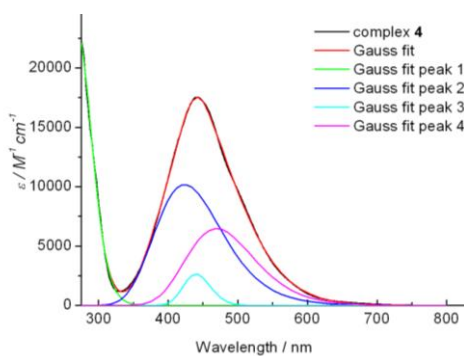


Fig. S6. UV/Vis absorption spectra of **6** in THF and band deconvolution (linear correlation coefficient $R^2 = 0.9999$), with Gaussian line shapes (357, 403, 446, 488, 564, 667, 817 and 904 nm) [left] and of **7** in THF and band deconvolution (linear correlation coefficient $R^2 = 0.9997$), with Gaussian line shapes (407, 443, 495, 662, 779, 864 and 949 nm) [right].

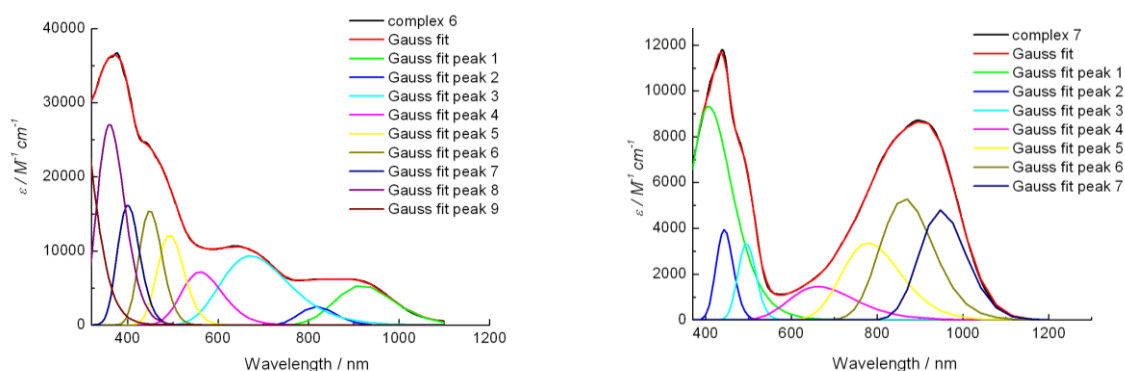


Fig. S7. UV/Vis absorption spectra of **1**, after reaction with P_1 -*t*-Bu and upon reacidification with CH_3COOH (4×10^{-5} M) in THF.

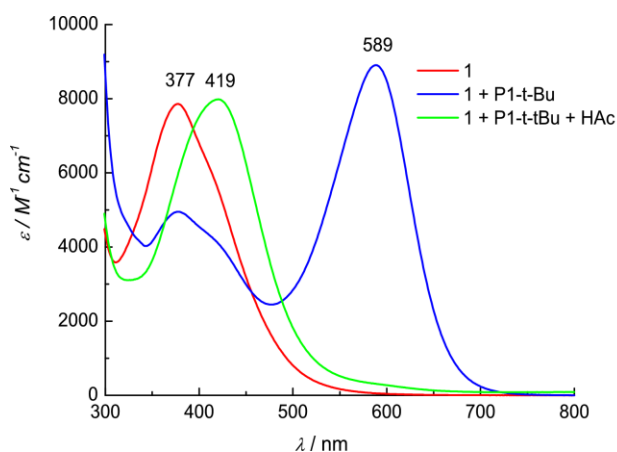


Fig. S8. UV/Vis absorption spectra of **3**, after reaction with P_1 -*t*-Bu and upon reacidification with CH_3COOH (4×10^{-5} M) in THF.

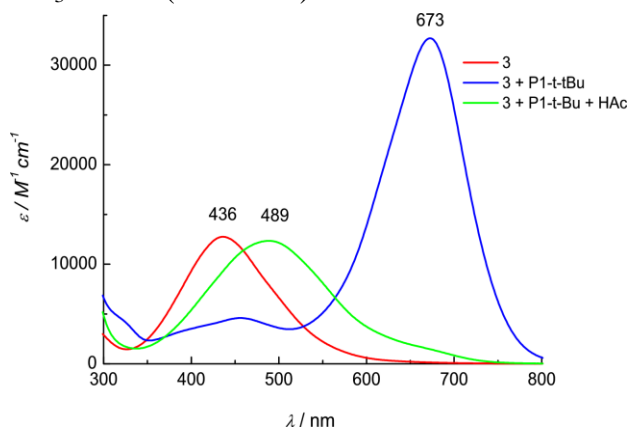


Fig. S9. Emission spectrum of **4** in a THF matrix at 77 K (10^{-7} M, $\lambda_{\text{exc}} = 388$ nm).

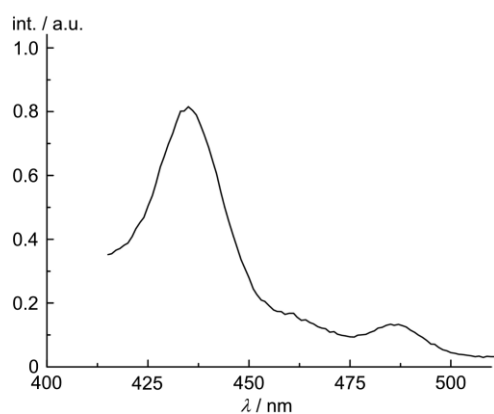


Fig. S10. Experimental (black) and simulated (red) EPR spectra of complex **6**^{•+} (10^{-3} M) in a mixture of THF/CH₃CN (v/v, 9/1) at room temperature, freq = 9.413686 GHz, $g = 1.9965$, $A_{\text{iso}}(^{195}\text{Pt}) = 23$ G, $A_{\text{iso}}(2\times^1\text{H}) = 3.3$ G. (* = unknown species / impurity).

