

Is the origin of green fluorescence in unsymmetrical four-ring bent-core liquid crystals single or double proton transfer?

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Kumar Biradha^{*a}

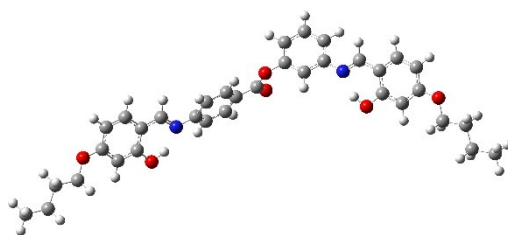
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Table of contents

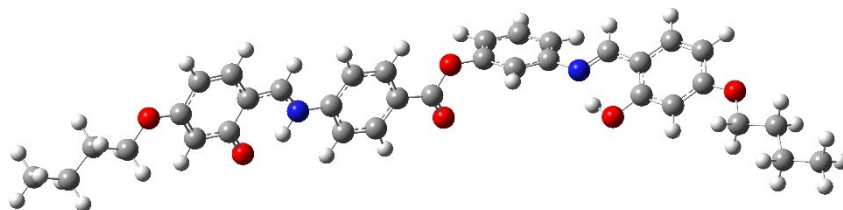
	Description	Page No
S3	The optimized (ground, excited and transition state) structure coordinates of various tautomers such as DE, MK-C, MK-O and DK using B3LYP functional	3-20
S4	The optimized (ground, excited and transition state) structure coordinates of various tautomers such as DE, MK-C, MK-O and DK using PBEPBE functional	21-38
S5	The optimized (ground, excited and transition state) structure coordinates of various tautomers such as DE, MK-C, MK-O and DK using mPW1PW91 functional	39-56
S6	The optimized (ground and excited) structure coordinates of various tautomers such as DE, MK-C, MK-O and DK using mPW1PW91 functional and 6-311++G(d) basis set.	57-64
S7	The optimized (excited state) structure coordinates of MK-C using mPW1PW91 functional and DZVP basis set.	65

Fig. S3: S_0 ; **4-4 (DE)** $E = -1916.422784$ hartree (B3LYP)



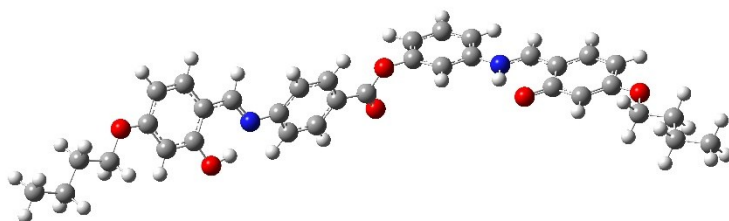
O	0.62969600	-2.69331800	2.17154100	O	0.77565400	-2.61243200	-0.09426400
N	-5.22727800	-0.54190000	0.57687000	N	5.47514200	-1.62069400	-0.13777100
C	-1.26739400	-1.95649200	0.90235800	C	2.09816100	-3.07895400	-0.06757600
C	-2.06184100	-1.74010800	2.04158900	C	3.13103400	-2.15026900	-0.07522000
H	-1.64383700	-1.94116400	3.02199400	H	2.91597500	-1.08776800	-0.04143000
C	-3.36235300	-1.27037300	1.91430500	C	4.46152400	-2.59717200	-0.14403800
H	-3.97669300	-1.09872800	2.79230400	C	4.72071500	-3.98035900	-0.16779300
C	-3.91194900	-1.02417200	0.64133000	H	5.74384500	-4.34156200	-0.16586100
C	-3.10769700	-1.22150800	-0.49894300	C	3.66336200	-4.89142900	-0.15568300
H	-3.49468400	-0.98277500	-1.48422600	H	3.87345500	-5.95655400	-0.16838300
C	-1.80255300	-1.68582500	-0.36800200	C	2.33783900	-4.45096800	-0.11261100
H	-1.19128100	-1.82824500	-1.25160800	H	1.50859600	-5.14980500	-0.10055400
C	0.11674300	-2.45097100	1.09549600	O	6.45521500	0.62640500	0.75627200
O	-7.12363300	1.01183500	1.47772000	H	5.81078100	-0.12796400	0.60416900
H	-6.24180700	0.53778800	1.42015000	O	10.86040000	1.84133100	-0.67362400
O	-11.21288600	1.16953700	-1.00455200	C	7.66430800	-0.83915600	-0.73102500
C	-7.34650200	-0.31656200	-0.52486700	C	7.56387700	0.35047100	0.04357200
C	-7.86154800	0.60965200	0.42616900	C	8.62096500	1.26929800	0.08186000
C	-9.15681600	1.12551800	0.29130300	H	8.49987500	2.15973600	0.68489300
H	-9.50608600	1.82672000	1.03788400	C	9.78532800	1.01465100	-0.64894900
C	-9.95102900	0.72608800	-0.78787400	C	9.90449800	-0.15980700	-1.42752300
C	-9.45967600	-0.19522800	-1.74277800	H	10.81869400	-0.33109700	-1.98463500
H	-10.09873500	-0.48736700	-2.56840000	C	8.85691400	-1.05842600	-1.45890700
C	-8.18309300	-0.69855300	-1.60059900	H	8.94385700	-1.96302400	-2.05520200
H	-7.80076900	-1.40661000	-2.33117600	C	6.58843100	-1.79935900	-0.78070200
C	-6.01718600	-0.85803600	-0.40580600	H	6.74782800	-2.68710600	-1.40425100
H	-5.70383700	-1.57162600	-1.17687900	C	10.83389400	3.06025800	0.09236000
C	-11.80348500	2.10863400	-0.08565100	H	10.68128600	2.81825900	1.15196100
H	-11.18742900	3.01624500	-0.05119400	H	9.99576400	3.68245700	-0.24700400
H	-11.82758000	1.66503800	0.91788700	C	12.16084800	3.77404200	-0.11644800
C	-13.20852600	2.42251100	-0.57664300	H	12.97554500	3.10827500	0.19528900
H	-13.14705300	2.82660800	-1.59499600	H	12.29648100	3.96669100	-1.18819300
H	-13.78127800	1.48843200	-0.63625200	C	12.23812200	5.09343900	0.66453800
C	-13.93273600	3.42071100	0.33764100	H	12.08955200	4.89370100	1.73429900
H	-13.34724000	4.34767700	0.40268800	H	11.41331900	5.74957600	0.35549600
H	-13.98121700	3.01381900	1.35665800	C	13.57135300	5.82289400	0.46356500
C	-15.34973600	3.74701600	-0.14782800	H	14.41386700	5.20491700	0.79520400
H	-15.33207700	4.18766500	-1.15142100	H	13.59953600	6.75896200	1.03116400
H	-15.84271200	4.45977600	0.52157800	H	13.73303200	6.06713800	-0.59280800
H	-15.97037900	2.84446500	-0.19127800				

S₀; **MK-C**, E= -1916.421285 hartree (B3LYP)



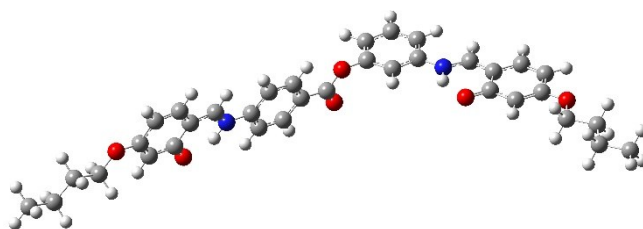
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C	-1.28435800	-1.99963000	0.73974300	H	2.93337400	-1.11134100	-0.08182100
C	-2.13222100	-1.80790000	1.84311900	C	4.48486400	-2.61814400	-0.11388600
H	-1.76500300	-2.03202300	2.83848800	C	4.74738800	-4.00079600	-0.10640300
C	-3.42505700	-1.33617300	1.66591900	H	5.77082200	-4.35922400	-0.06867500
H	-4.07437400	-1.19012500	2.52373500	C	3.69195800	-4.91429400	-0.10988900
C	-3.90280300	-1.04352200	0.37475500	H	3.90457600	-5.97891500	-0.09829700
C	-3.05893400	-1.23385300	-0.73383100	C	2.36480900	-4.47689300	-0.11420300
H	-3.39715100	-1.01706200	-1.74025200	H	1.53739300	-5.17795500	-0.11565800
C	-1.76476300	-1.70698700	-0.54733900	O	6.45282600	0.62200900	0.78858600
H	-1.12142000	-1.84960200	-1.40749100	H	5.81293400	-0.13523600	0.63252300
C	0.08791600	-2.50249400	0.98565000	O	10.88833800	1.82294500	-0.55695100
O	-11.11492700	1.64019900	-1.00766800	C	7.69773700	-0.86282100	-0.64923700
C	-7.19726100	0.23308900	-0.82230100	C	7.57804500	0.33763300	0.10564400
C	-7.93072000	0.37721500	0.44488800	C	8.63280800	1.25855300	0.15507600
C	-9.27897200	0.86282500	0.36812500	H	8.49690800	2.15733900	0.74238900
H	-9.81413200	0.96704400	1.30333100	C	9.81397500	0.99523500	-0.54511400
C	-9.85264000	1.17812200	-0.84860300	C	9.95238700	-0.19001700	-1.30395600
C	-9.12908400	1.03498100	-2.08170100	H	10.87932800	-0.36776500	-1.83748900
H	-9.62774000	1.29733200	-3.00787300	C	8.90698000	-1.09063400	-1.34645600
C	-7.84485500	0.57638900	-2.05464300	H	9.00865900	-2.00346900	-1.92767700
H	-7.28985200	0.46487500	-2.98302400	C	6.62455100	-1.82525000	-0.71008400
C	-5.88421000	-0.23084900	-0.84311400	H	6.79939400	-2.72159300	-1.31699200
H	-5.36966000	-0.32605100	-1.79463400	C	10.84326500	3.05268100	0.19073600
C	-11.94989200	1.82735300	0.15150200	H	10.66657400	2.82564200	1.24989000
H	-11.46689700	2.54195500	0.82977500	H	10.01265400	3.66899200	-0.17667900
H	-12.05659700	0.86882300	0.67484000	C	12.17415800	3.76474700	0.00212800
C	-13.29910900	2.34681600	-0.32095500	H	12.98191800	3.10442900	0.34220600
H	-13.14692300	3.28305200	-0.87279900	H	12.33427300	3.94184100	-1.06892300
H	-13.73137000	1.62553600	-1.02601300	C	12.23263000	5.09552000	0.76526400
C	-14.26955100	2.58132900	0.84529500	H	12.05960100	4.91136700	1.83414200
H	-13.82523300	3.29516900	1.55190300	H	11.41478700	5.74630700	0.42772400
H	-14.40747500	1.64330700	1.39972100	C	13.56972300	5.82313400	0.58429200
C	-15.63430400	3.10488600	0.38345200	H	14.40471900	5.21089800	0.94436300
H	-15.53306700	4.05992200	-0.14511400	H	13.58428300	6.76751200	1.13847400
H	-16.30566700	3.26309800	1.23399700	H	13.75556100	6.05187200	-0.47157500
H	-16.11924600	2.39665300	-0.29843900	O	-7.38722000	0.08220000	1.55779200
O	0.80043600	-2.63778800	-0.17526900	N	-5.21564200	-0.56990700	0.26579100
N	5.49607800	-1.63938600	-0.09623000	H	-5.79984200	-0.44150900	1.11626300
C	2.12149200	-3.10483200	-0.09939300				

S₀; **MK-O**, E= -1916.421104 hartree (B3LYP)



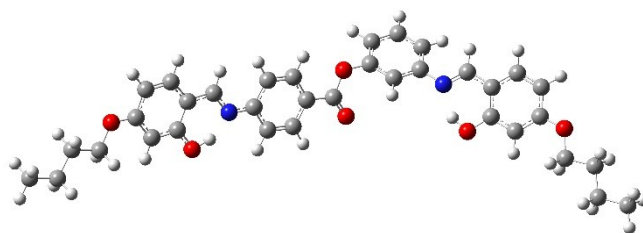
O	0.54917300	-3.42298600	1.91341700	O	0.86601900	-2.76786900	-0.23972200
N	-5.15267400	-0.77672500	0.51058600	C	2.17524800	-3.26053600	-0.24840200
C	-1.24407500	-2.34299600	0.74205400	C	3.21125700	-2.33624700	-0.20651100
C	-2.11842000	-2.39545100	1.84165000	H	2.98785600	-1.27888500	-0.11066000
H	-1.77576500	-2.84499100	2.76730300	C	4.53813300	-2.78620900	-0.29802300
C	-3.40117900	-1.87272000	1.74653400	C	4.79904500	-4.15970200	-0.42282400
H	-4.07655700	-1.90707400	2.59530000	H	5.81382400	-4.53526900	-0.48078500
C	-3.85275500	-1.30118200	0.54113700	C	3.73579400	-5.06234200	-0.46681100
C	-2.96902500	-1.23269300	-0.55463800	H	3.94501900	-6.12283200	-0.56465100
H	-3.27985500	-0.74582500	-1.47318800	C	2.41114900	-4.62698000	-0.38396400
C	-1.68189700	-1.75110800	-0.45459800	H	1.58333500	-5.32586800	-0.41881700
H	-1.00895800	-1.68602200	-1.30169100	O	10.66422600	2.08040400	-0.17747400
C	0.11776100	-2.90338900	0.90222500	C	7.77247700	-0.91633000	-0.34200200
O	-7.08619700	0.56410800	1.64373600	C	7.31602700	0.45611100	-0.08733200
H	-6.21099500	0.08818700	1.52904000	C	8.32077500	1.47913900	-0.03210300
O	-10.96260300	1.50688900	-1.00044400	H	7.97892000	2.48887400	0.15672200
C	-7.17582000	-0.20167100	-0.64330500	C	9.65680900	1.17479700	-0.21378000
C	-7.74650900	0.47133200	0.47449500	C	10.09386400	-0.16903200	-0.46388200
C	-9.01692800	1.05438400	0.38456000	H	11.15363200	-0.35333500	-0.59902900
H	-9.41024700	1.55571300	1.25928800	C	9.16953300	-1.17220400	-0.52397500
C	-9.73097700	0.97382600	-0.81486800	H	9.49141300	-2.19363400	-0.71231000
C	-9.18391200	0.30680300	-1.93651200	C	6.86336400	-1.97363300	-0.41286600
H	-9.76139400	0.25976600	-2.85284900	H	7.23070000	-2.97694100	-0.60926100
C	-7.93247400	-0.26511600	-1.83780200	C	10.35845500	3.46649700	0.06521000
H	-7.50742600	-0.77780100	-2.69672900	H	9.85492000	3.55893700	1.03587300
C	-5.86942600	-0.80355100	-0.57365900	H	9.67612000	3.82620500	-0.71538900
H	-5.50869300	-1.30744600	-1.47804400	C	11.66536000	4.24470200	0.05060500
C	-11.60226500	2.21187300	0.08072300	H	12.33515300	3.82990300	0.81451900
H	-10.96919000	3.05457800	0.38651700	H	12.15627900	4.09818500	-0.91987100
H	-11.71783300	1.53372600	0.93581000	C	11.45026000	5.74329000	0.30470200
C	-12.95552400	2.69901500	-0.41429600	H	10.94858600	5.88109900	1.27198300
H	-12.80340500	3.34059800	-1.29141700	H	10.77001500	6.14868700	-0.45638000
H	-13.54453000	1.83504200	-0.74708600	C	12.76007200	6.53969000	0.29270100
C	-13.72507900	3.46916800	0.66803300	H	13.44854500	6.17974800	1.06614400
H	-13.12409400	4.32471600	1.00449900	H	12.57787200	7.60379800	0.47632600
H	-13.86347300	2.82436300	1.54633700	H	13.26882400	6.44928100	-0.67413500
C	-15.09098600	3.96683700	0.18164900	O	6.07961500	0.72148300	0.07528900
H	-14.98339000	4.64141200	-0.67570700	N	5.54853700	-1.80916300	-0.25471800
H	-15.61758400	4.51202000	0.97197500	H	5.30880200	-0.81122400	-0.08378900
H	-15.72814400	3.13105900	-0.13008500				

S₀; **DK**, E= -1916.419611 hartree (B3LYP)



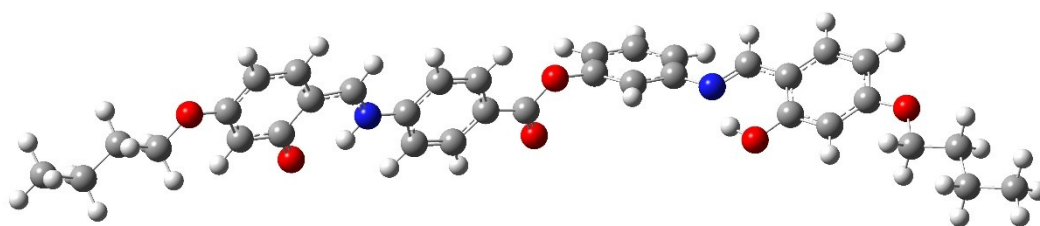
O	0.52303800	-3.30878600	1.80107900	H	3.01567600	-1.27578700	-0.18026200
C	-1.23977300	-2.26068400	0.55948500	C	4.55279300	-2.80192900	-0.31616400
C	-2.13617700	-2.27076800	1.64111500	C	4.80063600	-4.17866700	-0.43238700
H	-1.81828000	-2.69093900	2.58887000	H	5.81183100	-4.56561000	-0.47511000
C	-3.41431100	-1.74907600	1.50276700	C	3.72872300	-5.06927100	-0.50137000
H	-4.10130500	-1.75990500	2.34335000	H	3.92828000	-6.13213500	-0.59328800
C	-3.82815900	-1.20163000	0.27376400	C	2.40738000	-4.61811500	-0.45887100
C	-2.93535000	-1.18908600	-0.81265900	H	1.57227800	-5.30686700	-0.51632800
H	-3.22352100	-0.77340700	-1.77091800	O	10.72757400	1.99062900	0.04076700
C	-1.65645500	-1.71420300	-0.66575200	C	7.81016600	-0.97823900	-0.16604900
H	-0.97536700	-1.69877600	-1.50832000	C	8.37060100	1.43088200	-0.03614800
C	0.11352500	-2.82672700	0.76268100	H	8.03123300	2.45798200	0.00871300
O	-10.92167200	1.87896300	-0.87245900	C	9.71175300	1.09627900	-0.02557900
C	-7.04377300	0.35705600	-0.79483400	C	10.14561500	-0.27037000	-0.08529500
C	-7.83618600	0.26737600	0.44157300	H	11.20962200	-0.47794600	-0.07420800
C	-9.17032200	0.79473600	0.40248300	C	9.21295800	-1.26524200	-0.15243500
H	-9.74858200	0.72721300	1.31513400	H	9.53182100	-2.30384500	-0.19682200
C	-9.67795300	1.35880500	-0.75210600	C	6.89320200	-2.02880300	-0.23317300
C	-8.89791600	1.44046000	-1.95619200	H	7.25965600	-3.05062700	-0.27407000
H	-9.34622500	1.89287300	-2.83343900	C	10.42599800	3.39695400	0.11165500
C	-7.62457300	0.95216000	-1.96297400	H	9.81180400	3.58835500	1.00068300
H	-7.02612700	1.01094200	-2.86886900	H	9.85060900	3.68658800	-0.77680000
C	-5.73813700	-0.12392300	-0.84777300	C	11.74218500	4.15613800	0.18240400
H	-5.17954500	-0.04137800	-1.77535700	H	12.30567900	3.81081400	1.05845900
C	-11.80671600	1.86504100	0.26448700	H	12.34307400	3.91066000	-0.70246500
H	-11.33952700	2.41783400	1.08921700	C	11.53143300	5.67454600	0.26433600
H	-11.96204600	0.82726000	0.58530900	H	10.91962100	5.91099100	1.14531200
C	-13.11830800	2.51123100	-0.15454400	H	10.95746700	6.01116300	-0.60948600
H	-12.91639600	3.53096200	-0.50606000	C	12.85056500	6.45205600	0.33740100
H	-13.53353100	1.95523400	-1.00463400	H	13.43205900	6.16147100	1.22011300
C	-14.13827900	2.54800300	0.99226200	H	12.67138800	7.53083300	0.39541500
H	-13.71116600	3.09544500	1.84325000	H	13.47048400	6.26287700	-0.54673300
H	-14.32686200	1.52551500	1.34616000	O	6.11610400	0.71002400	-0.11737400
C	-15.46507200	3.19789400	0.58330000	C	7.35705100	0.41752800	-0.10679400
H	-15.31384700	4.23327000	0.25641600	N	5.57260500	-1.83650500	-0.24702900
H	-16.17306000	3.21112800	1.41862000	H	5.33635300	-0.82444600	-0.19747900
H	-15.93390900	2.65257800	-0.24408200	O	-7.35299300	-0.25565800	1.49690200
O	0.87939800	-2.74328100	-0.37165300	N	-5.12878400	-0.68989000	0.20141100
C	2.18437800	-3.24832200	-0.33868100	H	-5.75168300	-0.71806500	1.03337900
C	3.22911500	-2.33586400	-0.26867200				

S₁; **4-4 (DE)***, E= -1916.313287 hartree (B3LYP)



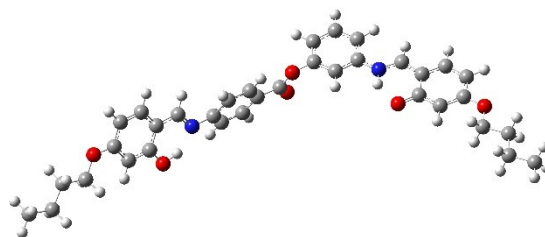
O	-0.93533200	-1.50945900	-2.04473100	O	-0.75188900	-2.84668700	-0.19602500
N	5.14062700	-0.45908800	-0.28572700	N	-5.44973100	-1.72986100	-0.03853800
C	1.13739600	-1.59617400	-0.85261400	C	-2.08968900	-3.22376800	-0.22499500
C	1.79735700	-0.69908400	-1.73912700	C	-3.11580400	-2.28313100	-0.16481400
H	1.24602200	-0.29847500	-2.58251200	H	-2.89887700	-1.22206100	-0.16402100
C	3.11046400	-0.34413400	-1.52938800	C	-4.44852900	-2.71841600	-0.09076000
H	3.61210700	0.34180200	-2.20549300	C	-4.73155400	-4.09828200	-0.11375900
C	3.85431500	-0.86308200	-0.41897100	H	-5.76025700	-4.44322100	-0.11428500
C	3.17909200	-1.77210300	0.46938900	C	-3.68736700	-5.02134900	-0.17647300
H	3.69894000	-2.19272700	1.32233100	H	-3.91000200	-6.08383600	-0.20002200
C	1.86317000	-2.11981900	0.25002200	C	-2.35801900	-4.59446000	-0.22677700
H	1.36967900	-2.80426000	0.93043600	H	-1.53698600	-5.30119200	-0.28031100
C	-0.25714800	-1.93935600	-1.11909900	O	-6.41553100	0.56440900	-0.82109400
O	7.01049400	0.99517900	-1.25219100	H	-5.77778700	-0.20363600	-0.71264300
H	6.10537000	0.52898400	-1.10700100	O	-10.77389800	1.77893800	0.74577400
O	11.25147700	1.04461400	0.95665000	C	-7.61545700	-0.94435400	0.63000300
C	7.30741400	-0.35246800	0.73281700	C	-7.51333000	0.27453900	-0.09806500
C	7.80769300	0.58384900	-0.26751800	C	-8.55810500	1.20810500	-0.07784100
C	9.11960600	1.06582300	-0.21683900	H	-8.43622100	2.12058300	-0.64679300
H	9.43412700	1.75923700	-0.98614100	C	-9.71122800	0.93966700	0.66557000
C	9.97085600	0.64656800	0.80738700	C	-9.83171700	-0.26388400	1.39835700
C	9.50677900	-0.26963300	1.79757700	H	-10.73700400	-0.44531100	1.96672600
H	10.19244500	-0.57665800	2.57974900	C	-8.79648500	-1.17696900	1.37226600
C	8.20990400	-0.74735500	1.74962200	H	-8.88448100	-2.10377100	1.93328600
H	7.86780100	-1.44425300	2.50890300	C	-6.55214200	-1.91999800	0.61942100
C	5.96688800	-0.85371200	0.69673100	H	-6.71150400	-2.82988900	1.21012900
H	5.66008600	-1.54734700	1.47811100	C	-10.74494700	3.02825400	0.03059900
C	11.82392600	1.97345400	0.01229200	H	-10.62010000	2.82834100	-1.04137800
H	11.23148600	2.89718900	0.01915500	H	-9.88952600	3.62296100	0.37594900
H	11.77555900	1.53412900	-0.99217500	C	-12.05504900	3.75285400	0.29989700
C	13.26207000	2.23889100	0.42806800	H	-12.88740300	3.11430100	-0.02197000
H	13.26927600	2.63619900	1.45071600	H	-12.16392700	3.90041600	1.38181100
H	13.80820900	1.28752600	0.44826500	C	-12.12726500	5.10637000	-0.42081900
C	13.96340600	3.22311800	-0.51910300	H	-12.00533700	4.95161900	-1.50130800
H	13.40444500	4.16814900	-0.54291000	H	-11.28505100	5.73513100	-0.10200800
H	13.94072900	2.82426800	-1.54208900	C	-13.44332700	5.84738600	-0.15828100
C	15.41522100	3.50019700	-0.11264800	H	-14.30320300	5.25822200	-0.49772500
H	15.46863000	3.93152300	0.89365400	H	-13.46794700	6.80793400	-0.68357400
H	15.89100300	4.20378900	-0.80367300	H	-13.57792700	6.04729500	0.91113900
H	16.00842300	2.57844200	-0.11230600				

S₁; **MK-C***, E= -1916.324092 hartree (B3LYP)



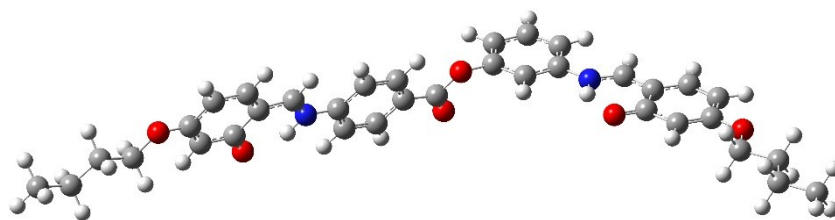
O	-0.37556700	-3.22383900	-1.91395200	C	-3.18720300	-2.08939400	0.10760200
C	1.33548200	-2.12148700	-0.65428200	H	-2.98716800	-1.02473300	0.05319100
C	2.30026600	-2.21697600	-1.68778900	C	-4.51197700	-2.55535300	0.16169300
H	2.02429900	-2.69285600	-2.62223100	C	-4.75092600	-3.94081900	0.20921000
C	3.57475100	-1.71372700	-1.51442100	H	-5.76778400	-4.31916300	0.19446800
H	4.30578200	-1.79298400	-2.31424400	C	-3.67742200	-4.83352300	0.23712100
C	3.93998700	-1.09064900	-0.29450600	H	-3.87037700	-5.90168200	0.26744500
C	2.98048100	-0.99025100	0.74572300	C	-2.35893600	-4.37346500	0.21415200
H	3.22843900	-0.51836600	1.68945800	H	-1.52212300	-5.06239400	0.23476800
C	1.70667000	-1.49857600	0.55992300	O	-6.53502500	0.62189900	-0.83360600
H	0.98054500	-1.41693100	1.36033600	H	-5.88352600	-0.12140500	-0.65578900
C	-0.00120200	-2.66917300	-0.89012400	O	-10.98212600	1.80074100	0.49629500
O	11.15802300	1.89289800	0.93016800	C	-7.75112100	-0.83400400	0.65685600
C	7.18400800	0.46499300	0.80912100	C	-7.65297600	0.34320300	-0.13638500
C	8.02883700	0.27343300	-0.36577100	C	-8.72177600	1.24642100	-0.20971300
C	9.37981700	0.76469400	-0.31226500	H	-8.60210300	2.12785300	-0.82615800
H	9.98000400	0.60718300	-1.19943200	C	-9.89543000	0.98835500	0.50484900
C	9.89437300	1.41395400	0.83165200	C	-10.01252600	-0.17387100	1.30142300
C	9.07018000	1.58573500	1.94339700	H	-10.93409700	-0.34836800	1.84525700
H	9.45434000	2.08256700	2.82673700	C	-8.95328100	-1.05724400	1.36702500
C	7.73184700	1.10836700	1.90934800	H	-9.03854800	-1.95248100	1.97756000
H	7.11757400	1.26088900	2.79322400	C	-6.66234100	-1.77791000	0.74283300
C	5.81250300	0.01232800	0.85897200	H	-6.82048300	-2.65699600	1.37883700
H	5.23341100	0.17688400	1.75924600	C	-10.95787200	3.00681100	-0.28938600
C	12.06276100	1.74990300	-0.18416900	H	-10.78517700	2.74944000	-1.34230100
H	11.63652100	2.25150600	-1.06210100	H	-10.13302700	3.64506100	0.05276100
H	12.18677100	0.68415400	-0.41443600	C	-12.29656100	3.70753700	-0.11374600
C	13.38983800	2.37893200	0.21069200	H	-13.09804700	3.02674100	-0.42727900
H	13.22085100	3.43150800	0.47049200	H	-12.45178500	3.91605700	0.95238000
H	13.76401600	1.88118900	1.11414500	C	-12.37728000	5.01292000	-0.91756500
C	14.43387600	2.27903400	-0.91056000	H	-12.20990300	4.79750500	-1.98150300
H	14.04713900	2.76832000	-1.81457600	H	-11.56509000	5.68386100	-0.60684600
H	14.58861400	1.22371200	-1.17243900	C	-13.72194500	5.72943000	-0.74886900
C	15.77668800	2.91014500	-0.52524800	H	-14.55189600	5.09595700	-1.08293100
H	15.66033200	3.97456400	-0.29049900	H	-13.75259300	6.65573700	-1.33214800
H	16.50173900	2.82515400	-1.34139600	H	-13.90261100	5.98878100	0.30080400
H	16.20578400	2.41946400	0.35607700	O	7.59657500	-0.31010500	-1.41524300
O	-0.83825600	-2.48445000	0.19479000	N	5.22903200	-0.60374700	-0.17384500
N	-5.54042400	-1.59420700	0.11728100	H	5.87289100	-0.71061400	-0.97605000
C	-2.13525100	-2.99753400	0.14379000				

S₁; **MK-O***, E= -1916.318568 hartree (B3LYP)



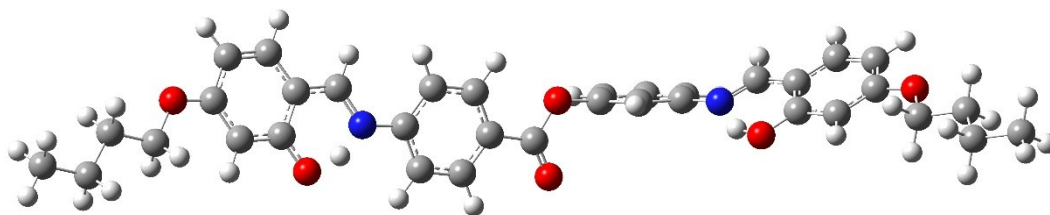
O	0.53276800	-3.40823400	1.89118100	O	0.84866100	-2.74677900	-0.26012300
N	-5.17020800	-0.75907100	0.50289500	C	2.15639100	-3.25227000	-0.27709700
C	-1.25971600	-2.32383400	0.72409300	C	3.19780100	-2.34338600	-0.22132200
C	-2.13049200	-2.37438400	1.82639000	H	2.98646400	-1.28522400	-0.10489000
H	-1.78472000	-2.82289800	2.75138900	C	4.53147300	-2.80798500	-0.31980900
C	-3.41367100	-1.85162200	1.73488500	C	4.76996200	-4.19519600	-0.47350800
H	-4.08630600	-1.88491300	2.58591000	H	5.77888400	-4.58154400	-0.55332000
C	-3.86933700	-1.28222500	0.53016000	C	3.69299400	-5.07652300	-0.52828300
C	-2.98917700	-1.21519700	-0.56844300	H	3.88517000	-6.13843700	-0.64842400
H	-3.30313100	-0.73003900	-1.48687100	C	2.37133600	-4.62586600	-0.43479700
C	-1.70158700	-1.73351100	-0.47173100	H	1.53339800	-5.31173500	-0.47930000
H	-1.03129900	-1.67026900	-1.32108400	O	10.76196700	2.07725500	-0.09018900
C	0.10336900	-2.88568600	0.87998700	C	7.81271600	-0.95878000	-0.25819500
O	-7.10219300	0.57716800	1.64212800	C	7.38142200	0.43184000	-0.13330700
H	-6.22622300	0.10315000	1.52384900	C	8.39318900	1.45033700	-0.07681900
O	-10.99184600	1.50824800	-0.98718900	H	8.03737200	2.46884900	0.01577100
C	-7.19850500	-0.18917600	-0.64432000	C	9.77409700	1.14529700	-0.13959700
C	-7.76681500	0.48242400	0.47542600	C	10.16570600	-0.18371700	-0.25840500
C	-9.03925700	1.06185100	0.39023500	H	11.21898000	-0.43533100	-0.30692600
H	-9.43068900	1.56214400	1.26640100	C	9.17615000	-1.20837200	-0.31461500
C	-9.75770500	0.97893200	-0.80638800	H	9.52089600	-2.23549000	-0.40640800
C	-9.21295300	0.31344900	-1.92995700	C	6.88043300	-2.06187900	-0.32417900
H	-9.79376800	0.26445300	-2.84409000	H	7.25701500	-3.07163400	-0.42299200
C	-7.95941400	-0.25489900	-1.83586900	C	10.41793100	3.47060600	0.03229300
H	-7.53621600	-0.76659300	-2.69631000	H	9.84215600	3.62347500	0.95414000
C	-5.89028800	-0.78816000	-0.57892800	H	9.79559100	3.76801600	-0.82153500
H	-5.53154100	-1.29177900	-1.48425700	C	11.71235200	4.26891000	0.06335000
C	-11.62973800	2.21019900	0.09687100	H	12.32498000	3.91988900	0.90418400
H	-10.99864800	3.05512800	0.40066700	H	12.27892200	4.06300100	-0.85358100
H	-11.73938800	1.53122000	0.95209900	C	11.45977600	5.77753300	0.19298900
C	-12.98681300	2.69259400	-0.39234100	H	10.88194900	5.97374100	1.10616400
H	-12.84071300	3.33489000	-1.26996400	H	10.83698000	6.11682300	-0.64561700
H	-13.57412200	1.82658400	-0.72283500	C	12.75707100	6.59353500	0.22646600
C	-13.75455100	3.45977200	0.69338100	H	13.38644700	6.30042400	1.07479800
H	-13.15535500	4.31759100	1.02725700	H	12.54836100	7.66449700	0.31932800
H	-13.88662000	2.81442000	1.57225600	H	13.34150400	6.44461700	-0.68894800
C	-15.12447100	3.95224600	0.21303100	O	6.14404900	0.75108200	-0.07513600
H	-15.02321000	4.62716700	-0.64482700	N	5.54616100	-1.87236300	-0.26171000
H	-15.64964600	4.49547900	1.00564800	H	5.29939100	-0.87473200	-0.16539100
H	-15.75982600	3.11404100	-0.09585400				

S₁; **DK***, E= -1916.322663 hartree (B3LYP)



