Supporting Information

N-(*p*-toluenesulfonyl)-1-(4′-Acetylphenoxy)acrylimidate: Synthesis, Crystal Structure and Theoretical Studies

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Figure S1. FTIR spectrum for imidate **3**

Figure S2. MS (EI^+) spectrum for imidate **3**

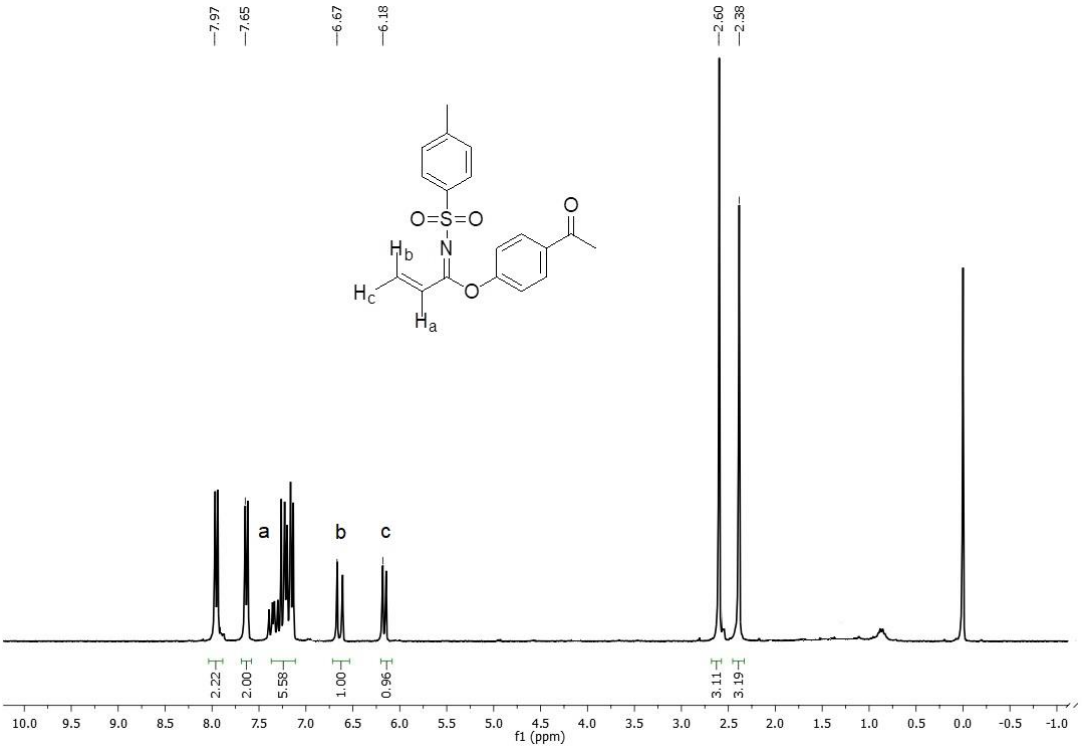

Figure S3. ^1H NMR spectrum for imidate **3** ($CDCl_3$, 300 MHz)

