

Phototransformation of Tetrazoline Oxime Ethers – Part 2: Theoretical Investigation

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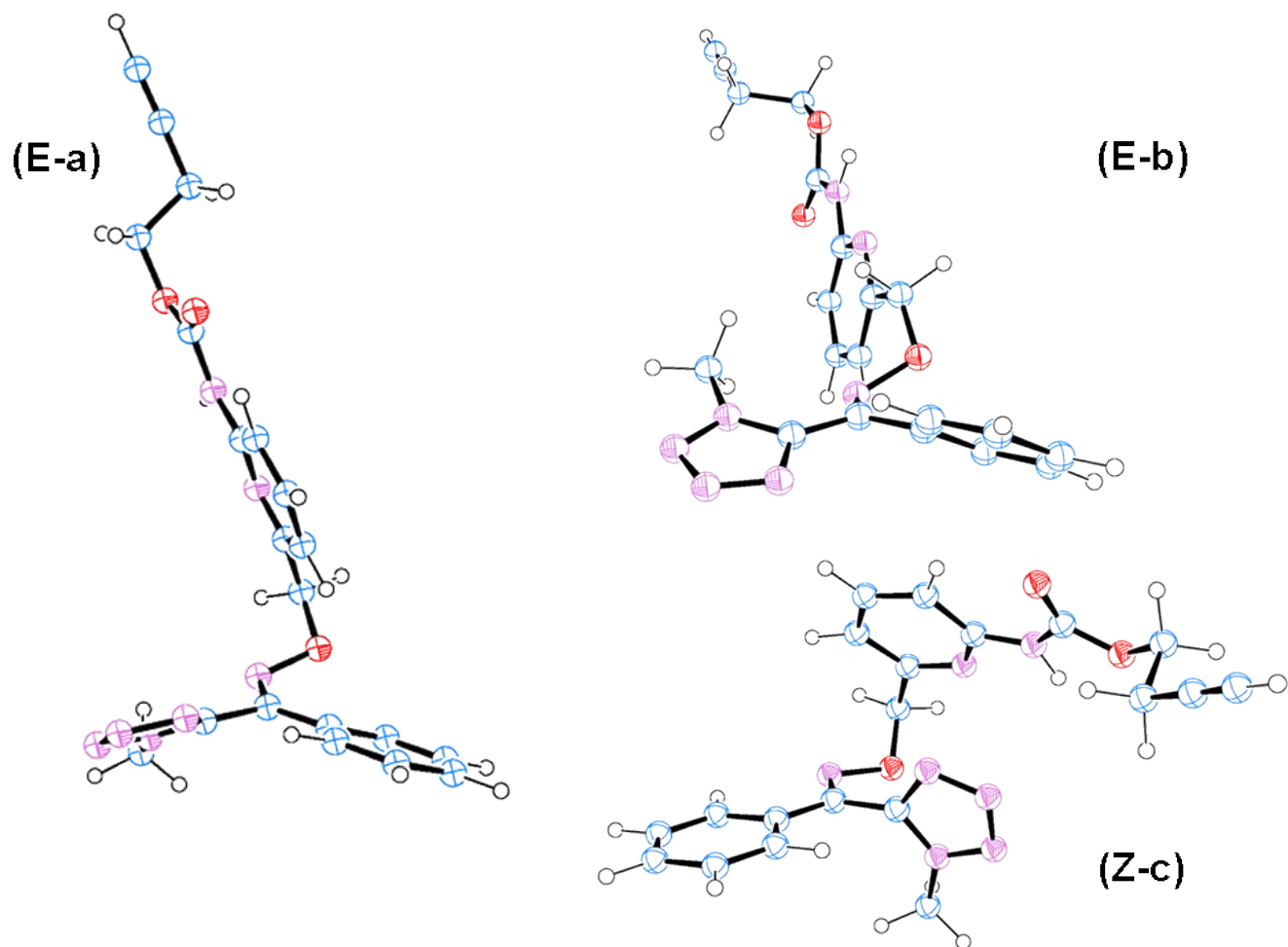
Z-a			S ₀	Z-b			S ₀	Z-c			S ₀	Z-d			S ₀
C	-1.75900900	-0.62389300	1.33546700	C	3.34878700	1.65348300	0.39398500	C	3.06117700	1.59444000	0.10407200	C	-3.05259200	-0.87641200	1.01994400
C	-2.91370500	-1.36901300	-0.83602000	C	4.41314400	-0.46922900	-0.59660300	C	4.57645400	-0.43067100	0.57756600	C	-4.99565900	-0.25989000	-0.54436900
C	-3.81694100	-1.10846200	-1.88560200	C	4.35889700	-1.85700700	-0.83440100	C	5.14748000	-1.62920700	0.10618400	C	-5.58165100	0.61223700	-1.48323400
C	-4.14811000	-2.10893000	-2.79442700	C	5.27638900	-2.46302100	-1.68723500	C	6.22350800	-2.20855500	0.77294800	C	-6.85610800	0.35962400	-1.98092500
C	-3.59207300	-3.38841300	-2.67281200	C	6.26488000	-1.70007700	-2.32126400	C	6.75392200	-1.60317200	1.91832300	C	-7.57367200	-0.76478300	-1.55384900
C	-2.70143400	-3.65672200	-1.63279200	C	6.32487000	-0.32521900	-2.09245300	C	6.19727800	-0.41291100	2.38872500	C	-7.00268100	-1.63183200	-0.62208700
C	-2.36365300	-2.65679300	-0.71785800	C	5.40581200	0.28999700	-1.23867500	C	5.11829300	0.17483200	1.72427300	C	-5.72315800	-1.38387000	-0.11904800
H	-4.25180200	-0.11958000	-1.97602900	H	3.59136300	-2.44794000	-0.34784400	H	4.74464400	-2.09314000	-0.78715500	H	-5.02943700	1.48502800	-1.81242300
H	-4.84528700	-1.89292700	-3.59871900	H	5.21997100	-3.53359100	-1.86192900	H	6.65555900	-3.13043900	0.39450100	H	-7.29476000	1.04314900	-2.70211500
H	-3.85484600	-4.16739500	-3.38247000	H	6.97893600	-2.17606900	-2.98690400	H	7.59582600	-2.05494100	2.43468800	H	-8.56948300	-0.95725200	-1.94219000
H	-2.26215300	-4.64442900	-1.53018200	H	7.08986100	0.27633300	-2.57417000	H	6.59867300	0.06388100	3.27795700	H	-7.55157700	-2.50306900	-0.27747500
N	-0.48651100	-1.00039700	1.35741700	N	4.29292600	2.46898800	0.84316000	N	2.62872100	2.10828900	1.24741400	N	-3.53769500	-1.05289200	2.24161400
N	-0.17339500	-1.18767400	2.66400600	N	3.78486200	3.372180900	0.73429600	N	2.42937000	3.42885100	1.01118200	N	-2.70064600	-1.92664000	2.85218500
N	-1.19320500	-0.95177400	3.42252500	N	2.59140500	3.69674600	0.23398400	N	2.72995100	3.73288900	-0.20994800	N	-1.74717300	-2.29072900	2.05514000
N	-2.21115000	-0.59516500	2.60611200	N	2.28904700	2.39961700	0.00833400	N	3.13420500	2.59007300	-0.80829000	N	-1.94422400	-1.64099800	0.88760300
C	-3.51595600	-0.22783300	3.14103200	C	0.99938100	2.01162000	-0.54852100	C	3.53723000	2.57890600	-2.20778900	C	-1.02872700	-1.81738700	-0.23237700
H	-3.49693300	-0.43918300	4.20951400	H	0.49656100	2.92716200	-0.85843400	H	3.69076300	3.61454100	-2.50910900	H	-0.43432200	-2.70691300	-0.02603700
H	-3.69698500	0.83404100	2.96470200	H	1.15213700	1.36351300	-1.41460000	H	4.46793200	2.01859600	-2.31815200	H	-1.59972300	-1.95827200	-1.15252400
H	-4.29590500	-0.82202900	2.65986500	H	0.41172500	1.48632500	0.20717200	H	2.75615400	2.11626200	-2.81362800	H	-0.38796900	-0.93880400	-0.32926200
H	-1.65461900	-2.87544000	0.02739000	H	5.47882600	1.35521300	-1.05320200	H	4.68100900	1.08781100	2.11158000	H	-5.30286800	-2.05635800	0.61964300
C	-2.55565700	-0.29618700	0.12415500	C	3.43007300	0.17304700	0.31167700	C	3.42300600	0.17482700	-0.13599200	C	-3.62900700	0.00104000	-0.02882400
N	-2.92937200	0.91099600	-0.13835000	N	2.65926400	-0.58879000	0.10150200	N	2.76373500	-0.57189900	-0.95914300	N	-2.97336400	1.00346100	-0.51525700
O	-2.60886400	1.80885800	0.88644800	O	1.79599400	0.13132800	1.83471500	O	1.74494300	0.10694000	-1.61733000	O	-1.71964000	1.15903900	0.06371800
C	-2.27884700	3.07945500	0.32733300	C	0.97572800	-0.77356800	2.59916800	C	0.87655300	-0.83185200	-2.29404900	C	-1.07250000	2.32318800	-0.49458700