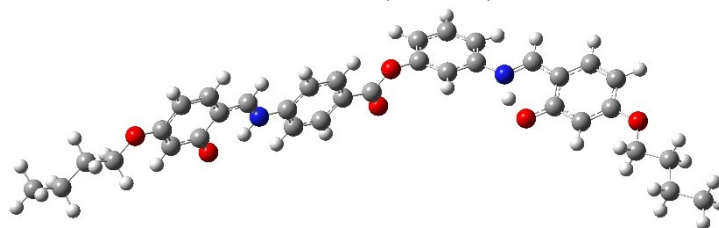
O	0.43202100	-3.47109100	1.71564900	H	3.05698000	-1.21047800	-0.17419900
C	-1.26254900	-2.27836300	0.51652700	C	4.56992700	-2.75895100	-0.32317300
C	-2.22744200	-2.40661800	1.54699300	C	4.79803000	-4.13842400	-0.44104900
H	-1.95881000	-2.93222800	2.45656900	H	5.80296100	-4.54056400	-0.49151200
C	-3.49243600	-1.87201400	1.40154600	C	3.71094900	-5.01191100	-0.50105900
H	-4.22361100	-1.97642700	2.19841200	H	3.89337100	-6.07792400	-0.59390200
C	-3.84783800	-1.18352100	0.21438500	C	2.39734400	-4.54127700	-0.44866600
C	-2.88886100	-1.05051000	-0.82263900	H	1.55372000	-5.21981900	-0.49809800
H	-3.12966600	-0.52798700	-1.74125000	O	10.82279600	1.93465200	0.06252700
C	-1.62437700	-1.59009000	-0.66533400	C	7.85622700	-0.98396800	-0.17099500
H	-0.89828300	-1.48211800	-1.46261000	C	8.45692700	1.41422400	-0.02909800
C	0.06309600	-2.85900900	0.72313400	H	8.13480200	2.44673900	0.01898100
O	-11.01346900	1.98436900	-0.83641800	C	9.79226500	1.05713900	-0.01376900
C	-7.06564400	0.48264900	-0.80061500	C	10.20318100	-0.31585900	-0.07826600
C	-7.90745800	0.25560000	0.37001600	H	11.26339200	-0.54188300	-0.06350400
C	-9.24967800	0.77288000	0.34606500	C	9.25344400	-1.29447900	-0.15330100
H	-9.84764400	0.58871100	1.22962500	H	9.55481400	-2.33820500	-0.20040000
C	-9.75831500	1.47960500	-0.76580700	C	6.92164100	-2.01994600	-0.24148100
C	-8.93686300	1.68452800	-1.87419400	H	7.27214500	-3.04744600	-0.28160000
H	-9.31677200	2.22564400	-2.73300300	C	10.54344600	3.34468400	0.14387900
C	-7.60744300	1.18237600	-1.86899700	H	9.92690000	3.53846000	1.03080800
H	-6.99566200	1.36135100	-2.74958200	H	9.97822200	3.65161600	-0.74534600
C	-5.70301000	0.00752000	-0.87790900	C	11.87122400	4.08191500	0.22956500
H	-5.12411500	0.20282400	-1.77225700	H	12.42378700	3.71883500	1.10540400
C	-11.91504800	1.80906300	0.27599300	H	12.47340100	3.83538700	-0.65415300
H	-11.47588100	2.26588300	1.17177500	C	11.68484100	5.60268500	0.32544600
H	-12.05544400	0.73666300	0.46150200	H	11.07125000	5.84035500	1.20486400
C	-13.23345200	2.47599300	-0.08404800	H	11.12215500	5.95744800	-0.54853700
H	-13.04841400	3.53584700	-0.29954100	C	13.01599400	6.35769300	0.41478300
H	-13.62041900	2.02358600	-1.00576000	H	13.58685300	6.04885500	1.29825200
C	-14.27322400	2.34508000	1.03801800	H	12.85414000	7.43865600	0.48248500
H	-13.87355200	2.78819100	1.96003700	H	13.63857000	6.16715000	-0.46719300
H	-14.44448900	1.28213500	1.25491300	O	6.19060400	0.73224700	-0.12412200
C	-15.60712300	3.01463300	0.68830800	C	7.42640900	0.41845500	-0.10889600
H	-15.47406800	4.08623800	0.49970400	N	5.60513500	-1.80780100	-0.25784500
H	-16.32943200	2.90595500	1.50407500	H	5.38316800	-0.79302800	-0.20769100
H	-16.04873100	2.57022400	-0.21119200	O	-7.48033000	-0.38026800	1.39059500
O	0.90521500	-2.63189800	-0.35398400	N	-5.12804100	-0.66694700	0.12159700
C	2.19032600	-3.16689300	-0.32860000	H	-5.77058600	-0.79770000	0.92143200
C	3.25392100	-2.27352300	-0.26638800				

S₀; DE to MK-C, TS, E= -1916.416594 hartree (B3LYP)



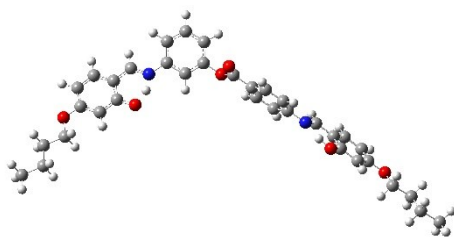
O	-0.40349700	2.55235500	2.26346600	C	-3.09177900	2.20670600	0.10028800
C	1.37472200	1.91720500	0.78477900	H	-2.88704400	1.15054300	-0.03707200
C	2.25899000	1.60365200	1.83030600	C	-4.41895800	2.66343600	0.17197000
H	1.92817900	1.72176800	2.85629400	C	-4.66236800	4.03531800	0.37041800
C	3.54185800	1.14888400	1.55559200	H	-5.67929900	4.39631900	0.48332000
H	4.22542500	0.91206700	2.36457700	C	-3.59499100	4.93047300	0.45945100
C	3.97546600	1.00124100	0.22444400	H	-3.79288700	5.98617400	0.61787800
C	3.08482200	1.29887200	-0.82464600	C	-2.27440800	4.48446000	0.36139100
H	3.37991900	1.15350000	-1.85793500	H	-1.43826700	5.17155700	0.43078300
C	1.80223000	1.75665100	-0.54415800	O	-6.39360600	-0.65972800	0.66707800
H	1.12327900	1.97962200	-1.35878700	H	-5.75117100	0.10849000	0.60073700
C	0.01540900	2.39695300	1.13221500	O	-10.88022100	-1.62956300	-0.69595400
O	11.07927800	-1.55754700	-1.42888800	C	-7.66698500	1.02341600	-0.50221700
C	7.26210000	0.07318700	-1.18003400	C	-7.53636800	-0.27380900	0.06823800
C	7.79817400	-0.59894300	-0.01699700	C	-8.59836500	-1.18635100	0.01809200
C	9.09621100	-1.15768300	-0.08909800	H	-8.45369600	-2.16128200	0.46501300
H	9.47962800	-1.65685600	0.79133300	C	-9.79771800	-0.81826400	-0.59899000
C	9.83293600	-1.05390700	-1.26519500	C	-9.94735400	0.46465500	-1.17476600
C	9.30943600	-0.38912400	-2.41260900	H	-10.88828000	0.72241600	-1.64773300
H	9.92135700	-0.33293800	-3.30571600	C	-8.89452200	1.35589900	-1.12093800
C	8.05216700	0.15939800	-2.35796400	H	-9.00407800	2.34313100	-1.56231300
H	7.64408500	0.66831200	-3.22759300	C	-6.58630700	1.97837400	-0.45962100
C	5.96535000	0.63561000	-1.10465300	H	-6.77128700	2.95294500	-0.92685000
H	5.55352800	1.16058800	-1.96740800	C	-10.82431900	-2.95574900	-0.13802300
C	11.71328400	-2.25266900	-0.33788200	H	-10.61516600	-2.88719500	0.93726000
H	11.09332000	-3.11082600	-0.04921400	H	-10.01004900	-3.51517200	-0.61631400
H	11.79375600	-1.57588900	0.52218200	C	-12.16632200	-3.62642000	-0.38974300
C	13.08769500	-2.70512700	-0.80675000	H	-12.95803400	-3.02119300	0.06968900
H	12.96943100	-3.34590200	-1.68968700	H	-12.35960000	-3.64056000	-1.46984900
H	13.66298500	-1.82591300	-1.12330700	C	-12.21343000	-5.05620500	0.16717800
C	13.85257900	-3.46212000	0.28809100	H	-12.00749900	-5.03500500	1.24581700
H	13.26518900	-4.33326700	0.60811800	H	-11.41140500	-5.65224100	-0.28870100
H	13.95699200	-2.81854500	1.17195400	C	-13.56126900	-5.74349200	-0.07987100
C	15.23986600	-3.92484300	-0.17154000	H	-14.38025500	-5.18896800	0.39286500
H	15.16635300	-4.59765800	-1.03388400	H	-13.56728900	-6.76012800	0.32708000
H	15.76272900	-4.46115100	0.62730500	H	-13.78002000	-5.81088900	-1.15193800
H	15.86329000	-3.07266200	-0.46622000	O	7.08302700	-0.67700700	1.07698400
O	-0.73808900	2.65145000	0.01791900	N	5.27912800	0.53450000	0.01722400
N	-5.44135000	1.70007300	0.08482400	H	6.02800700	-0.07744700	0.78726900
C	-2.04924500	3.12012200	0.18833900				

S₀; **MK-C to DK**, TS, E= -1916.415140 hartree (B3LYP)



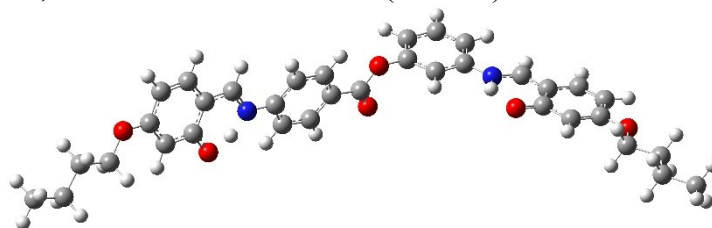
O	-0.44986200	2.70137800	2.37687100	H	-2.97111100	1.27555400	-0.07113400
C	1.31073800	1.92189200	0.94801700	C	-4.44935100	2.84748000	0.12851800
C	2.18879200	1.65902800	2.01259600	C	-4.64697100	4.22112900	0.35091300
H	1.86435400	1.85577900	3.02840600	H	-5.64929900	4.62829900	0.42646400
C	3.45847500	1.15393400	1.77145100	C	-3.54704900	5.06556000	0.50554400
H	4.13245000	0.95526500	2.59903400	H	-3.70768800	6.12503900	0.67866600
C	3.88193000	0.89785700	0.45382400	C	-2.24307400	4.56601300	0.45543500
C	3.00555100	1.15413400	-0.61555800	H	-1.38421200	5.21650300	0.57677100
H	3.29868500	0.95870100	-1.64019500	O	-10.61111100	-1.74657800	-0.75890500
C	1.73579300	1.66215300	-0.36546300	C	-7.70728000	1.22203000	-0.51409900
H	1.06780100	1.85646500	-1.19613100	C	-8.31849400	-1.14643000	-0.23256100
C	-0.03267400	2.46298700	1.25982000	H	-8.02383800	-2.15076800	0.04316500
O	10.95894100	-1.92115500	-1.30694400	C	-9.60889400	-0.83944200	-0.65431400
C	7.10123400	-0.39664800	-0.91512000	C	-9.97365900	0.48903000	-1.01599200
C	7.85917900	-0.65836400	0.31847900	H	-10.99036300	0.68057100	-1.33996500
C	9.18664200	-1.18342800	0.17061300	C	-9.03340700	1.48855900	-0.94455600
H	9.74004900	-1.37490700	1.08102100	H	-9.30243600	2.50593900	-1.21763100
C	9.71904700	-1.42796600	-1.08064800	C	-6.72329700	2.24087200	-0.43473700
C	8.97230400	-1.16840700	-2.28051400	H	-6.97877500	3.26351600	-0.71628700
H	9.43903000	-1.37853000	-3.23615800	C	-10.36077300	-3.12144200	-0.41195100
C	7.70682700	-0.66890700	-2.18598000	H	-10.03045800	-3.17518800	0.63322200
H	7.13418200	-0.46937000	-3.08843600	H	-9.55950500	-3.51471900	-1.05049300
C	5.80579400	0.11195400	-0.86836800	C	-11.65223500	-3.89867500	-0.61633100
H	5.27451000	0.29699400	-1.79733100	H	-12.43852000	-3.45156100	0.00499300
C	11.81475100	-2.22436500	-0.18817900	H	-11.97017700	-3.79248000	-1.66125600
H	11.32129100	-2.96835600	0.44977900	C	-11.49536800	-5.38545800	-0.26782000
H	11.97257600	-1.31166600	0.40016600	H	-11.16646400	-5.48297500	0.77554800
C	13.12949900	-2.75786700	-0.73612100	H	-10.69900200	-5.82309200	-0.88474600
H	12.92567700	-3.64475000	-1.34939700	C	-12.79056300	-6.18025700	-0.46957300
H	13.57066500	-2.00352200	-1.39984300	H	-13.59726900	-5.78765400	0.16037000
C	14.12134300	-3.11329800	0.38032200	H	-12.65082800	-7.23599200	-0.21440900
H	13.66864400	-3.85964200	1.04686700	H	-13.12716900	-6.12951400	-1.51162500
H	14.31158200	-2.22409800	0.99625000	O	-6.11500400	-0.38792600	0.23466200
C	15.45089400	-3.65259800	-0.15951100	C	-7.33906300	-0.12765900	-0.15355200
H	15.29708600	-4.56169000	-0.75249900	N	-5.50571300	1.93563400	-0.03983900
H	16.13877900	-3.89806500	0.65642300	H	-5.53964300	0.72226600	0.17219800
H	15.94453600	-2.91495400	-0.80290300	O	7.35395500	-0.42644800	1.46378900
O	-0.77637200	2.66934100	0.12755600	N	5.17489600	0.39088400	0.27898800
C	-2.06714200	3.19789300	0.25793400	H	5.77431000	0.18485800	1.10300200
C	-3.14240500	2.33363600	0.09475200				

S₀; DE to MK-O, TS, E= -1916.416667 hartree (B3LYP)



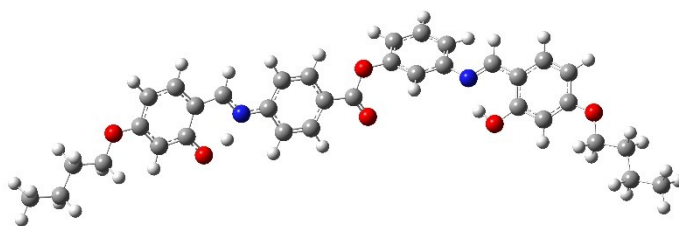
O	-0.50346800	2.76452600	2.39283200	O	-0.76706000	2.77067000	0.13587800
N	5.20373400	0.52869800	0.41210800	C	-2.06952800	3.27417500	0.24381500
C	1.30712300	2.03104300	1.00038300	C	-3.12733600	2.38721700	0.08736000
C	2.15228800	1.74709000	2.08724300	H	-2.93526900	1.32957700	-0.05724600
H	1.79073200	1.91661800	3.09564800	C	-4.44364000	2.87727800	0.10000200
C	3.43116600	1.25022400	1.87359200	C	-4.66876700	4.25102700	0.29431300
H	4.08412400	1.02598900	2.71090400	H	-5.67919600	4.64065500	0.35296200
C	3.90829700	1.04325500	0.56483500	C	-3.58614800	5.11852500	0.44281600
C	3.05289000	1.30893500	-0.52317400	H	-3.76787200	6.17792700	0.59432000
H	3.38220700	1.10144400	-1.53605000	C	-2.27280200	4.64213000	0.41408000
C	1.76955300	1.80050900	-0.30604500	H	-1.42677300	5.31016700	0.53083600
H	1.11857800	1.99513600	-1.15042700	O	-10.51391000	-1.84271600	-0.75874900
C	-0.05129200	2.55068700	1.28428400	C	-7.66552600	1.18149600	-0.54284700
O	7.09311200	-1.11982100	1.14327700	C	-7.27777600	-0.15384200	-0.15081500
H	6.22564200	-0.61693200	1.15379100	C	-8.23830100	-1.19125800	-0.21951400
O	11.03565100	-1.29871300	-1.56423700	H	-7.92910700	-2.18439800	0.07984800
C	7.25396500	0.28812900	-0.81039700	C	-9.52905700	-0.91585900	-0.66136700
C	7.78716900	-0.69502900	0.07101800	C	-9.91306400	0.39835600	-1.05377200
C	9.05497200	-1.24547800	-0.15629600	H	-10.92927900	0.56519700	-1.39264000
H	9.41937700	-1.98956600	0.53985700	C	-8.99126200	1.41567700	-0.99279400
C	9.80366200	-0.82440000	-1.25949300	H	-9.27508000	2.42227800	-1.28982500
C	9.29425800	0.15405300	-2.14564400	C	-6.70010800	2.21886800	-0.47415600
H	9.89806100	0.46175200	-2.99188000	H	-6.96983900	3.23094900	-0.77953900
C	8.04502200	0.69095000	-1.91276600	C	-10.24245800	-3.20643600	-0.38483200
H	7.64884500	1.44214200	-2.59103700	H	-9.92320800	-3.23603300	0.66473700
C	5.95089400	0.86341600	-0.59759300	H	-9.42686800	-3.59587600	-1.00740300
H	5.62017000	1.61832500	-1.32058000	C	-11.51704700	-4.01093300	-0.58990300
C	11.63788600	-2.30277000	-0.72494100	H	-12.31823400	-3.56855900	0.01558800
H	10.98847100	-3.18706300	-0.69764300	H	-11.82549300	-3.92784000	-1.63976400
H	11.73540300	-1.90963600	0.29507700	C	-11.33621800	-5.48857900	-0.21519400
C	12.99992500	-2.64521700	-1.30913800	H	-11.01659900	-5.56280400	0.83296500
H	12.86654300	-2.99477200	-2.34070500	H	-10.52532800	-5.92110700	-0.81659300
H	13.60673100	-1.73214300	-1.35577100	C	-12.61409500	-6.31091100	-0.41706300
C	13.73076200	-3.71563200	-0.48642600	H	-13.43466900	-5.92336300	0.19792900
H	13.11257900	-4.62202500	-0.43537600	H	-12.45732200	-7.35949200	-0.14298200
H	13.84952600	-3.36401500	0.54730200	H	-12.94049100	-6.28364200	-1.46323400
C	15.10571500	-4.06944400	-1.06464100	O	-6.05376800	-0.38454200	0.25569100
H	15.01705800	-4.45679600	-2.08629800	N	-5.48186600	1.94323900	-0.06029400
H	15.60444100	-4.83375400	-0.45945400	H	-5.49694600	0.73398400	0.17632300
H	15.75894400	-3.18973200	-1.09753700				

S₀; **MK-O to DK**, TS, E= -1916.414951 hartree (B3LYP)



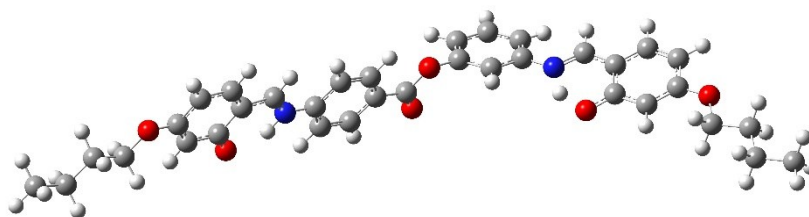
O	-0.46314700	2.80381800	2.07019200	H	-2.91581000	1.35508400	-0.19640200
C	1.32078100	2.08523100	0.63650000	C	-4.44271500	2.88935400	-0.04345000
C	2.18557300	1.78695400	1.70284200	C	-4.68267100	4.26763100	0.07313200
H	1.84566700	1.94560600	2.72035900	H	-5.69241300	4.65990700	0.10207800
C	3.46066900	1.29478300	1.45897300	C	-3.60602500	5.15270100	0.13633700
H	4.12903200	1.06899300	2.28363900	H	-3.79930400	6.21710000	0.22374300
C	3.90607900	1.09329800	0.13869900	C	-2.28749900	4.69425500	0.07859000
C	3.03490100	1.37674700	-0.93057900	H	-1.44742500	5.37826600	0.12095400
H	3.33867600	1.19060800	-1.95471400	O	-10.66168800	-1.85135500	-0.30870000
C	1.75989900	1.87175600	-0.68127900	C	-7.71102600	1.08038000	-0.04929200
H	1.09570100	2.08203100	-1.51128700	C	-8.30896100	-1.28828000	-0.45756800
C	-0.03151700	2.60218700	0.95150000	H	-7.98876300	-2.29520600	-0.69348900
O	10.95319200	-1.70913500	-1.35082100	C	-9.63672700	-0.96717300	-0.24633000
C	7.18309500	0.03848300	-1.19577600	C	-10.04496100	0.37244200	0.06711600
C	7.68589300	-0.61513400	-0.00738600	H	-11.09928500	0.57040600	0.22372300
C	8.96768600	-1.21314500	-0.04753800	C	-9.10076500	1.35429800	0.16029500
H	9.32574300	-1.69831800	0.85122200	H	-9.40033800	2.37211600	0.39826100
C	9.72075200	-1.16445400	-1.21679000	C	-6.78065500	2.11553100	0.06021900
C	9.23056700	-0.51729600	-2.38887500	H	-7.12578400	3.11604900	0.30563700
H	9.85427900	-0.50433900	-3.27546500	C	-10.38507800	-3.23256900	-0.60775100
C	7.98934000	0.06846200	-2.36565200	H	-9.69955700	-3.63388800	0.14938300
H	7.60650000	0.56369500	-3.25442600	H	-9.89600300	-3.29727900	-1.58802800
C	5.90180600	0.63791700	-1.15324300	C	-11.70609800	-3.98672200	-0.60433600
H	5.51446500	1.14778500	-2.03618100	H	-12.18214900	-3.86598700	0.37701500
C	11.55155500	-2.39469000	-0.23383100	H	-12.37734500	-3.53250300	-1.34421800
H	10.90128700	-3.22529400	0.06838400	C	-11.52254400	-5.47905900	-0.91413900
H	11.64228200	-1.69843300	0.60948900	H	-10.84101800	-5.92391800	-0.17659500
C	12.91690700	-2.90182800	-0.67215700	H	-11.03529000	-5.59173100	-1.89200200
H	12.78985600	-3.56158800	-1.53975200	C	-12.84700100	-6.25096300	-0.91354500
H	13.52378200	-2.04964400	-1.00334100	H	-13.34206100	-6.18570700	0.06237200
C	13.64324300	-3.65347800	0.45225200	H	-12.68725600	-7.31103900	-1.13706500
H	13.02447100	-4.49717900	0.78634800	H	-13.53794900	-5.85099300	-1.66480000
H	13.75644300	-2.99065000	1.32067800	O	-6.05488800	-0.56874600	-0.55920500
C	15.02107300	-4.17113800	0.02384900	C	-7.28407300	-0.28772600	-0.36993500
H	14.93760700	-4.86337200	-0.82205800	N	-5.47050100	1.93235800	-0.11579400
H	15.51618500	-4.70274500	0.84325500	H	-5.25114500	0.93710700	-0.32563600
H	15.67496200	-3.34678700	-0.28368500	O	6.95620600	-0.64127200	1.07926100
O	-0.76873200	2.83382400	-0.18135000	N	5.19987600	0.58882300	-0.03731900
C	-2.07262200	3.32331000	-0.04012600	H	5.92183400	-0.02055400	0.75921900
C	-3.12244600	2.41606400	-0.10363700				

S₁; DE* to MK-C*, TS, E= -1916.307345 hartree (B3LYP)



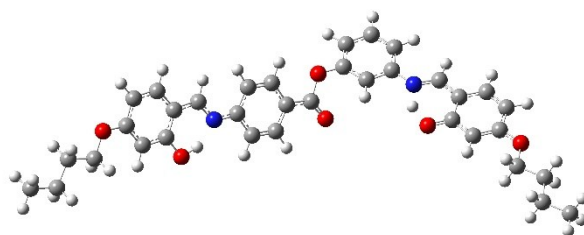
O	0.86581000	-1.66181700	2.06423000	O	0.77611800	-2.86154500	0.12111100
N	-5.14721900	-0.55247100	0.11237100	N	5.46518200	-1.71868600	0.07144500
C	-1.15591900	-1.67763100	0.78369400	C	2.11394500	-3.23915700	0.21047200
C	-1.86110300	-0.85408800	1.70010400	C	3.13230200	-2.29186400	0.14422900
H	-1.35206600	-0.50915400	2.59329700	H	2.90276300	-1.23414300	0.09200300
C	-3.17160200	-0.49520300	1.46229800	C	4.47094700	-2.71478500	0.13133900
H	-3.70453800	0.13598300	2.16748500	C	4.76423700	-4.08928600	0.21949800
C	-3.84882900	-0.94246500	0.29205100	H	5.79536000	-4.42399300	0.26534400
C	-3.14072700	-1.77132500	-0.62969600	C	3.72666200	-5.01951200	0.28771200
H	-3.62420000	-2.13077700	-1.53108400	H	3.95824700	-6.07778200	0.36197000
C	-1.82842500	-2.12434000	-0.38133800	C	2.39205000	-4.60476400	0.27888000
H	-1.30213200	-2.75354500	-1.08984400	H	1.57618100	-5.31721600	0.33576700
C	0.23088800	-2.02877300	1.08400100	O	6.39406200	0.60896000	0.79930100
O	-7.02422200	0.83548400	1.22014900	H	5.76534300	-0.16774000	0.70111300
H	-5.87770400	0.22602100	0.93947300	O	10.78396600	1.80390000	-0.69508500
O	-11.27679900	1.14497700	-0.96256600	C	7.64254200	-0.93890200	-0.56686700
C	-7.32087200	-0.31276900	-0.87317000	C	7.51273300	0.30314300	0.11522800
C	-7.80342900	0.53147500	0.22204700	C	8.55113500	1.24383300	0.08977500
C	-9.13504800	1.02828000	0.20257600	H	8.40797700	2.17446900	0.62330600
H	-9.43765700	1.64700500	1.03765500	C	9.72527300	0.95905000	-0.61361600
C	-9.99310400	0.72047100	-0.85278500	C	9.87335500	-0.26775200	-1.30073100
C	-9.52937100	-0.09390300	-1.91068500	H	10.79445800	-0.46172200	-1.83876400
H	-10.20372400	-0.32779000	-2.72709800	C	8.84402200	-1.18764200	-1.26963600
C	-8.21282500	-0.59294500	-1.90378400	H	8.95309200	-2.13257200	-1.79568000
H	-7.88912300	-1.21609000	-2.73255200	C	6.58601800	-1.92251500	-0.54945300
C	-5.97032700	-0.84079500	-0.89283600	H	6.76800000	-2.85167700	-1.10257300
H	-5.65699800	-1.46172800	-1.72771800	C	10.72733400	3.07614700	-0.02389300
C	-11.82663600	1.97972600	0.07452100	H	10.57509600	2.91189700	1.05063800
H	-11.22278900	2.89270600	0.15880500	H	9.87753000	3.65252500	-0.41173800
H	-11.78055700	1.44223300	1.03079500	C	12.03932200	3.80124400	-0.28282000
C	-13.26374300	2.30893800	-0.29797400	H	12.86696100	3.18053300	0.08316100
H	-13.27246600	2.80825500	-1.27500700	H	12.17648600	3.91223400	-1.36590200
H	-13.82573100	1.37321200	-0.41018000	C	12.08308500	5.17935500	0.39205700
C	-13.94175600	3.20244000	0.75052100	H	11.93290400	5.06124500	1.47363000
H	-13.36602700	4.13053200	0.86656800	H	11.24577000	5.79044500	0.02901800
H	-13.91925200	2.70063800	1.72718800	C	13.40094600	5.92061500	0.13934200
C	-15.39106800	3.54464600	0.38698900	H	14.25511900	5.34993800	0.52203200
H	-15.44323600	4.07775800	-0.56940400	H	13.40514500	6.89893800	0.63135900
H	-15.84997800	4.18164200	1.15031100	H	13.56318600	6.08435800	-0.93239800
H	-16.00071600	2.63810300	0.29689300				

S₁; **MK-C*** to **DK***, TS, E= -1916.304775 hartree (B3LYP)



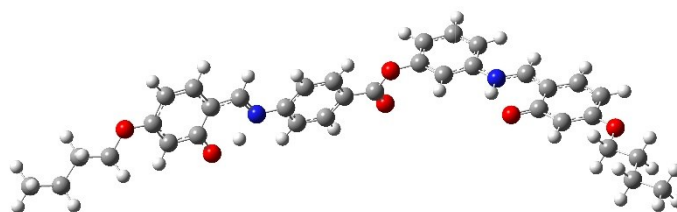
O	-0.39737600	-3.33884000	-1.85598700	C	-3.23121000	-2.18659100	0.17240500
C	1.29625600	-2.18110400	-0.62229200	H	-3.04546700	-1.11899500	0.12505000
C	2.26625700	-2.29350300	-1.64966200	C	-4.54523300	-2.67825300	0.23006000
H	1.99868300	-2.79540100	-2.57284700	C	-4.76484600	-4.06544900	0.28003300
C	3.53516000	-1.77420600	-1.48400300	H	-5.77208400	-4.46687100	0.27868400
H	4.27029300	-1.86688800	-2.27862600	C	-3.67522900	-4.93722300	0.30220600
C	3.88969000	-1.11778800	-0.27855100	H	-3.85063700	-6.00796500	0.33865200
C	2.92490000	-0.99914000	0.75484700	C	-2.36448000	-4.45621700	0.26381100
H	3.16448900	-0.50060200	1.68699400	H	-1.51736400	-5.13220900	0.27731800
C	1.65659300	-1.52336700	0.57713800	O	-6.33903200	0.70086500	-0.48426400
H	0.92648000	-1.42767900	1.37232600	H	-5.56291800	-0.44701600	-0.25618500
C	-0.03218000	-2.74897400	-0.84872600	O	-10.91306200	1.86091700	0.29711700
O	11.08562700	1.93290100	0.90582600	C	-7.82122400	-0.92821100	0.50436000
C	7.11925800	0.48417200	0.80065300	C	-7.53204500	0.37590600	-0.05236400
C	7.96873100	0.27286900	-0.36740300	C	-8.58293500	1.32606700	-0.12413200
C	9.31719000	0.77187800	-0.31970500	H	-8.34609800	2.29468200	-0.54535200
H	9.92086800	0.59987100	-1.20180500	C	-9.85757200	1.01009600	0.33268400
C	9.82472900	1.44635400	0.81255100	C	-10.14422800	-0.26935500	0.88576100
C	8.99586700	1.63682300	1.91797900	H	-11.14990900	-0.47853500	1.23230400
H	9.37484900	2.15330700	2.79222600	C	-9.13941100	-1.20212600	0.96310100
C	7.66014800	1.15241600	1.88945100	H	-9.34841600	-2.18328000	1.38254100
H	7.04234300	1.31945200	2.76820300	C	-6.82349400	-1.93457200	0.60918000
C	5.75021500	0.02483400	0.85550800	H	-7.10273600	-2.89337700	1.05069200
H	5.16687900	0.20572300	1.74995000	C	-10.73954000	3.18246200	-0.24702500
C	11.99574200	1.76976900	-0.20146900	H	-10.39990300	3.10273500	-1.28757000
H	11.57177800	2.25200200	-1.09124700	H	-9.97083000	3.71247200	0.32979500
H	12.12370200	0.69988300	-0.40918900	C	-12.07726300	3.90195800	-0.16366000
C	13.31928100	2.41063700	0.18605800	H	-12.82766200	3.32220200	-0.71597800
H	13.14642000	3.46805400	0.42260200	H	-12.40159200	3.92982800	0.88434100
H	13.69055200	1.93320300	1.10158700	C	-12.00485000	5.32902100	-0.72487600
C	14.36870500	2.28956200	-0.92807400	H	-11.66963900	5.29366600	-1.77020800
H	13.98470600	2.75798900	-1.84422300	H	-11.24355000	5.89926900	-0.17567600
H	14.52760900	1.22925800	-1.16627300	C	-13.34734900	6.06484000	-0.64555100
C	15.70794700	2.93279500	-0.55049700	H	-14.12178700	5.53653500	-1.21379100
H	15.58755400	4.00174600	-0.33961800	H	-13.26761700	7.07861500	-1.05193400
H	16.43699900	2.83206800	-1.36127100	H	-13.69271400	6.14629200	0.39167900
H	16.13430100	2.46272100	0.34329900	O	7.54272900	-0.33402200	-1.40596100
O	-0.87894500	-2.53887900	0.22704900	N	5.17481600	-0.61817800	-0.16454400
N	-5.58919400	-1.73798400	0.21026600	H	5.82213700	-0.73820800	-0.96219300
C	-2.16334600	-3.07720400	0.19111300				

S₁; DE* to MK-O*, TS, E= -1916.300569 hartree (B3LYP)



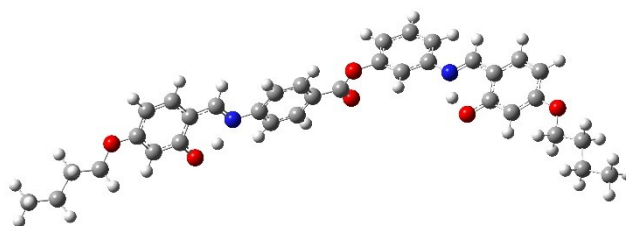
O	1.25151300	-1.89436800	1.95726900	O	0.89253200	-3.35810000	0.21419800
N	-4.86557300	-0.57745200	0.33060900	N	5.50257800	-2.08208000	-0.17278400
C	-0.88180900	-1.92076700	0.85835800	C	2.21278900	-3.66078000	0.08510600
C	-1.48090100	-0.93125500	1.70175500	C	3.22163100	-2.69829200	0.04658300
H	-0.89023200	-0.50741700	2.50720100	H	2.98958900	-1.65040900	0.18068000
C	-2.77790900	-0.51873800	1.50213000	C	4.55493300	-3.10066500	-0.15907900
H	-3.21763300	0.23426500	2.15089500	C	4.88652000	-4.46206600	-0.34303300
C	-3.58896000	-1.05146300	0.45350300	H	5.90977800	-4.77859100	-0.50327400
C	-2.98704700	-2.04607900	-0.38620100	C	3.86658800	-5.40238900	-0.31525000
H	-3.55501300	-2.48974800	-1.19724800	H	4.09841900	-6.45260300	-0.45609500
C	-1.68822100	-2.46082500	-0.18847100	C	2.53812900	-5.01420300	-0.09568100
H	-1.26654200	-3.21498800	-0.84402500	H	1.74249600	-5.75045700	-0.06299400
C	0.46897300	-2.31275500	1.10050900	O	5.81012500	0.53661300	0.03073500
O	-6.67320000	1.01996700	1.24798500	H	5.23239800	-0.74239000	-0.01515600
H	-5.79915800	0.51544200	1.11940000	O	10.23800400	2.22662000	-0.29311600
O	-10.97126600	1.11577200	-0.91827100	C	7.62372700	-1.01297400	-0.30821300
C	-7.06250100	-0.41898300	-0.65095500	C	7.06946900	0.34795200	-0.12309400
C	-7.50485800	0.56995900	0.27777400	C	7.95376000	1.46125700	-0.11707100
C	-8.80034600	1.09782300	0.21200400	H	7.51356100	2.43926300	0.02033400
H	-9.07926200	1.84535300	0.94412400	C	9.31053800	1.26624800	-0.28129600
C	-9.68644600	0.65633000	-0.77774400	C	9.84949900	-0.06060000	-0.46057000
C	-9.27713300	-0.31743500	-1.70735200	H	10.92101100	-0.16112000	-0.58465600
H	-9.97573200	-0.64919700	-2.46839400	C	9.01882100	-1.15575700	-0.47102300
C	-7.99184200	-0.83462300	-1.63414800	H	9.43725000	-2.14771800	-0.60541700
H	-7.68061100	-1.58747100	-2.35465900	C	6.80021100	-2.17528200	-0.32575400
C	-5.73299200	-0.97227800	-0.59484300	H	7.27775800	-3.14334800	-0.46668900
H	-5.47851600	-1.72467500	-1.34475900	C	9.83886700	3.61111000	-0.11772600
C	-11.45632000	2.10495500	-0.00294100	H	9.32910400	3.70480500	0.84794200
H	-10.82689100	3.00360500	-0.06321000	H	9.13738000	3.87351600	-0.91791200
H	-11.40022100	1.71668500	1.02340900	C	11.09160400	4.46850000	-0.17127200
C	-12.89559200	2.42986800	-0.37730600	H	11.78395900	4.13781600	0.61267100
H	-12.92116400	2.78495700	-1.41558900	H	11.59265800	4.30905200	-1.13402200
H	-13.48878100	1.50706400	-0.34094700	C	10.77035200	5.95927800	0.01041200
C	-13.51631200	3.48457900	0.54897900	H	10.25867700	6.10803700	0.97056200
H	-12.91129200	4.40080700	0.51599900	H	10.06578600	6.27854100	-0.76894700
H	-13.47746100	3.12697000	1.58686200	C	12.02289200	6.84111300	-0.04176500
C	-14.96631100	3.81926000	0.18052400	H	12.73253500	6.56696400	0.74728900
H	-15.03396400	4.21169500	-0.84094800	H	11.76638600	7.89703600	0.09126800
H	-15.38363000	4.57324100	0.85652700	H	12.53782300	6.74031000	-1.00406700
H	-15.60396100	2.92925500	0.23759000				

S₁; **MK-O*** to **DK***, TS, E= -1916.298588 hartree (B3LYP)



