Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Understanding M−ligand bonding and *mer*-/*fac*- isomerism in tris(8-hydroxyquinolinate) metallic complexes

(Supplementary Information)

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Section S1. Synthesis and characterization

S1.1. Synthesis

Table S1. Detailed results for the synthesis of the Al(III) metallic complexes.

Compound	*m*(8-Hq) / g	*m*(Al^{3+}) [a] / g	*m*(KOH) / g	*m*(Mq_3) / g	Yield %
Alq_3	1.42	0.65	1.22	0.65	52
$Al(qCH_3)_3$	0.72	0.38	0.09	0.54	68
$Al(qNO_2)_3$	0.90	0.38	0.09	0.66	70
$Al(qCl)_3$	0.69	0.14	0.24	0.52	71
$Al(qBr)_3$	0.91	0.14	0.29	0.59	75

[a] Corresponds to $AlCl_3 \cdot 6H_2O$.

Table S2. Detailed results for the synthesis of the In(III) metallic complexes.

Compound	*m*(8-Hq) / g	*m*(Al^{3+}) [a] / g	*m*(KOH) / g	*m*(Mq_3) / g	Yield %
Inq_3	0.97	0.41	1.06	1.01	84
$In(qCH_3)_3$	0.72	0.23	0.29	0.56	68
$In(qNO_2)_3$	0.97	0.21	0.29	0.70	72
$In(qCl)_3$	0.78	0.22	0.31	0.67	76
$In(qBr)_3$	1.01	0.21	0.27	0.74	69

[a] Corresponds to $InCl_3$.

S1.2. FTIR

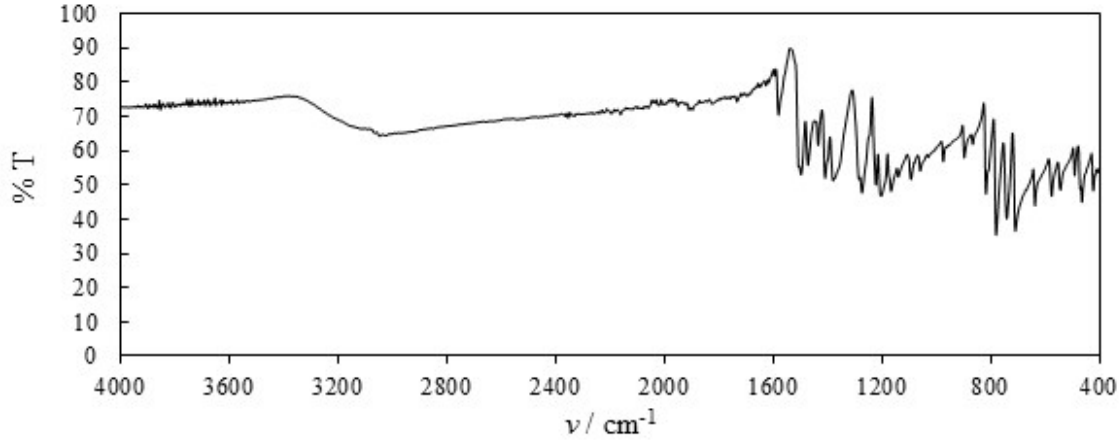


Figure S1. FTIR spectrum of 8-hydroxyquinoline (8-Hq).

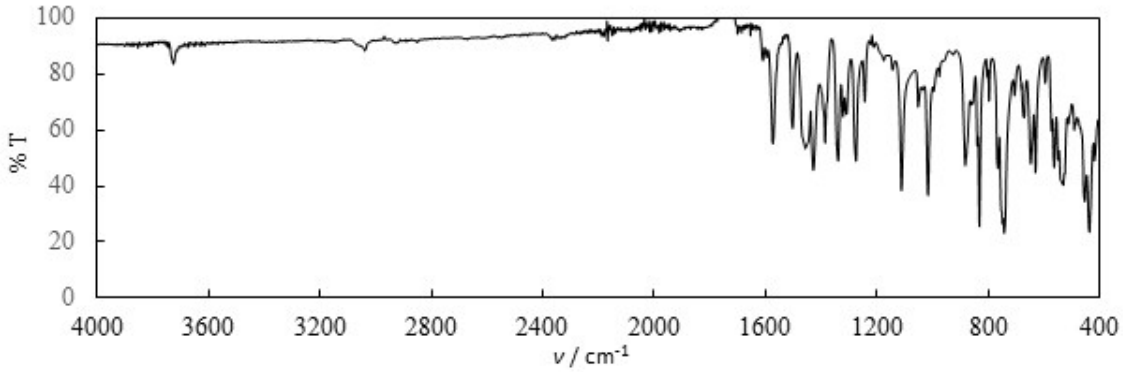


Figure S2. FTIR spectrum of $Al(qCH_3)_3$.

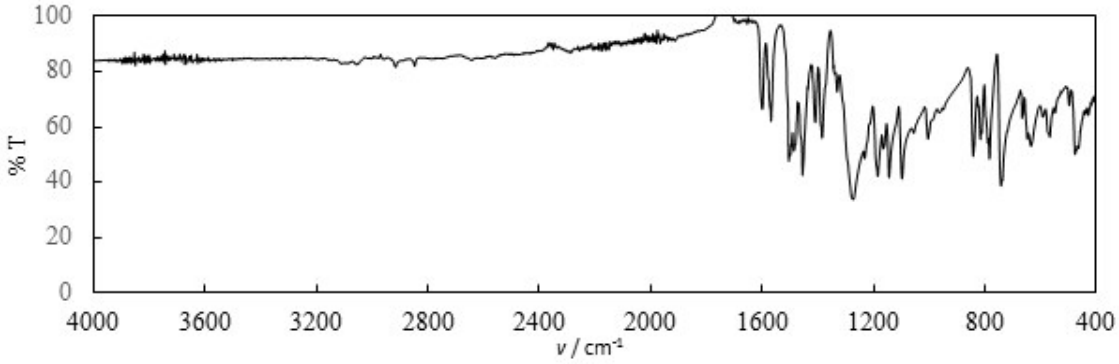


Figure S3. FTIR spectrum of $Al(qNO_2)_3$.

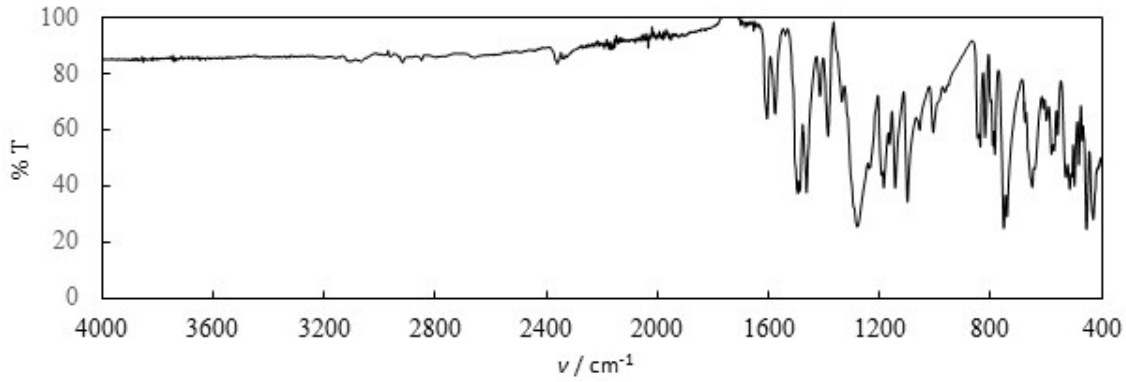


Figure S4. FTIR spectrum of $Al(qCl)_3$.

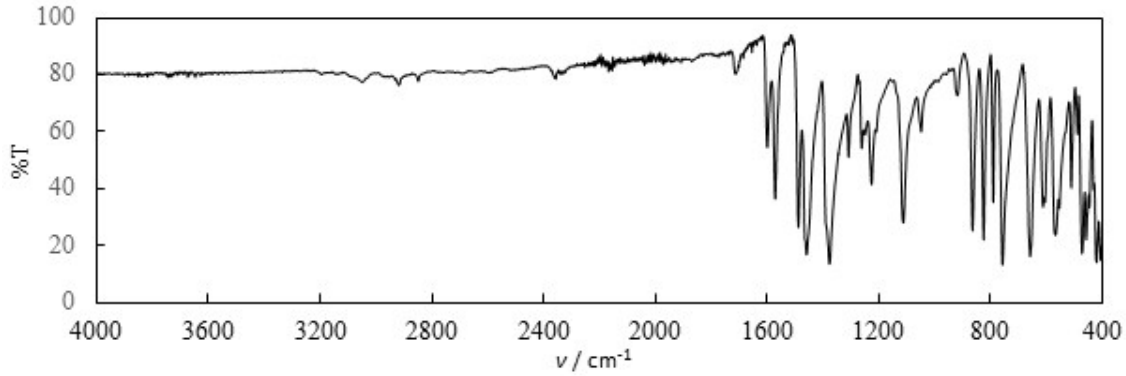


Figure S5. FTIR spectrum of $Al(qBr)_3$.

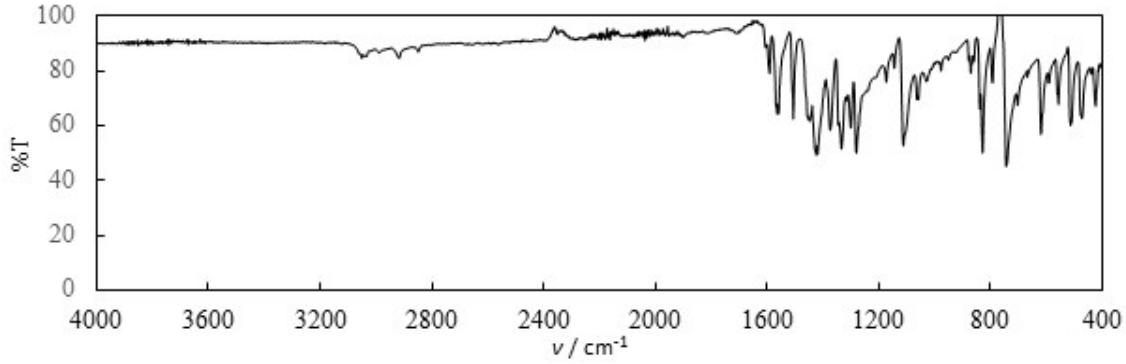


Figure S6. FTIR spectrum of $In(qCH_3)_3$.

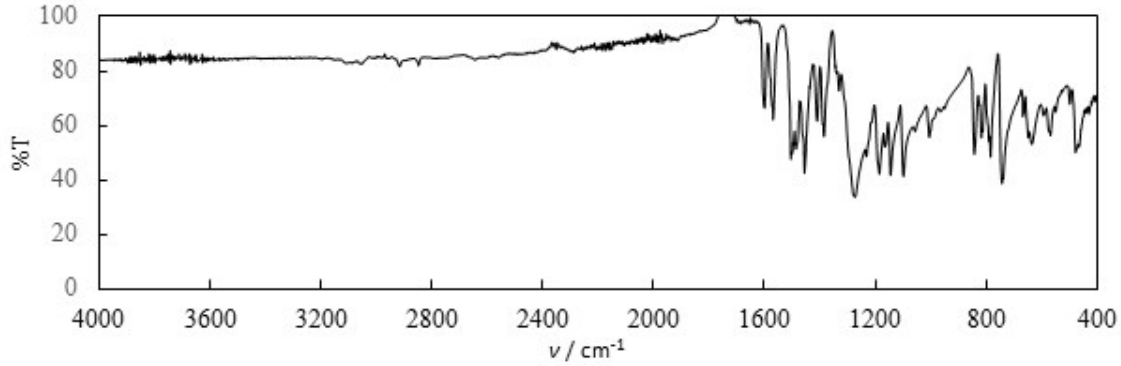


Figure S7. FTIR spectrum of $In(qNO_2)_3$.

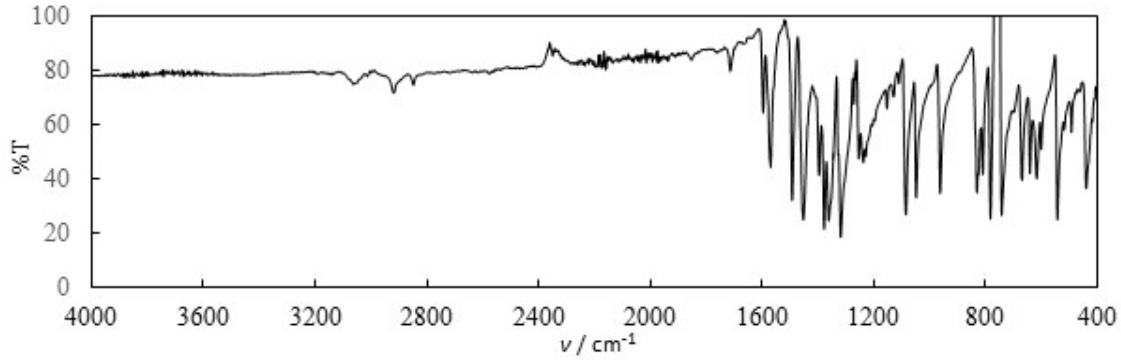


Figure S8. FTIR spectrum of $In(qCl)_3$.

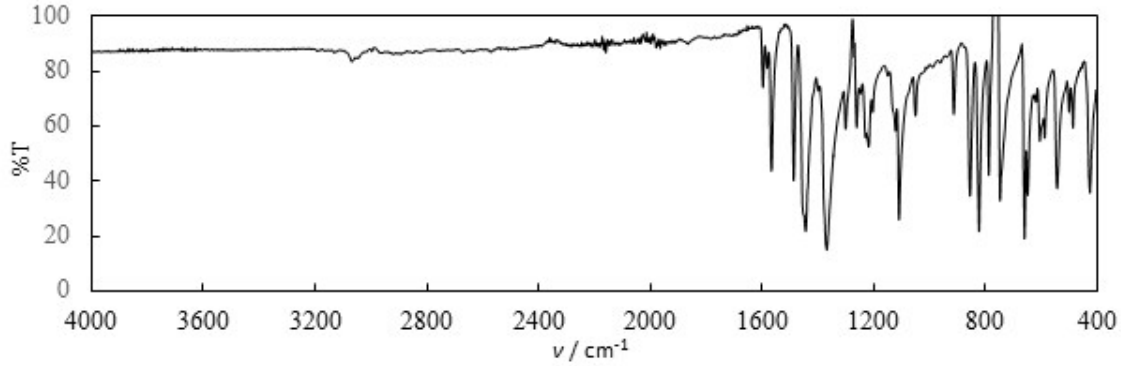


Figure S9. FTIR spectrum of $In(qBr)_3$.

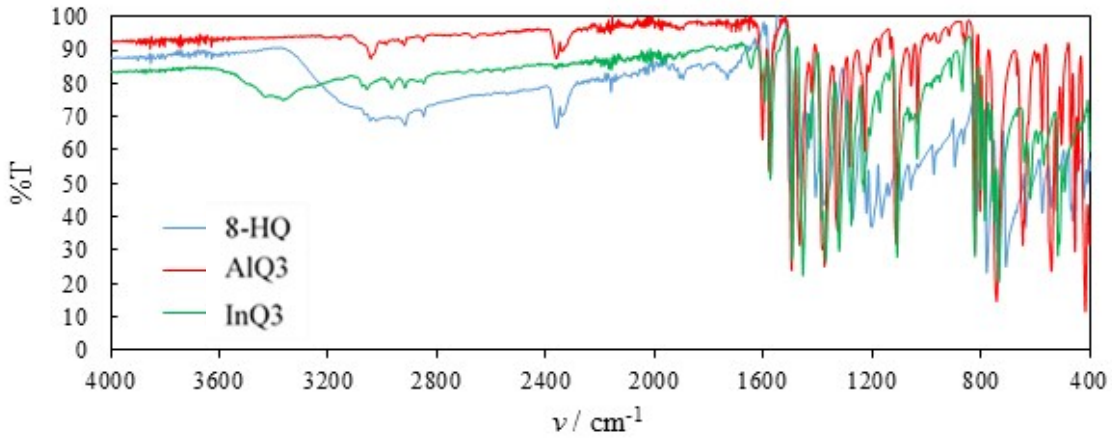


Figure S10. Comparison between the FTIR spectra of 8-Hq(blue), Alq_3 (red), and Inq_3 (blue) in the selected region.

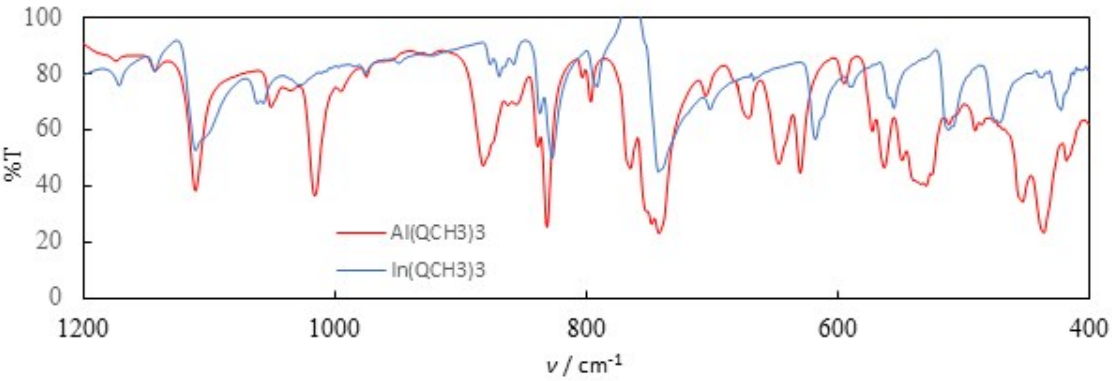


Figure S11. Comparison between the FTIR spectra of $Al(qCH_3)_3$ (red) and $In(qCH_3)_3$ (blue) in the selected region.

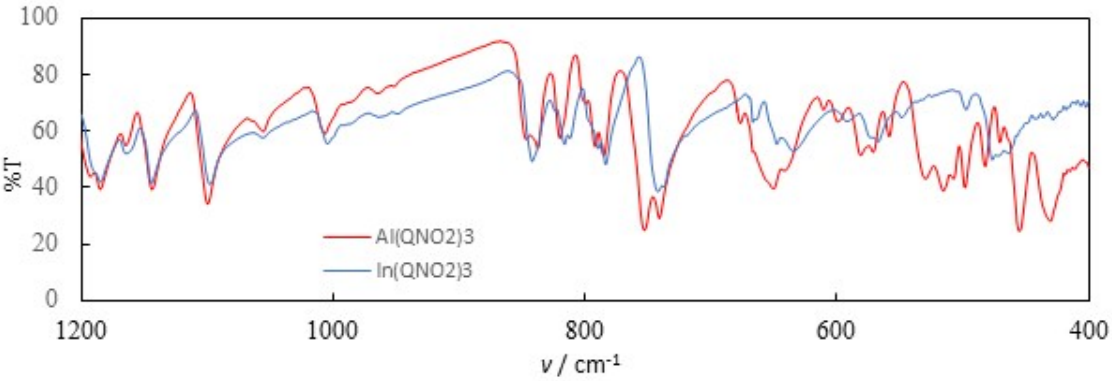


Figure S12. Comparison between the FTIR spectra of $Al(qNO_2)_3$ (red) and $In(qNO_2)_3$ (blue) in the selected region.

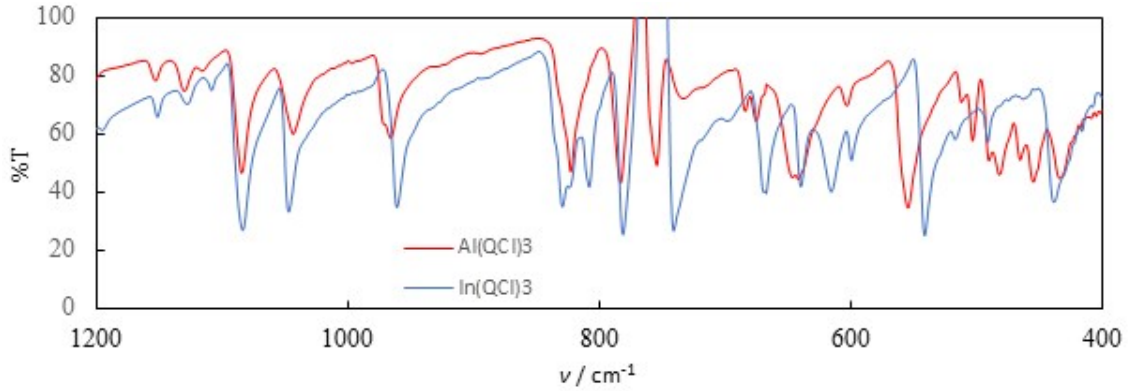


Figure S13. Comparison between the FTIR spectra of $Al(qCl)_3$ (red) and $In(qCl)_3$ (blue) in the selected region.

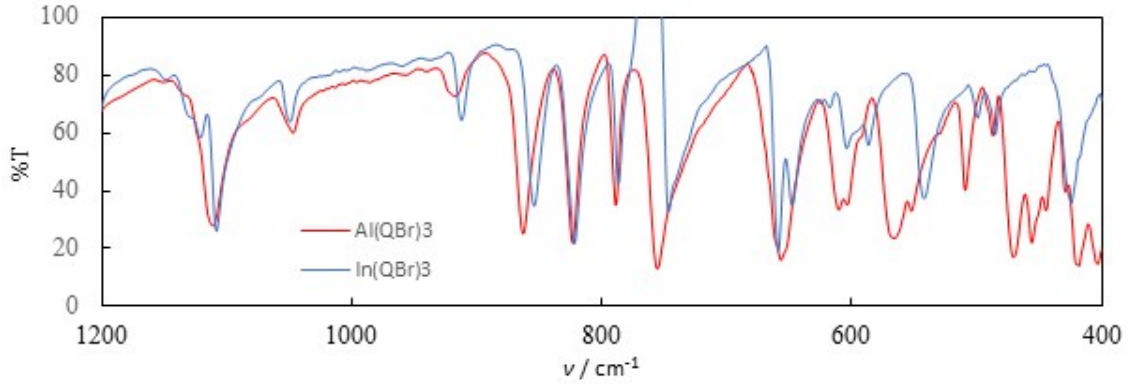


Figure S14. Comparison between the FTIR spectra of $Al(qBr)_3$ (red) and $In(qBr)_3$ (blue) in the selected region.

S1.3. UV-Vis

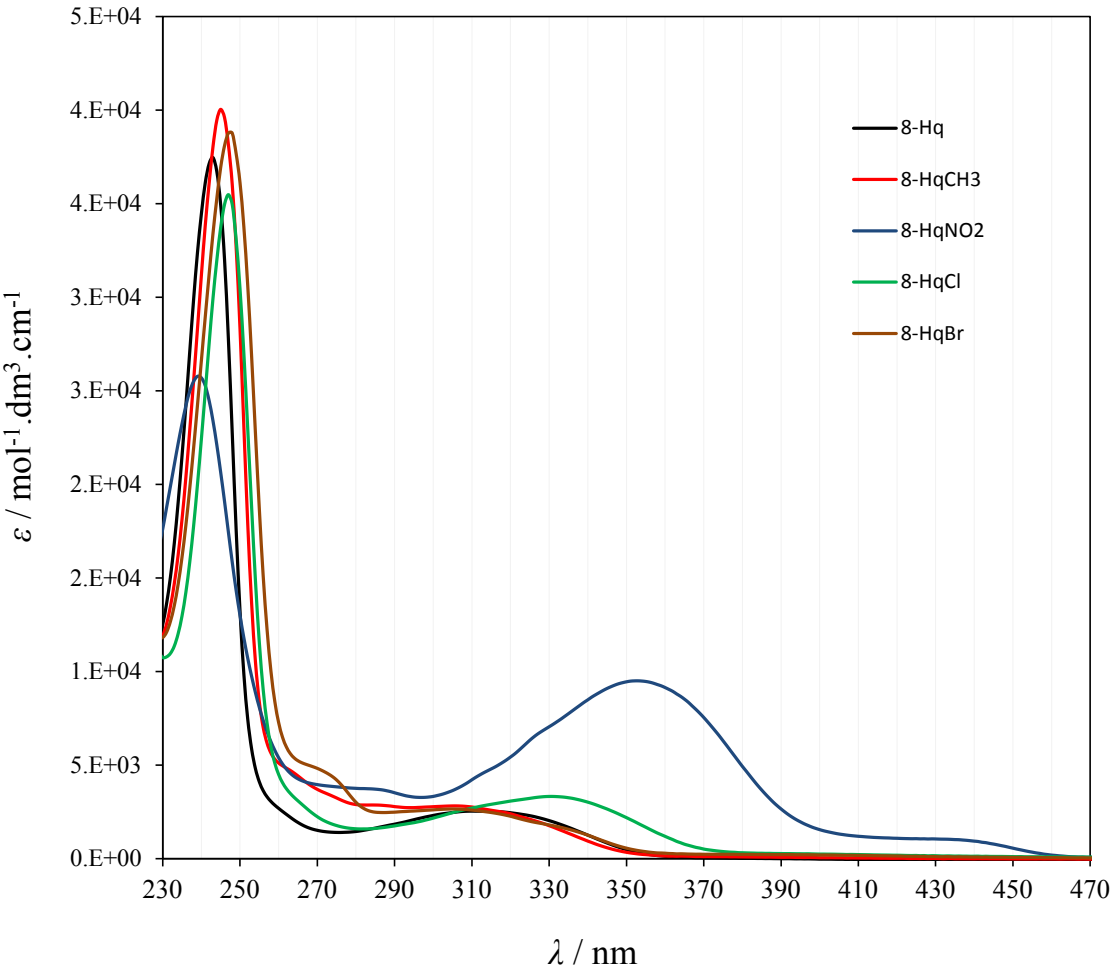


Figure S15. UV-Vis spectra of the 8-hydroxyquinolines studied in CH_2Cl_2.

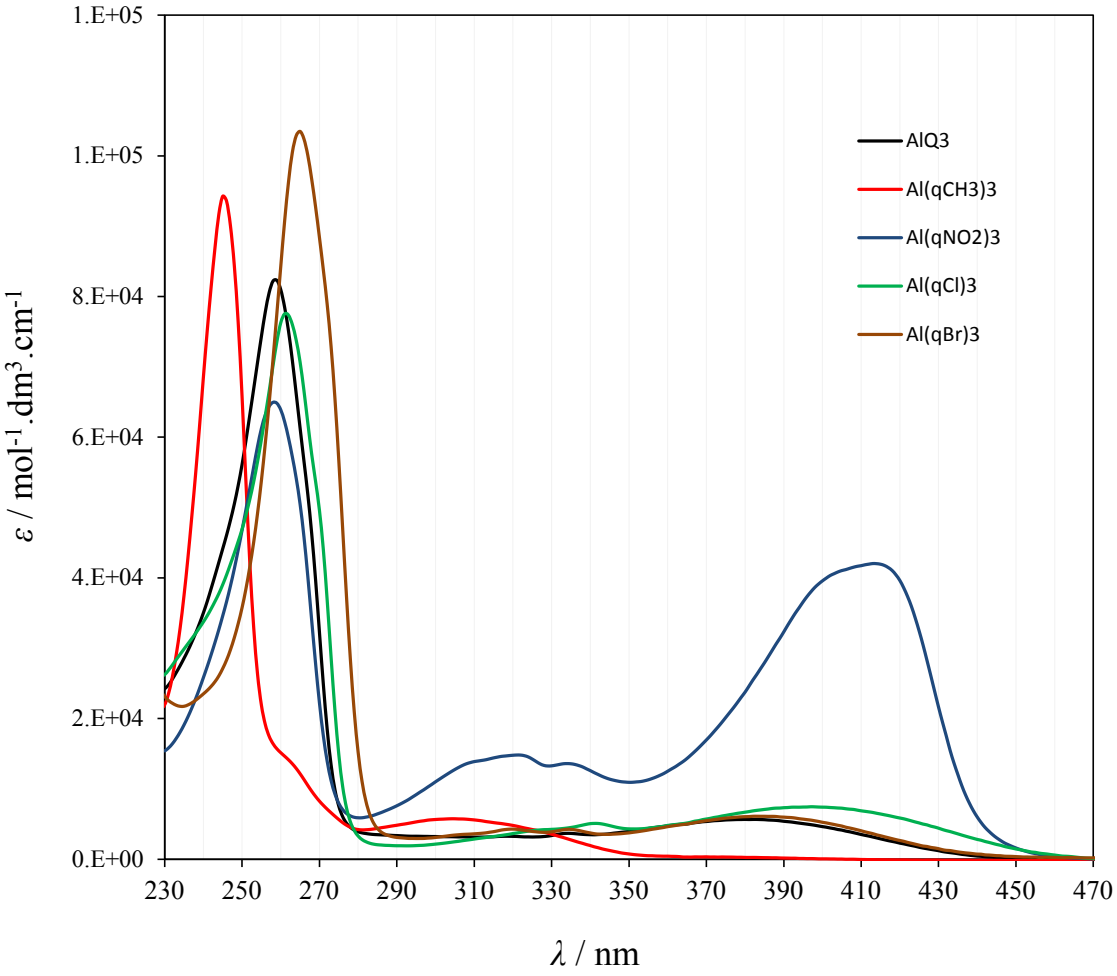


Figure S16. UV-Vis spectra of the Al(III) complexes studied in CH_2Cl_2.

