

Electronic Supplementary Information (ESI)

A high-efficient blue-light excitable red phosphor: intramolecular π -stacking interactions in one dinuclear europium(III) complex

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The molecular coordinate of [Eu₂(2,7-BTFDBC)(DBM)₄(Phen)₂] from theoretical calculations.

C	2.38113400	0.10506900	-2.32227100
C	1.12426500	-0.43278200	-2.58225800
C	0.87077100	-1.22342200	-3.73014300
C	1.91949900	-1.48751100	-4.61520800
C	3.17558700	-0.96284800	-4.35555500
C	3.41606500	-0.16665300	-3.21541900
C	-0.52052300	-1.61806500	-3.65859600
C	-1.36270100	-2.40782500	-4.45001700
C	-1.03631300	-1.02430900	-2.48122400
C	-2.68300900	-2.59352600	-4.06316600
C	-2.37448100	-1.15069700	-2.11930000
N	-0.03188100	-0.34213700	-1.82712200
C	-0.17725800	0.33403500	-0.55428000
C	-0.57284400	1.79907400	-0.71692100
C	4.78286000	0.34241000	-2.86589000
C	5.85042600	0.19953200	-3.78446000
C	7.16435800	0.49546300	-3.43019800
O	7.63934500	0.75145300	-2.29626400
O	4.92460800	0.87804300	-1.73005300
C	8.19950900	0.57052300	-4.56307400
F	7.76268600	0.02112700	-5.70775200
F	9.33110600	-0.04221700	-4.22618900
F	8.49064900	1.85281000	-4.82194900
Eu	6.67976300	0.50268200	-0.17814400
O	8.15633700	-1.30401700	-0.13167900
C	8.07971200	-2.56311400	-0.02108400
C	6.91213500	-3.31977100	-0.21486800
C	9.36050700	-3.25469100	0.33846000
C	5.66666500	-2.71592900	-0.47493100
C	9.38741200	-4.48878200	0.99430600
C	10.56584200	-2.60286400	0.05636200
C	4.49892400	-3.53170700	-0.94642800
O	5.44439800	-1.48003800	-0.34169000
C	10.60175800	-5.06850200	1.34984900
C	11.77886200	-3.18729100	0.40332300
C	3.24543100	-2.91172600	-0.96644800
C	4.61813300	-4.83607500	-1.43560500
C	11.79901000	-4.42172100	1.05086900
C	2.13389700	-3.57396400	-1.47285200
C	3.50246300	-5.50680300	-1.92805700
C	2.25927500	-4.87740200	-1.95142900

O	6.50537200	2.83161700	-0.00701100
C	7.07889100	3.75347200	0.64377000
C	8.25851400	3.59728400	1.39332800
C	6.42386600	5.10094800	0.57330900
C	8.91866000	2.36298200	1.51842700
C	6.58721600	6.07312800	1.56406900
C	5.59480600	5.37428500	-0.51956500
C	10.16243900	2.24894900	2.35051300
O	8.54487900	1.29231700	0.95861000
C	5.94081800	7.30092800	1.45880500
C	4.95913000	6.60552400	-0.63091800
C	10.52668000	3.18831500	3.31931500
C	10.97159400	1.12408300	2.15598500
C	5.13029500	7.57196000	0.35882000
C	11.68571100	3.01240000	4.06908600
C	12.13268400	0.95173200	2.90004800
C	12.49376200	1.89726800	3.85827800
N	6.54044900	-0.47778500	2.26907700
C	5.35802700	-0.45434500	2.92227000
C	7.54195100	-1.16512400	2.79246300
C	5.13588600	-1.15311300	4.12548900
C	4.30080100	0.36877000	2.37418400
C	7.41739600	-1.90419100	3.98460800
C	6.21060700	-1.90519700	4.64415400
C	3.85951300	-1.05760700	4.77880500
C	3.07524500	0.47564400	3.06417400
N	4.55348200	1.04164400	1.23079100
C	2.87426900	-0.27333500	4.27413000
C	2.10535400	1.34701000	2.52750900
C	3.64215400	1.87909600	0.76473800
C	2.39617700	2.06844300	1.39128900
C	-3.18721000	-1.95443100	-2.91356200
C	-4.59717300	-2.10499000	-2.43392200
C	-5.15985000	-3.39206500	-2.32677500
O	-5.17878600	-1.04669300	-2.07101900
C	-6.33599300	-3.60749800	-1.60700000
Eu	-6.59919800	-0.55981200	-0.27913800
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O	-4.46701300	-1.10827700	0.59051700
O	-6.79072100	-1.15036800	1.96885400
O	-8.90849200	-0.62558100	0.18757100
O	-7.73494700	0.69118700	-1.86892900
N	-5.36160000	1.75665200	-0.93207200

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F	-8.10120400	-5.14365700	-1.19087100
F	-6.10015000	-5.75807900	-0.65600900
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C	-6.05791800	-1.31048300	2.98607500
C	-9.81537600	0.24205300	0.05699300
C	-8.69345800	1.50847300	-1.73164900
C	-5.95331600	2.90604000	-0.52457800
C	-4.48850400	1.82189300	-1.92467300
C	-6.92705200	2.83878100	0.54592000
C	-8.07091300	1.55891800	2.08255800
C	-4.65879600	-1.44469800	2.93374900
C	-2.51961300	-1.80194400	1.69024700
C	-6.78548800	-1.38663200	4.29448400
C	-9.76760400	1.32509300	-0.84542300
C	-10.97832100	0.10486600	0.99688300
C	-8.58258800	2.76198000	-2.54904000
C	-5.67999700	4.15653100	-1.11875300
C	-4.13081900	3.02612600	-2.56258900
C	-7.58636400	4.01733600	0.95804600
C	-8.78650200	2.67442200	2.55508700
C	-1.58591700	-1.32562600	2.61415500
C	-2.10138400	-2.65995900	0.66892200
C	-6.15150700	-1.21491300	5.52820400
C	-8.16902600	-1.59804200	4.26124400
C	-11.77313100	1.18975500	1.37919400
C	-11.21974700	-1.15077400	1.56472900
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C	-7.71622300	2.75780100	-3.64794300
C	-6.36643500	5.33442300	-0.67053400
C	-4.73227600	4.19362800	-2.16140000
C	-8.54333000	3.90252800	1.98716500
C	-7.28268000	5.26874000	0.32583800
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C	-0.76678500	-3.03436800	0.56880900
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C	-8.90267800	-1.64931200	5.44068500
C	-12.80047200	1.01862400	2.30268900
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C	-7.50473300	3.91898200	-4.38140500
C	0.17041900	-2.53450700	1.47237100
C	-8.26217100	-1.48481400	6.66749000

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H	1.75607900	-2.10742900	-5.49157800
H	3.98984400	-1.20107700	-5.02898900
H	-0.98502200	-2.87512700	-5.35461200
H	-3.34622300	-3.21144600	-4.66071900
H	-2.78725900	-0.69666400	-1.22152500
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H	-1.52279600	1.88087200	-1.25483600
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H	12.74551000	-4.87718600	1.32584700
H	1.17396000	-3.06566200	-1.50150800
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H	3.70793500	-1.61482300	5.69885900
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H	-13.40709500	1.86888900	2.59911300
H	-12.44347800	-2.30596100	2.90054800
H	-9.48801800	6.04076400	-2.61859600
H	-6.83483100	3.90368500	-5.23603600
H	1.21666000	-2.81145700	1.37495100
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