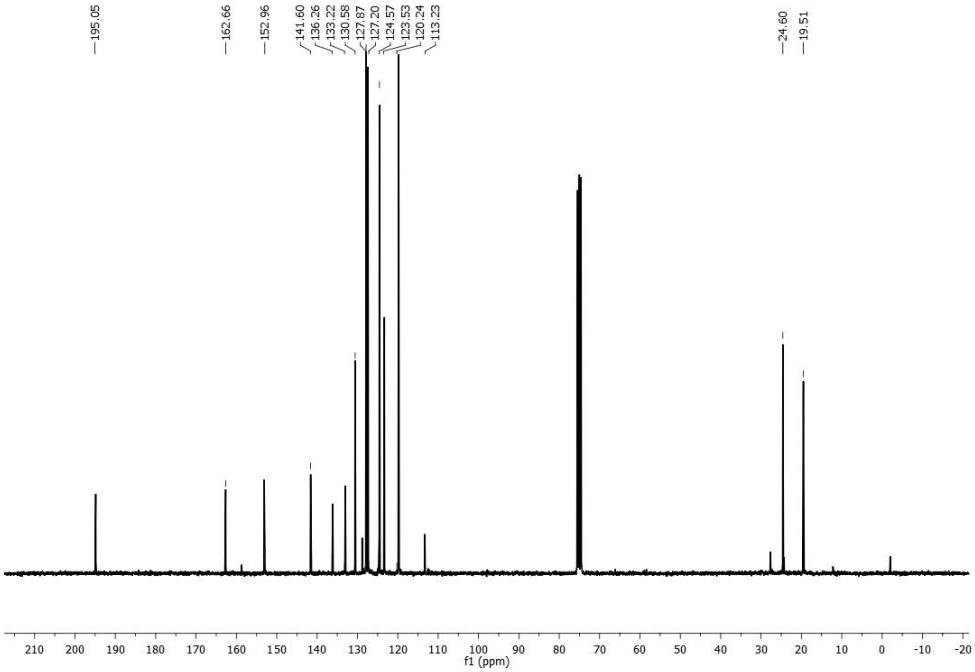

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum for imidate **3** ($CDCl_3$, 75 MHz)

Monomer

Optimized (Opt=ReadOpt; atoms=H notatoms=S,O,N,C) cartesian coordinates (Å) for Monomer at PBE1PBE/cc-pVDZ level theory

S	6.48930050	9.34030071	3.48430026
O	5.42400039	7.10840052	0.59620005
O	9.86060075	2.62950020	1.20300009
O	5.26240040	9.60810076	4.19540032
O	7.13600055	10.46910082	2.86570022
N	6.29530047	8.12030061	2.41790019
C	5.48980041	8.17020065	1.42390011
C	4.59570035	9.25980068	1.02130008
H	4.45347048	10.04746340	1.76332972
C	4.04510031	9.30790073	-0.18090001
H	4.21011709	8.51864678	-0.91643511
H	3.40723782	10.14564641	-0.46969854
C	6.24980049	6.00920047	0.90820007
C	7.34930058	5.77570043	0.10400001
H	7.56781776	6.44639708	-0.72713728
C	8.16680063	4.70030036	0.41380003
H	9.06575647	4.48495020	-0.16602803
C	7.88440059	3.87920029	1.51110012
C	6.73380050	4.11530031	2.26990017
H	6.48126785	3.47351018	3.11462565
C	5.90750044	5.18580040	1.96330015
H	5.01218066	5.39905714	2.54808384
C	8.85870068	2.80680021	1.87450015
C	8.60610067	1.98500015	3.11250024
H	7.65039042	1.44243938	3.04344825
H	8.55407456	2.62890903	4.00426807
H	9.42534288	1.26633805	3.22849183
C	7.64220061	8.56660066	4.57960035
C	7.73100057	7.18110053	4.68070036
H	7.12156190	6.55034226	4.03582270
C	8.63580064	6.62430049	5.57640042
H	8.71907848	5.53649321	5.64594913
C	9.45300070	7.42780058	6.37350048
C	9.33290070	8.81600068	6.26480049
H	9.96562931	9.45995256	6.88033201
C	8.43440065	9.39540071	5.37340041
H	8.36454888	10.47908518	5.26863927
C	10.41550078	6.79370050	7.34510055
H	10.99947851	5.99527898	6.86295017
H	9.87400121	6.33844217	8.19022085
H	11.11876898	7.53056723	7.75706123

E(RPBE1PBE) = -1448.618189 a.u.

Dimer A

Optimized (Opt=ReadOpt; atoms=H notatoms=S,O,N,C) cartesian coordinates (Å) for Dimer A at PBE1PBE/cc-pVDZ level theory