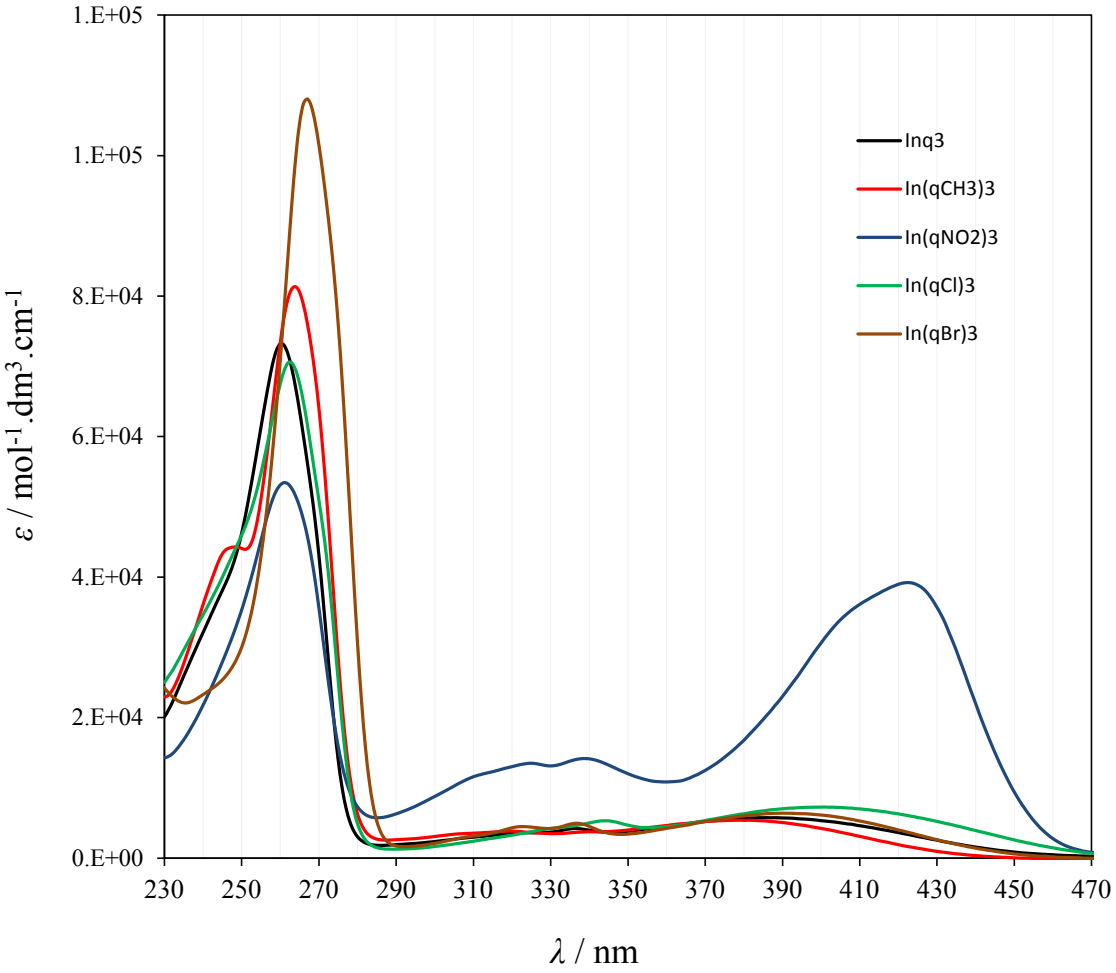


Figure S17. UV-Vis spectra of the In(III) complexes studied in CH_2Cl_2.

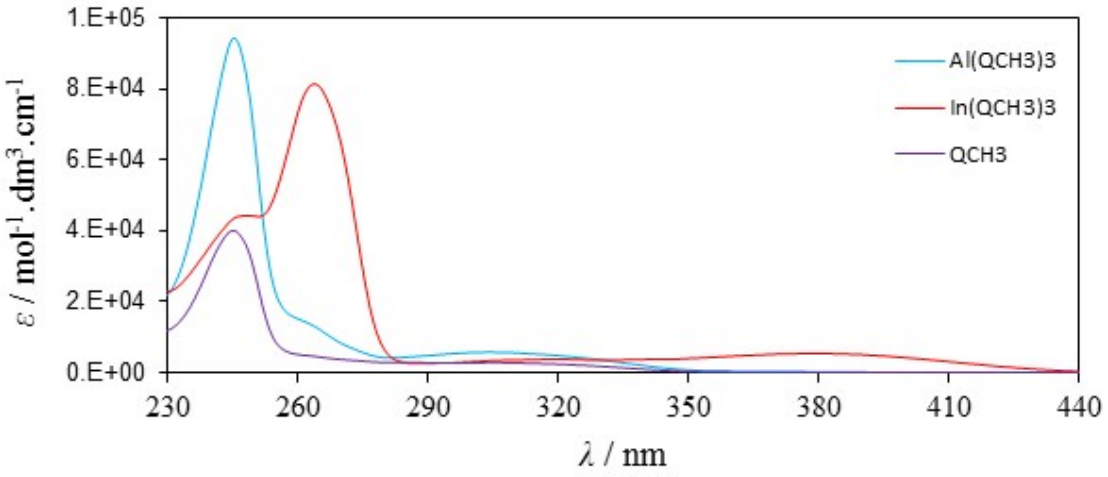


Figure S18. Comparison between the UV-Vis spectra of $Al(qCH_3)_3$ (blue), $In(qCH_3)_3$ (red), and QCH_3 (purple) in CH_2Cl_2.

Table S3. Sample concentrations used in the complexation study of $In(qCH_3)_3$ by UV-Vis spectroscopy.

Entry	$[In(qCH_3)_3] \cdot 10^5$ / mol·dm^{-3}
1	0.229
2	0.460
3	0.611
4	0.881
5	1.03
6	1.20
7	1.35
8	1.53

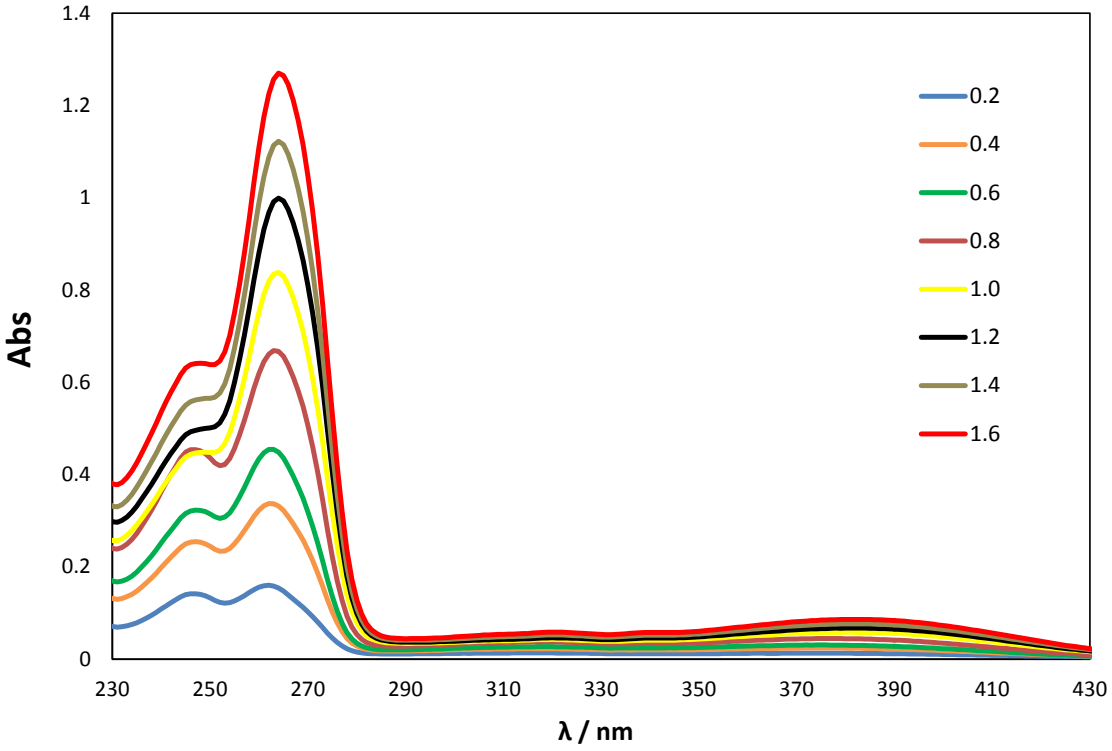


Figure S19. Complexation study of $In(qCH_3)_3$ in CH_2Cl_2.

S1.4. NMR spectroscopy

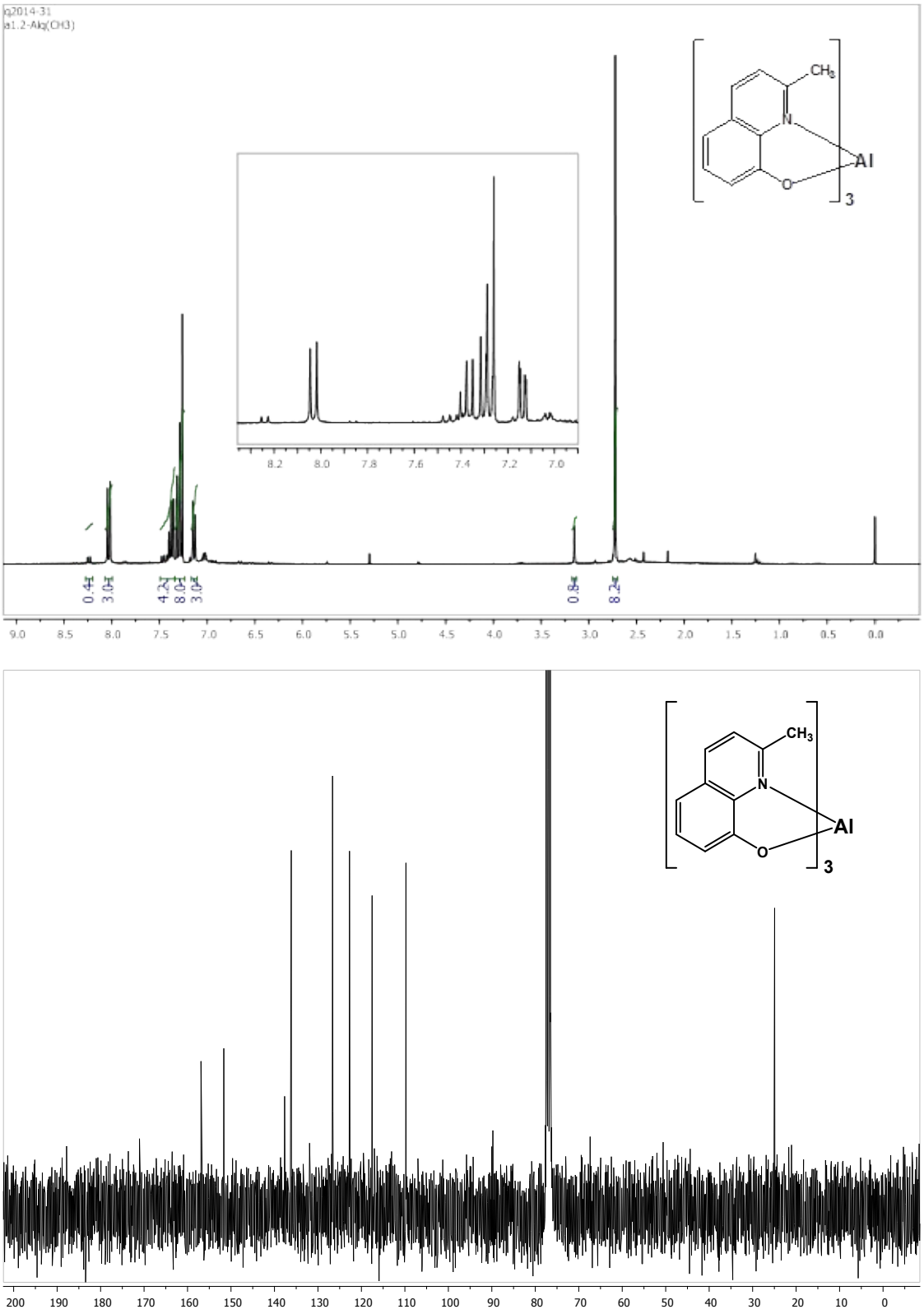


Figure S20. ^{1}H and ^{13}C NMR spectra of $Al(qCH_3)_3$ in $CDCl_3$.

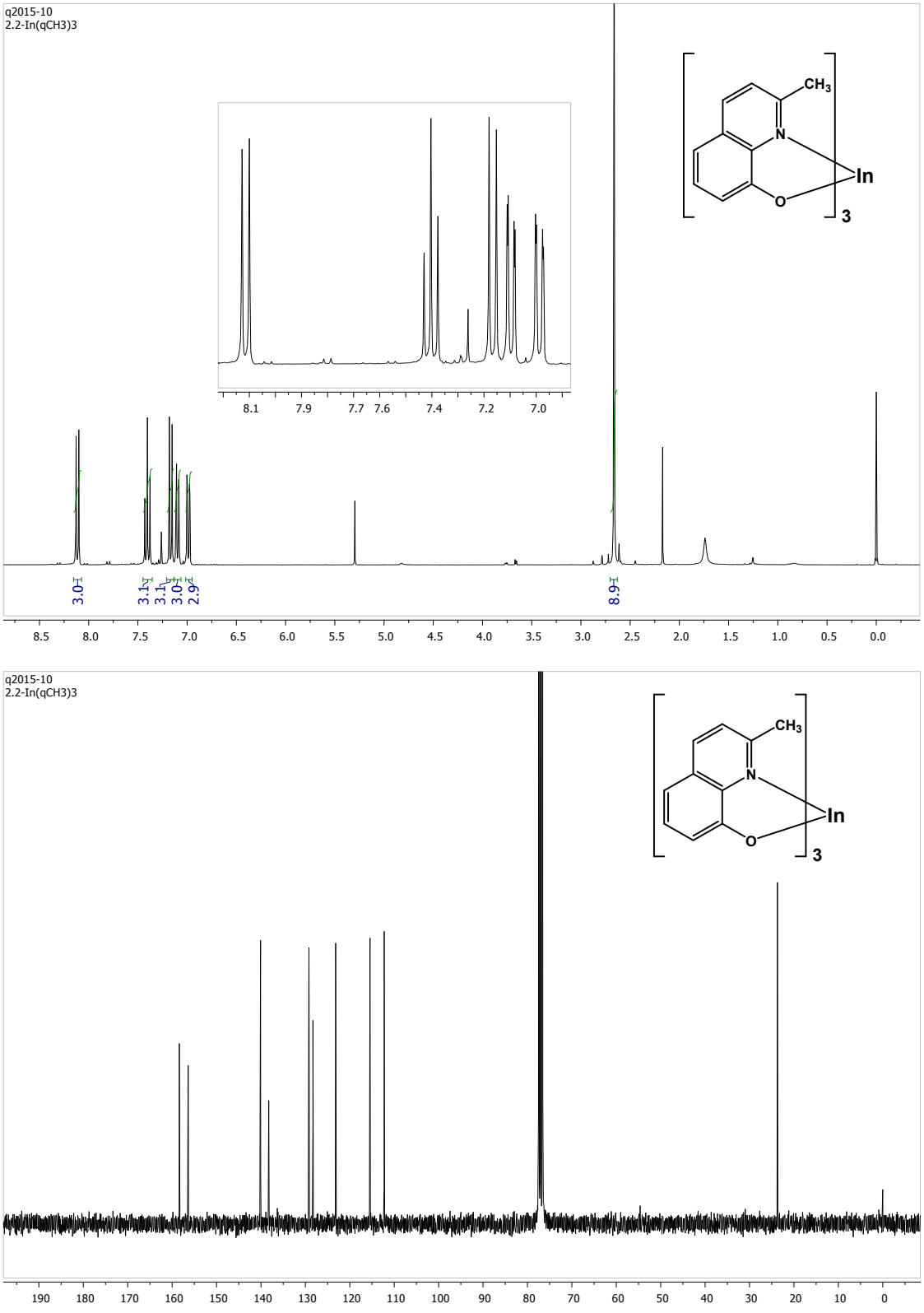


Figure S21. ^{1}H and ^{13}C NMR spectra of $In(qCH_3)_3$ in $CDCl_3$.

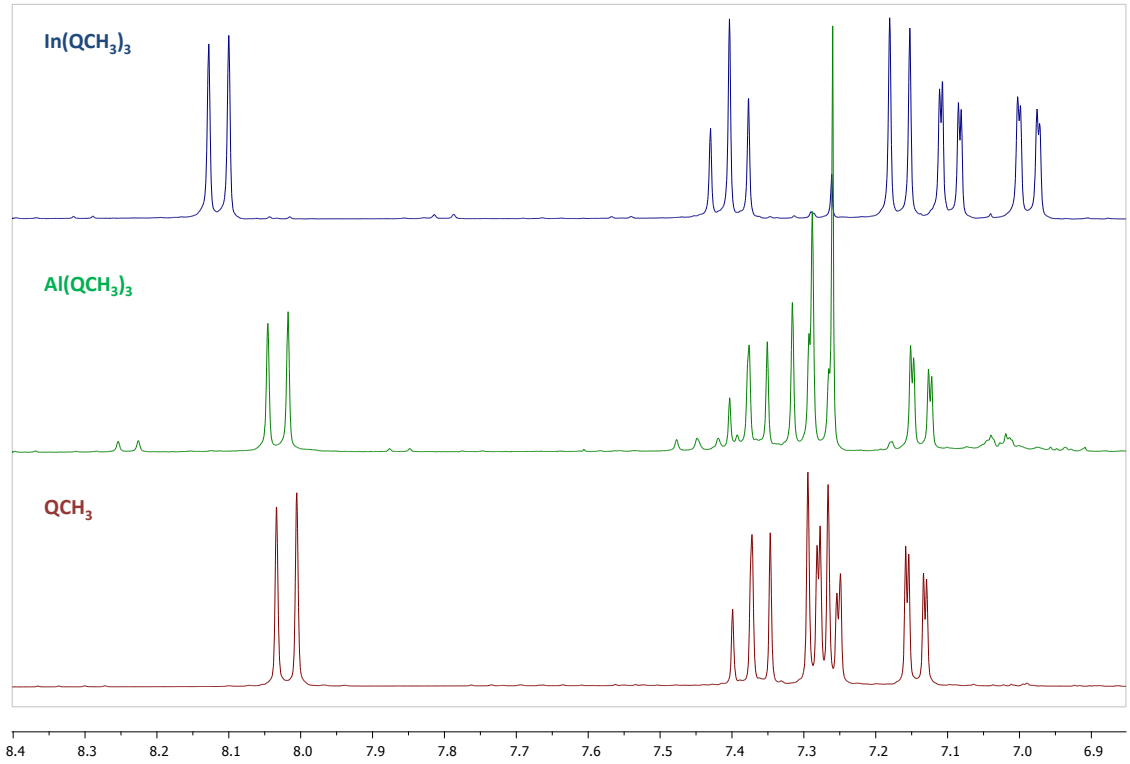


Figure S22. Comparison between the ^{1}H NMR spectra of qCH_3 (8-hydroxyquinaldine), $Al(qCH_3)_3$ and $In(qCH_3)_3$ in $CDCl_3$.

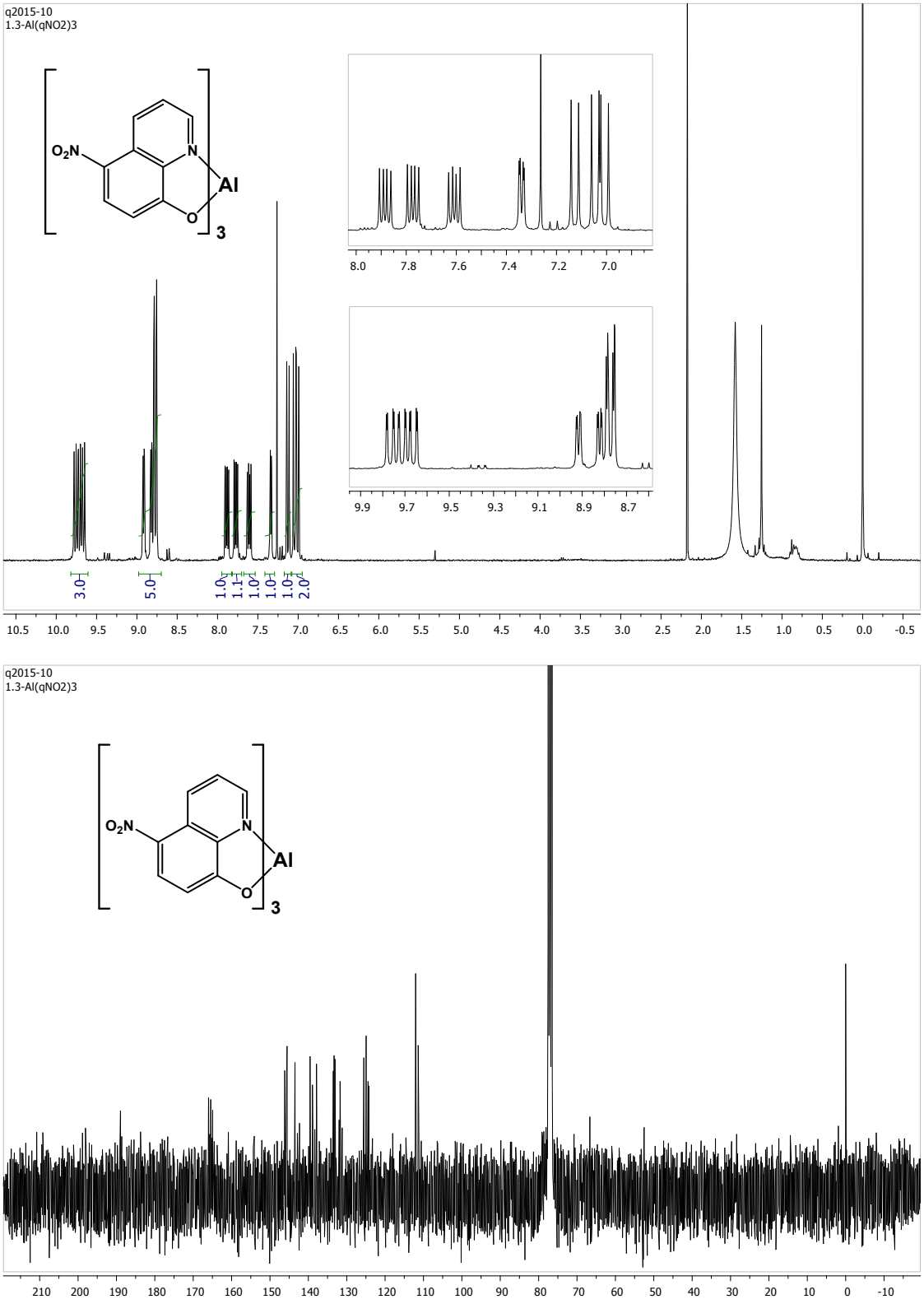


Figure S23. ^{1}H and ^{13}C NMR spectra of $Al(qNO_2)_3$ in $CDCl_3$.

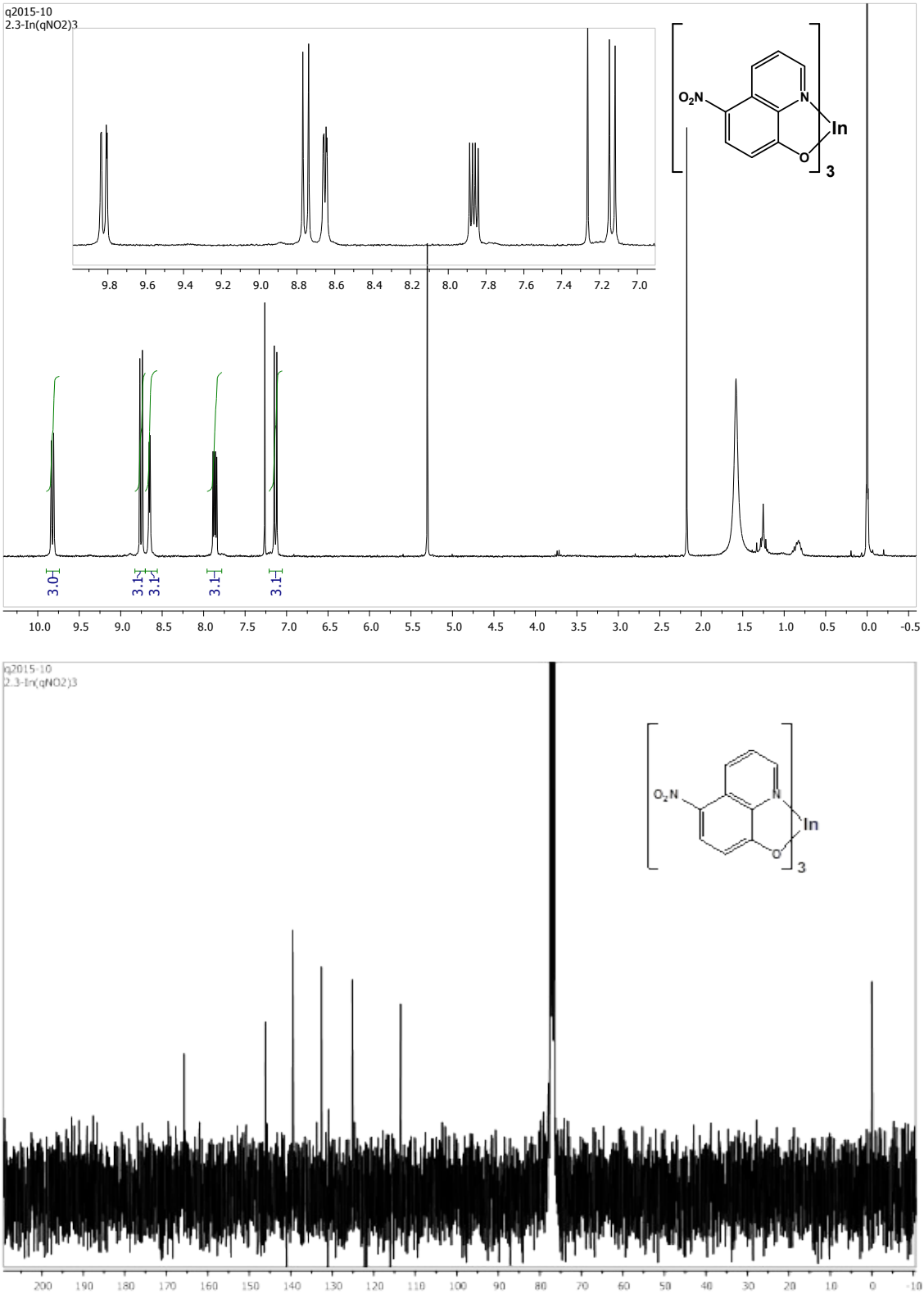


Figure S24. ^{1}H and ^{13}C NMR spectra of $In(qNO_2)_3$ in $CDCl_3$.