H	-3.01563000	3.34309300	-0.44132300	H	1.61367400	-1.54297000	3.04285500	H	0.41549900	-0.25344000	-3.09599000	H	-1.02266200	2.21716400	-1.58205000
H	-2.37245900	3.78221000	1.16179200	H	0.55609900	-0.14054700	3.38409700	H	1.49605100	-1.63357000	-2.70600700	H	-1.65593500	3.21234200	-0.23511800
C	-0.86534700	3.11067000	-0.24172100	C	-0.13531000	-1.38937900	1.77816000	C	-0.20292900	-1.36686400	-1.38067200	C	0.31376700	2.38162900	0.09512300
C	-0.37090500	4.24543100	-0.89214800	C	-0.12446000	-2.73996000	1.42710700	C	0.04521200	-2.40814300	-0.48227500	C	0.60440300	3.19220400	1.19310600
C	1.11281000	1.96427600	-0.54325800	C	-2.13304400	-1.04286300	0.67919100	C	-2.38928900	-1.17579900	-0.67649600	C	2.47908000	1.59704100	0.00267300
C	0.94157300	4.19803900	-1.36734800	C	-1.18567300	-3.23312800	0.66221000	C	-0.99800300	-2.82181000	0.34868300	C	1.90852600	3.18018400	1.69574800
H	-0.98604100	5.13088800	-1.02298000	H	0.69384300	-3.38081000	1.73647600	H	1.02631000	-2.86692500	-0.43167000	H	-0.16782400	3.80681800	1.64307200
C	1.71362300	3.04968100	-1.20174800	C	-2.21604300	-2.38576700	0.27117000	C	-2.24402600	-2.20794500	0.26464100	C	2.87582000	2.37671600	1.10305400
H	1.36854500	5.05828400	-1.87497900	H	-1.21074700	-4.27831400	0.36830200	H	-0.84387400	-3.62519600	1.06296400	H	2.17288800	3.79638300	2.54983200
H	2.72987300	2.97967600	-1.56293000	H	-3.05484600	-2.72733400	-0.31894200	H	-3.07701400	-2.50173100	0.88783400	H	3.89601200	2.34179100	1.45876900
N	-0.14029800	2.00680400	-0.07186400	N	-1.12345300	-0.55735600	1.40984000	N	-1.39821200	-0.76611200	-1.47767700	N	1.23468700	1.59782600	-0.48862800
N	1.72918800	0.72971100	-0.30808100	N	-3.09991700	-0.07372500	0.37361900	N	-3.58116700	-0.46575100	-0.88164300	N	3.34148100	0.74295600	-0.69970600
H	1.14218600	0.04422600	0.17021400	H	-2.91342300	0.84124200	0.76495300	H	-3.51887000	0.25965900	-1.58512700	H	2.91064700	0.26196100	-1.47924100
C	3.00392300	0.35865800	-0.64243000	C	-4.26134000	-0.22333800	-0.34163400	C	-4.78886300	-0.62967100	-0.25488300	C	4.67337400	0.50261900	-0.47499100
O	3.83972100	1.04906000	-1.20354800	O	-4.65725400	-1.24392500	-0.87580700	O	-5.05463700	-1.44832400	0.60745800	O	5.36362200	1.00198600	0.39526200
O	3.20865100	-0.92713400	-0.25159600	O	-4.91432700	0.96848800	-0.36811400	O	-5.66930900	0.27852900	-0.75610300	O	5.11598500	-0.39734300	-1.39317100
C	4.51103500	-1.48146300	-0.51672700	C	-6.16590100	1.00334100	-1.08848000	C	-7.00645600	0.24601900	-0.21379100	C	6.51098400	-0.76397100	-1.31545300
H	4.34956600	-2.55947900	-0.56644000	H	-6.28925900	2.04805600	-1.37721200	H	-7.63299900	0.67597400	-0.99667000	H	6.76514200	-1.09640800	-2.32291900
H	4.87932000	-1.11561300	-1.47719300	H	-6.09203100	0.37738000	-1.97956800	H	-7.30053200	-0.78873400	-0.02846000	H	7.10499100	0.11325000	-1.05266200
C	5.49159100	-1.12910200	0.61361300	C	-7.32391100	0.54252300	-0.19006400	C	-7.09257600	1.07855000	1.07491400	C	6.72273600	-1.89347000	-0.29561900
H	5.63039700	-0.04245100	0.64073400	H	-7.17110800	-0.50785700	0.08231600	H	-6.45995800	0.61898500	1.84251200	H	6.46146300	-1.52843700	0.70393900
H	5.05211600	-1.42932300	1.57260500	H	-7.31250900	1.12898500	0.73692600	H	-6.69616200	2.08239300	0.87891200	H	6.04355900	-2.72173000	-0.53251000
C	6.78313600	-1.78958900	0.42877000	C	-8.61350200	0.69932500	-0.86131200	C	-8.46982400	1.17368100	1.55705900	C	8.10608800	-2.36727200	-0.30607000
C	7.84326200	-2.34750800	0.25702700	C	-9.66998600	0.83885000	-1.43418900	C	-9.61652300	1.24148800	1.93724100	C	9.25508000	-2.74540700	-0.33193200
H	8.78190600	-2.83216200	0.11363500	H	-10.60600500	0.95530400	-1.93145000	H	-10.62294000	1.30510700	2.28346200	H	10.26605600	-3.08411300	-0.34356200