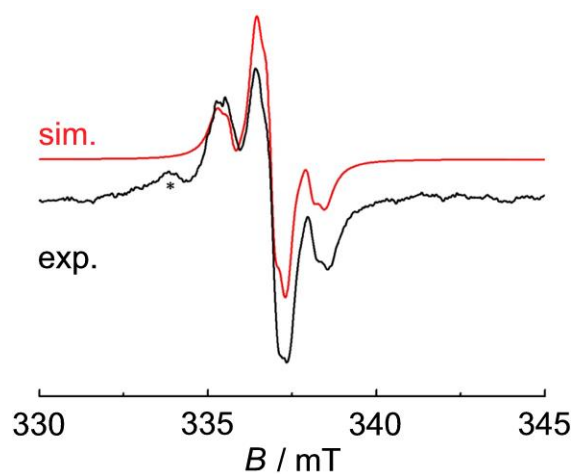


Fig. S11. UV/Vis absorption spectra of **1**, after reaction with P_1 -*t*-Bu and upon reacidification with HCl in dioxan and after addition of a mixture of P_1 -*t*-Bu/HCl to **1**.

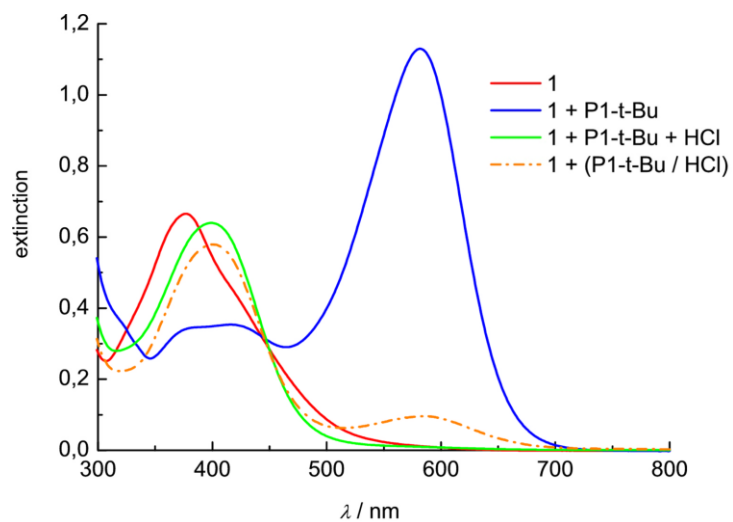


Fig. S12. FD mass spectrum of **1** after reaction with P_1 -*t*-Bu and HCl.

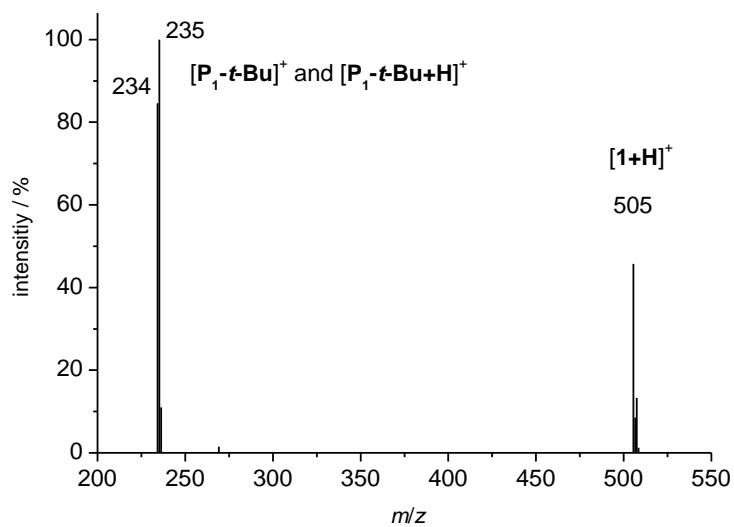
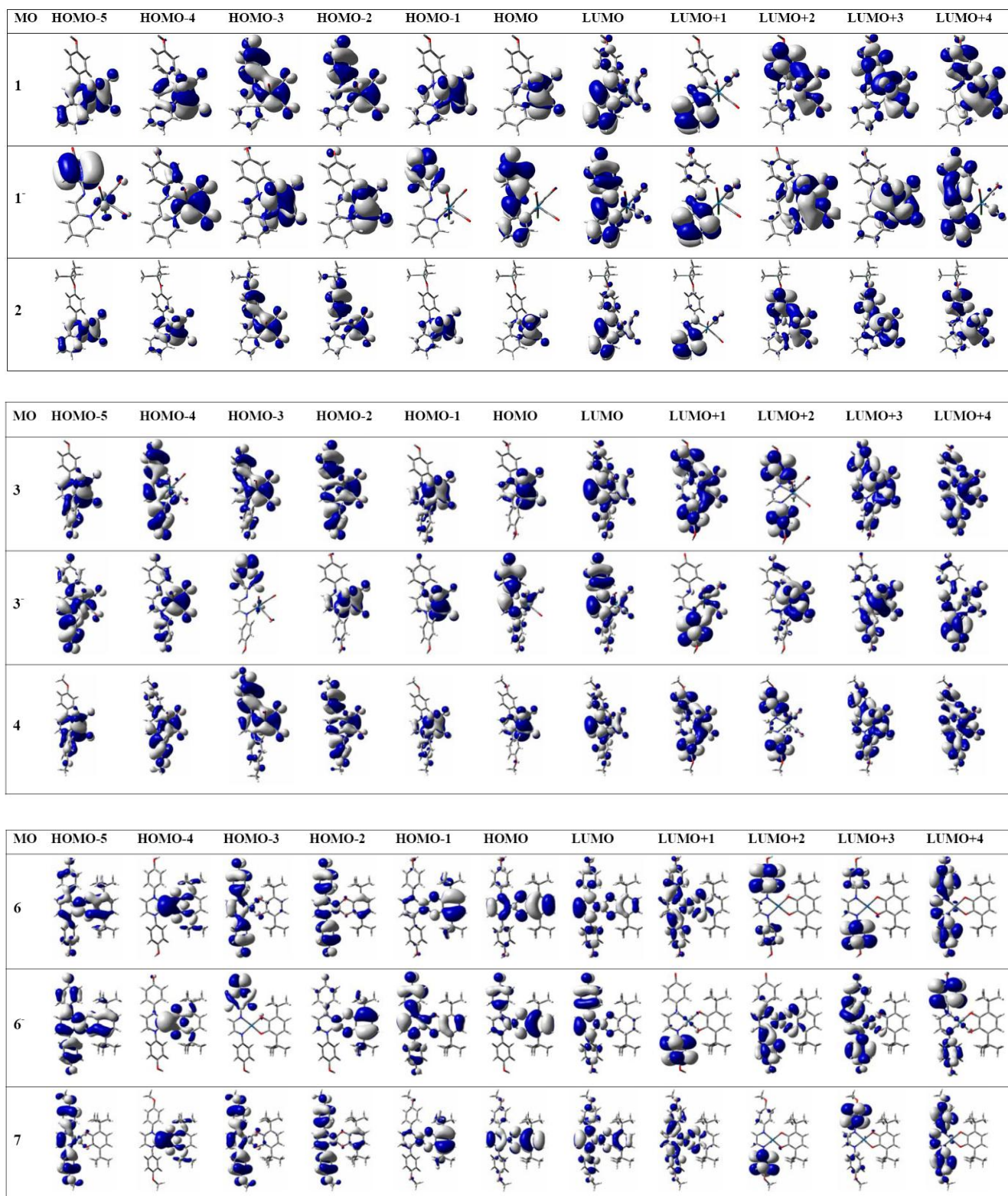