S	6.48930000	9.34030000	3.48430000
O	5.42400000	7.10840000	0.59620000
O	9.86060000	2.62950000	1.20300000
O	5.26240000	9.60810000	4.19540000
O	7.13600000	10.46910000	2.86570000
N	6.29530000	8.12030000	2.41790000
C	5.48980000	8.17020000	1.42390000
C	4.59570000	9.25980000	1.02130000
H	4.46175900	10.05699100	1.75453800
C	4.04510000	9.30790000	-0.18090000
H	4.20751300	8.51563300	-0.91388400
H	3.41302700	10.14900300	-0.47287700
C	6.24980000	6.00920000	0.90820000
C	7.34930000	5.77570000	0.10400000
H	7.56935300	6.44531700	-0.72797400
C	8.16680000	4.70030000	0.41380000
H	9.06525900	4.48495800	-0.16698700
C	7.88440000	3.87920000	1.51110000
C	6.73380000	4.11530000	2.26990000
H	6.49724200	3.49840200	3.13684300
C	5.90750000	5.18580000	1.96330000
H	5.01545000	5.39806200	2.55061500
C	8.85870000	2.80680000	1.87450000
C	8.60610000	1.98500000	3.11250000
H	7.70844800	1.35934100	2.97903600
H	8.41805600	2.61614200	3.99417800
H	9.47261300	1.33605200	3.28329500
C	7.64220000	8.56660000	4.57960000
C	7.73100000	7.18110000	4.68070000
H	7.11740500	6.54054900	4.04949400
C	8.63580000	6.62430000	5.57640000
H	8.69174700	5.53602700	5.65040500
C	9.45300000	7.42780000	6.37350000
C	9.33290000	8.81600000	6.26480000
H	9.96449400	9.46105400	6.88033300

C	8.43440000	9.39540000	5.37340000
H	8.36970400	10.47958200	5.26670200
C	10.41550000	6.79370000	7.34510000
H	11.00650100	6.00438700	6.85716800
H	9.87052800	6.32475800	8.18052100
H	11.10990700	7.53258400	7.76817500
S	5.47470000	4.11640000	6.35610000
O	6.54000000	6.34830000	9.24410000
O	2.10340000	10.82720000	8.63730000
O	6.70160000	3.84850000	5.64490000
O	4.82800000	2.98760000	6.97460000
N	5.66870000	5.33630000	7.42250000
C	6.47420000	5.28650000	8.41640000
C	7.36830000	4.19690000	8.81900000
H	7.50222800	3.39970300	8.08576500
C	7.91890000	4.14880000	10.02120000
H	7.75650000	4.94107600	10.75417700
H	8.55095100	3.30768400	10.31318800
C	5.71420000	7.44750000	8.93220000
C	4.61470000	7.68100000	9.73630000
H	4.39462300	7.01139300	10.56827800
C	3.79720000	8.75640000	9.42650000
H	2.89871900	8.97170300	10.00726700
C	4.07960000	9.57750000	8.32920000
C	5.23020000	9.34140000	7.57050000
H	5.46692000	9.95854000	6.70376800
C	6.05650000	8.27090000	7.87700000
H	6.94863500	8.05890100	7.28973300
C	3.10520000	10.64980000	7.96580000
C	3.35790000	11.47170000	6.72780000
H	4.25538900	12.09753600	6.86154900
H	3.54627600	10.84066100	5.84612200
H	2.49130400	12.12050200	6.55686600
C	4.32170000	4.89010000	5.26070000
C	4.23300000	6.27560000	5.15960000
H	4.84658300	6.91613400	5.79083600
C	3.32820000	6.83240000	4.26390000
H	3.27205300	7.92067000	4.18998000
C	2.51100000	6.02890000	3.46680000
C	2.63100000	4.64070000	3.57550000
H	1.99927800	3.99565500	2.96009400
C	3.52960000	4.06130000	4.46690000
H	3.59428300	2.97712100	4.57364300
C	1.54850000	6.66300000	2.49520000
H	0.95740600	7.45225100	2.98314400
H	2.09346800	7.13202800	1.65982600
H	0.85414700	5.92409100	2.07204200

E(RPBE1PBE) = -2897.261523 a.u.

Dimer B

Optimized (Opt=ReadOpt; atoms=H notatoms=S,O,N,C) cartesian coordinates (Å) for Dimer B at PBE1PBE/cc-pVDZ level theory