SI-I: Cartesian coordinates of the Z isomers in the ground state at the B3LYP/6-31+G(d,p) level

E-a			S ₀	E-b			S ₀	E-c			S ₀	E-d			S ₀
C	-4.04371000	1.68134300	-0.08791800	C	3.94352200	1.76253300	0.13494400	C	-4.26415600	-0.43834800	0.84356700	C	3.96755400	-0.25308200	1.13091300
C	-4.55428500	-0.81553200	-0.07345400	C	4.68225200	-0.66489400	-0.11205900	C	-3.29109600	1.66603500	-0.21387100	C	3.17280600	1.61073600	-0.40937800
C	-4.81205000	-1.83315500	-1.00694500	C	4.45433400	-1.89863300	0.51955400	C	-2.06285100	2.34768600	-0.24864200	C	3.41544100	2.05323100	-1.72008600
C	-5.68851000	-2.87105500	-0.69167800	C	5.47026600	-2.85098300	0.59399700	C	-2.03451500	3.73986800	-0.32121100	C	3.37934300	3.41441000	-2.02109100
C	-6.30387900	-2.91711100	0.56249900	C	6.71994900	-2.59307000	0.02395900	C	-3.22639700	4.46801300	-0.37885900	C	3.08391800	4.34878800	-1.02452200
C	-6.05013000	-1.91010200	1.49697600	C	6.95314100	-1.37039400	-0.61022000	C	-4.45083800	3.79639500	-0.35013300	C	2.83822200	3.91583300	0.28081500
C	-5.19057700	-0.85883300	1.17798800	C	5.94620100	-0.40707300	-0.66807100	C	-4.48448500	2.40505400	-0.25609700	C	2.89393400	2.55698400	0.59010200
H	-4.33313900	-1.80668100	-1.97843900	H	3.48561700	-2.11144500	0.95510400	H	-1.13562700	1.78821900	-0.21734100	H	3.63772200	1.33359500	-2.49883800
H	-5.88928900	-3.64521800	-1.42632700	H	5.28354200	-3.79622700	1.09496000	H	-1.07921800	4.25630300	-0.33595400	H	3.58000300	3.74464900	-3.03602800
H	-6.98216300	-3.72935100	0.80715500	H	7.50812400	-3.33836100	0.07820900	H	-3.20053600	5.55214100	-0.44062600	H	3.05170700	5.40802400	-1.26273800
H	-6.53113300	-1.93350000	2.47013600	H	7.92330200	-1.15882400	-1.04947600	H	-5.38161800	4.35432300	-0.38732100	H	2.61603600	4.63563200	1.06284100
N	-5.29602300	2.05661900	0.15515500	N	5.04860500	2.14612000	0.76770100	N	-4.84588900	0.20184300	1.85392600	N	4.88609900	0.48822600	1.74385900
N	-5.25813900	3.38830800	0.37416500	N	4.96538400	3.48689500	0.90143200	N	-5.59544100	-0.71323900	2.50472600	N	5.34484700	-0.25064700	2.77654200
N	-4.04675700	3.83926100	0.27840900	N	3.86689600	3.93664600	0.38177000	N	-5.50074800	-1.87577300	1.94080100	N	4.75029600	-1.40117100	2.82369400
N	-3.25374600	2.78432300	-0.01097500	N	3.19794800	2.87171800	-0.11281700	N	-4.66753300	-1.73560800	0.88551900	N	3.87132200	-1.43306600	1.79745300
C	-1.81779300	2.98537100	-0.17190100	C	1.91102900	3.07415000	-0.76910600	C	-4.37272100	-2.89043700	0.04685600	C	3.04171300	-2.61444700	1.59716100
H	-1.60482400	3.99921700	0.16597200	H	1.76525200	4.15160800	-0.84167100	H	-5.05590900	-3.68208000	0.35390400	H	3.13502600	-3.21995500	2.49851400
H	-1.27157500	2.25726600	0.42851000	H	1.92522900	2.62247600	-1.76195700	H	-4.52771600	-2.63572400	-1.00235200	H	2.00514800	-2.31689900	1.43771700
H	-1.53350900	2.86324300	-1.21810000	H	1.11243800	2.61613400	-0.18442700	H	-3.33699700	-3.20338400	0.18619400	H	3.38580600	-3.17426500	0.72563600
H	-5.02028700	-0.06661500	1.89871000	H	6.14480700	0.54907300	-1.13882800	H	-5.43932400	1.89377800	-0.20637100	H	2.72746900	2.23160400	1.61114000
C	-3.62642000	0.30270600	-0.39644200	C	3.61127200	0.36602100	-0.19817800	C	-3.33690300	0.18082800	-0.11961700	C	3.21819300	0.16259500	-0.06727000
N	-2.45217800	0.21485900	-0.93523700	N	2.37617900	0.18625100	-0.54427100	N	-2.63234800	-0.66771000	-0.79956700	N	2.66703200	-0.81330500	-0.71725300
O	-2.05780300	-1.08793900	-1.21143500	O	2.07100800	-1.12828400	-0.87081100	O	-1.80033400	-0.07249500	-1.73347600	O	1.96014400	-0.40348000	-1.83569400
C	-0.69826600	-1.09086000	-1.66043000	C	0.73166700	-1.20255500	-1.36789000	C	-1.00539900	-1.07372100	-2.39566600	C	1.28045200	-1.52510500	-2.42846800
H	-0.58077700	-2.05954300	-2.15783000	H	0.56406100	-0.42364900	-2.11836100	H	-1.65398100	-1.89351700	-2.72004400	H	0.97709900	-1.15045500	-3.40886800
H	-0.54067200	-0.29678300	-2.39583600	H	0.68501400	-2.17638900	-1.86600400	H	-0.60716500	-0.54940300	-3.26710900	H	1.98692700	-2.35216600	-2.54891300
C	0.31047400	-0.95927700	-0.53604300	C	-0.34067200	-1.12130100	-0.29864400	C	0.12907400	-1.58363500	-1.53485400	C	0.06187300	-1.96056900	-1.64422600
C	0.00002800	-1.26442200	0.79074800	C	-0.07371800	-1.23478000	1.06612000	C	0.13543100	-2.88233500	-1.02355600	C	0.00271100	-3.20453100	-1.01286300
C	2.49729100	-0.46822300	-0.00095800	C	-2.60614300	-0.91950600	0.07535100	C	2.14935700	-1.10076400	-0.53631200	C	-2.05630200	-1.40963500	-0.92319600
C	1.01655900	-1.14575900	1.74138400	C	-1.15524200	-1.17817700	1.94907900	C	1.21841100	-3.27689000	-0.23209300	C	-1.16250500	-3.53714100	-0.31456500
H	-0.99974000	-1.58273900	1.06052800	H	0.94158300	-1.35721000	1.42174800	H	-0.68328200	-3.56125000	-1.02365000	H	0.84112500	-3.89079200	-1.06890500
C	2.29327300	-0.74213100	1.36087400	C	-2.45097100	-1.01992500	1.46728300	C	2.25115700	-2.38433500	0.02945500	C	-2.21921700	-2.63282000	-0.25381500
H	0.81660600	-1.37103800	2.78497000	H	-0.98942700	-1.25851200	3.01944400	H	1.25792300	-4.27917100	0.18421900	H	-1.24822900	-4.49807500	0.18444100
H	3.10323300	-0.63812800	2.06896500	H	-3.31070500	-0.97357400	2.12064000	H	3.10502100	-2.64869600	0.63734400	H	-3.13654100	-2.85401400	0.27498000
N	1.53147900	-0.56767000	-0.92352200	N	-1.58010600	-0.96443200	-0.78305900	N	1.12202500	-0.71240900	-1.29867300	N	-0.95358500	-1.08542700	-1.60539300
N	3.72372200	-0.05603000	-0.54207300	N	-3.84315600	-0.75854000	-0.56553500	N	3.11345000	-0.09664400	-0.36944500	N	-3.03147400	-0.40344400	-0.95586800
H	3.70660500	0.10439200	-1.54156800	H	-3.78760700	-0.71373000	-1.57541400	H	2.89169900	0.77573400	-0.83309800	H	-2.76201200	0.42099300	-1.47867600
C	4.91570200	1.44966000	0.10509700	C	-5.08939400	-0.66396700	-0.00176400	C	4.29869900	-0.15879700	0.31794500	C	-4.27588200	-0.40478500	-0.37930700
O	5.12658000	0.00753500	1.29693600	O	-5.35403600	-0.70481100	1.18651900	O	4.73146600	-1.11771700	0.93203100	O	-4.76969400	-1.30464900	0.27720400
O	5.84842200	0.53294300	-0.80589000	O	-6.00814300	-0.51545300	-0.99413000	O	4.93118000	1.03984600	0.20938300	O	-4.88993800	0.77503800	-0.65940100
C	7.17425200	0.79627700	-0.29844900	C	-7.38813700	-0.40881000	-0.58356300	C	6.20095100	1.16172000	0.88636800	C	-6.22537600	0.94683400	-0.13756100
H	7.61179800	1.49254300	-1.01535800	H	-7.96080700	-0.74496000	-1.44914900	H	6.31378100	2.23079800	1.07189200	H	-6.68836500	1.67931700	-0.80026700
H	7.10299500	1.26856100	0.68294500	H	-7.56999800	-1.07292400	0.26336700	H	6.16276100	0.62165300	1.83408100	H	-6.76487400	-0.00026700	-0.19524500
C	7.99522900	-0.50044800	-0.22338500	C	-7.73939100	1.04345700	-0.22481000	C	7.34195700	0.63551200	0.00193600	C	-6.18343100	1.46559000	1.30812600
H	7.53334500	-1.17642400	0.50502500	H	-7.15210700	1.34971300	0.64813700	H	7.20066600	-0.43822400	-0.16501000	H	-5.71862800	0.70755400	1.94843800
H	7.96607900	-0.99850300	-1.20033100	H	-7.45547300	1.69637000	-1.05939400	H	7.29381400	1.13071900	-0.97572000	H	-5.55329400	2.36264200	1.34781700
C	9.38157300	-0.23294500	0.15705600	C	-9.16610200	1.19282200	0.05891200	C	8.64711200	0.87507700	0.61635400	C	-7.52417000	1.77795200	1.80126000
C	10.52422100	0.01039400	0.47177200	C	-10.34968900	1.29523000	0.28816400	C	9.71693300	1.08418600	1.14136800	C	-8.64180400	2.03162600	2.18912700
H	11.53269700	0.21407500	0.75177900	H	-11.39078300	1.39533700	0.49555500	H	10.66427400	1.26082700	1.59771400	H	-9.62280600	2.25543500	2.54191600

