

# Theoretically elucidating high photoluminescence performance of dimethylacridan-based blue-color thermally activated delayed fluorescent materials

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The Marcus–Levich equation<sup>1</sup> can be expressed as:

$$k = \frac{1}{\hbar^2} |\xi_{if}|^2 \sqrt{\frac{\pi}{\lambda_{reorg} k_B T}} \exp \left[ -\frac{(\Delta E_{if} - \lambda_{reorg})^2}{4\lambda_{reorg} k_B T} \right] \quad (S1)$$

where  $\xi_{if}$  is the spin-orbit coupling constant.  $\lambda_{reorg}$  is the reorganization energy.  $\Delta E_{if}$  is the energy gap between initial and final electronic states.

**Table S1.** Calculated the intersystem crossing rates and reverse intersystem crossing rates ( $K_{ISC}$ ,  $K_{RISC}$ ) with the calculated and experimental  $\Delta E_{ST}$ . We also list the experimental value (doped film)<sup>2, 3</sup> for a comparison.

	$K_{ISC}$ ( $\times 10^6 s^{-1}$ )	$K_{RISC}$ ( $\times 10^6 s^{-1}$ )
AC-OSO (Cal. $\Delta E_{ST}=0.03eV$ )	498	658
AC-OSO (Exp. $\Delta E_{ST}=0.06eV$ )	198	82.5
AC-OSO (exp.)	7.00	0.81
ACRXTN (Cal. $\Delta E_{ST}=0.02eV$ )	3.45	4.08
ACRXTN (Exp. $\Delta E_{ST}=0.06eV$ )	1.02	0.26
ACRXTN (exp.)	20.0	0.46

### Coordinates (unit: Å)

AC-OSO-S<sub>0</sub>

C	3.92108700	-1.31117800	2.77268100
C	2.76914500	-1.96657100	3.19925000

C	1.55327100	-1.88931900	2.50684100
C	1.51301800	-1.10964900	1.33281400
C	2.67724900	-0.44657800	0.89658400
C	3.86654900	-0.54670500	1.60869200
C	0.33297900	-2.64799000	3.04352700
C	-0.89548300	-2.43768100	2.14925500
C	-0.86680500	-1.64146400	0.98556600
N	0.31928100	-0.99034700	0.59225300
C	-2.10560900	-3.05738500	2.48824200
C	-3.26291900	-2.91635700	1.72713300
C	-3.21931600	-2.12626100	0.57988500
C	-2.03638500	-1.49535700	0.21335000
C	0.01007700	-2.14129000	4.47560900
C	0.66472000	-4.16414200	3.09903900
C	0.31978400	-0.19936700	-0.60185800
C	0.02050500	1.15948500	-0.52513900
C	0.02549900	1.93634000	-1.68624500
C	0.33986900	1.34546500	-2.91571300
C	0.61419600	-0.02405300	-2.99221000

C	0.60627300	-0.79730700	-1.83873500
O	-0.30524800	3.25744900	-1.53100600
C	-0.77233600	4.01055800	-2.58193000
C	-0.55725300	3.69487100	-3.92847600
S	0.53447600	2.36260300	-4.35992500
C	-1.51861200	5.14242700	-2.24516300
C	-2.04833900	5.93912600	-3.25447800
C	-1.85715200	5.61104800	-4.60273100
C	-1.11183900	4.48766300	-4.93960400
O	1.91877200	2.86941700	-4.39525900
O	0.01934500	1.65340900	-5.54306400
H	4.84233500	-1.39862500	3.33972400
H	2.81656900	-2.56227600	4.10557300
H	2.65168900	0.15041300	-0.00601900
H	4.74733900	-0.02428300	1.24736500
H	-2.14350400	-3.67357900	3.38112800
H	-4.17924600	-3.41499700	2.02640700
H	-4.10410000	-1.99551800	-0.03615400
H	-2.01859900	-0.88411400	-0.67987100

H	-0.22682900	-1.07344600	4.46365600
H	-0.84618500	-2.67472700	4.89843100
H	0.85932800	-2.29358200	5.14793800
H	-0.17815600	-4.73731300	3.49597400
H	0.89540600	-4.54620000	2.10037700
H	1.52769600	-4.35434400	3.74356600
H	-0.22727800	1.62086100	0.42382900
H	0.83493700	-0.46526600	-3.95814600
H	0.82330800	-1.85859900	-1.88023900
H	-1.67929200	5.36756800	-1.19667900
H	-2.62918100	6.81613300	-2.98752900
H	-2.28640100	6.23022300	-5.38282100
H	-0.94863900	4.21081600	-5.97568700