S	6.48930100	9.34030000	3.48429900
O	5.42399100	7.10839600	0.59620800
O	9.86063600	2.62947700	1.20301200
O	5.26240000	9.60810000	4.19540000
O	7.13600000	10.46910000	2.86570000
N	6.29531300	8.12030700	2.41789000
C	5.48980600	8.17021200	1.42391900
C	4.59567600	9.25975200	1.02128900
H	4.45361600	10.04728500	1.76349700
C	4.04511400	9.30793500	-0.18090500
H	4.21009400	8.51882000	-0.91659500
H	3.40725600	10.14568300	-0.46971000
C	6.24979800	6.00920500	0.90819600
C	7.34930600	5.77569600	0.10399700
H	7.56874000	6.44735200	-0.72607400
C	8.16678400	4.70030600	0.41380800
H	9.06716900	4.48934700	-0.16524300
C	7.88441000	3.87919000	1.51109700
C	6.73379900	4.11530000	2.26989800
H	6.48141900	3.47291500	3.11402600
C	5.90750000	5.18579900	1.96330000
H	5.01257400	5.39902400	2.54858100
C	8.85860900	2.80683300	1.87452300
C	8.60625400	1.98493200	3.11239400
H	7.69265700	1.38003000	2.99776300
H	8.46154100	2.63218500	3.99060400
H	9.46396200	1.32567900	3.29214800
C	7.64219600	8.56660200	4.57959800
C	7.73100200	7.18110200	4.68070300
H	7.12150500	6.55017000	4.03617300
C	8.63579900	6.62430000	5.57639800
H	8.72027700	5.53663200	5.64570600
C	9.45300200	7.42779900	6.37350100
C	9.33290000	8.81600100	6.26479900
H	9.96571400	9.45992000	6.88024700
C	8.43440000	9.39539700	5.37340100
H	8.36463300	10.47908600	5.26861800

C	10.41550000	6.79370000	7.34510000
H	11.00426800	6.00009200	6.86089900
H	9.87322600	6.33173400	8.18604000
H	11.11395400	7.53206200	7.76249400
S	13.63670100	0.10410000	3.48429900
O	12.57150400	-2.12779800	0.59619700
O	17.00800000	-6.60670000	1.20300000
O	12.40980000	0.37190000	4.19540000
O	14.28340000	1.23290000	2.86570000
N	13.44269000	-1.11580500	2.41790800
C	12.63717900	-1.06601400	1.42390800
C	11.74315800	0.02368300	1.02133700
H	11.60708600	0.83855800	1.73390500
C	11.19257300	0.07169600	-0.18087600
H	11.34551800	-0.72136400	-0.91530000
H	10.56886200	0.92512100	-0.45205200
C	13.39719800	-3.22699500	0.90819700
C	14.49670500	-3.46050400	0.10399800
H	14.71481300	-2.78924500	-0.72675400
C	15.31418600	-4.53589500	0.41380700
H	16.21329000	-4.75113800	-0.16584800
C	15.03191000	-5.35700700	1.51109900
C	13.88119900	-5.12090000	2.26989900
H	13.62899900	-5.76281300	3.11468800
C	13.05490000	-4.05040100	1.96330000
H	12.15967500	-3.83661000	2.54792500
C	16.00620000	-6.42940000	1.87450000
C	15.75350000	-7.25120000	3.11250000
H	14.79779600	-7.79374700	3.04327600
H	15.70134700	-6.60725400	4.00422300
H	16.57273400	-7.96988900	3.22862900
C	14.78969600	-0.66959800	4.57959700
C	14.87840200	-2.05509800	4.68070400
H	14.26924800	-2.68499500	4.03469600
C	15.78319900	-2.61190000	5.57639800
H	15.86683900	-3.69973000	5.64569900
C	16.60040300	-1.80840100	6.37350100
C	16.48040000	-0.42019900	6.26479900
H	17.11374600	0.22355000	6.87998700
C	15.58180000	0.15919700	5.37340200
H	15.51250400	1.24279400	5.26721100
C	17.56290000	-2.44250000	7.34510000
H	18.15171800	-3.23630400	6.86108900
H	17.02135900	-2.90393600	8.18686700
H	18.26209400	-1.70446200	7.76193900

E(RPBE1PBE) = -2897.243107 a.u.