E-a				E-b				Z-c			
S _I				S _I				S _I			
C	-3.47270600	1.60851200	0.35576600	C	4.11948700	1.66158900	-0.00031800	C	-1.40503300	0.51083100	0.97357500
C	-4.16396000	-0.82628000	0.12449900	C	4.70533900	-0.77489400	-0.19646400	C	-3.46604700	1.03378600	-0.38474600
C	-4.52496100	-1.88147300	-0.76709100	C	4.70309000	-1.97560800	0.54854500	C	-4.76491900	0.68151400	-0.87498400
C	-5.29381800	-2.96010600	-0.34233000	C	5.63453900	-2.98142100	0.30008400	C	-5.51344400	1.57800900	-1.62622500
C	-5.74553400	-3.05434700	0.98090100	C	6.59815000	-2.82760800	-0.70300100	C	-5.02760800	2.85883000	-1.93457000
C	-5.41375100	-2.02282800	1.87022000	C	6.61624000	-1.64360700	-1.44819600	C	-3.75434700	3.22268000	-1.45961100
C	-4.64635600	-0.93622000	1.46330000	C	5.68716300	-0.63464400	-1.20115100	C	-2.99065000	2.34181100	-0.70705200
H	-4.21656500	-1.83025200	-1.80229800	H	3.96982700	-2.10594700	1.33565200	H	-5.16374200	-0.29706800	-0.63262900
H	-5.55769700	-3.73278800	-1.06092900	H	5.61486800	-3.88816900	0.89977900	H	-6.49931500	1.27878100	-1.97560100
H	-6.34651100	-3.89843700	1.30544200	H	7.32483900	-3.61187300	-0.89514700	H	-5.62074400	3.55301200	-2.52120900
H	-5.76069500	-2.06267700	2.90010300	H	7.36177000	-1.50169600	-2.22626100	H	-3.35556600	4.20927400	-1.68337800
N	-3.52934600	1.85017500	1.67485900	N	5.39202200	2.12522100	-0.01429100	N	-0.21364500	0.53879400	0.37661800
N	-3.54336300	3.19445400	1.82576000	N	5.32126900	3.46546100	-0.04296900	N	0.68760400	0.89979200	1.32372800
N	-3.49095400	3.79674000	0.68387100	N	4.09793700	3.88664600	-0.03475900	N	0.10516400	1.09709200	2.46746800
N	-3.44569100	2.82409000	-0.26590000	N	3.30644000	2.77007600	0.00237900	N	-1.20711500	0.86876000	2.26465200
C	-3.50556300	3.18530800	-1.67274900	C	1.87408500	2.93201600	-0.11801900	C	-2.17677600	0.94328200	3.34747000
H	-3.75199500	4.24662200	-1.71832200	H	1.68473600	4.00386100	-0.19582500	H	-1.73325400	1.52549600	4.15473400
H	-2.55290000	2.98669800	-2.16509900	H	1.50468900	2.42921200	-1.01728300	H	-3.08133700	1.42951800	2.97872600
H	-4.27893700	2.59623900	-2.16998200	H	1.36256100	2.51834600	0.75137000	H	-2.42220800	-0.06432800	3.69041600
H	-4.41137600	-0.15254700	2.17262300	H	5.72669400	0.28139000	-1.77871300	H	-2.00777000	2.65358800	-0.36664300
C	-3.38600600	0.31951100	-0.32683300	C	3.71634700	0.28496500	0.07254300	C	-2.70517300	0.10796800	0.39795000
N	-2.55213500	0.41869100	-1.41023600	N	2.45427800	0.06927200	0.54940100	N	-3.17655700	-1.15861600	0.60455400
O	-2.19315900	-0.91424600	-1.92529000	O	1.99274000	-1.29334500	0.15877500	O	-2.28728200	-1.83727000	1.56928500
C	-0.86123800	-0.82272500	-2.30776200	C	0.84629100	-1.16709000	-0.61330100	C	-1.87839100	-3.05837100	1.00662100
H	-0.62015500	-1.71677700	-2.90210000	H	0.93628000	-0.39075200	-1.38765200	H	-1.42073600	-3.64701900	1.80676800
H	-0.66468200	0.06075500	-2.93082700	H	0.66914600	-2.12355200	-1.12523800	H	-2.73503100	-3.59931300	0.58446000
C	0.09342300	-0.78589800	-1.13160600	C	-0.38238400	-0.86737400	0.22044400	C	-0.83320300	-2.77601900	-0.06239000
C	-0.37059500	-1.14764300	0.18932200	C	-0.23401000	-0.53390400	1.61950300	C	-1.20185900	-2.65014700	-1.44849000
C	2.20440500	-0.42181200	-0.31102100	C	-2.66390500	-0.68528800	0.39297200	C	1.28034200	-2.03405200	-0.54887000
C	0.51747000	-1.11153500	1.26101900	C	-1.37167500	-0.26872900	2.38023700	C	-0.24909800	-2.26108700	-2.38790500
H	-1.40893200	-1.42267600	0.30949500	H	0.77110000	-0.47468000	2.01344800	H	-2.22830800	-2.84044500	-1.73251000
C	1.83544500	-0.74577900	1.03728100	C	-2.62092900	-0.34282100	1.78618400	C	1.02382800	-1.93125400	-1.95655200
H	0.17965700	-1.35815700	2.26076500	H	-1.28289800	-0.00945400	3.42915000	H	-0.51028100	-2.17211500	-3.43603300
H	2.57350100	-0.69470900	1.82524000	H	-3.54053400	-0.16016600	2.32391300	H	1.79364600	-1.56273200	-2.61938900
N	1.34704500	-0.44367200	-1.35916900	N	-1.56769200	-0.94087400	-0.35734500	N	0.38928300	-2.52458100	0.35077500
N	3.46019100	-0.04472400	-0.67197600	N	-3.82143400	-0.78852100	-0.31498200	N	2.42366900	-1.61194600	0.03652000
H	3.55990300	0.17975500	-1.65949900	H	-3.69241700	-1.04465200	-1.29125400	H	2.39551600	-1.62319000	1.05475000
C	4.61736000	0.08884800	0.12881400	C	-5.15154800	-0.59041100	0.11864900	C	3.52111400	-0.93621200	-0.54995600
O	4.66815000	-0.14876800	1.31237300	O	-5.47186300	-0.29049800	1.24502600	O	3.67720100	-0.78082800	-1.73824200
O	5.60528700	0.51481000	-0.65897900	O	-5.95266600	-0.79949600	-0.92600600	O	4.32504100	-0.54927000	0.43647300
C	6.90636400	0.73846300	-0.03423800	C	-7.38986100	-0.66376700	-0.70217100	C	5.49310200	0.24373700	0.07342500
H	7.37221200	1.49999600	-0.65872400	H	-7.83683100	-1.31436100	-1.45308600	H	6.20603700	0.04870400	0.87401700
H	6.75224500	1.12155500	0.97526300	H	-7.62657200	-1.02573300	0.29912400	H	5.88652700	-0.11753700	-0.87783600
C	7.72476600	-0.55849800	-0.02702300	C	-7.82581500	0.79401000	-0.89236100	C	5.11978400	1.73009300	0.00505400
H	7.22115500	-1.30776000	0.59479600	H	-7.34142500	1.42444300	-0.13771500	H	4.38521700	1.88971900	-0.79246500
H	7.77781000	-0.95699700	-1.04747600	H	-7.49535800	1.14454600	-1.87764500	H	4.64362400	2.02667600	0.94672100
C	9.07217700	-0.31403500	0.48492500	C	-9.27856000	0.91409900	-0.78027400	C	6.30844400	2.54513500	-0.24127400
C	10.18125900	-0.09089300	0.91115300	C	-10.48111300	0.99217500	-0.68392500	C	7.30570100	3.19824900	-0.44472300
H	11.16240800	0.09408700	1.28694400	H	-11.54149600	1.07484300	-0.60090400	H	8.17462200	3.79015800	-0.62370900

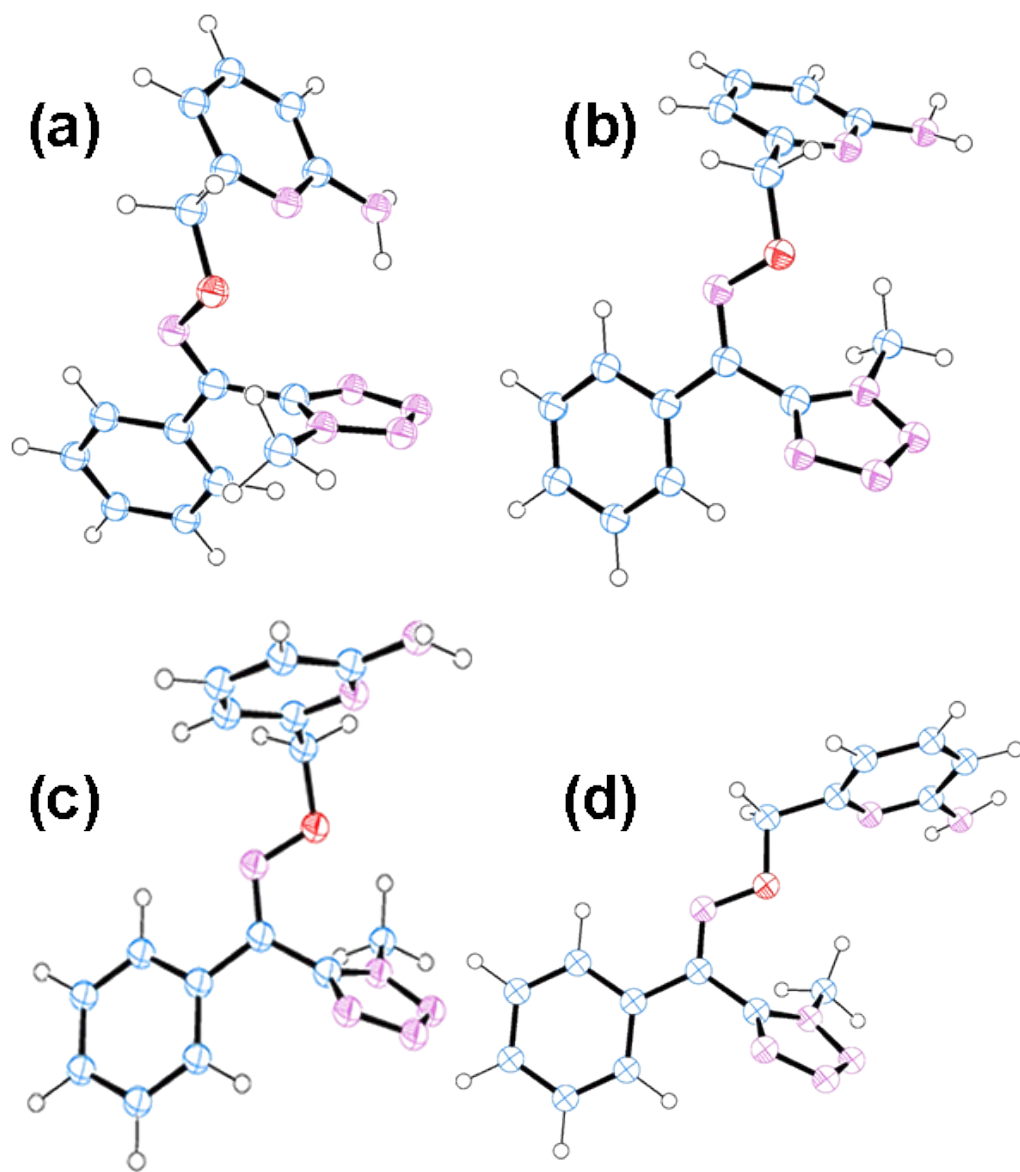
Figure SI-1: Geometries of **E-a**, **E-b** and **Z-c** in S_1 .