AC-OSO-S<sub>1</sub>

C	3.89321500	-1.26045800	2.63086000
C	2.78530400	-1.95115300	3.11988200
C	1.54456000	-1.90303200	2.48313100

C	1.43897400	-1.12132500	1.29907100
C	2.56913300	-0.41717800	0.80542700
C	3.77840900	-0.48858800	1.46704800
C	0.36462100	-2.67493100	3.05660700
C	-0.89277500	-2.48148200	2.22072700
C	-0.90916400	-1.67973200	1.04647700
N	0.23849400	-1.02920000	0.60446100
C	-2.08272700	-3.10796200	2.59480300
C	-3.25728700	-2.96177500	1.85885600
C	-3.26431300	-2.16700900	0.70506700
C	-2.10681300	-1.53344500	0.29928900
C	0.09000900	-2.17644600	4.50610500
C	0.72168400	-4.19066300	3.08844700
C	0.18007500	-0.23307800	-0.60955600
C	-0.15279500	1.15891200	-0.51659700
C	-0.10016200	1.92392600	-1.65509800
C	0.23190500	1.36683500	-2.92771700
C	0.51082900	-0.04948400	-2.99682500
C	0.49180400	-0.81822400	-1.85686100

O	-0.43659300	3.26318300	-1.50872600
C	-0.81702600	4.02077700	-2.58657300
C	-0.41810000	3.75184900	-3.90275500
S	0.72583600	2.41989600	-4.20558800
C	-1.63604900	5.12087700	-2.32232100
C	-2.05079500	5.94204800	-3.37071400
C	-1.67421100	5.66079000	-4.68696100
C	-0.85827200	4.56220400	-4.95170100
O	2.10220300	2.97055800	-4.05759400
O	0.42658900	1.79785200	-5.51870600
H	4.84085000	-1.32331200	3.15519400
H	2.89695800	-2.54245800	4.02189600
H	2.46593300	0.17405900	-0.09216600
H	4.63395000	0.05429600	1.08103300
H	-2.09928400	-3.72927800	3.48317300
H	-4.16179600	-3.46550100	2.18297100
H	-4.17352000	-2.04705900	0.12637900
H	-2.09348700	-0.91923500	-0.58890500
H	-0.16685000	-1.11400800	4.51053900

H	-0.73647900	-2.73192100	4.95554000
H	0.97053100	-2.32003100	5.13650700
H	-0.09932600	-4.77099000	3.51612300
H	0.92006300	-4.56593200	2.08111000
H	1.60971700	-4.36403400	3.70078400
H	-0.48091500	1.60515600	0.41487000
H	0.72310000	-0.49010800	-3.96338900
H	0.70357400	-1.88222700	-1.91388500
H	-1.93934400	5.30960900	-1.29808000
H	-2.68412500	6.79771400	-3.15713900
H	-2.01221900	6.29404000	-5.50080000
H	-0.55389900	4.31668600	-5.96371400

AC-OSO-T<sub>1</sub>

C	3.88734600	-1.24622800	2.61717300
C	2.78597900	-1.94591300	3.10767100
C	1.54136600	-1.90003900	2.47787700
C	1.42570200	-1.11272600	1.29876000
C	2.54901400	-0.39902700	0.80385800



C	3.76199600	-0.46729700	1.45910000
C	0.36835100	-2.68090500	3.05346500
C	-0.89484900	-2.48809600	2.22625700
C	-0.92152300	-1.68086600	1.05604300
N	0.22167300	-1.02625100	0.60812700
C	-2.08007500	-3.12133900	2.60427100
C	-3.25989500	-2.97507400	1.87687600
C	-3.27746800	-2.17332200	0.72801000
C	-2.12451100	-1.53436100	0.31767500
C	0.09987600	-2.19189300	4.50729700
C	0.73235300	-4.19514600	3.07437800
C	0.15450700	-0.23544300	-0.60764000
C	-0.17492100	1.15820800	-0.51661600
C	-0.10827600	1.92401200	-1.65424400
C	0.23439100	1.36705200	-2.92303100
C	0.51050500	-0.05008200	-2.99124200
C	0.48006100	-0.81941100	-1.85203300
O	-0.44331600	3.26379700	-1.50978200
C	-0.81299200	4.02302300	-2.59017400

C	-0.40437000	3.75375100	-3.90320600
S	0.73864300	2.41925500	-4.19791500
C	-1.63145100	5.12499200	-2.33182600
C	-2.03591800	5.94755400	-3.38296700
C	-1.64958500	5.66598500	-4.69643800
C	-0.83431100	4.56566500	-4.95527700
O	2.11526000	2.96612100	-4.03999400
O	0.44692000	1.79768000	-5.51285900
H	4.83818300	-1.30727400	3.13591800
H	2.90555300	-2.54251200	4.00518400
H	2.43821000	0.19728300	-0.08947000
H	4.61224100	0.08343200	1.07249200
H	-2.08842300	-3.74813900	3.48892200
H	-4.16039000	-3.48419400	2.20375900
H	-4.19109800	-2.05260700	0.15648500
H	-2.11820900	-0.91583900	-0.56765900
H	-0.16245100	-1.13084400	4.51906800
H	-0.72097500	-2.75410400	4.95867700
H	0.98495700	-2.33427200	5.13151300