Fig. S11. Graphical representation of relevant molecular orbitals of **1**, **1⁻**, **2**, **3**, **3⁻**, **4**, **6**, **6⁻** and **7**

(contour value 0.02 a.u.)



Optimised Cartesian Coordinates of **1**

6	-0.047082000	-0.107119000	0.186525000
6	0.163281000	0.730802000	1.287449000
6	1.404452000	0.747518000	1.920844000
6	2.446626000	-0.057623000	1.447033000
6	2.237810000	-0.886526000	0.333576000
6	0.995005000	-0.920324000	-0.282609000
1	-0.635032000	1.379019000	1.642894000
1	1.576197000	1.420907000	2.755696000
1	3.044203000	-1.526651000	-0.008094000
1	0.812418000	-1.568226000	-1.133380000
7	3.723218000	-0.053371000	2.083572000
6	7.357619000	0.035318000	3.784592000
6	7.566457000	-0.169978000	5.147245000
7	6.135137000	0.030300000	3.231718000
6	3.773967000	-0.218577000	3.365654000
6	5.061949000	-0.197272000	4.035670000
1	2.870468000	-0.398850000	3.947913000
75	5.673193000	0.236200000	1.078434000
17	5.766716000	-2.281118000	1.091972000
6	5.543719000	2.151583000	1.167676000
6	5.073971000	0.244305000	-0.758729000
6	7.504325000	0.335157000	0.484776000
8	4.703099000	0.232431000	-1.856034000
8	5.461149000	3.311682000	1.231157000
8	8.624696000	0.375276000	0.185658000
6	5.196564000	-0.409273000	5.410595000
6	6.467928000	-0.395275000	5.976748000
1	4.312621000	-0.588830000	6.014363000
1	6.599807000	-0.560270000	7.041548000
1	8.577429000	-0.155403000	5.539881000
1	8.186663000	0.205386000	3.107918000
8	-1.236349000	-0.173301000	-0.474201000
1	-1.866724000	0.441431000	-0.066809000

