Electronic Supplementary Information

8-Quinolinolate complexes of yttrium and ytterbium: molecular arrangement and fragmentation under laser impact

Evgeny V. Baranov,*[a] Georgy K. Fukin,[a] Tatyana V. Balashova,[a] Anatoly P. Pushkarev,[a] Ivan D. Grishin[b] and Mikhail N. Bochkarev*[a]

[a] G. A. Razuvaev Institute of Organometallic Chemistry of Russian Academy of Sciences, Tropinina 49, 603950 Nizhny Novgorod, Russian Federation.
Fax: +7 (831) 4627497; Tel: +7 (831) 4627709; E-mail: mboch@iomc.ras.ru, bar@iomc.ras.ru

[b] Nizhny Novgorod State University, Gagarina 23/2, 603950 Nizhny Novgorod, Russian Federation.

Table S1. X-ray data collection and refinement parameters for complexes **1** and **2**.

Complex	1	2
Empirical formula	$C_{85}H_{64}N_9O_{11}Y_3$	$C_{86}H_{66.5}N_9O_{11.5}Yb_3$
Formula weight	1654.18	1929.10
Temperature (K)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073
Crystal system, space group	Monoclinic, P2(1)/n	Monoclinic, P2(1)/n
Unit cell dimensions		
a (Å)	16.9402(19)	16.4688(9)
b (Å)	24.619(3)	24.5129(13)
c (Å)	18.248(2)	18.2696(10)
β (°)	91.536(2)	91.7790(10)
Volume (Å^3)	7607.7(15)	7371.8(7)
Z, Calculated density (Mg/m^3)	4, 1.444	4, 1.738
Absorption coefficient (mm^{-1})	2.337	3.846
F(000)	3368	3790
Crystal size (mm)	0.61 × 0.18 × 0.05	0.37 × 0.08 × 0.03
θ Range for data collection (°)	1.82 – 26.06	1.84 – 27.00
Limiting indices	$-20 \leq h \leq 20$ $-30 \leq k \leq 30$ $-22 \leq l \leq 22$	$-21 \leq h \leq 21$ $-31 \leq k \leq 31$ $-23 \leq l \leq 23$
Reflections collected/unique [R_{int}]	63970 /14889 [0.1564]	67420 / 16015 [0.0552]
Completeness	0.99 (to θ = 26.06°)	99.6 (to θ = 27.00°)
Max. and min. transmission	0.8921, 0.3298	0.8933, 0.3303
Refinement method	full-matrix least-squares on F^2	full-matrix least-squares on F^2
Data / restraints / parameters	14889 / 177 / 1063	16015 / 344 / 1315
Goodness-of-fit on F^2	1.017	1.016
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0827, wR2 = 0.1815	R1 = 0.0397, wR2 = 0.0811
R indices (all data)	R1 = 0.1904, wR2 = 0.2285	R1 = 0.0697, wR2 = 0.0876
Largest diff. peak and hole (eÅ^{-3})	1.406, -0.825	2.229, -1.220

Table S2. Selected bond lengths and angles in **1** (Ln=Y) and **2** (Ln=Yb).