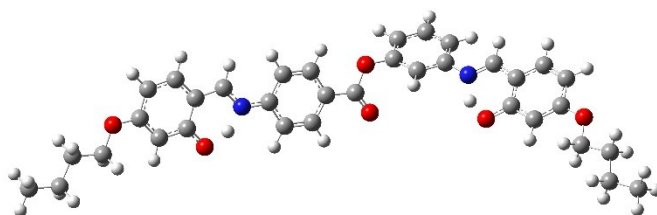
O	0.51819300	-3.27592500	1.88167500	O	0.86199000	-2.72784000	-0.29736200
N	-5.16347900	-0.72347300	0.27639600	C	2.16759000	-3.24031400	-0.27326600
C	-1.25631700	-2.25067300	0.63741400	C	3.21402900	-2.33741100	-0.21704900
C	-2.14160400	-2.24345100	1.72808100	H	3.00838800	-1.27519300	-0.13133700
H	-1.81040400	-2.64270500	2.68041800	C	4.54590300	-2.81399800	-0.27433100
C	-3.42548300	-1.73318200	1.59031300	C	4.77681900	-4.20635900	-0.38870600
H	-4.11005600	-1.73250900	2.43249300	H	5.78423500	-4.60171200	-0.43703100
C	-3.85909700	-1.22195400	0.35280700	C	3.69474000	-5.08113000	-0.44574400
C	-2.96748000	-1.21150600	-0.73730700	H	3.88137700	-6.14699500	-0.53575500
H	-3.26293800	-0.78424100	-1.68905800	C	2.37479800	-4.61879300	-0.39249900
C	-1.68383700	-1.72610400	-0.59412100	H	1.53242400	-5.29915000	-0.43893200
H	-1.00404900	-1.71055900	-1.43788800	O	10.80888100	2.02832100	-0.03095100
C	0.10376500	-2.80616200	0.83905300	C	7.83959300	-0.98856500	-0.18475100
O	-7.23353500	0.23891000	1.61638200	C	7.41686600	0.40784700	-0.10378600
H	-5.98648800	-0.32537500	1.30837800	C	8.43540800	1.41983000	-0.05166200
O	-11.00545600	1.64731900	-0.95861200	H	8.08592800	2.44297500	0.00821000
C	-7.16201800	0.04540200	-0.78994200	C	9.81491700	1.10291600	-0.07749100
C	-7.81224100	0.40444800	0.45458100	C	10.19823400	-0.23161100	-0.15438100
C	-9.12021600	0.94945300	0.39904200	H	11.25024600	-0.49224900	-0.17406800
H	-9.58727600	1.21180000	1.33953000	C	9.20186500	-1.24980500	-0.20592500
C	-9.76084200	1.13208800	-0.82107100	H	9.54003000	-2.28151100	-0.26474600
C	-9.12740000	0.77581400	-2.04657300	C	6.90026000	-2.08600400	-0.24298800
H	-9.66088400	0.93233800	-2.97716600	H	7.27093700	-3.10079600	-0.30637200
C	-7.86263600	0.24645900	-2.01378800	C	10.47370200	3.42691100	0.05020900
H	-7.37017700	-0.02845800	-2.94332100	H	9.88146800	3.60692300	0.95659600
C	-5.85722500	-0.50587700	-0.82023100	H	9.87044600	3.70761000	-0.82273700
H	-5.43165000	-0.76892200	-1.79031800	C	11.77368800	4.21587000	0.08662500
C	-11.74162200	2.04729400	0.21345800	H	12.36759200	3.88264900	0.94707700
H	-11.17118200	2.81455700	0.75202800	H	12.35567300	3.98345200	-0.81418000
H	-11.86724900	1.17944300	0.87318400	C	11.53096600	5.72909700	0.17511100
C	-13.08883100	2.58732600	-0.24155300	H	10.93879300	5.95191000	1.07286300
H	-12.92201200	3.42561600	-0.92976300	H	10.92575500	6.05261300	-0.68240000
H	-13.61244300	1.80674300	-0.80787900	C	12.83400700	6.53575800	0.21183200
C	-13.95703000	3.04650300	0.93834500	H	13.44614200	6.25840700	1.07788800
H	-13.42142000	3.81852600	1.50703800	H	12.63231900	7.61020300	0.27529900
H	-14.11022800	2.20551400	1.62795700	H	13.43306600	6.36036300	-0.68932800
C	-15.31789000	3.59432300	0.49349600	O	6.18114100	0.73763900	-0.07954500
H	-15.19821100	4.45826500	-0.17058700	N	5.56655500	-1.88486800	-0.21661800
H	-15.91587100	3.91399000	1.35339100	H	5.32592600	-0.88326800	-0.15067700
H	-15.89174500	2.83410800	-0.04915500				

S₀; **DE to DK**, TS, E= -1916.394989 hartree (B3LYP)



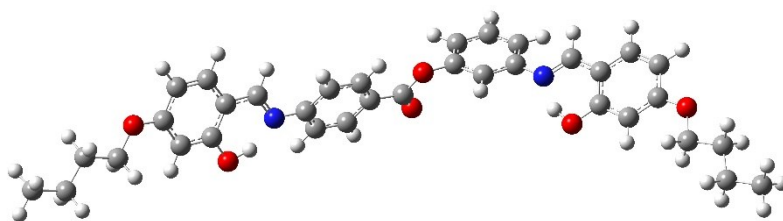
O	0.50372000	-3.17601000	2.01981100	O	0.86063900	-2.67698000	-0.16860800
N	-5.18328400	-0.69348700	0.32293500	N	5.55802300	-1.75239500	-0.17223400
C	-1.26761200	-2.18808100	0.74097300	C	2.16939300	-3.17415500	-0.11938300
C	-2.16585900	-2.17818500	1.82124600	C	3.21151000	-2.25566300	-0.12455800
H	-1.84273500	-2.56628400	2.78095700	H	3.00176000	-1.19169400	-0.10955500
C	-3.45164800	-1.67872900	1.66324900	C	4.53731300	-2.71796300	-0.16738700
H	-4.14694300	-1.67440300	2.49648700	C	4.78640600	-4.10171800	-0.17611300
C	-3.87551900	-1.18293400	0.41589700	H	5.80332600	-4.47804000	-0.15977400
C	-2.96918300	-1.17300900	-0.66245000	C	3.71910800	-5.00054300	-0.17478300
H	-3.25639200	-0.75155000	-1.61954700	H	3.91958300	-6.06739100	-0.17920200
C	-1.68316000	-1.67642600	-0.50008000	C	2.39719500	-4.54862800	-0.15267500
H	-0.99254000	-1.66093500	-1.33507000	H	1.56370300	-5.24193600	-0.14893200
C	0.09306200	-2.73152700	0.96515300	O	6.25142100	0.63803500	0.51293300
O	-7.21657800	0.33798600	1.59106000	H	5.57598400	-0.44113900	0.30622800
H	-6.06905700	-0.19753800	1.32670100	O	10.75435600	1.97994300	-0.40833400
O	-11.02611100	1.57306200	-1.02381900	C	7.75955800	-0.91343800	-0.54446900
C	-7.17734900	-0.00562400	-0.79683700	C	7.45087600	0.36905800	0.03586300
C	-7.81671000	0.43020700	0.42014500	C	8.46013600	1.35731200	0.08750100
C	-9.12224900	0.96592800	0.35343200	H	8.20328500	2.31172000	0.52879900
H	-9.57925500	1.28527600	1.28106400	C	9.73047700	1.09125500	-0.41765100
C	-9.77807800	1.07032100	-0.87073900	C	10.04106600	-0.16998600	-0.99444700
C	-9.15615000	0.64005400	-2.07498300	H	11.04082700	-0.33964300	-1.37778900
H	-9.69860100	0.73598700	-3.00863000	C	9.06677200	-1.13858900	-1.05068900
C	-7.88760100	0.11523700	-2.02210800	H	9.29504500	-2.10648100	-1.49020600
H	-7.40397100	-0.21693000	-2.93735400	C	6.77354600	-1.93956100	-0.62212700
C	-5.86601300	-0.55803700	-0.78860600	H	7.05101900	-2.88959400	-1.08513900
H	-5.44221800	-0.88859800	-1.73987500	C	10.55055300	3.29082700	0.15147700
C	-11.75176400	2.03649700	0.13136100	H	10.25456900	3.19203200	1.20366300
H	-11.17970100	2.83566500	0.61948500	H	9.74045200	3.79357200	-0.39206500
H	-11.86690500	1.20710500	0.84066100	C	11.85496400	4.06266200	0.02185300
C	-13.10612600	2.54411900	-0.33938000	H	12.64816200	3.51023900	0.54135600
H	-12.95048400	3.34404000	-1.07426400	H	12.13733000	4.10842600	-1.03759000
H	-13.63076000	1.73091600	-0.85671100	C	11.74804300	5.48298600	0.59455500
C	-13.96545100	3.06317400	0.82202800	H	11.45543700	5.42931400	1.65182600
H	-13.42866100	3.86788200	1.34223300	H	10.94402400	6.02512400	0.07878600
H	-14.10748000	2.26052000	1.55815500	C	13.05629000	6.27195800	0.46797200
C	-15.33344800	3.57909600	0.36122500	H	13.87256900	5.77210700	1.00236000
H	-15.22481200	4.40587700	-0.35035000	H	12.95239100	7.27974400	0.88364500
H	-15.92485800	3.94252900	1.20817500	H	13.35743300	6.37216200	-0.58131900
H	-15.90836100	2.78746600	-0.13324000				

S₁; **DE* to DK***, TS, E=-1916.296317 hartree (B3LYP)



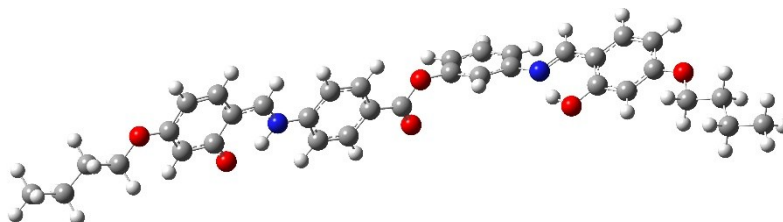
O -0.91775100	-1.80202400	-2.02032100	O -0.82339800	-2.97381900	-0.06060900
N 5.07603200	-0.60091300	-0.06062700	N -5.51383200	-1.86323500	-0.01099000
C 1.09988900	-1.77876400	-0.73258800	C -2.15664800	-3.36066400	-0.15458200
C 1.80239000	-0.96588000	-1.66064000	C -3.18008000	-2.41877000	-0.08365600
H 1.29518700	-0.64251800	-2.56286900	H -2.95284100	-1.36122200	-0.01762600
C 3.10813500	-0.59027400	-1.42254200	C -4.51498200	-2.85032800	-0.08513600
H 3.63881600	0.03244000	-2.13687400	C -4.80447500	-4.22405400	-0.18025400
C 3.78213800	-1.00838300	-0.23994200	H -5.83186500	-4.56771100	-0.23098100
C 3.07734100	-1.82635000	0.69336500	C -3.76161600	-5.14759400	-0.24273300
H 3.55932900	-2.16398900	1.60396800	H -3.98824100	-6.20658400	-0.31908000
C 1.77014500	-2.19726100	0.44442900	C -2.42866200	-4.72668600	-0.22835000
H 1.24610800	-2.81830800	1.16175100	H -1.60974500	-5.43561900	-0.28338000
C -0.28117800	-2.14758500	-1.03354100	O -6.17340700	0.58886000	-0.53731300
O 6.90251400	0.76206400	-1.19816800	H -5.50740700	-0.51460400	-0.40922500
H 5.78511100	0.14517900	-0.88258600	O -10.64413500	1.93984700	0.51510300
O 11.16921300	1.21232500	0.93889400	C -7.69649600	-1.00546000	0.43477400
C 7.23889700	-0.31149700	0.92229900	C -7.37187300	0.30621100	-0.06537700
C 7.69906800	0.50642800	-0.20157800	C -8.36539700	1.31177800	-0.04318800
C 9.02239000	1.02562900	-0.20743900	H -8.09640500	2.28810100	-0.42539100
H 9.30996100	1.62335700	-1.06283900	C -9.63520700	1.03501300	0.45716300
C 9.89182800	0.76411700	0.85169100	C -9.96128300	-0.25492200	0.95549600
C 9.44836400	-0.02364200	1.93758800	H -10.95983100	-0.43295000	1.33828400
H 10.13169500	-0.22061400	2.75626700	C -9.00224700	-1.24074800	0.93911700
C 8.13960300	-0.54495900	1.95567100	H -9.24262000	-2.23081300	1.31883800
H 7.83135000	-1.14683600	2.80575700	C -6.72840800	-2.05318200	0.43711000
C 5.89557700	-0.85713500	0.95598100	H -7.02076400	-3.02553800	0.84132100
H 5.58566400	-1.46046800	1.80472000	C -10.42098700	3.28047800	0.04023200
C 11.70081300	2.01716800	-0.13092900	H -10.13519400	3.24586000	-1.01885900
H 11.08403700	2.91839300	-0.24368000	H -9.59750400	3.73236600	0.60783500
H 11.65607600	1.44531800	-1.06716100	C -11.70976400	4.06561300	0.23184800
C 13.13561400	2.37860000	0.22004700	H -12.51673900	3.56460300	-0.31770800
H 13.14357300	2.91313800	1.17827100	H -11.98432600	4.04458100	1.29414600
H 13.71058700	1.45496500	0.36250600	C -11.57973800	5.51937300	-0.24392400
C 13.79563200	3.24207600	-0.86441900	H -11.29368500	5.53244500	-1.30425600
H 13.20748000	4.15812800	-1.00992500	H -10.76313200	6.01058900	0.30217500
H 13.77343400	2.70511300	-1.82220800	C -12.87251600	6.32145600	-0.05573300
C 15.24275000	3.61505500	-0.52308100	H -13.70054200	5.87409400	-0.61786400
H 15.29420600	4.18251800	0.41337700	H -12.75208100	7.35323200	-0.40240800
H 15.68876000	4.23005700	-1.31166800	H -13.16658700	6.35524300	0.99980500
H 15.86434100	2.71991900	-0.40489200			

Fig. S4: S₀; 4-4 (DE) E= -1914.091597 hartree (Using PBE)



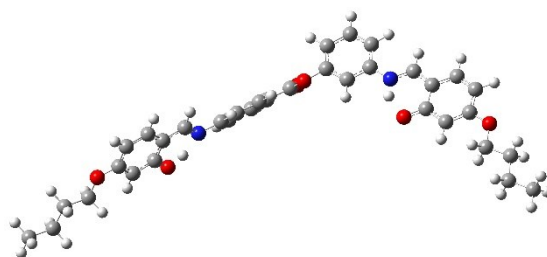
O	0.42129000	-3.25679600	2.04760800	O	0.81680600	-2.50651900	-0.08629600
N	-5.30159000	-0.71158300	0.45686600	N	5.53057200	-1.59752600	-0.16877600
C	-1.34726600	-2.16834400	0.82288700	C	2.12580900	-3.01763300	-0.06531200
C	-2.26834400	-2.26538300	1.88958100	C	3.17555100	-2.09784700	-0.07722500
H	-1.94607100	-2.72904800	2.82583900	H	2.97059900	-1.02496100	-0.03617400
C	-3.56565400	-1.77478500	1.75106200	C	4.50726600	-2.56216600	-0.16497500
H	-4.28110000	-1.84735900	2.57520900	C	4.75016700	-3.95559900	-0.19801700
C	-3.98768200	-1.19040100	0.53197900	H	5.77677100	-4.33216900	-0.20686500
C	-3.05567400	-1.07395100	-0.52986400	C	3.67651800	-4.85628400	-0.17803700
H	-3.34412800	-0.57245100	-1.45807100	H	3.87450600	-5.93211100	-0.19637200
C	-1.75501100	-1.56043100	-0.38526300	C	2.35045800	-4.40024000	-0.12056900
H	-1.04294800	-1.45971500	-1.20778000	H	1.50981800	-5.09753600	-0.10426400
C	0.01988300	-2.70615100	1.02824900	O	6.44345700	0.62138100	0.70610500
O	-7.26753300	0.45764800	1.59759000	H	5.82040800	-0.18571300	0.50904700
H	-6.35598700	-0.00680900	1.42782600	O	10.90745200	1.89011900	-0.57828700
O	-11.12400800	1.51321300	-1.08128100	C	7.73789700	-0.84161200	-0.71861100
C	-7.28228800	-0.11247400	-0.75274500	C	7.58788500	0.36511600	0.04455300
C	-7.90506900	0.45241400	0.41242500	C	8.63718500	1.30231700	0.10991400
C	-9.19711800	1.00598400	0.33218500	H	8.48295600	2.20618600	0.70114300
H	-9.63449100	1.42432200	1.23990600	C	9.83526600	1.05030500	-0.57909300
C	-9.87637800	1.00339200	-0.89766500	C	10.00088900	-0.13747300	-1.34348400
C	-9.27677800	0.44661600	-2.06213900	H	10.94534900	-0.30145200	-1.86758200
H	-9.83451200	0.46109700	-3.00138100	C	8.96403100	-1.05514900	-1.40416800
C	-8.00674600	-0.09850800	-1.97640500	H	9.08409600	-1.97266900	-1.99028300
H	-7.53837000	-0.52930600	-2.86780100	C	6.67067300	-1.80339600	-0.78701600
C	-5.96669000	-0.68145600	-0.67773600	H	6.83769800	-2.71125500	-1.39451300
H	-5.54340300	-1.11645700	-1.60087500	C	10.82472100	3.12100900	0.17767000
C	-11.81213500	2.09472200	0.05193700	H	10.63223300	2.88332100	1.24127600
H	-11.21115200	2.93419200	0.45025300	H	9.98086200	3.72709900	-0.20383500
H	-11.91634200	1.33020100	0.84513600	C	12.14605100	3.85980500	0.01393800
C	-13.17567400	2.57557300	-0.42515800	H	12.96758700	3.20959600	0.36673000
H	-13.03432000	3.30857400	-1.24049100	H	12.32261800	4.04746100	-1.06113200
H	-13.72912600	1.71972500	-0.85327600	C	12.16546600	5.18886800	0.78532500
C	-13.99383000	3.20985900	0.71065500	H	11.97607600	4.99397800	1.85783500
H	-13.42879900	4.05802100	1.14120600	H	11.33339700	5.82881800	0.43573700
H	-14.11867400	2.47472500	1.52802200	C	13.49199900	5.94326600	0.62871200
C	-15.37208400	3.69670800	0.24513400	H	14.33884500	5.34124000	1.00129100
H	-15.27835200	4.45696600	-0.54958600	H	13.48162300	6.89199400	1.19016500
H	-15.93878700	4.14772900	1.07627300	H	13.69198400	6.18144900	-0.43037300
H	-15.97318100	2.86367000	-0.15871900				

S₀; **MK-C**, E= -1914.091225 hartree (Using PBE)



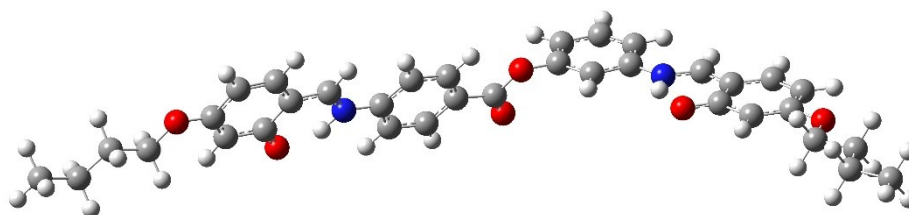
O	0.33895000	-3.23790900	1.91539600	C	3.19214200	-2.08678600	-0.12398400
C	-1.35834100	-2.09187000	0.64628500	H	3.00230900	-1.01071300	-0.09565200
C	-2.32520300	-2.20212500	1.66920500	C	4.51859000	-2.57125100	-0.17532300
H	-2.05359600	-2.69785900	2.60480700	C	4.74115700	-3.96833000	-0.19235200
C	-3.60757700	-1.68834700	1.49076500	H	5.76180600	-4.36024200	-0.17320500
H	-4.35240900	-1.77732700	2.28722100	C	3.65394100	-4.85276300	-0.19260800
C	-3.95750800	-1.04816300	0.27799500	H	3.83614400	-5.93150200	-0.19844900
C	-2.99247200	-0.93314000	-0.74939600	C	2.33370200	-4.37707600	-0.17135200
H	-3.23231200	-0.44263900	-1.69555600	H	1.48304500	-5.06215900	-0.17102400
C	-1.71023800	-1.45085900	-0.56212600	O	6.47625800	0.59242000	0.71811200
H	-0.97102100	-1.35850100	-1.36090100	H	5.84738600	-0.20781000	0.51180200
C	-0.01116900	-2.66182500	0.89137100	O	10.99035000	1.78651800	-0.45804000
O	-11.10448300	1.88728100	-0.91812900	C	7.78740700	-0.90217500	-0.65770200
C	-7.15603000	0.51144600	-0.84097300	C	7.63422100	0.31388700	0.08992500
C	-7.98341100	0.28163400	0.35987100	C	8.69454900	1.23697100	0.17477900
C	-9.33737100	0.75705500	0.32531400	H	8.53739600	2.14845300	0.75344900
H	-9.94432900	0.58495400	1.21583700	C	9.90684100	0.96177500	-0.47968900
C	-9.83729200	1.40620900	-0.80046200	C	10.07587900	-0.23543900	-1.22850300
C	-9.02419800	1.62578100	-1.96639800	H	11.03149400	-0.41747600	-1.72572500
H	-9.46611600	2.14075400	-2.82257400	C	9.02823200	-1.13922300	-1.30830100
C	-7.72249800	1.18564300	-1.97290100	H	9.15089700	-2.06383100	-1.88260500
H	-7.09441200	1.34807200	-2.85595500	C	6.70897500	-1.84963700	-0.74576700
C	-5.82367700	0.07667800	-0.88153700	H	6.87945400	-2.76576400	-1.33977000
H	-5.21950300	0.25245400	-1.77815800	C	10.90528800	3.02524400	0.28479500
C	-12.01337800	1.72056700	0.19622300	H	10.68287400	2.79966000	1.34518100
H	-11.58604700	2.21592600	1.08860100	H	10.07959400	3.63898100	-0.12321200
H	-12.12320400	0.64140200	0.41478000	C	12.24009000	3.74503600	0.14811200
C	-13.34871700	2.34139600	-0.19027800	H	13.04378800	3.08722600	0.52692200
H	-13.19281200	3.40796500	-0.43585200	H	12.44599400	3.92096900	-0.92371800
H	-13.72212600	1.85049600	-1.10775800	C	12.25781700	5.08039900	0.90859000
C	-14.39149400	2.21165600	0.93124100	H	12.03934100	4.89728700	1.97764100
H	-14.00520700	2.69289100	1.84954100	H	11.44313200	5.72796200	0.53302900
H	-14.53327500	1.14266500	1.17874400	C	13.59761000	5.81620200	0.77878400
C	-15.74269000	2.83407200	0.55689200	H	14.42695900	5.20655500	1.17740500
H	-15.63796100	3.91067900	0.33697900	H	13.58575600	6.76983700	1.33183100
H	-16.47276100	2.72815000	1.37616000	H	13.82694100	6.04253500	-0.27694300
H	-16.16967500	2.35024300	-0.33865900	O	-7.50347300	-0.32106400	1.39171600
O	0.82952400	-2.45721200	-0.18871600	N	-5.26164200	-0.55688700	0.16176500
N	5.55560200	-1.62161000	-0.16062400	H	-5.97419600	-0.65180800	0.95183000
C	2.12880800	-2.99085500	-0.13161900				

S₀; **MK-O**, E= -1914.091108 hartree (using PBE)



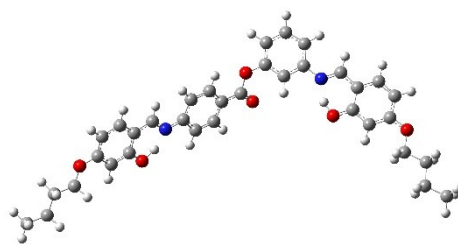
O	0.38136300	-3.88181400	1.69882500	O	0.91916900	-2.72196600	-0.21111000
N	-5.18719600	-0.89740600	0.34874500	C	2.21514100	-3.25284500	-0.23449000
C	-1.29141500	-2.51994000	0.62256900	C	3.26776600	-2.33668900	-0.18265500
C	-2.27569500	-2.80262400	1.59598800	H	3.05455500	-1.27137700	-0.05963900
H	-2.01773200	-3.45440400	2.43507400	C	4.59642100	-2.80000000	-0.29234500
C	-3.55312700	-2.25578300	1.49000700	C	4.84343900	-4.18066700	-0.44858000
H	-4.31689500	-2.47094500	2.24283400	H	5.86131300	-4.56746800	-0.53399600
C	-3.89121000	-1.42480700	0.39403700	C	3.76535000	-5.07393700	-0.49768800
C	-2.89665500	-1.12624700	-0.57120500	H	3.96321900	-6.14253700	-0.62090400
H	-3.12108600	-0.43989800	-1.39262900	C	2.43905600	-4.62731300	-0.39472200
C	-1.61587700	-1.67008200	-0.45821800	H	1.60122500	-5.32577200	-0.43713300
H	-0.85503600	-1.42696100	-1.20369000	O	10.64696900	2.15820300	-0.05596200
C	0.05073800	-3.12561400	0.79271600	C	7.83218800	-0.93118200	-0.24631100
O	-7.18279300	0.08751300	1.60280800	C	7.32647900	0.44304600	-0.08197800
H	-6.27507600	-0.36602000	1.38709900	C	8.29857400	1.49721100	-0.01829300
O	-10.85197200	1.80622600	-0.99290600	H	7.91809400	2.51282800	0.10393400
C	-7.08079800	0.00226700	-0.81222500	C	9.66066100	1.21999700	-0.10886900
C	-7.75227900	0.34461300	0.41132100	C	10.14470700	-0.12282700	-0.26937900
C	-9.02214600	0.95181700	0.38106700	H	11.22283300	-0.28726800	-0.33510700
H	-9.49807300	1.19559100	1.33197000	C	9.24335300	-1.16003600	-0.33495800
C	-9.63150300	1.22209700	-0.85555800	H	9.60248500	-2.18824100	-0.45666100
C	-8.98372800	0.88675400	-2.07781300	C	6.93939300	-2.01462100	-0.31726800
H	-9.48779500	1.11017200	-3.02097600	H	7.32646600	-3.03229700	-0.44024100
C	-7.73566200	0.28812000	-2.04192900	C	10.27105500	3.54564900	0.10632200
H	-7.23047600	0.02715200	-2.97809100	H	9.69766900	3.65841600	1.04618800
C	-5.78597700	-0.61647300	-0.78854600	H	9.62044700	3.84650000	-0.73695200
H	-5.32144200	-0.87140300	-1.75809800	C	11.54610500	4.37745700	0.13914500
C	-11.58143600	2.18380800	0.19940100	H	12.18592300	4.02365800	0.96849200
H	-10.97645200	2.90410800	0.78246900	H	12.10987800	4.21032200	-0.79713400
H	-11.75192800	1.28439000	0.82122000	C	11.25300400	5.87626900	0.31048100
C	-12.90137100	2.80484100	-0.23701300	H	10.67680700	6.03350000	1.24187900
H	-12.69254600	3.67412100	-0.88733100	H	10.60358800	6.22018500	-0.51666500
H	-13.45949400	2.07161300	-0.84775100	C	12.52861700	6.72765900	0.34793000
C	-13.75729000	3.24372000	0.96168700	H	13.18236100	6.42855500	1.18560400
H	-13.18836100	3.96885400	1.57375100	H	12.29246000	7.79750300	0.47156700
H	-13.94973500	2.37142300	1.61456900	H	13.10886700	6.61688600	-0.58459000
C	-15.09218800	3.86903300	0.53675000	O	6.06186200	0.68262900	0.00097900
H	-14.93147800	4.76342700	-0.08989100	N	5.61442600	-1.83332600	-0.23638700
H	-15.68725800	4.17524200	1.41289700	H	5.40099300	-0.79252100	-0.11749900
H	-15.69785400	3.15543300	-0.04841900				

S₀; **DK**, E= -1914.090734 hartree (using PBE)



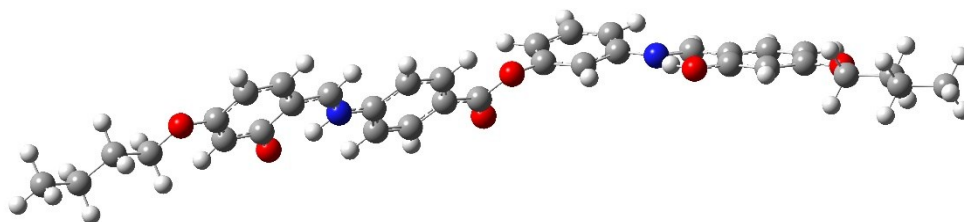
O	0.33741900	-3.69512600	1.62183700	H	3.08869800	-1.22994700	-0.12674900
C	-1.29207000	-2.33937800	0.47647200	C	4.59511500	-2.80057600	-0.30886700
C	-2.29772500	-2.57465700	1.43941400	C	4.80890200	-4.18830200	-0.45077900
H	-2.07028400	-3.20840300	2.30051000	H	5.81827200	-4.60124700	-0.50944400
C	-3.56228000	-2.00904000	1.29578500	C	3.70950400	-5.05354900	-0.52371200
H	-4.33756800	-2.19580200	2.04480400	H	3.88227100	-6.12759600	-0.63619900
C	-3.85507900	-1.18939200	0.17948200	C	2.39341600	-4.57084500	-0.45997200
C	-2.85084000	-0.94843700	-0.78686800	H	1.53782100	-5.24611600	-0.52181700
H	-3.04525200	-0.31612300	-1.65620800	O	10.76882100	1.99354700	0.05883900
C	-1.58680500	-1.51956700	-0.63551900	C	7.87816000	-1.02164200	-0.17540400
H	-0.81696100	-1.32797000	-1.38623500	C	8.40305000	1.39826600	0.01327400
C	0.03327200	-2.96992100	0.68177600	H	8.04670300	2.42664500	0.09506300
O	-10.89322400	2.07292400	-0.78409800	C	9.75932400	1.08164500	-0.01315700
C	-6.98325600	0.58908600	-0.80197900	C	10.21159500	-0.27743700	-0.12130000
C	-7.84743900	0.22564900	0.33863500	H	11.28642700	-0.47253200	-0.13812600
C	-9.18766900	0.73933000	0.33722000	C	9.28478000	-1.29104900	-0.19919100
H	-9.82180400	0.46838600	1.18303800	H	9.61907700	-2.33139100	-0.28124300
C	-9.64206700	1.54498400	-0.70346200	C	6.95880100	-2.08180100	-0.25542000
C	-8.79404300	1.89292900	-1.81191200	H	7.32143400	-3.11277500	-0.33531800
H	-9.20085300	2.52811500	-2.60223100	C	10.42658500	3.39427700	0.17545300
C	-7.50389200	1.42145100	-1.84748600	H	9.81720400	3.54408800	1.08698900
H	-6.84971900	1.68123900	-2.68717200	H	9.82154500	3.69427000	-0.70131800
C	-5.66108500	0.12732400	-0.86873500	C	11.72283300	4.19012300	0.24567600
H	-5.02858900	0.40220800	-1.71986400	H	12.31630400	3.83643200	1.10876700
C	-11.83301400	1.78920500	0.27994000	H	12.32067900	3.98640000	-0.66171200
H	-11.41515100	2.15329300	1.23767200	C	11.46711100	5.70005000	0.37330900
H	-11.97492300	0.69438800	0.35462300	H	10.85658100	5.89383100	1.27542400
C	-13.14269100	2.49154900	-0.05085700	H	10.86396200	6.04439200	-0.48791600
H	-12.95370000	3.57567000	-0.15641400	C	12.76444100	6.51528600	0.44856700
H	-13.50758600	2.13099100	-1.03017800	H	13.37258800	6.21612600	1.31983000
C	-14.21386700	2.25154500	1.02477700	H	12.55489100	7.59383300	0.53966600
H	-13.83685400	2.60351000	2.00358600	H	13.38068800	6.36764900	-0.45526100
H	-14.38804500	1.16437000	1.13339100	O	6.14524900	0.64479500	-0.04177300
C	-15.54011500	2.95299600	0.70485000	C	7.40507500	0.36962200	-0.06583100
H	-15.40343700	4.04529300	0.62363100	N	5.63723900	-1.86164100	-0.23401500
H	-16.29125800	2.76596800	1.48984500	H	5.44957700	-0.81239200	-0.14863600
H	-15.95831800	2.59661300	-0.25248800	O	-7.41006000	-0.52193600	1.29163300
O	0.91775800	-2.62921900	-0.33008600	N	-5.14369900	-0.65384300	0.09478500
C	2.20276000	-3.19004800	-0.31383100	H	-5.88124800	-0.83336300	0.84685300
C	3.27660500	-2.30126900	-0.23790800				

S₁; DE* E= -1914.021877 hartree (Using PBE)



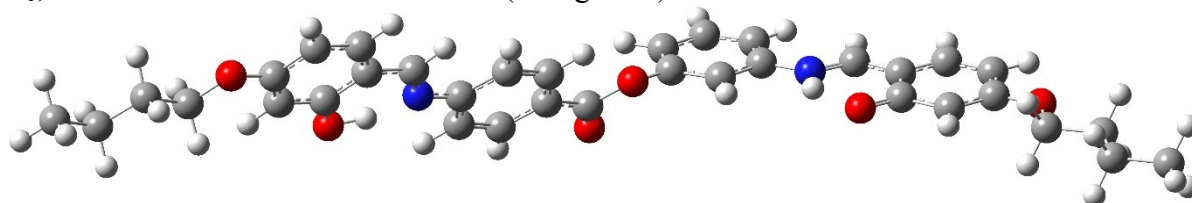
O 1.25694900	-1.83614100	1.91640600	O 0.91376200	-3.33301500	0.17090100
N -4.89767700	-0.61877600	0.27143900	N 5.53817400	-2.03975400	-0.14481700
C -0.88730800	-1.90660100	0.81354600	C 2.24428700	-3.63714000	0.08223200
C -1.49777400	-0.91500300	1.65113300	C 3.25976100	-2.67241200	0.04077300
H -0.90470400	-0.47407600	2.45754700	H 3.02952000	-1.61136700	0.14045900
C -2.80636600	-0.51814100	1.44948600	C 4.60832600	-3.07701100	-0.12711300
H -3.25928900	0.24094700	2.09625700	C 4.93890800	-4.45229800	-0.27353700
C -3.61388900	-1.07372100	0.40128100	H 5.97181000	-4.77765300	-0.41174200
C -2.99772100	-2.07157700	-0.43328500	C 3.91382300	-5.39606600	-0.24526900
H -3.56606600	-2.53221700	-1.24606700	H 4.14772600	-6.45760900	-0.36033700
C -1.68598500	-2.46892900	-0.23044600	C 2.57621800	-5.00095000	-0.05814000
H -1.24902400	-3.22946500	-0.88331300	H 1.77341600	-5.74203000	-0.02332700
C 0.47885900	-2.27508900	1.06014900	O 5.80799900	0.46366800	-0.05992900
O -6.64273500	0.95307000	1.18716700	H 5.39934900	-0.51718900	-0.07068300
H -5.75145200	0.39694700	1.00428300	O 10.23946000	2.24300100	-0.25648200
O -11.01042000	1.09547400	-0.89903700	C 7.68734400	-1.04218800	-0.24476800
C -7.09675800	-0.48606300	-0.70487400	C 7.11539000	0.30792000	-0.14941000
C -7.50785100	0.51852600	0.24135900	C 7.95026900	1.43922600	-0.15149500
C -8.80753300	1.06094300	0.19717700	H 7.48687400	2.42289400	-0.07750500
H -9.06722600	1.81958700	0.93801500	C 9.33353700	1.25863700	-0.24651100
C -9.72076700	0.62250600	-0.77868500	C 9.91212800	-0.06211600	-0.34326000
C -9.34131800	-0.36346000	-1.71929800	H 10.99859800	-0.14244900	-0.41497200
H -10.06615000	-0.69067700	-2.46959200	C 9.09809400	-1.17549600	-0.34023000
C -8.05483400	-0.89714300	-1.67201100	H 9.53450700	-2.17544100	-0.41053700
H -7.76311400	-1.66102100	-2.40201100	C 6.84399400	-2.19885500	-0.23752300
C -5.77153000	-1.04050800	-0.66299800	H 7.32310400	-3.18678600	-0.30383200
H -5.50672100	-1.80449000	-1.40952600	C 9.79216200	3.63121200	-0.15509500
C -11.44918700	2.10169600	0.03023300	H 9.22479500	3.74305800	0.78592700
H -10.79556100	2.99312200	-0.04879400	H 9.12209800	3.84086900	-1.00783700
H -11.37327800	1.71248100	1.06505000	C 11.02557400	4.51901400	-0.17554100
C -12.89187900	2.45950700	-0.30652700	H 11.69133000	4.23066100	0.65791400
H -12.93925100	2.81433900	-1.35281500	H 11.58248900	4.34398700	-1.11373800
H -13.51111400	1.54509200	-0.25003600	C 10.65500800	6.00668500	-0.05678100
C -13.46156000	3.53293500	0.63346400	H 10.08807400	6.17046700	0.87875500
H -12.83027400	4.44015200	0.57995400	H 9.97575000	6.28402400	-0.88444800
H -13.39967800	3.17564100	1.67889200	C 11.88692400	6.92023800	-0.07629700
C -14.91409700	3.90067200	0.30393300	H 12.56833700	6.68832200	0.76025200
H -15.00194500	4.29298200	-0.72422900	H 11.59686500	7.97990700	0.01044300
H -15.29934600	4.67179400	0.99159500	H 12.45563300	6.80273500	-1.01472000
H -15.57518600	3.02001300	0.38210900			

S₁; **MK-C*** E= -1914.023873 hartree (Using PBE)