Optimised Cartesian Coordinates of **2**

6	0.157869000	0.096094000	0.713706000
6	0.445266000	0.769059000	1.910588000
6	1.724474000	0.702185000	2.459844000
6	2.735186000	-0.020586000	1.815497000
6	2.454492000	-0.686357000	0.612581000
6	1.174901000	-0.637284000	0.078816000
1	-0.321829000	1.348964000	2.412492000
1	1.949305000	1.252065000	3.369579000
1	3.234073000	-1.269064000	0.133698000
1	0.937983000	-1.161372000	-0.841200000
7	4.048651000	-0.095595000	2.365930000
6	7.783579000	-0.207547000	3.835694000
6	8.075754000	-0.587411000	5.144413000
7	6.529160000	-0.145274000	3.363688000
6	4.179713000	-0.422759000	3.610670000
6	5.507136000	-0.481297000	4.195807000
1	3.313990000	-0.679647000	4.220953000
75	5.934973000	0.336386000	1.288209000
17	6.033637000	-2.160145000	0.969192000
6	5.804482000	2.221729000	1.635373000
6	5.226425000	0.576772000	-0.493298000
6	7.725068000	0.534491000	0.602516000
8	4.792221000	0.704487000	-1.559693000
8	5.721310000	3.362472000	1.856220000
8	8.824604000	0.629413000	0.243533000
6	5.726013000	-0.869589000	5.520635000
6	7.029916000	-0.923203000	6.004169000
1	4.880343000	-1.130500000	6.149049000
1	7.226911000	-1.224534000	7.028307000
1	9.109202000	-0.619854000	5.472110000
1	8.570042000	0.051748000	3.136836000
8	-1.061163000	0.101297000	0.122134000
14	-2.459450000	1.045150000	0.325415000
6	-3.259151000	0.678563000	1.994833000
1	-3.451608000	-0.394801000	2.108061000
1	-2.644042000	0.996845000	2.843915000
1	-4.222845000	1.197455000	2.075105000
6	-2.024849000	2.871127000	0.154663000
1	-1.322758000	3.212121000	0.923453000
1	-1.569610000	3.073515000	-0.821765000
1	-2.928096000	3.489054000	0.234225000
6	-3.571802000	0.474952000	-1.075107000
1	-4.531301000	1.006218000	-1.059148000
1	-3.103969000	0.656298000	-2.049250000
1	-3.781900000	-0.598036000	-1.000334000

75	-0.041985000	0.006935000	0.186739000
8	0.198365000	0.185342000	3.259536000
8	3.033935000	-0.161003000	-0.104795000
8	-0.228775000	-3.078889000	0.292852000
17	-0.260027000	-0.076492000	-2.321320000
8	3.824405000	5.956663000	-0.285017000
8	-6.154535000	-3.571092000	0.411183000
7	-2.212956000	0.367086000	0.139248000
7	-0.276723000	2.178297000	-0.080121000
6	-2.552516000	1.596944000	-0.129549000
1	-3.595125000	1.884050000	-0.254333000
6	-1.509207000	2.578518000	-0.220566000
1	-1.746853000	3.624469000	-0.406874000
6	-3.224006000	-0.628428000	0.178889000
6	-4.221889000	-0.683588000	-0.804900000
1	-4.189056000	0.004538000	-1.643494000
6	-5.208095000	-1.664028000	-0.750126000
1	-5.960633000	-1.717790000	-1.534007000
6	-5.215728000	-2.592705000	0.297720000
6	-4.217489000	-2.542975000	1.281844000
1	-4.234651000	-3.272903000	2.084157000
6	-3.221734000	-1.580380000	1.211931000
1	-2.449297000	-1.540778000	1.972124000
6	1.883606000	-0.103727000	0.012357000
6	-0.140731000	-1.925292000	0.263730000
6	2.797317000	5.067265000	-0.199109000
6	1.694271000	5.260602000	0.641041000
1	1.636737000	6.143319000	1.274583000
6	0.674751000	4.312550000	0.678610000
1	-0.164894000	4.449156000	1.353897000
6	0.757861000	3.154411000	-0.105772000
6	1.872587000	2.958755000	-0.937617000
1	1.914300000	2.078312000	-1.568795000
6	2.876708000	3.914235000	-0.993794000
1	3.733674000	3.784613000	-1.646276000
6	0.111210000	0.119431000	2.100212000
1	-6.768002000	-3.519763000	-0.338846000
1	3.659595000	6.700147000	0.316154000

75	-0.092886000	0.019191000	0.220283000
8	0.234878000	0.140003000	3.287569000
8	2.970706000	-0.185389000	-0.161629000
8	-0.316805000	-3.065483000	0.276044000
17	-0.381647000	-0.016793000	-2.282296000
8	3.857844000	5.904029000	-0.243153000
8	-6.217548000	-3.508084000	0.569040000
7	-2.260208000	0.408368000	0.237631000
7	-0.306082000	2.198296000	0.001455000
6	-2.590151000	1.647231000	0.000530000
1	-3.631848000	1.949589000	-0.091555000
6	-1.536380000	2.616870000	-0.099048000
1	-1.764329000	3.669516000	-0.257658000
6	-3.281858000	-0.575416000	0.285155000
6	-4.302785000	-0.605124000	-0.672752000
1	-4.281414000	0.096989000	-1.500306000
6	-5.302261000	-1.576167000	-0.617944000
1	-6.062274000	-1.595359000	-1.390088000
6	-5.295247000	-2.523776000	0.414555000
6	-4.268491000	-2.496302000	1.375482000
1	-4.277410000	-3.241191000	2.164242000
6	-3.264772000	-1.546145000	1.302254000
1	-2.474733000	-1.528476000	2.044970000
6	1.824999000	-0.114030000	-0.010479000
6	-0.215162000	-1.912578000	0.265347000
6	3.883998000	7.071528000	0.565461000
1	3.024632000	7.722682000	0.359128000
1	4.804861000	7.594744000	0.303344000
1	3.900728000	6.819507000	1.633652000
6	2.804748000	5.054303000	-0.123272000
6	1.723170000	5.242238000	0.747514000
1	1.676753000	6.100775000	1.407083000
6	0.693304000	4.301240000	0.781735000
1	-0.128583000	4.432204000	1.479931000
6	0.740135000	3.161430000	-0.028404000
6	1.833896000	2.969622000	-0.890582000
1	1.851125000	2.103530000	-1.542434000
6	2.845254000	3.913852000	-0.945356000
1	3.686594000	3.791104000	-1.619366000
6	-7.265011000	-3.614509000	-0.385302000
1	-7.886645000	-2.709942000	-0.401697000
1	-7.871431000	-4.464081000	-0.067699000
1	-6.871617000	-3.804294000	-1.392029000
6	0.114447000	0.095840000	2.130063000