Dimer C

Optimized (Opt=ReadOpt; atoms=H notatoms=S,O,N,C) cartesian coordinates (Å) for Dimer C at PBE1PBE/cc-pVDZ level theory

S	6.48930000	9.34030000	3.48430000
O	5.42401100	7.10840600	0.59619300
O	9.86061800	2.62952400	1.20302000
O	5.26240000	9.60810000	4.19540000
O	7.13600000	10.46910000	2.86570000
N	6.29532100	8.12031100	2.41788400
C	5.48974600	8.17015800	1.42390500
C	4.59573100	9.25982500	1.02131600
H	4.44851600	10.04468900	1.76522800
C	4.04504200	9.30781700	-0.18105900
H	4.21782000	8.51717000	-0.91205800
H	3.40049900	10.13962100	-0.47094300
C	6.24980500	6.00919500	0.90820200
C	7.34929600	5.77570200	0.10400000
H	7.56971500	6.44846100	-0.72484700
C	8.16680600	4.70029300	0.41379200
H	9.06690500	4.48554800	-0.16456700
C	7.88439100	3.87920400	1.51109900
C	6.73379900	4.11529500	2.26989700
H	6.48313900	3.47638300	3.11744300
C	5.90749500	5.18580200	1.96330200
H	5.01257700	5.40050200	2.54785300
C	8.85870000	2.80678900	1.87449300
C	8.60608500	1.98496500	3.11244200
H	7.62716900	1.48286600	3.08214900
H	8.61079900	2.62868100	4.00642400
H	9.40057800	1.23537400	3.20415000
C	7.64221000	8.56659500	4.57961000
C	7.73098900	7.18108900	4.68069000
H	7.12106600	6.55049900	4.03617300
C	8.63580300	6.62431100	5.57640200
H	8.71885200	5.53650100	5.64652500
C	9.45300000	7.42779900	6.37350000
C	9.33289800	8.81599400	6.26479800
H	9.96548000	9.45994500	6.88045200
C	8.43439900	9.39541200	5.37339900
H	8.36438900	10.47909800	5.26885800
C	10.41550000	6.79370000	7.34510000
H	10.99896400	5.99472300	6.86323400

H	9.87402700	6.33932100	8.19069400
H	11.11931900	7.53038400	7.75640700
S	4.63110000	-0.10410000	-3.48430000
O	5.69629500	2.12779800	-0.59619200
O	1.25977400	6.60666400	-1.20302900
O	5.85800000	-0.37190000	-4.19540000
O	3.98440000	-1.23290000	-2.86570000
N	4.82508700	1.11579300	-2.41789000
C	5.63062800	1.06602400	-1.42389700
C	6.52462200	-0.02363200	-1.02133300
H	6.67273200	-0.80784000	-1.76578600
C	7.07517400	-0.07165200	0.18096600
H	6.90056800	0.71785900	0.91271500
H	7.71999700	-0.90326200	0.47081100
C	4.87059300	3.22700400	-0.90820400
C	3.77109800	3.46049200	-0.10400600
H	3.55068100	2.78774800	0.72485200
C	2.95360900	4.53592400	-0.41377600
H	2.05351300	4.75062200	0.16461000
C	3.23589900	5.35698600	-1.51111200
C	4.38661600	5.12092200	-2.26987900
H	4.63729200	5.75985300	-3.11740800
C	5.21290000	4.05039200	-1.96330800
H	6.10783500	3.83571500	-2.54784200
C	2.26154700	6.42938100	-1.87452300
C	2.51441100	7.25131700	-3.11230300
H	3.49295900	7.75425500	-3.08157800
H	2.51083500	6.60758900	-4.00632900
H	1.71940100	8.00030500	-3.20467000
C	3.47809000	0.66960500	-4.57961000
C	3.38941100	2.05511100	-4.68069000
H	3.99931700	2.68567400	-4.03613300
C	2.48459700	2.61188900	-5.57640300
H	2.40149500	3.69969500	-5.64649500
C	1.66740000	1.80840100	-6.37350000
C	1.78740200	0.42020600	-6.26479800
H	1.15475200	-0.22374800	-6.88037600
C	2.68600100	-0.15921200	-5.37339900
H	2.75599200	-1.24289500	-5.26881900
C	0.70490000	2.44250000	-7.34510000
H	0.12486500	3.24474700	-6.86457900
H	1.24609800	2.89255200	-8.19320200
H	-0.00195200	1.70670900	-7.75280600

E(RPBE1PBE) = -2897.235407 a.u.