Zm-a			S ₀	Zm-b			S ₀	Zm-c			S ₀	Zm-d			S ₀
C	-0.91155300	1.35565900	0.17084200	C	1.59403600	1.49780200	0.30241500	C	-1.25531600	1.43353400	-0.31415700	C	-1.22942000	1.18482000	-0.43526300
C	-2.11082700	-0.89350700	-0.15559700	C	2.36937200	-0.93945100	0.03576300	C	-2.43389700	-0.83275800	-0.00162600	C	-3.05903500	-0.55087700	0.04057400
C	-2.26597200	-2.10844700	-0.85239000	C	2.11472400	-2.32184300	0.13391800	C	-2.64970200	-1.96733700	0.80508400	C	-3.46888000	-1.89622100	0.11968300
C	-3.27306000	-3.00100400	-0.49826200	C	3.05862500	-3.24615400	-0.30274700	C	-3.71634900	-2.82420300	0.54771100	C	-4.81123700	-2.21534500	0.30143300
C	-4.14904500	-2.70073500	0.55242900	C	4.27524500	-2.81417800	-0.84579300	C	-4.59084900	-2.56541700	-0.51447700	C	-5.77238100	-1.20230900	0.40601100
C	-4.00528300	-1.49856600	1.24540500	C	4.53824900	-1.44757100	-0.94588700	C	-4.38680700	-1.44094900	-1.31538600	C	-5.37605900	0.13296300	0.32400300
C	-2.99488100	-0.59914700	0.89594500	C	3.59206400	-0.51430600	-0.51021200	C	-3.31922500	-0.57625800	-1.06246400	C	-4.03023900	0.45902700	0.14135600
H	-1.59050900	-2.33973900	-1.66793700	H	1.17336700	-2.65793200	0.55323500	H	-1.97842700	-2.16307500	1.63366100	H	-2.72664900	-2.68140500	0.03157700
H	-3.37798300	-3.93405200	-1.04430600	H	2.84649300	-4.30828700	-0.22040900	H	-3.87121500	-3.69274200	1.18136200	H	-5.11162100	-3.25779500	0.35514800
H	-4.93522600	-3.39889200	0.82461200	H	5.01022900	-3.53841600	-1.18471800	H	-5.42446000	-3.23335200	-0.71082300	H	-6.81973200	-1.45489300	0.54315700
H	-4.67620000	-1.25543000	2.06392400	H	5.47813000	-1.09945000	-1.35929600	H	-5.05669000	-1.23172900	-2.14411000	H	-6.11274400	0.92750500	0.39599500
N	-0.62072200	1.51637800	1.45595900	N	2.55240200	2.21537400	0.87288600	N	-1.18414100	1.72611400	-1.60575300	N	-1.62742200	1.89139900	-1.48545600
N	-0.60634200	2.85486800	1.67120500	N	2.38845300	3.48227000	0.41836800	N	-1.18454200	3.08005300	-1.68258000	N	-1.03433000	3.10319000	-1.36604500
N	-0.88422800	3.50263800	0.58634200	N	1.38917200	3.55522600	-0.40204300	N	-1.26299300	3.61160700	-0.50551700	N	-0.31228300	3.16298900	-0.29176600
N	-1.08365200	2.57710500	-0.37840100	N	0.86677100	2.31329200	-0.49400200	N	-1.30998400	2.59257000	0.38065800	N	-0.41587000	1.96248400	0.31653100
C	-1.40891600	2.97161500	-1.74280000	C	-0.28705700	2.03951100	-1.34277400	C	-1.39540200	2.84616000	1.81233800	C	0.29489100	1.69073600	1.56008900
H	-1.58466300	4.04667800	-1.73328400	H	-0.49757800	2.95319900	-1.89765900	H	-1.60250700	3.90805200	1.94014000	H	0.51594900	2.65141800	2.02455600
H	-0.57633600	2.72416300	-2.40327100	H	-0.04841200	1.23283800	-2.03994900	H	-2.20644700	2.25571300	2.24426700	H	-0.34408000	1.09764100	2.21726100
H	-2.31069300	2.45166000	-2.07386800	H	-1.14425600	1.75553100	-0.72871000	H	-0.45111000	2.57944500	2.28992000	H	1.21487300	1.14013000	1.35394300
H	-2.88448200	0.32090200	1.45790800	H	3.81940900	0.54335700	-0.57465100	H	-3.15881900	0.28173000	-1.70491300	H	-3.74210800	1.50080800	0.06044400
C	-1.03434900	0.05531900	-0.53753600	C	1.35546700	0.04444500	0.49068300	C	-1.28817700	0.07133900	0.27567500	C	-1.62493500	-0.21151900	-0.12996600
N	-0.21245000	-0.29863000	-1.46852700	N	0.27673000	-0.39992000	1.04587400	N	-0.34195700	-0.36975600	1.03727500	N	-0.75571300	-1.16166200	-0.01165100
O	0.70566700	0.70390300	-1.79040200	O	-0.57698900	0.61911000	1.45060600	O	0.64808100	0.57203100	1.28013800	O	0.54400000	-0.73124300	-0.23882700
C	1.95835000	0.11213300	-2.14635900	C	-1.77206700	0.05997100	2.02761100	C	1.80600500	-0.06252200	1.87712000	C	1.45725300	-1.83973100	-0.08993500
H	1.80071800	-0.65782200	-2.91084000	H	-1.49187400	-0.70232100	2.76018600	H	2.32039200	0.74800900	2.39576500	H	1.32434100	-2.27810700	0.90370200
H	2.52578500	0.93997800	-2.58454100	H	-2.23165000	0.91103800	2.53606600	H	1.45376800	-0.81424000	2.58886300	H	1.23636900	-2.58816900	-0.85764000
C	2.68866500	-0.45901900	-0.93986900	C	-2.71936400	-0.50021300	0.98925600	C	2.72369800	-0.65771900	0.83446600	C	2.85120400	-1.28492700	-0.24199500
C	3.66621500	-1.44455400	-1.08753800	C	-3.02934400	-1.85813600	0.94919800	C	2.56252000	-1.96959000	0.38790600	C	3.56509300	-1.44363800	-1.42783200
C	2.93250800	-0.40043700	1.35496200	C	-4.08654700	-0.03546500	-0.81304200	C	4.49488700	-0.27969800	-0.59612100	C	4.56486500	-0.09711000	0.74862000
C	4.31051300	-1.89379800	0.07315200	C	-3.92441400	-2.30147500	-0.03445400	C	3.42927600	-2.43308700	-0.61016500	C	4.85011800	-0.88831800	-1.50182400
H	3.91071500	-1.85363800	-2.06278300	H	-2.58186000	-2.54788600	1.65606900	H	1.77967000	-2.59948100	0.79485500	H	3.13140200	-1.97508600	-2.26765700
C	3.95193300	-1.37869800	1.31075500	C	-4.46220600	-1.39283900	-0.93134700	C	4.40927300	-1.59155700	-1.11304500	C	5.36421700	-0.20518800	-0.41218100
H	5.08305600	-2.65511700	0.00859400	H	-4.19296400	-3.35199800	-0.09906400	H	3.33743000	-3.44687400	-0.98931500	H	5.43988000	-0.98793200	-2.40836600
H	4.43226600	-1.71961000	2.22296000	H	-5.15169800	-1.70798700	-1.70867800	H	5.10068800	-1.92716900	-1.88010900	H	6.35303200	0.24221200	-0.44295200
N	2.33837500	0.05449100	0.24159900	N	-3.23959500	0.39533100	0.13056600	N	3.66868100	0.17012300	0.35810100	N	3.33841000	-0.63041800	0.82771500
N	2.51133900	0.17241000	2.53345500	N	-4.54979700	0.91682400	-1.70288200	N	5.47790900	0.59609200	-1.01819700	N	5.00104100	0.60627100	1.85477300
H	1.62596600	0.66464900	2.48092900	H	-4.44100400	1.87427500	-1.39735800	H	5.31647500	1.56316500	-0.77192400	H	4.48591900	0.43401600	2.70669500
H	2.69021600	-0.32065900	3.39485800	H	-5.40807500	0.72178500	-2.19679900	H	5.87617900	0.44906400	-1.93380000	H	5.99360900	0.74565300	1.96941000

SI-IV: Cartesian coordinates of the Zm isomers in the ground state at the B3LYP/6-31G+(d,p) level.

Figure SI-2: Geometries of the **Zm** conformers in S_0 .



SI-V: The Conical Intersection Structure in Figure 3 (CI).

Z-b is the low energy **Z** isomer species. The search for the CI structure was performed on **Z_m-b**, a model structure with a geometry similar to that of **Z-b**. UHF/STO-3G natural orbitals were selected initially for active space. Ground state CAS(8,7) optimization was performed and the conical intersection was found at the CAS(8,7)/STO-3G level. State averaged single point calculations were performed on this CI structure to enlarge the basis set progressively. Then, the conical intersection was found (opt=conical) from the above starting geometry at the CAS(8,7)/6-31G level. Active Space and structure of the conical intersection are given below.

Figure SI-3: Active space (bonding (top) and antibonding (bottom)) for location of the conical intersection at the CAS(8,7)/6-31G for **Z_m-b**.