Optimised Cartesian Coordinates of **6**

6	-0.060394000	-0.269304000	0.438020000
6	0.293656000	-1.191810000	1.429869000
6	1.526473000	-1.088599000	2.068056000
6	2.422188000	-0.065137000	1.723464000
6	2.065047000	0.847292000	0.717876000
6	0.833666000	0.750170000	0.085112000
1	-0.386020000	-2.000006000	1.692798000
1	1.811404000	-1.827992000	2.810472000
1	2.761371000	1.631641000	0.449658000
1	0.548263000	1.455330000	-0.688298000
7	3.665014000	0.067255000	2.391240000
6	7.311838000	0.396614000	3.982080000
6	7.544066000	1.150884000	5.146236000
6	8.394082000	-0.222395000	3.342912000
6	8.825919000	1.274901000	5.665765000
1	6.719579000	1.673846000	5.621642000
6	9.677629000	-0.104125000	3.864856000
1	8.216193000	-0.797235000	2.443105000
6	9.901240000	0.642999000	5.027781000
1	9.016153000	1.870240000	6.552787000
1	10.508860000	-0.593836000	3.361925000
7	6.002765000	0.241553000	3.463879000
6	3.716670000	-0.075833000	3.714474000
6	4.987806000	0.024274000	4.298889000
78	5.461584000	0.391482000	1.519125000
8	4.899640000	0.536200000	-0.389959000
8	7.246300000	0.711415000	0.681248000
6	5.913445000	0.753350000	-1.243275000
6	5.720879000	0.861332000	-2.645979000
6	7.203396000	0.858866000	-0.652784000
6	6.875475000	1.101510000	-3.387601000
6	8.363077000	1.116686000	-1.430305000
6	8.146479000	1.230889000	-2.801764000
1	6.810341000	1.196379000	-4.465403000
1	8.983022000	1.428770000	-3.462116000
6	4.331350000	0.734986000	-3.292701000
6	4.401645000	0.799652000	-4.831481000
1	4.800809000	1.756491000	-5.187224000
1	5.019641000	-0.005158000	-5.246268000
1	3.392557000	0.689829000	-5.245774000
6	3.437107000	1.903002000	-2.812531000
1	2.427968000	1.812431000	-3.235401000
1	3.357485000	1.911238000	-1.724006000
1	3.853440000	2.865619000	-3.132674000
6	3.684535000	-0.618584000	-2.910422000

1	3.578344000	-0.718055000	-1.828763000
1	2.690633000	-0.704543000	-3.368247000
1	4.296164000	-1.452976000	-3.274677000
6	9.759065000	1.249143000	-0.798747000
6	10.833076000	1.616100000	-1.842102000
1	10.615181000	2.571051000	-2.333989000
1	11.804599000	1.714286000	-1.343379000
1	10.937360000	0.847318000	-2.616400000
6	9.755980000	2.360267000	0.279011000
1	9.500069000	3.328294000	-0.168327000
1	9.034891000	2.147525000	1.070305000
1	10.753023000	2.451819000	0.729650000
6	10.164379000	-0.102175000	-0.163173000
1	9.434042000	-0.416293000	0.584718000
1	10.230218000	-0.885808000	-0.927310000
1	11.146813000	-0.017773000	0.320608000
8	-1.252988000	-0.314900000	-0.221513000
8	11.137626000	0.796824000	5.581373000
1	5.158904000	-0.089507000	5.364190000
1	2.811890000	-0.236009000	4.291502000
1	-1.771089000	-1.067571000	0.104259000
1	11.792829000	0.342113000	5.028859000

Optimised Cartesian Coordinates of 7

6	-0.121375000	0.231515000	0.442779000
6	0.149576000	-0.703991000	1.450240000
6	1.383751000	-0.681724000	2.099812000
6	2.359627000	0.262761000	1.756218000
6	2.085859000	1.188144000	0.734607000
6	0.858757000	1.175013000	0.092027000
1	-0.578417000	-1.458418000	1.724861000
1	1.603299000	-1.431646000	2.854068000
1	2.843910000	1.912214000	0.463824000
1	0.634184000	1.888622000	-0.693765000
7	3.602486000	0.305783000	2.435124000
6	7.251699000	0.360783000	4.053215000
6	7.536928000	1.099573000	5.217313000
6	8.284861000	-0.342887000	3.425381000
6	8.821005000	1.121835000	5.738547000
1	6.755127000	1.688819000	5.687306000
6	9.576183000	-0.328101000	3.948723000
1	8.066078000	-0.906015000	2.526978000
6	9.853270000	0.404770000	5.110726000
1	9.056648000	1.703443000	6.623962000
1	10.352823000	-0.887166000	3.440651000
7	5.938044000	0.307386000	3.527044000