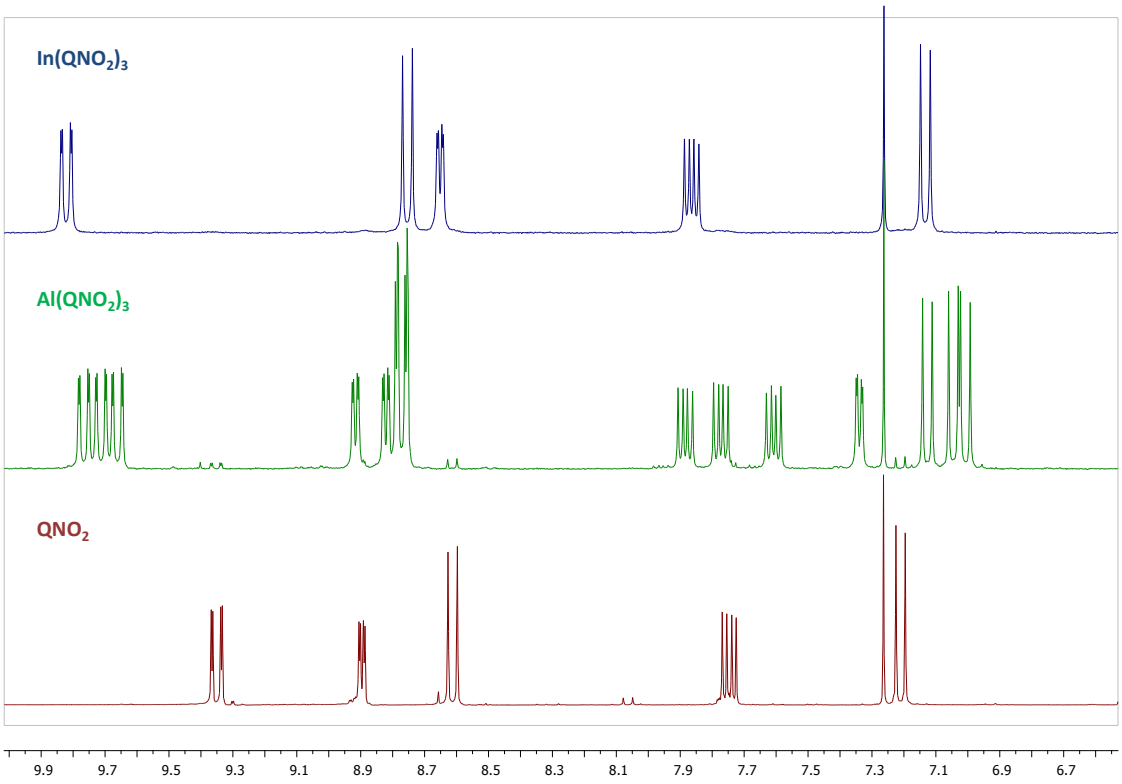


Figure S25. Comparison between the ^{1}H NMR spectra of qNO_2 (5-nitro-8-hydroxyquinoline), $Al(qNO_2)_3$ and $In(qNO_2)_3$ in $CDCl_3$.

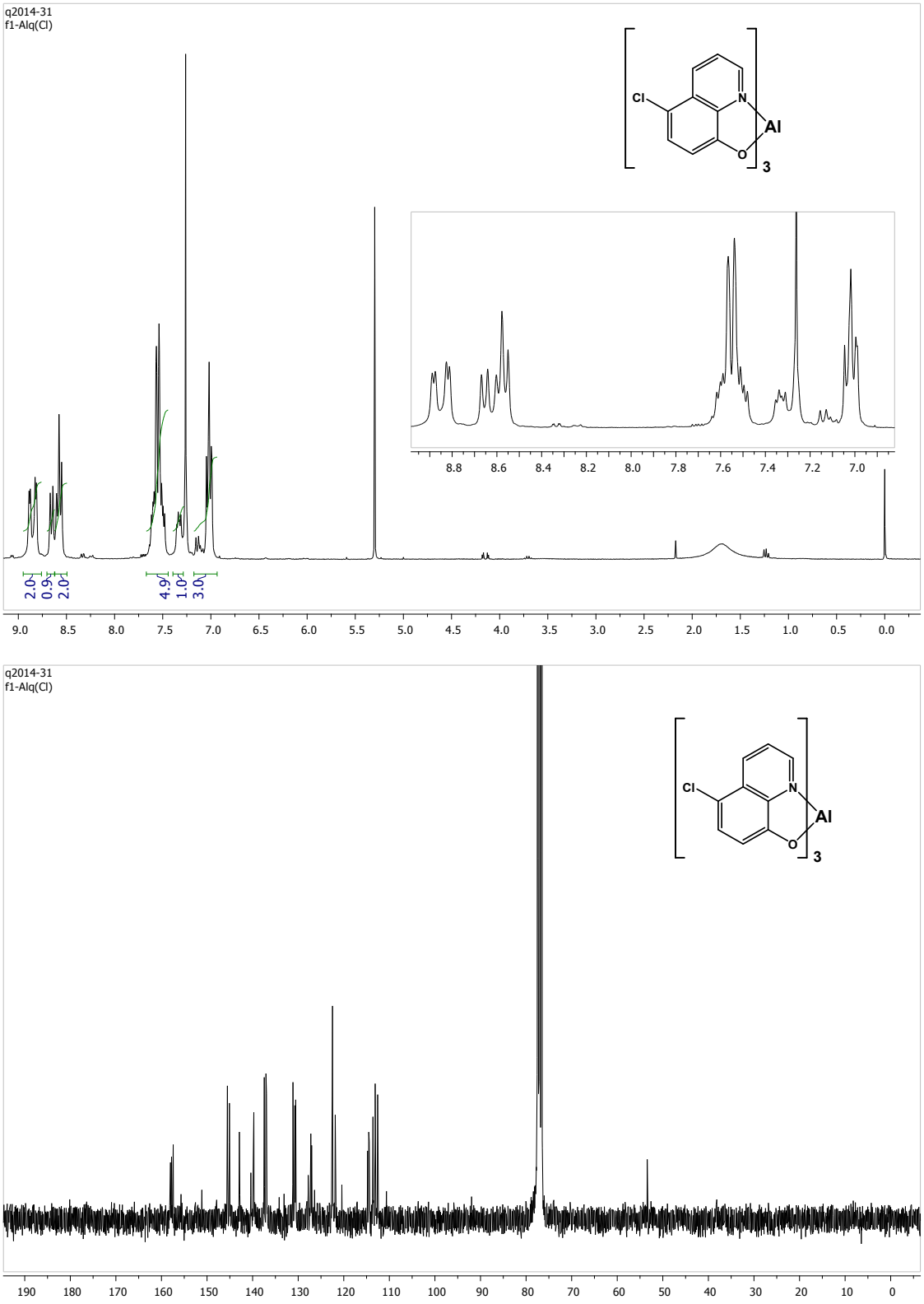


Figure S26. ^{1}H and ^{13}C NMR spectra of $Al(qCl)_3$ in $CDCl_3$.

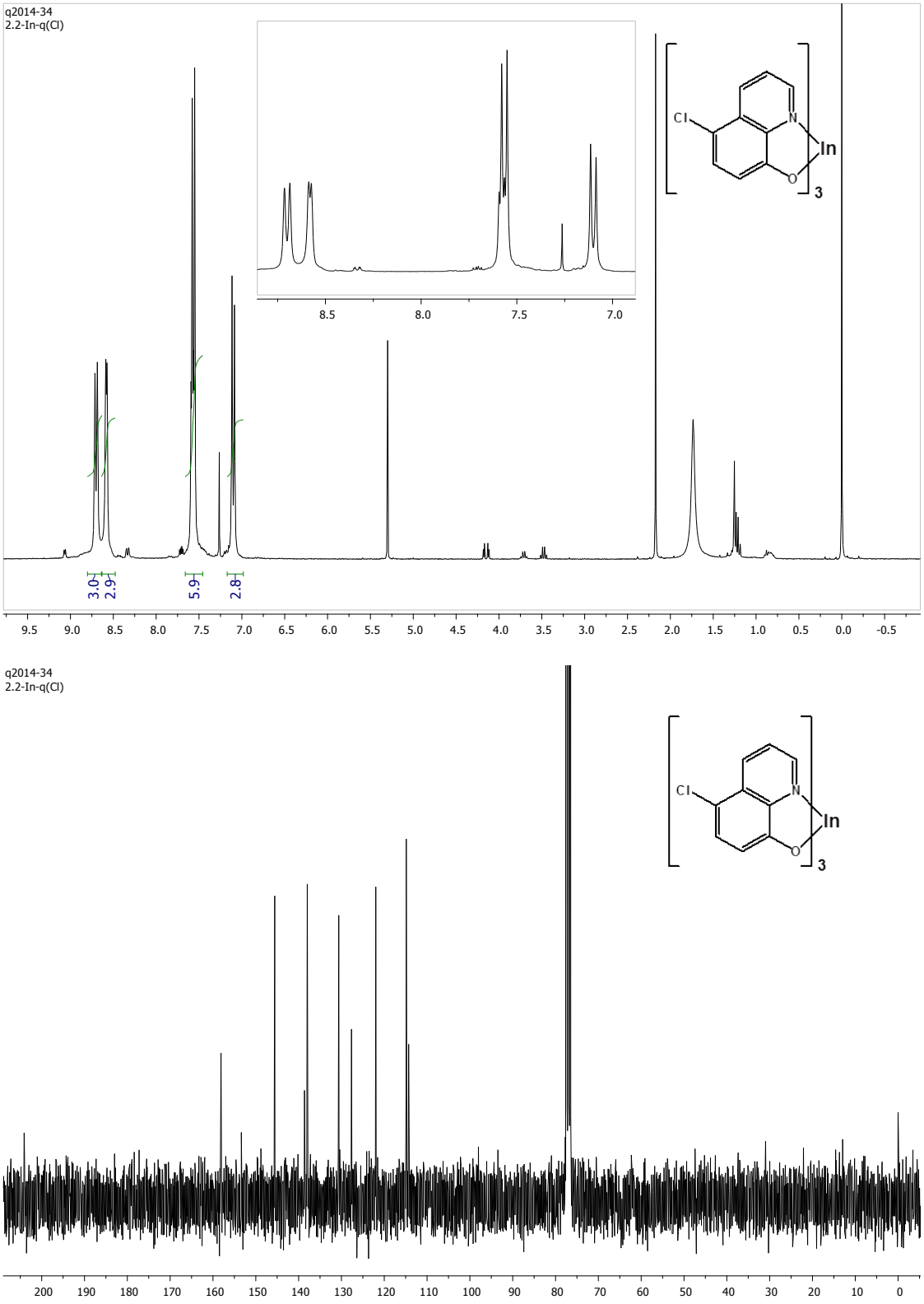


Figure S27. ^{1}H and ^{13}C NMR spectra of $In(qCl)_3$ in $CDCl_3$.

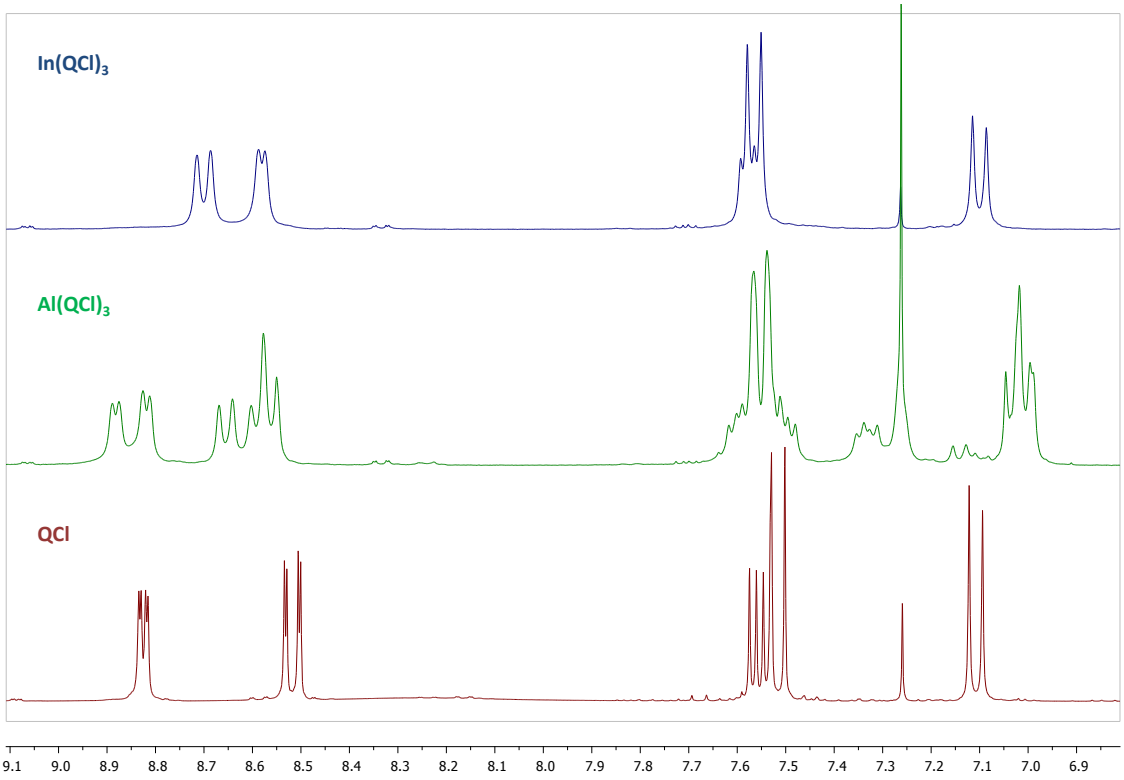


Figure S28. Comparison between the ^{1}H NMR spectra of qCl (5-chloro-8-hydroxyquinoline), $Al(qCl)_3$ and $In(qCl)_3$ in $CDCl_3$.

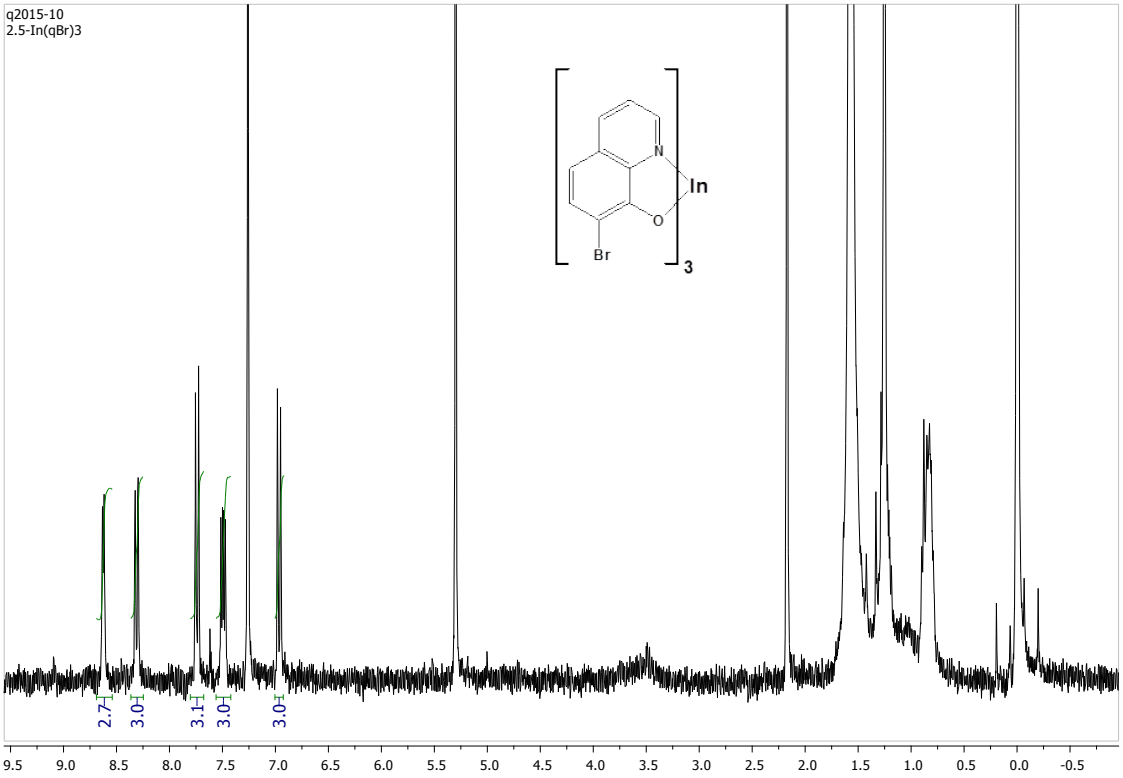


Figure S29. ^{1}H NMR spectrum of $In(qBr)_3$ in $CDCl_3$.

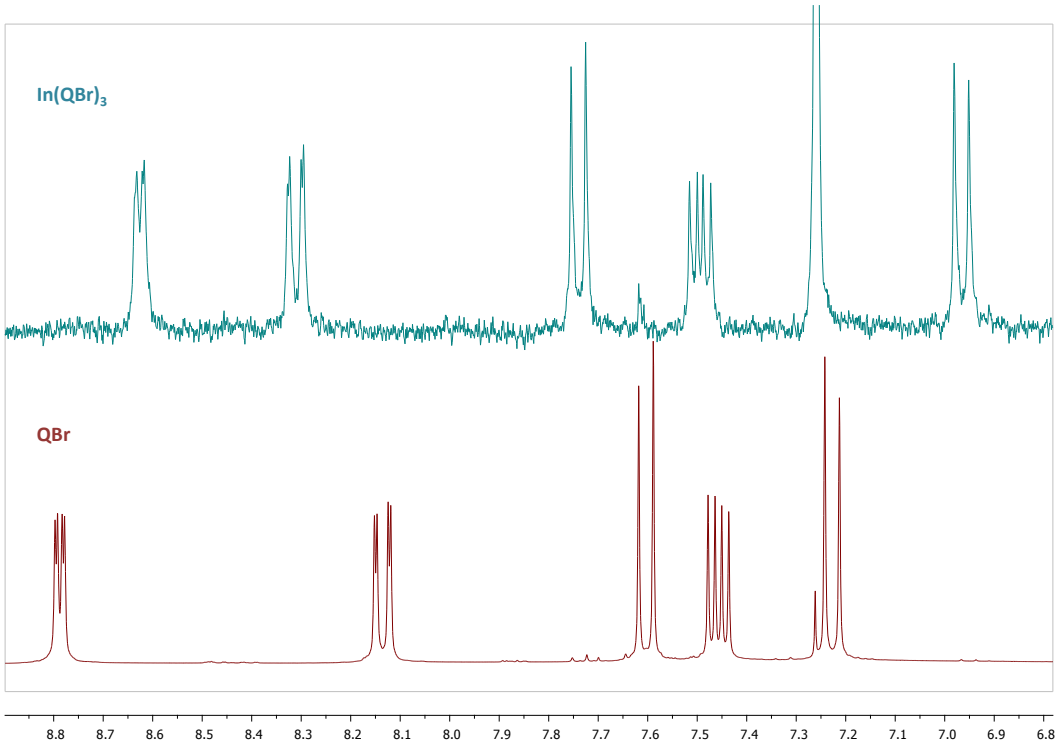


Figure S30. Comparison between the ^{1}H NMR spectra of qBr (7-bromo-8-hydroxyquinoline) and $In(qBr)_3$ in $CDCl_3$.

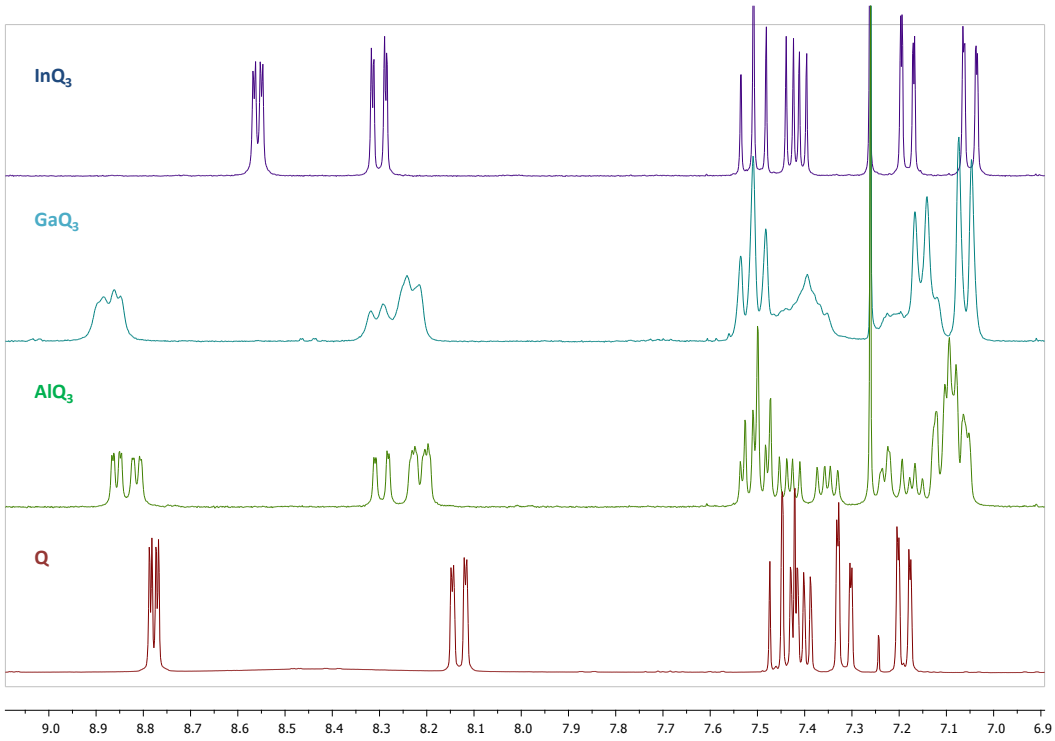


Figure S31. Comparison between the ^{1}H NMR spectra of q (8-hydroxyquinoline), Alq_3, Gaq_3 and Inq_3 in $CDCl_3$.

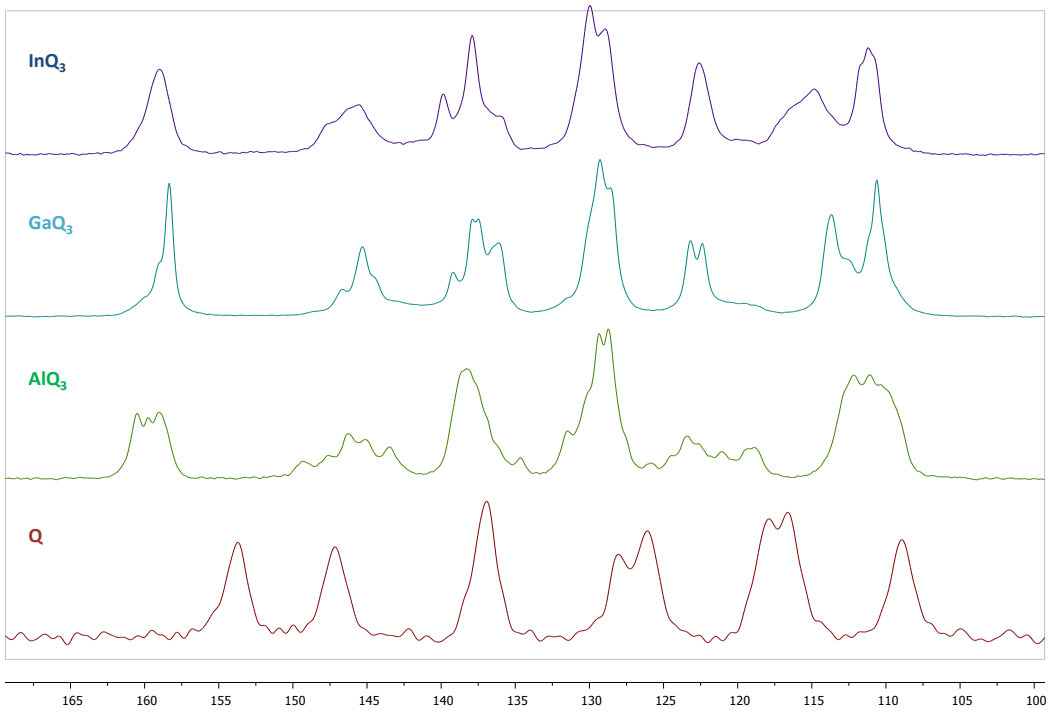


Figure S32. Comparison between the ^{13}C CPMAS NMR spectra of solid q (8-hydroxyquinoline), Alq_3, Gaq_3 and Inq_3.

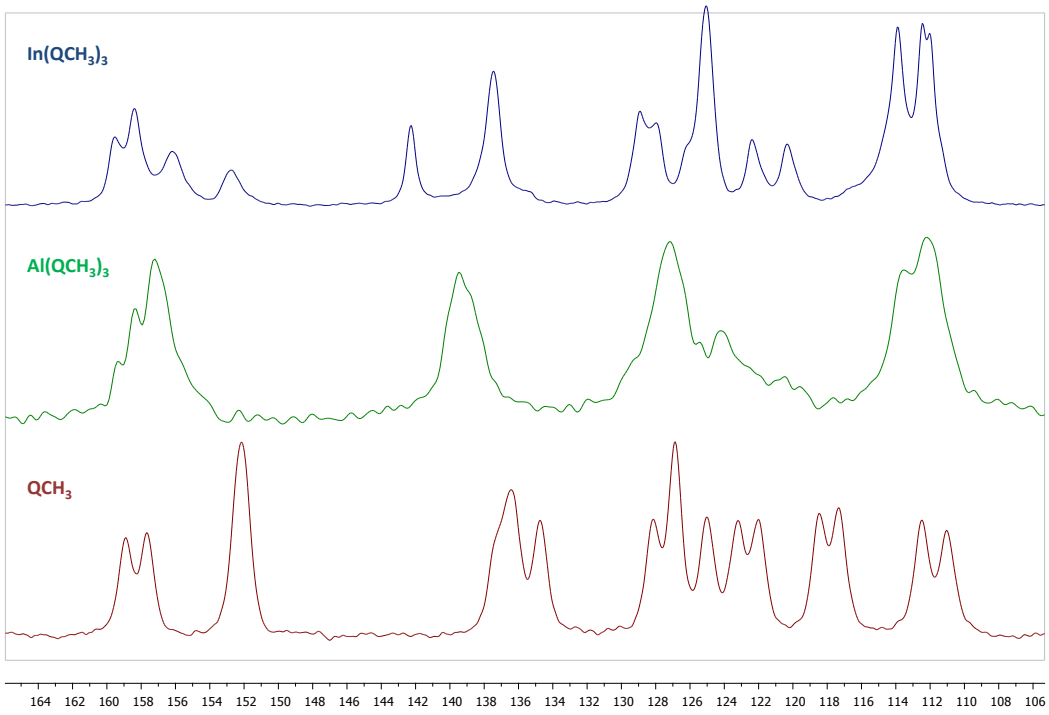


Figure S33. Comparison between the ^{13}C CPMAS NMR spectra of solid qCH_3 (8-hydroxyquinaldine), $Al(qCH_3)_3$ and $In(qCH_3)_3$.

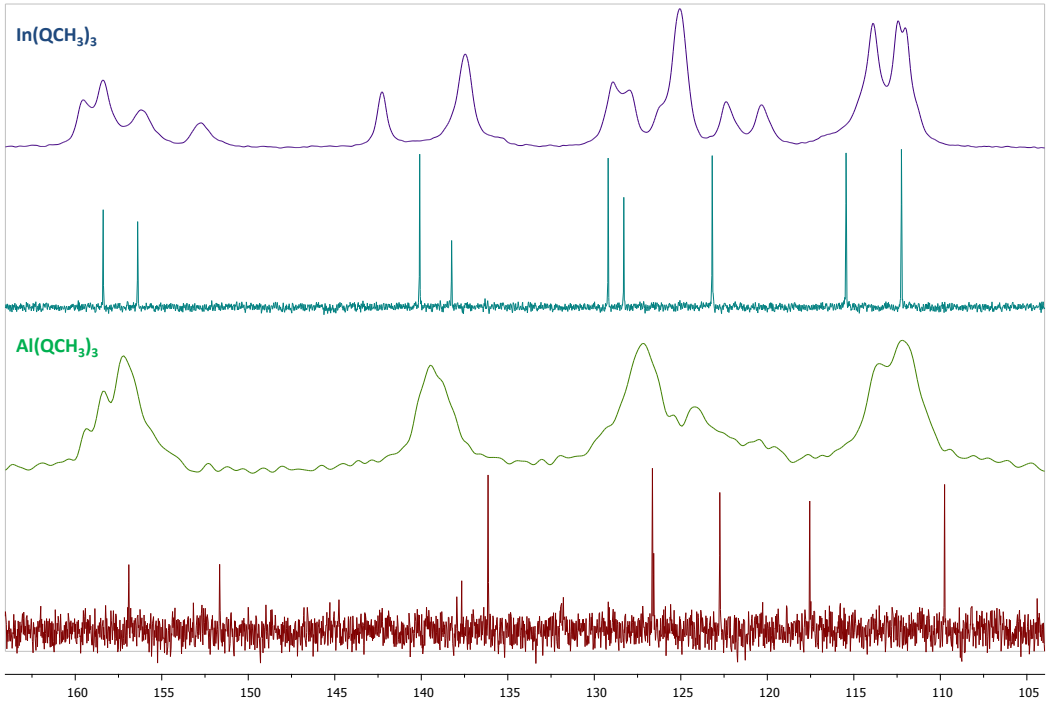


Figure S34. Comparison between the solid ^{13}C CPMAS and solution ($CDCl_3$) ^{13}C NMR spectra of $Al(qCH_3)_3$ and $In(qCH_3)_3$.