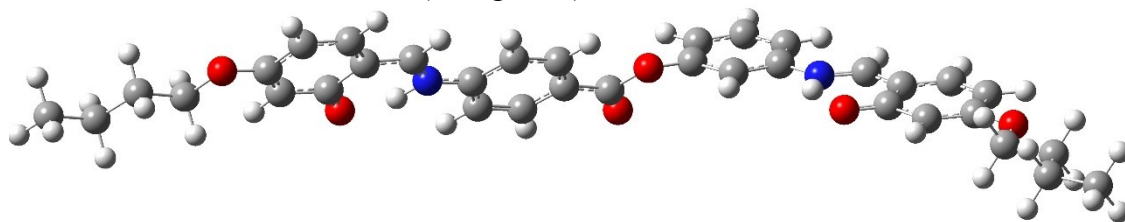
O	-0.22294900	-3.75018300	-1.38151100	C	-3.29355800	-2.01400900	0.20572000
C	1.36738500	-2.19020400	-0.45819700	H	-3.20453100	-0.95169300	-0.03415600
C	2.47131200	-2.65535000	-1.24329600	C	-4.57450800	-2.58926100	0.40294100
H	2.30225600	-3.46482000	-1.95885400	C	-4.69575500	-3.97234600	0.71314900
C	3.73013700	-2.10006100	-1.10745500	H	-5.67084200	-4.42697000	0.90032300
H	4.56214100	-2.46874900	-1.71635500	C	-3.54042800	-4.74575100	0.81279100
C	3.97339500	-1.04076600	-0.17649600	H	-3.61810300	-5.80660100	1.06447400
C	2.87204600	-0.57014000	0.60862100	C	-2.26759600	-4.18026700	0.61103200
H	3.01623500	0.23807700	1.32992400	H	-1.37102900	-4.79429300	0.70753200
C	1.61204700	-1.13125900	0.46640100	O	-6.34567800	0.70627700	0.14960600
H	0.78791100	-0.75518200	1.07797100	H	-5.77519300	-0.18256400	0.20823900
C	0.08110800	-2.81265000	-0.63578100	O	-11.01491100	1.67691200	-0.16700100
O	11.08416600	2.17048100	0.64775000	C	-7.94055900	-1.10879900	0.11876400
C	7.07082400	0.85942800	0.67376500	C	-7.60817800	0.32113400	0.08758800
C	8.00534600	0.20502000	-0.24989800	C	-8.62301000	1.28784600	-0.01139500
C	9.36363700	0.66004600	-0.24954100	H	-8.33568300	2.33889200	-0.03243100
H	10.04542700	0.16404800	-0.94394300	C	-9.95543300	0.86608200	-0.07564100
C	9.79103600	1.68715500	0.59914400	C	-10.30002300	-0.53696400	-0.04787800
C	8.88518900	2.31657000	1.49440400	H	-11.35608500	-0.80781800	-0.10493600
H	9.24668000	3.11575600	2.14678700	C	-9.30787400	-1.48939200	0.04599500
C	7.55939400	1.89980800	1.51751000	H	-9.56504200	-2.55183300	0.06484200
H	6.85715600	2.38404500	2.20708300	C	-6.91412000	-2.10006600	0.21378600
C	5.70554400	0.46980000	0.73094400	H	-7.21660700	-3.15761100	0.21763400
H	5.01358800	0.96149800	1.41987100	C	-10.81255200	3.12462700	-0.20833000
C	12.05619000	1.58096000	-0.23187000	H	-10.18547500	3.35978000	-1.08669600
H	11.73023200	1.70300600	-1.28398000	H	-10.27629400	3.42440200	0.70945100
H	12.13743300	0.49534000	-0.02459600	C	-12.18022700	3.78119600	-0.29977700
C	13.39172100	2.27708600	0.00343400	H	-12.69841800	3.41380400	-1.20387400
H	13.27020800	3.36047100	-0.18251900	H	-12.78665700	3.47436800	0.57147800
H	13.67353000	2.16469200	1.06694800	C	-12.07128200	5.31432600	-0.34628500
C	14.50780300	1.71792400	-0.89206100	H	-11.45545800	5.61341600	-1.21500500
H	14.21373500	1.82283900	-1.95364800	H	-11.53545200	5.67221600	0.55271500
H	14.61618700	0.63211800	-0.70849400	C	-13.44274600	5.99596100	-0.43122800
C	15.85678500	2.41223400	-0.66413700	H	-13.98878600	5.68110700	-1.33706700
H	15.78781300	3.49416500	-0.87268800	H	-13.33967700	7.09266000	-0.46510700
H	16.64016300	1.99361200	-1.31767500	H	-14.06820100	5.74356700	0.44226700
H	16.19303900	2.29535100	0.38089400	O	7.61346200	-0.75559100	-1.04234600
O	-0.93438600	-2.18046200	0.16956000	N	5.23951000	-0.52712300	-0.07777200
N	-5.65212900	-1.71878900	0.27503600	H	6.05131900	-0.88823200	-0.67754100
C	-2.14752000	-2.80674100	0.30024800				

S₁; **MK-O*** E= - 1914.027971 hartree (Using PBE)



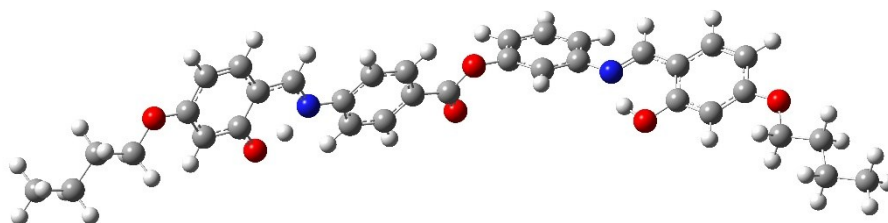
O	0.16796700	-3.71471300	1.57968900	O	0.90194600	-2.12131000	0.05389100
N	-5.31752600	-0.53631000	0.20412200	C	2.08504400	-2.77541300	-0.15178800
C	-1.41514200	-2.15844100	0.63452100	C	3.25342400	-1.99786700	-0.10566400
C	-2.53307000	-2.62529000	1.40326700	H	3.18052500	-0.93773700	0.15337900
H	-2.37146500	-3.43162700	2.12451000	C	4.49439400	-2.59226600	-0.39695700
C	-3.79045100	-2.07437300	1.24080800	C	4.59546500	-3.95832500	-0.72144900
H	-4.63480900	-2.44154800	1.83397200	H	5.55344800	-4.43264300	-0.94342200
C	-4.03913700	-1.01739400	0.30347900	C	3.42040200	-4.71708000	-0.75658200
C	-2.91385900	-0.54886100	-0.46124200	H	3.47711500	-5.77900400	-1.00983000
H	-3.04451400	0.25687000	-1.18899500	C	2.16950200	-4.14395900	-0.48002200
C	-1.65356300	-1.10048200	-0.29803600	H	1.26386300	-4.75059100	-0.51900800
H	-0.82018400	-0.72260600	-0.89670400	O	11.14827900	1.63548000	-0.12484600
C	-0.13389100	-2.77361700	0.83354400	C	7.92751500	-1.04224400	-0.43862800
O	-7.67591300	-0.72664500	1.07691800	C	7.64082600	0.35525100	-0.03809700
H	-6.63401100	-0.85019800	0.89208400	C	8.74384100	1.27907700	0.07083700
O	-11.09783300	2.17649600	-0.74125200	H	8.49716400	2.29872300	0.36786000
C	-7.08265400	0.86631400	-0.64508800	C	10.04858300	0.86340600	-0.19682800
C	-8.05152100	0.25889900	0.22893000	C	10.30014700	-0.49053300	-0.58787900
C	-9.39675300	0.67855000	0.21560900	H	11.33102900	-0.78589500	-0.79437400
H	-10.09041400	0.18527200	0.89923000	C	9.25578600	-1.41316900	-0.70331100
C	-9.80643600	1.70090200	-0.65901500	H	9.48412200	-2.43956700	-1.00509200
C	-8.87374300	2.31207800	-1.52925900	C	6.89123200	-2.01924400	-0.55962700
H	-9.21285000	3.10429500	-2.20208800	H	7.15787800	-3.03996300	-0.84868700
C	-7.54436200	1.89395900	-1.51197200	C	10.99660600	3.03046700	0.26858100
H	-6.82317400	2.36906700	-2.18701300	H	10.52790000	3.06559700	1.26916300
C	-5.70827300	0.44198500	-0.63166600	H	10.32902000	3.53067800	-0.45693000
H	-5.00703300	0.94032400	-1.31847800	C	12.37952200	3.66292700	0.27969600
C	-12.08826500	1.59300900	0.12344000	H	13.02544500	3.10416900	0.98105200
H	-11.78647200	1.72844200	1.18112300	H	12.82913000	3.56430900	-0.72502800
H	-12.16247200	0.50519300	-0.07482600	C	12.32746200	5.14489400	0.68552500
C	-13.41962800	2.28275600	-0.14964200	H	11.86361400	5.23638700	1.68555100
H	-13.30532100	3.36809000	0.02875700	H	11.66968700	5.69486000	-0.01334500
H	-13.67581600	2.15899200	-1.21825000	C	13.71556000	5.79749900	0.70339600
C	-14.55439700	1.72834500	0.72517900	H	14.38563600	5.28952800	1.41821300
H	-14.28533800	1.84398700	1.79224700	H	13.65274800	6.85788000	0.99725900
H	-14.65574100	0.64065400	0.54901600	H	14.19059200	5.75181600	-0.29171900
C	-15.89941400	2.41686800	0.45952900	O	6.45023100	0.72912800	0.20333000
H	-15.83811500	3.50077700	0.65981500	N	5.62463700	-1.73811900	-0.33129100
H	-16.69645100	2.00186400	1.09860600	H	5.48458200	-0.73407900	-0.05939000
H	-16.21102200	2.28943600	-0.59184500				

S₁; **DK*** E= -1914.029747 hartree (Using PBE)



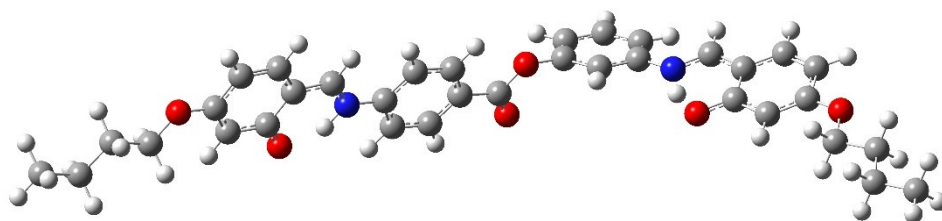
O	0.17365600	-3.90850600	1.45989500	H	3.13777500	-1.10887500	0.00739000
C	-1.38350000	-2.35472400	0.47282800	C	4.55175000	-2.73787500	-0.33014400
C	-2.50005700	-2.77784500	1.26420600	C	4.72738700	-4.11848600	-0.54070000
H	-2.35004900	-3.57324500	1.99947700	H	5.71603600	-4.56402700	-0.66727700
C	-3.74631100	-2.19868400	1.11143000	C	3.58898800	-4.93037500	-0.59115700
H	-4.58766200	-2.53467600	1.72642500	H	3.70526800	-6.00424000	-0.75900000
C	-3.96341200	-1.15533500	0.15708500	C	2.30007500	-4.39541100	-0.43831900
C	-2.85170200	-0.73060800	-0.63887800	H	1.42344600	-5.04222800	-0.48822700
H	-2.97706500	0.06212100	-1.38070200	O	10.96183500	1.84227700	0.01200100
C	-1.60440400	-1.31507300	-0.47989600	C	7.90668600	-1.02761300	-0.26161100
H	-0.77136400	-0.97240900	-1.09890400	C	8.56846000	1.37680500	0.05035700
C	-0.10866300	-2.99132200	0.68055100	H	8.24995200	2.40708400	0.21081300
O	-10.97979300	2.25144000	-0.68538900	C	9.90935300	1.00762400	-0.06174000
C	-7.01145000	0.81330600	-0.71836300	C	10.25584400	-0.36506000	-0.27450200
C	-7.95746400	0.20661800	0.22514400	H	11.31329800	-0.62428500	-0.35915400
C	-9.30104500	0.70385700	0.22665400	C	9.26866600	-1.35060500	-0.37141800
H	-9.99211500	0.24318100	0.93604600	H	9.56897900	-2.38948800	-0.53356900
C	-9.70280400	1.72738700	-0.63849200	C	6.93046900	-2.06717400	-0.36063500
C	-8.78551500	2.31014200	-1.55369500	H	7.26639200	-3.09606300	-0.52196500
H	-9.12740500	3.10765300	-2.21853100	C	10.71266800	3.26154700	0.23097600
C	-7.47383200	1.85139500	-1.57905200	H	10.15812600	3.37960900	1.18002800
H	-6.76234200	2.30007200	-2.28302400	H	10.08828400	3.64143700	-0.59844100
C	-5.65846300	0.38150400	-0.77590300	C	12.05851000	3.96739900	0.28215500
H	-4.95673700	0.83944300	-1.47833500	H	12.66576600	3.52732900	1.09389100
C	-11.96096400	1.71507600	0.21793000	H	12.59845100	3.78349100	-0.66439700
H	-11.61809500	1.84842100	1.26325300	C	11.90174500	5.47999300	0.50872100
H	-12.08215800	0.62878000	0.03550800	H	11.34810700	5.65530700	1.45018100
C	-13.27434800	2.45214300	-0.01726800	H	11.28271500	5.91085500	-0.30045600
H	-13.11268200	3.53448500	0.14237400	C	13.25088500	6.20765200	0.56470300
H	-13.57362800	2.32588300	-1.07442900	H	13.87844600	5.82082000	1.38597300
C	-14.39759000	1.95286800	0.90431100	H	13.11321900	7.28892100	0.72778100
H	-14.08579500	2.07016000	1.95952600	H	13.81301100	6.07822600	-0.37618200
H	-14.54703300	0.86793200	0.74621100	O	6.30001100	0.71907500	0.05830100
C	-15.72391900	2.69006500	0.67813800	C	7.52281000	0.38713100	-0.04356700
H	-15.61375500	3.77304000	0.86215900	N	5.63817500	-1.82952900	-0.26131000
H	-16.51292100	2.31386500	1.35043700	H	5.43575000	-0.81052200	-0.10570900
H	-16.07801400	2.56299400	-0.35978500	O	-7.58858100	-0.74960500	1.03353400
O	0.92049500	-2.39635700	-0.13670600	N	-5.21703400	-0.61064800	0.04913200
C	2.14239000	-3.01244600	-0.22142400	H	-6.03569700	-0.93614800	0.66069700
C	3.27084700	-2.18058400	-0.16474400				

S₀; DE to MK-C, TS, E= -1914.089164 hartree (PBE)



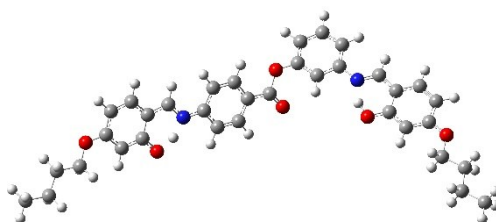
O	-0.22501000	2.86454200	2.33498400	C	-3.13467400	2.13437200	0.17283100
C	1.43045100	1.95778600	0.83729500	H	-2.95591100	1.07238100	-0.01424000
C	2.41600900	1.86132700	1.84390400	C	-4.45665500	2.62819100	0.24610200
H	2.16660000	2.17480200	2.86107400	C	-4.66443700	4.00290200	0.50832700
C	3.68764000	1.37597100	1.54529300	H	-5.68006800	4.39051500	0.62618500
H	4.45193800	1.30734000	2.32472700	C	-3.56788500	4.86273700	0.65837900
C	4.01238100	0.97847600	0.22565300	H	-3.73852600	5.92279400	0.86831200
C	3.01923900	1.05771100	-0.78094900	C	-2.25267800	4.38330800	0.55811100
H	3.23045100	0.71746500	-1.79798600	H	-1.39487300	5.04901900	0.67588600
C	1.74796000	1.54620900	-0.47649200	O	-6.42097500	-0.63996400	0.54332200
H	0.98752200	1.60007300	-1.25893700	H	-5.78999700	0.18295400	0.48262500
C	0.09604800	2.48496900	1.21423600	O	-10.97738200	-1.55594100	-0.71536400
O	11.05353300	-1.76405200	-1.51488600	C	-7.75358000	1.10415800	-0.47073100
C	7.19403300	-0.18567000	-1.26164500	C	-7.59256000	-0.23683500	0.01626400
C	7.86462600	-0.57062300	-0.02800200	C	-8.65968900	-1.15329900	-0.05317600
C	9.17681600	-1.10745700	-0.10045600	H	-8.49638800	-2.16222700	0.32839000
H	9.66225500	-1.38982300	0.83492700	C	-9.88647300	-0.74813100	-0.60488800
C	9.80249000	-1.25825600	-1.34325700	C	-10.06347800	0.57453200	-1.09665600
C	9.14855100	-0.87793100	-2.55765400	H	-11.03036000	0.85606100	-1.52027900
H	9.67822400	-1.01365700	-3.50343000	C	-9.00915000	1.47131800	-1.02572800
C	7.87346500	-0.35253100	-2.50423100	H	-9.13802400	2.49217700	-1.40141100
H	7.36385600	-0.05792100	-3.42805400	C	-6.66859100	2.04547200	-0.39853900
C	5.88589300	0.35749100	-1.19127800	H	-6.84617800	3.06237500	-0.79284800
H	5.37337000	0.67048600	-2.11258200	C	-10.88460200	-2.91683700	-0.23281200
C	11.80077000	-2.17942600	-0.34643900	H	-10.63159000	-2.90458000	0.84456900
H	11.23252900	-2.96510700	0.18674900	H	-10.07600900	-3.44204000	-0.77625200
H	11.92276600	-1.31409600	0.33241300	C	-12.22927900	-3.59073500	-0.47030800
C	13.15129000	-2.70286000	-0.81562300	H	-13.01614600	-3.01860400	0.05471900
H	12.98837100	-3.53811300	-1.52127100	H	-12.46674300	-3.54995700	-1.54923800
H	13.67242500	-1.90465100	-1.37546800	C	-12.23701800	-5.05030000	0.01064300
C	14.02627400	-3.17397500	0.35665300	H	-11.98615300	-5.08349900	1.08768700
H	13.49250300	-3.96290800	0.91945600	H	-11.43928600	-5.61290400	-0.51011800
H	14.17474000	-2.33626500	1.06394100	C	-13.58630700	-5.74227200	-0.22180400
C	15.39059800	-3.70559500	-0.10080500	H	-14.39862300	-5.22130100	0.31404400
H	15.27451800	-4.56590100	-0.78256000	H	-13.56660500	-6.78642600	0.13143800
H	15.99914600	-4.03646200	0.75686100	H	-13.84797900	-5.75494700	-1.29407600
H	15.96112300	-2.92824900	-0.63803000	O	7.25525900	-0.41427500	1.12857100
O	-0.77012500	2.49277100	0.13453800	N	5.30713400	0.50184000	-0.00264800
N	-5.50275100	1.70025100	0.09774600	H	6.15715500	0.08700000	0.81037100
C	-2.06181100	3.01491300	0.32062300				

S₀; **MK-C to DK**, TS, E= -1914.088816 hartree (PBE)



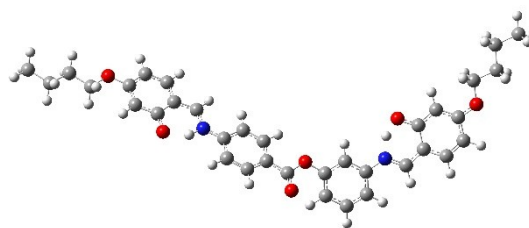
O	-0.26743800	2.97933000	2.39466000	H	-2.99477800	1.24145200	-0.04794800
C	1.38266800	2.00577800	0.93400900	C	-4.46744100	2.82935300	0.20738100
C	2.35105600	1.89395000	1.95549100	C	-4.65200400	4.20392900	0.47900100
H	2.09894700	2.22939800	2.96479600	H	-5.65781400	4.62169200	0.57018200
C	3.61012800	1.36423300	1.68352300	C	-3.53861500	5.03363700	0.66463800
H	4.35608100	1.28042600	2.47944200	H	-3.68971700	6.09581500	0.87773100
C	3.93484500	0.93118000	0.37577500	C	-2.23264900	4.52372900	0.59649800
C	2.96772500	1.03790400	-0.65061300	H	-1.36350400	5.16826100	0.74328200
H	3.18703100	0.70492300	-1.66755700	O	-10.68705700	-1.71846000	-0.73651400
C	1.70884500	1.57011500	-0.36945400	C	-7.75606500	1.24442000	-0.42520000
H	0.96742200	1.64795900	-1.16771400	C	-8.36018700	-1.14952400	-0.26343000
C	0.06045900	2.57798600	1.28381600	H	-8.05351000	-2.17666600	-0.05957400
O	10.94460200	-2.07909400	-1.33166700	C	-9.67330800	-0.81658000	-0.61611500
C	7.06993200	-0.53712200	-1.01286200	C	-10.05153100	0.53573900	-0.88269600
C	7.88740100	-0.59198500	0.21533600	H	-11.08799500	0.74748600	-1.15557200
C	9.21564900	-1.12293200	0.09729100	C	-9.10270900	1.53536800	-0.78738000
H	9.81459700	-1.16173100	1.00866300	H	-9.38269600	2.57542400	-0.98787000
C	9.70183100	-1.56319800	-1.13082900	C	-6.77009800	2.26258700	-0.32030000
C	8.89947500	-1.50425300	-2.32309700	H	-7.03873200	3.30883100	-0.52851500
H	9.32973000	-1.86278100	-3.26111700	C	-10.40631600	-3.11413300	-0.47883500
C	7.62196400	-1.00318300	-2.25178700	H	-10.02679700	-3.22368000	0.55494600
H	7.00250800	-0.95491900	-3.15424500	H	-9.62188700	-3.46255900	-1.17745200
C	5.76168700	-0.03387500	-0.97534200	C	-11.69849200	-3.89584500	-0.67283600
H	5.16440100	0.00426600	-1.89299200	H	-12.46851000	-3.49358400	0.01087100
C	11.83881600	-2.18876600	-0.19843100	H	-12.06618000	-3.73446000	-1.70286100
H	11.36862800	-2.82850100	0.57232100	C	-11.50845400	-5.39917100	-0.41677000
H	12.00019800	-1.18293400	0.23364200	H	-11.12948800	-5.55144000	0.61146400
C	13.14750300	-2.79213400	-0.68962500	H	-10.72750600	-5.79149800	-1.09522700
H	12.94058500	-3.77601400	-1.14935800	C	-12.80283500	-6.19977800	-0.60895500
H	13.56636000	-2.14681800	-1.48353000	H	-13.59204700	-5.85213300	0.08003300
C	14.17082600	-2.95243500	0.44570600	H	-12.64108600	-7.27379100	-0.41979300
H	13.73966000	-3.58878500	1.24145100	H	-13.18759600	-6.09377400	-1.63810600
H	14.36312900	-1.96621000	0.90875600	O	-6.12938900	-0.42074200	0.16458100
C	15.49547400	-3.55967200	-0.03379600	C	-7.37343800	-0.13327900	-0.16078400
H	15.33930800	-4.56091600	-0.47143200	N	-5.52865000	1.93081400	0.00992200
H	16.21171100	-3.66459200	0.79771600	H	-5.56082400	0.69639100	0.14653700
H	15.96702900	-2.92745300	-0.80603400	O	7.42181200	-0.17843300	1.34254700
O	-0.78832100	2.59876400	0.18917400	N	5.21600900	0.41048600	0.16957800
C	-2.06804200	3.15422700	0.34777800	H	5.92165000	0.31318500	0.96603600
C	-3.15770400	2.30311100	0.15499200				

S₁; DE* to MK-C*, TS, E= -1914.019221 hartree (PBE)



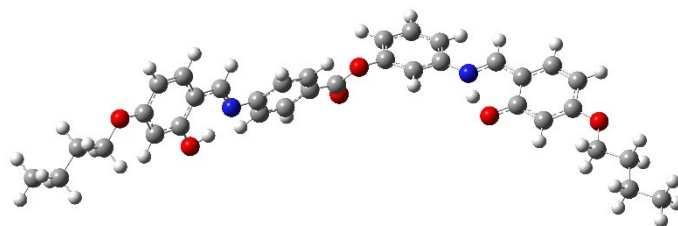
O	1.23725900	-1.84760300	1.90052200	O	0.91895400	-3.34037900	0.14900000
N	-4.90753600	-0.68544300	0.20552500	N	5.54275900	-2.03754100	-0.12340000
C	-0.89883900	-1.93392500	0.78431600	C	2.25228200	-3.64383500	0.08202800
C	-1.52106500	-0.95080000	1.62178500	C	3.26441200	-2.67600300	0.04283200
H	-0.93667100	-0.50899800	2.43386900	H	3.02897800	-1.61461500	0.12598500
C	-2.83097500	-0.56101500	1.41467400	C	4.61624100	-3.07775800	-0.10366300
H	-3.29142800	0.19187500	2.06301400	C	4.95255800	-4.45373800	-0.22825800
C	-3.62117800	-1.12106700	0.35764100	H	5.98833400	-4.77745700	-0.34735600
C	-2.99813600	-2.11002500	-0.47794100	C	3.93045800	-5.40072300	-0.20153700
H	-3.56057400	-2.56836800	-1.29587000	H	4.16950800	-6.46280400	-0.29952300
C	-1.68468200	-2.49835700	-0.26694900	C	2.58903600	-5.00787200	-0.03750400
H	-1.23789300	-3.25261800	-0.92012000	H	1.78809000	-5.75098500	-0.00419800
C	0.47041000	-2.29241700	1.03825300	O	5.80338200	0.46695500	-0.04655800
O	-6.62126500	0.91297800	1.16351100	H	5.39833900	-0.51553400	-0.05477100
H	-5.58754000	0.22727800	0.90881600	O	10.22825200	2.26174900	-0.24693400
O	-11.00485600	1.12327900	-0.88069700	C	7.68852600	-1.03279600	-0.22173800
C	-7.11302600	-0.50902100	-0.73624200	C	7.11140100	0.31574200	-0.13336100
C	-7.48857700	0.50105800	0.23538200	C	7.94202500	1.45011900	-0.13981500
C	-8.79319900	1.05415400	0.19371500	H	7.47488300	2.43240100	-0.07126800
H	-9.03905700	1.81183700	0.94059300	C	9.32604100	1.27422700	-0.23236700
C	-9.71916400	0.63399300	-0.77436400	C	9.90969800	-0.04496300	-0.32154800
C	-9.36578900	-0.35167600	-1.72824600	H	10.99654600	-0.12159400	-0.39152300
H	-10.10360000	-0.66312500	-2.47244100	C	9.09984100	-1.16139000	-0.31438400
C	-8.08688700	-0.90117600	-1.69663800	H	9.54003800	-2.16002000	-0.37957800
H	-7.81190500	-1.66397800	-2.43467200	C	6.84932200	-2.19250000	-0.21197900
C	-5.80354900	-1.08755000	-0.72469000	H	7.33209200	-3.17890000	-0.27439800
H	-5.54442900	-1.84867100	-1.47214700	C	9.77576000	3.64908000	-0.15508300
C	-11.42308200	2.12903900	0.05802600	H	9.20855200	3.76525400	0.78551300
H	-10.75862900	3.01241900	-0.02061900	H	9.10439200	3.85003600	-1.00887000
H	-11.34335400	1.73273600	1.08984100	C	11.00579500	4.54136600	-0.18271300
C	-12.86385400	2.50737400	-0.26462200	H	11.67360000	4.26098700	0.65181900
H	-12.91543900	2.86871700	-1.30852200	H	11.56226300	4.36230900	-1.12041100
H	-13.49451900	1.60076800	-0.20811400	C	10.62974500	6.02840500	-0.07325600
C	-13.41201200	3.58271500	0.68589300	H	10.06394900	6.19630800	0.86223200
H	-12.76959900	4.48207800	0.63206700	H	9.94792900	6.29766900	-0.90148700
H	-13.34596200	3.21893400	1.72883100	C	11.85809900	6.94653900	-0.10124200
C	-14.86242900	3.97085700	0.37067300	H	12.54196400	6.72297500	0.73557500
H	-14.95386000	4.36982300	-0.65463000	H	11.56404300	8.00562500	-0.02112800
H	-15.23206800	4.74309900	1.06564400	H	12.42552000	6.82493400	-1.03992100
H	-15.53410400	3.09829900	0.44967800				

S₁; **MK-C*** to **DK***, TS, E= -1914.020770 hartree (PBE)



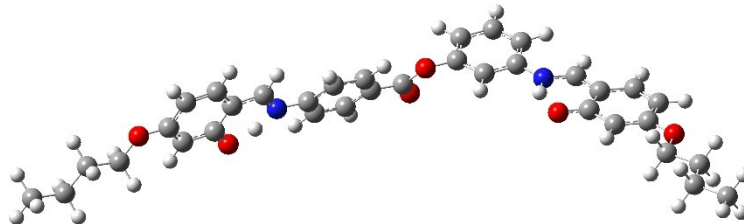
O	0.23222700	-3.80400800	1.42969800	C	3.31634400	-2.09540700	-0.19122300
C	-1.34344200	-2.23883700	0.49022100	H	3.22712600	-1.03113500	0.04080900
C	-2.45229700	-2.68727900	1.27827300	C	4.58694900	-2.67836500	-0.39920000
H	-2.29099000	-3.49228100	2.00061800	C	4.70853200	-4.05857600	-0.69399000
C	-3.70603800	-2.12181600	1.13667300	H	5.68183300	-4.51624700	-0.88326900
H	-4.54186600	-2.47808100	1.74774200	C	3.54904800	-4.83186100	-0.77099500
C	-3.93893500	-1.06818800	0.19696700	H	3.62461400	-5.89599400	-1.00920000
C	-2.83307200	-0.61443700	-0.59150300	C	2.27977000	-4.26363500	-0.56365100
H	-2.96956000	0.18870500	-1.31996300	H	1.38175900	-4.87821600	-0.64069400
C	-1.57831500	-1.18566900	-0.44377200	O	6.29865200	0.64478900	-0.12768800
H	-0.75052700	-0.82253000	-1.05818800	H	5.68287000	-0.44902200	-0.20784600
C	-0.06273200	-2.87049700	0.67501800	O	10.94056800	1.77334700	0.11775700
O	-11.02271600	2.19142600	-0.66817500	C	7.94574100	-1.11605900	-0.17427100
C	-7.01954800	0.85095700	-0.67276500	C	7.55635100	0.30882900	-0.10206500
C	-7.96081500	0.21130700	0.25405800	C	8.55673000	1.30983400	-0.00146200
C	-9.31586400	0.67601000	0.24624700	H	8.23029000	2.34838800	0.05053100
H	-10.00326100	0.19079200	0.94272100	C	9.89743100	0.93569300	0.02586000
C	-9.73335600	1.69920300	-0.61197000	C	10.28115700	-0.45572600	-0.04499700
C	-8.82058500	2.31485400	-1.50984600	H	11.34603400	-0.69555500	-0.01850800
H	-9.17456300	3.11127800	-2.16966500	C	9.31806900	-1.44694800	-0.14140500
C	-7.49793900	1.88806700	-1.52613400	H	9.61874400	-2.49664700	-0.19272600
H	-6.79030800	2.36136800	-2.21777500	C	6.95440600	-2.14876400	-0.26850400
C	-5.65717900	0.44990700	-0.72390200	H	7.28344700	-3.19609000	-0.30442100
H	-4.96022600	0.93046000	-1.41574600	C	10.68862600	3.20849800	0.20456600
C	-12.00198000	1.61504000	0.21218800	H	10.06494500	3.39778900	1.09692500
H	-11.67910200	1.74265500	1.26458200	H	10.12910400	3.51809600	-0.69663400
H	-12.08980500	0.52851100	0.01257100	C	12.03272000	3.91218100	0.29976300
C	-13.33182500	2.31849700	-0.03328400	H	12.57677200	3.53354500	1.18393500
H	-13.20368400	3.40234100	0.14541400	H	12.63766700	3.65707900	-0.58910400
H	-13.61024400	2.20039000	-1.09706900	C	11.86989200	5.43782200	0.40060400
C	-14.45516700	1.77333700	0.86175800	H	11.25273600	5.68406700	1.28492000
H	-14.16448700	1.88371400	1.92372300	H	11.31205700	5.80705300	-0.48026200
H	-14.57033300	0.68703700	0.68539200	C	13.21664200	6.16562900	0.49683500
C	-15.79842300	2.47529600	0.62366800	H	13.78245600	5.84064800	1.38686700
H	-15.72277600	3.55817400	0.82486500	H	13.07477900	7.25619000	0.56858500
H	-16.58720200	2.06671200	1.27706100	H	13.84234900	5.96538600	-0.38991500
H	-16.13143200	2.35334700	-0.42182400	O	-7.57773100	-0.74541500	1.05540400
O	0.95821600	-2.25232000	-0.13469600	N	-5.20070400	-0.54370800	0.09304300
N	5.68259400	-1.81567000	-0.29448500	H	-6.01640300	-0.89336500	0.69459200
C	2.16580900	-2.88814400	-0.26898600				

S₀; DE to MK-O, TS, E= -1914.089192 hartree (PBE)



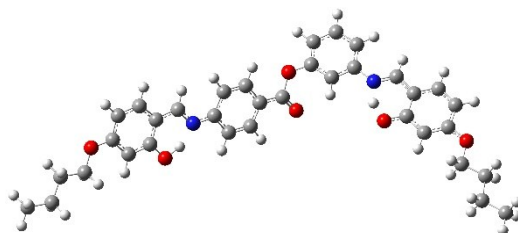
O	-0.28397900	3.14195500	2.47809300	O	-0.78537100	2.72305900	0.27536100
N	5.27753700	0.67369000	0.30864700	C	-2.07935800	3.24613700	0.42125200
C	1.39882900	2.19616200	1.03482000	C	-3.14482900	2.36772700	0.21497900
C	2.36306200	2.11675000	2.06435300	H	-2.95222500	1.31106100	0.01194200
H	2.09376400	2.45606400	3.06817800	C	-4.46812000	2.85993100	0.25321000
C	3.63480500	1.60930400	1.80487900	C	-4.69156900	4.22859300	0.52529600
H	4.38310100	1.54454000	2.59998900	H	-5.70903300	4.61946700	0.60657200
C	3.98787200	1.18357300	0.50097200	C	-3.60200600	5.08635700	0.72484200
C	3.01292700	1.24556900	-0.52648000	H	-3.78284500	6.14382700	0.93830200
H	3.24662700	0.86746000	-1.52580000	C	-2.28262200	4.61056200	0.67035200
C	1.73785300	1.74881600	-0.26162100	H	-1.43226600	5.27719800	0.82795800
H	0.99178500	1.78423700	-1.05899300	O	-10.56335500	-1.83706500	-0.76940700
C	0.06017700	2.73644200	1.37358000	C	-7.70694100	1.19460700	-0.42759100
O	7.23160900	-0.69842500	1.21399000	C	-7.29769400	-0.17199700	-0.14619100
H	6.33412500	-0.18294100	1.13952500	C	-8.25906200	-1.21135600	-0.25870600
O	10.94124200	-1.55531000	-1.72870500	H	-7.93273500	-2.22968600	-0.04159000
C	7.18591400	0.16064900	-1.04660400	C	-9.57275300	-0.91123900	-0.63761200
C	7.82572200	-0.56859800	0.01372100	C	-9.97681100	0.43001500	-0.92143400
C	9.08952800	-1.15570100	-0.18683800	H	-11.01262300	0.61595600	-1.21487700
H	9.54118600	-1.70005300	0.64369900	C	-9.05293900	1.45188100	-0.81648600
C	9.72396300	-1.02515100	-1.43340100	H	-9.35282700	2.48373100	-1.03016900
C	9.10759700	-0.30447300	-2.49473600	C	-6.74649800	2.23591300	-0.31208600
H	9.63037400	-0.22230000	-3.45045200	H	-7.03481600	3.27452600	-0.53196100
C	7.86565400	0.27303600	-2.29092000	C	-10.25575800	-3.22407500	-0.49636900
H	7.38529000	0.82943500	-3.10286000	H	-9.89234200	-3.31779000	0.54473200
C	5.89850300	0.76315500	-0.84782000	H	-9.45134300	-3.55957300	-1.17840000
H	5.45943000	1.32568200	-1.69112700	C	-11.52636600	-4.03623700	-0.70731000
C	11.64102800	-2.30362500	-0.70565200	H	-12.31719300	-3.64693200	-0.04005300
H	11.01752000	-3.16306800	-0.39382000	H	-11.87935300	-3.89019300	-1.74473700
H	11.80471000	-1.65168900	0.17339500	C	-11.30692600	-5.53305700	-0.43718100
C	12.96522100	-2.77249900	-1.29284600	H	-10.94233900	-5.66962700	0.59843000
H	12.76386300	-3.38841200	-2.18848400	H	-10.50579700	-5.91216500	-1.09940700
H	13.54105300	-1.89121900	-1.63026500	C	-12.57940000	-6.36416900	-0.64552900
C	13.79294300	-3.57952500	-0.28018900	H	-13.38796300	-6.02983700	0.02743000
H	13.20536400	-4.45210000	0.06247600	H	-12.39667300	-7.43291100	-0.44588700
H	13.97990200	-2.96065100	0.61765300	H	-12.94877300	-6.27399700	-1.68180500
C	15.13046400	-4.05861000	-0.85888400	O	-6.05345400	-0.42858200	0.20323200
H	14.97455600	-4.70777500	-1.73788000	N	-5.50395000	1.93501300	0.04220600
H	15.70533400	-4.63366900	-0.11443400	H	-5.50995900	0.70142900	0.18673600
H	15.75383400	-3.20603900	-1.17966600				

S₀; **MK-O to DK**, TS, E= -1914.088727 hartree (PBE)