6	3.631928000	0.173592000	3.759867000
6	4.902454000	0.179463000	4.354850000
78	5.426035000	0.481950000	1.576043000
8	4.892897000	0.652301000	-0.339897000
8	7.236765000	0.660623000	0.752098000
6	5.927948000	0.784144000	-1.185381000
6	5.757102000	0.891677000	-2.590819000
6	7.216777000	0.798822000	-0.583573000
6	6.933087000	1.038919000	-3.323475000
6	8.399387000	0.962931000	-1.351935000
6	8.204680000	1.079749000	-2.726592000
1	6.884781000	1.127447000	-4.402681000
1	9.059545000	1.208012000	-3.380695000
6	4.368207000	0.860359000	-3.250939000
6	4.458587000	0.900718000	-4.789348000
1	4.930548000	1.821314000	-5.151513000
1	5.020239000	0.047771000	-5.187754000
1	3.448466000	0.860186000	-5.213681000
6	3.557237000	2.096376000	-2.793913000
1	2.548567000	2.074696000	-3.227166000
1	3.466651000	2.122968000	-1.706579000
1	4.046162000	3.022165000	-3.120000000
6	3.618991000	-0.436789000	-2.860025000
1	3.492511000	-0.512880000	-1.778677000
1	2.627238000	-0.455139000	-3.330045000
1	4.171605000	-1.319000000	-3.205479000
6	9.795654000	0.995340000	-0.707564000
6	10.903414000	1.275426000	-1.742288000
1	10.761481000	2.241172000	-2.240846000
1	11.875055000	1.303605000	-1.234977000
1	10.956456000	0.496487000	-2.511516000
6	9.864410000	2.109847000	0.364709000
1	9.681652000	3.091374000	-0.089138000
1	9.124139000	1.952766000	1.151099000
1	10.862057000	2.132521000	0.822766000
6	10.091824000	-0.378737000	-0.060778000
1	9.330452000	-0.633145000	0.678833000
1	10.108915000	-1.168986000	-0.820775000
1	11.071443000	-0.365439000	0.435835000
8	-1.288058000	0.304490000	-0.253992000
8	11.076277000	0.491346000	5.700329000
1	-1.989412000	-1.659810000	-0.143884000
6	-2.314713000	-0.628448000	0.045395000
1	-2.648443000	-0.539865000	1.087749000
1	-3.143910000	-0.384196000	-0.620711000
1	12.011464000	-1.259974000	5.049622000
6	12.170161000	-0.174333000	5.085654000

1	13.039488000	0.042895000	5.708547000
1	12.347403000	0.199547000	4.069103000
1	5.055007000	0.063052000	5.422738000
1	2.712476000	0.090772000	4.329951000

Optimised Cartesian Coordinates of 1^-

6	0.211465000	-0.190380000	-0.045610000
6	1.555716000	0.049549000	0.479698000
6	2.141262000	1.283761000	0.460015000
6	1.456884000	2.435895000	-0.051599000
6	0.125523000	2.239834000	-0.531550000
6	-0.459437000	1.003555000	-0.548347000
1	2.064813000	-0.803869000	0.921572000
1	3.121183000	1.412381000	0.913962000
1	-0.391822000	3.088120000	-0.962298000
1	-1.458828000	0.869113000	-0.953859000
7	2.049965000	3.673976000	-0.120894000
6	3.777907000	7.370101000	-0.026668000
6	5.147094000	7.574708000	-0.129263000
7	3.212705000	6.151674000	-0.014768000
6	3.374013000	3.777707000	-0.153053000
6	4.012449000	5.046459000	-0.132078000
1	3.994795000	2.891953000	-0.255828000
75	1.054478000	5.721376000	0.070350000
17	1.199756000	5.858774000	-2.451695000
6	1.055193000	5.532730000	1.976087000
6	-0.821519000	5.271494000	-0.022375000
6	0.552652000	7.560488000	0.197017000
8	-1.960434000	5.047837000	-0.085918000
8	1.060266000	5.421454000	3.138895000
8	0.300816000	8.697945000	0.268581000
6	5.416901000	5.189959000	-0.238248000
6	5.982211000	6.449958000	-0.235341000
1	6.029253000	4.297619000	-0.327800000
1	7.059820000	6.568022000	-0.317914000
1	5.545060000	8.583711000	-0.128305000
1	3.093059000	8.207074000	0.051118000
8	-0.315489000	-1.322180000	-0.042148000

Optimised Cartesian Coordinates of 3^-

75	-0.004054000	-0.069618000	0.024186000
8	0.531150000	0.152071000	3.051243000
8	2.990511000	-0.525224000	-0.595351000
8	-0.272197000	-3.130943000	0.205339000
17	-0.515668000	-0.108469000	-2.460520000

8	3.686046000	6.119022000	-0.211190000
8	-6.236575000	-3.534679000	0.438616000
7	-2.168310000	0.306123000	0.200591000
7	-0.216508000	2.216956000	-0.132623000
6	-2.494629000	1.569764000	0.013021000
1	-3.546765000	1.858177000	-0.018834000
6	-1.512574000	2.560872000	-0.115829000
1	-1.817137000	3.596040000	-0.232847000
6	-3.197715000	-0.661065000	0.229242000
6	-4.218481000	-0.670995000	-0.733390000
1	-4.179047000	0.039998000	-1.552320000
6	-5.240471000	-1.618632000	-0.678556000
1	-6.016498000	-1.622202000	-1.443325000
6	-5.254119000	-2.578002000	0.336535000
6	-4.233215000	-2.588247000	1.293201000
1	-4.249804000	-3.343562000	2.072865000
6	-3.215011000	-1.643574000	1.234084000
1	-2.424631000	-1.647572000	1.977422000
6	1.869989000	-0.322608000	-0.354790000
6	-0.161235000	-1.973787000	0.138714000
6	2.810701000	5.232570000	-0.180991000
6	1.456671000	5.487589000	0.317022000
1	1.262108000	6.484339000	0.705618000
6	0.491000000	4.525665000	0.335177000
1	-0.477708000	4.759508000	0.768250000
6	0.749178000	3.181096000	-0.111529000
6	2.079508000	2.896546000	-0.561604000
1	2.290354000	1.903041000	-0.932718000
6	3.046982000	3.858491000	-0.613253000
1	4.038556000	3.628631000	-0.993833000
6	0.331663000	0.070857000	1.902410000
1	-6.840748000	-3.429073000	-0.312273000