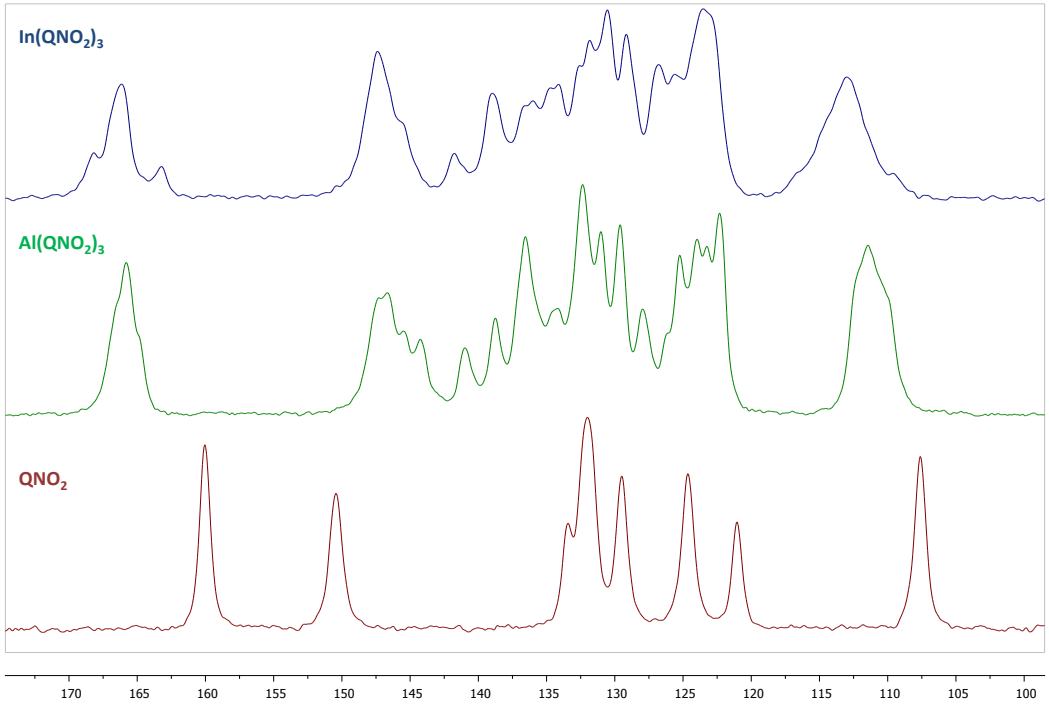


Figure S35. Comparison between the ^{13}C CPMAS NMR spectra of solid qNO_2 (5-nitro-8-hydroxyquinoline), $Al(qNO_2)_3$ and $In(qNO_2)_3$.

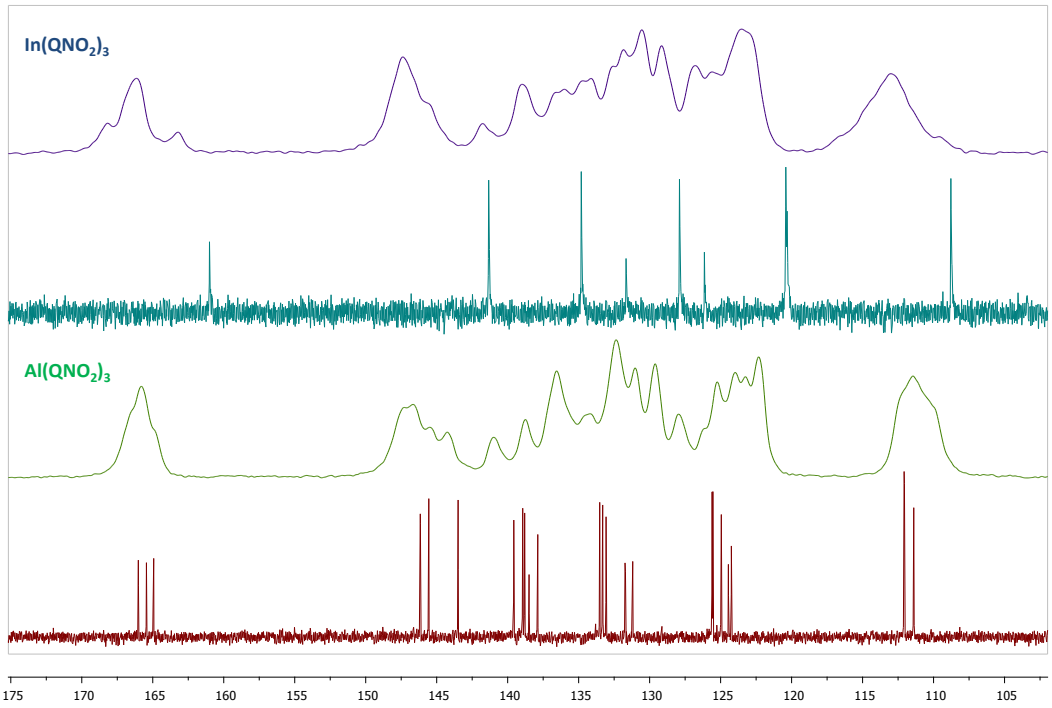


Figure S36. Comparison between the solid ^{13}C CPMAS and solution ($CDCl_3$) ^{13}C NMR spectra of $Al(qNO_2)_3$ and $In(qNO_2)_3$.

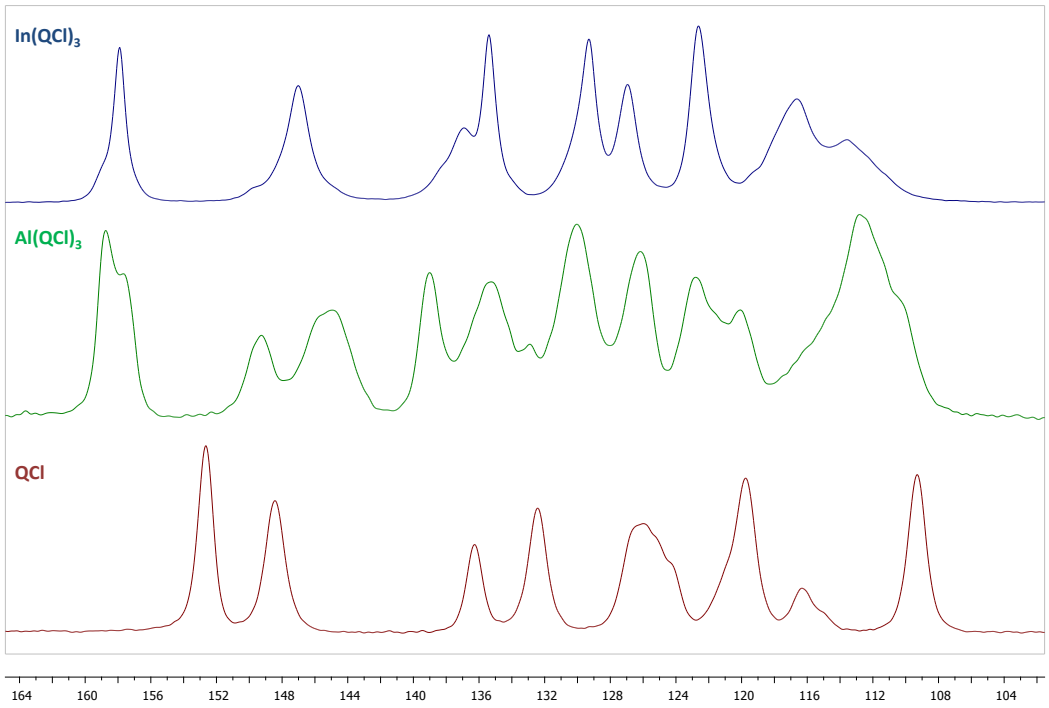


Figure S37. Comparison between the ^{13}C CPMAS NMR spectra of solid qCl (5-chloro-8-hydroxyquinoline), $Al(qCl)_3$ and $In(qCl)_3$.

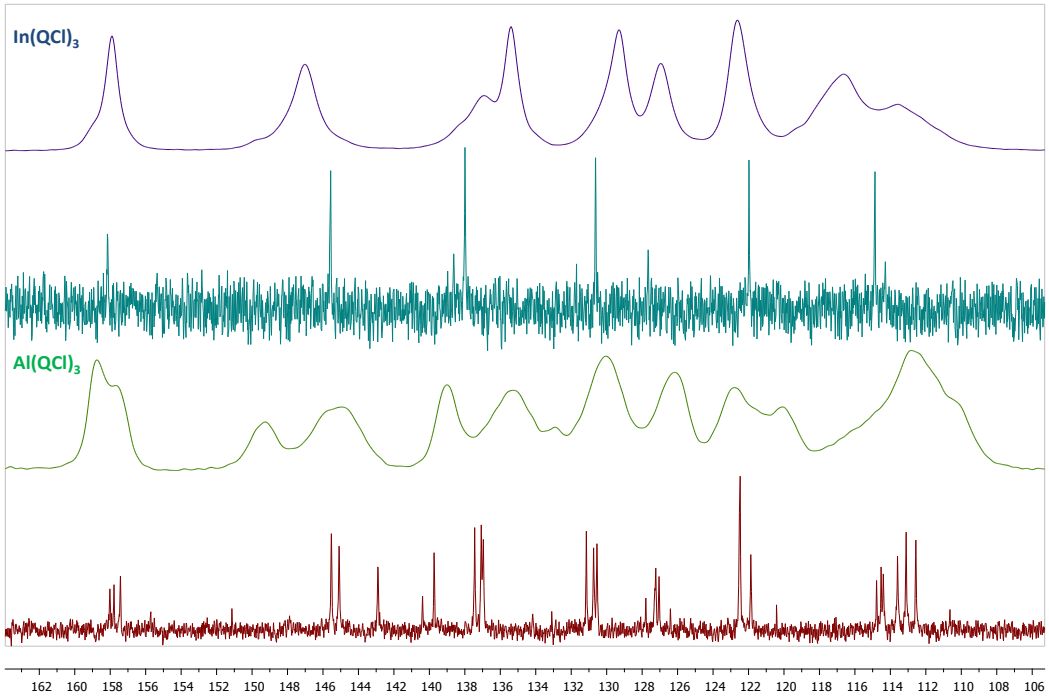


Figure S38. Comparison between the solid ^{13}C CPMAS and solution ($CDCl_3$) ^{13}C NMR spectra of $Al(qCl)_3$ and $In(qCl)_3$.

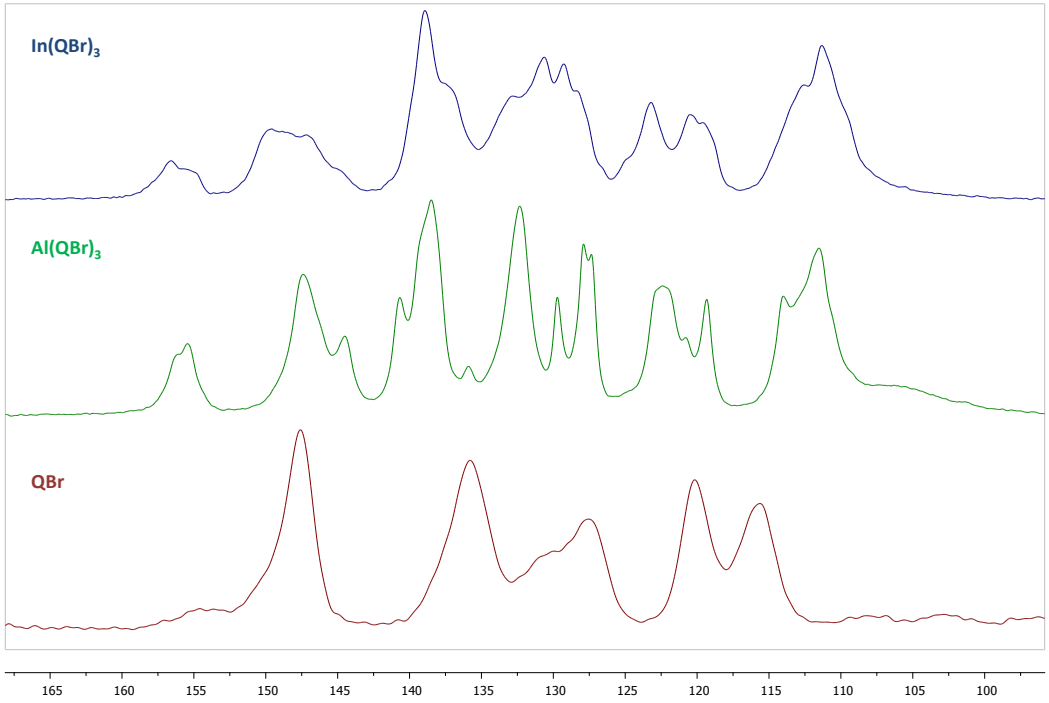


Figure S39. Comparison between the ^{13}C CPMAS NMR spectra of solid qBr (7-bromo-8-hydroxyquinoline), $Al(qBr)_3$ and $In(qBr)_3$.

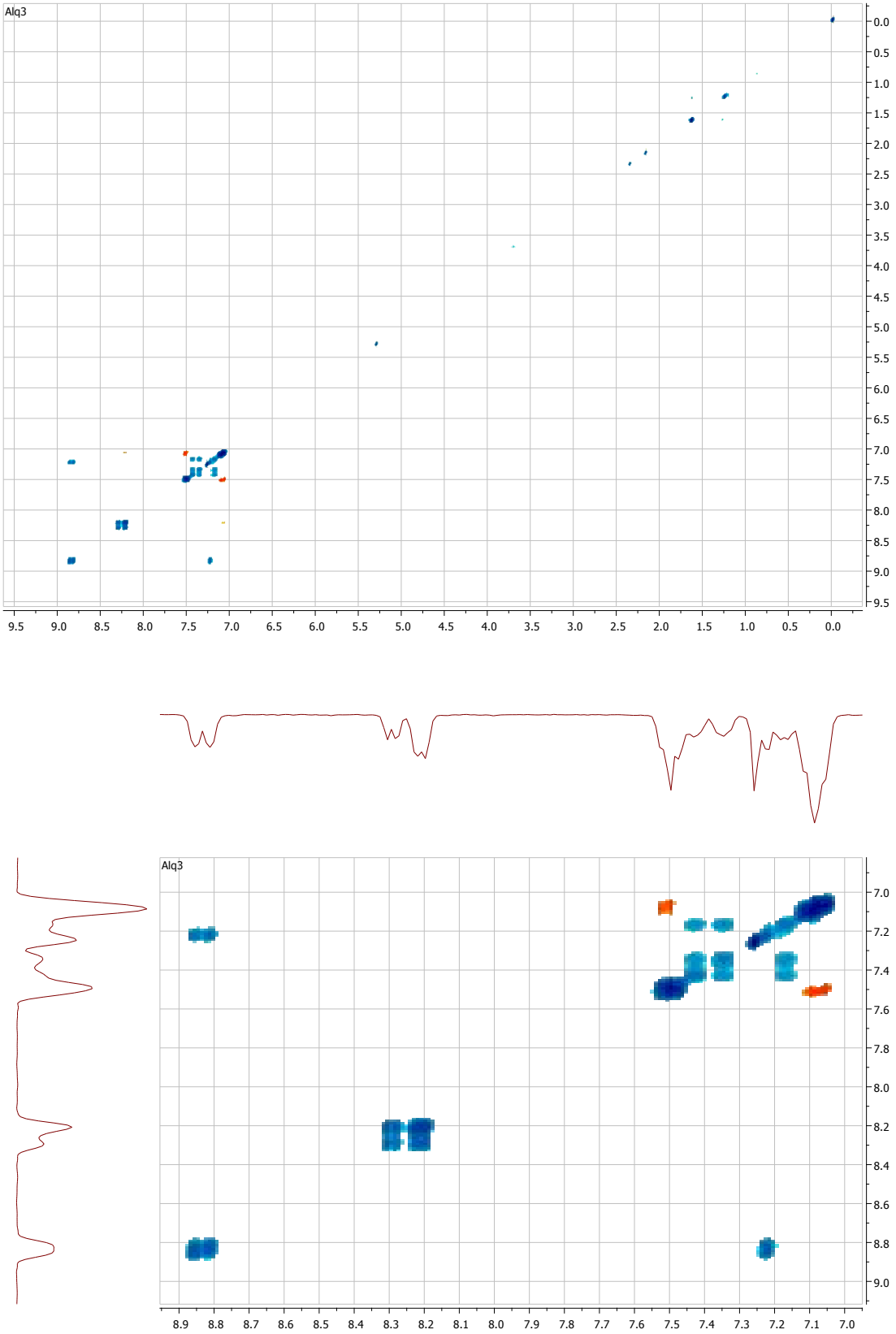


Figure S40. 2D ^{1}H NOESY NMR spectrum of Alq_3 in $CDCl_3$.

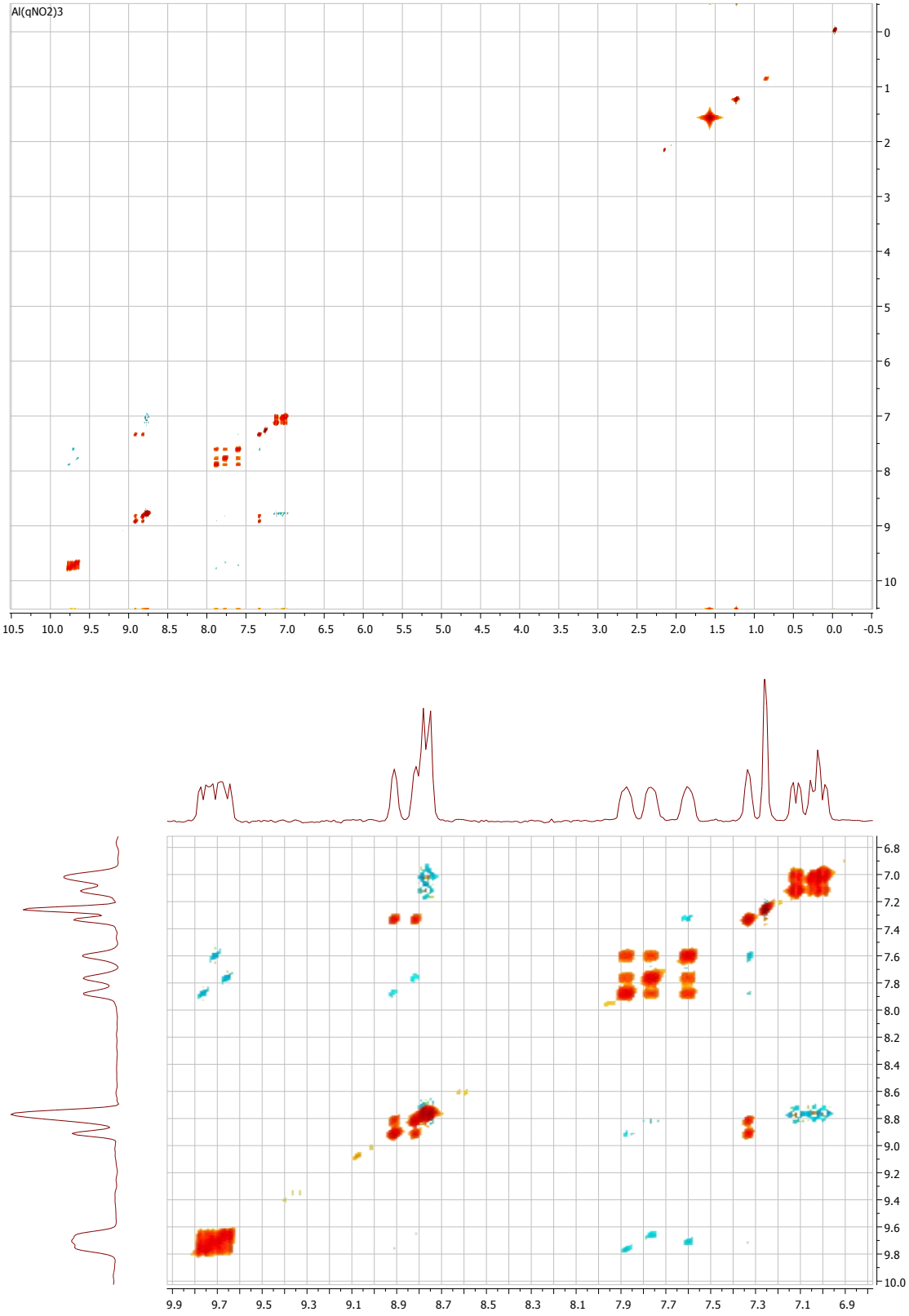


Figure S41. 2D ^{1}H NOESY NMR spectrum of $Al(qNO_2)_3$ in $CDCl_3$.

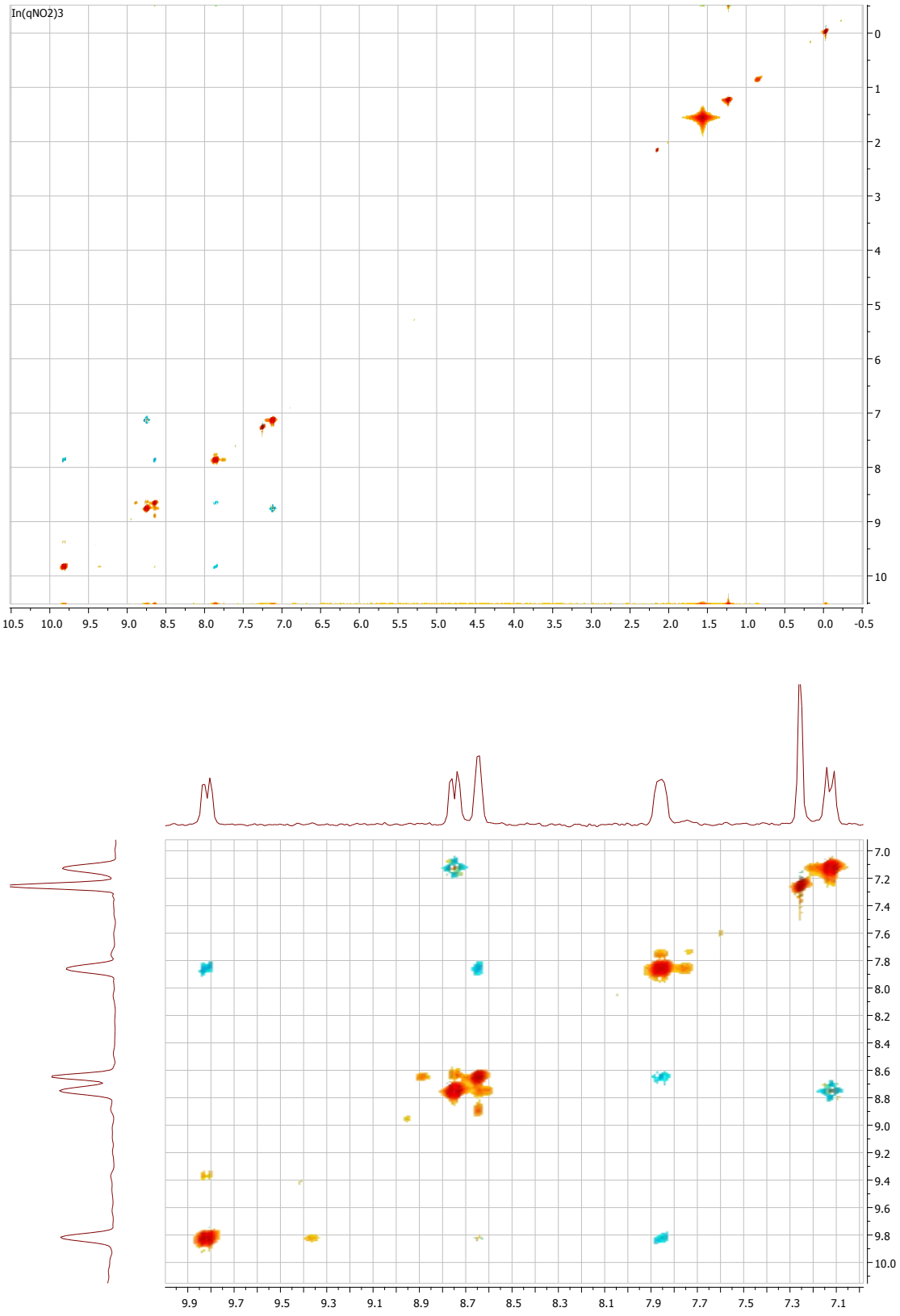


Figure S42. 2D ^{1}H NOESY NMR spectrum of $In(qNO_2)_3$ in $CDCl_3$.

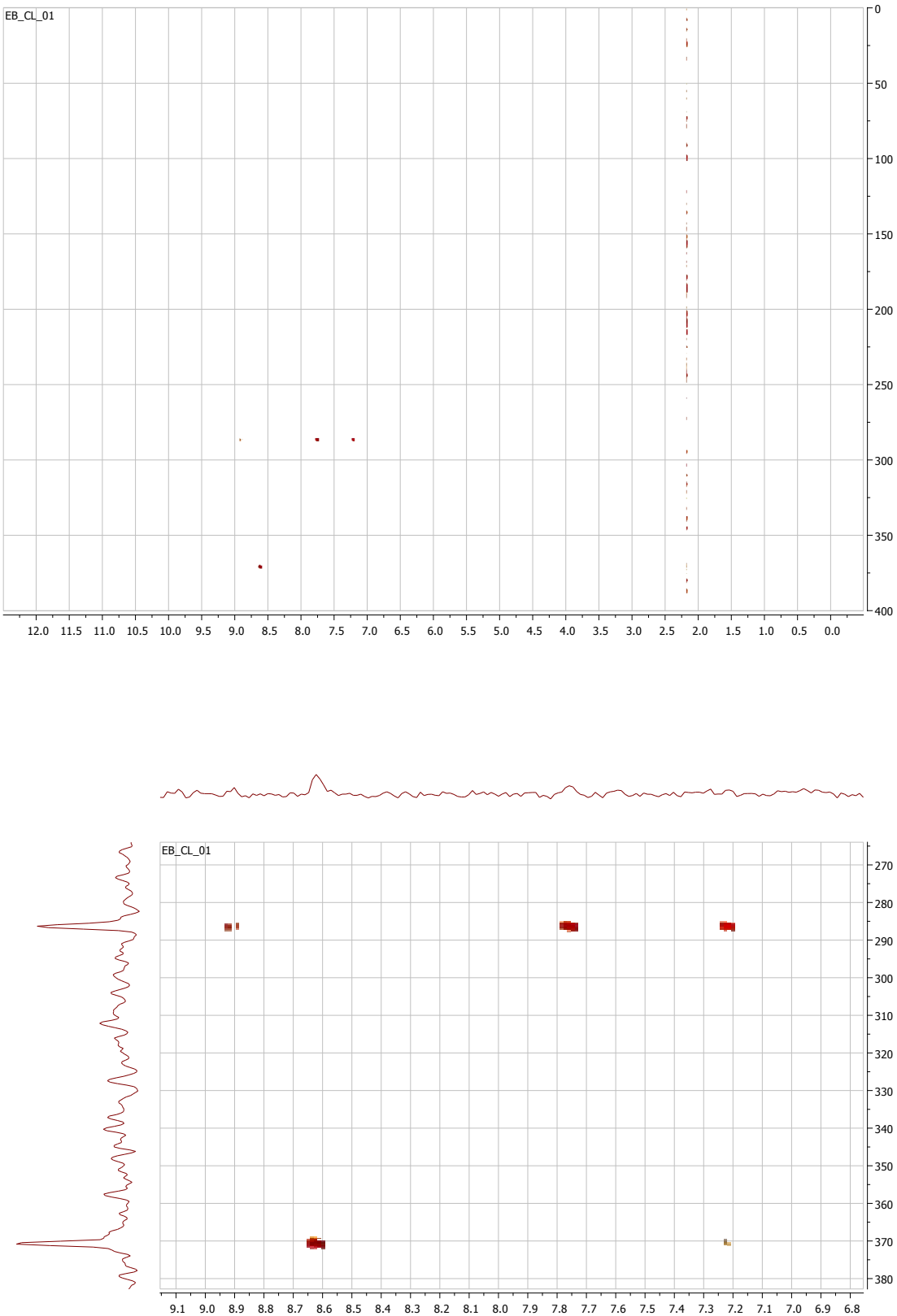


Figure S43. 2D ^{15}N HMBC NMR spectrum of 8-HqNO$_2$ in CDCl$_3$.

