

**Internal conversion rate constant calculations considering
Duschinsky, Anharmonic and Herzberg-Teller effects**

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Table S1. Calculated excitation energies of S_1 and triplet states (cm^{-1}) for poly[n]fluorenes with $n=2..14$.

poly[n]fluorene	S_1	T_1	T_2	T_3	T_4
2	25514.32	16095.97	23047.82	29055.18	29482.66
3	22967.97	15557.99	19852.18	23836.65	27346.05
4	21927.49	15460.39	18760.89	21583.89	24223.81
5	21487.91	15538.63	18197.09	20476.47	21487.91
6	21311.27	15653.16	17969.64	19755.39	21500.01
7	21247.55	15745.11	17872.04	19408.57	20721.67
8	21241.91	15823.35	17847.04	19207.73	20296.6
9	21243.52	15868.52	17827.68	19102.87	19989.3

10	21232.23	15883.04	17823.65	19041.58	19806.21
11	21235.45	15896.75	17825.26	19018.18	19687.64
12	21277.4	15952.4	17844.62	19002.05	19611.82
13	16947.71	12976.95	13297.16	13811.76	14487.66
14	21262.07	15943.53	17837.36	18991.57	19514.23

Table S1. Cartesian coordinates (Å) for ground and excited states of 4B.

S₀

O	3.880119420072	-0.014774011083	0.000000000000
C	3.043331737436	-1.118261242991	0.000000000000
C	1.700237077131	-0.722119989325	0.000000000000
C	0.709169915374	-1.705668365562	0.000000000000
C	1.095084263331	-3.051750039029	0.000000000000
O	-0.014760085043	-3.880106604034	0.000000000000
C	-1.118258679974	-3.043329756461	0.000000000000
C	-0.722107910325	-1.700225056129	0.000000000000
C	-1.705680622524	-0.709182207367	0.000000000000
C	-3.051752278031	-1.095087005316	0.000000000000
O	-3.880119565067	0.014746177048	0.000000000000
C	-3.043329883464	1.118228194019	0.000000000000
C	-1.700233472164	0.722107469309	0.000000000000
C	-0.709178274363	1.705648265558	0.000000000000
C	-1.095094553341	3.051744290047	0.000000000000
C	1.118268877007	3.043323919424	0.000000000000
C	0.722116011288	1.700204908129	0.000000000000
C	1.705676865525	0.709169673381	0.000000000000
C	3.051750071044	1.095053961319	0.000000000000
C	3.451858044036	2.437578110551	0.000000000000
C	2.463767923466	3.433168333669	0.000000000000
H	2.737406319257	4.482188426677	0.000000000000

C	-2.437584506558	3.451815135011	0.000000000000
C	-3.433211118655	2.463761684466	0.000000000000
H	-2.703232275829	4.502884734151	0.000000000000
C	-3.451849413049	-2.437602226587	0.000000000000
C	-2.463758152472	-3.433198890691	0.000000000000
H	-4.502899853168	-2.703239669811	0.000000000000
C	2.437574413560	-3.451845609006	0.000000000000
C	3.433202261656	-2.463785728481	0.000000000000
H	4.482203234644	-2.737413578299	0.000000000000
O	0.014760009053	3.880093668032	0.000000000000
H	4.502912344185	2.703182851786	0.000000000000
H	-4.482216215680	2.737356928287	0.000000000000
H	-2.737372026296	-4.482214194646	0.000000000000
H	2.703197679808	-4.502910244145	0.000000000000

S₁

O	3.895007463138	-0.014793470095	0.000000000000
C	3.061303610716	-1.121061844206	0.000000000000
C	1.702545489317	-0.703562069970	0.000000000000
C	0.690581199014	-1.707901739726	0.000000000000
C	1.097791922500	-3.069761392371	0.000000000000
O	-0.014812226095	-3.894880459116	0.000000000000
C	-1.121109690190	-3.061325768743	0.000000000000
C	-0.703553802951	-1.702602321313	0.000000000000
C	-1.707845586718	-0.690591105000	0.000000000000
C	-3.069739276361	-1.097745344530	0.000000000000
O	-3.895007347142	0.014831346063	0.000000000000
C	-3.061347667738	1.121084575226	0.000000000000
C	-1.702641392321	0.703523650961	0.000000000000
C	-0.690577603995	1.707839170708	0.000000000000
C	-1.097767052492	3.069740367365	0.000000000000
C	1.121084778219	3.061304501744	0.000000000000
C	0.703549240967	1.702539079340	0.000000000000
C	1.707941131734	0.690551915033	0.000000000000