Optimised Cartesian Coordinates of $\mathbf{6}^-$

6	-5.797789000	-2.014256000	-0.103789000
6	-5.072822000	-3.232480000	-0.472258000
6	-3.711356000	-3.308462000	-0.450266000
6	-2.899333000	-2.181468000	-0.073986000
6	-3.579074000	-0.959785000	0.232059000
6	-4.942651000	-0.880959000	0.233784000
1	-5.675274000	-4.078538000	-0.794264000
1	-3.233253000	-4.224877000	-0.784126000
1	-2.974028000	-0.097701000	0.481278000
1	-5.441975000	0.048352000	0.494846000
7	-1.536898000	-2.261718000	0.021867000
6	2.528741000	-2.331244000	0.053852000

6	3.239521000	-3.158191000	0.942119000
6	3.254064000	-1.510307000	-0.820648000
6	4.631834000	-3.183471000	0.942331000
1	2.692732000	-3.764404000	1.658600000
6	4.645702000	-1.529060000	-0.818930000
1	2.709913000	-0.857411000	-1.490698000
6	5.341706000	-2.366637000	0.058729000
1	5.180242000	-3.813642000	1.636105000
1	5.191969000	-0.881701000	-1.503386000
7	1.117825000	-2.335565000	0.014902000
6	-0.924610000	-3.469675000	0.085414000
6	0.462697000	-3.491213000	0.086521000
78	-0.126657000	-0.712248000	-0.013622000
8	-1.286422000	0.947287000	0.036517000
8	1.313521000	0.685496000	-0.089098000
6	-0.569518000	2.092140000	0.030365000
6	-1.181634000	3.367548000	0.083757000
6	0.839023000	1.952057000	-0.037935000
6	-0.317600000	4.470353000	0.073425000
6	1.694999000	3.079012000	-0.041884000
6	1.070104000	4.331948000	0.014247000
1	-0.725976000	5.474589000	0.113152000
1	1.670893000	5.235371000	0.016780000
6	-2.710334000	3.525627000	0.163321000
6	-3.146652000	5.004735000	0.164808000
1	-2.747813000	5.550789000	1.028170000
1	-2.826409000	5.526057000	-0.745338000
1	-4.241426000	5.062186000	0.213668000
6	-3.226135000	2.888249000	1.476267000
1	-4.322817000	2.934507000	1.526366000
1	-2.916828000	1.844577000	1.554663000
1	-2.824427000	3.425798000	2.344548000
6	-3.377779000	2.847417000	-1.057578000
1	-3.101793000	1.793953000	-1.123455000
1	-4.471683000	2.920664000	-0.987840000
1	-3.064485000	3.342397000	-1.985686000
6	3.225058000	2.931857000	-0.115904000
6	3.950318000	4.290253000	-0.035875000
1	3.731644000	4.814310000	0.902033000
1	5.035107000	4.128155000	-0.081793000
1	3.679417000	4.952480000	-0.866808000
6	3.734338000	2.062347000	1.058479000
1	3.509427000	2.547939000	2.016385000
1	3.258074000	1.080685000	1.051540000
1	4.823764000	1.929205000	0.994866000
6	3.609141000	2.276726000	-1.463845000
1	3.097247000	1.320655000	-1.581912000

1	3.322186000	2.924570000	-2.301487000
1	4.694470000	2.108132000	-1.520818000
8	-7.043318000	-1.958441000	-0.102844000
8	6.715105000	-2.419372000	0.097092000
1	1.013831000	-4.428623000	0.122755000
1	-1.499546000	-4.382887000	0.166632000
1	7.058772000	-1.757409000	-0.522502000

Optimised Cartesian Coordinates of $\mathbf{6}^{+}$

6	0.000000000	0.000000000	0.000000000
6	1.405242000	0.000000000	0.000000000
6	2.097459000	1.202190000	0.000000000
6	1.397374000	2.422583000	-0.014471000
6	-0.008797000	2.417028000	-0.041074000
6	-0.700492000	1.218673000	-0.018993000
1	1.952109000	-0.939412000	-0.017012000
1	3.182455000	1.194894000	-0.038745000
1	-0.545251000	3.357109000	-0.049555000
1	-1.784719000	1.198613000	-0.016512000
7	2.093054000	3.651496000	0.035379000
6	3.922925000	7.221029000	-0.154648000
6	4.383289000	7.866662000	1.011870000
6	4.074897000	7.849325000	-1.400477000
6	4.994102000	9.105137000	0.930210000
1	4.216371000	7.415439000	1.985212000
6	4.707078000	9.081272000	-1.485942000
1	3.722586000	7.353730000	-2.295879000
6	5.170829000	9.718441000	-0.323295000
1	5.329674000	9.626193000	1.820261000
1	4.841313000	9.551674000	-2.456715000
7	3.347655000	5.932959000	-0.084708000
6	3.150589000	3.785619000	0.803072000
6	3.834306000	5.033110000	0.739939000
78	1.682785000	5.305804000	-1.090061000
8	0.000540000	4.697970000	-2.053201000
8	1.296791000	6.936970000	-2.239985000
6	-0.491437000	5.567538000	-2.899596000
6	-1.652335000	5.298851000	-3.695229000
6	0.226627000	6.837679000	-2.988731000
6	-2.035831000	6.345810000	-4.507216000
6	-0.224664000	7.900547000	-3.835932000
6	-1.354849000	7.600238000	-4.567746000
1	-2.904610000	6.235150000	-5.144858000
1	-1.769402000	8.344426000	-5.237105000
6	-2.407461000	3.962311000	-3.630706000
6	-3.552620000	3.910339000	-4.661574000