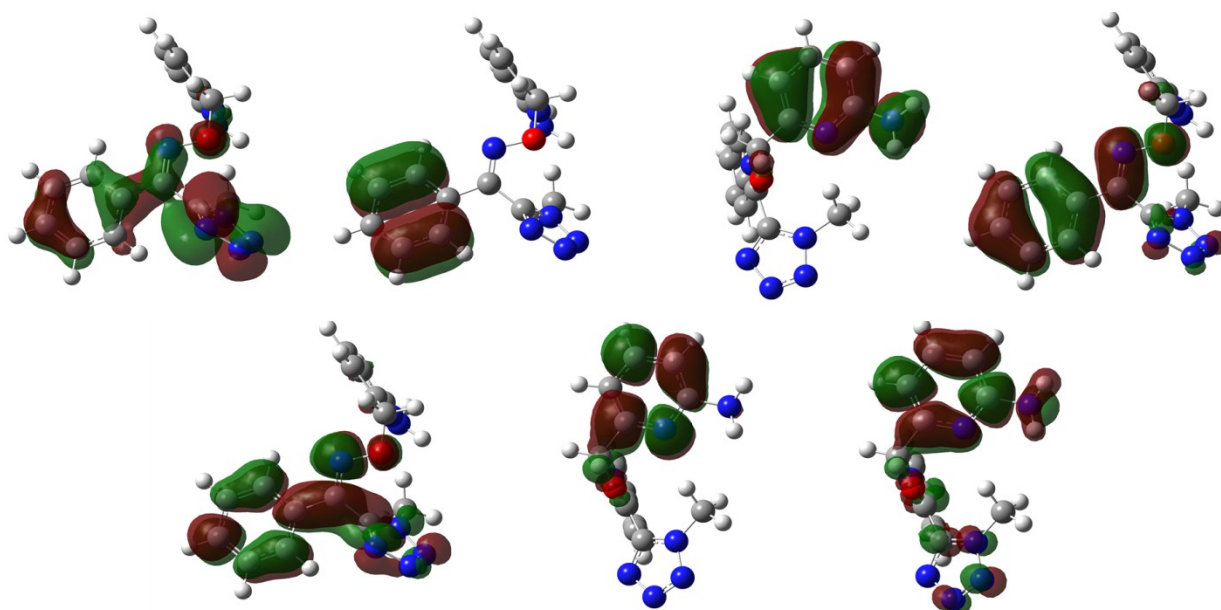
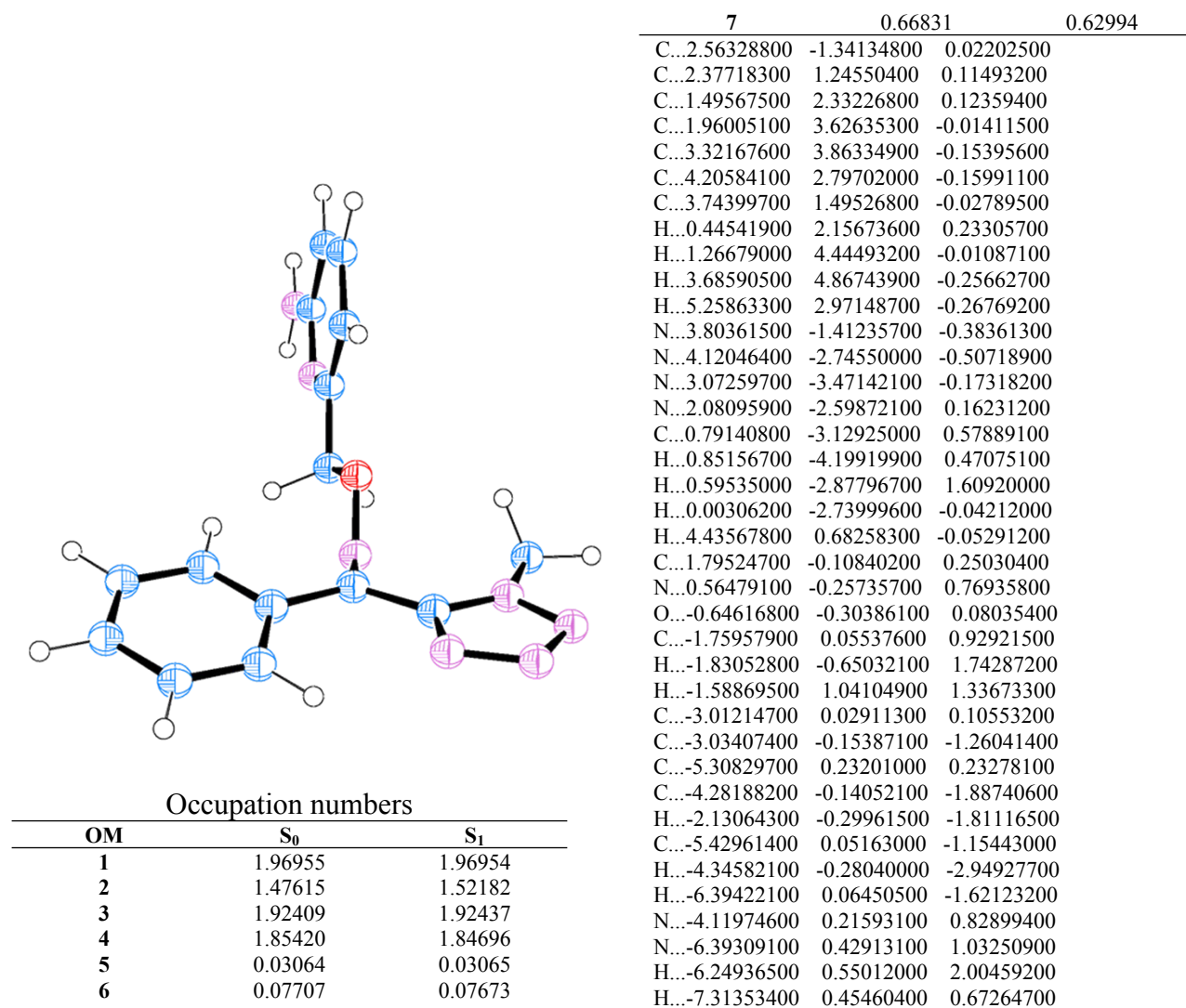
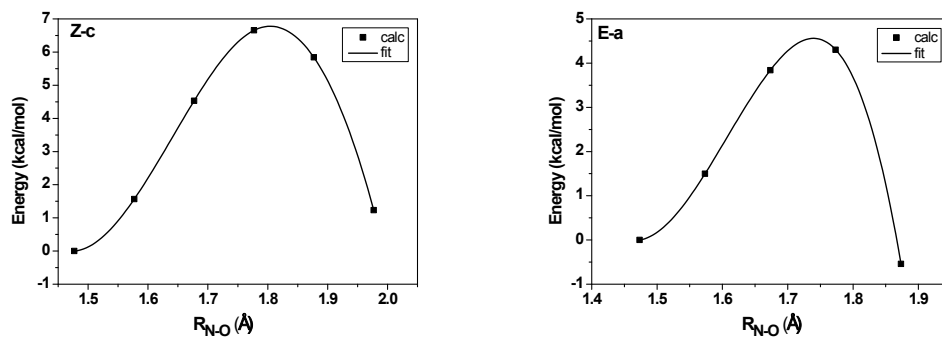


Figure SI-4: Geometry of the conical intersection (CI in Figure 3) for **Z_m-b**.



SI-VI: MEP data vs the N-O bond length for Z-c and E-a in S_1 at the 6-31+G(d,p) level.



SI-VII: The Photoreactivity of Z-a.

The photoreactivity of **Z-a** was investigated from CASSCF calculations. The model structure **Z_m-a** was used in this section. The procedure was similar to that described in SI-V.

Figure SI-5 : Active space (bonding (top) and antibonding (bottom)) for location of the minimum energy biradical structure **Z_m-a** at the CAS(8,7)/6-31G.

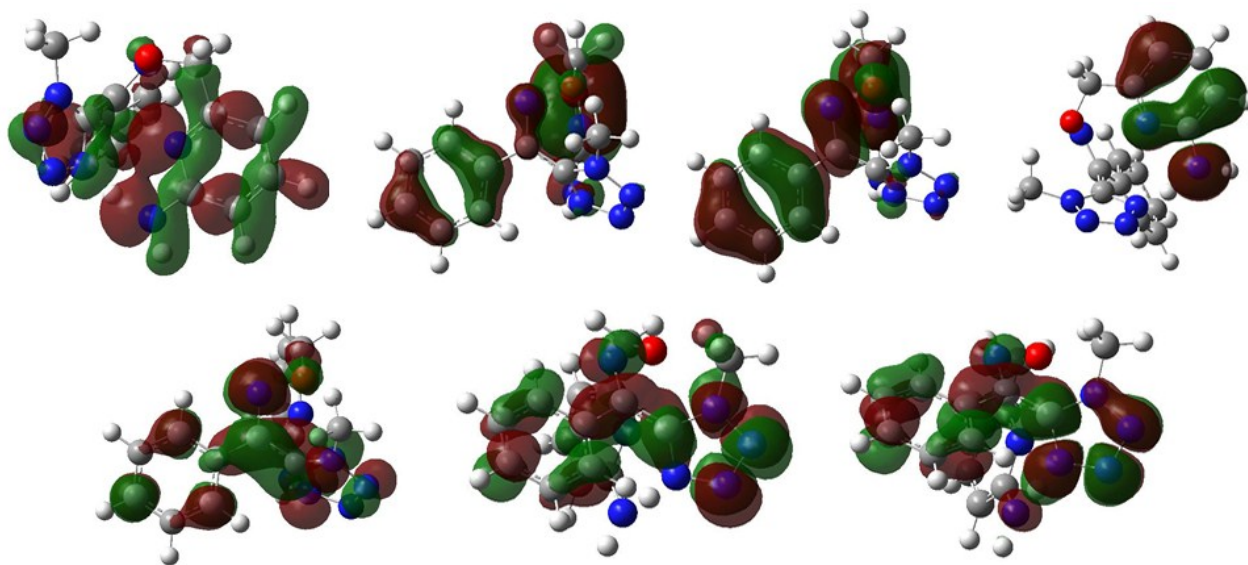
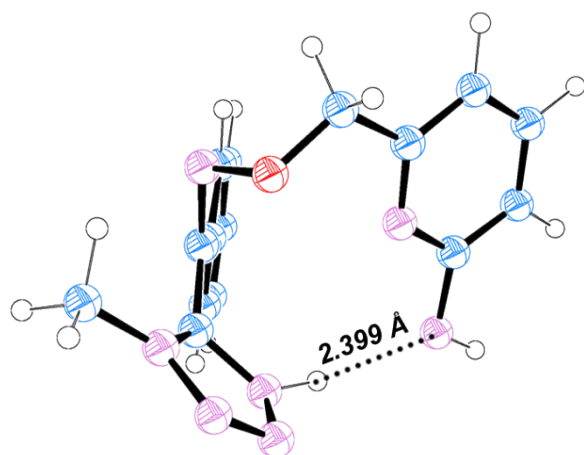


Figure SI-6 : Geometry of the minimum energy biradical structure Z_m -a in S_1 at the CAS(8,7)/6-31G level.