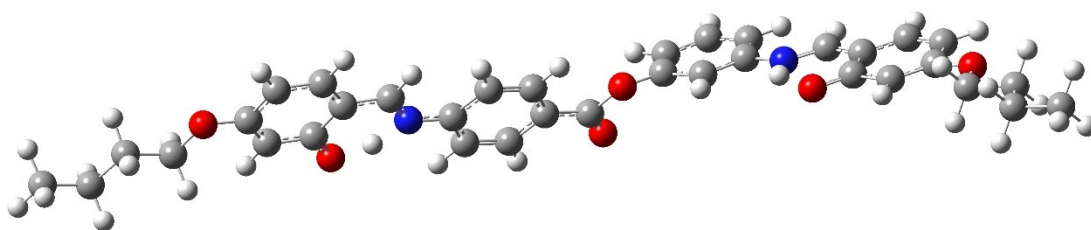
O -0.16774200	3.43043100	2.10090600	H -2.99353400	1.31997300	-0.02855000
C 1.40511200	2.26267400	0.69674500	C -4.49121700	2.90176600	0.12446800
C 2.43770500	2.30951700	1.65906400	C -4.69766600	4.29132900	0.25899300
H 2.24395700	2.79072700	2.62135800	H -5.70534200	4.71211600	0.28177700
C 3.68497100	1.75136900	1.38630800	C -3.59330000	5.14893500	0.34613200
H 4.48540400	1.79273600	2.13059300	H -3.75987500	6.22519300	0.44622100
C 3.93739800	1.13321500	0.13744200	C -2.27972400	4.65769500	0.29570300
C 2.89752400	1.07199000	-0.82228700	H -1.42092700	5.32876000	0.35601700
H 3.05199600	0.56505100	-1.77813600	O -10.70575100	-1.82570800	-0.38292700
C 1.65127300	1.63443200	-0.54486100	C -7.78555000	1.14296300	0.02219100
H 0.85464700	1.57745500	-1.29008600	C -8.33987000	-1.23270700	-0.44141700
C 0.09829800	2.87025300	1.04374600	H -7.99757100	-2.24051500	-0.68269400
O 10.80700600	-2.10085700	-1.43331300	C -9.68800200	-0.92711700	-0.26947700
C 7.00983200	-0.36776300	-1.27484300	C -10.12127800	0.40409200	0.05182200
C 7.73756700	-0.55055700	-0.02706600	H -11.19020200	0.59174000	0.17756200
C 9.02966400	-1.13705400	-0.06731000	C -9.18412000	1.40157400	0.19162400
H 9.55858100	-1.26540200	0.87830000	H -9.50405300	2.42062000	0.43651300
C 9.58137800	-1.52806900	-1.29272600	C -6.85465900	2.18548500	0.17236400
C 8.87157700	-1.34594900	-2.52177300	H -7.20074700	3.19495200	0.42192700
H 9.34483000	-1.66584600	-3.45299700	C -10.38101800	-3.19789900	-0.70614000
C 7.61530700	-0.77529500	-2.50004200	H -9.71235200	-3.60622900	0.07549100
H 7.06277100	-0.63169600	-3.43496700	H -9.84366500	-3.22518200	-1.67322700
C 5.71984900	0.21931500	-1.23768900	C -11.68285000	-3.98423800	-0.78018400
H 5.16472500	0.37710200	-2.17373300	H -12.20846300	-3.90368700	0.18908200
C 11.60595400	-2.33094600	-0.24798400	H -12.33885000	-3.52381400	-1.54173000
H 11.04599700	-2.98762300	0.44450400	C -11.44530900	-5.46342300	-1.12278300
H 11.79011800	-1.36427300	0.25798600	H -10.77904700	-5.91397400	-0.36305700
C 12.91281300	-2.98033100	-0.68197200	H -10.90741200	-5.53516200	-2.08696600
H 12.68719300	-3.92052200	-1.21793300	C -12.74858000	-6.26871700	-1.20262500
H 13.42517700	-2.31446900	-1.40046300	H -13.29188300	-6.24326100	-0.24210100
C 13.83698000	-3.26946000	0.51146800	H -12.55199800	-7.32510900	-1.44935000
H 13.31229300	-3.92516600	1.23176800	H -13.42121700	-5.86194700	-1.97758000
H 14.04831500	-2.32604600	1.04938000	O -6.07916300	-0.48669500	-0.45861500
C 15.15807100	-3.92564500	0.09029100	C -7.33180800	-0.22023300	-0.30464400
H 14.97971100	-4.88804200	-0.41996000	N -5.54003000	1.97216900	0.02604300
H 15.80304600	-4.12235900	0.96247100	H -5.36599800	0.94038300	-0.19586700
H 15.72046700	-3.27829600	-0.60469800	O 7.19648700	-0.17095300	1.11153500
O -0.81811000	2.71882800	0.01400000	N 5.20948200	0.59000100	-0.06654800
C -2.09626800	3.27465900	0.16066800	H 6.09394700	0.29971500	0.76418200
C -3.17564200	2.39306600	0.07464500			

S₁; **DE*** to **MK-O***, TS, E= -1914.019301 hartree (PBE)



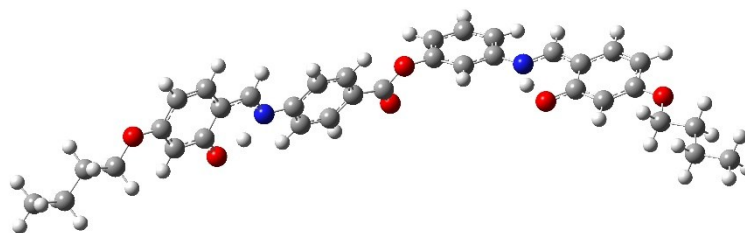
O	1.27952900	-1.77989700	1.87937300	O	0.92373200	-3.31034200	0.16486000
N	-4.88643200	-0.59458800	0.25241700	N	5.58080400	-2.10013500	-0.13534200
C	-0.87045400	-1.86901000	0.78888600	C	2.24998500	-3.63668500	0.09066900
C	-1.47565200	-0.86202900	1.61186100	C	3.28035200	-2.68464000	0.04384800
H	-0.87722900	-0.40620200	2.40592100	H	3.05944600	-1.62000500	0.12712900
C	-2.78605400	-0.46979900	1.41228200	C	4.61757500	-3.11617500	-0.10856000
H	-3.23499700	0.30049600	2.04849600	C	4.93459100	-4.49108200	-0.23166600
C	-3.60054600	-1.04522900	0.38058800	H	5.96478800	-4.83128000	-0.35405300
C	-2.98953300	-2.05751100	-0.44006400	C	3.89451100	-5.42092600	-0.19696000
H	-3.56331000	-2.53331000	-1.24022400	H	4.11661400	-6.48687400	-0.29311500
C	-1.67627700	-2.45070000	-0.23908900	C	2.56221100	-5.00560600	-0.02770600
H	-1.24357800	-3.22301700	-0.88083800	H	1.74863100	-5.73456400	0.01122500
C	0.49634300	-2.23514800	1.03553200	O	5.82340900	0.42201800	-0.04062300
O	-6.63078300	0.98320800	1.16033900	H	5.38010000	-0.76009300	-0.05862700
H	-5.73857500	0.42893200	0.97772100	O	10.23430200	2.26091500	-0.25813300
O	-11.01901100	1.07016500	-0.88524200	C	7.71070900	-1.06309300	-0.24037700
C	-7.09455700	-0.48559100	-0.70619200	C	7.11312300	0.28606800	-0.13624500
C	-7.50230000	0.53013300	0.22920500	C	7.95119300	1.43227000	-0.14064500
C	-8.80552600	1.06445000	0.18975000	H	7.47285500	2.40839600	-0.06055600
H	-9.06267200	1.83195600	0.92227600	C	9.32950800	1.27025700	-0.24396500
C	-9.72534800	0.60679500	-0.77092900	C	9.91528700	-0.04635600	-0.34772000
C	-9.34893300	-0.38999300	-1.70125200	H	11.00197500	-0.11856000	-0.42679900
H	-10.07888700	-0.73208600	-2.43984500	C	9.11342700	-1.17740900	-0.34406200
C	-8.05891100	-0.91558000	-1.65852500	H	9.56892400	-2.16840600	-0.42139800
H	-7.76961600	-1.68826500	-2.38017400	C	6.88417100	-2.23684400	-0.23370700
C	-5.76609900	-1.03335800	-0.66776700	H	7.36393000	-3.22182900	-0.30668900
H	-5.50456600	-1.80737400	-1.40510900	C	9.76967600	3.64034000	-0.15345500
C	-11.45578300	2.08476900	0.03582800	H	9.20716600	3.74689300	0.79174600
H	-10.80966100	2.97990600	-0.06097700	H	9.08925400	3.84292300	-1.00037300
H	-11.36648200	1.70909300	1.07457500	C	10.98991300	4.54647000	-0.18381000
C	-12.90444900	2.42778000	-0.29053300	H	11.66597700	4.26847100	0.64496700
H	-12.96508100	2.76952900	-1.34048300	H	11.54259700	4.37755900	-1.12572800
H	-13.51620300	1.50957400	-0.21669800	C	10.60081900	6.02926000	-0.06473400
C	-13.47265200	3.50827300	0.64223300	H	10.03846700	6.18724600	0.87457200
H	-12.84871200	4.41938200	0.57148900	H	9.91195200	6.29623800	-0.88788400
H	-13.39762200	3.16404200	1.69117700	C	11.82010000	6.95940100	-0.09468000
C	-14.93112800	3.86134500	0.32305400	H	12.51062300	6.73830300	0.73735300
H	-15.03220400	4.24070800	-0.70874300	H	11.51660400	8.01532900	-0.00782300
H	-15.31523200	4.63775500	1.00538800	H	12.38373400	6.84773300	-1.03691000
H	-15.58479100	2.97683500	0.41833800				

S₁; **MK-O*** to **DK***, TS, E= -1914.025220 hartree (PBE)



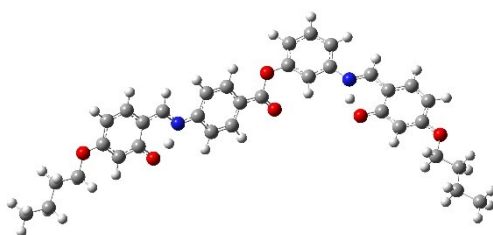
O	0.14683300	-3.70759600	1.56583200	O	0.89979300	-2.12816900	0.03625400
N	-5.29212800	-0.48476700	0.13755900	C	2.08531300	-2.78531500	-0.15134100
C	-1.41833700	-2.14251000	0.60659700	C	3.25293700	-2.00737600	-0.10079900
C	-2.54321100	-2.60042800	1.36914600	H	3.17773600	-0.94493400	0.14780600
H	-2.39167000	-3.40691600	2.09221900	C	4.49641300	-2.60457600	-0.37534900
C	-3.79657000	-2.04243800	1.19959900	C	4.59968800	-3.97357600	-0.68634100
H	-4.64564900	-2.40492900	1.78857300	H	5.55948600	-4.45023100	-0.89504600
C	-4.02511900	-0.98611600	0.25844400	C	3.42483200	-4.73236800	-0.72608800
C	-2.89698200	-0.52409100	-0.50134300	H	3.48361900	-5.79647200	-0.96941700
H	-3.02119900	0.28129200	-1.23031100	C	2.17147400	-4.15635000	-0.46705200
C	-1.64192600	-1.08529500	-0.32911500	H	1.26585500	-4.76270700	-0.51025800
H	-0.80253400	-0.71451900	-0.92338600	O	11.14526500	1.63087200	-0.10948000
C	-0.14157900	-2.76754000	0.81440100	C	7.92914400	-1.05391500	-0.40894000
O	-7.64522700	-0.71498000	1.04577300	C	7.63889300	0.34779800	-0.02610100
H	-6.41036400	-0.82627500	0.79306300	C	8.74027800	1.27408400	0.07793000
O	-11.11042300	2.16606700	-0.72229200	H	8.49092200	2.29686700	0.36160100
C	-7.08508100	0.89440000	-0.67674100	C	10.04691800	0.85674300	-0.17780100
C	-8.03298500	0.25827000	0.21782600	C	10.30203300	-0.50153300	-0.55121800
C	-9.38670000	0.67960300	0.20891300	H	11.33435100	-0.79820400	-0.74845600
H	-10.07114300	0.17878800	0.89670800	C	9.25925400	-1.42656600	-0.66172500
C	-9.81368900	1.70033500	-0.65499300	H	9.49021300	-2.45611000	-0.95050000
C	-8.89863300	2.32798200	-1.53548000	C	6.89435900	-2.03285600	-0.52571600
H	-9.25427500	3.11992400	-2.19988700	H	7.16354300	-3.05651000	-0.80171200
C	-7.56676600	1.92217500	-1.53396100	C	10.99005300	3.03081600	0.26479200
H	-6.85694400	2.40719900	-2.21450100	H	10.51531100	3.07855600	1.26197200
C	-5.70885700	0.49618200	-0.69142800	H	10.32646200	3.52081400	-0.47128600
H	-5.01181100	0.99564500	-1.37731900	C	12.37239600	3.66451100	0.27594500
C	-12.08705900	1.57121400	0.14986800	H	13.01445700	3.11568400	0.98859300
H	-11.77515300	1.70405400	1.20490400	H	12.82819600	3.55292000	-0.72461900
H	-12.15467100	0.48369200	-0.05214400	C	12.31678900	5.15173500	0.66160900
C	-13.42663500	2.25170300	-0.10620000	H	11.84690600	5.25624600	1.65752800
H	-13.31901100	3.33718400	0.07564600	H	11.66283000	5.69176100	-0.04850200
H	-13.69331300	2.13060800	-1.17259000	C	13.70429400	5.80561600	0.67905900
C	-14.54782000	1.68481200	0.77806100	H	14.37040000	5.30781600	1.40465700
H	-14.26842200	1.79810900	1.84273000	H	13.63894800	6.86979300	0.95827100
H	-14.64236000	0.59706600	0.59845300	H	14.18534500	5.74696000	-0.31247600
C	-15.90102500	2.36362700	0.52954000	O	6.44659800	0.72305400	0.20451200
H	-15.84624000	3.44717300	0.73372800	N	5.62607600	-1.74977300	-0.30901000
H	-16.68803200	1.93966600	1.17517200	H	5.48399900	-0.74287500	-0.04878600
H	-16.22268200	2.23811700	-0.51905200				

S₀; **DE to DK**, TS, E=-1914.080641 hartree (PBE)



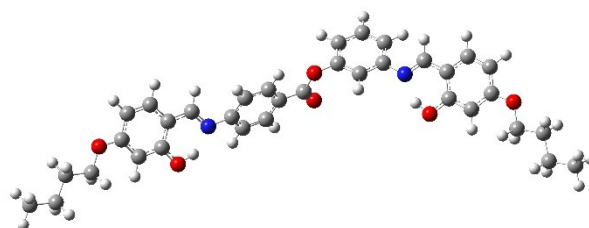
O	0.42393400	-3.51857400	1.86340100	O	0.92738100	-2.70571900	-0.22572900
N	-5.15109500	-0.75834200	0.14445300	N	5.63604300	-1.84071300	-0.19853800
C	-1.26282200	-2.34230400	0.60675200	C	2.22629400	-3.23446900	-0.16585200
C	-2.23172400	-2.45742100	1.62751900	C	3.28399600	-2.32349600	-0.16529400
H	-1.96540500	-2.96987400	2.55571200	H	3.08134300	-1.24944500	-0.14907900
C	-3.50817300	-1.92627900	1.45450700	C	4.61277900	-2.80110500	-0.19938100
H	-4.25934300	-2.01919200	2.24418900	C	4.84835900	-4.19462300	-0.21302100
C	-3.85473200	-1.26823300	0.24965900	H	5.86729700	-4.58906800	-0.20159100
C	-2.87952800	-1.13987900	-0.76982100	C	3.76596600	-5.08367800	-0.21727300
H	-3.10705500	-0.60447300	-1.69505700	H	3.95671700	-6.16069500	-0.22618100
C	-1.60342200	-1.67496800	-0.59125600	C	2.44149800	-4.61880300	-0.19892100
H	-0.85695900	-1.56656200	-1.38140400	H	1.59680300	-5.31088500	-0.20100900
C	0.07949100	-2.92399000	0.84835400	O	6.12768900	0.58358400	0.26156600
O	-7.24142200	-0.10336500	1.47442000	H	5.55573100	-0.60738000	0.08515900
H	-6.03950200	-0.55756900	1.10178000	O	10.67819700	2.09420700	-0.19954600
O	-10.91434600	1.82345200	-0.96069900	C	7.84692900	-0.97817300	-0.39020500
C	-7.05747000	0.20789900	-0.91785700	C	7.39296200	0.35342900	-0.01058500
C	-7.77920400	0.30520200	0.34514900	C	8.35070400	1.40327500	0.05577400
C	-9.09124600	0.85219600	0.33735300	H	7.99203500	2.39338000	0.34176200
H	-9.61447600	0.91639300	1.29270600	C	9.69481200	1.15250500	-0.23857400
C	-9.66958900	1.28473200	-0.86036000	C	10.14208400	-0.15271500	-0.61363300
C	-8.96688400	1.18609100	-2.10255100	H	11.20126700	-0.30314000	-0.83502500
H	-9.45750700	1.53473100	-3.01420100	C	9.22721000	-1.18398600	-0.68528900
C	-7.69342200	0.65685300	-2.11519700	H	9.55931700	-2.18840900	-0.97061100
H	-7.14500200	0.57776200	-3.06039200	C	6.91808400	-2.04906200	-0.47031100
C	-5.74650100	-0.33091400	-0.96339400	H	7.27000800	-3.04600300	-0.77281400
H	-5.23542100	-0.40510500	-1.93443600	C	10.32585600	3.44812200	0.16925200
C	-11.70524400	1.97332400	0.24281700	H	9.87766500	3.44414200	1.18108100
H	-11.15686600	2.61421600	0.95895900	H	9.57357000	3.83508300	-0.54425600
H	-11.85375000	0.97912000	0.70522600	C	11.59509100	4.28868600	0.13614800
C	-13.03637000	2.60130800	-0.14661300	H	12.33558300	3.85000800	0.82998700
H	-12.84560200	3.57055500	-0.64291300	H	12.03401000	4.23867500	-0.87730900
H	-13.53788500	1.95255000	-0.88804800	C	11.32815400	5.75344100	0.51689700
C	-13.95358000	2.81000700	1.06875500	H	10.87759300	5.79418900	1.52656100
H	-13.43995400	3.45026300	1.81060700	H	10.57755800	6.18159000	-0.17403700
H	-14.12912800	1.83831800	1.56783200	C	12.59869600	6.61266800	0.48843400
C	-15.29939900	3.44222100	0.69147300	H	13.35533700	6.22815900	1.19417800
H	-15.15711000	4.43045500	0.22081100	H	12.38162900	7.65754100	0.76517300
H	-15.93869500	3.58170200	1.57873700	H	13.05296600	6.61868600	-0.51756900
H	-15.85080100	2.80781500	-0.02396000				

S₁; **DE* to DK***, TS, E=-1914.019400 hartree (PBE)



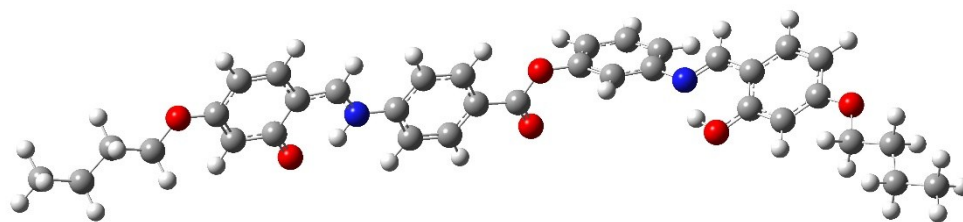
O	1.27589000	-1.79970000	1.84517900	O	0.94868000	-3.33115200	0.12836500
N	-4.87951500	-0.68530600	0.15937400	N	5.60919500	-2.11593400	-0.10972300
C	-0.86434200	-1.91012800	0.73903500	C	2.27754100	-3.65788600	0.08015700
C	-1.48248400	-0.90902600	1.55785100	C	3.30538000	-2.70281100	0.03817500
H	-0.89344600	-0.44838200	2.35594100	H	3.07914100	-1.63806700	0.10491600
C	-2.79456100	-0.52599800	1.35125200	C	4.64465900	-3.13378200	-0.08594200
H	-3.25148800	0.24042200	1.98602900	C	4.96762300	-4.50769200	-0.18648000
C	-3.58976900	-1.11210700	0.31289700	H	6.00056500	-4.84603300	-0.28925300
C	-2.97154600	-2.11744700	-0.50522300	C	3.92935400	-5.44030600	-0.15749600
H	-3.53910800	-2.59440900	-1.30882700	H	4.15624400	-6.50655100	-0.23730700
C	-1.65599300	-2.49891900	-0.29434500	C	2.59345200	-5.02685600	-0.01589100
H	-1.21234800	-3.26677300	-0.93357600	H	1.78100200	-5.75724600	0.01820500
C	0.50578500	-2.26435600	0.99562400	O	5.79812400	0.37194300	-0.07383300
O	-6.56447600	0.91721600	1.11270500	H	5.39435300	-0.84819300	-0.07473200
H	-5.51917200	0.20772300	0.83766500	O	10.16760300	2.32676700	-0.20761400
O	-10.98921900	1.09733500	-0.84800300	C	7.72473700	-1.05880100	-0.17962200
C	-7.09555600	-0.53040500	-0.75286800	C	7.08911400	0.27762700	-0.12774400
C	-7.45030300	0.49564800	0.21282100	C	7.90157500	1.44563700	-0.13671500
C	-8.75805400	1.04661900	0.18580300	H	7.39780600	2.41120500	-0.09570700
H	-8.99111600	1.81526500	0.92561300	C	9.28522300	1.31503700	-0.19398000
C	-9.70090600	0.61110800	-0.75821000	C	9.90366600	0.01076600	-0.24448500
C	-9.36554200	-0.38863600	-1.70468300	H	10.99373900	-0.03735400	-0.28801600
H	-10.11761200	-0.71080600	-2.42976500	C	9.12994900	-1.14222300	-0.23655100
C	-8.08618900	-0.93747400	-1.68935700	H	9.61350100	-2.12217800	-0.27417800
H	-7.82477500	-1.71120700	-2.42099600	C	6.91605900	-2.24472200	-0.16780800
C	-5.78651300	-1.10704900	-0.75292800	H	7.40317000	-3.22745500	-0.20216700
H	-5.53226900	-1.88071200	-1.48813600	C	9.66588600	3.69584300	-0.15899600
C	-11.39142700	2.11618600	0.08348100	H	9.07454900	3.81730700	0.76676200
H	-10.72981500	2.99909900	-0.02030500	H	9.00426400	3.85491600	-1.02984200
H	-11.29192600	1.73514800	1.11933100	C	10.86322100	4.63234900	-0.18571800
C	-12.83850600	2.48801900	-0.21787300	H	11.52026800	4.40236700	0.67254200
H	-12.90993400	2.83430100	-1.26570400	H	11.44875100	4.44402000	-1.10381900
H	-13.46667500	1.58154000	-0.13677200	C	10.43376000	6.10786300	-0.13355600
C	-13.37078700	3.57614000	0.72710200	H	9.83742300	6.28517500	0.78099400
H	-12.73078200	4.47542200	0.64877500	H	9.76564700	6.32704500	-0.98740300
H	-13.28516100	3.22732200	1.77372300	C	11.62981300	7.06788300	-0.15937000
C	-14.82729800	3.95800200	0.43299300	H	12.29800400	6.89559000	0.70191000
H	-14.93802400	4.34231900	-0.59599900	H	11.29734300	8.11797500	-0.12180400
H	-15.18538000	4.73952300	1.12363500	H	12.22669800	6.93665800	-1.07832900
H	-15.49611500	3.08580700	0.53653400				

Fig. S5: S_0 ; DE, $E = -1915.959515$ hartree (mPW1PW91)



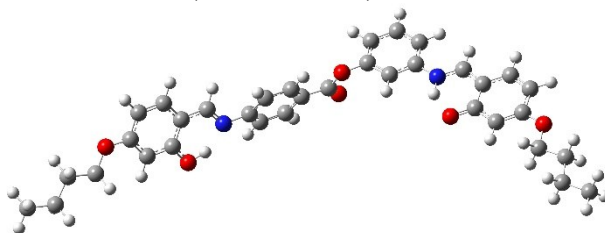
O	0.63215300	-2.64380200	2.16051700	O	0.76967200	-2.57875100	-0.09420800
N	-5.20565200	-0.52056800	0.56729500	N	5.45264500	-1.60578100	-0.12704100
C	-1.26020200	-1.91881500	0.89516900	C	2.08171300	-3.04460400	-0.05813500
C	-2.04744400	-1.69657500	2.03191900	C	3.11408800	-2.12132000	-0.06977500
H	-1.62479500	-1.89148100	3.01079900	H	2.90212900	-1.05878900	-0.04901300
C	-3.34501800	-1.23021800	1.90537600	C	4.43878800	-2.57212800	-0.12584900
H	-3.95804800	-1.05366600	2.78205500	C	4.69450000	-3.95112800	-0.13259100
C	-3.89456400	-0.99500200	0.63547400	H	5.71642500	-4.31333800	-0.11853100
C	-3.09656200	-1.19703400	-0.50233700	C	3.63794800	-4.85654400	-0.11726800
H	-3.48698500	-0.96314900	-1.48662300	H	3.84503300	-5.92114700	-0.11672400
C	-1.79456500	-1.65821800	-0.37193700	C	2.31770200	-4.41365500	-0.08737700
H	-1.18423200	-1.80593500	-1.25456200	H	1.48703700	-5.10914000	-0.07277000
C	0.12020000	-2.41048300	1.08786200	O	6.43375700	0.61129700	0.74959900
O	-7.08022900	1.02340300	1.44051900	H	5.79350600	-0.14655700	0.59327800
H	-6.20068000	0.54504900	1.37631900	O	10.81671000	1.81813300	-0.68264400
O	-11.17152600	1.13738100	-0.99874300	C	7.63195800	-0.84403800	-0.73332600
C	-7.31824500	-0.32791200	-0.52740100	C	7.53327900	0.34059600	0.04082500
C	-7.82338700	0.60956200	0.41092600	C	8.59012700	1.25470100	0.07594000
C	-9.11758200	1.11929800	0.27694600	H	8.47281300	2.14442500	0.67968900
H	-9.46268700	1.83165500	1.01398100	C	9.74778200	0.99846400	-0.65643900
C	-9.91576200	0.70189000	-0.78660000	C	9.86300200	-0.17212100	-1.43460800
C	-9.43211200	-0.23143000	-1.72801600	H	10.77468000	-0.34352400	-1.99368000
H	-10.07684900	-0.53696700	-2.54286700	C	8.81694200	-1.06584900	-1.46316500
C	-8.15758600	-0.72848000	-1.58749000	H	8.89948800	-1.96956900	-2.05966800
H	-7.77907900	-1.44714600	-2.30821400	C	6.55520300	-1.79601200	-0.77591800
C	-5.99071400	-0.85999500	-0.40529900	H	6.70166900	-2.68611000	-1.39759500
H	-5.67354300	-1.58596800	-1.16177500	C	10.78648800	3.02380100	0.08165100
C	-11.74350200	2.08256200	-0.09334200	H	10.63496900	2.78013200	1.14021400
H	-11.12752000	2.98978700	-0.07772500	H	9.94823900	3.64661400	-0.25373000
H	-11.75757300	1.65556800	0.91672500	C	12.10492100	3.74006800	-0.12214300
C	-13.14765500	2.39251700	-0.56759600	H	12.92100400	3.07719800	0.18695300
H	-13.09922800	2.78209500	-1.59071400	H	12.24102000	3.93750400	-1.19145000
H	-13.72331700	1.46089000	-0.60708300	C	12.17412400	5.04913200	0.66101000
C	-13.85102100	3.39986700	0.33922700	H	12.02436900	4.84431400	1.72805900
H	-13.26219100	4.32409600	0.38397100	H	11.34791900	5.70203000	0.35436400
H	-13.88577000	3.00744100	1.36280400	C	13.49825100	5.77955800	0.46510200
C	-15.26595100	3.72146700	-0.12960800	H	14.34092600	5.16369200	0.79434300
H	-15.26032400	4.14699400	-1.13790600	H	13.52440400	6.71228600	1.03473400
H	-15.74877400	4.44351100	0.53420900	H	13.65997100	6.02741600	-0.58856200
H	-15.88811700	2.82138600	-0.15263500				

S₀; MK-C, E= -1915.957018 hartree (mPW1PW91)



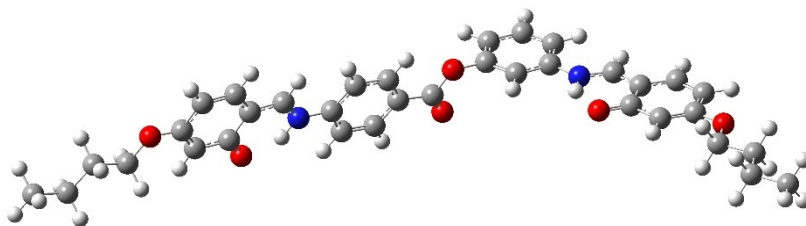
O	0.42936500	-3.04403200	1.96305800	C	3.14310600	-2.11325900	-0.11094900
C	-1.32292300	-2.06867400	0.66827600	H	2.93271000	-1.05046300	-0.08830200
C	-2.23003500	-2.06507800	1.73388500	C	4.46782200	-2.56788700	-0.13419600
H	-1.91616200	-2.45237600	2.69607500	C	4.71887600	-3.94731700	-0.14209600
C	-3.51193600	-1.57318000	1.56312100	H	5.73867600	-4.31353500	-0.10176200
H	-4.21087700	-1.57260700	2.39251600	C	3.65871400	-4.84896700	-0.16263000
C	-3.91561700	-1.07148800	0.31667200	H	3.86214800	-5.91426900	-0.16277400
C	-3.01082800	-1.07283100	-0.75400100	C	2.33974400	-4.40269600	-0.16948600
H	-3.29259600	-0.69178000	-1.72761300	H	1.50855800	-5.09722500	-0.18454900
C	-1.72846400	-1.56791000	-0.57417100	O	6.45030300	0.60559800	0.80808300
H	-1.03486600	-1.56533200	-1.40584700	H	5.81212000	-0.14975100	0.63284200
C	0.03320400	-2.60447000	0.90643600	O	10.86807300	1.80854100	-0.51695100
O	-11.02903100	1.78907800	-0.95032400	C	7.67954500	-0.84581300	-0.65300000
C	-7.13235100	0.38073200	-0.82585700	C	7.56565800	0.33554100	0.12402800
C	-7.92243100	0.29530900	0.40363600	C	8.62340500	1.24700500	0.18786500
C	-9.26521700	0.78415200	0.34882800	H	8.49422500	2.13433900	0.79274200
H	-9.84596600	0.72030500	1.25939500	C	9.79710000	0.99131900	-0.51881000
C	-9.78028500	1.30884000	-0.81672200	C	9.92770300	-0.17611400	-1.29931100
C	-9.00012600	1.38647200	-2.01527800	H	10.85170200	-0.34710000	-1.83790800
H	-9.45591800	1.80791300	-2.90274200	C	8.88062400	-1.06722300	-1.35619800
C	-7.71773200	0.93302700	-2.00555800	H	8.97492000	-1.96834400	-1.95488600
H	-7.11643500	0.98806400	-2.90861600	C	6.60150300	-1.79436700	-0.72610800
C	-5.81755100	-0.06818500	-0.85617700	H	6.76000600	-2.68145500	-1.34914600
H	-5.25008900	0.00598400	-1.77847200	C	10.82310700	3.01162200	0.25071600
C	-11.90363200	1.76895300	0.17918500	H	10.64767100	2.76462800	1.30479500
H	-11.45356700	2.34758400	0.99464000	H	9.99370400	3.63722400	-0.10105200
H	-12.03075900	0.73417500	0.51899500	C	12.14716900	3.72578100	0.07850400
C	-13.22838600	2.36772600	-0.24373100	H	12.95487500	3.05994400	0.40284300
H	-13.05762000	3.38591000	-0.61127100	H	12.30701400	3.92682600	-0.98685200
H	-13.62950400	1.78794900	-1.08273900	C	12.20226900	5.03184900	0.86779200
C	-14.23881400	2.39173600	0.90098800	H	12.02954900	4.82349900	1.93068900
H	-13.82524800	2.96318800	1.74082800	H	11.38406300	5.68758100	0.54607100
H	-14.39537300	1.37121200	1.27102800	C	13.53172700	5.76013800	0.70254500
C	-15.57769800	2.99327400	0.48777700	H	14.36597800	5.14132000	1.04732800
H	-15.45729800	4.02549400	0.14448800	H	13.54776900	6.69081300	1.27589600
H	-16.28369100	2.99982800	1.32245400	H	13.71617600	6.01128900	-0.34658800
H	-16.03147200	2.42276600	-0.32857000	O	-7.43137600	-0.19111600	1.46635900
O	0.80526400	-2.54497900	-0.20987900	N	-5.21836700	-0.59045800	0.21160600
N	5.48403300	-1.60452200	-0.10302400	H	-5.86463500	-0.60625600	1.03008600
C	2.10770800	-3.03255100	-0.13712000				

S₀; MK-O, E= -1915.956849 hartree (mPW1PW91)



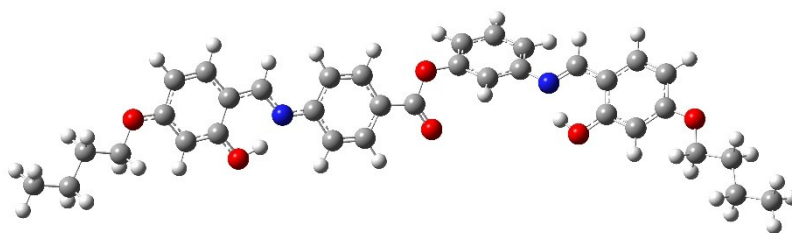
O	0.54484800	-3.43107200	1.88726700	O	0.87386800	-2.74608200	-0.24189400
N	-5.11961500	-0.76909800	0.49221800	C	2.17145000	-3.24217300	-0.24217600
C	-1.23102800	-2.33422400	0.72504400	C	3.20809900	-2.32429600	-0.20695200
C	-2.10632800	-2.40136400	1.81647800	H	2.98837100	-1.26605500	-0.12382400
H	-1.76678500	-2.86454600	2.73569900	C	4.52921200	-2.77909200	-0.28693700
C	-3.38420000	-1.87706300	1.72276200	C	4.78463300	-4.15055600	-0.39345200
H	-4.06443800	-1.92203000	2.56582900	H	5.79717000	-4.53114500	-0.44192900
C	-3.82578800	-1.29109000	0.52609800	C	3.72123900	-5.04658100	-0.43086200
C	-2.94040900	-1.20738900	-0.56098900	H	3.92660300	-6.10787600	-0.51456400
H	-3.24677300	-0.70588600	-1.47230700	C	2.40200900	-4.60707400	-0.35991800
C	-1.65812800	-1.72740000	-0.46189600	H	1.57254100	-5.30260300	-0.38964800
H	-0.97977200	-1.65172600	-1.30299000	O	10.59320400	2.08776300	-0.16966500
C	0.12471900	-2.89785400	0.88465200	C	7.74721500	-0.92312500	-0.33290100
O	-7.03130200	0.55053800	1.61455100	C	7.27599600	0.43952300	-0.09443400
H	-6.15822600	0.07282300	1.48666600	C	8.26610200	1.46952000	-0.03955000
O	-10.90002700	1.49971600	-0.99907300	H	7.91357700	2.47694400	0.13792500
C	-7.13000800	-0.20049300	-0.66191300	C	9.60291800	1.17686000	-0.20725200
C	-7.69349500	0.46526300	0.45803700	C	10.05416900	-0.15996100	-0.44218900
C	-8.96155400	1.04620500	0.37310300	H	11.11575900	-0.33463900	-0.56694800
H	-9.35279300	1.54383100	1.25010700	C	9.14182700	-1.16924700	-0.50125100
C	-9.67577500	0.96963600	-0.82123200	H	9.47358500	-2.18844500	-0.67831300
C	-9.13372600	0.30917700	-1.94437700	C	6.84511500	-1.98297200	-0.39947900
H	-9.71381000	0.26594900	-2.85796400	H	7.21469100	-2.98727000	-0.58350900
C	-7.88558900	-0.26054100	-1.85128500	C	10.26415100	3.45835200	0.05917300
H	-7.46235400	-0.76956800	-2.71208100	H	9.74871600	3.55069800	1.02268900
C	-5.82721100	-0.79863800	-0.59236000	H	9.58533800	3.80421100	-0.72963800
H	-5.46091100	-1.30232400	-1.49347100	C	11.55105700	4.25626300	0.05480100
C	-11.52388000	2.19140100	0.08389700	H	12.21838300	3.85964600	0.82834600
H	-10.88992100	3.03175500	0.39150200	H	12.05591300	4.11269900	-0.90725300
H	-11.63368400	1.50955200	0.93578500	C	11.30466600	5.74398900	0.29493200
C	-12.87533500	2.68164700	-0.39126700	H	10.78816900	5.87812300	1.25313500
H	-12.73215800	3.32897400	-1.26381600	H	10.62734900	6.13073800	-0.47615800
H	-13.46841700	1.82244300	-0.72430700	C	12.59346600	6.55901500	0.29420900
C	-13.62675100	3.43992700	0.70064200	H	13.27714700	6.21655400	1.07724200
H	-13.02126500	4.29028100	1.03716900	H	12.39204500	7.61941100	0.46795600
H	-13.75563100	2.78926800	1.57413100	H	13.11535700	6.47109300	-0.66378600
C	-14.98965700	3.94007100	0.23422100	O	6.04057500	0.69147000	0.05511800
H	-14.88992800	4.61954200	-0.61791600	N	5.53769900	-1.81060700	-0.25068700
H	-15.50800000	4.47917500	1.03158900	H	5.31274700	-0.80326300	-0.09150100
H	-15.62958500	3.10866200	-0.07723500				

S₀; DK, E= -1915.954289 hartree (mPW1PW91)