Bond	*d*, Å		Angle	ω, °	
	1	**2**		**1**	**2**
Ln(1)-O(1A)	2.336(3)	2.299(2)	N(1I)-Ln(1)-O(1I)	64.94(17)	66.99(15)
Ln(1)-O(1B)	2.300(3)	2.261(2)	O(1A)-Ln(1)-O(1B)	76.04(12)	76.03(8)
Ln(1)-O(1C)	2.474(3)	2.453(2)	O(1B)-Ln(1)-O(1C)	69.07(11)	68.63(7)
Ln(1)-O(1E)	2.316(3)	2.276(2)	O(1C)-Ln(1)-O(1A)	64.05(11)	64.00(7)
Ln(1)-O(1F)	2.330(4)	2.307(2)	O(1E)-Ln(1)-O(1F)	76.24(12)	75.84(8)
Ln(1)-O(1G)	2.465(3)	2.430(2)	O(1F)-Ln(1)-O(1G)	64.33(12)	64.16(8)
Ln(1)-O(1I)	2.301(5)	2.236(4)	O(1G)-Ln(1)-O(1E)	69.10(12)	68.29(8)
Ln(1)-N(1I)	2.644(4)	2.587(5)	N(1A)-Ln(2)-O(1A)	67.42(14)	68.27(9)
			N(1B)-Ln(2)-O(1B)	65.52(12)	66.56(8)
Ln(2)-O(1A)	2.350(3)	2.332(2)	N(1C)-Ln(2)-O(1C)	66.60(13)	68.04(8)
Ln(2)-O(1B)	2.322(3)	2.286(2)	N(1D)-Ln(2)-O(1D)	69.12(13)	70.70(19)
Ln(2)-O(1C)	2.342(3)	2.307(2)	O(1A)-Ln(2)-O(1B)	75.35(12)	74.92(8)
Ln(2)-O(1D)	2.240(4)	2.038(8)	O(1B)-Ln(2)-O(1C)	71.04(11)	70.85(8)
Ln(2)-N(1A)	2.504(5)	2.448(3)	O(1C)-Ln(2)-O(1A)	65.96(11)	65.86(8)
Ln(2)-N(1B)	2.555(4)	2.527(3)	N(1E)-Ln(3)-O(1E)	65.43(13)	67.10(9)
Ln(2)-N(1C)	2.502(4)	2.457(3)	N(1F)-Ln(3)-O(1F)	67.32(15)	68.77(10)
Ln(2)-N(1D)	2.493(4)	2.469(5)	N(1G)-Ln(3)-O(1G)	67.15(14)	68.62(9)
			N(1H)-Ln(3)-O(1H)	69.10(14)	72.46(13)
Ln(3)-O(1E)	2.331(3)	2.295(2)	O(1E)-Ln(3)-O(1F)	75.40(12)	75.39(8)
Ln(3)-O(1F)	2.359(4)	2.311(2)	O(1F)-Ln(3)-O(1G)	66.19(13)	66.18(8)
Ln(3)-O(1G)	2.320(4)	2.301(2)	O(1G)-Ln(3)-O(1E)	71.41(12)	70.26(8)
Ln(3)-O(1H)	2.247(4)	2.163(4)			
Ln(3)-N(1E)	2.549(4)	2.511(3)	Ln(2)-O(1A)-Ln(1)	96.62(12)	96.65(8)
Ln(3)-N(1F)	2.481(5)	2.438(3)	Ln(2)-O(1B)-Ln(1)	98.42(12)	99.06(8)
Ln(3)-N(1G)	2.484(5)	2.419(3)	Ln(2)-O(1C)-Ln(1)	93.17(11)	93.20(7)
Ln(3)-N(1H)	2.491(4)	2.487(4)	Ln(1)-O(1E)-Ln(3)	97.57(12)	98.33(8)
			Ln(1)-O(1F)-Ln(3)	96.40(13)	96.98(8)
Ln(1)-Ln(2)	3.4994(8)	3.4594(3)	Ln(1)-O(1G)-Ln(3)	93.81(13)	93.88(8)
Ln(1)-Ln(3)	3.4957(9)	3.4578(3)			
			Ln(2)-Ln(1)-Ln(3)	139.87(2)	140.32(1)

Table S3. X-ray and DFT (B3LYP/DZVP level) distances and angles in complex **1**.