1	-4.311411000	4.679612000	-4.478921000
1	-3.185957000	4.020398000	-5.688556000
1	-4.052965000	2.938774000	-4.594373000
6	-3.028599000	3.795596000	-2.222424000
1	-3.552108000	2.834664000	-2.155966000
1	-2.266620000	3.825677000	-1.440475000
1	-3.756770000	4.589157000	-2.019957000
6	-1.443901000	2.788852000	-3.935993000
1	-0.628762000	2.729377000	-3.212039000
1	-1.996437000	1.842758000	-3.908189000
1	-1.010321000	2.892431000	-4.937452000
6	0.499699000	9.252782000	-3.923292000
6	-0.254153000	10.239746000	-4.836648000
1	-1.267687000	10.443746000	-4.473204000
1	0.284498000	11.192867000	-4.857069000
1	-0.320605000	9.882019000	-5.870347000
6	0.601408000	9.894904000	-2.517795000
1	-0.395566000	10.064104000	-2.094956000
1	1.168792000	9.272809000	-1.822537000
1	1.099922000	10.868436000	-2.592685000
6	1.912113000	9.040168000	-4.520240000
1	2.505420000	8.350739000	-3.915410000
1	1.850899000	8.635713000	-5.536866000
1	2.442696000	9.998411000	-4.572400000
8	-0.737036000	-1.129952000	0.003794000
8	5.780299000	10.921647000	-0.333502000
1	4.724870000	5.233686000	1.327048000
1	3.468195000	2.986053000	1.464892000
1	-0.163235000	-1.913594000	0.021260000
1	5.846729000	11.263441000	-1.240346000

Optimised Cartesian Coordinates of $7^{•+}$

6	0.000000000	0.000000000	0.000000000
6	1.407125000	0.000000000	0.000000000
6	2.095901000	1.206652000	0.000000000
6	1.400271000	2.427706000	-0.015273000
6	-0.007224000	2.423862000	-0.043428000
6	-0.695600000	1.226447000	-0.020868000
1	1.964747000	-0.928450000	-0.017439000
1	3.181098000	1.199596000	-0.038774000
1	-0.542961000	3.364409000	-0.052813000
1	-1.779924000	1.204764000	-0.019002000
7	2.097828000	3.654600000	0.033044000
6	3.934495000	7.220760000	-0.162464000
6	4.420771000	7.859878000	0.999340000
6	4.067407000	7.856255000	-1.405122000

6	5.033562000	9.093725000	0.908063000
1	4.270145000	7.406880000	1.974530000
6	4.702866000	9.087854000	-1.503828000
1	3.696991000	7.365294000	-2.295811000
6	5.192674000	9.719681000	-0.346670000
1	5.388170000	9.611660000	1.792688000
1	4.812895000	9.547137000	-2.478507000
7	3.357192000	5.935223000	-0.090209000
6	3.156530000	3.788628000	0.799885000
6	3.842535000	5.033704000	0.734539000
78	1.689529000	5.308042000	-1.093826000
8	0.006591000	4.697531000	-2.056856000
8	1.298065000	6.939302000	-2.243979000
6	-0.485830000	5.565264000	-2.904478000
6	-1.643985000	5.293202000	-3.703280000
6	0.228743000	6.837103000	-2.993033000
6	-2.030467000	6.339547000	-4.514714000
6	-0.224778000	7.898791000	-3.841014000
6	-1.353578000	7.595981000	-4.573898000
1	-2.897761000	6.226028000	-5.153814000
1	-1.769170000	8.338551000	-5.244457000
6	-2.392725000	3.952526000	-3.644497000
6	-3.534229000	3.897848000	-4.679022000
1	-4.297265000	4.662912000	-4.496369000
1	-3.164803000	4.012946000	-5.704474000
1	-4.030077000	2.923634000	-4.616301000
6	-3.016889000	3.776852000	-2.238786000
1	-3.535548000	2.812844000	-2.178241000
1	-2.256934000	3.806531000	-1.455011000
1	-3.749689000	4.565753000	-2.034782000
6	-1.421958000	2.785177000	-3.950149000
1	-0.610211000	2.727373000	-3.222369000
1	-1.970020000	1.836253000	-3.928130000
1	-0.984497000	2.894460000	-4.949349000
6	0.499649000	9.251038000	-3.931405000
6	-0.258436000	10.238371000	-4.840682000
1	-1.269675000	10.443156000	-4.471343000
1	0.281032000	11.190959000	-4.865168000
1	-0.331042000	9.879308000	-5.873409000
6	0.609763000	9.892469000	-2.526118000
1	-0.384534000	10.057705000	-2.095333000
1	1.184788000	9.271351000	-1.836540000
1	1.104115000	10.867950000	-2.603735000
6	1.908511000	9.035818000	-4.535606000
1	2.501506000	8.341736000	-3.935776000
1	1.840748000	8.635213000	-5.553370000
1	2.443217000	9.991874000	-4.586955000

8	-0.767286000	-1.104089000	0.004982000
8	5.809028000	10.913854000	-0.324990000
1	0.468852000	-2.553647000	-0.855700000
6	-0.146237000	-2.390656000	0.036831000
1	0.464888000	-2.510807000	0.938717000
1	-0.964894000	-3.109945000	0.051779000
1	6.618496000	11.055997000	-2.246458000
6	5.996685000	11.628015000	-1.548309000
1	6.509039000	12.549658000	-1.272976000
1	5.034266000	11.867303000	-2.015095000
1	4.734397000	5.232193000	1.320258000
1	3.472208000	2.989377000	1.462946000