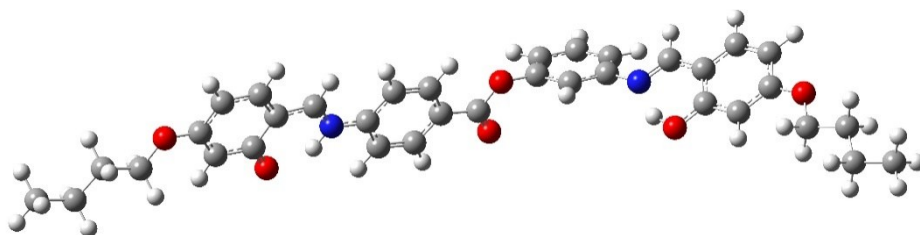
O	0.48648900	-3.35186900	1.74421700	H	3.02141700	-1.24359100	-0.18673300
C	-1.24083400	-2.24542500	0.52214700	C	4.53987400	-2.78320800	-0.30728900
C	-2.15271200	-2.30179100	1.58239000	C	4.77390500	-4.15841100	-0.41501000
H	-1.85073800	-2.76292200	2.51538800	H	5.78028000	-4.55619600	-0.45013700
C	-3.42433700	-1.77493400	1.44311400	C	3.69663200	-5.03559900	-0.48481100
H	-4.12684900	-1.82033400	2.26821700	H	3.88583100	-6.09975200	-0.57007600
C	-3.81308600	-1.17777300	0.23439700	C	2.38379600	-4.57311200	-0.45237500
C	-2.90332000	-1.11885800	-0.83052800	H	1.54338700	-5.25357100	-0.51052700
H	-3.17347900	-0.66364000	-1.77506100	O	10.68097900	1.97325000	0.06085200
C	-1.63104900	-1.64876800	-0.68241100	C	7.79084100	-0.99204400	-0.14753000
H	-0.93369400	-1.59868700	-1.50940900	C	8.33817600	1.40913700	-0.02649400
C	0.10287900	-2.82244000	0.72524000	H	7.99554700	2.43476800	0.01148200
O	-10.86366500	1.90448300	-0.84648400	C	9.67681900	1.07960500	-0.00671600
C	-6.99645900	0.41283500	-0.81180800	C	10.11514000	-0.28105500	-0.05723500
C	-7.79352800	0.25527600	0.40615400	H	11.17881300	-0.48427700	-0.03907300
C	-9.12615300	0.77351500	0.38259100	C	9.18820000	-1.27623100	-0.12484200
H	-9.71192900	0.65650300	1.28465600	H	9.50935200	-2.31331500	-0.16247400
C	-9.62545000	1.39090900	-0.74374800	C	6.87435700	-2.03913400	-0.21541900
C	-8.83855700	1.53880100	-1.93134100	H	7.23605800	-3.06236700	-0.24998300
H	-9.28194900	2.03227100	-2.78739400	C	10.36608800	3.36467900	0.12239200
C	-7.56554800	1.06024900	-1.95046600	H	9.74494300	3.55628500	1.00558200
H	-6.95908200	1.16794800	-2.84521400	H	9.79360300	3.64608900	-0.76961600
C	-5.69055100	-0.05806300	-0.87039000	C	11.66658900	4.13656900	0.19711400
H	-5.11776000	0.07096700	-1.78335600	H	12.22813900	3.80356700	1.07734000
C	-11.74381000	1.82128200	0.27584600	H	12.27568600	3.89414400	-0.68112200
H	-11.28661000	2.33201400	1.13166600	C	11.43572000	5.64430300	0.26880100
H	-11.89215300	0.76770500	0.54103700	H	10.81531200	5.87708100	1.14278600
C	-13.05483700	2.47391600	-0.10827100	H	10.86367900	5.96802100	-0.60921000
H	-12.86263700	3.51150500	-0.40388300	C	12.73824000	6.43340500	0.34592600
H	-13.46365500	1.96167200	-0.98659000	H	13.31630000	6.15456500	1.23245100
C	-14.06945900	2.43867100	1.03244600	H	12.54793900	7.50876400	0.39673200
H	-13.64852900	2.94281300	1.91083700	H	13.36531900	6.24658200	-0.53141600
H	-14.24716000	1.39834000	1.33085800	O	6.09577400	0.68001200	-0.11644100
C	-15.39473000	3.09319900	0.65771600	C	7.33281500	0.39493700	-0.09765000
H	-15.25299600	4.14404700	0.38671200	N	5.56343300	-1.83279200	-0.23708000
H	-16.10405200	3.05607300	1.48876300	H	5.34877400	-0.81192800	-0.19282000
H	-15.85587700	2.58918000	-0.19734500	O	-7.31669500	-0.31573400	1.43258400
O	0.88522500	-2.68684200	-0.37982800	N	-5.10615500	-0.66680600	0.15944000
C	2.17426400	-3.20447700	-0.34084200	H	-5.75667900	-0.72889300	0.97239300
C	3.22502500	-2.30507100	-0.26962800				

S₁; DE*, E= -1915.846356 hartree (mPW1PW91)



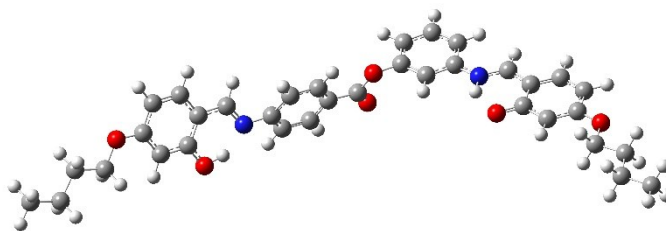
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N	-5.11854400	-0.47546600	0.26276000	N	5.42650800	-1.71728100	0.05148800
C	-1.13614700	-1.60474700	0.83214800	C	2.07995200	-3.21009500	0.22501500
C	-1.79408500	-0.71688900	1.72010800	C	3.10013400	-2.26969800	0.16134700
H	-1.24316600	-0.32237000	2.56574500	H	2.87970400	-1.21015100	0.14060300
C	-3.10292200	-0.36277700	1.51042600	C	4.43012900	-2.70117900	0.10955400
H	-3.60750700	0.31785400	2.18805700	C	4.71657800	-4.07423900	0.15705400
C	-3.84028400	-0.87561900	0.39749900	H	5.74598100	-4.41440800	0.17567500
C	-3.16488100	-1.77607500	-0.49265100	C	3.67767300	-4.99684800	0.22195900
H	-3.68157500	-2.19143500	-1.34898600	H	3.90308800	-6.05696200	0.26475100
C	-1.85288300	-2.12194000	-0.27186300	C	2.35062300	-4.57515600	0.25094000
H	-1.35520000	-2.80095200	-0.95371300	H	1.53171500	-5.28259800	0.30655900
C	0.25635700	-1.94577500	1.09879200	O	6.37822400	0.55366100	0.81438300
O	-6.95717100	0.96439400	1.22441300	H	5.74975700	-0.22219800	0.70206100
H	-6.05546000	0.48578300	1.06375900	O	10.71212900	1.78107800	-0.74498700
O	-11.18940300	1.05047400	-0.95284500	C	7.58057600	-0.94215800	-0.62414200
C	-7.27059100	-0.36424500	-0.75447400	C	7.47094300	0.27311000	0.09932700
C	-7.75812000	0.56845600	0.25143300	C	8.51009700	1.20795600	0.07633100
C	-9.06445400	1.05605300	0.20730800	H	8.38482400	2.12096600	0.64258000
H	-9.37143100	1.74749000	0.98056500	C	9.66033600	0.94234100	-0.66419300
C	-9.91900500	0.64691800	-0.81236800	C	9.78619500	-0.25883700	-1.39219900
C	-9.46609700	-0.26510800	-1.80656100	H	10.69167300	-0.43714600	-1.95918300
H	-10.15748800	-0.56346800	-2.58571000	C	8.75758100	-1.17293900	-1.36364800
C	-8.17718200	-0.74905100	-1.76756000	H	8.84838700	-2.10021600	-1.92161900
H	-7.84204700	-1.44374700	-2.53048600	C	6.52145000	-1.91528900	-0.60718900
C	-5.93944900	-0.86789800	-0.72264500	H	6.67495200	-2.82874000	-1.19223200
H	-5.63089600	-1.55934000	-1.50364300	C	10.66892800	3.01885500	-0.03496100
C	-11.73942500	1.96995800	-0.00500400	H	10.54313900	2.81997800	1.03631900
H	-11.14148000	2.88921900	-0.00990200	H	9.81048500	3.60749500	-0.38082700
H	-11.68675500	1.52624400	0.99648900	C	11.96631800	3.75429400	-0.29730500
C	-13.17286500	2.25084400	-0.40119700	H	12.80337600	3.12558800	0.02676900
H	-13.18801100	2.65617900	-1.41905200	H	12.07820200	3.90377200	-1.37715800
H	-13.72778600	1.30631200	-0.42336900	C	12.01874300	5.10040500	0.42163700
C	-13.84872600	3.22847000	0.55799300	H	11.89331500	4.94341900	1.49984900
H	-13.27962700	4.16558000	0.58516300	H	11.17178400	5.71882500	0.10048000
H	-13.81922000	2.82050200	1.57555600	C	13.32126900	5.85091600	0.16586000
C	-15.29374700	3.52249600	0.17012200	H	14.18432300	5.27109000	0.50755000
H	-15.35210400	3.96241700	-0.83022200	H	13.33547700	6.81016200	0.69008900
H	-15.75627100	4.22328900	0.87003700	H	13.45784400	6.05182000	-0.90129500
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S₁; MK-C*, E= -1915.855298 hartree (mPW1PW91)



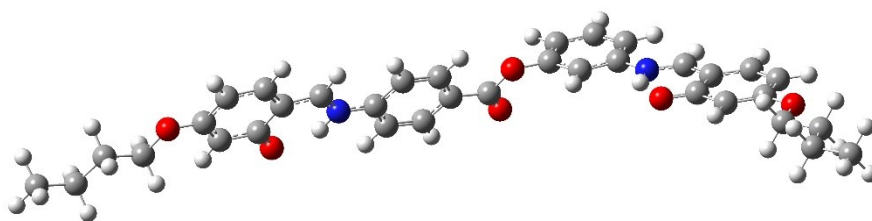
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C	1.33406400	-2.08284500	-0.63527600	H	-2.97519600	-0.99100800	0.06619800
C	2.29846800	-2.18748600	-1.65975500	C	-4.48847600	-2.52845300	0.14467500
H	2.02487000	-2.67067400	-2.59035100	C	-4.72138500	-3.91048300	0.17168900
C	3.56873700	-1.68559700	-1.48455700	H	-5.73616100	-4.29154700	0.14318900
H	4.30374300	-1.77121800	-2.27854400	C	-3.64731900	-4.79599600	0.19477200
C	3.92644900	-1.05540900	-0.27021500	H	-3.83531600	-5.86416800	0.20917200
C	2.96413400	-0.94628400	0.76112700	C	-2.33503600	-4.33151800	0.18654100
H	3.20691800	-0.46788500	1.70187400	H	-1.49587400	-5.01606000	0.20288800
C	1.69483700	-1.45377800	0.57198000	O	-6.51439700	0.60719200	-0.82427500
H	0.96347800	-1.36636300	1.36620100	H	-5.86650800	-0.13897300	-0.64148900
C	0.00141500	-2.63261000	-0.87374900	O	-10.94416300	1.77031600	0.49828100
O	11.11727500	1.88476400	0.91984300	C	-7.72117000	-0.84174400	0.65744600
C	7.14767400	0.49177800	0.82996400	C	-7.62443500	0.33145100	-0.13391200
C	7.98746000	0.28179600	-0.34402800	C	-8.69411900	1.22848900	-0.20577600
C	9.33721200	0.76170200	-0.30121700	H	-8.57789300	2.10990200	-0.82183800
H	9.93148600	0.58924400	-1.18909700	C	-9.86250800	0.96656900	0.50728200
C	9.85718500	1.41586900	0.82736100	C	-9.97591500	-0.19259800	1.30224500
C	9.03815800	1.60633800	1.93861900	H	-10.89609600	-0.36895800	1.84564700
H	9.43145300	2.11024400	2.81293600	C	-8.91715000	-1.06970100	1.36667300
C	7.70172400	1.14216700	1.91859600	H	-8.99826200	-1.96468000	1.97642300
H	7.09256000	1.30926600	2.80202700	C	-6.63053600	-1.77619500	0.73754200
C	5.78074000	0.04879600	0.88415400	H	-6.77583200	-2.65863500	1.37034600
H	5.19942800	0.22281000	1.78028400	C	-10.91645300	2.96315600	-0.28564200
C	12.00339900	1.71557600	-0.18865300	H	-10.74103100	2.70420100	-1.33688900
H	11.57977300	2.20827700	-1.07218200	H	-10.09392900	3.60389900	0.05488600
H	12.11449200	0.64635400	-0.40639000	C	-12.24870700	3.66333800	-0.11911800
C	13.33621200	2.33005400	0.18277700	H	-13.04913500	2.98340400	-0.43206800
H	13.18463800	3.38782700	0.42564500	H	-12.40802100	3.87678200	0.94391500
H	13.71077900	1.84374500	1.09053600	C	-12.32196000	4.95786800	-0.92571100
C	14.36260800	2.19598700	-0.94001200	H	-12.14978900	4.73728800	-1.98622500
H	13.97457700	2.67255600	-1.84839700	H	-11.51080900	5.62768300	-0.61532500
H	14.50038400	1.13556100	-1.18369900	C	-13.65965300	5.67223900	-0.76626200
C	15.70919900	2.81321200	-0.57829800	H	-14.48732300	5.03873800	-1.10006700
H	15.60828900	3.88128900	-0.36208700	H	-13.68869300	6.59479700	-1.35209700
H	16.42673600	2.70497400	-1.39588800	H	-13.84408100	5.93530400	0.27995400
H	16.13772800	2.33407500	0.30743500	O	7.54610400	-0.30750200	-1.37780600
O	-0.83208600	-2.44278600	0.19671900	N	5.20580000	-0.57265300	-0.14632100
N	-5.51829900	-1.57875800	0.10824500	H	5.86143800	-0.68293300	-0.93930400
C	-2.11810200	-2.95781800	0.13560100				

S₁; MK-O*, E= -1915.850074 hartree (mPW1PW91)



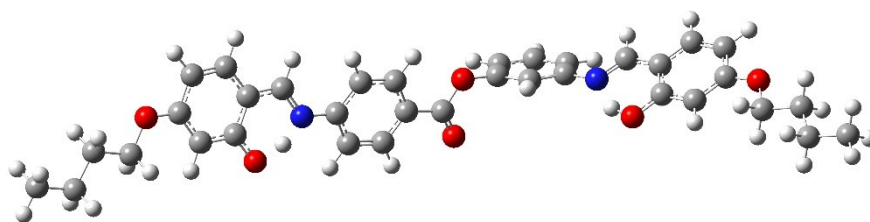
O	0.52909100	-3.39774800	1.86542700	O	0.85170600	-2.71430200	-0.26518700
N	-5.14216900	-0.74374000	0.48644200	C	2.14705700	-3.22367300	-0.27460600
C	-1.24958300	-2.30196600	0.70767000	C	3.19019300	-2.32277000	-0.22006800
C	-2.11926100	-2.36444300	1.80368400	H	2.98360700	-1.26381400	-0.11166500
H	-1.77447900	-2.82326300	2.72315200	C	4.51779400	-2.79412300	-0.30790900
C	-3.39827400	-1.84186400	1.71407100	C	4.74875600	-4.17943000	-0.44996600
H	-4.07425400	-1.88373300	2.56074900	H	5.75494300	-4.57204300	-0.52207400
C	-3.84667800	-1.26250700	0.51683800	C	3.67065600	-5.05225900	-0.50310500
C	-2.96682100	-1.18278400	-0.57489800	H	3.85746100	-6.11491200	-0.61430700
H	-3.27850200	-0.68631000	-1.48719100	C	2.35507800	-4.59549500	-0.42026000
C	-1.68332800	-1.70086200	-0.47964900	H	1.51445200	-5.27655900	-0.46356500
H	-1.00915800	-1.62906000	-1.32445700	O	10.70505300	2.07083600	-0.08326900
C	0.10792700	-2.86552900	0.86214100	C	7.78562800	-0.96986100	-0.24225000
O	-7.05301800	0.57337700	1.61224800	C	7.34810500	0.41890300	-0.12979100
H	-6.17866800	0.09847900	1.48176400	C	8.35030000	1.43976000	-0.07622000
O	-10.94009000	1.49333300	-0.98483500	H	7.98708300	2.45600400	0.00723700
C	-7.16042200	-0.18812100	-0.66024200	C	9.72440600	1.14245700	-0.12979000
C	-7.72094800	0.48010800	0.45962100	C	10.12261500	-0.18525500	-0.23677900
C	-8.99207100	1.05498800	0.37880500	H	11.17749300	-0.42792000	-0.27801200
H	-9.38095200	1.55466700	1.25569500	C	9.14735400	-1.21357000	-0.29042000
C	-9.71229000	0.96983300	-0.81131800	H	9.49775400	-2.23833000	-0.37304000
C	-9.17309300	0.30703600	-1.93436400	C	6.85929500	-2.06796700	-0.30397400
H	-9.75775200	0.25703700	-2.84469000	H	7.23382900	-3.07896800	-0.39144500
C	-7.92185500	-0.25667600	-1.84530300	C	10.34837300	3.44861900	0.02718200
H	-7.50090800	-0.76767500	-2.70606100	H	9.76631800	3.60414200	0.94394100
C	-5.85486300	-0.78115600	-0.59439900	H	9.72731400	3.73629000	-0.83015700
H	-5.49129800	-1.28793500	-1.49489100	C	11.62663500	4.25973500	0.05947100
C	-11.56177300	2.18565200	0.09882900	H	12.23871300	3.92467200	0.90449100
H	-10.93070300	3.03048600	0.40009100	H	12.20021600	4.05529000	-0.85167900
H	-11.66349500	1.50642900	0.95384100	C	11.35403400	5.75754900	0.17703600
C	-12.91831300	2.66700600	-0.37092200	H	10.76911100	5.95180000	1.08424800
H	-12.78321100	3.31174100	-1.24667600	H	10.73174400	6.08244600	-0.66562900
H	-13.50859500	1.80343200	-0.69758400	C	12.63456100	6.58474000	0.21153700
C	-13.66796500	3.42544900	0.72206100	H	13.26202200	6.30489000	1.06345500
H	-13.06528600	4.28032800	1.05211400	H	12.41464000	7.65228200	0.29595100
H	-13.78868300	2.77749400	1.59872000	H	13.22466300	6.43651900	-0.69820400
C	-15.03599200	3.91645900	0.26101100	O	6.11510900	0.72572300	-0.08026100
H	-14.94445800	4.59313600	-0.59426800	N	5.53126300	-1.86960100	-0.25157300
H	-15.55301700	4.45587000	1.05903300	H	5.29726200	-0.86760100	-0.16446600
H	-15.67307900	3.08042800	-0.04383100				

S₁; DK*, E= -1915.852858 hartree (mPW1PW91)



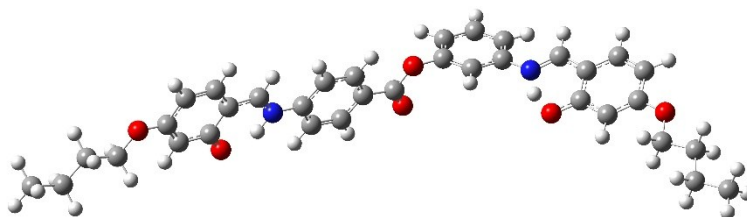
O	0.30361800	-3.81452200	1.52150400	H	3.05209600	-1.22814800	-0.11576900
C	-1.28528600	-2.40564400	0.43808300	C	4.56674000	-2.76306100	-0.30804700
C	-2.31701500	-2.70044000	1.35495100	C	4.79989500	-4.13404200	-0.45728000
H	-2.11423500	-3.38444300	2.17060700	H	5.80513500	-4.53142900	-0.51980300
C	-3.56278500	-2.13017700	1.21953900	C	3.71889900	-5.00678800	-0.53318400
H	-4.34997700	-2.36317800	1.92952700	H	3.90481100	-6.06850200	-0.65157100
C	-3.82748200	-1.23704600	0.15560300	C	2.40700700	-4.54653400	-0.46618900
C	-2.79776500	-0.93584700	-0.76671700	H	1.56945700	-5.22889800	-0.52879100
H	-2.96850100	-0.25286600	-1.58973400	O	10.71604400	1.98613000	0.07831400
C	-1.55388500	-1.51433100	-0.61952000	C	7.82068200	-0.97279000	-0.15855600
H	-0.77043300	-1.27760700	-1.32899600	C	8.37158500	1.42343400	0.02043600
C	0.01672500	-3.03576600	0.63148900	H	8.03013300	2.44749500	0.09461400
O	-10.85566500	2.16171600	-0.73635600	C	9.71033400	1.09384800	0.00472200
C	-6.93967100	0.62370000	-0.75547900	C	10.14684700	-0.26428800	-0.09333600
C	-7.85174500	0.19651200	0.29956000	H	11.21051300	-0.46823400	-0.10184500
C	-9.18285600	0.72788000	0.29536800	C	9.21763400	-1.25719100	-0.17145000
H	-9.83222500	0.38983200	1.09231400	H	9.53755700	-2.29274900	-0.24536600
C	-9.61756800	1.63251300	-0.68632600	C	6.90210500	-2.01843300	-0.23898400
C	-8.73066900	2.02643700	-1.68688900	H	7.26307400	-3.04003600	-0.31068200
H	-9.05863200	2.72364300	-2.44804000	C	10.40199500	3.37473200	0.18477200
C	-7.41134000	1.51637200	-1.70195500	H	9.79744900	3.54131100	1.08445300
H	-6.74776000	1.84778300	-2.49512100	H	9.81272500	3.68082700	-0.68803200
C	-5.58374000	0.15136700	-0.83387800	C	11.70338800	4.14545700	0.25677500
H	-4.94622200	0.49147600	-1.63968400	H	12.28098900	3.78902300	1.11721900
C	-11.80705100	1.79721800	0.26614300	H	12.29647800	3.92750300	-0.63867100
H	-11.41860900	2.07282600	1.25410700	C	11.47351800	5.65048700	0.37374300
H	-11.96200100	0.71172900	0.24388300	H	10.86842300	5.85881900	1.26448300
C	-13.09809100	2.53096900	-0.02834600	H	10.88611200	5.99768600	-0.48494400
H	-12.90071000	3.60884200	-0.03494500	C	12.77695300	6.43820300	0.44965200
H	-13.43826100	2.26170000	-1.03464000	H	13.37042800	6.13582600	1.31809900
C	-14.18714000	2.20809900	0.99232900	H	12.58730400	7.51166200	0.53293600
H	-13.83449900	2.46912000	1.99749800	H	13.38875300	6.27571300	-0.44319000
H	-14.36987400	1.12672600	1.00145500	O	6.12716300	0.69724500	-0.04534700
C	-15.49294400	2.94153700	0.70585900	C	7.36432100	0.41156200	-0.05969500
H	-15.34815700	4.02617900	0.72312600	N	5.59185000	-1.81323400	-0.22892900
H	-16.25650700	2.69527100	1.44838300	H	5.37655800	-0.79499400	-0.15099600
H	-15.88732300	2.67476100	-0.27953800	O	-7.48787500	-0.62119100	1.19918900
O	0.92418800	-2.63776900	-0.31883100	N	-5.08652800	-0.69586900	0.06681400
C	2.19511300	-3.17985600	-0.31219700	H	-5.79187600	-0.95127500	0.77998600
C	3.25342300	-2.28684900	-0.23354600				

S₀; DE to MK-C, TS, E= -1915.953825 hartree (mPW1PW91)



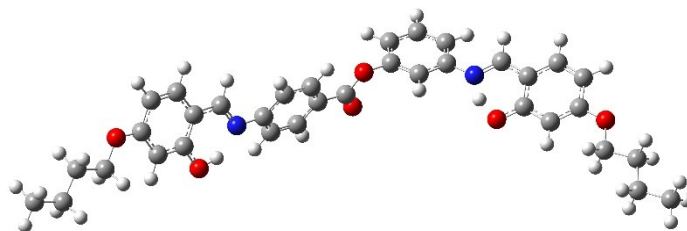
O	-0.32298400	2.61137800	2.27705100	C	-3.08218700	2.11952100	0.13968200
C	1.39648700	1.87531500	0.79205700	H	-2.89082700	1.06576500	-0.02552400
C	2.31619100	1.65420800	1.82356200	C	-4.39863000	2.58964100	0.23012200
H	2.01894300	1.85216200	2.84674600	C	-4.62447900	3.95333200	0.46556600
C	3.58957000	1.19072000	1.54007600	H	-5.63594100	4.32153300	0.59594300
H	4.30434300	1.02482300	2.33828900	C	-3.54887400	4.83031100	0.57115900
C	3.97418900	0.94277300	0.21371000	H	-3.73278400	5.88253000	0.75893500
C	3.04699200	1.14624400	-0.81983000	C	-2.23884800	4.37346600	0.45291800
H	3.30595100	0.92064700	-1.84760800	H	-1.39568600	5.04863200	0.53534300
C	1.77418400	1.61354600	-0.53043100	O	-6.40702500	-0.67677200	0.65860000
H	1.06329900	1.76543000	-1.33328900	H	-5.76154000	0.09037000	0.59960000
C	0.05111400	2.37167300	1.15045300	O	-10.88136900	-1.57473500	-0.71729000
O	11.03198500	-1.61378800	-1.46952200	C	-7.65347000	1.02460600	-0.48347600
C	7.20929000	-0.04750400	-1.22464000	C	-7.53699400	-0.27695700	0.06855500
C	7.79369800	-0.60738000	-0.03143000	C	-8.60772400	-1.17303600	0.00362000
C	9.09779400	-1.14428600	-0.10424900	H	-8.47604300	-2.15506700	0.43729900
H	9.52140800	-1.56032700	0.79992100	C	-9.79710500	-0.78262100	-0.60887100
C	9.78910500	-1.12581000	-1.30650600	C	-9.93057000	0.50595400	-1.16642000
C	9.21488100	-0.57256300	-2.48388300	H	-10.86679600	0.78021200	-1.63694000
H	9.79483900	-0.58121600	-3.39848300	C	-8.87051500	1.38077000	-1.09838200
C	7.95301900	-0.04641600	-2.43022800	H	-8.96664200	2.37451000	-1.52574200
H	7.50451900	0.37917200	-3.32311400	C	-6.56223000	1.95875100	-0.42176300
C	5.91036300	0.49716900	-1.15016500	H	-6.72426100	2.94380300	-0.87303400
H	5.45896100	0.94430600	-2.03537200	C	-10.83460800	-2.89542700	-0.17667300
C	11.70687100	-2.18775800	-0.34891100	H	-10.62548800	-2.84146200	0.89865400
H	11.12067700	-3.03186300	0.03360800	H	-10.02579200	-3.45781200	-0.65893100
H	11.79234900	-1.43708200	0.44584200	C	-12.17454200	-3.55279700	-0.43247000
C	13.07489900	-2.64384600	-0.81045000	H	-12.96167100	-2.94796500	0.03181100
H	12.95334500	-3.36438000	-1.62712200	H	-12.36858800	-3.55646500	-1.51102800
H	13.61671900	-1.78409900	-1.22057100	C	-12.22738700	-4.97924600	0.10992800
C	13.88194200	-3.27392400	0.32245600	H	-12.01992300	-4.96816900	1.18685500
H	13.32837800	-4.12627800	0.73467500	H	-11.42978300	-5.57466100	-0.35077700
H	13.98772300	-2.55127900	1.14070000	C	-13.57268700	-5.65190800	-0.14097000
C	15.26323100	-3.73578200	-0.12908900	H	-14.38635600	-5.09686000	0.33616500
H	15.18859200	-4.48353300	-0.92475900	H	-13.58655300	-6.67051800	0.25576600
H	15.82133700	-4.18326200	0.69760300	H	-13.79225800	-5.70780800	-1.21169800
H	15.85264300	-2.89820400	-0.51492000	O	7.12286700	-0.60632800	1.08150500
O	-0.73899900	2.53081600	0.05663500	N	5.26947000	0.47725400	-0.00354200
N	-5.43064400	1.64880200	0.12272800	H	6.04306700	-0.04793800	0.77655700
C	-2.03104900	3.01507100	0.24410900				

S₀; **MK-C to DK**, TS, E= -1915.951381 hartree (mPW1PW91)



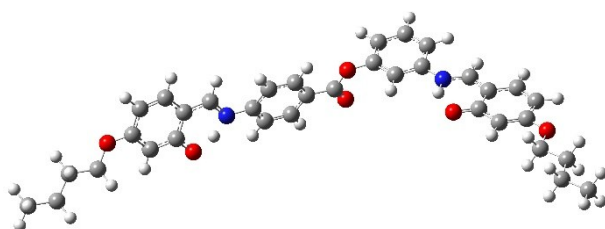
O	-0.41082800	2.69979800	2.35616800	H	-2.95226300	1.23976400	-0.09126600
C	1.32283600	1.90456400	0.91959400	C	-4.42377700	2.80472700	0.15786400
C	2.21086200	1.66185700	1.97373200	C	-4.61989800	4.16753300	0.41412100
H	1.89684400	1.87351400	2.98905600	H	-5.62117900	4.57070200	0.51116500
C	3.47515900	1.15818500	1.72456400	C	-3.52182800	5.00573300	0.57800400
H	4.16025400	0.97339000	2.54479600	H	-3.68074900	6.05948800	0.77826700
C	3.88023800	0.88517300	0.40936300	C	-2.22260100	4.50977000	0.50465800
C	2.99281500	1.12217800	-0.64953000	H	-1.36375300	5.15688400	0.63435100
H	3.27336600	0.91317200	-1.67415100	O	-10.58006100	-1.72705700	-0.76294100
C	1.72841300	1.62822800	-0.39123200	C	-7.67342000	1.20951400	-0.50391500
H	1.04841700	1.80846500	-1.21454200	C	-8.29696600	-1.14746100	-0.23177400
C	-0.01353400	2.44477900	1.24119500	H	-8.00972500	-2.15388800	0.04175700
O	10.91579200	-1.92788000	-1.31437900	C	-9.57975900	-0.83188700	-0.65468700
C	7.07245200	-0.41580500	-0.96083600	C	-9.93545000	0.49598200	-1.01331900
C	7.82450400	-0.64844200	0.27366800	H	-10.94926600	0.69349300	-1.33915500
C	9.14903400	-1.17049800	0.13933300	C	-8.99220500	1.48586900	-0.93636700
H	9.70182400	-1.34186200	1.05335800	H	-9.25334500	2.50489300	-1.20683700
C	9.68186900	-1.43771100	-1.10312800	C	-6.68779400	2.21905100	-0.41731900
C	8.93874600	-1.20607800	-2.30534600	H	-6.93279800	3.24438500	-0.69488900
H	9.40699000	-1.43410000	-3.25493900	C	-10.33181300	-3.09036500	-0.41873700
C	7.67503800	-0.71001900	-2.22173800	H	-10.00209400	-3.14670400	0.62566600
H	7.10243400	-0.53063900	-3.12720500	H	-9.53134400	-3.48588600	-1.05556300
C	5.77841100	0.08884800	-0.91835400	C	-11.61655900	-3.86552400	-0.62184300
H	5.24028000	0.25620000	-1.84624900	H	-12.40246000	-3.42011100	-0.00140400
C	11.75579300	-2.19896200	-0.19099100	H	-11.93487900	-3.76018300	-1.66519000
H	11.26266300	-2.93008800	0.46062400	C	-11.45643100	-5.34382400	-0.27445600
H	11.90593300	-1.27422600	0.37886800	H	-11.12649300	-5.44009800	0.76707900
C	13.07255000	-2.73632700	-0.71038800	H	-10.66042900	-5.77939700	-0.89056700
H	12.88011200	-3.63728900	-1.30386500	C	-12.74438300	-6.13525600	-0.47442500
H	13.51689200	-1.99703000	-1.38638200	H	-13.54975900	-5.74334700	0.15454400
C	14.04718300	-3.05775100	0.42029600	H	-12.60557800	-7.18935800	-0.21990200
H	13.59074100	-3.78873900	1.09866800	H	-13.08107900	-6.08461300	-1.51457000
H	14.22512100	-2.15442300	1.01627700	O	-6.10013900	-0.40541900	0.24082000
C	15.37787000	-3.59993300	-0.09008600	C	-7.31207300	-0.13832700	-0.14681300
H	15.23486100	-4.52188900	-0.66224500	N	-5.47880000	1.90388700	-0.02085000
H	16.05826700	-3.82253100	0.73615000	H	-5.51675100	0.70975500	0.18258300
H	15.87351800	-2.87646500	-0.74488300	O	7.31805400	-0.39551400	1.40796000
O	-0.76911700	2.62563400	0.12498700	N	5.16569200	0.38173100	0.22674100
C	-2.04843000	3.15052400	0.27428000	H	5.78636600	0.18479400	1.04158700
C	-3.12210900	2.29276400	0.10046800				

S₀; **DE to MK-P**, TS, E= -1915.953912 hartree (mPW1PW91)



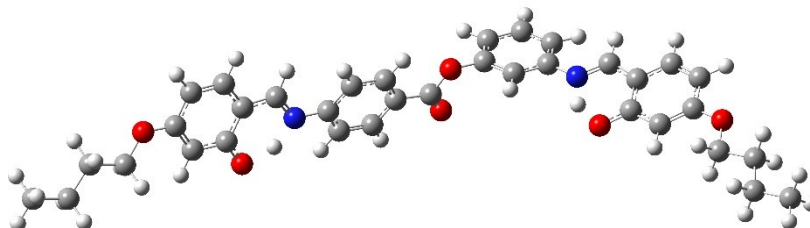
O	-0.46980300	2.78466400	2.38021300	O	-0.76115500	2.72761800	0.13958400
N	5.19563700	0.53106200	0.39186300	C	-2.05258700	3.22921800	0.25938900
C	1.31723000	2.02418000	0.98862000	C	-3.10835200	2.34759400	0.09471900
C	2.17164500	1.77247100	2.06952400	H	-2.91712100	1.29337700	-0.06800200
H	1.81913300	1.96707600	3.07583700	C	-4.41964300	2.83673000	0.12318000
C	3.44612400	1.27623600	1.85428800	C	-4.64390600	4.20184500	0.34162800
H	4.11032300	1.07589500	2.68748600	H	-5.65359500	4.58862900	0.41574000
C	3.90541400	1.03951400	0.54921400	C	-3.56351400	5.06418200	0.49719600
C	3.04014700	1.27260600	-0.53216000	H	-3.74412900	6.11961800	0.66814100
H	3.35910500	1.03884500	-1.54183600	C	-2.25467200	4.59037900	0.45242000
C	1.76127800	1.76362500	-0.31299000	H	-1.40895200	5.25589300	0.57564800
H	1.09863900	1.93434700	-1.15268400	O	-10.47914200	-1.82957900	-0.76961200
C	-0.03533600	2.54446200	1.27569700	C	-7.63102100	1.16632800	-0.54031400
O	7.07533400	-1.07476100	1.12970200	C	-7.25028400	-0.16553600	-0.14551100
H	6.20857000	-0.56940600	1.12687500	C	-8.21521500	-1.19466700	-0.21971500
O	10.98762600	-1.29970000	-1.57975500	H	-7.91348200	-2.18871800	0.08204300
C	7.22431800	0.28471800	-0.84147200	C	-9.49728000	-0.91335400	-0.66813900
C	7.76082400	-0.67590300	0.05527700	C	-9.87216700	0.39873000	-1.06331700
C	9.02612200	-1.22520100	-0.16821100	H	-10.88461200	0.56938300	-1.40808200
H	9.39666600	-1.95376300	0.54007000	C	-8.94835000	1.40761500	-0.99741300
C	9.76433500	-0.82495300	-1.28048000	H	-9.22421300	2.41470600	-1.29649400
C	9.24955800	0.13173500	-2.18110200	C	-6.66478900	2.19553900	-0.46574100
H	9.84793100	0.42323100	-3.03550000	H	-6.92395900	3.20902300	-0.77240100
C	8.00390900	0.66773900	-1.95258700	C	-10.20969400	-3.18049200	-0.39400800
H	7.60159700	1.40371200	-2.64231400	H	-9.89549100	-3.20955000	0.65628500
C	5.92447200	0.85507000	-0.62869200	H	-9.39164400	-3.57260700	-1.01027400
H	5.57961100	1.59584000	-1.35823700	C	-11.47559800	-3.98506500	-0.60130300
C	11.58328500	-2.27772600	-0.72586100	H	-12.27955700	-3.54425500	-0.00103100
H	10.93458600	-3.16067300	-0.67701900	H	-11.78008800	-3.90552500	-1.65105600
H	11.68386900	-1.86474500	0.28514100	C	-11.29110300	-5.45311100	-0.22388100
C	12.93824500	-2.63543100	-1.29923300	H	-10.97473000	-5.52339900	0.82392100
H	12.80472000	-3.00747900	-2.32131100	H	-10.47749500	-5.88367400	-0.82018500
H	13.54712600	-1.72681500	-1.36663200	C	-12.55977500	-6.27419800	-0.42753400
C	13.66022700	-3.68337200	-0.45519600	H	-13.38211500	-5.88730400	0.18230500
H	13.03940600	-4.58464800	-0.38303500	H	-12.40354300	-7.32038400	-0.15135400
H	13.77901500	-3.30887600	0.56880500	H	-12.88197200	-6.24960300	-1.47320000
C	15.02665700	-4.05212700	-1.02273400	O	-6.03933900	-0.40066100	0.26516800
H	14.93650200	-4.46138100	-2.03374900	N	-5.45599200	1.91244600	-0.04550100
H	15.52392300	-4.80254100	-0.40247500	H	-5.47531100	0.72298900	0.18708300
H	15.68102300	-3.17650300	-1.07619100				

S₀; **MK-P to DK**, TS, E= -1915.951175 hartree (mPW1PW91)