Bond	d, Å		Angle	ω, °	
	Xray	**DFT**		**Xray**	**DFT**
Ln(1)-O(1A)	2.336(3)	2.420	N(1I)-Ln(1)-O(1I)	64.94(17)	65.63
Ln(1)-O(1B)	2.300(3)	2.390	O(1A)-Ln(1)-O(1B)	76.04(12)	76.60
Ln(1)-O(1C)	2.474(3)	2.535	O(1B)-Ln(1)-O(1C)	69.07(11)	67.74
Ln(1)-O(1E)	2.316(3)	2.404	O(1C)-Ln(1)-O(1A)	64.05(11)	62.99
Ln(1)-O(1F)	2.330(4)	2.431	O(1E)-Ln(1)-O(1F)	76.24(12)	72.36
Ln(1)-O(1G)	2.465(3)	2.463	O(1F)-Ln(1)-O(1G)	64.33(12)	63.58
Ln(1)-O(1I)	2.301(5)	2.253	O(1G)-Ln(1)-O(1E)	69.10(12)	71.29
Ln(1)-N(1I)	2.644(4)	2.666	N(1A)-Ln(2)-O(1A)	67.42(14)	66.43
			N(1B)-Ln(2)-O(1B)	65.52(12)	65.56
Ln(2)-O(1A)	2.350(3)	2.415	N(1C)-Ln(2)-O(1C)	66.60(13)	67.15
Ln(2)-O(1B)	2.322(3)	2.365	N(1D)-Ln(2)-O(1D)	69.12(13)	67.55
Ln(2)-O(1C)	2.342(3)	2.361	O(1A)-Ln(2)-O(1B)	75.35(12)	77.17
Ln(2)-O(1D)	2.240(4)	2.298	O(1B)-Ln(2)-O(1C)	71.04(11)	71.10
Ln(2)-N(1A)	2.504(5)	2.545	O(1C)-Ln(2)-O(1A)	65.96(11)	65.68
Ln(2)-N(1B)	2.555(4)	2.586	N(1E)-Ln(3)-O(1E)	65.43(13)	65.23
Ln(2)-N(1C)	2.502(4)	2.531	N(1F)-Ln(3)-O(1F)	67.32(15)	66.66
Ln(2)-N(1D)	2.493(4)	2.540	N(1G)-Ln(3)-O(1G)	67.15(14)	66.62
			N(1H)-Ln(3)-O(1H)	69.10(14)	67.97
Ln(3)-O(1E)	2.331(3)	2.406	O(1E)-Ln(3)-O(1F)	75.40(12)	73.48
Ln(3)-O(1F)	2.359(4)	2.365	O(1F)-Ln(3)-O(1G)	66.19(13)	66.01
Ln(3)-O(1G)	2.320(4)	2.369	O(1G)-Ln(3)-O(1E)	71.41(12)	72.89
Ln(3)-O(1H)	2.247(4)	2.296			
Ln(3)-N(1E)	2.549(4)	2.587	Ln(2)-O(1A)-Ln(1)	96.62(12)	95.84
Ln(3)-N(1F)	2.481(5)	2.549	Ln(2)-O(1B)-Ln(1)	98.42(12)	97.97
Ln(3)-N(1G)	2.484(5)	2.544	Ln(2)-O(1C)-Ln(1)	93.17(11)	94.19
Ln(3)-N(1H)	2.491(4)	2.524	Ln(1)-O(1E)-Ln(3)	97.57(12)	96.96
			Ln(1)-O(1F)-Ln(3)	96.40(13)	97.33
Ln(1)-Ln(2)	3.4994(8)	3.5884	Ln(1)-O(1G)-Ln(3)	93.81(13)	96.35
Ln(1)-Ln(3)	3.4957(9)	3.6015			
			Ln(2)-Ln(1)-Ln(3)	139.87(2)	138.71

Table S4. Main topological parameters of Y-N and Y-O bonds in complex **1**.