H	-0.08393500	-4.78176400	3.50252500
H	0.92739500	-4.56344000	2.06381600
H	1.62420600	-4.36831900	3.68120400
H	-0.51279500	1.60418400	0.41148600
H	0.72852300	-0.49065600	-3.95653900
H	0.69201800	-1.88349300	-1.90746900
H	-1.94237500	5.31389700	-1.30990400
H	-2.66889000	6.80462800	-3.17405200
H	-1.97965800	6.30047200	-5.51256200
H	-0.52257700	4.31988900	-5.96497900

ACRXTN-S<sub>0</sub>

C	3.51219200	-3.71742500	-0.15298600
C	4.21142400	-2.52304000	-0.30559400
C	3.59991100	-1.26744800	-0.19170100
C	2.21772000	-1.23028300	0.08623900
C	1.50676600	-2.43720300	0.24116600
C	2.14703100	-3.66499500	0.12334600
C	4.44393400	-0.00010500	-0.37946000
C	3.59996700	1.26732500	-0.19200400

C	2.21777600	1.23027700	0.08596400
N	1.54310000	0.00002500	0.20771000
C	4.21153600	2.52286900	-0.30615900
C	3.51236200	3.71731500	-0.15379900
C	2.14720200	3.66500500	0.12257000
C	1.50688100	2.43727500	0.24065900
C	5.04408300	-0.00029700	-1.81196800
C	5.59835600	-0.00002000	0.65928400
C	0.14179000	0.00009600	0.51243800
C	-0.78554300	-0.00011500	-0.52380200
C	-2.15064400	-0.00001500	-0.21704800
C	-2.59704300	0.00031700	1.11388500
C	-1.63935400	0.00053300	2.14292300
C	-0.28506300	0.00042100	1.85393600
O	-3.00813100	-0.00021600	-1.28003800
C	-4.36033000	-0.00022000	-1.06159600
C	-4.91568800	0.00009600	0.22824300
C	-4.04289800	0.00041500	1.41772100
C	-5.17151300	-0.00053300	-2.20101300

C	-6.55108000	-0.00052800	-2.04446600
C	-7.12982300	-0.00022000	-0.76382300
C	-6.31613600	0.00008700	0.35751700
O	-4.47928700	0.00071000	2.56841200
H	4.02571100	-4.66873700	-0.24910800
H	5.27411400	-2.56714300	-0.52293700
H	0.44603400	-2.41175600	0.45532900
H	1.57235400	-4.57799200	0.24864400
H	5.27422900	2.56687400	-0.52349600
H	4.02591800	4.66858600	-0.25013700
H	1.57258000	4.57806000	0.24770400
H	0.44616000	2.41192800	0.45487700
H	4.24979500	-0.00017100	-2.56410400
H	5.66802400	0.88301300	-1.97697900
H	5.66766600	-0.88387300	-1.97690500
H	6.23393400	0.88222900	0.54182200
H	5.20145900	0.00032300	1.67859900
H	6.23363600	-0.88254500	0.54230700
H	-0.46458000	-0.00035700	-1.55908100

H	-2.00051800	0.00078100	3.16564700
H	0.45677600	0.00057800	2.64503400
H	-4.70639700	-0.00077300	-3.18062100
H	-7.18584300	-0.00077100	-2.92522000
H	-8.20955300	-0.00022100	-0.65672600
H	-6.72676700	0.00033200	1.36155800

ACRXTN-S<sub>1</sub>

C	-3.48786500	3.69561800	-0.16372500
C	-4.21432900	2.51640900	-0.32067700
C	-3.61935900	1.26001400	-0.19818400
C	-2.22905300	1.21464600	0.09764000
C	-1.49135700	2.41732400	0.25520200
C	-2.11759100	3.64015800	0.12469400
C	-4.45373800	0.00009300	-0.38432600
C	-3.61940400	-1.25990600	-0.19850800
C	-2.22909300	-1.21466500	0.09731000
N	-1.56978400	-0.00004000	0.23924900
C	-4.21442200	-2.51624700	-0.32132000