Occupation numbers		
OM	S_0	S_1
1	1.77433	1.17598
2	0.11736	0.11812
3	1.88767	1.88772
4	1.00772	1.31977
5	1.99165	1.99419
6	0.22106	0.50502
7	1.00021	0.99919

C	-2.08893100	-0.33594100	0.33264500
C	-0.16232100	-1.78947800	-0.48863800
C	0.86518500	-2.03401200	-1.40699300
C	1.72667200	-3.10468200	-1.23688100
C	1.58172900	-3.95577900	-0.15053100
C	0.56097000	-3.72953100	0.76263400
C	-0.30554500	-2.66303900	0.59594600
H	0.97756600	-1.39346500	-2.25810000
H	2.50571800	-3.27717000	-1.95468200
H	2.24834800	-4.78670600	-0.02157800
H	0.43494100	-4.38671600	1.60149100
N	-1.75639300	0.07944800	1.64430800
N	-2.60441800	1.10803500	2.03843600
N	-3.46312700	1.30416000	1.13284400
N	-3.21866200	0.45160900	0.07912900
C	-4.02849100	0.49577500	-1.10731600
H	-4.84056500	1.18249400	-0.92929500
H	-3.45286800	0.83935500	-1.95812200
H	-4.43597100	-0.48274200	-1.32707100
H	-1.09604700	-2.50801400	1.30233000
C	-1.07904000	-0.66983900	-0.66641600
N	-0.92843500	0.13304600	-1.82780200
O	-0.82003800	1.49381900	-1.40197000
C	0.40604000	2.11656600	-1.76534800
H	0.71909400	1.77426500	-2.74407900
H	0.18072500	3.17186100	-1.82334200
C	1.48571200	1.87211900	-0.73580900
C	2.79817100	2.29233000	-0.94991400
C	2.03127700	1.03597600	1.34378600
C	3.73842500	2.06659000	0.03841000
H	3.07138500	2.78089200	-1.86484300
C	3.35564900	1.42657900	1.21104400
H	4.75472700	2.37969700	-0.09823000
H	4.06590900	1.23783900	1.99156400
N	1.13650500	1.26488400	0.38362200
N	1.51028400	0.38059000	2.47192400
H	-0.82753400	0.11100800	2.00354600
H	2.21158600	0.21263300	3.17922400

Z-a			T ₁	Z-b			T ₁	Z-c			T ₁	Z-d			T ₁
C	0.00000000	0.00000000	0.00000000	C	-3.15592600	1.66287800	0.37219400	C	4.81396400	0.14998400	-0.58493500	C	-2.83236500	-1.89631200	-0.32470900
C	0.00000000	0.00000000	2.55778472	C	-4.83710000	-0.10939500	-0.42941000	C	2.92554400	1.60482100	0.37922800	C	-4.68247300	-0.21847100	0.29460700
C	0.75892232	0.00000000	3.75926892	C	-5.10658700	-1.49819500	-0.57812500	C	1.65357800	1.61690800	1.01560000	C	-5.18757500	1.09786700	0.10707500
C	0.14478604	-0.20690025	4.98801320	C	-6.32399900	-1.94615000	-1.07486900	C	1.03878600	2.81168900	1.36752100	C	-6.36295500	1.51034800	0.72144500
C	-1.24032082	-0.40720515	5.06796373	C	-7.31781500	-1.03138500	-1.44413900	C	1.66436500	4.03606200	1.10140300	C	-7.07862000	0.63023300	1.54306600
C	-2.00874143	-0.38730617	3.89671884	C	-7.07313200	0.33947300	-1.30243600	C	2.91806900	4.04422700	0.47838100	C	-6.59976300	-0.67113600	1.73547000
C	-1.40515008	-0.18524115	2.66090553	C	-5.86082900	0.80319500	-0.80238400	C	3.54768100	2.85662600	0.12159200	C	-5.42590700	-1.10001900	1.12489700
H	1.83037158	0.15694024	3.70701056	H	-4.35405300	-2.22126200	-0.28745200	H	1.15720600	0.67970100	1.23531100	H	-4.65173800	1.78532900	-0.53718900
H	0.74564624	-0.21026214	5.89280548	H	-6.50178900	-3.01322600	-1.17308600	H	0.06737300	2.79005900	1.85301800	H	-6.72723100	2.52044200	0.55732300
H	-1.71607500	-0.56369476	6.03118273	H	-8.26871000	-1.38234500	-1.83397900	H	1.18217800	4.96929400	1.37704800	H	-7.99746800	0.95347900	2.02324500
H	-3.08605256	-0.51440134	3.95177283	H	-7.83656000	1.05854100	-1.58518900	H	3.41263200	4.98797200	0.26729800	H	-7.14759800	-1.36186900	2.36998000
N	-0.05149356	0.83358687	-1.04282740	N	-3.86311300	2.77409000	0.10195300	N	5.62209100	1.11288400	-1.06022100	N	-3.20460900	-2.94122400	0.43397600
N	-0.70703694	0.17554678	-0.23403300	N	-3.13195300	3.81697300	0.52647600	N	6.71106800	0.50212900	-1.55528500	N	-2.34959500	-3.94203500	0.16704100
N	-1.04768190	-1.01558176	-1.64604832	N	-2.01283800	3.42144500	1.04864100	N	6.63124100	-0.78369700	-1.41457300	N	-1.47011500	-3.58278900	-0.71568800
N	-0.61641972	-1.15657426	-0.37272213	N	-1.99339600	2.07292100	0.96940600	N	5.45073200	-1.04318000	-0.80803400	N	-1.74146600	-2.30154500	-1.04785300
C	-0.75109684	-2.43760979	0.30865509	C	-0.83460200	1.35782700	1.48992600	C	5.10938800	-2.42958000	-0.51461300	C	-0.90775800	-1.64580900	-2.05062000
H	-0.80926643	-3.21076751	-0.45716594	H	-0.21878900	2.09726700	2.00138000	H	5.98032700	-3.02597200	-0.78585600	H	-0.23053800	-2.41002000	-2.43225500
H	0.12274102	-2.60085441	0.94071642	H	-1.15171700	0.58193500	2.18715800	H	4.88641700	-2.54867800	0.54650300	H	-1.52847600	-1.25871700	-2.86007300
H	-1.65269228	-2.45960307	0.92503164	H	-0.26983100	0.90424900	0.67381000	H	4.24787000	-2.74382200	-1.10714900	H	-0.33740100	-0.82889800	-1.60370200
H	-2.02106563	-0.12755902	1.76887775	H	-5.68601500	1.86556300	-0.70012700	H	4.51474500	2.87845100	-0.36226900	H	-5.06483300	-2.10711700	1.28524000
C	0.64054862	0.23593186	1.29101719	C	-3.55027800	0.30465600	0.09277300	C	3.52499200	0.33321000	0.03527600	C	-3.45276000	-0.59547700	-0.35733800
N	1.89887165	0.86299050	1.24269247	N	-2.63860600	-0.71740400	0.45866800	N	2.84877400	-0.84990400	0.42323800	N	-2.82986200	0.36279900	-1.20331000
O	2.88944298	-0.09710802	1.15082110	O	-1.91305400	-1.07127900	-0.66118900	O	1.99869600	-1.22355400	-0.59845300	O	-1.92529000	1.07382700	-0.44053600
C	4.16536243	0.51450515	0.84996974	C	-1.10667000	-2.25630700	-0.41521500	C	1.22637700	-2.40218700	-0.23118900	C	-1.29448500	2.12036100	-1.22678700
H	4.18127099	1.50561629	1.31395782	H	-1.73828100	-2.99961200	0.07758200	H	0.94526000	-2.84666700	-1.18672700	H	-1.17501600	1.75402500	-2.24893600
H	4.91474753	-0.12886460	1.31665058	H	-0.83933700	-2.59049900	-1.41911100	H	1.87984500	-3.07188900	0.33346200	H	-1.95373600	2.99390500	-1.22184200
C	4.37670155	0.61193351	-0.64742019	C	0.14061700	-1.97949200	0.38890300	C	-0.01287500	-2.04277200	0.55262900	C	0.03800600	2.42974600	-0.59692900
C	5.55488976	0.18383092	-1.26147626	C	0.24218700	-2.35288200	1.73014400	C	-0.00135300	-1.97927900	1.94820200	C	0.22901800	3.57221100	0.17968900
C	3.46164454	1.28524268	-2.65312162	C	2.26975500	-1.09427900	0.39013600	C	-2.23184700	-1.42853500	0.46070100	C	2.21483200	1.74596200	-0.27516100
C	5.66155964	0.35318937	-2.64725831	C	1.43396700	-2.06833900	2.40446000	C	-1.18395000	-1.61642400	2.59871700	C	1.49272800	3.78413200	0.73990300
H	6.35779875	-0.26462503	-0.68494841	H	-0.58569000	-2.84416400	2.22950900	H	0.90497000	-2.19895400	2.50157500	H	-0.58499600	4.26995700	0.34450200
C	4.61184333	0.90648122	-3.37265783	C	2.47458500	-1.42739800	1.74194000	C	-2.32742000	-1.33112400	1.86020100	C	2.51338300	2.86784600	0.52026200
H	6.56291961	0.04069348	-3.16660015	H	1.55266800	-2.34454600	3.44801600	H	-1.21695900	-1.55672700	3.68254900	H	1.68202100	4.66215700	1.35001400
H	4.65584687	1.04014740	-4.44450613	H	3.41066900	-1.18943700	2.22749900	H	-3.26158000	-1.05006200	2.32605100	H	3.50365300	2.99492700	0.93458400
N	3.36522076	1.15348725	-1.32772475	N	1.13760900	-1.36641700	-0.26840600	N	-1.10780800	-1.77843400	-0.17541600	N	1.01329800	1.53459600	-0.82332500
N	2.30760584	1.82994841	-3.22227800	N	3.22358100	-0.45081600	-0.40811900	N	-3.29670000	-1.17793700	-0.41433300	N	3.14164100	0.74104300	-0.57915800
H	1.53995637	1.95960692	-2.56591482	H	2.92513700	-0.27763400	-1.36032000	H	-3.06710100	-1.28642200	-1.39461600	H	2.77835400	-0.00726200	-1.15570700
C	2.07326048	2.10489473	-4.54445941	C	4.48257000	-0.02871600	-0.05768400	C	-4.58108900	-0.80552100	-0.10710800	C	4.45294700	0.64144600	-0.18291600
O	2.84874103	1.92631970	-5.46982403	O	5.00384600	-0.14161600	1.03738200	O	-5.03654800	-0.62983400	1.00907100	O	5.06410100	1.44059400	0.50324300
O	0.82781564	2.62764724	-4.67143835	O	5.06697000	0.54708800	-1.13909000	O	-5.28342600	-0.66309100	-1.26124500	O	4.97447600	-0.50607500	-0.68766500
C	0.37510140	2.90908963	-6.00926161	C	6.39936700	1.07374700	-0.94996700	C	-6.66989200	-0.27955200	-1.12965400	C	6.35870300	-0.77913000	-0.37447800
H	-0.37537585	3.69202571	-5.89011544	H	6.50068900	1.84629000	-1.71333700	H	-7.14417100	-0.64291300	-2.04233800	H	6.69740900	-1.43656200	-1.17629200
H	1.20756737	3.27938483	-6.61070406	H	6.47748600	1.51954400	-0.34203000	H	-7.10513600	-0.77675600	-0.26089100	H	6.92697900	0.15259500	-0.39213800
C	-0.24378508	1.65187630	-6.64146271	C	7.45290100	-0.02800400	-1.14080000	C	-6.80459000	1.24644100	-1.01219900	C	6.48284200	-1.47088100	0.99160100
H	0.53286728	0.88623120	-6.75008463	H	7.32511000	-0.78700900	-0.36078900	H	-6.32099800	1.57972600	-0.08715700	H	6.13283200	-0.78781700	1.77367200
H	-1.00565189	1.25125887	-5.96208047	H	7.28722400	-0.51764900	-2.10836400	H	-6.27533500	1.71755400	-1.84962500	H	5.83081000	-2.35285200	1.00765600
C	-0.83755636	1.94374707	-7.94552165	C	8.80861900	0.51729300	-1.08558400	C	-8.20751900	1.65883100	-1.01569000	C	7.86387100	-1.86879800	1.26133700
C	-1.32440042	2.20831116	-9.02150738	C	9.92144300	0.98961200	-1.03801200	C	-9.37441400	1.97843800	-1.02163400	C	9.01233800	-2.19093600	1.46385400
H	-1.75473662	2.43035726	-9.97122077	H	10.90627300	1.39608200	-0.99466100	H	-10.39986500	2.27065300	-1.02338900	H	10.02159400	-2.47748100	1.65419000