C	3.069783795355	1.097767570504	0.000000000000
C	3.458120452486	2.421596679390	0.000000000000
C	2.447771304282	3.439530709152	0.000000000000
H	2.730674395805	4.485782041911	0.000000000000
C	-2.421537480384	3.458048856498	0.000000000000
C	-3.439601214136	2.447830448307	0.000000000000
H	-2.696473742329	4.506421953430	0.000000000000
C	-3.458141430501	-2.421525999408	0.000000000000
C	-2.447823115286	-3.439498451142	0.000000000000
H	-4.506496365436	-2.696509816342	0.000000000000
C	2.421589442415	-3.458016835454	0.000000000000
C	3.439622650154	-2.447759691276	0.000000000000
H	4.485855376935	-2.730710835797	0.000000000000
O	0.014812488090	3.894869722110	0.000000000000
H	4.506530238442	2.696270280292	0.000000000000
H	-4.485891141908	2.730471790770	0.000000000000
H	-2.730541751760	-4.485788178938	0.000000000000
H	2.696340493328	-4.506427024430	0.000000000000

Table S2. Cartesian coordinates (Å) for ground and excited states of H2P.

S₀

C	2.896354329664	-1.130550891511	0.000000000000
N	2.117541269044	0.000000627022	0.000000000000
C	2.896354623675	1.130551968493	0.000000000000
C	0.678273643717	-4.259283209071	0.000000000000
C	-0.678274931681	-4.259281385050	0.000000000000
C	-1.084926645498	-2.856461652707	0.000000000000
N	-0.000000752014	-2.030326446103	0.000000000000
C	1.084925365524	-2.856462665711	0.000000000000
C	-0.678274857702	4.259279951086	0.000000000000
C	0.678273162695	4.259281000074	0.000000000000
C	1.084925227515	2.856460504710	0.000000000000
N	-0.000001018984	2.030326751068	0.000000000000
C	-1.084926518496	2.856460253721	0.000000000000

C	-4.261030718086	-0.686225140702	0.000000000000
C	-4.261029736092	0.686226475710	0.000000000000
C	-2.896352570679	1.130551790478	0.000000000000
N	-2.117541486059	0.000000532987	0.000000000000
C	-2.896353192674	-1.130550759482	0.000000000000
C	4.261032419073	0.686227139669	0.000000000000
C	4.261032644079	-0.686225477682	0.000000000000
C	2.422276986910	-2.441740599900	0.000000000000
C	-2.422277027921	2.441740132901	0.000000000000
C	-2.422277574879	-2.441739572873	0.000000000000
C	2.422276868903	2.441740893911	0.000000000000
H	1.101940356478	0.000000365979	0.000000000000
H	1.352449786396	-5.107614093702	0.000000000000
H	-1.352448474407	-5.107614003689	0.000000000000
H	-1.352447263384	5.107613014709	0.000000000000
H	1.352448254375	5.107612557659	0.000000000000
H	-5.117785995668	-1.347611070383	0.000000000000
H	-5.117786317673	1.347610467386	0.000000000000
H	-1.101940915501	-0.000001444019	0.000000000000
H	5.117789090667	1.347611694389	0.000000000000
H	5.117787756665	-1.347612467411	0.000000000000
H	3.180061554543	-3.220358706543	0.000000000000
H	-3.180059484560	3.220358513552	0.000000000000
H	-3.180059637545	-3.220359002564	0.000000000000
H	3.180061085533	3.220358632564	0.000000000000
S ₁			
C	1.133128732494	2.897384997662	0.000000000000
N	-0.000000335022	2.115405741023	0.000000000000
C	-1.133129267493	2.897385750681	0.000000000000
C	4.278097582062	0.681431677705	0.000000000000
C	4.278096855079	-0.681431870696	0.000000000000
C	2.882699673669	-1.089114672518	0.000000000000
N	2.051636079057	0.000000135999	0.000000000000