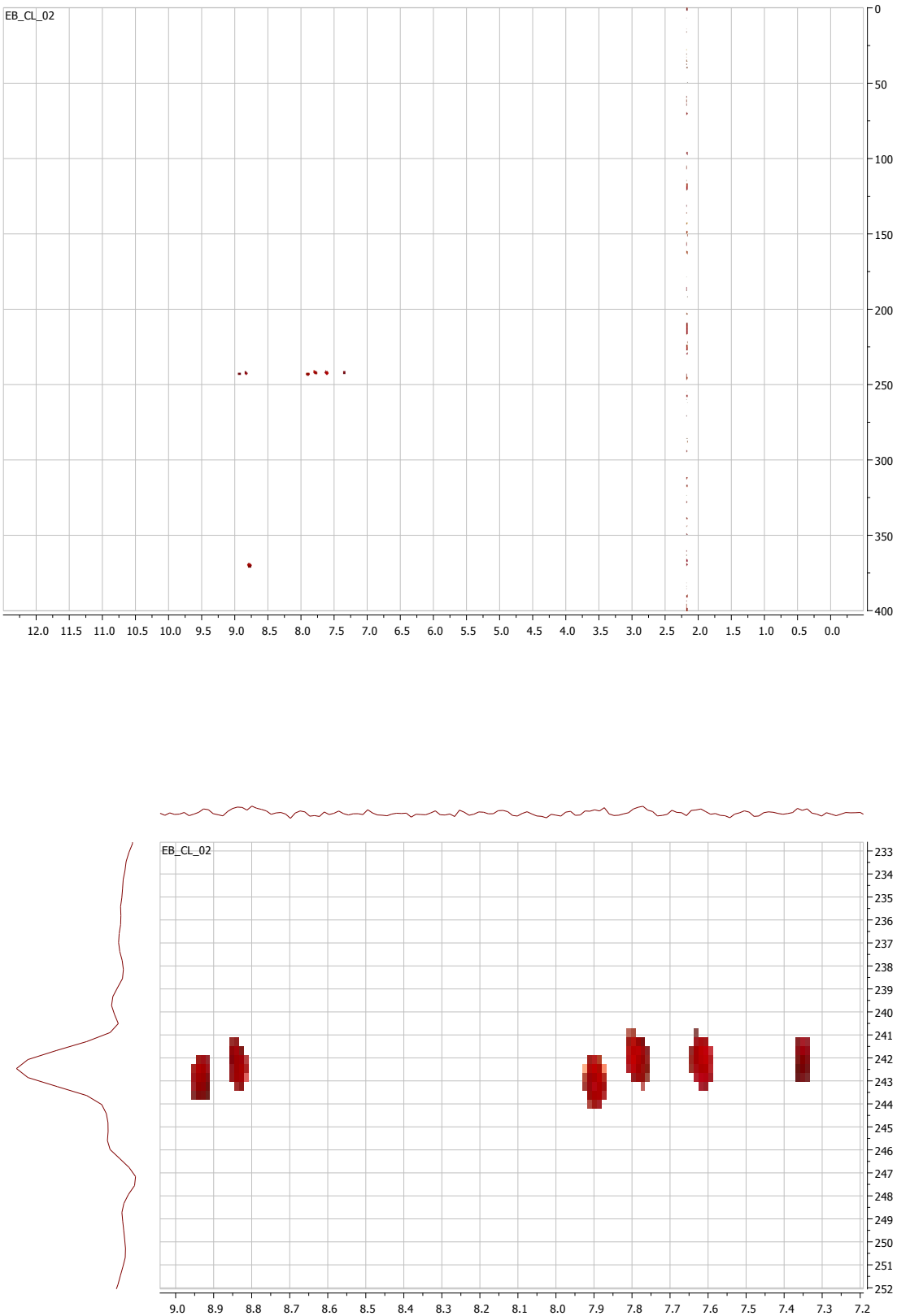


Figure S44. 2D ^{15}N HMBC NMR spectrum of $Al(qNO_2)_3$ in $CDCl_3$.

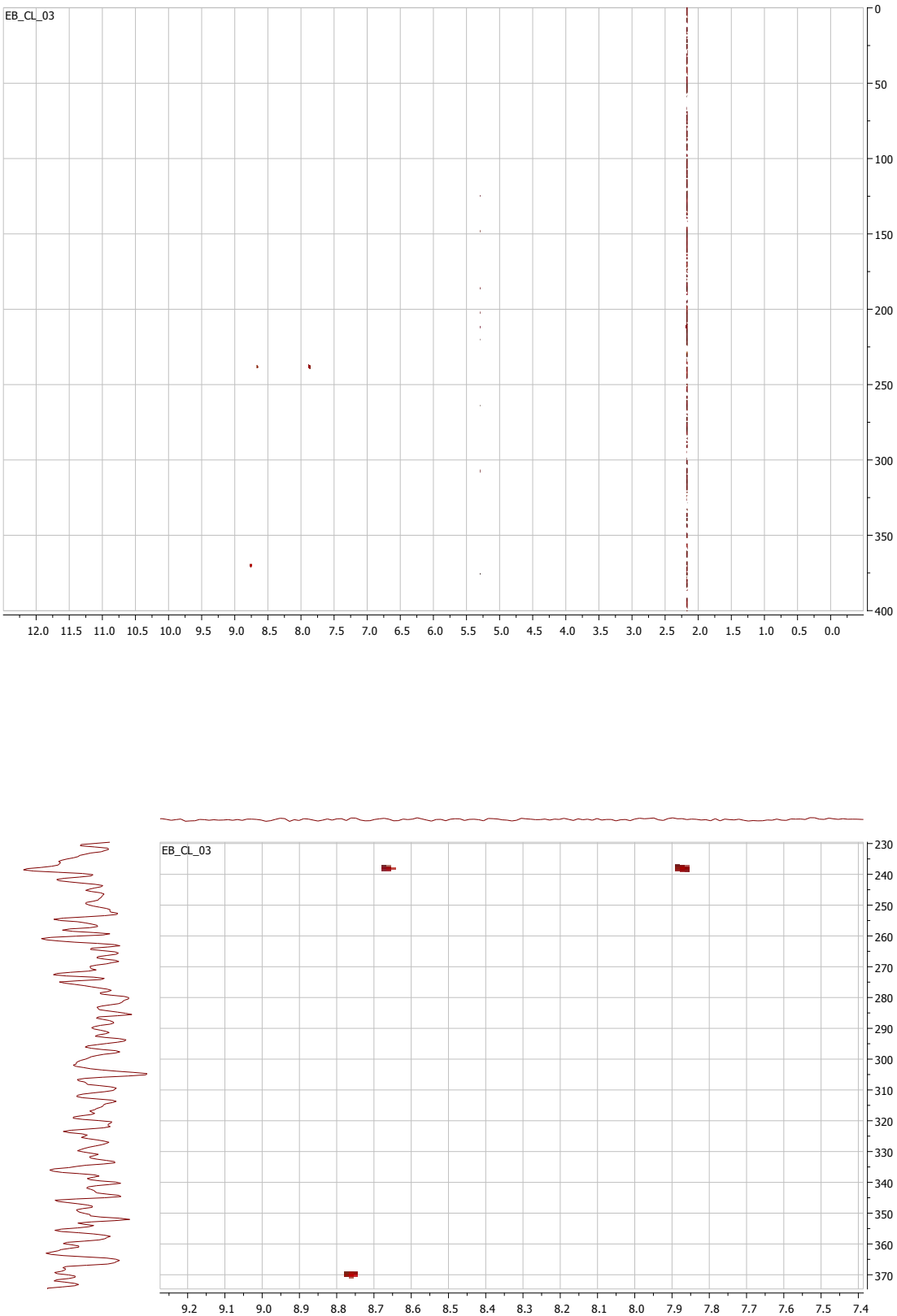
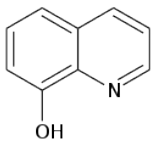


Figure S45. 2D ^{15}N HMBC NMR spectrum of $In(qNO_2)_3$ in $CDCl_3$.

Section S2. Mass spectrometry analysis

Table S4. Electrospray ionization mass spectra data (ESI-MS) of the tris(8-hidroxiquinolinate)metallic complexes.



= qH M-metal

	M(III)	$[Mq_3+H]^+$	$[Mq_3+Na]^+$	$[Mq_2]^+$	$[Mq_2+18]^+$	$[(Mq_3)_2+Na]^+$	$[q_2M-Mq_3]^+$
Mq_3	Al	460 15%	482 21%	315 100%	333 21%	941 2.8%	774 21%
	Ga	502 0.18%	524 13%	357 100%	-	1025 4.4%	858 6%
	In	548 46%	570 34%	403 100%	421 4.8%	1117 17%	950 54%
$M(qCH_3)_3$	Al	502 16%	524 2.9%	343 100%	-	-	-
	In	590 1.9%	612 3.9%	431 100%	449 0.5%	-	1020 3.0%
$M(qNO_2)_3$	Al	595 15%	617 16%	405 100%	423 43%	1211 2.4%	999 11%
	In	683 12%	705 46%	493 100%	511 28%	1387 11%	1175 26%
$M(qCl)_3$	Al	562 12%	584 4.0%	383 100%	401 18%	1147 3,5%	944 10%
	In	650 34%	672 8,6%	471 100%	489 7%	1321 1,7%	1120 31%
$M(qBr)_3$	Al	694 4,1%	716 2,8%	471 53%(1)	-	-	-
	In	782 100%	804 25%	559 54%	577 4.6%	-	-

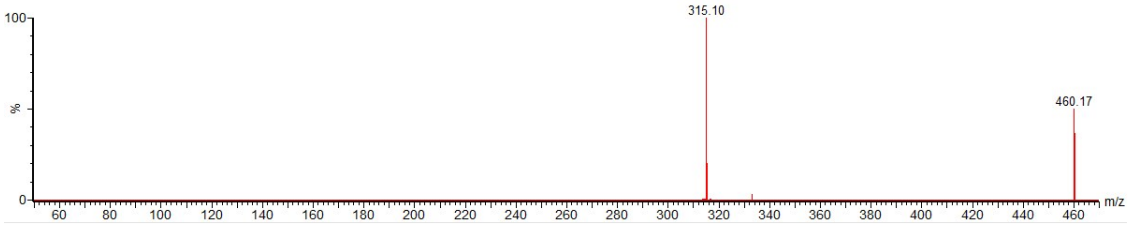


Figure S46. Electrospray ionization tandem mass spectra (ESI-MS-MS) of ion $[Alq_3+H]^+$ at 14 eV collision energy.

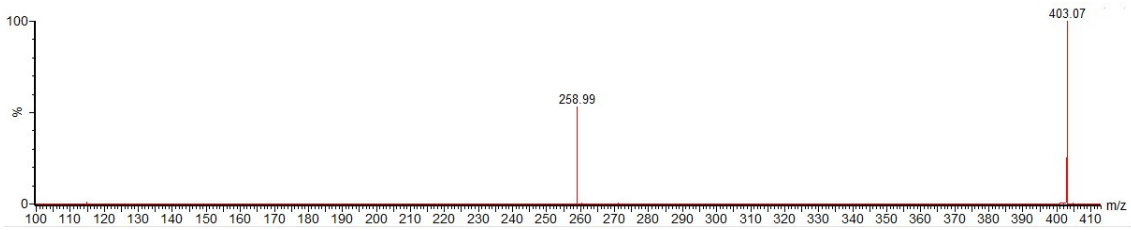


Figure S47. Electrospray ionization tandem mass spectra (ESI-MS-MS) of ion $[Inq_2]^+$ at 20 eV collision energy.

Section S3. Quantum chemistry calculations

S3.1. Calculated energies for the systems studied

Table S5. Electronic energies, E_{el} and unscaled enthalpies at T = 298.15 K, H_{298K}, obtained at the M06-2X/6-31+G(d,p)/SDD level of theory for the systems studied (the SDD Effective Core Potential basis set was used for the heavy atoms of Ga, In and Br, and 6-31+G(d,p) was used for the other atoms). All optimized geometries were obtained at the same level of theory.

Molecular system	E_{el} / hartree	H_{298K} / hartree
Hq	−476.986421	---
$HqCH_3$	−516.289171	---
$HqNO_2$	−681.417832	---
HqCl	−936.554034	---
HqBr	−489.708928	---
mer-Alq_3	−1671.807273	−1671.384047
mer-$Al(qCH_3)_3$	−1789.705794	---
mer-$Al(qNO_2)_3$	−2285.107782	−2284.667180
mer-$Al(qCl)_3$	−3050.502918	---
mer-$Al(qBr)_3$	−1709.995357	---
fac-Alq_3	−1671.799618	−1671.376926
fac-$Al(qCH_3)_3$	−1789.689161	---
fac-$Al(qNO_2)_3$	−2285.100015	---
fac-$Al(qCl)_3$	−3050.494798	---
fac-$Al(qBr)_3$	−1709.983875	---
mer-Gaq_3	−1431.390124	−1430.968326
fac-Gaq_3	−1431.383849	−1430.963356
mer-Inq_3	−1431.223614	−1430.802554
mer-$In(qCH_3)_3$	−1549.126855	---
mer-$In(qNO_2)_3$	−2044.522217	---
mer-$In(qCl)_3$	−2809.918581	---

mer-$In(qBr)_3$	−1469.411455	---
fac-Inq_3	−1431.218609	−1430.797823
fac-$In(qCH_3)_3$	−1549.115266	---
fac-$In(qNO_2)_3$	−2044.516749	−2044.078392
fac-$In(qCl)_3$	−2809.913314	---
fac-$In(qBr)_3$	−1469.402793	---
q^-	−476.417758	−476.282361
qCH_3^-	−515.718076	---
qNO_2^-	−680.886035	−680.744252
qCl^-	−935.9948074	---
qBr^-	−489.153474	---
Alq_2^+	−1195.135331	−1194.852010
$Al(qCH_3)_2^+$	−1273.750443	---
$Al(qNO_2)_2^+$	−1603.970346	−1603.675716
$Al(qCl)_2^+$	−2114.255895	---
$Al(qBr)_2^+$	−1220.582758	---
Gaq_2^+	−954.733702	---
Inq_2^+	−954.550314	−954.268551
$In(qCH_3)_2^+$	−1033.164014	---
$In(qNO_2)_2^+$	−1363.385476	−1363.092466
$In(qCl)_2^+$	−1873.671062	---
$In(qBr)_2^+$	−979.998549	---

Table S6. Electronic energies, E_{el}, obtained at the M06-2X/6-31+G(d,p) level of theory for the systems studied.

Isolated ligands [a]	E_{el} / Hartree	ΔE_{el}(dist.) / kJ·mol^{-1}
q• optimized	−476.330029	
q• 1 (*mer*-Alq_3)	−476.318124	31
q• 2 (*mer*-Alq_3)	−476.316707	35
q• 3 (*mer*-Alq_3)	−476.316584	35
q• (*fac*-Alq_3)	−476.318532	30
q• 1 (*mer*-Inq_3)	−476.320430	25
q• 2 (*mer*-Inq_3)	−476.319726	27
q• 3 (*mer*-Inq_3)	−476.319729	27
q• (*fac*-Inq_3)	−476.320769	24

Intermolecular complexes without the metal [b]		ΔE_{el}(int.) [c] / kJ·mol^{-1} (with ΔE_{el}(dist.))	ΔE_{el}(int.) [c] / kJ·mol^{-1} (no ΔE_{el}(dist.))
[q•$_3$] (*mer*-Alq_3)	−1428.878542	293	191
[q•$_3$] (*fac*-Alq_3)	−1428.874311	304	213
[q•$_3$] (*mer*-Inq_3)	−1428.945314	118	38
[q•$_3$] (*fac*-Inq_3)	−1428.946170	115	42

[a] The values of E_{el} presented are for the radical ligands with various geometries; for the fully optimized isolated 8-hydroxyquinoline ligand (q• optimized) and for the isolated ligands with the geometry they adopt in the respective metallic complexes (obtained from a single-point energy calculation) – in the *mer*-isomers the three ligands have slightly different structures, whereas in the *fac*-isomer they are all equivalent due to symmetry; ΔE_{el}(dist.) is the geometry distortion energy of each ligand relative to its optimized structure (q• optimized) – it translates the energy required for the structural rearrangement of the isolated ligand upon complexation with the metal.

[b] The intermolecular complexes formed between three 8-hydroxyquinoline radicals considering the geometry they adopt in the respective Mq_3 complexes (E_{el} obtained from a single-point energy calculation).

[c] The values of ΔE_{el}(int.) refer to the total interaction energy (not corrected for BSSE) between the three 8-hydroxyquinoline radicals in the intermolecular complexes, as translated by the equation: 3q• → [q•$_3$], both considering and not considering the contribution of the geometry distortion energy on complexation, ΔE_{el}(dist.).

Table S7. Calculated HOMO and LUMO orbital energies, at the M06-2X/6-31+G(d,p)/SDD level of theory, for the Al(III) and In(III) complexes studied.

Molecular system	E_{HOMO} / Hartree	E_{LUMO} / Hartree	$\Delta_{(LUMO-HOMO)}$ / hartree
mer-Alq_3	-0.24012	-0.04459	**0.196**
mer-$Al(qCH_3)_3$	-0.23294	-0.04044	**0.193**
mer-$Al(qNO_2)_3$	-0.28658	-0.09075	**0.196**
mer-$Al(qCl)_3$	-0.24909	-0.05906	**0.190**
mer-$Al(qBr)_3$	-0.25023	-0.05626	**0.194**
fac-Alq_3	-0.24735	-0.04228	**0.205**
fac-$Al(qCH_3)_3$	-0.24003	-0.04028	**0.200**
fac-$Al(qNO_2)_3$	-0.29038	-0.08336	**0.207**
fac-$Al(qCl)_3$	-0.25633	-0.05700	**0.199**
fac-$Al(qBr)_3$	-0.25623	-0.05447	**0.202**
mer-Inq_3	-0.24247	-0.0425	**0.200**
mer-$In(qCH_3)_3$	-0.23316	-0.03965	**0.194**
mer-$In(qNO_2)_3$	-0.28772	-0.08839	**0.199**
mer-$In(qCl)_3$	-0.25120	-0.05682	**0.194**
mer-$In(qBr)_3$	-0.25250	-0.05384	**0.199**
fac-Inq_3	-0.24755	-0.0428	**0.205**
fac-$In(qCH_3)_3$	-0.24050	-0.04189	**0.199**
fac-$In(qNO_2)_3$	-0.29225	-0.08760	**0.205**
fac-$In(qCl)_3$	-0.25609	-0.05710	**0.199**
fac-$In(qBr)_3$	-0.25619	-0.05453	**0.202**

S3.2. Optimized geometries

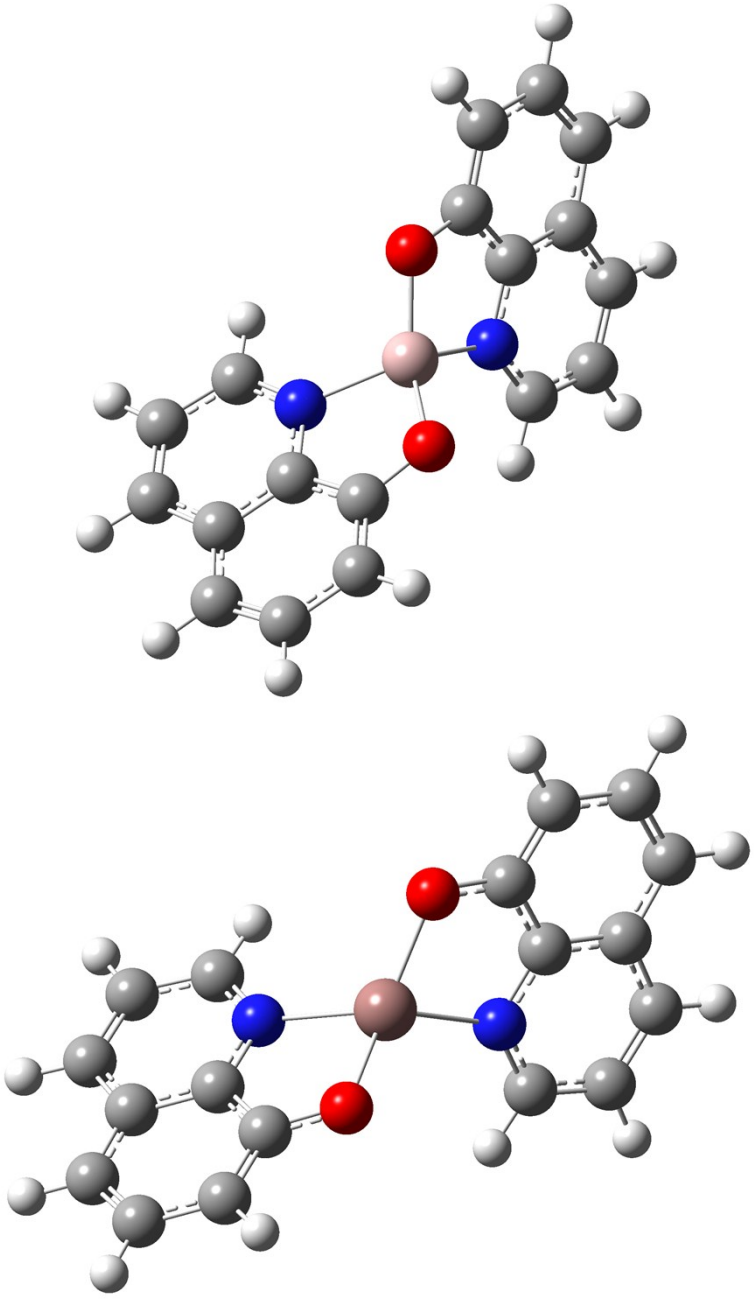


Figure S48. Optimized geometries for the Alq_2^+ (top) and Inq_2^+(bottom) complexes, obtained at the M06-2X/6-31+G(d,p)/SDD level of theory.

Table S8. Optimized geometries in Cartesian coordinates for the molecular systems considered, obtained at the M06-2X/6-31+G(d,p)/SDD level of theory.

A) *mer*-Alq_3

1	7	0	-0.622502	1.381701	0.774673
2	7	0	-1.690989	-0.851385	-0.906397
3	7	0	2.021787	0.071592	0.534104
4	8	0	1.012201	-1.631683	-1.176158
5	8	0	0.309827	1.002799	-1.609449
6	8	0	-0.345740	-1.297033	1.275799
7	6	0	-2.294113	-0.577173	-2.045325
8	6	0	-3.561705	-1.120401	-2.350208
9	6	0	-4.177096	-1.953340	-1.443753
10	6	0	-3.542992	-2.266493	-0.214604
11	6	0	-2.278398	-1.676103	-0.001179
12	6	0	-4.070847	-3.110838	0.794201
13	6	0	-3.330783	-3.323673	1.938034
14	6	0	-2.062580	-2.734904	2.150456
15	6	0	-1.505087	-1.903962	1.188488
16	6	0	-1.098013	1.477661	2.001623
17	6	0	-1.573942	2.707251	2.510053
18	6	0	-1.541727	3.829405	1.713057
19	6	0	-1.038704	3.750526	0.389614
20	6	0	-0.589839	2.476699	-0.026852
21	6	0	-0.956971	4.825070	-0.530087
22	6	0	-0.446318	4.584573	-1.789432
23	6	0	0.000640	3.310600	-2.207129
24	6	0	-0.059647	2.228025	-1.338810
25	6	0	2.466149	0.967225	1.392928
26	6	0	3.822643	1.018566	1.778470
27	6	0	4.708097	0.108907	1.248914
28	6	0	4.260014	-0.865523	0.323181
29	6	0	2.884275	-0.832793	-0.004470
30	6	0	5.078040	-1.847994	-0.285681
31	6	0	4.503731	-2.733984	-1.173799
32	6	0	3.132251	-2.701556	-1.506182
33	6	0	2.291603	-1.754578	-0.936264
34	1	0	-1.757197	0.080502	-2.723489
35	1	0	-4.031488	-0.876131	-3.295886
36	1	0	-5.152273	-2.382026	-1.661243
37	1	0	-5.040458	-3.577587	0.654720
38	1	0	-3.730975	-3.973320	2.711315
39	1	0	-1.504538	-2.935482	3.058674
40	1	0	-1.093195	0.562809	2.587462
41	1	0	-1.958273	2.749741	3.522640
42	1	0	-1.903220	4.783427	2.088458
43	1	0	-1.294497	5.813831	-0.237521
44	1	0	-0.382285	5.406637	-2.496841
45	1	0	0.398560	3.161922	-3.205049
46	1	0	1.740061	1.668613	1.793726
47	1	0	4.146382	1.773292	2.485779
48	1	0	5.757260	0.128507	1.532886
49	1	0	6.135880	-1.891184	-0.048136
50	1	0	5.127934	-3.489901	-1.642164
51	1	0	2.714683	-3.411674	-2.211227
52	13	0	0.149781	-0.283473	-0.238752

B) *mer*-$Al(qCH_3)_3$

1	7	0	0.182923	1.783328	-0.535910
2	7	0	1.995078	-0.217563	0.871343
3	7	0	-1.782483	-0.865730	-0.755517
4	8	0	-0.115584	-1.941612	1.006436
5	8	0	-0.921847	0.522039	1.464828
6	8	0	0.907824	-0.925784	-1.406146

7	6	0	2.479942	0.186853	2.034966
8	6	0	3.840523	-0.055686	2.363093
9	6	0	4.664076	-0.713296	1.485061
10	6	0	4.161437	-1.151922	0.235582
11	6	0	2.801144	-0.873837	-0.015058
12	6	0	4.919212	-1.826487	-0.755137
13	6	0	4.306481	-2.186842	-1.934809
14	6	0	2.944992	-1.907001	-2.192397
15	6	0	2.169229	-1.257410	-1.245479
16	6	0	0.828495	2.399952	-1.519084
17	6	0	0.589590	3.775142	-1.789331
18	6	0	-0.298124	4.497318	-1.034673
19	6	0	-0.965284	3.874552	0.046759
20	6	0	-0.673832	2.506097	0.248143
21	6	0	-1.869652	4.527701	0.920578
22	6	0	-2.432568	3.813390	1.955808
23	6	0	-2.139249	2.449961	2.172396
24	6	0	-1.267032	1.774476	1.329452
25	6	0	-2.540166	-0.345341	-1.705218
26	6	0	-3.830583	-0.873385	-1.972744
27	6	0	-4.301701	-1.943501	-1.257631
28	6	0	-3.488998	-2.545309	-0.265907
29	6	0	-2.219398	-1.959025	-0.057125
30	6	0	-3.860977	-3.682873	0.491301
31	6	0	-2.965123	-4.198647	1.403469
32	6	0	-1.690422	-3.631473	1.605315
33	6	0	-1.287621	-2.511212	0.888820
34	1	0	4.211084	0.285929	3.323221
35	1	0	5.704251	-0.903396	1.737925
36	1	0	5.965498	-2.048207	-0.570977
37	1	0	4.881702	-2.703546	-2.697603
38	1	0	2.483875	-2.201692	-3.129210
39	1	0	1.125892	4.240556	-2.609002
40	1	0	-0.485759	5.546566	-1.248824
41	1	0	-2.097227	5.577632	0.767213
42	1	0	-3.122443	4.309389	2.632528
43	1	0	-2.588868	1.905659	2.995839
44	1	0	-4.428962	-0.415300	-2.753065
45	1	0	-5.290290	-2.351054	-1.454627
46	1	0	-4.835900	-4.134120	0.337152
47	1	0	-3.241741	-5.073811	1.984566
48	1	0	-0.995542	-4.060891	2.318726
49	13	0	0.054746	-0.317112	0.125769
50	6	0	1.828664	1.662338	-2.361512
51	1	0	2.632510	1.258858	-1.738411
52	1	0	1.370920	0.811648	-2.871483
53	1	0	2.267350	2.339681	-3.095925
54	6	0	-2.012598	0.803753	-2.517965
55	1	0	-2.107081	1.749309	-1.972676
56	1	0	-0.957158	0.640643	-2.748037
57	1	0	-2.570185	0.892972	-3.452396
58	6	0	1.577841	0.901280	2.998163
59	1	0	1.204013	1.830783	2.556008
60	1	0	0.703267	0.287963	3.229155
61	1	0	2.117524	1.142107	3.915547

C) *mer*-Al(qNO$_2$)$_3$

1	7	0	0.582238	1.381049	-0.781126
2	7	0	1.700063	-0.779464	0.994013
3	7	0	-1.988182	-0.077490	-0.578912
4	8	0	-0.945640	-1.651660	1.197489
5	8	0	-0.394299	1.017390	1.568365
6	8	0	0.482098	-1.337471	-1.211311
7	6	0	2.218618	-0.436183	2.155998
8	6	0	3.473188	-0.930398	2.554920
9	6	0	4.173243	-1.786848	1.734883