SI-VIII: Energies and geometries (cartesian coordinates) of the Z isomers in T₁ ($\delta \sim 90$ deg.) at the B3LYP/6-31+G(d,p) level. SI. 12

Figure SI-7 : Energies and geometries of the Z isomers in T_1 at the B3LYP/6-31+G(d,p) level.

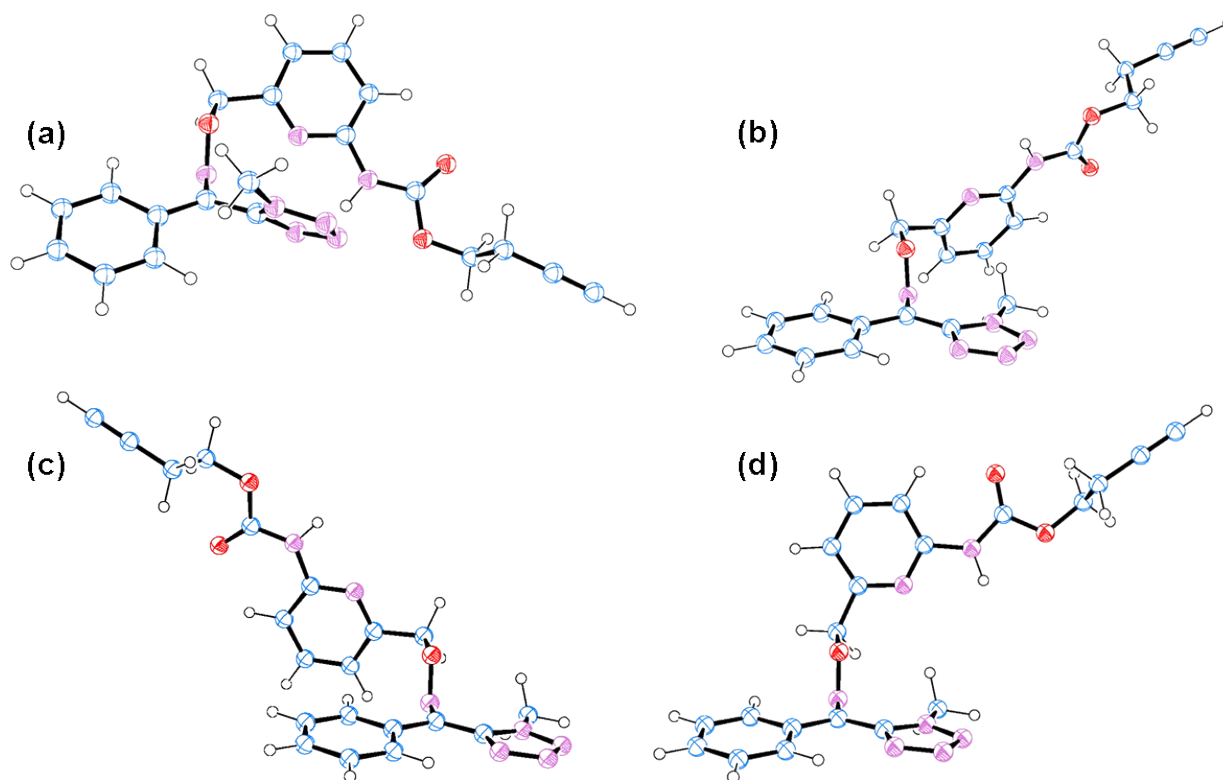
Z-a: 46.09 kcal/mol ($\delta=-96.8$ deg)

Z-b: 42.62 kcal/mol ($\delta=-87.1$ deg)

Z-c: 42.62 kcal/mol ($\delta=-90.6$ deg)

Z-d: 41.63 kcal/mol ($\delta=-91.7$ deg)

Energies are given with respect to the energy of the most stable Z isomer (Z-b(S_0)) in the ground state. δ is $C_{Ph}C-NO$ (see Figure 1).



SI-IX: Investigation of excited state destabilizing effects.

Figure SI-8 : $\pi_{py}-\pi_{ox}$ for E-a. The electronic density is more diffuse on C** than on N_{py}. The geometry is that of the ground state energy structure with $\delta_3=-161.3$ deg.

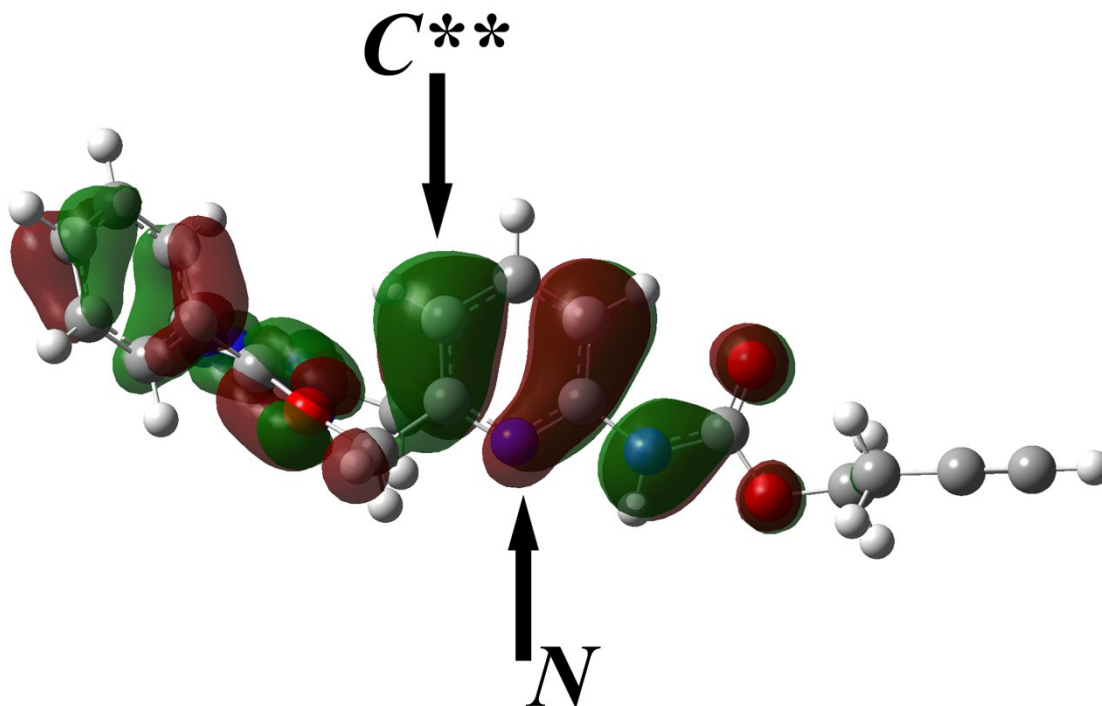


Figure SI-9 : The antibonding molecular orbital π_{ox} for E-a. The geometry is that of a structure where $\delta_3=-61.3$ deg.