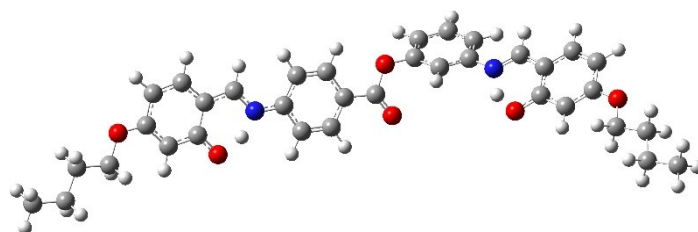
O	-0.45686500	2.83248000	2.04483700	H	-2.91843800	1.35174900	-0.20448800
C	1.30707600	2.08570100	0.61721200	C	-4.43272600	2.88976800	-0.03123500
C	2.17469600	1.81148900	1.68086700	C	-4.66477700	4.26392600	0.09513100
H	1.84019300	1.99366500	2.69546200	H	-5.67141800	4.66112800	0.13353000
C	3.44400900	1.31440800	1.43961300	C	-3.58676300	5.14059400	0.15621900
H	4.11844400	1.10648900	2.26267700	H	-3.77426600	6.20419500	0.25145200
C	3.87655600	1.08530800	0.12460000	C	-2.27493600	4.67841400	0.08604400
C	3.00131700	1.34290500	-0.94155700	H	-1.43229500	5.35768900	0.12676900
H	3.29696200	1.13062500	-1.96215700	O	-10.59325200	-1.84746800	-0.29546500
C	1.73238700	1.84351600	-0.69455800	C	-7.68494100	1.09533200	-0.02570200
H	1.06107600	2.03516900	-1.52257000	C	-8.25871900	-1.26460600	-0.45157700
C	-0.03797200	2.60967300	0.93094900	H	-7.93076300	-2.26570500	-0.69838600
O	10.88193700	-1.72464600	-1.35743200	C	-9.58470500	-0.95851300	-0.23041500
C	7.13306900	0.02193500	-1.20754500	C	-10.00324500	0.36952500	0.09693700
C	7.63291200	-0.62178700	-0.01791300	H	-11.05754200	0.55546600	0.26100400
C	8.91141000	-1.22021900	-0.05861800	C	-9.06972900	1.35619400	0.19383400
H	9.27083500	-1.69968900	0.84190600	H	-9.37614900	2.36821200	0.44290100
C	9.65889700	-1.18039000	-1.22610500	C	-6.76002900	2.13127400	0.08622700
C	9.16942900	-0.54213100	-2.39887200	H	-7.10396300	3.12887800	0.34276000
H	9.79122700	-0.53657800	-3.28557900	C	-10.29631300	-3.20894000	-0.60737500
C	7.93325800	0.04365300	-2.37641700	H	-9.60160500	-3.60837000	0.14123200
H	7.54915200	0.53343900	-3.26640500	H	-9.81051000	-3.25760300	-1.58934800
C	5.85744800	0.62190800	-1.16642400	C	-11.59700400	-3.98416900	-0.60740600
H	5.46741900	1.12856300	-2.04892300	H	-12.07124200	-3.88368400	0.37545500
C	11.46900800	-2.39437800	-0.24044100	H	-12.27893500	-3.53547900	-1.33863000
H	10.81739100	-3.21987500	0.06999200	C	-11.38504200	-5.46094100	-0.93296200
H	11.56026200	-1.69175300	0.59651800	H	-10.69272200	-5.89952600	-0.20407400
C	12.82829700	-2.90875700	-0.66498200	H	-10.89925400	-5.55267000	-1.91201200
H	12.70338300	-3.57696600	-1.52451400	C	-12.68794800	-6.25319600	-0.93621800
H	13.43903600	-2.06387900	-1.00283900	H	-13.17973000	-6.20773300	0.04047100
C	13.54160600	-3.64574300	0.46634100	H	-12.51111400	-7.30605800	-1.17162300
H	12.91878800	-4.48184200	0.80688800	H	-13.38802700	-5.85820000	-1.67899500
H	13.65211400	-2.97437900	1.32655900	O	-6.02121500	-0.52320300	-0.55744000
C	14.91219500	-4.16953800	0.05127700	C	-7.24716200	-0.25830800	-0.36012900
H	14.82994800	-4.86930700	-0.78619300	N	-5.45975600	1.94294900	-0.10150900
H	15.40284300	-4.69301700	0.87612500	H	-5.25832200	0.94218300	-0.32186700
H	15.56854700	-3.35192400	-0.26256500	O	6.91133500	-0.63937400	1.06235700
O	-0.77683700	2.81767200	-0.19255200	N	5.16279900	0.57988200	-0.05185600
C	-2.06785000	3.31123900	-0.04241400	H	5.87296900	-0.01475000	0.73616200
C	-3.11952200	2.41214200	-0.10405500				

S₀; **DE to DK**, TS, E= -1915.924409 hartree (mPW1PW91)



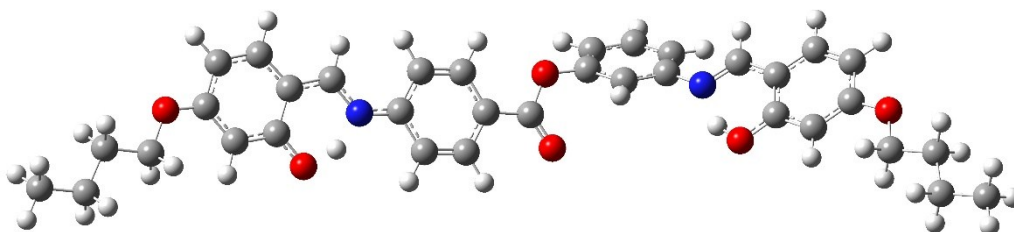
O	0.49262300	-3.18470700	1.96268800	O	0.85831300	-2.66300900	-0.20637700
N	-5.15605000	-0.68942800	0.27072300	N	5.53679000	-1.76032400	-0.17116500
C	-1.26316400	-2.18429800	0.69070400	C	2.15520600	-3.16138900	-0.14580000
C	-2.15835900	-2.17827300	1.76667700	C	3.19708400	-2.24867600	-0.14621300
H	-1.83576800	-2.57183800	2.72349000	H	2.98922000	-1.18513900	-0.13975200
C	-3.43932800	-1.67781000	1.60985600	C	4.51654200	-2.71508700	-0.16978500
H	-4.13559000	-1.67784600	2.44105500	C	4.76259700	-4.09407600	-0.16909800
C	-3.85591600	-1.17647300	0.36770900	H	5.77665500	-4.47440400	-0.14060500
C	-2.95370600	-1.16385500	-0.70732300	C	3.69543900	-4.98621500	-0.17547600
H	-3.23820500	-0.74076300	-1.66336200	H	3.89302300	-6.05237100	-0.17306300
C	-1.67304100	-1.66934800	-0.54498700	C	2.37880100	-4.53256400	-0.16928400
H	-0.98118900	-1.65303800	-1.37809500	H	1.54413900	-5.22277300	-0.17045000
C	0.09124600	-2.73032400	0.91475200	O	6.20700000	0.69080000	0.43489900
O	-7.21805000	0.25020300	1.57618500	H	5.47517900	-0.49101100	0.23506800
H	-5.96731300	-0.30465600	1.26480700	O	10.73118900	1.95457800	-0.34090200
O	-10.97771700	1.60715600	-1.00466500	C	7.74132800	-0.91703900	-0.47225300
C	-7.13935600	0.05023200	-0.81556200	C	7.40514400	0.39315800	0.03187500
C	-7.79292800	0.40631200	0.42342600	C	8.42567500	1.37312700	0.07725900
C	-9.10313500	0.93744800	0.35862400	H	8.15639300	2.34904700	0.45867200
H	-9.57672100	1.19928100	1.29527800	C	9.70927000	1.07800600	-0.35328200
C	-9.73726000	1.10786900	-0.86123500	C	10.04026800	-0.20957300	-0.85286600
C	-9.09783300	0.75370600	-2.08054400	H	11.05495200	-0.39973200	-1.18014400
H	-9.62944500	0.90170900	-3.01234800	C	9.06782200	-1.17046600	-0.90557100
C	-7.83265300	0.23820100	-2.04049300	H	9.30904900	-2.15927500	-1.28530000
H	-7.33369400	-0.03614200	-2.96558900	C	6.77520300	-1.94658200	-0.55075300
C	-5.83528500	-0.48750500	-0.83306900	H	7.07710100	-2.91348000	-0.95532100
H	-5.39627400	-0.75530000	-1.79455800	C	10.50413400	3.27965800	0.14037600
C	-11.70941600	1.99743200	0.15870100	H	10.15687300	3.23401000	1.17959900
H	-11.14782400	2.77012300	0.69720200	H	9.72329700	3.75656100	-0.46420500
H	-11.82706700	1.13077600	0.82016000	C	11.80761900	4.04357300	0.03908900
C	-13.05676200	2.52229200	-0.29042200	H	12.57280100	3.52086300	0.62410400
H	-12.90055600	3.36134200	-0.97784600	H	12.14332600	4.03739300	-1.00412100
H	-13.57411100	1.73836000	-0.85501100	C	11.67022100	5.48239400	0.53179500
C	-13.91965900	2.96956700	0.88737800	H	11.32352300	5.48034200	1.57233400
H	-13.38960900	3.74431300	1.45459300	H	10.89413200	5.99473700	-0.04972900
H	-14.06211300	2.12775300	1.57582200	C	12.97674200	6.26247700	0.43332100
C	-15.27927800	3.50223600	0.44823000	H	13.76309400	5.79210100	1.03183300
H	-15.16913400	4.36615500	-0.21457600	H	12.85400200	7.28817100	0.79119800
H	-15.87848900	3.81545400	1.30729300	H	13.33073300	6.31010500	-0.60121000
H	-15.84600800	2.73845300	-0.09329200				

S₁; DE* to DK*, TS, E= -1915.828874 hartree (mPW1PW91)



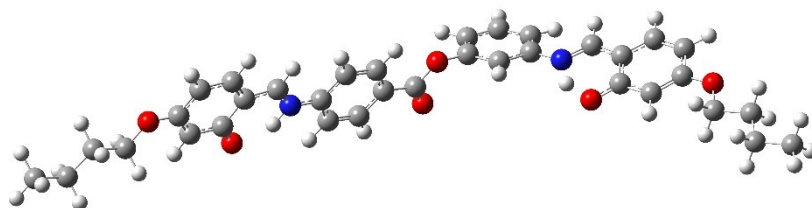
O	-0.89444900	-1.77135000	-1.99621800	O	-0.80438000	-2.94020900	-0.05129400
N	5.07042000	-0.59592000	-0.03618000	N	-5.47425500	-1.83360600	-0.03488700
C	1.11394100	-1.75798800	-0.71174900	C	-2.12859100	-3.32416800	-0.16041400
C	1.81319600	-0.94763100	-1.63523200	C	-3.14780200	-2.38406300	-0.08920400
H	1.30501300	-0.62300300	-2.53561500	H	-2.92040100	-1.32843900	-0.00702000
C	3.11543700	-0.57571100	-1.39706500	C	-4.47825400	-2.81334200	-0.11106900
H	3.64796800	0.04676400	-2.10858100	C	-4.76811600	-4.18032900	-0.22728200
C	3.78488900	-0.99720400	-0.21714100	H	-5.79493300	-4.52006000	-0.29677800
C	3.08078500	-1.81357300	0.71186600	C	-3.72911300	-5.10190700	-0.28860200
H	3.56112900	-2.15360200	1.62126700	H	-3.95597300	-6.15829600	-0.38167300
C	1.77706200	-2.18012200	0.46078300	C	-2.40014300	-4.68464400	-0.25340300
H	1.24990100	-2.80144800	1.17463700	H	-1.58199000	-5.39286100	-0.30828200
C	-0.26594700	-2.12183200	-1.01376800	O	-6.17053300	0.61849500	-0.56359500
O	6.86735200	0.75129100	-1.16583700	H	-5.47819800	-0.48058300	-0.44070500
H	5.75639300	0.12745700	-0.83183800	O	-10.62617100	1.89883100	0.52651400
O	11.12928000	1.20597000	0.93221700	C	-7.65313500	-0.99288300	0.42358900
C	7.21995300	-0.31491100	0.94270200	C	-7.35049000	0.31670500	-0.08129300
C	7.66916000	0.50235200	-0.18502100	C	-8.35663100	1.30457700	-0.05019100
C	8.98809500	1.02024900	-0.19757400	H	-8.10512100	2.28317000	-0.43679500
H	9.27012600	1.61750000	-1.05448100	C	-9.61349100	1.01258100	0.46170200
C	9.85989500	0.76021800	0.85291600	C	-9.91653800	-0.27659300	0.96462000
C	9.42579100	-0.02619100	1.94175300	H	-10.90766500	-0.46744400	1.35730100
H	10.11667600	-0.21958800	2.75380200	C	-8.94614100	-1.24481600	0.93990400
C	8.12627500	-0.54689800	1.97058100	H	-9.16770500	-2.23669000	1.32357400
H	7.82305800	-1.14814000	2.82158300	C	-6.67864300	-2.02903500	0.42134300
C	5.88684200	-0.85713400	0.98115700	H	-6.95885200	-3.00162900	0.83199800
H	5.57378300	-1.46119000	1.82655900	C	-10.41799000	3.22739800	0.04725700
C	11.64183100	2.00342800	-0.13574800	H	-10.14049000	3.19225100	-1.01320300
H	11.02379000	2.90338000	-0.24470300	H	-9.59459600	3.69017900	0.60460900
H	11.58883600	1.43259100	-1.07131200	C	-11.70432400	4.00193500	0.24333600
C	13.07336300	2.36797500	0.19508500	H	-12.51143400	3.49372200	-0.29637800
H	13.09211700	2.90347000	1.15095300	H	-11.97082900	3.98532900	1.30624100
H	13.65224600	1.44769100	0.33210000	C	-11.58548600	5.44568900	-0.23958100
C	13.71249000	3.22662900	-0.89413900	H	-11.30688700	5.45401400	-1.30035000
H	13.12041600	4.13918200	-1.03397700	H	-10.76858300	5.94378800	0.29664400
H	13.67914900	2.68874300	-1.84932200	C	-12.87546100	6.23572500	-0.04710200
C	15.15502400	3.60135200	-0.57207700	H	-13.70323300	5.77998000	-0.59929900
H	15.21607000	4.16900500	0.36160400	H	-12.76639800	7.26490400	-0.39939300
H	15.59101500	4.21521900	-1.36460200	H	-13.16148200	6.27292800	1.00867700
H	15.77874500	2.70913100	-0.45969900				

S₁; DE* to MK-C*, TS, E= -1915.841877 hartree (mPW1PW91)



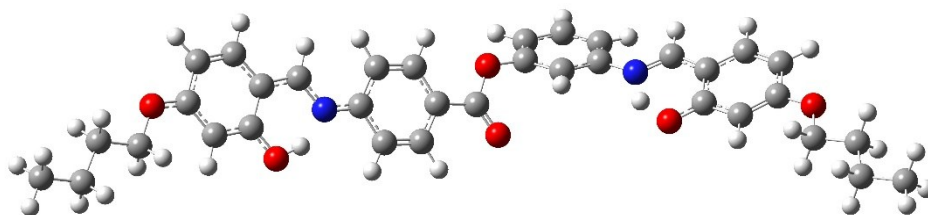
O	0.89739400	-1.53041700	2.01542100	O	0.76121600	-2.83698500	0.16038800
N	-5.12565900	-0.53083100	0.14816000	N	5.43474100	-1.70924200	0.07676100
C	-1.14417600	-1.62162500	0.78901000	C	2.09095200	-3.20994200	0.23829500
C	-1.82008000	-0.73921900	1.66462300	C	3.10837300	-2.26784700	0.16443100
H	-1.28576200	-0.34005400	2.51874200	H	2.88363200	-1.21015400	0.11194700
C	-3.12989700	-0.39247200	1.43610300	C	4.44065200	-2.69500800	0.14473200
H	-3.64574600	0.28573200	2.10780300	C	4.73078800	-4.06513100	0.23293400
C	-3.83814800	-0.91282100	0.31575500	H	5.76095400	-4.40085900	0.27562800
C	-3.15296600	-1.80402900	-0.56385600	C	3.69420600	-4.98963800	0.30727400
H	-3.65764000	-2.22100600	-1.42677300	H	3.92271100	-6.04734200	0.38175100
C	-1.84049000	-2.14218200	-0.32429100	C	2.36527700	-4.57245700	0.30556100
H	-1.33023100	-2.81808200	-0.99980300	H	1.54811300	-5.28133600	0.36818800
C	0.24666800	-1.95542400	1.07719400	O	6.37196900	0.57987600	0.80266200
O	-6.94837200	0.91745400	1.16757200	H	5.74656500	-0.19959500	0.69885600
H	-5.89274900	0.32740200	0.92503900	O	10.72443800	1.78207500	-0.72461200
O	-11.22029600	1.07448700	-0.93702800	C	7.59606000	-0.94402100	-0.58718900
C	-7.29547100	-0.37733700	-0.82200300	C	7.47461400	0.28629300	0.10826300
C	-7.75437300	0.54789500	0.21488700	C	8.51237500	1.22252000	0.07899200
C	-9.07259700	1.04524200	0.18892800	H	8.37802300	2.14726000	0.62371600
H	-9.35823900	1.72669800	0.97915800	C	9.67291500	0.94327800	-0.64015000
C	-9.94575500	0.66052000	-0.81896800	C	9.81045700	-0.27288800	-1.34055600
C	-9.51057400	-0.23715500	-1.82704100	H	10.72372900	-0.46156900	-1.89145400
H	-10.21038500	-0.52360800	-2.60321500	C	8.78313400	-1.18827200	-1.30590000
C	-8.21279700	-0.73552300	-1.81496100	H	8.88291800	-2.12717800	-1.84249000
H	-7.90300800	-1.42097100	-2.59697200	C	6.53884800	-1.91919400	-0.56245300
C	-5.95939600	-0.89945900	-0.82500700	H	6.70237000	-2.84544500	-1.12421700
H	-5.65922900	-1.58075500	-1.61592200	C	10.67023600	3.03405800	-0.04083400
C	-11.74079500	1.98250200	0.03533200	H	10.52974300	2.85707500	1.03246800
H	-11.13493700	2.89700700	0.03464800	H	9.81613800	3.61449300	-0.41053100
H	-11.67339400	1.52363200	1.02949500	C	11.97049200	3.76551500	-0.30020400
C	-13.17934600	2.28502600	-0.32558200	H	12.80351500	3.14458800	0.04835800
H	-13.21149500	2.70722100	-1.33625100	H	12.09729000	3.89285800	-1.38124800
H	-13.74461700	1.34666800	-0.35195300	C	12.01173400	5.12620900	0.39149800
C	-13.82537500	3.25333000	0.66308100	H	11.87138500	4.99133600	1.47086400
H	-13.24609700	4.18410700	0.69378200	H	11.16883800	5.73694300	0.04586700
H	-13.77907300	2.82845700	1.67311600	C	13.31709500	5.87274300	0.13852000
C	-15.27496900	3.56844500	0.31038600	H	14.17576700	5.30098700	0.50402800
H	-15.34936700	4.02542300	-0.68123500	H	13.32322800	6.84255700	0.64309700
H	-15.71578900	4.26218100	1.03107800	H	13.46838800	6.05184300	-0.93053200
H	-15.88592800	2.66049400	0.30447200				

S₁; **MK-C* to DK***, TS, E= -1915.838386 hartree (mPW1PW91)



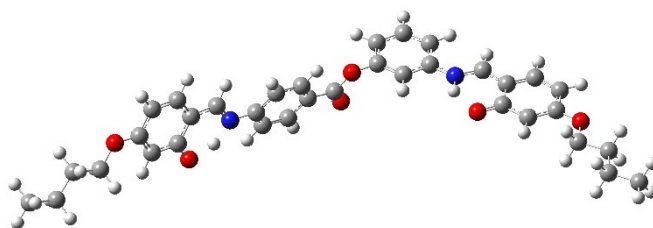
O	-0.38951400	-3.31793200	-1.83211400	C	-3.21868000	-2.17045500	0.17220900
C	1.28878700	-2.15507600	-0.60063300	H	-3.03661300	-1.10253000	0.14050300
C	2.25752500	-2.27284500	-1.62000200	C	-4.52633600	-2.66715900	0.21382300
H	1.99212800	-2.78030600	-2.53997400	C	-4.74118800	-4.05062200	0.24311800
C	3.52163600	-1.75342100	-1.45274300	H	-5.74619500	-4.45520300	0.22718000
H	4.26007100	-1.84949900	-2.24236000	C	-3.65170300	-4.91583200	0.26148400
C	3.86892000	-1.09215000	-0.25199100	H	-3.82317800	-5.98643500	0.28181600
C	2.90217100	-0.96877100	0.77362700	C	-2.34665800	-4.43151800	0.23877000
H	3.13678700	-0.46561700	1.70349200	H	-1.49777900	-5.10371000	0.24857600
C	1.63894800	-1.49364300	0.59271900	O	-6.30598600	0.67531700	-0.47572600
H	0.90428800	-1.39513300	1.38256200	H	-5.54374600	-0.48214800	-0.24518600
C	-0.03512400	-2.72639000	-0.82950600	O	-10.85698500	1.84831600	0.29096400
O	11.03316200	1.92671900	0.89642000	C	-7.79220100	-0.93951500	0.49593700
C	7.07395000	0.50480600	0.82368100	C	-7.49338500	0.36102300	-0.05389300
C	7.91738200	0.27978400	-0.34478800	C	-8.53964300	1.31224200	-0.12429300
C	9.26370800	0.76998600	-0.30814800	H	-8.29868400	2.28121600	-0.54079500
H	9.86079200	0.58636900	-1.19191100	C	-9.81206400	0.99914100	0.32625400
C	9.77671500	1.44763500	0.80963100	C	-10.10558700	-0.27816000	0.87249900
C	8.95407900	1.65211000	1.91586700	H	-11.11245800	-0.48347300	1.21448600
H	9.34218000	2.17423200	2.78176500	C	-9.10788700	-1.21174600	0.94885900
C	7.62112300	1.17822900	1.90171300	H	-9.32074000	-2.19308400	1.36338600
H	7.00919600	1.35631500	2.78105700	C	-6.79904800	-1.94213500	0.59697200
C	5.71031100	0.05250400	0.88334400	H	-7.07217500	-2.90390700	1.03299900
H	5.12531500	0.23980600	1.77442300	C	-10.66944400	3.15850900	-0.24428700
C	11.92301600	1.74404400	-0.20702000	H	-10.32574000	3.08092700	-1.28282600
H	11.49808300	2.21837200	-1.09989900	H	-9.89967100	3.68142700	0.33605600
H	12.04158100	0.67192900	-0.40568900	C	-11.99374400	3.88873200	-0.16682300
C	13.25086100	2.37378600	0.15648700	H	-12.74658100	3.31954900	-0.72386300
H	13.09165200	3.43452500	0.38081700	H	-12.32357100	3.91763400	0.87788500
H	13.62678900	1.90569200	1.07321500	C	-11.90090300	5.30840300	-0.72154300
C	14.28045800	2.22735700	-0.96182100	H	-11.56008300	5.27147900	-1.76338000
H	13.89115400	2.68569600	-1.87899900	H	-11.13678000	5.86741200	-0.16781000
H	14.42579300	1.16385600	-1.18702400	C	-13.22893900	6.05410900	-0.64767400
C	15.62215800	2.85966200	-0.60807400	H	-14.00465100	5.53595100	-1.22005200
H	15.51372800	3.93061100	-0.41051700	H	-13.13810100	7.06656200	-1.05003600
H	16.34212800	2.74212500	-1.42223200	H	-13.57835700	6.13600000	0.38626800
H	16.05194900	2.39871400	0.28665500	O	7.48218500	-0.33095300	-1.36855700
O	-0.87716200	-2.51590900	0.23314800	N	5.14355800	-0.59486900	-0.13500600
N	-5.56988700	-1.73661300	0.19987100	H	5.80199200	-0.71496700	-0.92434800
C	-2.15117700	-3.05503600	0.18568100				

S₁; DE* to MK-O*, TS, E= -1915.829211 hartree (mPW1PW91)



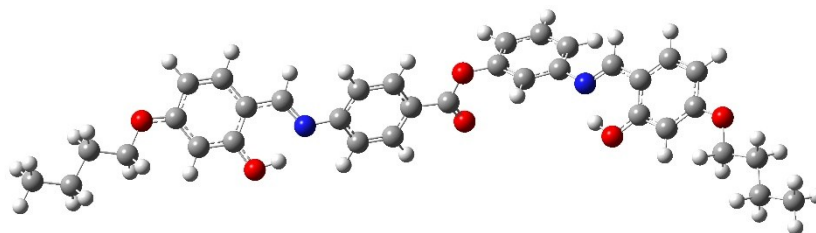
O	0.99643500	-1.60404200	1.95467800	O	0.79022900	-2.93094600	0.11856000
N	-5.04960900	-0.49862900	0.23654500	N	5.47442000	-1.87322000	-0.02131600
C	-1.07545700	-1.67035100	0.77887900	C	2.11342800	-3.32064900	0.16090500
C	-1.71474800	-0.76724500	1.66532100	C	3.14411000	-2.39126100	0.09380800
H	-1.15163000	-0.37218100	2.50261100	H	2.93149200	-1.33020600	0.06733600
C	-3.02111400	-0.39933200	1.46419100	C	4.46708500	-2.84067200	0.04903800
H	-3.51141800	0.29284100	2.14059000	C	4.74308000	-4.21461800	0.09070500
C	-3.77419900	-0.91234700	0.36232200	H	5.76579900	-4.57219600	0.10690100
C	-3.11768100	-1.82731900	-0.52673900	C	3.69294300	-5.12370100	0.14575800
H	-3.64699600	-2.24294600	-1.37521200	H	3.90725000	-6.18617100	0.18004000
C	-1.80813800	-2.18751900	-0.31490600	C	2.37032600	-4.68806700	0.17940300
H	-1.32504200	-2.87789700	-0.99582500	H	1.54443300	-5.38743000	0.23091900
C	0.31357100	-2.02639300	1.03743400	O	6.15989200	0.58884100	0.51674600
O	-6.86500700	0.96280900	1.21094800	H	5.42547000	-0.60010900	0.37401600
H	-5.96956200	0.47603900	1.04336000	O	10.61796200	1.88099200	-0.54542100
O	-11.11985800	1.07401500	-0.91982400	C	7.65039500	-1.01649200	-0.46387900
C	-7.21107100	-0.37189900	-0.75824400	C	7.33389300	0.29640100	0.04563000
C	-7.67968300	0.56921700	0.24847100	C	8.34707200	1.28509100	0.01857200
C	-8.98228300	1.06760700	0.21647700	H	8.09283900	2.26296500	0.40534200
H	-9.27490200	1.76494000	0.98998200	C	9.60448700	0.99568100	-0.48629700
C	-9.85129300	0.66105400	-0.79188000	C	9.91541800	-0.29433200	-0.99177300
C	-9.41664600	-0.25873300	-1.78712100	H	10.90967800	-0.48004500	-1.37891100
H	-10.11884400	-0.55456100	-2.55750700	C	8.94959600	-1.26383600	-0.97475300
C	-8.13134800	-0.75329100	-1.75986100	H	9.17586300	-2.25444300	-1.35913500
H	-7.81034200	-1.45402300	-2.52336700	C	6.68861700	-2.05428100	-0.47259200
C	-5.88380400	-0.88756100	-0.73780100	H	6.97157800	-3.02382900	-0.88461400
H	-5.58991800	-1.58543600	-1.51880300	C	10.40828000	3.20893100	-0.06490300
C	-11.65208300	2.00097200	0.03100000	H	10.12515500	3.17167300	0.99395800
H	-11.04788300	2.91599500	0.01520100	H	9.58773900	3.67275900	-0.62551300
H	-11.59029000	1.56063900	1.03345700	C	11.69604700	3.98302700	-0.25307500
C	-13.08831900	2.29042300	-0.34846800	H	12.50018400	3.47329900	0.28965500
H	-13.11331200	2.69387600	-1.36687500	H	11.96788500	3.96844600	-1.31466400
H	-13.64966200	1.34952600	-0.36186300	C	11.57566600	5.42587600	0.23217300
C	-13.74578500	3.27433800	0.61711800	H	11.29175200	5.43219200	1.29154400
H	-13.16998800	4.20756100	0.63573600	H	10.76173300	5.92554100	-0.30709400
H	-13.70667900	2.86788700	1.63497700	C	12.86705600	6.21552600	0.04777300
C	-15.19338100	3.57764400	0.24640200	H	13.69179300	5.75812600	0.60314300
H	-15.26096100	4.01633800	-0.75389500	H	12.75686800	7.24404100	0.40165700
H	-15.64247500	4.28273800	0.95072900	H	13.15836900	6.25474600	-1.00648800
H	-15.80111500	2.66755900	0.25198500				

S₁; **MK-O* to DK***, TS, E= -1915.832456 hartree (mPW1PW91)



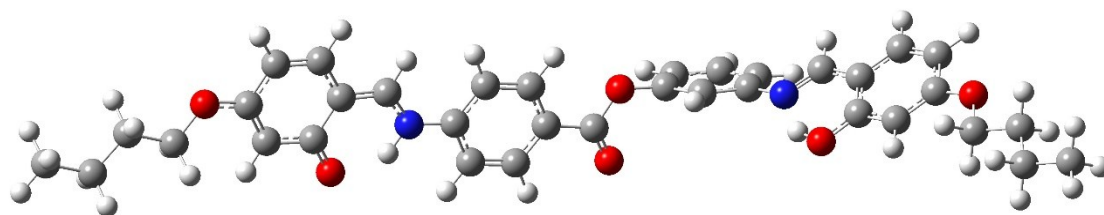
O	0.49605200	-3.30711500	1.84009500	O	0.86534200	-2.68190400	-0.30115500
N	-5.14236300	-0.71673500	0.25390700	C	2.15687000	-3.20136300	-0.27278800
C	-1.25449600	-2.24098800	0.61469400	C	3.20635500	-2.30818800	-0.21530000
C	-2.14776100	-2.27037400	1.69180300	H	3.00710100	-1.24543400	-0.13355300
H	-1.82511200	-2.70018400	2.63289900	C	4.53116300	-2.79293300	-0.26498900
C	-3.42711000	-1.75910000	1.55593900	C	4.75226900	-4.18298200	-0.37249100
H	-4.12195300	-1.78639200	2.38792100	H	5.75611700	-4.58572500	-0.41490900
C	-3.84381700	-1.21210300	0.33334500	C	3.66775600	-5.04746100	-0.43009600
C	-2.94340700	-1.16357700	-0.74201200	H	3.84721200	-6.11380500	-0.51478400
H	-3.22815300	-0.70411800	-1.68109100	C	2.35493200	-4.57764300	-0.38504900
C	-1.66440500	-1.67939100	-0.60045600	H	1.50910200	-5.25198900	-0.43195900
H	-0.97365300	-1.63560500	-1.43345900	O	10.75934300	2.01810200	-0.01854100
C	0.09864600	-2.80193400	0.81365600	C	7.81413100	-0.99768900	-0.16957500
O	-7.19112200	0.21124100	1.58556400	C	7.38795300	0.39716000	-0.09700700
H	-5.94603600	-0.34727300	1.25744400	C	8.39883900	1.40957300	-0.04557200
O	-10.95021100	1.65101300	-0.95203700	H	8.04399100	2.43078100	0.00799000
C	-7.12436400	0.05893600	-0.80967300	C	9.77078500	1.09824500	-0.06426700
C	-7.76979100	0.39545500	0.43888400	C	10.15807600	-0.23523600	-0.13318700
C	-9.07579600	0.93876900	0.39020600	H	11.21114400	-0.48860200	-0.14714200
H	-9.54333900	1.18607500	1.33385800	C	9.17408500	-1.25525000	-0.18402600
C	-9.71339400	1.13846000	-0.82342800	H	9.51582800	-2.28489700	-0.23655300
C	-9.08211800	0.80288000	-2.05211300	C	6.87876000	-2.08827000	-0.22636300
H	-9.61634900	0.97352900	-2.97853700	H	7.24540800	-3.10436300	-0.28304100
C	-7.82097700	0.27640900	-2.02763500	C	10.41433300	3.40144400	0.05288900
H	-7.32803400	0.01630700	-2.96004500	H	9.81623000	3.58389600	0.95422400
C	-5.82415000	-0.48772000	-0.84287200	H	9.81291800	3.67482200	-0.82292200
H	-5.39024900	-0.73964600	-1.81097900	C	11.69982100	4.20078600	0.09124300
C	-11.67378100	2.02571700	0.22136400	H	12.29241600	3.87926600	0.95519900
H	-11.10360400	2.78367300	0.77167300	H	12.28843900	3.96995800	-0.80387800
H	-11.79609800	1.14805800	0.86728800	C	11.44013800	5.70345900	0.16952300
C	-13.01842900	2.56991200	-0.21266400	H	10.84087200	5.92414800	1.06119400
H	-12.85772100	3.41975400	-0.88565200	H	10.83648600	6.01487700	-0.69159100
H	-13.54452400	1.80059800	-0.78916000	C	12.72805800	6.51889500	0.20859200
C	-13.87315500	3.00334600	0.97620500	H	13.33724300	6.25259000	1.07793400
H	-13.33468600	3.76369600	1.55485100	H	12.51732900	7.59014300	0.26474900
H	-14.01991700	2.15075700	1.65033800	H	13.33293600	6.34427600	-0.68664800
C	-15.23000900	3.55464100	0.55170300	O	6.15724100	0.71636800	-0.07957000
H	-15.11525200	4.42891500	-0.09659200	N	5.55195200	-1.87658000	-0.20701100
H	-15.82334800	3.85792200	1.41837500	H	5.32600100	-0.87074800	-0.14680800
H	-15.80509200	2.80498700	-0.00065200				

Fig. S6: S_0 ; **4-4 (DE)** $E = -1916.269659$ hartree (6-311++G(d)-mPW1PW91)



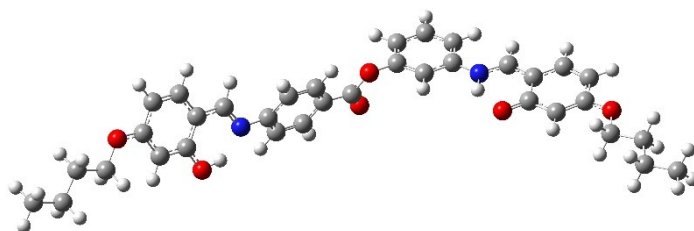
O	0.65081300	-2.56075800	2.16019300	O	0.75065800	-2.55737200	-0.09027800
N	-5.19676800	-0.46172600	0.61051300	N	5.43151800	-1.58324300	-0.11502900
C	-1.25745700	-1.86639800	0.91370900	C	2.06293100	-3.01922200	-0.06531400
C	-2.02130300	-1.60326700	2.05426500	C	3.09371700	-2.09852400	-0.06498000
H	-1.58301300	-1.76696300	3.03126500	H	2.88206600	-1.03667700	-0.03046300
C	-3.31588100	-1.13506300	1.93763000	C	4.41603300	-2.54613000	-0.12742200
H	-3.90966200	-0.92612400	2.81987900	C	4.67099200	-3.92177300	-0.15185700
C	-3.88831600	-0.94063200	0.67424800	H	5.69292000	-4.28289500	-0.14136100
C	-3.11466200	-1.18542000	-0.46793400	C	3.61755000	-4.82609200	-0.14642600
H	-3.52350500	-0.98274400	-1.45124400	H	3.82481600	-5.89022300	-0.15893100
C	-1.81456000	-1.64629800	-0.34774000	C	2.30037900	-4.38449600	-0.10988300
H	-1.22369400	-1.82557300	-1.23682700	H	1.47069700	-5.08083300	-0.10332600
C	0.12343400	-2.35603500	1.09711600	O	6.48657900	0.61581000	0.81140000
O	-7.08221200	1.16567000	1.39804300	H	5.82003300	-0.10809200	0.67085600
H	-6.20280100	0.70474800	1.37807300	O	10.83116600	1.77955100	-0.72831400
O	-11.19966600	1.05196800	-0.97282000	C	7.60152300	-0.81902100	-0.75452500
C	-7.33656800	-0.34966100	-0.44443800	C	7.55194000	0.33972900	0.05598600
C	-7.83172700	0.65842400	0.41723800	C	8.62504300	1.22956400	0.08274600
C	-9.12771900	1.14740000	0.26074000	H	8.54312200	2.10109000	0.71749700
H	-9.46361000	1.91745700	0.94147000	C	9.75165600	0.97890500	-0.69298700
C	-9.94097900	0.64107100	-0.74745700	C	9.81710500	-0.16651300	-1.50775600
C	-9.46668200	-0.36414800	-1.61160800	H	10.70535100	-0.33829500	-2.10264000
H	-10.12113700	-0.74160100	-2.38717600	C	8.75603600	-1.03752200	-1.52771500
C	-8.19000900	-0.84002600	-1.45049400	H	8.80278200	-1.92288800	-2.15408400
H	-7.82038700	-1.61546000	-2.11398800	C	6.51152800	-1.75535800	-0.79636500
C	-6.00575500	-0.86926400	-0.30821100	H	6.63267600	-2.62460500	-1.45131600
H	-5.70672000	-1.65122400	-1.01388400	C	10.84495100	2.95833500	0.07390600
C	-11.75826100	2.06756000	-0.14133900	H	10.72094000	2.68197200	1.12651300
H	-11.14419700	2.97174400	-0.21180600	H	10.00621300	3.60200800	-0.21265100
H	-11.75078500	1.72768900	0.89985700	C	12.16443300	3.66164500	-0.14670500
C	-13.16922400	2.33486200	-0.61250300	H	12.97960700	2.97807500	0.11209600
H	-13.14181700	2.63347300	-1.66550600	H	12.27178800	3.89160700	-1.21177000
H	-13.74296100	1.40364400	-0.56364800	C	12.27678800	4.94028100	0.67583600
C	-13.85664100	3.41391300	0.21653700	H	12.15598700	4.70319000	1.73893900
H	-13.27069200	4.33888800	0.17157500	H	11.45106400	5.61379600	0.41994600
H	-13.86879000	3.11380400	1.27044200	C	13.60192200	5.65827200	0.46344500
C	-15.27913400	3.69131300	-0.24847900	H	14.44690200	5.02354600	0.74408300
H	-15.29847000	4.02812300	-1.28857500	H	13.66085600	6.57009900	1.06207300
H	-15.75192900	4.46678600	0.35842800	H	13.73684100	5.94142500	-0.58405300
H	-15.90094600	2.79439100	-0.18150800				

