Supplementary Material for Dalton Transactions
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Experimental and Computational Evidences of the Intermolecular Motifs in the Crystal Packing of Luminescent Pentacoordinated Gallium(III) Complexes

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Complex **1** optimised geometry at the B3LYP/6-31G(d) level of approximation.
The Cartesian coordinates are reported in Ångstrom.

Al	-0.294268	-0.090843	-0.090060
O	-1.310713	-1.179256	-1.282109
N	-2.172004	0.374783	0.674611
N	1.458945	-1.069753	-0.696072
8	0.271290	-0.694733	1.628789
C	-2.623827	-1.106578	-1.109825
C	-3.552702	-1.791516	-1.881947
C	-4.936711	-1.659892	-1.625280
C	-5.425672	-0.859454	-0.611669
C	-4.511744	-0.142570	0.201938
C	-3.121772	-0.273750	-0.054441
C	-4.861134	0.714801	1.273822
C	-3.881835	1.361790	1.996128
C	-2.513172	1.179473	1.678160
C	-1.420639	1.867502	2.447405
H	-4.144964	2.020330	2.817403
H	-5.910506	0.858146	1.520919
H	-6.492555	-0.770226	-0.429344
H	-5.633102	-2.211524	-2.251683
H	-3.199042	-2.429838	-2.685451
C	1.990053	-1.207868	-1.908828
C	3.217209	-1.899882	-2.063903
C	3.864756	-2.432879	-0.970907
C	3.311300	-2.293747	0.325510
C	2.085354	-1.583129	0.399135
C	1.416235	-1.365548	1.646826
C	2.005913	-1.874649	2.795836
C	3.227801	-2.582278	2.720558
C	3.881042	-2.796850	1.523033
C	1.256598	-0.621869	-3.082152
H	3.637212	-2.002764	-3.059014
H	4.805697	-2.963959	-1.094567
H	4.819585	-3.341876	1.483784
H	3.660278	-2.966838	3.640655
H	1.511978	-1.723395	3.750443
O	0.059927	1.603513	-0.738789
C	1.124997	2.407452	-0.567468
C	1.283682	3.487691	-1.455979
C	2.357326	4.363896	-1.322898
C	3.300030	4.187182	-0.305723
C	3.144680	3.119903	0.579798

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C	2.073838	2.233517	0.457170
H	0.541500	3.617824	-2.238617
H	2.457976	5.192682	-2.020165
H	4.137372	4.871775	-0.203810
H	3.866221	2.971718	1.380196
H	1.959573	1.423018	1.171368
H	0.253804	-1.054596	-3.152166
H	1.131539	0.458722	-2.955031
H	1.797965	-0.806661	-4.013468
H	-0.821887	2.501931	1.784482
H	-1.835621	2.489627	3.244577
H	-0.742982	1.126156	2.882651

Complex **1** TD-DFT electronic transitions at the B3LYP/6-31G(d) level of approximation. Each line lists the transition energy (eV), the relative transition wavelength (nm) and the oscillator strength of all the computed transitions.

2.8598 , 433.54 , 0.0007
2.9763 , 416.58 , 0.0005
3.1037 , 399.47 , 0.0819
3.1837 , 389.43 , 0.0052
3.2834 , 377.60 , 0.0044
3.3544 , 369.62 , 0.0040
3.9129 , 316.86 , 0.0001
4.0615 , 305.27 , 0.0004
4.1148 , 301.31 , 0.0003
4.1823 , 296.45 , 0.0025
4.1944 , 295.59 , 0.0012
4.2106 , 294.46 , 0.0011
4.5015 , 275.43 , 0.0015
4.5683 , 271.40 , 0.0024
4.7065 , 263.43 , 0.0018
4.7441 , 261.34 , 0.0019
4.8525 , 255.50 , 0.0040
4.9221 , 251.89 , 0.0022
5.0143 , 247.26 , 0.1096
5.0259 , 246.69 , 0.0949
5.1104 , 242.61 , 0.6850
5.1531 , 240.60 , 0.0093
5.1611 , 240.23 , 0.0203
5.2493 , 236.19 , 0.0011
5.2885 , 234.44 , 0.0004
5.4125 , 229.07 , 0.0036
5.4240 , 228.58 , 0.0203
5.4865 , 225.98 , 0.0067
5.5217 , 224.54 , 0.0009
5.5313 , 224.15 , 0.0191

Complex **2** optimised geometry at the B3LYP/6-31G(d) level of approximation.
The Cartesian coordinates are reported in Ångstrom.