Bond	distance, Å	$\rho(r)$	$\nabla^2\rho(r)$	$h_e(r)$	$v(r)$
Ln(1)-O(1A)	2.420	0.0399	0.1803	0.0021	-0.0409
Ln(1)-O(1B)	2.390	0.0433	0.1948	0.0016	-0.0455
Ln(1)-O(1C)	2.535	0.0301	0.1370	0.0032	-0.0278
Ln(1)-O(1E)	2.404	0.0413	0.1911	0.0021	-0.0436
Ln(1)-O(1F)	2.431	0.0389	0.1754	0.0023	-0.0393
Ln(1)-O(1G)	2.463	0.0358	0.1634	0.0027	-0.0354
Ln(1)-O(1I)	2.253	0.0624	0.2648	-0.0041	-0.0743
Ln(1)-N(1I)	2.666	0.0287	0.1026	0.0015	-0.0226
Ln(2)-O(1A)	2.415	0.0429	0.1845	0.0011	-0.0439
Ln(2)-O(1B)	2.365	0.0480	0.2097	-0.00002	-0.0525
Ln(2)-O(1C)	2.361	0.0489	0.2092	-0.0003	-0.0528
Ln(2)-O(1D)	2.298	0.0568	0.2408	-0.0025	-0.0652
Ln(2)-N(1A)	2.545	0.0376	0.1321	-0.00006	-0.0332
Ln(2)-N(1B)	2.586	0.0342	0.1221	0.0007	-0.0290
Ln(2)-N(1C)	2.531	0.0387	0.1362	-0.0003	-0.0346
Ln(2)-N(1D)	2.540	0.0381	0.1342	-0.0002	-0.0339
Ln(3)-O(1E)	2.406	0.0436	0.1909	0.0010	-0.0458
Ln(3)-O(1F)	2.365	0.0483	0.2074	-0.00004	-0.0519
Ln(3)-O(1G)	2.369	0.0479	0.2056	0.00002	-0.0514
Ln(3)-O(1H)	2.296	0.0572	0.2412	-0.0026	-0.0655
Ln(3)-N(1E)	2.587	0.0342	0.1224	0.0007	-0.0291
Ln(3)-N(1F)	2.549	0.0372	0.1312	0.00003	-0.0328
Ln(3)-N(1G)	2.544	0.0378	0.1327	-0.0001	-0.0334
Ln(3)-N(1H)	2.524	0.0395	0.1381	-0.0005	-0.0354

Table S5. Optimized Cartesians of the computed minima of complex **1**.

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
Y	39	-0.0174475606	-0.0286495174	-0.1791325599
Y	39	-3.3114258376	1.3607518674	0.1307346992
Y	39	3.4035061075	1.0972049069	-0.1978241340
O	8	-2.0181535035	-0.4204370973	1.1244660378
N	7	-4.5492502413	-0.8610225202	0.2326523306
C	6	-5.7663008774	-1.0852572803	-0.2448088877
H	1	-6.1847600106	-0.3120462356	-0.8829338078
C	6	-6.5129406053	-2.2441737474	0.0627572989
H	1	-7.5012339770	-2.3756629319	-0.3692763995
C	6	-5.9745283859	-3.1723143772	0.9299856035
H	1	-6.5334570643	-4.0647302822	1.2063826305
C	6	-4.6841448404	-2.9631443863	1.4801745547
C	6	-3.9845154706	-1.7839880859	1.0702289649
C	6	-2.6583494125	-1.5094850633	1.5591202786
C	6	-2.1275423125	-2.3882784193	2.5017102057
H	1	-1.1404869011	-2.1894372497	2.9059438082
C	6	-2.8314557740	-3.5428498167	2.9148144280
H	1	-2.3627186150	-4.2060743325	3.6388834657
C	6	-4.0807811556	-3.8477730549	2.4124651253
H	1	-4.6100446259	-4.7456085758	2.7228099455
O	8	-1.7626042836	0.8223389794	-1.5737249347
N	7	-4.2689050591	1.4994132949	-2.2678992433
C	6	-5.4970350762	1.8822197350	-2.5997480471
H	1	-6.1217528753	2.2143778485	-1.7733891536
C	6	-5.9771714192	1.8508299860	-3.9296456732
H	1	-6.9916682849	2.1795883369	-4.1393122011
C	6	-5.1456707064	1.3955848570	-4.9327190557
H	1	-5.4899443603	1.3537871505	-5.9648109551