S₀; **MK-C** E= -1916.270369 hartree (6-311++G(d)-mPW1PW91)



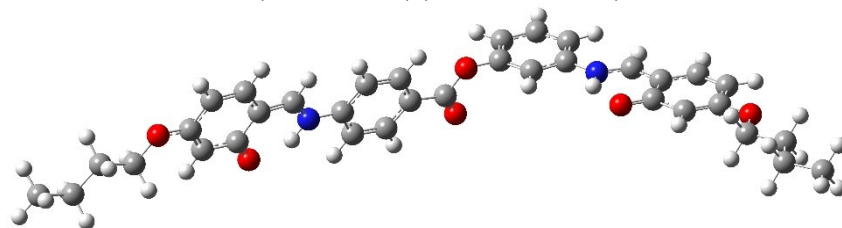
O	-0.42314000	-3.11157800	-1.92947200	C	-3.13068700	-2.10153800	0.11648300
C	1.32846800	-2.10197100	-0.67249700	H	-2.91422600	-1.04130400	0.06688300
C	2.23485100	-2.13489900	-1.73435700	C	-4.45564900	-2.54546000	0.15349600
H	1.92316500	-2.55215800	-2.68389100	C	-4.71355500	-3.91962000	0.19567000
C	3.51479000	-1.64127400	-1.57977200	H	-5.73528100	-4.28003900	0.16443700
H	4.21240200	-1.67001700	-2.40934800	C	-3.66137900	-4.82520600	0.23601300
C	3.91958600	-1.10037100	-0.35350600	H	-3.87090500	-5.88862700	0.26244600
C	3.01605600	-1.06608600	0.71344300	C	-2.34309700	-4.38730200	0.22965600
H	3.29691500	-0.65579900	1.67482600	H	-1.51710000	-5.08702000	0.26111600
C	1.73524900	-1.56270400	0.54974400	O	-6.49141500	0.61095100	-0.87983400
H	1.04357100	-1.53102300	1.38142800	H	-5.83184300	-0.11400900	-0.71420700
C	-0.02753700	-2.64141700	-0.89412400	O	-10.86670500	1.81077000	0.54166200
O	11.00755300	1.82723300	0.94886900	C	-7.65039100	-0.80062200	0.67488500
C	7.12785600	0.39528400	0.76382600	C	-7.57628600	0.34832100	-0.14759100
C	7.95057800	0.27393500	-0.44146600	C	-8.64442000	1.24227800	-0.21053700
C	9.28815100	0.77311800	-0.36062000	H	-8.54355400	2.10612500	-0.85304000
H	9.89415600	0.68338800	-1.25208700	C	-9.79044200	1.00522000	0.54072500
C	9.76818000	1.33671200	0.79651300	C	-9.88074200	-0.13071700	1.36635900
C	8.95451500	1.44815900	1.96857300	H	-10.78390300	-0.29193400	1.94140800
H	9.38280300	1.90053800	2.85406200	C	-8.82426200	-1.00563700	1.42222600
C	7.67933500	0.98893900	1.93866400	H	-8.88996600	-1.88342000	2.05750600
H	7.05449800	1.07032500	2.82299100	C	-6.56503900	-1.73963400	0.75590000
C	5.81820500	-0.05485900	0.78386000	H	-6.70501200	-2.59909100	1.41993100
H	5.23681400	0.05240100	1.69278100	C	-10.85536800	2.98313600	-0.26998700
C	11.91166300	1.77538400	-0.15369600	H	-10.70994500	2.69778800	-1.31745300
H	11.47998300	2.32179800	-0.99882100	H	-10.01921800	3.62402000	0.03005800
H	12.05064500	0.73210800	-0.45615500	C	-12.17515600	3.69568700	-0.08350900
C	13.21986600	2.39406300	0.28213200	H	-12.98846400	3.01497900	-0.35539100
H	13.03507600	3.42097400	0.61392900	H	-12.30448000	3.93358200	0.97738100
H	13.60160900	1.84618700	1.14984100	C	-12.26235600	4.96934800	-0.91679100
C	14.25764400	2.38752200	-0.83468600	H	-12.12012900	4.72455900	-1.97548700
H	13.86384300	2.92719000	-1.70335900	H	-11.43851700	5.63999200	-0.64758200
H	14.42850400	1.35819200	-1.16963400	C	-13.58765600	5.69597500	-0.73748200
C	15.58009000	3.00869500	-0.40815100	H	-14.42998400	5.06411900	-1.03218800
H	15.44914900	4.05003400	-0.10135400	H	-13.62863100	6.60426200	-1.34294200
H	16.30780200	2.99363300	-1.22269400	H	-13.74336400	5.98650700	0.30508800
H	16.01823200	2.46958900	0.43627100	O	7.49704100	-0.24455900	-1.49504000
O	-0.79756000	-2.54231200	0.21911800	N	5.22295300	-0.61843400	-0.26475600
N	-5.46780500	-1.58044900	0.09921900	H	5.84863000	-0.67680400	-1.08232100
C	-2.10198000	-3.02294300	0.16425500				

S₀; **MK-O** E= -1916.270129 hartree (6-311++G(d)-mPW1PW91)



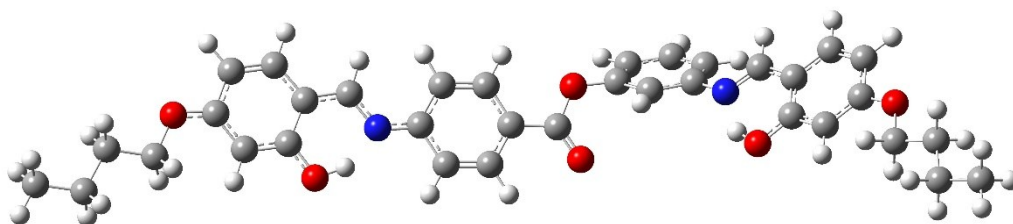
O	0.51912900	-3.43917700	1.87205900	O	0.84566700	-2.72037900	-0.23892100
N	-5.13244200	-0.74399300	0.53478400	C	2.14290100	-3.21206100	-0.25126000
C	-1.25342800	-2.32209600	0.73736100	C	3.17592100	-2.29472800	-0.21048500
C	-2.12912200	-2.41269800	1.82320500	H	2.95270300	-1.23841700	-0.11703300
H	-1.79384800	-2.89770700	2.73190400	C	4.49591300	-2.74195200	-0.29834500
C	-3.40285400	-1.88449200	1.74133300	C	4.75419500	-4.10834100	-0.41813500
H	-4.08285400	-1.94856300	2.58278700	H	5.76682800	-4.48675100	-0.47168800
C	-3.84170800	-1.27059900	0.56122700	C	3.69588300	-5.00538200	-0.46059200
C	-2.95633700	-1.16388300	-0.51962200	H	3.90447000	-6.06476700	-0.55451800
H	-3.26064600	-0.63922300	-1.41802100	C	2.37859900	-4.57185300	-0.38113600
C	-1.67763400	-1.68717900	-0.43203600	H	1.55257200	-5.27079300	-0.41546000
H	-0.99991500	-1.59197200	-1.27068400	O	10.64719100	2.02885000	-0.18957800
C	0.09972100	-2.89105200	0.88589000	C	7.72443600	-0.89929500	-0.35501900
O	-7.07467800	0.60272200	1.64290800	C	7.29152700	0.46981100	-0.08089400
H	-6.20176200	0.13781800	1.55141800	C	8.31324600	1.46864000	-0.02604900
O	-10.91672500	1.48548200	-1.01069800	H	7.99142500	2.48097600	0.17855700
C	-7.14732300	-0.18991600	-0.62046900	C	9.63451500	1.14738700	-0.22522800
C	-7.72070200	0.49060000	0.48076700	C	10.04445900	-0.19503800	-0.49538800
C	-8.98756300	1.06249100	0.37573100	H	11.09795400	-0.39511800	-0.64503600
H	-9.38578500	1.57211300	1.24225500	C	9.10821900	-1.17570700	-0.55560700
C	-9.69392800	0.96454500	-0.81822000	H	9.41061400	-2.19857000	-0.75965200
C	-9.14083400	0.28919900	-1.92299400	C	6.80640400	-1.93857200	-0.42576600
H	-9.71266000	0.22709900	-2.84030200	H	7.16041400	-2.94217000	-0.63525800
C	-7.89388800	-0.27183900	-1.81098600	C	10.35913000	3.40096500	0.07104200
H	-7.46360900	-0.79312100	-2.66031400	H	9.86564100	3.48716300	1.04493200
C	-5.84408300	-0.78507400	-0.54086800	H	9.67184500	3.77686300	-0.69433700
H	-5.48043600	-1.29957800	-1.43635200	C	11.66250800	4.16605400	0.05312600
C	-11.54831300	2.18868700	0.05771400	H	12.33677900	3.73849400	0.80240500
H	-10.91910100	3.03377900	0.35695000	H	12.14409100	4.02651200	-0.92027400
H	-11.65639100	1.51947100	0.91797000	C	11.45950100	5.65242600	0.32434100
C	-12.89770400	2.66558300	-0.42793200	H	10.96622600	5.78340100	1.29410400
H	-12.75502300	3.30011100	-1.30868800	H	10.77507700	6.07060900	-0.42240900
H	-13.48453900	1.80070400	-0.75403500	C	12.76563300	6.43375100	0.30968400
C	-13.65618800	3.43297900	0.64910300	H	13.45864800	6.06313900	1.06998700
H	-13.05690900	4.28898800	0.97938000	H	12.59687600	7.49499800	0.50615500
H	-13.78504800	2.79508500	1.53083000	H	13.26618500	6.35264300	-0.65911300
C	-15.01682800	3.92015200	0.17174100	O	6.07577900	0.75156500	0.09637500
H	-14.91992600	4.58946900	-0.68746300	N	5.50136000	-1.77044400	-0.25477400
H	-15.54211100	4.46662800	0.95829500	H	5.25689500	-0.78469200	-0.07383200
H	-15.65366100	3.08485800	-0.13211100				

S₀; **DK** E= -1916.270843 hartree (6-311++G(d)-mPW1PW91)



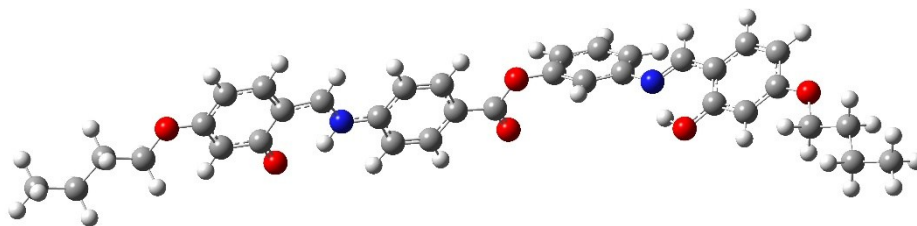
O -0.48696400	-3.36175200	-1.73617500	H -2.98615500	-1.23130900	0.19892500
C 1.25179100	-2.26076800	-0.53812100	C -4.51591400	-2.75361000	0.33173000
C 2.15379800	-2.32353900	-1.60258400	C -4.76069800	-4.12308700	0.44528300
H 1.84560200	-2.78685400	-2.53167800	H -5.76937400	-4.51318700	0.48707200
C 3.42504200	-1.80071400	-1.47611100	C -3.69340400	-5.00777700	0.51242400
H 4.11933700	-1.85222300	-2.30735900	H -3.89192000	-6.06943900	0.60219000
C 3.82567600	-1.20062300	-0.27611100	C -2.37966200	-4.55841900	0.47135700
C 2.92597100	-1.13528800	0.79271200	H -1.54638700	-5.24725300	0.52808800
H 3.20314500	-0.67723300	1.73327500	O -10.71299300	1.94241100	-0.05664300
C 1.65367800	-1.66092400	0.65734600	C -7.76759300	-0.95873400	0.16733700
H 0.96506300	-1.60434700	1.49022700	C -8.36508700	1.42615400	0.03594300
C -0.09402400	-2.83323800	-0.72878200	H -8.04399300	2.45835200	-0.00589800
O 10.86312000	1.91058100	0.85995900	C -9.69282600	1.07203800	0.01586800
C 7.01336000	0.39220400	0.76159000	C -10.10215800	-0.29639200	0.07142000
C 7.82767400	0.24688100	-0.44699100	H -11.16096400	-0.52186100	0.05263900
C 9.15499400	0.77649600	-0.39626400	C -9.15855000	-1.26898000	0.14405300
H 9.75451200	0.66955400	-1.29023900	H -9.45984400	-2.31147000	0.18499700
C 9.63342000	1.38894900	0.73641000	C -6.84256800	-1.99150300	0.23876100
C 8.82842900	1.52265300	1.91226900	H -7.19737800	-3.01571800	0.27605800
H 9.25517900	2.01368200	2.77768100	C -10.42632400	3.33773800	-0.12407600
C 7.56308800	1.03638300	1.91046800	H -9.80660900	3.53613800	-1.00497200
H 6.94465400	1.13461800	2.79755400	H -9.85978300	3.63298800	0.76547500
C 5.71341600	-0.08257400	0.80921700	C -11.73846100	4.08351600	-0.20452200
H 5.13809800	0.04358800	1.71959500	H -12.29326800	3.73433100	-1.08151400
C 11.75755300	1.84243700	-0.24964200	H -12.34494200	3.83348300	0.67217100
H 11.30608200	2.35224700	-1.10720500	C -11.53713000	5.59257000	-0.28420300
H 11.91599100	0.79318700	-0.52010400	H -10.91933700	5.83365200	-1.15664500
C 13.05622200	2.50229700	0.15294300	H -10.97177200	5.93313500	0.59061500
H 12.85233000	3.53476200	0.45494000	C -12.85203500	6.35465400	-0.36728000
H 13.45847900	1.98990100	1.03297100	H -13.42508400	6.06236000	-1.25150600
C 14.08271600	2.48361100	-0.97412900	H -12.68451900	7.43263000	-0.42399000
H 13.66850300	2.98759900	-1.85466100	H -13.47816900	6.16321100	0.50850600
H 14.27272900	1.44835300	-1.27916000	O -6.11419200	0.74783500	0.13217800
C 15.39538700	3.14607500	-0.58084300	C -7.33552200	0.43685400	0.11275100
H 15.24466600	4.19331300	-0.30475400	N -5.53053500	-1.79361000	0.26116700
H 16.11517100	3.12159200	-1.40217200	H -5.28820700	-0.79195700	0.21482300
H 15.85352800	2.64289000	0.27505800	O 7.37589300	-0.31709400	-1.47758000
O -0.86472500	-2.69022200	0.38225900	N 5.12048500	-0.69306900	-0.21457600
C -2.15722300	-3.19537700	0.35570100	H 5.74105500	-0.76857800	-1.03464800
C -3.19923300	-2.29020600	0.28666300			

S₁; DE* E= -1916.155405 hartree (6-311++G(d)-mPW1PW91)



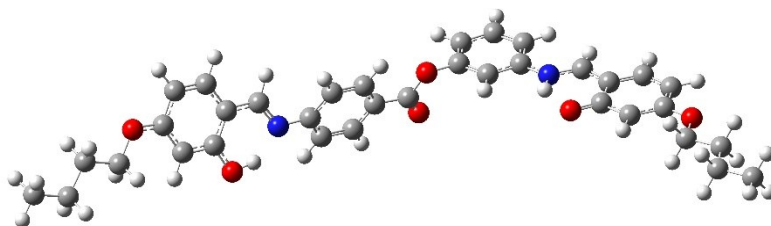
O	0.90688300	-1.50998300	2.03287100	O	0.73807100	-2.77211500	0.15689300
N	-5.12643400	-0.42770700	0.29884800	N	5.41569700	-1.68401600	0.06325200
C	-1.14813500	-1.56345900	0.84038400	C	2.06339200	-3.15771000	0.20743500
C	-1.80662200	-0.69649300	1.74479300	C	3.08696400	-2.22522600	0.15348400
H	-1.25823200	-0.31872400	2.59889100	H	2.87134300	-1.16506700	0.13287200
C	-3.11250400	-0.34046900	1.54334100	C	4.41293700	-2.66034700	0.10897100
H	-3.61707700	0.32492100	2.23519100	C	4.69097500	-4.03183900	0.15379100
C	-3.85095700	-0.82815200	0.42185600	H	5.71834800	-4.37642100	0.17952200
C	-3.17275300	-1.70733700	-0.48521700	C	3.64993300	-4.94802400	0.20991200
H	-3.68680100	-2.10618700	-1.35036300	H	3.87011300	-6.00892800	0.25140500
C	-1.86370900	-2.05609700	-0.27187900	C	2.32784500	-4.52095600	0.23154200
H	-1.36717800	-2.72005700	-0.96810300	H	1.50637400	-5.22540500	0.27999700
C	0.24303700	-1.90896700	1.10063900	O	6.44077700	0.57827700	0.86004800
O	-7.03015700	0.98147900	1.27825100	H	5.78436700	-0.16259300	0.76403200
H	-6.12379900	0.54411400	1.15004500	O	10.75735800	1.72399600	-0.77025000
O	-11.20841700	1.03000000	-0.97418500	C	7.56963700	-0.92325600	-0.63156100
C	-7.27436500	-0.31608800	-0.73314600	C	7.50588300	0.27758700	0.11412100
C	-7.79751200	0.58480000	0.27880000	C	8.56489900	1.18436800	0.08454700
C	-9.10783400	1.04722500	0.21910100	H	8.47239400	2.08841600	0.67049700
H	-9.44051800	1.71644000	1.00078400	C	9.69098500	0.90912500	-0.68339000
C	-9.93692700	0.64629800	-0.82102100	C	9.77047200	-0.27849100	-1.43369000
C	-9.44895100	-0.23519300	-1.82264200	H	10.65795100	-0.46897100	-2.02407400
H	-10.11908000	-0.53029800	-2.62073500	C	8.72313500	-1.16583200	-1.39873500
C	-8.15674100	-0.69452400	-1.76890600	H	8.78073600	-2.08369900	-1.97548900
H	-7.79542400	-1.36690400	-2.53924300	C	6.49366400	-1.87719200	-0.61503200
C	-5.94050800	-0.80170600	-0.69702500	H	6.62412000	-2.77884500	-1.22268900
H	-5.62065500	-1.47129300	-1.49188500	C	10.75548600	2.94632500	-0.03642500
C	-11.78928300	1.91856000	-0.01784400	H	10.64397800	2.72834900	1.03124800
H	-11.20530900	2.84464200	0.00896100	H	9.90324200	3.55785900	-0.35209600
H	-11.74446800	1.45478900	0.97329500	C	12.06038900	3.65917000	-0.30773000
C	-13.21753500	2.18604200	-0.43101100	H	12.88974000	3.00633500	-0.01660300
H	-13.22301500	2.60928400	-1.44055800	H	12.15596500	3.82888100	-1.38514700
H	-13.75744900	1.23517800	-0.48341600	C	12.15524400	4.98512300	0.43849200
C	-13.92260000	3.13263100	0.53423500	H	12.04636000	4.80803500	1.51445800
H	-13.36917500	4.07669700	0.59087800	H	11.31550200	5.62781300	0.15092000
H	-13.90205000	2.70775200	1.54406800	C	13.46539300	5.71336400	0.17414800
C	-15.36302200	3.41191100	0.12979300	H	14.32395900	5.11150400	0.48444100
H	-15.41547400	3.87083600	-0.86121100	H	13.51158700	6.65943700	0.71829700
H	-15.84865800	4.09089200	0.83417500	H	13.58783700	5.93749500	-0.88907600
H	-15.95239900	2.49153900	0.09818000				

S₁; **MK-C*** E= -1916.168643 hartree (6-311++G(d)-mPW1PW91)



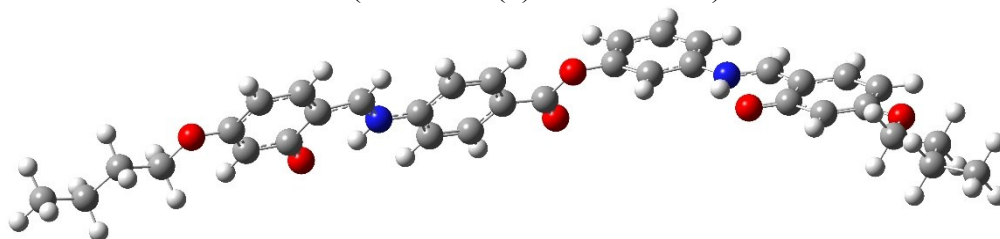
O	-0.37116100	-3.18698500	-1.88222500	C	-3.15532200	-2.04694400	0.10541200
C	1.33515300	-2.08828800	-0.64310100	H	-2.95381300	-0.98385300	0.05255800
C	2.29046600	-2.19360900	-1.67214500	C	-4.47390100	-2.50865600	0.14704800
H	2.01163800	-2.67484500	-2.60146900	C	-4.71392800	-3.88567900	0.19156000
C	3.56007300	-1.69526900	-1.50646000	H	-5.73064400	-4.26037700	0.16318700
H	4.28764900	-1.78231800	-2.30668400	C	-3.64807100	-4.77577400	0.22910100
C	3.92877300	-1.06750800	-0.29769700	H	-3.84241200	-5.84218700	0.25673500
C	2.97596900	-0.95861600	0.73813700	C	-2.33633400	-4.31969100	0.21879600
H	3.22533900	-0.48302800	1.67812800	H	-1.50202000	-5.00940000	0.24798500
C	1.70679000	-1.46227000	0.55863600	O	-6.55114400	0.61820100	-0.88888000
H	0.98373600	-1.37351500	1.35928900	H	-5.88224700	-0.09829300	-0.72095000
C	0.00105700	-2.63487900	-0.87215000	O	-10.94354600	1.76299600	0.52693200
O	11.11055700	1.88728300	0.92960000	C	-7.69184200	-0.80478100	0.66870700
C	7.15211000	0.48250900	0.79528400	C	-7.63279900	0.34291600	-0.15648300
C	8.00239700	0.27823500	-0.36977800	C	-8.71306400	1.22215900	-0.22232800
C	9.34810700	0.76342200	-0.30743900	H	-8.62350900	2.08542400	-0.86729400
H	9.95242500	0.59573900	-1.18891600	C	-9.85610600	0.97180500	0.52908000
C	9.85537300	1.41590200	0.82535800	C	-9.93119500	-0.16263400	1.35791000
C	9.02499700	1.59920800	1.92452300	H	-10.83217200	-0.33455100	1.93331200
H	9.40498900	2.10184000	2.80484200	C	-8.86284200	-1.02329000	1.41622400
C	7.69269000	1.13044000	1.88807500	H	-8.91687100	-1.90018500	2.05383800
H	7.07496300	1.29313000	2.76584800	C	-6.59390600	-1.72994200	0.75093800
C	5.78827300	0.03746800	0.84024600	H	-6.72271100	-2.59074100	1.41553600
H	5.20337700	0.21261900	1.73264500	C	-10.94742500	2.93171500	-0.28965100
C	12.00545300	1.72277400	-0.17018900	H	-10.79734900	2.64393600	-1.33583300
H	11.58690900	2.21351900	-1.05545000	H	-10.12024800	3.58524300	0.00803900
H	12.11900000	0.65559600	-0.38941500	C	-12.27673500	3.62753300	-0.10743300
C	13.33171200	2.33860900	0.21097900	H	-13.08073400	2.93510100	-0.37741300
H	13.17632000	3.39426400	0.45617400	H	-12.41037900	3.86803600	0.95234300
H	13.70000900	1.85412700	1.12108300	C	-12.37965700	4.89651900	-0.94600400
C	14.36521200	2.20902400	-0.90237100	H	-12.23251300	4.64934600	-2.00347200
H	13.98367600	2.68365500	-1.81341600	H	-11.56521100	5.57912700	-0.67828100
H	14.50707400	1.15066900	-1.14858800	C	-13.71478400	5.60619900	-0.77173500
C	15.70518200	2.82783200	-0.53077400	H	-14.54814400	4.96201700	-1.06527100
H	15.60348500	3.89465600	-0.31373100	H	-13.76684300	6.51145800	-1.38088700
H	16.42966700	2.72356600	-1.34156700	H	-13.87608500	5.89874600	0.26942800
H	16.13088900	2.35062000	0.35613700	O	7.57806000	-0.30572700	-1.40534600
O	-0.82092100	-2.44689300	0.20617400	N	5.20954900	-0.58671500	-0.18468300
N	-5.49956600	-1.55691900	0.09367800	H	5.84722300	-0.70532700	-0.98238400
C	-2.11005800	-2.95133700	0.15154200				

S₁; **MK-O*** E= -1916.163498 hartree (6-311++G(d)-mPW1PW91)



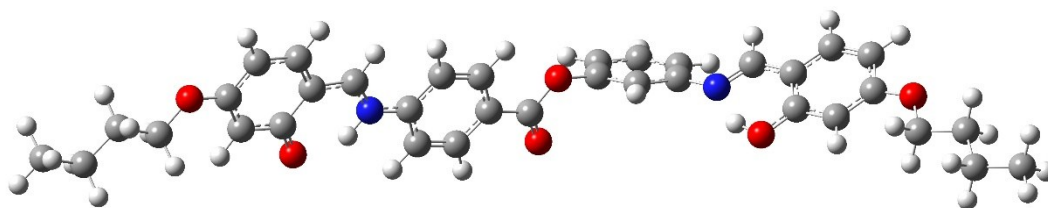
O	0.52140800	-3.42270100	1.84995300	O	0.83676900	-2.71794500	-0.26736300
N	-5.13532700	-0.73142400	0.52950600	C	2.13289200	-3.22062900	-0.28769600
C	-1.25534200	-2.31054300	0.71808000	C	3.17085200	-2.31846400	-0.23142900
C	-2.12323000	-2.39053900	1.81081000	H	2.95928800	-1.26151600	-0.11619400
H	-1.78164700	-2.86815400	2.72108300	C	4.49817400	-2.77954200	-0.32605500
C	-3.39717000	-1.86170400	1.73374500	C	4.73452400	-4.15950700	-0.47681200
H	-4.07112000	-1.91792600	2.58064600	H	5.74135500	-4.54822100	-0.55473600
C	-3.84415800	-1.25802200	0.55155300	C	3.66296900	-5.03574700	-0.53097000
C	-2.96653100	-1.16148100	-0.53641400	H	3.85495600	-6.09635800	-0.64889400
H	-3.27696600	-0.64462700	-1.43726300	C	2.34854300	-4.58740700	-0.44065000
C	-1.68762000	-1.68536100	-0.45348800	H	1.51251000	-5.27352600	-0.48588700
H	-1.01579800	-1.59862500	-1.29779300	O	10.71541500	2.05054100	-0.08745700
C	0.09919400	-2.88050000	0.86105600	C	7.76575300	-0.95270400	-0.25773700
O	-7.07087000	0.62253800	1.64027100	C	7.34318800	0.43770400	-0.13433400
H	-6.19820200	0.15734900	1.54616400	C	8.35886500	1.44295800	-0.07741800
O	-10.93230500	1.48119100	-0.99342800	H	8.00800200	2.46241200	0.01412100
C	-7.15847700	-0.18773400	-0.61630200	C	9.72804600	1.13355100	-0.13722200
C	-7.72486600	0.50084500	0.48344100	C	10.10807300	-0.19456900	-0.25415500
C	-8.99294900	1.07085000	0.38273900	H	11.15900200	-0.45100400	-0.30054500
H	-9.38565500	1.58681700	1.24800700	C	9.12151800	-1.20916500	-0.31147800
C	-9.70752400	0.96290800	-0.80545000	H	9.46117400	-2.23646300	-0.40212400
C	-9.16145000	0.27951800	-1.90864400	C	6.83288700	-2.04165000	-0.32424700
H	-9.73953200	0.20961800	-2.82146100	H	7.20235100	-3.05273600	-0.42051700
C	-7.91315100	-0.27956500	-1.80086100	C	10.37190700	3.42905800	0.03148900
H	-7.48834100	-0.80714400	-2.64906300	H	9.79217700	3.58321200	0.94822800
C	-5.85413600	-0.78157400	-0.54086200	H	9.75065900	3.72543600	-0.82089900
H	-5.49632100	-1.30296900	-1.43469400	C	11.65398000	4.22884500	0.06574900
C	-11.55716300	2.19177200	0.07397500	H	12.26583200	3.88375300	0.90559400
H	-10.92673100	3.03963200	0.36265400	H	12.22519300	4.02400300	-0.84561200
H	-11.65879900	1.52891700	0.93994200	C	11.39410800	5.72568600	0.19185900
C	-12.91028400	2.66391400	-0.40597800	H	10.81124300	5.92071900	1.09912100
H	-12.77412000	3.29218200	-1.29223500	H	10.77223100	6.06105800	-0.64579900
H	-13.49842100	1.79613800	-0.72187400	C	12.67868500	6.54124500	0.22884100
C	-13.66234600	3.43834700	0.67053000	H	13.30673800	6.25456000	1.07677100
H	-13.06171600	4.29725200	0.99068400	H	12.46931300	7.60951700	0.31941000
H	-13.78477600	2.80666900	1.55763100	H	13.26779200	6.39597000	-0.68083300
C	-15.02659000	3.92085300	0.19870200	O	6.12081900	0.75803200	-0.07862200
H	-14.93599000	4.58399100	-0.66596400	N	5.50568400	-1.84871400	-0.26655000
H	-15.54714600	4.47256000	0.98474700	H	5.25668000	-0.85747500	-0.17129700
H	-15.66462800	3.08280100	-0.09484700				

S₁; **DK*** E= -1916.169424 hartree (6-311++G(d)-mPW1PW91)



O	-0.30988000	-3.81303500	-1.51682000	H	-3.01097400	-1.22866300	0.13931500
C	1.29418100	-2.42655100	-0.44032600	C	-4.54249600	-2.74281400	0.32232900
C	2.31485400	-2.71476000	-1.36735200	C	-4.79138300	-4.10816300	0.46671500
H	2.10548500	-3.39136300	-2.18665800	H	-5.80046300	-4.49506600	0.52610700
C	3.55980100	-2.14817900	-1.24062500	C	-3.72359500	-4.99220000	0.54271300
H	4.33823100	-2.37755000	-1.96091900	H	-3.92276800	-6.05148400	0.65756400
C	3.83727700	-1.26473300	-0.17588700	C	-2.40917000	-4.54845100	0.48068900
C	2.81917000	-0.97123900	0.75687000	H	-1.58111500	-5.24165900	0.54542500
H	2.99761500	-0.29579600	1.58390600	O	-10.73167500	1.96613100	-0.08837700
C	1.57560400	-1.54571500	0.61842300	C	-7.79090400	-0.93900700	0.15444700
H	0.80177700	-1.31250700	1.33841900	C	-8.38406700	1.44433600	-0.00988500
C	-0.00988600	-3.05111100	-0.62641900	H	-8.06076800	2.47488000	-0.07156100
O	10.84659300	2.17170500	0.74607900	C	-9.71293000	1.09355900	-0.01159300
C	6.94968200	0.60039300	0.72920400	C	-10.12487900	-0.27225500	0.06986700
C	7.86914100	0.19078300	-0.32374600	H	-11.18428800	-0.49568900	0.06486600
C	9.19326200	0.73554700	-0.30316000	C	-9.18226600	-1.24592000	0.14937400
H	9.85047800	0.41092500	-1.09868600	H	-9.48567300	-2.28687100	0.21028700
C	9.61563600	1.63428500	0.68638100	C	-6.86710400	-1.97355900	0.23496700
C	8.72052800	2.00919300	1.68157100	H	-7.22433800	-2.99598900	0.29335700
H	9.03525800	2.70232700	2.45128800	C	-10.44114000	3.35898300	-0.18011800
C	7.40812100	1.48688400	1.68330900	H	-9.82910000	3.54192000	-1.06972900
H	6.73823000	1.80570300	2.47575800	H	-9.86524000	3.66625200	0.69934000
C	5.59932100	0.11905300	0.80115900	C	-11.75147000	4.10809200	-0.25978600
H	4.96058100	0.45105600	1.60809000	H	-12.31552800	3.74763000	-1.12625700
C	11.80323000	1.82400300	-0.25487600	H	-12.35069000	3.87342600	0.62610800
H	11.41441400	2.10184300	-1.24044600	C	-11.54587600	5.61504800	-0.36412800
H	11.96525800	0.74087200	-0.24152700	H	-10.93507300	5.84074600	-1.24556500
C	13.08543600	2.56436100	0.04726800	H	-10.97159000	5.96683800	0.50037700
H	12.88002400	3.63962500	0.06296200	C	-12.85887700	6.38044000	-0.44707500
H	13.42428200	2.29301500	1.05236600	H	-13.44074300	6.07692700	-1.32171500
C	14.17800500	2.25776900	-0.97094300	H	-12.68825700	7.45686600	-0.52145900
H	13.82688600	2.52046700	-1.97520600	H	-13.47787400	6.20434900	0.43697100
H	14.36912500	1.17889500	-0.98914600	O	-6.13362000	0.76220100	0.07491700
C	15.47491300	2.99815800	-0.67697600	C	-7.35601400	0.45373700	0.07282100
H	15.32502500	4.08119300	-0.68715800	N	-5.55536200	-1.77994900	0.24193000
H	16.24285200	2.76420000	-1.41768600	H	-5.30936500	-0.78053300	0.17604400
H	15.87138000	2.72996200	0.30609200	O	7.52192000	-0.61727900	-1.22902000
O	-0.90278700	-2.66324300	0.34094100	N	5.09723400	-0.72476500	-0.09795700
C	-2.17942300	-3.18733000	0.33251900	H	5.78315700	-0.98287700	-0.81929300
C	-3.22563700	-2.28476000	0.25373300				

Fig. S7: S₁; MK-C* E= -1915.882285 hartree (DZVP-mPW1PW91)



O	-0.38195500	-3.19934600	-1.88143700	C	-3.16951700	-2.07843000	0.10597500
C	1.32737300	-2.10310000	-0.62854900	H	-2.96741500	-1.01391100	0.06241500
C	2.28323200	-2.19777600	-1.66188000	C	-4.49116500	-2.54148200	0.13393900
H	2.00372400	-2.67344300	-2.59501500	C	-4.73169000	-3.92216400	0.16662300
C	3.55450700	-1.69570600	-1.49322500	H	-5.74806400	-4.29942600	0.12808900
H	4.28188200	-1.77430000	-2.29547800	C	-3.66310400	-4.81393000	0.20621100
C	3.92291700	-1.07464600	-0.27762900	H	-3.85762000	-5.88116400	0.22412200
C	2.96908800	-0.97599600	0.76280200	C	-2.34801500	-4.35717900	0.21027100
H	3.21726800	-0.50615900	1.70688300	H	-1.51307200	-5.04746200	0.24053700
C	1.69853900	-1.48372800	0.58017900	O	-6.52481200	0.62822300	-0.86092600
H	0.97505700	-1.40321500	1.38268200	H	-5.87060600	-0.11287300	-0.68728200
C	-0.00796500	-2.65224400	-0.85965300	O	-10.94425600	1.78497700	0.51156900
O	11.12058300	1.89557600	0.93164800	C	-7.71405000	-0.82764300	0.64110200
C	7.15502900	0.47986600	0.81401800	C	-7.62668400	0.34348300	-0.15319700
C	7.99907900	0.28194000	-0.35815400	C	-8.69819300	1.23941100	-0.21490900
C	9.34680200	0.76953200	-0.30390500	H	-8.58625400	2.11955200	-0.83476700
H	9.94497100	0.60561900	-1.19140600	C	-9.86008100	0.98053200	0.51015900
C	9.86104600	1.42013100	0.83202800	C	-9.96325800	-0.17740000	1.30828200
C	9.03646000	1.59798300	1.93950000	H	-10.87759400	-0.35412300	1.86264600
H	9.42225600	2.09820800	2.81994000	C	-8.90299200	-1.05350800	1.36299200
C	7.70150300	1.12547700	1.90878300	H	-8.97946300	-1.94674300	1.97630900
H	7.08873500	1.28370000	2.79164100	C	-6.62508400	-1.76720100	0.71989200
C	5.78905000	0.03104100	0.86505000	H	-6.77172500	-2.64134800	1.36376900
H	5.20862900	0.20019200	1.76278600	C	-10.91773300	2.97671700	-0.27854200
C	12.00737300	1.73462600	-0.18098400	H	-10.75177500	2.71407500	-1.32901100
H	11.58254300	2.23029700	-1.06053900	H	-10.09201700	3.61577000	0.05303100
H	12.12248000	0.66840100	-0.40422900	C	-12.24689000	3.68166000	-0.10438000
C	13.33845300	2.35197800	0.19321800	H	-13.05039200	3.00308100	-0.40817000
H	13.18248300	3.40637500	0.44259300	H	-12.39698000	3.89834400	0.95813700
H	13.71433600	1.86218600	1.09713400	C	-12.32142700	4.97303700	-0.91515700
C	14.36343800	2.22796900	-0.93147100	H	-12.15790000	4.74878000	-1.97503100
H	13.97352800	2.70781000	-1.83587300	H	-11.50688100	5.64096400	-0.61396200
H	14.50475900	1.17080000	-1.18178800	C	-13.65517900	5.69376800	-0.74971400
C	15.70914700	2.84731700	-0.56937800	H	-14.48777200	5.06382700	-1.07539500
H	15.60676700	3.91333400	-0.34764900	H	-13.68291300	6.61333700	-1.33944800
H	16.42379100	2.74506100	-1.38965300	H	-13.83199000	5.96277900	0.29550000
H	16.14197500	2.36520600	0.31168500	O	7.56863900	-0.30190000	-1.40037400
O	-0.82976900	-2.47812500	0.22589600	N	5.20555400	-0.58950700	-0.16298600
N	-5.51537600	-1.58416400	0.08142700	H	5.84692000	-0.70044100	-0.96530900
C	-2.12173500	-2.98477700	0.15470700				