Al	0.613304	0.218968	-0.086089
O	1.929443	0.964968	-1.239634
N	2.234219	-0.834770	0.673733
N	-0.757858	1.683905	-0.682469
O	0.195372	0.888580	1.645839
C	3.152896	0.478986	-1.063647
C	4.258485	0.860824	-1.810712
C	5.528670	0.295789	-1.553137
C	5.728405	-0.645249	-0.562568
C	4.625479	-1.062196	0.225210
C	3.349532	-0.496048	-0.032530

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C	4.676575	-2.014311	1.272246
C	3.535481	-2.340871	1.972556
C	2.296361	-1.731813	1.655856
C	1.037361	-2.065955	2.405304
H	3.569654	-3.069666	2.775590
H	5.625323	-2.485328	1.518374
H	6.711161	-1.068871	-0.378200
H	6.370877	0.619162	-2.159307
H	4.132576	1.600347	-2.595139
C	-1.183830	2.023068	-1.898044
C	-2.154798	3.045145	-2.042632
C	-2.661864	3.693084	-0.937507
C	-2.217428	3.344538	0.361287
C	-1.248288	2.310005	0.424621
C	-0.712749	1.859034	1.673333
C	-1.172268	2.464644	2.834088
C	-2.140193	3.493781	2.769427
C	-2.662472	3.936995	1.570649
C	-0.607039	1.307240	-3.086810
H	-2.492306	3.308197	-3.039593
H	-3.407305	4.476181	-1.053724
H	-3.405693	4.728130	1.539324
H	-2.477921	3.945411	3.698457
H	-0.774539	2.138665	3.789916
O	-0.250669	-1.264360	-0.806325
C	-1.475447	-1.755144	-0.621621
C	-1.933870	-2.746366	-1.516753
C	-3.195450	-3.301571	-1.379652
C	-4.048276	-2.886042	-0.338480
C	-3.594403	-1.905018	0.560170
C	-2.330833	-1.346189	0.424196
H	-1.267065	-3.061701	-2.313419
H	-3.534703	-4.062274	-2.076378
C	-5.352546	-3.453731	-0.195420
H	-4.244072	-1.584638	1.369233
H	-1.994129	-0.604930	1.141847
H	0.475075	1.464282	-3.130245
H	-0.768644	0.227328	-3.003389
H	-1.063158	1.661095	-4.014695
H	0.277302	-2.468166	1.726438
H	1.231805	-2.807025	3.184616
H	0.618822	-1.163018	2.860701
N	-6.415446	-3.916346	-0.080869

Complex **2** TD-DFT electronic transitions at the B3LYP/6-31G(d) level of approximation. Each line lists the transition energy (eV), the relative transition wavelength (nm) and the oscillator strength of all the computed transitions.

3.1013 , 399.77 , 0.0805
3.1647 , 391.77 , 0.0049
3.1925 , 388.36 , 0.0031
3.2820 , 377.76 , 0.0019
3.2900 , 376.85 , 0.0039
3.3667 , 368.26 , 0.0041
4.1853 , 296.23 , 0.0016
4.1976 , 295.37 , 0.0007
4.3851 , 282.74 , 0.0003
4.4379 , 279.37 , 0.0006
4.5166 , 274.50 , 0.0020
4.5264 , 273.91 , 0.0029

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4.5277 , 273.83 , 0.0007
4.5932 , 269.93 , 0.0029
4.6922 , 264.24 , 0.0019
4.7278 , 262.24 , 0.0019
4.8056 , 258.00 , 0.0018
4.8856 , 253.77 , 0.0067
4.9320 , 251.39 , 0.0037
5.0143 , 247.26 , 0.4038
5.0257 , 246.70 , 0.0509
5.0897 , 243.60 , 0.1348
5.1217 , 242.08 , 0.7274
5.1311 , 241.63 , 0.1173
5.1560 , 240.47 , 0.0037
5.1969 , 238.57 , 0.0020
5.3007 , 233.90 , 0.0027
5.3450 , 231.96 , 0.0003
5.4602 , 227.07 , 0.0217
5.5399 , 223.80 , 0.0073

Complex **3** optimised geometry at the B3LYP/6-31G(d) level of approximation.
The Cartesian coordinates are reported in Ångstrom.