C	6	-3.8262174788	0.9756520446	-4.6227003588
C	6	-3.4255176440	1.0559352268	-3.2512653770
C	6	-2.0984795804	0.6720155859	-2.8504384468
C	6	-1.2302291442	0.2072081460	-3.8379315262
H	1	-0.2296090784	-0.1016189370	-3.5528823076
C	6	-1.6388559439	0.1195912617	-5.1877840860
H	1	-0.9286492984	-0.2538677036	-5.9230929217
C	6	-2.9069504564	0.4946754370	-5.5919756776
H	1	-3.2091731898	0.4283983523	-6.6345011728
O	8	-1.1499410577	2.0025755870	0.8309667423
N	7	-3.0019456783	3.8726544482	0.1871111806
C	6	-3.9160301413	4.7751783912	-0.1469345341
H	1	-4.8263764556	4.3918632453	-0.6007792426
C	6	-3.7523440291	6.1573940031	0.0933539040
H	1	-4.5340745945	6.8500156313	-0.2065896172
C	6	-2.6059374399	6.5920822933	0.7271194505
H	1	-2.4573110140	7.6491188086	0.9418367485
C	6	-1.6106694133	5.6591418784	1.1152396530
C	6	-1.8511372991	4.2835875300	0.8026844585
C	6	-0.8880572970	3.2652248263	1.1470657582
C	6	0.2603289672	3.6785852159	1.8239914087
H	1	0.9923999319	2.9324744373	2.1059441285
C	6	0.4840090223	5.0378425608	2.1392082682
H	1	1.3986427435	5.3043817023	2.6655391813
C	6	-0.4190876526	6.0250499712	1.7945960466
H	1	-0.2346910286	7.0693783638	2.0355000255
O	8	-5.4827884892	2.0706253895	0.3773164040
N	7	-3.9385710205	1.7373739980	2.5631013768
C	6	-3.1521371440	1.5873550696	3.6205715869
H	1	-2.1339251149	1.2666178441	3.4178236572
C	6	-3.5951975540	1.8342154842	4.9401722742

H	1	-2.9067539696	1.6990188068	5.7699882282
C	6	-4.8968018841	2.2456317745	5.1452468644
H	1	-5.2642910642	2.4404022070	6.1515633878
C	6	-5.7699668623	2.4228724623	4.0393487594
C	6	-5.2290324119	2.1540631504	2.7440507055
C	6	-6.0264737759	2.3169642874	1.5487719308
C	6	-7.3506445865	2.7415771769	1.7224544269
H	1	-7.9724394592	2.8710713924	0.8391506612
C	6	-7.8786959883	2.9987852913	3.0076908520
H	1	-8.9139921952	3.3257570517	3.0891785134
C	6	-7.1200534123	2.8492356469	4.1563482345
H	1	-7.5385078333	3.0536112188	5.1389961662
O	8	1.7127166941	0.4955193992	1.4053239023
N	7	4.1151132634	1.3532846723	2.2756474744
C	6	5.3094485655	1.7612914731	2.6906142065
H	1	6.0310389959	1.9695504717	1.9035406041
C	6	5.6342992778	1.9152949434	4.0585601253
H	1	6.6294879376	2.2522824360	4.3361754098
C	6	4.6772268586	1.6354539818	5.0120421150
H	1	4.8982753185	1.7475152536	6.0721468891
C	6	3.3881026124	1.1952388928	4.6130284070
C	6	3.1542403198	1.0646059132	3.2079484307
C	6	1.8763187190	0.6175187743	2.7167924087
C	6	0.8815019872	0.3343323239	3.6539651275
H	1	-0.0909920177	0.0089617198	3.2960599505
C	6	1.1230180163	0.4678567604	5.0404210775
H	1	0.3189929493	0.2310185574	5.7345316392
C	6	2.3466340198	0.8865237865	5.5284464940
H	1	2.5231808400	0.9847177265	6.5968496769
O	8	2.1127402604	-0.6163016419	-1.1930377568
N	7	4.5981095156	-1.1531590862	-0.2724871232