10	6	0	3.627110	-2.179065	0.478717
11	6	0	2.362328	-1.628406	0.167954
12	6	0	4.174753	-3.055601	-0.510335
13	6	0	3.483767	-3.330705	-1.677836
14	6	0	2.232035	-2.777042	-1.963336
15	6	0	1.636343	-1.916216	-1.048950
16	6	0	1.095375	1.449389	-1.995943
17	6	0	1.509300	2.680832	-2.534746
18	6	0	1.374973	3.839665	-1.802303
19	6	0	0.820649	3.792685	-0.491403
20	6	0	0.448576	2.506172	-0.034078
21	6	0	0.603247	4.860112	0.433898
22	6	0	0.071453	4.615827	1.689125
23	6	0	-0.287218	3.336738	2.122998
24	6	0	-0.110379	2.248659	1.274545
25	6	0	-2.433303	0.769447	-1.487218
26	6	0	-3.773707	0.751221	-1.906164
27	6	0	-4.651903	-0.162856	-1.370237
28	6	0	-4.201849	-1.090224	-0.388916
29	6	0	-2.835216	-0.989311	-0.030753
30	6	0	-4.945996	-2.107293	0.286814
31	6	0	-4.340041	-2.923656	1.228028
32	6	0	-2.992370	-2.809288	1.569631
33	6	0	-2.203622	-1.842893	0.953765
34	1	0	3.882141	-0.634238	3.513848
35	1	0	5.135895	-2.167691	2.042431
36	1	0	3.947220	-4.006474	-2.387259
37	1	0	1.712592	-3.020109	-2.882632
38	1	0	1.932843	2.710376	-3.531965
39	1	0	1.689891	4.786056	-2.217431
40	1	0	-0.068410	5.465429	2.347713
41	1	0	-0.707472	3.180751	3.109434
42	1	0	-4.109348	1.461771	-2.652396
43	1	0	-5.683229	-0.179794	-1.689912
44	1	0	-4.954774	-3.676269	1.707903
45	1	0	-2.546848	-3.463081	2.309540
46	13	0	-0.120078	-0.290629	0.237752
47	1	0	1.622316	0.231026	2.771396
48	1	0	1.166996	0.512675	-2.540770
49	1	0	-1.720723	1.479356	-1.895759
50	7	0	5.469927	-3.699481	-0.349465
51	8	0	5.854847	-4.449423	-1.231811
52	8	0	6.117690	-3.458217	0.661525
53	7	0	-6.357525	-2.341702	0.031324
54	8	0	-6.923842	-1.648222	-0.805689
55	8	0	-6.919488	-3.223042	0.661888
56	7	0	0.917823	6.243915	0.112773
57	8	0	0.791157	7.081542	0.990430
58	8	0	1.289401	6.506855	-1.024575

D) *mer*-Al(qCl)$_3$

1	7	0	0.630718	1.342761	-0.764966
2	7	0	1.662448	-0.870097	0.985391
3	7	0	-2.023749	0.043411	-0.529343
4	8	0	-1.041994	-1.619163	1.233009
5	8	0	-0.332456	1.019762	1.612723
6	8	0	0.347307	-1.345766	-1.206084
7	6	0	2.245655	-0.574758	2.129201
8	6	0	3.495899	-1.130689	2.475220
9	6	0	4.117638	-2.000074	1.608436
10	6	0	3.500495	-2.334234	0.376649
11	6	0	2.250718	-1.729630	0.114588
12	6	0	4.010781	-3.213478	-0.612520
13	6	0	3.296591	-3.451205	-1.763844
14	6	0	2.046462	-2.841238	-2.009607
15	6	0	1.491793	-1.973294	-1.081213

16	6	0	1.124891	1.404040	-1.986827
17	6	0	1.606469	2.618676	-2.522091
18	6	0	1.560529	3.765379	-1.761846
19	6	0	1.037054	3.719382	-0.445709
20	6	0	0.583431	2.458257	0.006339
21	6	0	0.927023	4.804487	0.459469
22	6	0	0.399093	4.608056	1.715539
23	6	0	-0.046755	3.342224	2.154003
24	6	0	0.033990	2.239268	1.315592
25	6	0	-2.449159	0.920179	-1.416724
26	6	0	-3.796961	0.965644	-1.828218
27	6	0	-4.697584	0.072564	-1.296971
28	6	0	-4.266091	-0.880094	-0.342052
29	6	0	-2.896227	-0.847502	0.014594
30	6	0	-5.076626	-1.856815	0.287480
31	6	0	-4.530063	-2.725268	1.204471
32	6	0	-3.164934	-2.680466	1.554505
33	6	0	-2.316820	-1.746991	0.976292
34	1	0	3.951081	-0.868478	3.423083
35	1	0	5.078580	-2.439234	1.858060
36	1	0	3.708124	-4.131864	-2.502258
37	1	0	1.503215	-3.058909	-2.922290
38	1	0	2.006401	2.633905	-3.529240
39	1	0	1.924683	4.708237	-2.157591
40	1	0	0.325849	5.456727	2.388279
41	1	0	-0.459264	3.222073	3.149399
42	1	0	-4.106369	1.704237	-2.558386
43	1	0	-5.739720	0.088298	-1.599393
44	1	0	-5.173346	-3.464808	1.670907
45	1	0	-2.762835	-3.376591	2.281489
46	13	0	-0.161707	-0.297642	0.277444
47	1	0	1.705159	0.109528	2.777545
48	1	0	1.129044	0.472836	-2.546248
49	1	0	-1.713892	1.610356	-1.819971
50	17	0	5.551142	-3.993676	-0.360008
51	17	0	1.467268	6.390776	-0.028176
52	17	0	-6.775294	-1.952551	-0.107312

E) *mer*-Al(qBr)$_3$

1	7	0	-0.524108	-1.872462	0.981533
2	7	0	0.496422	-0.949691	-1.693722
3	7	0	-0.322861	0.969797	1.816313
4	8	0	0.273390	1.637496	-0.635520
5	8	0	-1.843880	-0.119993	-0.393252
6	8	0	1.759836	-0.483414	0.530249
7	6	0	-0.214514	-1.113877	-2.791229
8	6	0	0.339898	-1.729638	-3.934606
9	6	0	1.641997	-2.175274	-3.900279
10	6	0	2.422367	-2.010717	-2.728777
11	6	0	1.787880	-1.367599	-1.646455
12	6	0	3.762846	-2.441429	-2.557931
13	6	0	4.388405	-2.229916	-1.350317
14	6	0	3.737968	-1.580630	-0.276652
15	6	0	2.439794	-1.104881	-0.394061
16	6	0	0.229383	-2.713060	1.666333
17	6	0	-0.305574	-3.900281	2.212965
18	6	0	-1.638405	-4.192412	2.027480
19	6	0	-2.464881	-3.308592	1.290308
20	6	0	-1.839530	-2.147165	0.786638
21	6	0	-3.843143	-3.495885	1.018655
22	6	0	-4.514018	-2.550875	0.275244
23	6	0	-3.874182	-1.394691	-0.224565
24	6	0	-2.528726	-1.148486	0.018665
25	6	0	-0.630790	0.561879	3.031685
26	6	0	-0.815151	1.467097	4.097013
27	6	0	-0.666167	2.815693	3.867913

28	6	0	-0.333944	3.283701	2.574117
29	6	0	-0.175018	2.300638	1.571786
30	6	0	-0.153304	4.643011	2.217659
31	6	0	0.170824	4.958674	0.917808
32	6	0	0.325060	3.967752	-0.075393
33	6	0	0.156321	2.619505	0.210640
34	1	0	-0.268942	-1.843398	-4.823850
35	1	0	2.083671	-2.656610	-4.768984
36	1	0	5.409426	-2.565245	-1.200776
37	1	0	0.342619	-4.565241	2.771753
38	1	0	-2.067033	-5.102210	2.439727
39	1	0	-5.568284	-2.683526	0.054981
40	1	0	-1.069970	1.087160	5.079319
41	1	0	-0.801869	3.532794	4.673192
42	1	0	0.314947	5.994960	0.630184
43	13	0	-0.016111	-0.055586	0.062256
44	1	0	-1.237757	-0.748372	-2.757533
45	1	0	1.272530	-2.431277	1.787133
46	1	0	-0.737800	-0.509076	3.178606
47	1	0	4.281741	-2.937166	-3.371341
48	1	0	-4.356349	-4.376227	1.390575
49	1	0	-0.269736	5.419415	2.966019
50	35	0	0.774373	4.469435	-1.833543
51	35	0	4.633262	-1.350429	1.366617
52	35	0	-4.853665	-0.155429	-1.248128

F) *fac*-Alq_3

1	7	0	-0.464892	-1.620584	0.450246
2	7	0	1.635795	0.402247	0.455891
3	7	0	-1.163209	1.210675	0.456556
4	8	0	0.255720	1.607743	-1.702193
5	8	0	-1.515330	-0.581502	-1.705891
6	8	0	1.268755	-1.022872	-1.704665
7	6	0	1.757770	1.157771	1.529999
8	6	0	2.992319	1.309819	2.198093
9	6	0	4.103408	0.655876	1.719285
10	6	0	4.007818	-0.154363	0.559854
11	6	0	2.728126	-0.239492	-0.040697
12	6	0	5.079503	-0.868499	-0.027157
13	6	0	4.837454	-1.618157	-1.160922
14	6	0	3.565601	-1.701324	-1.765172
15	6	0	2.483435	-1.014993	-1.226531
16	6	0	0.126539	-2.106511	1.524401
17	6	0	-0.361821	-3.251472	2.190687
18	6	0	-1.486819	-3.881547	1.712192
19	6	0	-2.142445	-3.387344	0.556466
20	6	0	-1.572297	-2.238209	-0.043369
21	6	0	-3.300379	-3.951908	-0.028724
22	6	0	-3.829119	-3.362278	-1.159670
23	6	0	-3.262028	-2.220638	-1.763316
24	6	0	-2.122371	-1.632931	-1.226255
25	6	0	-1.879509	0.936352	1.529464
26	6	0	-2.630810	1.927890	2.197262
27	6	0	-2.622375	3.217335	1.718127
28	6	0	-1.871188	3.542058	0.560565
29	6	0	-1.154509	2.477814	-0.038956
30	6	0	-1.788560	4.827649	-0.025997
31	6	0	-1.017555	4.993264	-1.159278
32	6	0	-0.305469	3.935121	-1.761113
33	6	0	-0.357399	2.655021	-1.222406
34	1	0	0.862230	1.659842	1.884836
35	1	0	3.045771	1.941989	3.077061
36	1	0	5.063206	0.757354	2.219611
37	1	0	6.069166	-0.816305	0.414647
38	1	0	5.659078	-2.164790	-1.615286
39	1	0	3.412992	-2.291329	-2.661847

40	1	0	1.010128	-1.584718	1.880943
41	1	0	0.158077	-3.617975	3.068309
42	1	0	-1.882136	-4.762345	2.211808
43	1	0	-3.753959	-4.832920	0.413595
44	1	0	-4.716819	-3.795092	-1.612418
45	1	0	-3.698342	-1.788413	-2.657097
46	1	0	-1.862522	-0.090210	1.884933
47	1	0	-3.204742	1.656827	3.075872
48	1	0	-3.194230	3.996000	2.216749
49	1	0	-2.330566	5.658102	0.414273
50	1	0	-0.954634	5.977961	-1.614159
51	1	0	0.285342	4.099116	-2.655442
52	13	0	0.003155	-0.001096	-0.820325

G) *fac*-Al(qCH$_3$)$_3$

1	7	0	1.966800	0.285249	0.547227
2	7	0	-1.180642	1.249761	0.562650
3	7	0	-0.609917	-1.815768	0.291066
4	8	0	-1.370579	-0.255884	-1.691577
5	8	0	1.298759	-1.137874	-1.579966
6	8	0	0.597447	1.566759	-1.397630
7	6	0	-2.051629	1.075192	1.545658
8	6	0	-2.992334	2.086249	1.881232
9	6	0	-3.005881	3.276308	1.205643
10	6	0	-2.071402	3.502538	0.167047
11	6	0	-1.182808	2.439021	-0.123649
12	6	0	-1.983969	4.712030	-0.561848
13	6	0	-1.022963	4.833046	-1.542812
14	6	0	-0.133241	3.784866	-1.843550
15	6	0	-0.196933	2.575456	-1.160892
16	6	0	2.271135	1.038591	1.593915
17	6	0	3.622325	1.248474	1.977161
18	6	0	4.644882	0.675669	1.268661
19	6	0	4.351361	-0.123121	0.138491
20	6	0	2.981773	-0.272546	-0.185190
21	6	0	5.331600	-0.764025	-0.657324
22	6	0	4.926959	-1.522311	-1.734443
23	6	0	3.567230	-1.671471	-2.072880
24	6	0	2.577087	-1.049325	-1.323516
25	6	0	-0.138003	-2.633961	1.221356
26	6	0	-0.873217	-3.779853	1.620602
27	6	0	-2.083074	-4.067993	1.043460
28	6	0	-2.588293	-3.234900	0.018555
29	6	0	-1.790106	-2.119701	-0.332089
30	6	0	-3.809893	-3.457375	-0.661216
31	6	0	-4.183793	-2.586314	-1.662703
32	6	0	-3.386041	-1.486027	-2.035519
33	6	0	-2.178191	-1.233846	-1.393937
34	1	0	-3.691754	1.895635	2.688202
35	1	0	-3.718775	4.055884	1.462707
36	1	0	-2.670502	5.521787	-0.336858
37	1	0	-0.947599	5.759138	-2.105529
38	1	0	0.613011	3.890988	-2.623059
39	1	0	3.825705	1.868877	2.843137
40	1	0	5.680334	0.828349	1.562629
41	1	0	6.381466	-0.646301	-0.409183
42	1	0	5.673425	-2.016734	-2.349436
43	1	0	3.266132	-2.260381	-2.932174
44	1	0	-0.458768	-4.419848	2.391689
45	1	0	-2.653921	-4.939451	1.354229
46	1	0	-4.423575	-4.311063	-0.392815
47	1	0	-5.118137	-2.752960	-2.191050
48	1	0	-3.687793	-0.824867	-2.840273
49	13	0	0.148234	-0.051274	-0.653712
50	6	0	1.183503	-2.349025	1.875735
51	1	0	1.179362	-1.380664	2.384930

52	1	0	1.413280	-3.123358	2.609366
53	1	0	1.983712	-2.324488	1.130651
54	6	0	1.185818	1.688783	2.404499
55	1	0	0.712737	2.497483	1.839160
56	1	0	0.405931	0.973228	2.669773
57	1	0	1.602319	2.106054	3.322919
58	6	0	-2.059427	-0.186975	2.366789
59	1	0	-2.637636	-0.975526	1.873095
60	1	0	-1.051276	-0.568576	2.531522
61	1	0	-2.518260	0.009913	3.337991

H) *fac*-Al(qNO$_2$)$_3$

1	7	0	1.692394	0.110042	0.366440
2	7	0	-0.945468	1.398082	0.359936
3	7	0	-0.741969	-1.530491	0.355462
4	8	0	-1.574426	-0.326938	-1.783926
5	8	0	1.081156	-1.211068	-1.778375
6	8	0	0.517325	1.530006	-1.774517
7	6	0	-1.701265	1.234043	1.429993
8	6	0	-2.298633	2.329210	2.076568
9	6	0	-2.099093	3.605492	1.601262
10	6	0	-1.293769	3.815428	0.445743
11	6	0	-0.746334	2.646762	-0.139942
12	6	0	-0.972438	5.044161	-0.208226
13	6	0	-0.184814	5.058086	-1.348921
14	6	0	0.344270	3.898542	-1.913766
15	6	0	0.078420	2.662612	-1.330238
16	6	0	1.923632	0.840727	1.441777
17	6	0	3.169680	0.808802	2.090173
18	6	0	4.177202	0.001756	1.611627
19	6	0	3.961633	-0.791483	0.449616
20	6	0	2.676646	-0.680889	-0.138343
21	6	0	4.868891	-1.678337	-0.206957
22	6	0	4.488458	-2.366083	-1.349387
23	6	0	3.222649	-2.240883	-1.919409
24	6	0	2.281379	-1.398256	-1.333397
25	6	0	-0.225684	-2.106457	1.425196
26	6	0	-0.881993	-3.167835	2.070907
27	6	0	-2.091524	-3.622597	1.596979
28	6	0	-2.673624	-3.024123	0.443731
29	6	0	-1.924336	-1.975180	-0.147167
30	6	0	-3.899797	-3.353071	-0.209361
31	6	0	-4.297131	-2.681096	-1.355346
32	6	0	-3.547240	-1.651702	-1.923901
33	6	0	-2.342020	-1.269035	-1.339673
34	1	0	-2.914725	2.160193	2.952041
35	1	0	-2.553490	4.451406	2.096870
36	1	0	0.021490	6.021429	-1.801484
37	1	0	0.956920	3.939924	-2.806041
38	1	0	3.330080	1.425020	2.967158
39	1	0	5.134291	-0.029112	2.110534
40	1	0	5.219454	-3.023715	-1.804396
41	1	0	2.956673	-2.786324	-2.816711
42	1	0	-0.428750	-3.620598	2.945113
43	1	0	-2.602724	-4.432487	2.095698
44	1	0	-5.233571	-2.980167	-1.811551
45	1	0	-3.883109	-1.143545	-2.819723
46	13	0	0.006646	-0.003863	-0.865948
47	1	0	1.111411	1.466830	1.799359
48	1	0	-1.838535	0.218080	1.788957
49	1	0	0.722961	-1.722188	1.787745
50	7	0	-4.789451	-4.392532	0.281748
51	8	0	-4.533917	-4.921662	1.357497
52	8	0	-5.762582	-4.681076	-0.395564
53	7	0	-1.442712	6.331072	0.277178
54	8	0	-2.061211	6.364700	1.334560

55	8	0	-1.191525	7.324104	-0.385765
56	7	0	6.219164	-1.913365	0.279048
57	8	0	6.567657	-1.369280	1.320672
58	8	0	6.944090	-2.652004	-0.367352

I) *fac*-Al(qCl)$_3$

1	7	0	1.423457	-0.960682	-0.333845
2	7	0	-1.491337	-0.729959	-0.352864
3	7	0	0.161215	1.668834	-0.312960
4	8	0	-1.203192	1.037316	1.824570
5	8	0	1.562637	0.479908	1.839201
6	8	0	-0.316438	-1.627272	1.800865
7	6	0	-2.053797	-0.205348	-1.424928
8	6	0	-3.122659	-0.840816	-2.091229
9	6	0	-3.598695	-2.040890	-1.618154
10	6	0	-3.018593	-2.623601	-0.464782
11	6	0	-1.954852	-1.909349	0.141722
12	6	0	-3.402559	-3.846794	0.135747
13	6	0	-2.755225	-4.298834	1.263954
14	6	0	-1.702000	-3.578102	1.861599
15	6	0	-1.277201	-2.370079	1.324076
16	6	0	1.273611	-1.705994	-1.411430
17	6	0	2.377818	-2.269833	-2.084915
18	6	0	3.649274	-2.039052	-1.614558
19	6	0	3.838623	-1.248803	-0.453592
20	6	0	2.669907	-0.734701	0.161659
21	6	0	5.080159	-0.929013	0.146749
22	6	0	5.121055	-0.154284	1.284933
23	6	0	3.951684	0.345620	1.891645
24	6	0	2.701692	0.068888	1.353493
25	6	0	0.898082	1.927354	-1.375997
26	6	0	0.830309	3.168127	-2.044660
27	6	0	-0.024979	4.141131	-1.583264
28	6	0	-0.820492	3.894050	-0.436812
29	6	0	-0.679319	2.621848	0.172436
30	6	0	-1.739264	4.796754	0.150978
31	6	0	-2.450640	4.429877	1.271961
32	6	0	-2.299436	3.163864	1.871620
33	6	0	-1.414671	2.231605	1.344547
34	1	0	-3.556751	-0.373327	-2.967211
35	1	0	-4.419142	-2.547624	-2.115679
36	1	0	-3.072102	-5.238551	1.705501
37	1	0	-1.216708	-3.955051	2.754538
38	1	0	2.208300	-2.878256	-2.965671
39	1	0	4.512894	-2.460752	-2.118970
40	1	0	6.086289	0.073694	1.726304
41	1	0	4.013120	0.946781	2.791487
42	1	0	1.453740	3.338386	-2.914713
43	1	0	-0.097266	5.100997	-2.084738
44	1	0	-3.147468	5.141377	1.703738
45	1	0	-2.868239	2.904398	2.756945
46	13	0	0.026934	-0.026669	0.941426
47	1	0	0.258598	-1.864897	-1.764453
48	1	0	-1.656165	0.741267	-1.779464
49	1	0	1.559237	1.137695	-1.722386
50	17	0	-1.966652	6.377305	-0.552477
51	17	0	-4.703676	-4.779431	-0.562613
52	17	0	6.560159	-1.518354	-0.567261

J) *fac*-Al(qBr)$_3$

1	7	0	1.680015	-0.123819	1.476215
2	7	0	-0.754668	1.516313	1.459492
3	7	0	-0.955554	-1.400041	1.466973
4	8	0	-1.620259	-0.084084	-0.688516
5	8	0	0.881162	-1.373562	-0.669753

6	8	0	0.749758	1.436500	-0.673899
7	6	0	-1.536751	1.485621	2.521938
8	6	0	-1.979315	2.664374	3.158696
9	6	0	-1.586327	3.886088	2.661962
10	6	0	-0.751890	3.952966	1.519485
11	6	0	-0.368468	2.716769	0.947344
12	6	0	-0.283020	5.147227	0.921262
13	6	0	0.529686	5.066893	-0.188553
14	6	0	0.903950	3.828511	-0.747317
15	6	0	0.466006	2.620236	-0.219837
16	6	0	2.032723	0.567885	2.542731
17	6	0	3.272617	0.366859	3.186211
18	6	0	4.143029	-0.577745	2.692016
19	6	0	3.796335	-1.332606	1.544596
20	6	0	2.536207	-1.050335	0.965875
21	6	0	4.602740	-2.330246	0.945329
22	6	0	4.136123	-2.989003	-0.171668
23	6	0	2.880186	-2.694652	-0.738166
24	6	0	2.045632	-1.719203	-0.209076
25	6	0	-0.542922	-2.053869	2.536311
26	6	0	-1.349927	-3.014688	3.181439
27	6	0	-2.605590	-3.281626	2.685455
28	6	0	-3.073958	-2.602543	1.534515
29	6	0	-2.188186	-1.664565	0.954213
30	6	0	-4.341423	-2.793060	0.933696
31	6	0	-4.668556	-2.063167	-0.188437
32	6	0	-3.774142	-1.135235	-0.757690
33	6	0	-2.511634	-0.908651	-0.225759
34	1	0	-2.622705	2.590150	4.027572
35	1	0	-1.911602	4.808437	3.136160
36	1	0	0.897450	5.973106	-0.658831
37	1	0	3.521022	0.960917	4.057807
38	1	0	5.103195	-0.748996	3.171603
39	1	0	4.742640	-3.755452	-0.643427
40	1	0	-0.967980	-3.528731	4.055768
41	1	0	-3.245835	-4.016899	3.166026
42	1	0	-5.636304	-2.196600	-0.660918
43	13	0	-0.003894	-0.006734	0.210174
44	1	0	1.321360	1.302534	2.910149
45	1	0	-1.826048	0.505541	2.891289
46	1	0	0.452056	-1.816959	2.903641
47	1	0	5.575609	-2.566110	1.362925
48	1	0	-0.565141	6.109237	1.335621
49	1	0	-5.040523	-3.507702	1.354547
50	35	0	2.298365	-3.648161	-2.294633
51	35	0	-4.292486	-0.157548	-2.321207
52	35	0	2.042145	3.795527	-2.287674

K) *mer*-Gaq_3

1	7	0	-0.660586	1.442007	0.794420
2	7	0	-1.730852	-0.927661	-0.917108
3	7	0	2.086241	0.099088	0.568665
4	8	0	1.128691	-1.655526	-1.194308
5	8	0	0.265167	1.073227	-1.656890
6	8	0	-0.395522	-1.322907	1.344529
7	6	0	-2.323149	-0.691394	-2.069370
8	6	0	-3.590639	-1.240443	-2.363328
9	6	0	-4.212802	-2.034683	-1.428213
10	6	0	-3.589621	-2.301689	-0.182395
11	6	0	-2.320403	-1.711110	0.020969
12	6	0	-4.141244	-3.102525	0.847363
13	6	0	-3.419713	-3.280586	2.008543
14	6	0	-2.150272	-2.696107	2.213385
15	6	0	-1.565012	-1.904383	1.232466
16	6	0	-1.126061	1.539603	2.023768
17	6	0	-1.620864	2.765209	2.524287

18	6	0	-1.615533	3.875828	1.711861
19	6	0	-1.125003	3.791162	0.383668
20	6	0	-0.654512	2.520287	-0.027538
21	6	0	-1.079482	4.864293	-0.538447
22	6	0	-0.579477	4.631392	-1.803134
23	6	0	-0.113182	3.365596	-2.218462
24	6	0	-0.137426	2.279384	-1.350210
25	6	0	2.500634	0.998121	1.436905
26	6	0	3.852532	1.075038	1.834680
27	6	0	4.758445	0.187838	1.302650
28	6	0	4.338833	-0.788545	0.365019
29	6	0	2.963280	-0.785702	0.025612
30	6	0	5.190225	-1.744026	-0.239026
31	6	0	4.650588	-2.638986	-1.139496
32	6	0	3.283375	-2.637464	-1.485551
33	6	0	2.406329	-1.719794	-0.919490
34	1	0	-1.781329	-0.058413	-2.766979
35	1	0	-4.053355	-1.031180	-3.320832
36	1	0	-5.188337	-2.468432	-1.633574
37	1	0	-5.113808	-3.563640	0.709695
38	1	0	-3.836235	-3.896316	2.800764
39	1	0	-1.606361	-2.867409	3.136117
40	1	0	-1.100444	0.629839	2.617811
41	1	0	-1.997047	2.813070	3.539746
42	1	0	-1.990318	4.828504	2.077577
43	1	0	-1.434776	5.845912	-0.242722
44	1	0	-0.540856	5.451389	-2.514783
45	1	0	0.274912	3.220129	-3.220758
46	1	0	1.753874	1.680254	1.833983
47	1	0	4.155721	1.830119	2.550762
48	1	0	5.805144	0.225541	1.593768
49	1	0	6.245762	-1.760070	0.011935
50	1	0	5.298971	-3.375386	-1.605965
51	1	0	2.890820	-3.352673	-2.199815
52	31	0	0.157687	-0.287146	-0.239817

L) *fac*-Gaq_3

1	7	0	1.517864	-0.772993	0.527822
2	7	0	-0.128755	1.731369	0.467286
3	7	0	-1.490079	-0.953449	0.500749
4	8	0	-1.651703	0.479227	-1.742923
5	8	0	0.363878	-1.712160	-1.690020
6	8	0	1.254499	1.101059	-1.729237
7	6	0	-0.855066	2.000367	1.532984
8	6	0	-0.738334	3.228005	2.222407
9	6	0	0.159225	4.166512	1.771067
10	6	0	0.949292	3.906666	0.622549
11	6	0	0.753743	2.649986	-0.005929
12	6	0	1.897131	4.805105	0.079854
13	6	0	2.599137	4.428952	-1.047415
14	6	0	2.407414	3.184468	-1.680015
15	6	0	1.485056	2.267024	-1.186272
16	6	0	2.066731	-0.251892	1.606725
17	6	0	3.112748	-0.902531	2.297703
18	6	0	3.571454	-2.112045	1.832499
19	6	0	3.004427	-2.693228	0.670546
20	6	0	1.962867	-1.961898	0.043579
21	6	0	3.405906	-3.928978	0.112439
22	6	0	2.771665	-4.380208	-1.027059
23	6	0	1.739840	-3.657106	-1.658945
24	6	0	1.310277	-2.435341	-1.151056
25	6	0	-1.346822	-1.681463	1.588994
26	6	0	-2.459882	-2.195594	2.290429
27	6	0	-3.726181	-1.927793	1.826387
28	6	0	-3.909686	-1.153559	0.652548
29	6	0	-2.730779	-0.689675	0.014507

30	6	0	-5.165437	-0.825018	0.091097
31	6	0	-5.199516	-0.067075	-1.062037
32	6	0	-4.032138	0.392217	-1.704231
33	6	0	-2.773278	0.093686	-1.193608
34	1	0	-1.547351	1.231020	1.865842
35	1	0	-1.355863	3.411088	3.094317
36	1	0	0.271813	5.117687	2.285238
37	1	0	2.055090	5.770467	0.549372
38	1	0	3.326921	5.115484	-1.470551
39	1	0	2.969460	2.920393	-2.568829
40	1	0	1.677335	0.703815	1.947799
41	1	0	3.538326	-0.438827	3.180134
42	1	0	4.375152	-2.633328	2.346206
43	1	0	4.202359	-4.497920	0.580809
44	1	0	3.077462	-5.327360	-1.462598
45	1	0	1.267614	-4.035055	-2.558959
46	1	0	-0.330758	-1.867135	1.927505
47	1	0	-2.298718	-2.791848	3.181305
48	1	0	-4.599312	-2.308909	2.350111
49	1	0	-6.076573	-1.173497	0.566239
50	1	0	-6.161016	0.186508	-1.499616
51	1	0	-4.091699	0.979447	-2.613885
52	31	0	-0.028568	-0.029001	-0.842338