Dimer D

Optimized (Opt=ReadOpt; atoms=H notatoms=S,O,N,C) cartesian coordinates (Å) for Dimer D at PBE1PBE/cc-pVDZ level theory

S	6.48930300	9.34029500	3.48432100
O	5.42401700	7.10841400	0.59620300
O	9.86059800	2.62949800	1.20299800
O	5.26240700	9.60810200	4.19541100
O	7.13603800	10.46911900	2.86564000
N	6.29527300	8.12029200	2.41791400
C	5.48979800	8.17019800	1.42389900
C	4.59575900	9.25990100	1.02126500
H	4.41277600	10.01650400	1.78703400
C	4.04515400	9.30790200	-0.18094700
H	4.26310300	8.55583400	-0.94339000
H	3.38991200	10.13657400	-0.45825300
C	6.24978900	6.00916400	0.90819400
C	7.34934700	5.77581200	0.10400900
H	7.53415300	6.43037800	-0.74742000
C	8.16683600	4.70031800	0.41379600
H	9.05991000	4.47872400	-0.17287600
C	7.88439400	3.87920600	1.51110100
C	6.73381000	4.11531000	2.26990900
H	6.47986500	3.47173100	3.11293300
C	5.90746200	5.18576800	1.96326500
H	5.01062300	5.39691900	2.54665800
C	8.85869700	2.80679600	1.87449500
C	8.60609900	1.98499800	3.11249900
H	7.65134400	1.44094400	3.04199600
H	8.55136000	2.62872600	4.00420900
H	9.42612900	1.26736700	3.22973400
C	7.64222400	8.56659100	4.57960400
C	7.73099300	7.18108600	4.68067500
H	7.12135700	6.55068100	4.03538000
C	8.63580400	6.62430800	5.57640700
H	8.71827000	5.53652000	5.64572000
C	9.45298700	7.42780400	6.37350500
C	9.33289600	8.81599500	6.26480500
H	9.96484100	9.45994800	6.88111500
C	8.43441100	9.39541200	5.37338500
H	8.36366300	10.47939600	5.27151600
C	10.41550000	6.79370000	7.34510000
H	11.00093100	5.99680700	6.86223300
H	9.87329000	6.33612900	8.18842400
H	11.11707800	7.53086300	7.75932400

S	6.61759700	9.13210500	-3.48432100
O	7.68278300	11.36398600	-0.59620300
O	3.24630200	15.84290200	-1.20299800
O	7.84439300	8.86419800	-4.19541100
O	5.97086200	8.00328100	-2.86564000
N	6.81152700	10.35200800	-2.41791400
C	7.61700200	10.30220200	-1.42389900
C	8.51104100	9.21249900	-1.02126500
H	8.69399600	8.45587000	-1.78701400
C	9.06164600	9.16449800	0.18094700
H	8.84371500	9.91657700	0.94338400
H	9.71686700	8.33581200	0.45826300
C	6.85711100	12.46323600	-0.90819400
C	5.75755300	12.69658800	-0.10400900
H	5.57275500	12.04201900	0.74742000
C	4.93996400	13.77208200	-0.41379600
H	4.04689100	13.99362900	0.17289100
C	5.22240600	14.59319400	-1.51110100
C	6.37299000	14.35709000	-2.26990900
H	6.62693500	15.00065300	-3.11294200
C	7.19933800	13.28663200	-1.96326500
H	8.09616000	13.07550500	-2.54669900
C	4.24810300	15.66560400	-1.87449500
C	4.50080100	16.48740200	-3.11249900
H	5.45555100	17.03145200	-3.04189900
H	4.55561300	15.84368000	-4.00420700
H	3.68078900	17.20504500	-3.22980400
C	5.46457600	9.90580900	-4.57960400
C	5.37590700	11.29131400	-4.68067500
H	5.98550600	11.92169500	-4.03532400
C	4.47109600	11.84809200	-5.57640700
H	4.38851800	12.93587300	-5.64563400
C	3.65391300	11.04459600	-6.37350500
C	3.77390400	9.65640500	-6.26480500
H	3.14182400	9.01246300	-6.88099000
C	4.67238900	9.07698700	-5.37338500
H	4.74307000	7.99300700	-5.27142800
C	2.69140000	11.67870000	-7.34510000
H	2.11212700	12.48147400	-6.86464000
H	3.23312800	12.12849600	-8.19294400
H	1.98436500	10.94312800	-7.75285500

E(RPBE1PBE) = -2897.250055 a.u.