C	6	5.8088479304	-1.4101056174	0.2057724260
H	1	6.2555550016	-0.6375506673	0.8264149427
C	6	6.5147689745	-2.5983816077	-0.0871997240
H	1	7.5007818869	-2.7559238259	0.3414081100
C	6	5.9411737028	-3.5230995025	-0.9367194601
H	1	6.4687961782	-4.4388498177	-1.1981469737
C	6	4.6573993535	-3.2795592498	-1.4884450919
C	6	4.0034198307	-2.0669355983	-1.1008513913
C	6	2.6922687674	-1.7470087800	-1.5997334196
C	6	2.1124966732	-2.6276342983	-2.5106855834
H	1	1.1263896582	-2.3972231291	-2.8999953404
C	6	2.7691629171	-3.8197565575	-2.8950060917
H	1	2.2664797704	-4.4860026989	-3.5928739691
C	6	4.0127096094	-4.1596493239	-2.3973244726
H	1	4.5045694430	-5.0837633162	-2.6919917973
O	8	1.3263066011	1.8362519115	-1.0647236092
N	7	3.2372395185	3.6274842516	-0.4005160343
C	6	4.1776759103	4.4965266208	-0.0499423612
H	1	5.0249816590	4.0922719270	0.4977298404
C	6	4.1225797922	5.8664997496	-0.3887399659
H	1	4.9218972779	6.5299619088	-0.0699098461
C	6	3.0588780085	6.3251649370	-1.1394005047
H	1	2.9958354768	7.3722871533	-1.4310572245
C	6	2.0376339616	5.4294021835	-1.5451555050
C	6	2.1655116795	4.0660142883	-1.1297083111
C	6	1.1647175589	3.0915422112	-1.4801236819
C	6	0.0923698636	3.5215634551	-2.2596512106
H	1	-0.6691855577	2.8029635908	-2.5349980227
C	6	-0.0199229096	4.8681359233	-2.6753539509
H	1	-0.8791983189	5.1537391608	-3.2790902977
C	6	0.9215042663	5.8188726619	-2.3313917392

H	1	0.8226602674	6.8536905290	-2.6509332734
O	8	5.6126819837	1.7185623134	-0.2818941643
N	7	4.2298085134	1.3377584388	-2.5709199573
C	6	3.5267891898	1.1500155520	-3.6802131365
H	1	2.4894679535	0.8535123134	-3.5467282205
C	6	4.0799602046	1.3240225095	-4.9694661630
H	1	3.4580019222	1.1581112890	-5.8448436196
C	6	5.4022631839	1.7022190671	-5.0867886495
H	1	5.8532339864	1.8415771171	-6.0680051613
C	6	6.1888333983	1.9141869828	-3.9232118524
C	6	5.5415565830	1.7157766191	-2.6648334873
C	6	6.2494304583	1.9079064594	-1.4185187068
C	6	7.5932893920	2.2940344873	-1.5046594883
H	1	8.1486581942	2.4440064242	-0.5811842409
C	6	8.2256387484	2.4868513068	-2.7539286954
H	1	9.2721599094	2.7867197745	-2.7671517887
C	6	7.5542557965	2.3058155708	-3.9509716358
H	1	8.0521416291	2.4592140698	-4.9054250700
O	8	-0.8332922902	-1.7733963401	-1.3475810946
N	7	0.6540853187	-2.4169031162	0.7972969581
C	6	1.4589301932	-2.7341643981	1.8036941682
H	1	1.9417049006	-1.9114625530	2.3211029147
C	6	1.6937614734	-4.0661265058	2.2169474740
H	1	2.3654539767	-4.2550411760	3.0504593408
C	6	1.0615157441	-5.0965968662	1.5512639964
H	1	1.2168511778	-6.1318274449	1.8515210879
C	6	0.2077263197	-4.8084395512	0.4556740771
C	6	0.0473746605	-3.4298506355	0.1074908548
C	6	-0.7615242199	-3.0397037102	-1.0242387634
C	6	-1.4123983036	-4.0597336196	-1.7320236381
H	1	-2.0319585673	-3.7807094752	-2.5809723873

C	6	-1.2645212456	-5.4147551899	-1.3640898535
H	1	-1.7890062414	-6.1726339534	-1.9441680551
C	6	-0.4694015390	-5.8033104649	-0.2984095745
H	1	-0.3544046674	-6.8518370793	-0.0333877949