M) *mer*-Inq_3

1	7	0	-0.459872	1.634259	0.788197
2	7	0	-1.981240	-0.833627	-0.915369
3	7	0	2.161801	-0.139755	0.576144
4	8	0	1.037096	-1.884328	-1.154307
5	8	0	0.253422	1.106188	-1.745895
6	8	0	-0.741752	-1.236883	1.444323
7	6	0	-2.539678	-0.600289	-2.086676
8	6	0	-3.860739	-1.009727	-2.367447
9	6	0	-4.577622	-1.665230	-1.394334
10	6	0	-4.000493	-1.922815	-0.124494
11	6	0	-2.669584	-1.476324	0.067434
12	6	0	-4.665471	-2.582993	0.937185
13	6	0	-3.994060	-2.770226	2.126509
14	6	0	-2.669768	-2.327748	2.325062
15	6	0	-1.969500	-1.674332	1.315994
16	6	0	-0.837140	1.826595	2.037645
17	6	0	-1.074240	3.123544	2.543562
18	6	0	-0.908053	4.206826	1.712273
19	6	0	-0.514994	4.025023	0.361386
20	6	0	-0.303068	2.686676	-0.057934
21	6	0	-0.332706	5.073704	-0.571418
22	6	0	0.042305	4.756639	-1.860502
23	6	0	0.248820	3.428296	-2.285992
24	6	0	0.084613	2.358824	-1.410598
25	6	0	2.674775	0.741617	1.411889
26	6	0	4.028591	0.698277	1.804677
27	6	0	4.836124	-0.292334	1.299098
28	6	0	4.315737	-1.251305	0.394357
29	6	0	2.943273	-1.126838	0.055512
30	6	0	5.076005	-2.299188	-0.176125
31	6	0	4.456679	-3.169614	-1.048031
32	6	0	3.095702	-3.052150	-1.392943
33	6	0	2.302464	-2.039616	-0.863459
34	1	0	-1.927507	-0.075028	-2.815419
35	1	0	-4.288162	-0.804728	-3.342131
36	1	0	-5.596640	-1.992494	-1.585522
37	1	0	-5.684190	-2.930831	0.800992
38	1	0	-4.496495	-3.278387	2.944704
39	1	0	-2.167019	-2.497465	3.271177
40	1	0	-0.947301	0.930828	2.644855
41	1	0	-1.382429	3.246368	3.575515

42	1	0	-1.081199	5.215424	2.079523
43	1	0	-0.491289	6.102291	-0.264344
44	1	0	0.184110	5.555713	-2.582647
45	1	0	0.541711	3.213890	-3.308179
46	1	0	2.003462	1.509232	1.788515
47	1	0	4.409295	1.441933	2.495012
48	1	0	5.883380	-0.351290	1.584807
49	1	0	6.125980	-2.401628	0.077543
50	1	0	5.032821	-3.977205	-1.490965
51	1	0	2.637491	-3.750840	-2.084338
52	49	0	0.075127	-0.319459	-0.240830

N) *mer*-In(qCH$_3$)$_3$

1	7	0	0.242280	1.966333	-0.436383
2	7	0	2.162617	-0.443135	0.924800
3	7	0	-1.908458	-0.855562	-0.843941
4	8	0	-0.422350	-2.106029	1.073460
5	8	0	-0.981001	0.697965	1.612836
6	8	0	1.088984	-0.954928	-1.511295
7	6	0	2.632085	-0.189214	2.135554
8	6	0	4.003335	-0.404027	2.428937
9	6	0	4.846263	-0.882186	1.458381
10	6	0	4.355671	-1.171199	0.160600
11	6	0	2.977453	-0.934021	-0.056573
12	6	0	5.154212	-1.670969	-0.897216
13	6	0	4.564622	-1.917977	-2.117036
14	6	0	3.191365	-1.687571	-2.342911
15	6	0	2.365730	-1.201528	-1.336280
16	6	0	0.902540	2.582600	-1.408299
17	6	0	0.660476	3.951973	-1.695951
18	6	0	-0.253881	4.661924	-0.962996
19	6	0	-0.941328	4.038543	0.105897
20	6	0	-0.646131	2.670120	0.332595
21	6	0	-1.873297	4.708001	0.934005
22	6	0	-2.472544	4.011408	1.960667
23	6	0	-2.183867	2.654923	2.204751
24	6	0	-1.280569	1.952879	1.411274
25	6	0	-2.573187	-0.264164	-1.821569
26	6	0	-3.876788	-0.693965	-2.174007
27	6	0	-4.455682	-1.737053	-1.499123
28	6	0	-3.750129	-2.402815	-0.466107
29	6	0	-2.450817	-1.917293	-0.172000
30	6	0	-4.266503	-3.508073	0.250577
31	6	0	-3.480359	-4.099048	1.216000
32	6	0	-2.183311	-3.636701	1.507582
33	6	0	-1.630019	-2.548372	0.838084
34	1	0	4.365477	-0.187658	3.427987
35	1	0	5.898338	-1.050617	1.674849
36	1	0	6.210771	-1.854040	-0.730371
37	1	0	5.168144	-2.302315	-2.934300
38	1	0	2.746749	-1.892606	-3.311237
39	1	0	1.210274	4.419261	-2.505649
40	1	0	-0.452088	5.707803	-1.184444
41	1	0	-2.094741	5.754590	0.751382
42	1	0	-3.187490	4.515868	2.604362
43	1	0	-2.664207	2.121902	3.018163
44	1	0	-4.398474	-0.187013	-2.978514
45	1	0	-5.456793	-2.073922	-1.756876
46	1	0	-5.262798	-3.874731	0.025489
47	1	0	-3.864641	-4.951117	1.769918
48	1	0	-1.578492	-4.123968	2.264813
49	49	0	0.053509	-0.326322	0.156202
50	6	0	1.924356	1.831641	-2.212442
51	1	0	2.700795	1.422724	-1.558068
52	1	0	1.476180	0.982676	-2.735254
53	1	0	2.397921	2.496954	-2.936059

54	6	0	-1.915934	0.873391	-2.551914
55	1	0	-2.000868	1.804350	-1.979265
56	1	0	-0.854982	0.656343	-2.705454
57	1	0	-2.387281	1.028505	-3.524505
58	6	0	1.681478	0.329511	3.175653
59	1	0	1.357183	1.345514	2.926891
60	1	0	0.780114	-0.288310	3.216478
61	1	0	2.157363	0.345655	4.157654

O) *mer*-In(qNO$_2$)$_3$

1	7	0	-0.432508	1.613159	0.807610
2	7	0	-1.960807	-0.805888	-1.031437
3	7	0	2.127610	-0.280527	0.595542
4	8	0	0.986011	-1.871010	-1.225854
5	8	0	0.317574	1.157906	-1.705936
6	8	0	-0.852646	-1.288008	1.347998
7	6	0	-2.432953	-0.521947	-2.229933
8	6	0	-3.719684	-0.934883	-2.613563
9	6	0	-4.503598	-1.641557	-1.730921
10	6	0	-4.019244	-1.953540	-0.428060
11	6	0	-2.706168	-1.502476	-0.133201
12	6	0	-4.686187	-2.672701	0.612129
13	6	0	-4.061299	-2.905763	1.824895
14	6	0	-2.771767	-2.452395	2.101993
15	6	0	-2.052356	-1.741685	1.144136
16	6	0	-0.843350	1.748994	2.055348
17	6	0	-1.062531	3.022394	2.608281
18	6	0	-0.841201	4.147584	1.847271
19	6	0	-0.402103	4.027622	0.497301
20	6	0	-0.222428	2.701469	0.021843
21	6	0	-0.145251	5.072966	-0.441647
22	6	0	0.240715	4.780788	-1.738908
23	6	0	0.406811	3.473585	-2.194825
24	6	0	0.186091	2.394404	-1.340366
25	6	0	2.633174	0.552049	1.485761
26	6	0	3.968911	0.451197	1.904425
27	6	0	4.774059	-0.535487	1.385124
28	6	0	4.258255	-1.450376	0.423541
29	6	0	2.898866	-1.262531	0.054281
30	6	0	4.949292	-2.517556	-0.228547
31	6	0	4.309001	-3.303805	-1.171707
32	6	0	2.975685	-3.110302	-1.525044
33	6	0	2.227521	-2.094553	-0.932795
34	1	0	-4.086172	-0.695438	-3.604933
35	1	0	-5.493336	-1.960820	-2.021244
36	1	0	-4.610807	-3.460034	2.576744
37	1	0	-2.308284	-2.650916	3.061222
38	1	0	-1.404760	3.110049	3.632915
39	1	0	-1.001556	5.128495	2.269891
40	1	0	0.419199	5.612712	-2.410338
41	1	0	0.713981	3.276121	-3.215069
42	1	0	4.357110	1.153156	2.633020
43	1	0	5.802217	-0.621018	1.704023
44	1	0	4.880773	-4.096472	-1.639876
45	1	0	2.498133	-3.743003	-2.263558
46	49	0	0.056419	-0.314264	-0.255904
47	1	0	-1.777772	0.041047	-2.889480
48	1	0	-0.995668	0.828871	2.614136
49	1	0	1.970361	1.319378	1.876877
50	7	0	-6.036802	-3.194409	0.465500
51	8	0	-6.490516	-3.876716	1.370031
52	8	0	-6.662333	-2.924575	-0.552528
53	7	0	6.339377	-2.840338	0.051847
54	8	0	6.906813	-2.252098	0.965103
55	8	0	6.880754	-3.692753	-0.633895
56	7	0	-0.266079	6.481820	-0.098475

57	8	0	-0.157551	7.302211	-0.995052
58	8	0	-0.462240	6.783936	1.072633

P) *mer*-In(qCl)$_3$

1	7	0	-0.451107	1.569465	0.783863
2	7	0	-1.974884	-0.846325	-1.017620
3	7	0	2.148231	-0.234293	0.568577
4	8	0	1.027961	-1.921366	-1.215227
5	8	0	0.289320	1.092750	-1.748897
6	8	0	-0.799817	-1.310363	1.358062
7	6	0	-2.494765	-0.575623	-2.198371
8	6	0	-3.810227	-0.962550	-2.527184
9	6	0	-4.564786	-1.636434	-1.596156
10	6	0	-4.025401	-1.932653	-0.318797
11	6	0	-2.695187	-1.506713	-0.071602
12	6	0	-4.703672	-2.611463	0.724443
13	6	0	-4.074484	-2.837791	1.926094
14	6	0	-2.753533	-2.408898	2.163278
15	6	0	-2.025510	-1.737819	1.188328
16	6	0	-0.844754	1.730447	2.032895
17	6	0	-1.059603	3.015098	2.575307
18	6	0	-0.854316	4.122133	1.785494
19	6	0	-0.443290	3.970312	0.436966
20	6	0	-0.255450	2.641786	-0.027465
21	6	0	-0.212076	5.025254	-0.479263
22	6	0	0.174864	4.747315	-1.770003
23	6	0	0.351771	3.425984	-2.224697
24	6	0	0.146696	2.339058	-1.382152
25	6	0	2.654355	0.624787	1.431462
26	6	0	4.000753	0.562957	1.841698
27	6	0	4.811739	-0.420521	1.328599
28	6	0	4.295426	-1.354034	0.396108
29	6	0	2.928072	-1.215484	0.035840
30	6	0	5.033528	-2.404319	-0.201834
31	6	0	4.427536	-3.250845	-1.100721
32	6	0	3.073699	-3.105820	-1.456184
33	6	0	2.286825	-2.097583	-0.912615
34	1	0	-4.208413	-0.726602	-3.507068
35	1	0	-5.579384	-1.945433	-1.826042
36	1	0	-4.612084	-3.361650	2.710086
37	1	0	-2.280537	-2.606195	3.118913
38	1	0	-1.382260	3.113853	3.605236
39	1	0	-1.008566	5.120690	2.181792
40	1	0	0.346629	5.571731	-2.454772
41	1	0	0.656528	3.238000	-3.248173
42	1	0	4.378066	1.288336	2.552769
43	1	0	5.852490	-0.493034	1.627027
44	1	0	5.011797	-4.049591	-1.546691
45	1	0	2.620999	-3.785404	-2.169245
46	49	0	0.069716	-0.367431	-0.283726
47	1	0	-1.855449	-0.037656	-2.893746
48	1	0	-0.985262	0.818682	2.608919
49	1	0	1.982823	1.388383	1.815445
50	17	0	-6.343001	-3.160453	0.477501
51	17	0	-0.419735	6.681000	0.036025
52	17	0	6.718140	-2.621699	0.206243

Q) *mer*-In(qBr)$_3$

1	7	0	-0.208677	-1.927852	1.148115
2	7	0	0.885035	-0.776087	-1.855818
3	7	0	-0.590666	1.158571	1.865227
4	8	0	-0.149763	1.954640	-0.671833
5	8	0	-1.874629	-0.681545	-0.541886
6	8	0	2.016653	-0.165210	0.507885
7	6	0	0.276385	-1.042012	-2.995463

8	6	0	0.981560	-1.552971	-4.105138
9	6	0	2.330584	-1.792915	-3.986006
10	6	0	3.002218	-1.530039	-2.766177
11	6	0	2.219980	-0.998501	-1.714022
12	6	0	4.379143	-1.774975	-2.538837
13	6	0	4.912006	-1.505881	-1.299993
14	6	0	4.124482	-0.976952	-0.256676
15	6	0	2.775668	-0.676817	-0.419300
16	6	0	0.667392	-2.506354	1.949222
17	6	0	0.372517	-3.716197	2.613237
18	6	0	-0.853116	-4.308212	2.412168
19	6	0	-1.801599	-3.716899	1.540998
20	6	0	-1.421323	-2.500774	0.922437
21	6	0	-3.074355	-4.263155	1.247251
22	6	0	-3.894964	-3.605230	0.360438
23	6	0	-3.506801	-2.398719	-0.257703
24	6	0	-2.278578	-1.794467	-0.001432
25	6	0	-0.800958	0.726245	3.093424
26	6	0	-1.183856	1.592315	4.137283
27	6	0	-1.344126	2.930473	3.864892
28	6	0	-1.128252	3.424822	2.556165
29	6	0	-0.746060	2.480605	1.570882
30	6	0	-1.272308	4.783148	2.186000
31	6	0	-1.038484	5.149967	0.881163
32	6	0	-0.658852	4.207674	-0.095210
33	6	0	-0.499227	2.856145	0.198962
34	1	0	0.451530	-1.751678	-5.029047
35	1	0	2.896484	-2.192815	-4.823609
36	1	0	5.960909	-1.700715	-1.102292
37	1	0	1.113920	-4.159787	3.267510
38	1	0	-1.105122	-5.240379	2.911413
39	1	0	-4.869967	-4.013392	0.114817
40	1	0	-1.344645	1.191965	5.131292
41	1	0	-1.638975	3.623591	4.648577
42	1	0	-1.143439	6.186456	0.578035
43	49	0	-0.000822	0.028574	0.015266
44	1	0	-0.793545	-0.851690	-3.026143
45	1	0	1.621057	-1.995135	2.063731
46	1	0	-0.666335	-0.338246	3.267513
47	1	0	4.996362	-2.177792	-3.334697
48	1	0	-3.387084	-5.192516	1.711245
49	1	0	-1.564984	5.517964	2.928384
50	35	0	-0.354513	4.783570	-1.861684
51	35	0	4.908374	-0.670751	1.432294
52	35	0	-4.675526	-1.578344	-1.487814

R) *fac*-InQ_3

1	7	0	-1.565116	-0.946875	0.532744
2	7	0	1.574284	-0.858818	0.548514
3	7	0	-0.058944	1.811359	0.516401
4	8	0	1.318993	1.272818	-1.748565
5	8	0	-1.799020	0.482384	-1.750648
6	8	0	0.465167	-1.809292	-1.730600
7	6	0	2.110779	-0.351679	1.641461
8	6	0	3.101738	-1.036894	2.376874
9	6	0	3.520270	-2.270713	1.939523
10	6	0	2.968956	-2.840592	0.764341
11	6	0	1.981593	-2.074990	0.088513
12	6	0	3.346929	-4.098798	0.242182
13	6	0	2.743155	-4.545602	-0.915182
14	6	0	1.767226	-3.792897	-1.596058
15	6	0	1.359715	-2.546050	-1.128077
16	6	0	-1.408609	-1.669125	1.624557
17	6	0	-2.508349	-2.156672	2.363104
18	6	0	-3.780878	-1.867969	1.930618
19	6	0	-3.983149	-1.100446	0.755456

20	6	0	-2.815961	-0.660848	0.075365
21	6	0	-5.254070	-0.763902	0.235276
22	6	0	-5.320601	-0.018623	-0.924273
23	6	0	-4.170005	0.416316	-1.609383
24	6	0	-2.893789	0.111559	-1.143339
25	6	0	-0.771701	2.050648	1.599868
26	6	0	-0.637226	3.248610	2.334460
27	6	0	0.265782	4.192980	1.907855
28	6	0	1.041381	3.969790	0.742186
29	6	0	0.830479	2.739158	0.064547
30	6	0	1.986391	4.888373	0.230049
31	6	0	2.674492	4.560909	-0.920382
32	6	0	2.468161	3.347364	-1.603588
33	6	0	1.549117	2.407128	-1.144460
34	1	0	1.751739	0.624538	1.958617
35	1	0	3.516559	-0.581108	3.268424
36	1	0	4.281569	-2.822501	2.485215
37	1	0	4.102282	-4.687644	0.752037
38	1	0	3.029782	-5.510069	-1.324771
39	1	0	1.316577	-4.165412	-2.509371
40	1	0	-0.386757	-1.873250	1.935514
41	1	0	-2.332750	-2.749313	3.253473
42	1	0	-4.647196	-2.228191	2.479852
43	1	0	-6.150622	-1.097443	0.747382
44	1	0	-6.293128	0.241923	-1.332267
45	1	0	-4.252672	0.992940	-2.524187
46	1	0	-1.470163	1.276793	1.909657
47	1	0	-1.244826	3.404542	3.218497
48	1	0	0.393937	5.123500	2.455217
49	1	0	2.153017	5.830644	0.741529
50	1	0	3.401509	5.261580	-1.321069
51	1	0	3.018524	3.119679	-2.509727
52	49	0	-0.015327	-0.012048	-0.869757

S) *fac*-In(qCH$_3$)$_3$

1	7	0	-2.096657	-0.780680	0.513674
2	7	0	1.496679	-1.043755	0.717515
3	7	0	0.231502	1.980258	0.256565
4	8	0	1.433725	0.556896	-1.723385
5	8	0	-1.750498	0.759344	-1.693138
6	8	0	-0.073194	-2.020065	-1.298952
7	6	0	2.223665	-0.594363	1.726451
8	6	0	3.445550	-1.221045	2.090621
9	6	0	3.876624	-2.327383	1.411139
10	6	0	3.095189	-2.860032	0.356194
11	6	0	1.900392	-2.165161	0.035572
12	6	0	3.447022	-4.033017	-0.350886
13	6	0	2.605314	-4.494100	-1.340041
14	6	0	1.414594	-3.821501	-1.666673
15	6	0	1.036539	-2.651993	-1.013295
16	6	0	-2.238336	-1.603626	1.541807
17	6	0	-3.526061	-1.940028	2.032020
18	6	0	-4.645879	-1.424904	1.433064
19	6	0	-4.521721	-0.577805	0.305895
20	6	0	-3.202592	-0.294285	-0.129835
21	6	0	-5.626954	-0.029744	-0.387468
22	6	0	-5.394278	0.767420	-1.486953
23	6	0	-4.090600	1.044506	-1.941085
24	6	0	-2.972329	0.526690	-1.293867
25	6	0	-0.431182	2.703965	1.145085
26	6	0	0.088136	3.938201	1.608761
27	6	0	1.290670	4.396598	1.135385
28	6	0	2.001072	3.657158	0.159191
29	6	0	1.407650	2.440839	-0.270102
30	6	0	3.234289	4.073209	-0.394654
31	6	0	3.828698	3.285837	-1.357911

32	6	0	3.240362	2.091506	-1.812499
33	6	0	2.024129	1.638564	-1.302381
34	1	0	4.017089	-0.809601	2.916087
35	1	0	4.807846	-2.819174	1.681382
36	1	0	4.365639	-4.552846	-0.098638
37	1	0	2.862306	-5.397389	-1.885701
38	1	0	0.760752	-4.192217	-2.448541
39	1	0	-3.603069	-2.608802	2.882206
40	1	0	-5.637251	-1.670338	1.805871
41	1	0	-6.633821	-0.251539	-0.048865
42	1	0	-6.235172	1.190981	-2.028684
43	1	0	-3.924982	1.660203	-2.818617
44	1	0	-0.477350	4.503326	2.341483
45	1	0	1.705053	5.335372	1.494541
46	1	0	3.683886	5.003240	-0.062103
47	1	0	4.774639	3.597235	-1.792104
48	1	0	3.713730	1.498536	-2.587548
49	49	0	-0.204264	-0.089685	-0.662234
50	6	0	-1.744365	2.195900	1.668280
51	1	0	-1.636429	1.205715	2.122836
52	1	0	-2.148475	2.876879	2.418902
53	1	0	-2.470302	2.107364	0.853707
54	6	0	-1.015645	-2.194918	2.183275
55	1	0	-0.425834	-2.737698	1.438663
56	1	0	-0.374331	-1.419208	2.611699
57	1	0	-1.299696	-2.884601	2.979722
58	6	0	1.748363	0.581205	2.537651
59	1	0	2.147053	1.521994	2.141097
60	1	0	0.658942	0.649746	2.533744
61	1	0	2.087868	0.481086	3.571423

T) *fac*-In(qNO$_2$)$_3$

1	7	0	-1.588451	-0.984974	0.371568
2	7	0	1.583164	-0.850446	0.394296
3	7	0	-0.105417	1.816524	0.342466
4	8	0	1.260629	1.277987	-1.898170
5	8	0	-1.817196	0.406939	-1.904501
6	8	0	0.500696	-1.804422	-1.864474
7	6	0	2.101903	-0.309336	1.481242
8	6	0	3.138552	-0.938400	2.190196
9	6	0	3.622917	-2.150526	1.757190
10	6	0	3.081849	-2.762928	0.591621
11	6	0	2.052214	-2.040143	-0.071672
12	6	0	3.474127	-3.999014	-0.003578
13	6	0	2.883780	-4.439709	-1.176671
14	6	0	1.880175	-3.721576	-1.822283
15	6	0	1.429204	-2.508480	-1.301332
16	6	0	-1.404917	-1.700393	1.465253
17	6	0	-2.489430	-2.227076	2.186177
18	6	0	-3.774115	-1.986006	1.758404
19	6	0	-4.005401	-1.216092	0.583043
20	6	0	-2.845449	-0.747825	-0.092753
21	6	0	-5.259916	-0.893622	-0.014564
22	6	0	-5.318125	-0.182918	-1.202245
23	6	0	-4.175164	0.268809	-1.857689
24	6	0	-2.908404	0.009775	-1.333641
25	6	0	-0.839006	2.037185	1.417144
26	6	0	-0.757394	3.248479	2.123742
27	6	0	0.115315	4.225004	1.703813
28	6	0	0.925874	4.014941	0.551935
29	6	0	0.751120	2.770648	-0.113748
30	6	0	1.864798	4.919146	-0.028504
31	6	0	2.538600	4.589788	-1.193388
32	6	0	2.354038	3.371382	-1.842328
33	6	0	1.465476	2.423567	-1.333044
34	1	0	3.551178	-0.462677	3.072233

35	1	0	4.417206	-2.643569	2.297972
36	1	0	3.226518	-5.381235	-1.590184
37	1	0	1.435175	-4.088365	-2.739474
38	1	0	-2.304589	-2.820272	3.074251
39	1	0	-4.614454	-2.380863	2.310887
40	1	0	-6.297354	0.024553	-1.618411
41	1	0	-4.247039	0.825856	-2.784167
42	1	0	-1.383337	3.405011	2.994678
43	1	0	0.189542	5.156807	2.244594
44	1	0	3.234147	5.316755	-1.596353
45	1	0	2.894976	3.136665	-2.751102
46	49	0	-0.033482	-0.029416	-0.980787
47	1	0	-0.377927	-1.864434	1.781724
48	1	0	1.692143	0.644671	1.803339
49	1	0	-1.507871	1.239881	1.731229
50	7	0	2.172709	6.212889	0.560233
51	8	0	1.754629	6.458988	1.685953
52	8	0	2.847962	6.992790	-0.091205
53	7	0	4.493998	-4.859224	0.575935
54	8	0	4.907694	-4.603124	1.700945
55	8	0	4.884363	-5.808931	-0.083058
56	7	0	-6.529561	-1.276862	0.581406
57	8	0	-6.531832	-1.698218	1.732572
58	8	0	-7.540508	-1.147111	-0.089046

U) *fac*-In(qCl)$_3$

1	7	0	-1.621099	-0.942767	0.387396
2	7	0	1.533163	-0.877165	0.418879
3	7	0	-0.068552	1.804142	0.349636
4	8	0	1.305439	1.212300	-1.901632
5	8	0	-1.825282	0.473680	-1.901434
6	8	0	0.426344	-1.847539	-1.848990
7	6	0	2.064151	-0.353756	1.507249
8	6	0	3.081705	-1.008109	2.231333
9	6	0	3.537255	-2.227734	1.792024
10	6	0	2.990280	-2.811398	0.622472
11	6	0	1.971285	-2.079330	-0.047725
12	6	0	3.382891	-4.054836	0.073163
13	6	0	2.787867	-4.521830	-1.076669
14	6	0	1.785420	-3.791177	-1.739720
15	6	0	1.348512	-2.560178	-1.260589
16	6	0	-1.470805	-1.665770	1.479722
17	6	0	-2.574854	-2.140824	2.217191
18	6	0	-3.845641	-1.841178	1.788149
19	6	0	-4.037152	-1.073600	0.612015
20	6	0	-2.867169	-0.645280	-0.073834
21	6	0	-5.292071	-0.710411	0.068422
22	6	0	-5.356135	0.027864	-1.091749
23	6	0	-4.195611	0.440170	-1.771085
24	6	0	-2.927090	0.120797	-1.297628
25	6	0	-0.785089	2.066331	1.425250
26	6	0	-0.630938	3.265463	2.151167
27	6	0	0.295984	4.188295	1.729949
28	6	0	1.075053	3.936685	0.572743
29	6	0	0.844622	2.707138	-0.104052
30	6	0	2.051417	4.812641	0.042210
31	6	0	2.743285	4.468662	-1.097186
32	6	0	2.506889	3.254870	-1.766607
33	6	0	1.560909	2.344288	-1.305507
34	1	0	3.492239	-0.541391	3.119050
35	1	0	4.320472	-2.752721	2.329031
36	1	0	3.107596	-5.476642	-1.481997
37	1	0	1.339634	-4.176407	-2.649672
38	1	0	-2.407158	-2.734378	3.108375
39	1	0	-4.713365	-2.191000	2.338197
40	1	0	-6.329596	0.293255	-1.492135

41	1	0	-4.272024	1.012389	-2.688721
42	1	0	-1.242383	3.443432	3.028166
43	1	0	0.438818	5.117666	2.271758
44	1	0	3.486211	5.156656	-1.488086
45	1	0	3.059475	3.009468	-2.666268
46	49	0	-0.052031	-0.039888	-1.012188
47	1	0	-0.450942	-1.879476	1.790168
48	1	0	1.679382	0.611187	1.828083
49	1	0	-1.501621	1.309109	1.734793
50	17	0	2.374556	6.334976	0.834000
51	17	0	4.628688	-4.995418	0.855659
52	17	0	-6.761104	-1.206053	0.872535