C	-3.48799800	-3.69552300	-0.16469200
C	-2.11771700	-3.64018900	0.12371500
C	-1.49143600	-2.41741200	0.25453800
C	-5.04939000	0.00028500	-1.82379900
C	-5.61186900	-0.00001900	0.65662100
C	-0.14477000	-0.00010200	0.54675000
C	0.78529600	0.00005800	-0.51984700
C	2.13697700	-0.00000300	-0.21962200
C	2.61738900	-0.00023000	1.11755900
C	1.64128000	-0.00038900	2.15628700
C	0.28310200	-0.00032100	1.87789000
O	2.99512200	0.00016200	-1.29362700
C	4.36211300	0.00016200	-1.07410700
C	4.90316300	-0.00005700	0.22631200
C	4.03171700	-0.00029600	1.41040000
C	5.16720300	0.00038700	-2.20704700
C	6.56060200	0.00040000	-2.06082200
C	7.12516300	0.00019000	-0.78223400
C	6.30552500	-0.00003500	0.34441100

O	4.49220000	-0.00055700	2.58684300
H	-3.98739200	4.65295300	-0.26652800
H	-5.27280900	2.58279300	-0.54509900
H	-0.43611700	2.36044400	0.47725600
H	-1.54463400	4.55246100	0.24673800
H	-5.27290700	-2.58253200	-0.54574200
H	-3.98756200	-4.65281300	-0.26773700
H	-1.54479100	-4.55254600	0.24550700
H	-0.43619100	-2.36062800	0.47659500
H	-4.25498200	0.00036100	-2.57469000
H	-5.67228300	-0.88305400	-1.98277300
H	-5.67224700	0.88368800	-1.98255400
H	-6.24305400	-0.88265600	0.53084900
H	-5.21950300	-0.00015700	1.67687700
H	-6.24302100	0.88267500	0.53107500
H	0.46433300	0.00022900	-1.55527800
H	2.00715000	-0.00056200	3.17618000
H	-0.44653000	-0.00043900	2.68265500
H	4.69842200	0.00054900	-3.18584000



H	7.19297100	0.00057500	-2.94335000
H	8.20546300	0.00020400	-0.66619900
H	6.71477700	-0.00019500	1.34907600

ACRXTN-T<sub>1</sub>

C	-3.48817400	3.69564400	-0.16533700
C	-4.21557500	2.51649600	-0.31773200
C	-3.62002000	1.26004200	-0.19772400
C	-2.22843800	1.21476400	0.09165300
C	-1.48973300	2.41735900	0.24434600
C	-2.11633400	3.64022700	0.11569600
C	-4.45535900	0.00013200	-0.37955800
C	-3.62012000	-1.25988100	-0.19797700
C	-2.22852800	-1.21477300	0.09137600
N	-1.56877900	-0.00004500	0.23296200
C	-4.21577700	-2.51626200	-0.31823200
C	-3.48846300	-3.69550000	-0.16611500
C	-2.11660600	-3.64025000	0.11486900
C	-1.48990600	-2.41745800	0.24376400

C	-5.05771100	0.00029500	-1.81623100
C	-5.60852100	0.00007600	0.66680700
C	-0.14525700	-0.00013100	0.54260100
C	0.78687300	0.00009400	-0.52274600
C	2.13810400	0.00000200	-0.22009100
C	2.61625300	-0.00031600	1.11777100
C	1.63818400	-0.00053400	2.15527800
C	0.28069800	-0.00044100	1.87460800
O	2.99789900	0.00022800	-1.29270600
C	4.36434900	0.00021500	-1.07121100
C	4.90343300	-0.00009300	0.22983700
C	4.02979900	-0.00041500	1.41274400
C	5.17133000	0.00051700	-2.20298100
C	6.56427400	0.00052000	-2.05437300
C	7.12692600	0.00022400	-0.77485500
C	6.30544700	-0.00007700	0.35038500
O	4.48881700	-0.00077400	2.58954000
H	-3.98814100	4.65298300	-0.26602200
H	-5.27523400	2.58284700	-0.53655500

H	-0.43341600	2.36025200	0.46125900
H	-1.54253600	4.55255100	0.23359700
H	-5.27544800	-2.58248300	-0.53703700
H	-3.98850900	-4.65277800	-0.26698600
H	-1.54287300	-4.55264400	0.23254100
H	-0.43357500	-2.36048000	0.46064500
H	-4.26677300	0.00033500	-2.57078300
H	-5.68131900	-0.88305600	-1.97231200
H	-5.68124500	0.88372800	-1.97214300
H	-6.24037500	-0.88254100	0.54411100
H	-5.21132100	-0.00004100	1.68519400
H	-6.24030200	0.88276900	0.54428600
H	0.46760200	0.00033200	-1.55868200
H	2.00238700	-0.00077200	3.17575900
H	-0.45036900	-0.00060300	2.67807100
H	4.70418300	0.00074500	-3.18255100
H	7.19811600	0.00075400	-2.93585500
H	8.20703200	0.00023100	-0.65715900
H	6.71294500	-0.00030300	1.35577100

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