Al	0.853716	0.225104	-0.089652
O	2.262711	0.745566	-1.255600
N	2.297597	-1.049663	0.685505
N	-0.277693	1.872494	-0.708474
O	0.535329	0.967662	1.633193
C	3.401419	0.087188	-1.069016
C	4.551630	0.291584	-1.818013
C	5.724463	-0.450690	-1.548735
C	5.782210	-1.396623	-0.544537
C	4.629294	-1.634935	0.246050
C	3.450981	-0.890673	-0.023466
C	4.538959	-2.567842	1.307580
C	3.362156	-2.711051	2.010279
C	2.226715	-1.930313	1.682061
C	0.933014	-2.062357	2.435419
H	3.288633	-3.424164	2.824604
H	5.407570	-3.170071	1.563248
H	6.691511	-1.957930	-0.351319
H	6.605683	-0.263732	-2.156804
H	4.536608	1.030408	-2.612957
C	-0.646145	2.256972	-1.929580
C	-1.444577	3.416526	-2.090234
C	-1.841519	4.152924	-0.995462
C	-1.456227	3.757854	0.308849
C	-0.663520	2.583602	0.388876
C	-0.206948	2.071157	1.644896
C	-0.564906	2.757948	2.795944
C	-1.356049	3.927475	2.714710
C	-1.801024	4.431003	1.508636
C	-0.191555	1.442145	-3.107681
H	-1.737789	3.714431	-3.091369
H	-2.454176	5.042013	-1.124179
H	-2.409730	5.329156	1.464355
H	-1.617858	4.439953	3.636582
H	-0.225031	2.385867	3.757227
O	-0.227897	-1.121041	-0.793344
C	-1.504791	-1.429222	-0.592733

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C	-2.104163	-2.370265	-1.462256
C	-3.429784	-2.737751	-1.309322
C	-4.183311	-2.168196	-0.277063
C	-3.615345	-1.242485	0.600914
C	-2.287362	-0.873774	0.445961
H	-1.492575	-2.796429	-2.251337
H	-3.896788	-3.456867	-1.971430
H	-4.225361	-0.825822	1.393420
H	-1.843485	-0.168347	1.140727
H	0.901759	1.414995	-3.145774
H	-0.533014	0.405625	-3.015512
H	-0.577714	1.857559	-4.041756
H	0.121520	-2.363901	1.763865
H	1.018272	-2.807794	3.229945
H	0.650247	-1.099066	2.871186
N	-5.577556	-2.547801	-0.112744
O	-6.051833	-3.370927	-0.902365
O	-6.217260	-2.027576	0.807370

Complex **3** TD-DFT electronic transitions at the B3LYP/6-31G(d) level of approximation. Each line lists the transition energy (eV), the relative transition wavelength (nm) and the oscillator strength of all the computed transitions.

3.0980 , 400.21 , 0.0809
3.1822 , 389.62 , 0.0091
3.2890 , 376.96 , 0.0038
3.3555 , 369.49 , 0.0029
3.3733 , 367.54 , 0.0007
3.4848 , 355.78 , 0.0045
3.7081 , 334.36 , 0.0003
3.8133 , 325.13 , 0.0000
3.8494 , 322.09 , 0.0014
4.0825 , 303.70 , 0.4122
4.1854 , 296.23 , 0.0006
4.1976 , 295.37 , 0.0010
4.3806 , 283.03 , 0.0001
4.4245 , 280.22 , 0.0005
4.5266 , 273.90 , 0.0021
4.5412 , 273.02 , 0.0007
4.5677 , 271.44 , 0.0028
4.5875 , 270.26 , 0.0026
4.6464 , 266.84 , 0.0004
4.6944 , 264.11 , 0.0019
4.7160 , 262.90 , 0.0017
4.7314 , 262.04 , 0.0014
4.7428 , 261.42 , 0.0001
4.8542 , 255.41 , 0.0001
5.0134 , 247.31 , 0.1493
5.0823 , 243.95 , 0.0878
5.0947 , 243.36 , 0.0654
5.1063 , 242.81 , 0.4549
5.1299 , 241.69 , 0.0273
5.1551 , 240.50 , 0.0023
5.1677 , 239.92 , 0.0791
5.2140 , 237.79 , 0.0016
5.2773 , 234.94 , 0.0002
5.2784 , 234.89 , 0.0045
5.3091 , 233.53 , 0.0002