V) *fac*-In(qBr)$_3$

1	7	0	-1.604924	-0.922779	1.432348
2	7	0	1.549712	-0.784670	1.455277
3	7	0	-0.112896	1.872214	1.343843
4	8	0	1.290924	1.254729	-0.877685
5	8	0	-1.842371	0.471820	-0.864327
6	8	0	0.437066	-1.812216	-0.782868
7	6	0	2.087168	-0.237493	2.529336
8	6	0	3.132949	-0.856876	3.244875
9	6	0	3.609259	-2.069718	2.806515
10	6	0	3.058503	-2.680197	1.653999
11	6	0	2.013177	-1.981478	0.996244
12	6	0	3.491557	-3.921968	1.134124
13	6	0	2.886975	-4.421392	0.002281
14	6	0	1.853862	-3.721245	-0.647326
15	6	0	1.380258	-2.490205	-0.199744
16	6	0	-1.441879	-1.632723	2.532072
17	6	0	-2.533424	-2.161005	3.252305
18	6	0	-3.807945	-1.927776	2.792212
19	6	0	-4.016148	-1.176394	1.609790
20	6	0	-2.857897	-0.692410	0.948439
21	6	0	-5.288942	-0.895017	1.060967
22	6	0	-5.369238	-0.160436	-0.101084
23	6	0	-4.215890	0.311148	-0.753667
24	6	0	-2.929667	0.067363	-0.278927
25	6	0	-0.845868	2.151848	2.404488
26	6	0	-0.728586	3.375627	3.096414
27	6	0	0.182766	4.304562	2.652437
28	6	0	0.980625	4.036819	1.513156
29	6	0	0.783373	2.785368	0.874229
30	6	0	1.938665	4.934948	0.987881
31	6	0	2.655730	4.570770	-0.130231
32	6	0	2.450635	3.330775	-0.761481
33	6	0	1.517930	2.400197	-0.309134
34	1	0	3.545575	-0.368707	4.119971
35	1	0	4.415493	-2.572129	3.334572
36	1	0	3.206037	-5.371857	-0.412788
37	1	0	-2.351227	-2.741157	4.149357
38	1	0	-4.669871	-2.320917	3.325271
39	1	0	-6.336177	0.062963	-0.539894
40	1	0	-1.354782	3.564586	3.960536
41	1	0	0.299779	5.255678	3.165437
42	1	0	3.394737	5.246459	-0.548149
43	49	0	-0.057686	0.003499	0.030760
44	1	0	-0.418611	-1.793927	2.862807
45	1	0	1.683652	0.721714	2.845247
46	1	0	-1.548456	1.387671	2.728745
47	1	0	-6.184300	-1.260844	1.551965
48	1	0	4.292353	-4.464535	1.624976
49	1	0	2.097388	5.897022	1.463034
50	35	0	-4.403485	1.316427	-2.375038
51	35	0	3.480956	2.888797	-2.316297
52	35	0	1.063076	-4.472082	-2.223540

W) Alq_2^+

1	7	0	1.475755	-0.790531	-0.356019
2	7	0	-1.475789	0.790550	-0.356026
3	8	0	-1.115097	-1.160017	1.340688
4	8	0	1.115131	1.160184	1.340579
5	6	0	1.575013	-1.815567	-1.196600
6	6	0	2.813082	-2.202601	-1.731115
7	6	0	3.955523	-1.512731	-1.373767
8	6	0	3.884491	-0.425252	-0.472093
9	6	0	2.601313	-0.098723	0.015731
10	6	0	4.984774	0.348738	-0.022229
11	6	0	4.766712	1.372437	0.871308
12	6	0	3.474757	1.687171	1.365991
13	6	0	2.387675	0.957615	0.945911
14	6	0	-1.575064	1.815559	-1.196635
15	6	0	-2.813151	2.202554	-1.731147
16	6	0	-3.955569	1.512663	-1.373773
17	6	0	-3.884507	0.425202	-0.472076
18	6	0	-2.601323	0.098738	0.015765
19	6	0	-4.984761	-0.348832	-0.022215
20	6	0	-4.766650	-1.372523	0.871318
21	6	0	-3.474688	-1.687179	1.366045
22	6	0	-2.387644	-0.957554	0.945996
23	1	0	0.658287	-2.341902	-1.444857
24	1	0	2.854417	-3.043120	-2.412946
25	1	0	4.920263	-1.806574	-1.778707
26	1	0	5.982409	0.122261	-0.382727
27	1	0	5.608036	1.963076	1.218341
28	1	0	3.332005	2.491717	2.078657
29	1	0	-0.658340	2.341866	-1.444957
30	1	0	-2.854525	3.043052	-2.413002
31	1	0	-4.920317	1.806468	-1.778722
32	1	0	-5.982405	-0.122397	-0.382713
33	1	0	-5.607942	-1.963216	1.218337
34	1	0	-3.331931	-2.491721	2.078713
35	13	0	0.000008	0.000055	0.626175

X) $Al(qCH_3)_2^+$

1	7	0	1.419386	-0.797519	0.174233
2	7	0	-1.419403	0.797551	0.174205
3	8	0	-1.163185	-1.109161	-1.593711
4	8	0	1.163195	1.109214	-1.593661
5	6	0	1.436572	-1.804077	1.047048
6	6	0	2.657742	-2.179452	1.647276
7	6	0	3.825270	-1.518116	1.329717
8	6	0	3.821879	-0.452968	0.396087
9	6	0	2.570915	-0.128260	-0.161970
10	6	0	4.951837	0.298795	-0.015015
11	6	0	4.789451	1.303320	-0.942560
12	6	0	3.527295	1.616263	-1.508401
13	6	0	2.412066	0.906411	-1.126017
14	6	0	-1.436590	1.804090	1.047055
15	6	0	-2.657759	2.179431	1.647291
16	6	0	-3.825278	1.518072	1.329736
17	6	0	-3.821882	0.452942	0.396093
18	6	0	-2.570918	0.128275	-0.161993
19	6	0	-4.951829	-0.298842	-0.015005
20	6	0	-4.789432	-1.303346	-0.942569
21	6	0	-3.527274	-1.616255	-1.508431
22	6	0	-2.412054	-0.906387	-1.126052
23	1	0	2.659591	-2.998905	2.356704
24	1	0	4.761726	-1.815361	1.794580
25	1	0	5.927846	0.072897	0.401118
26	1	0	5.652939	1.877723	-1.261041
27	1	0	3.427806	2.403409	-2.247581

28	1	0	-2.659627	2.998879	2.356724
29	1	0	-4.761730	1.815286	1.794626
30	1	0	-5.927838	-0.072977	0.401145
31	1	0	-5.652910	-1.877762	-1.261050
32	1	0	-3.427780	-2.403391	-2.247621
33	13	0	0.000000	0.000017	-0.868839
34	6	0	0.141652	-2.506274	1.327127
35	1	0	-0.663984	-1.784667	1.502083
36	1	0	-0.142948	-3.123286	0.468209
37	1	0	0.224404	-3.149147	2.203644
38	6	0	-0.141659	2.506275	1.327135
39	1	0	0.663893	1.784629	1.502336
40	1	0	0.143093	3.123095	0.468132
41	1	0	-0.224464	3.149325	2.203515

Y) $Al(qNO_2)_2^+$

1	7	0	1.480794	0.812078	-0.229746
2	7	0	-1.478702	-0.801368	-0.253078
3	8	0	-1.128181	1.139513	1.431997
4	8	0	1.126309	-1.166785	1.409917
5	6	0	1.554191	1.864566	-1.037743
6	6	0	2.785027	2.291638	-1.548876
7	6	0	3.944594	1.618099	-1.219721
8	6	0	3.897652	0.487304	-0.357225
9	6	0	2.618341	0.131093	0.124446
10	6	0	4.973191	-0.322369	0.118409
11	6	0	4.759430	-1.354437	1.002159
12	6	0	3.471644	-1.682299	1.472524
13	6	0	2.393931	-0.948214	1.038915
14	6	0	-1.548400	-1.827393	-1.094805
15	6	0	-2.775514	-2.230720	-1.633066
16	6	0	-3.937498	-1.572180	-1.282608
17	6	0	-3.897629	-0.484214	-0.366444
18	6	0	-2.618038	-0.132838	0.118668
19	6	0	-4.973082	0.319933	0.118923
20	6	0	-4.756610	1.353389	1.000463
21	6	0	-3.470310	1.669366	1.482426
22	6	0	-2.394482	0.931459	1.050821
23	1	0	2.817488	3.157859	-2.198457
24	1	0	4.894781	1.950545	-1.615029
25	1	0	5.618438	-1.925811	1.336137
26	1	0	3.324431	-2.497690	2.170891
27	1	0	-2.803819	-3.066514	-2.321613
28	1	0	-4.885154	-1.889392	-1.696097
29	1	0	-5.613893	1.930335	1.329220
30	1	0	-3.323296	2.476138	2.190731
31	13	0	-0.000225	-0.006063	0.712730
32	1	0	0.625902	2.377530	-1.271150
33	1	0	-0.619270	-2.333551	-1.339513
34	7	0	6.361048	-0.097745	-0.316604
35	8	0	7.237429	-0.673860	0.291546
36	8	0	6.540906	0.643442	-1.269445
37	7	0	-6.366651	0.079405	-0.289025
38	8	0	-7.183131	0.932618	-0.013974
39	8	0	-6.614173	-0.964968	-0.869420

Z) $Al(qCl)_2^+$

1	7	0	-1.469910	-0.792954	-0.237045
2	7	0	1.469911	0.792955	-0.237045
3	8	0	1.123309	-1.153427	1.464188
4	8	0	-1.123310	1.153430	1.464187
5	6	0	-1.555397	-1.817121	-1.080044
6	6	0	-2.785172	-2.206316	-1.629324
7	6	0	-3.934673	-1.520885	-1.286714
8	6	0	-3.874723	-0.435323	-0.383128

9	6	0	-2.599782	-0.103141	0.124692
10	6	0	-4.973285	0.348928	0.066247
11	6	0	-4.770297	1.369630	0.965371
12	6	0	-3.483016	1.677344	1.470055
13	6	0	-2.391852	0.950323	1.058409
14	6	0	1.555398	1.817121	-1.080045
15	6	0	2.785173	2.206315	-1.629325
16	6	0	3.934674	1.520882	-1.286716
17	6	0	3.874724	0.435322	-0.383128
18	6	0	2.599782	0.103142	0.124693
19	6	0	4.973285	-0.348929	0.066248
20	6	0	4.770296	-1.369630	0.965373
21	6	0	3.483015	-1.677343	1.470056
22	6	0	2.391851	-0.950321	1.058410
23	1	0	-2.817970	-3.045991	-2.312582
24	1	0	-4.893237	-1.815193	-1.703340
25	1	0	-5.621926	1.953351	1.298308
26	1	0	-3.352114	2.480744	2.186112
27	1	0	2.817972	3.045990	-2.312583
28	1	0	4.893238	1.815191	-1.703341
29	1	0	5.621925	-1.953351	1.298310
30	1	0	3.352112	-2.480742	2.186114
31	13	0	0.000000	0.000001	0.754285
32	1	0	-0.633734	-2.339827	-1.317811
33	1	0	0.633736	2.339829	-1.317811
34	17	0	-6.563193	0.005400	-0.525948
35	17	0	6.563193	-0.005403	-0.525948

AA) $Al(qBr)_2^+$

1	7	0	1.053544	-1.336363	1.073659
2	7	0	-1.053541	1.336357	1.073663
3	8	0	-1.483121	-0.665283	-0.537738
4	8	0	1.483119	0.665280	-0.537739
5	6	0	0.741049	-2.363426	1.860208
6	6	0	1.726568	-3.226202	2.359294
7	6	0	3.051223	-3.014585	2.023732
8	6	0	3.412721	-1.942421	1.177920
9	6	0	2.362141	-1.120362	0.720217
10	6	0	4.729890	-1.634315	0.747636
11	6	0	4.937003	-0.569645	-0.095630
12	6	0	3.863692	0.235896	-0.555010
13	6	0	2.570241	-0.025031	-0.163198
14	6	0	-0.741044	2.363417	1.860215
15	6	0	-1.726562	3.226194	2.359302
16	6	0	-3.051217	3.014581	2.023740
17	6	0	-3.412717	1.942420	1.177925
18	6	0	-2.362139	1.120360	0.720220
19	6	0	-4.729887	1.634319	0.747640
20	6	0	-4.937003	0.569651	-0.095628
21	6	0	-3.863693	-0.235893	-0.555009
22	6	0	-2.570242	0.025030	-0.163196
23	1	0	1.433631	-4.051806	2.996015
24	1	0	3.823293	-3.678959	2.402279
25	1	0	5.939180	-0.327592	-0.432772
26	1	0	-1.433622	4.051795	2.996027
27	1	0	-3.823286	3.678956	2.402289
28	1	0	-5.939180	0.327600	-0.432770
29	13	0	0.000000	-0.000003	0.143523
30	1	0	-0.310549	-2.505694	2.090514
31	1	0	0.310554	2.505682	2.090521
32	1	0	5.562721	-2.243948	1.081004
33	1	0	-5.562717	2.243953	1.081010
34	35	0	4.203116	1.688748	-1.735280
35	35	0	-4.203121	-1.688742	-1.735281

AB) Gaq_2^+

1	7	0	1.542401	-0.797651	-0.430908
2	7	0	-1.542355	0.797490	-0.431028
3	8	0	-1.188768	-1.190820	1.307576
4	8	0	1.188672	1.190921	1.307398
5	6	0	1.644525	-1.818021	-1.274096
6	6	0	2.886393	-2.199342	-1.805733
7	6	0	4.021890	-1.504028	-1.441792
8	6	0	3.942742	-0.418952	-0.537035
9	6	0	2.655750	-0.097643	-0.048196
10	6	0	5.044463	0.351708	-0.089069
11	6	0	4.829423	1.373687	0.807143
12	6	0	3.539316	1.684592	1.303026
13	6	0	2.446099	0.958910	0.885876
14	6	0	-1.644427	1.817951	-1.274127
15	6	0	-2.886291	2.199438	-1.805637
16	6	0	-4.021821	1.504140	-1.441744
17	6	0	-3.942715	0.418981	-0.537095
18	6	0	-2.655738	0.097589	-0.048261
19	6	0	-5.044475	-0.351663	-0.089171
20	6	0	-4.829491	-1.373641	0.807045
21	6	0	-3.539404	-1.684565	1.302995
22	6	0	-2.446155	-0.958916	0.885889
23	1	0	0.730351	-2.345639	-1.528174
24	1	0	2.933578	-3.037344	-2.490351
25	1	0	4.990229	-1.790153	-1.843536
26	1	0	6.040561	0.124075	-0.453064
27	1	0	5.670903	1.963854	1.154608
28	1	0	3.396880	2.487480	2.017692
29	1	0	-0.730197	2.345447	-1.528254
30	1	0	-2.933444	3.037535	-2.490141
31	1	0	-4.990152	1.790372	-1.843431
32	1	0	-6.040555	-0.123958	-0.453171
33	1	0	-5.670985	-1.963810	1.154472
34	1	0	-3.397032	-2.487415	2.017718
35	31	0	-0.000006	-0.000047	0.574170

AC) Inq_2^+

1	7	0	1.683301	0.827603	0.475965
2	7	0	-1.683172	-0.827241	0.476378
3	8	0	-1.361904	1.237829	-1.279652
4	8	0	1.361793	-1.237665	-1.279855
5	6	0	1.803093	1.850607	1.315184
6	6	0	3.044038	2.221059	1.854904
7	6	0	4.168911	1.506844	1.501244
8	6	0	4.077947	0.415926	0.605103
9	6	0	2.789382	0.103569	0.102440
10	6	0	5.184835	-0.361074	0.185768
11	6	0	4.983014	-1.394342	-0.699841
12	6	0	3.699849	-1.703245	-1.206148
13	6	0	2.594449	-0.972908	-0.820480
14	6	0	-1.802950	-1.850473	1.315311
15	6	0	-3.043954	-2.221396	1.854584
16	6	0	-4.168887	-1.507277	1.500934
17	6	0	-4.077933	-0.416088	0.605123
18	6	0	-2.789361	-0.103430	0.102691
19	6	0	-5.184896	0.360790	0.185742
20	6	0	-4.983127	1.394203	-0.699712
21	6	0	-3.699973	1.703284	-1.205919
22	6	0	-2.594498	0.973029	-0.820273
23	1	0	0.897563	2.395272	1.565466
24	1	0	3.097033	3.062630	2.534691
25	1	0	5.140450	1.778174	1.905623
26	1	0	6.174202	-0.129081	0.565216
27	1	0	5.827199	-1.992102	-1.027177

28	1	0	3.561591	-2.516137	-1.910450
29	1	0	-0.897326	-2.394829	1.565925
30	1	0	-3.096881	-3.063265	2.534009
31	1	0	-5.140470	-1.778945	1.904979
32	1	0	-6.174268	0.128576	0.565043
33	1	0	-5.827359	1.991893	-1.027054
34	1	0	-3.561733	2.516184	-1.910217
35	49	0	0.000007	0.000067	-0.561558

AD) $In(qCH_3)_2^+$

1	7	0	1.661270	-0.825827	0.325628
2	7	0	-1.660713	0.825278	0.325865
3	8	0	-1.371015	-1.242583	-1.436191
4	8	0	1.369513	1.240951	-1.437371
5	6	0	1.739456	-1.857048	1.162952
6	6	0	2.985001	-2.210017	1.727482
7	6	0	4.112820	-1.489068	1.411583
8	6	0	4.046423	-0.392086	0.517409
9	6	0	2.772110	-0.089108	-0.015624
10	6	0	5.158888	0.392839	0.131034
11	6	0	4.973482	1.427420	-0.757729
12	6	0	3.702313	1.725946	-1.297199
13	6	0	2.592254	0.984316	-0.943416
14	6	0	-1.737767	1.856852	1.162877
15	6	0	-2.982896	2.211260	1.727367
16	6	0	-4.111487	1.491352	1.411758
17	6	0	-4.046276	0.394017	0.517952
18	6	0	-2.772286	0.089544	-0.015022
19	6	0	-5.159567	-0.389892	0.131829
20	6	0	-4.975235	-1.424941	-0.756596
21	6	0	-3.704364	-1.724997	-1.295951
22	6	0	-2.593544	-0.984442	-0.942388
23	1	0	3.032169	-3.055717	2.403916
24	1	0	5.072757	-1.761119	1.842693
25	1	0	6.139607	0.166926	0.536033
26	1	0	5.821477	2.032106	-1.061443
27	1	0	3.576170	2.537724	-2.005201
28	1	0	-3.029193	3.057226	2.403522
29	1	0	-5.071114	1.764576	1.842816
30	1	0	-6.140051	-0.162825	0.536754
31	1	0	-5.823854	-2.028840	-1.060129
32	1	0	-3.579075	-2.537182	-2.003641
33	49	0	-0.000209	-0.001121	-0.731793
34	6	0	0.477437	-2.595754	1.501024
35	1	0	-0.021705	-2.119045	2.352306
36	1	0	-0.215877	-2.613782	0.653444
37	1	0	0.694796	-3.627315	1.782172
38	6	0	-0.474902	2.594454	1.500267
39	1	0	0.025167	2.116397	2.350261
40	1	0	0.217229	2.613061	0.651736
41	1	0	-0.691306	3.625774	1.782997

AE) $In(qNO_2)_2^+$

1	7	0	-1.691854	0.856305	0.313137
2	7	0	1.689673	-0.837103	0.355618
3	8	0	1.375920	1.203579	-1.397019
4	8	0	-1.375042	-1.257134	-1.350622
5	6	0	-1.786119	1.921391	1.100917
6	6	0	-3.020981	2.343121	1.606748
7	6	0	-4.163668	1.639011	1.295402
8	6	0	-4.095166	0.487514	0.462300
9	6	0	-2.810454	0.137763	-0.029372
10	6	0	-5.177835	-0.330666	0.027874
11	6	0	-4.981390	-1.379637	-0.839553
12	6	0	-3.702006	-1.709708	-1.315967

13	6	0	-2.604431	-0.972050	-0.923773
14	6	0	1.779886	-1.856555	1.202269
15	6	0	3.009758	-2.238551	1.749507
16	6	0	4.155315	-1.557958	1.398685
17	6	0	4.095961	-0.475103	0.477760
18	6	0	2.810104	-0.138634	-0.020808
19	6	0	5.177321	0.332644	0.020922
20	6	0	4.974404	1.377833	-0.849646
21	6	0	3.696805	1.683726	-1.346170
22	6	0	2.603453	0.941673	-0.950543
23	1	0	-3.065506	3.223712	2.236061
24	1	0	-5.120224	1.959664	1.685151
25	1	0	-5.843554	-1.959694	-1.149315
26	1	0	-3.560209	-2.541772	-1.995785
27	1	0	3.049165	-3.069391	2.443554
28	1	0	5.108685	-1.852537	1.815724
29	1	0	5.832719	1.964915	-1.156897
30	1	0	3.553780	2.497132	-2.047851
31	49	0	0.000187	-0.013228	-0.665576
32	1	0	-0.868782	2.456674	1.327881
33	1	0	0.861986	-2.380631	1.451934
34	7	0	-6.555671	-0.102901	0.488444
35	8	0	-7.448315	-0.613876	-0.154464
36	8	0	-6.714173	0.567231	1.496554
37	7	0	6.563902	0.088762	0.445897
38	8	0	7.359532	0.990645	0.287414
39	8	0	6.831416	-1.005473	0.915858

AF) $In(qCl)_2^+$

1	7	0	-1.676374	0.831056	0.351553
2	7	0	1.676377	-0.831058	0.351566
3	8	0	1.372073	1.227394	-1.410070
4	8	0	-1.372081	-1.227413	-1.410065
5	6	0	-1.779702	1.853839	1.192906
6	6	0	-3.011343	2.228800	1.747538
7	6	0	-4.144916	1.520743	1.410057
8	6	0	-4.068629	0.431253	0.511411
9	6	0	-2.788263	0.110457	-0.010645
10	6	0	-5.173611	-0.356831	0.092022
11	6	0	-4.986674	-1.386228	-0.799775
12	6	0	-3.708761	-1.688797	-1.316562
13	6	0	-2.599720	-0.961361	-0.939397
14	6	0	1.779712	-1.853831	1.192931
15	6	0	3.011356	-2.228777	1.747568
16	6	0	4.144924	-1.520719	1.410076
17	6	0	4.068631	-0.431241	0.511416
18	6	0	2.788262	-0.110456	-0.010640
19	6	0	5.173609	0.356841	0.092014
20	6	0	4.986667	1.386227	-0.799796
21	6	0	3.708751	1.688787	-1.316582
22	6	0	2.599713	0.961353	-0.939403
23	1	0	-3.054232	3.070018	2.428404
24	1	0	-5.108479	1.795772	1.827619
25	1	0	-5.841169	-1.976441	-1.113209
26	1	0	-3.583075	-2.499885	-2.025069
27	1	0	3.054251	-3.069986	2.428445
28	1	0	5.108490	-1.795739	1.827640
29	1	0	5.841159	1.976437	-1.113239
30	1	0	3.583060	2.499866	-2.025098
31	49	0	0.000000	-0.000013	-0.697639
32	1	0	-0.868061	2.393530	1.431859
33	1	0	0.868075	-2.393525	1.431891
34	17	0	-6.755869	-0.013380	0.708048
35	17	0	6.755870	0.013404	0.708040

AG) $In(qBr)_2^+$

1	7	0	1.270266	-1.438740	1.023048
2	7	0	-1.270303	1.438808	1.023001
3	8	0	-1.722642	-0.705204	-0.591665
4	8	0	1.722674	0.705232	-0.591655
5	6	0	1.004559	-2.496281	1.784884
6	6	0	2.020487	-3.332477	2.267880
7	6	0	3.331024	-3.052555	1.939616
8	6	0	3.646679	-1.942524	1.124237
9	6	0	2.565852	-1.145686	0.672318
10	6	0	4.962100	-1.594194	0.729322
11	6	0	5.159708	-0.503782	-0.081388
12	6	0	4.072480	0.278595	-0.533375
13	6	0	2.769327	-0.012573	-0.177521
14	6	0	-1.004630	2.496372	1.784818
15	6	0	-2.020585	3.332547	2.267794
16	6	0	-3.331113	3.052578	1.939533
17	6	0	-3.646732	1.942521	1.124176
18	6	0	-2.565880	1.145708	0.672273
19	6	0	-4.962142	1.594141	0.729267
20	6	0	-5.159715	0.503705	-0.081420
21	6	0	-4.072462	-0.278646	-0.533392
22	6	0	-2.769318	0.012572	-0.177547
23	1	0	1.759530	-4.184338	2.883599
24	1	0	4.134988	-3.687999	2.301123
25	1	0	6.160318	-0.226299	-0.394777
26	1	0	-1.759655	4.184429	2.883495
27	1	0	-4.135097	3.688005	2.301023
28	1	0	-6.160317	0.226182	-0.394801
29	49	0	0.000005	0.000041	0.074218
30	1	0	-0.039062	-2.689791	2.014692
31	1	0	0.038984	2.689917	2.014627
32	1	0	5.800824	-2.194104	1.065582
33	1	0	-5.800885	2.194031	1.065513
34	35	0	4.399474	1.771359	-1.670596
35	35	0	-4.399409	-1.771440	-1.670587

S3.3. NBO charges

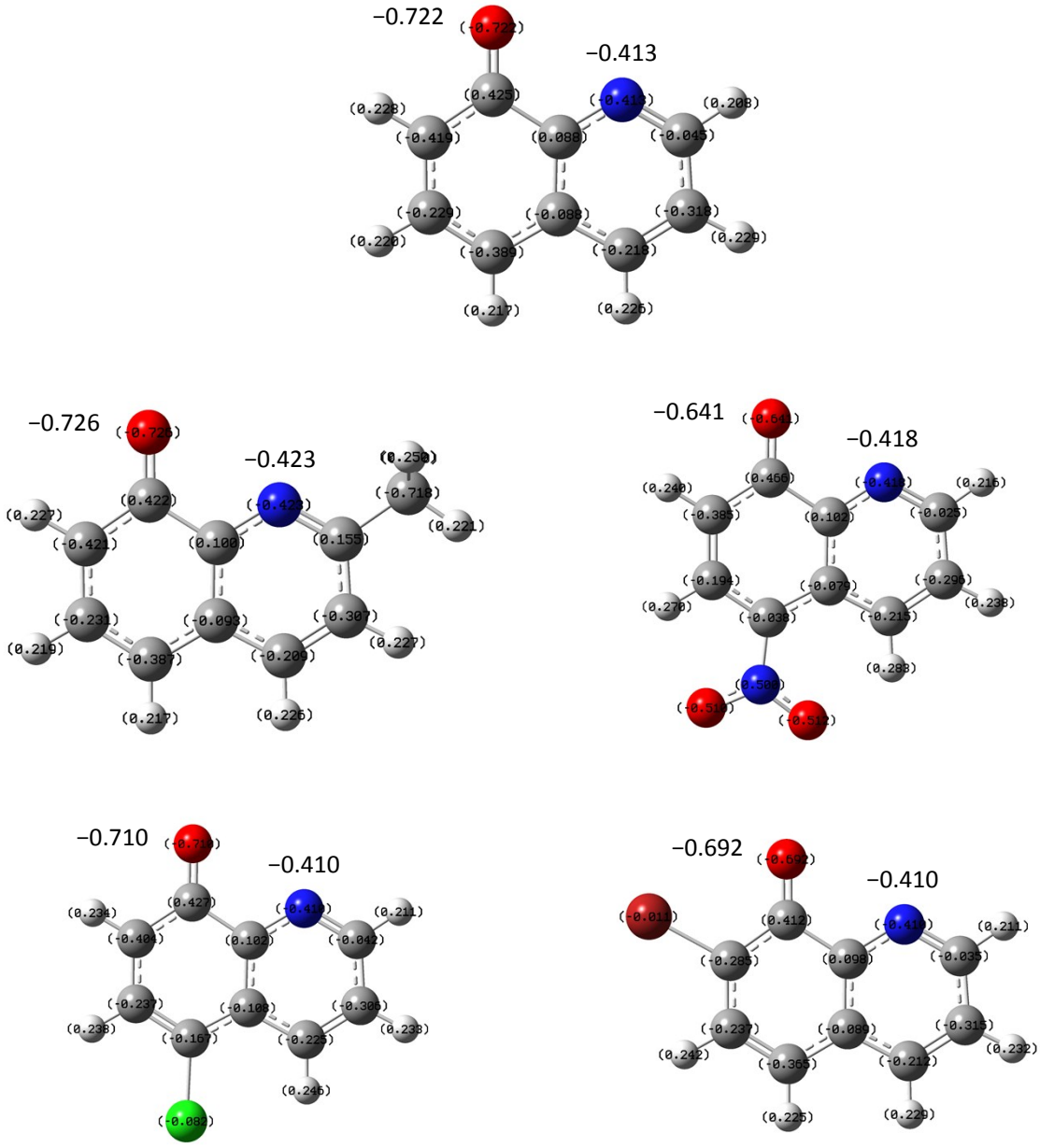


Figure S49. Calculated NBO partial point charges, at the M06-2X/6-31+G(d,p) level of theory, for the 8-hydroxyquinolinate ligands studied; the NBO charges of the coordinating N and O atoms are highlighted.