C	2.882700388693	1.089114658495	0.000000000000
C	-4.278096853068	-0.681431943669	0.000000000000
C	-4.278097036057	0.681431510697	0.000000000000
C	-2.882699919683	1.089114956527	0.000000000000
N	-2.051636435087	0.000000265012	0.000000000000
C	-2.882699625672	-1.089114417508	0.000000000000
C	0.687544455679	-4.262026968077	0.000000000000
C	-0.687544802713	-4.262026349046	0.000000000000
C	-1.133128953479	-2.897385409679	0.000000000000
N	0.000000161981	-2.115406118062	0.000000000000
C	1.133128946494	-2.897386050672	0.000000000000
C	-0.687545004700	4.262026595060	0.000000000000
C	0.687544381700	4.262026164045	0.000000000000
C	2.448962629910	2.428355172885	0.000000000000
C	-2.448962136876	-2.428354707897	0.000000000000
C	2.448962184872	-2.428355402918	0.000000000000
C	-2.448962850895	2.428355532884	0.000000000000
H	-0.000001257008	1.101289468514	0.000000000000
H	5.127789854648	1.353535595403	0.000000000000
H	5.127788904669	-1.353536259362	0.000000000000
H	-5.127788771687	-1.353536236396	0.000000000000
H	-5.127789593658	1.353535171373	0.000000000000
H	1.348388131401	-5.119123487673	0.000000000000
H	-1.348388314391	-5.119123053695	0.000000000000
H	0.000001466985	-1.101289970492	0.000000000000
H	-1.348387498399	5.119124068656	0.000000000000
H	1.348387890414	5.119122923676	0.000000000000
H	3.222070987540	3.191926147577	0.000000000000
H	-3.222071135551	-3.191924846541	0.000000000000
H	3.222071806547	-3.191925015561	0.000000000000
H	-3.222071324520	3.191926246533	0.000000000000

Table S3. Cartesian coordinates (Å) for ground and excited states of PM567.

S₀

C	-1.214925645100	0.889484143000	0.165885900500
N	-1.239395599100	-0.507131193500	0.152582182700
B	-0.007791267900	-1.447503538700	0.082166848600
N	1.225403805800	-0.520742449400	-0.079073805600
C	1.219993430100	0.875933334800	-0.057635216200
C	0.010723685400	1.579864224300	0.102709579700
C	2.487605330400	-0.954985231900	-0.244104775400
C	3.357893242000	0.155810762100	-0.364256956400
C	2.575053323800	1.308998765200	-0.240477994500
C	-2.576258345000	1.337557275400	0.229537414200
C	-3.379701700900	0.193724023100	0.274317830200
C	-2.515083855500	-0.926931482400	0.222148187500
C	3.109803875600	2.709066262400	-0.330384565900
C	-3.104720288400	2.743149662100	0.198626972000
C	-2.858338304900	-2.380595125100	0.225040627800
C	2.811296846500	-2.413021284900	-0.272229158100
C	5.617924514500	0.112205947600	0.786334161400
C	4.848049085500	0.077187244400	-0.546226082700
C	-5.511267439400	0.050101387300	-1.092701611200
C	-4.881493935000	0.128103727600	0.309832929300
C	0.028591356200	3.084509385300	0.211402410500
F	0.099888432600	-2.199299365200	1.253942997600
F	-0.118518564800	-2.292841576600	-1.024025072900
H	2.545614208400	3.324949424700	-1.037399036300
H	4.151071565100	2.698832389300	-0.661419278100
H	3.090703423000	3.223081897600	0.638848251400
H	-2.660270332700	3.331282172800	-0.610086720600
H	-4.185930690400	2.741149683500	0.041612084300
H	-2.916986405300	3.282468705000	1.135747806600
H	-2.303860270000	-2.896037572800	1.014783097700
H	-3.928803924500	-2.534669549500	0.370630073200
H	-2.552157662700	-2.839169003700	-0.720129440500
H	3.886130010900	-2.579680910700	-0.358650410400
H	2.443384650000	-2.890939812300	0.640778452700

H	2.296760373200	-2.899753721900	-1.106068243600
H	6.699415728800	0.053511795300	0.622986639000
H	5.322890180100	-0.725341426700	1.426840390500
H	5.404543715000	1.036195982600	1.333958679900
H	5.189853910600	0.901616664100	-1.183330008600
H	5.104247909100	-0.839308807000	-1.089758910600
H	-6.603892376000	-0.001748961300	-1.036545327900
H	-5.154070141000	-0.835125732800	-1.628795100800
H	-5.239903913800	0.927250100000	-1.689506226100
H	-5.195693396200	-0.743376233700	0.896402164500
H	-5.280637156800	0.999013767500	0.841770880400
H	0.948408257200	3.437253351100	0.672271919400
H	-0.797577036000	3.447834891100	0.818118027800
H	-0.050711693200	3.556113031100	-0.776244892200

S₁

C	1.228906559600	0.874243186300	-0.203464439400
N	1.254763717100	-0.539619287000	-0.254805896300
B	0.003266188800	-1.469637184300	-0.163586027300
N	-1.191573273900	-0.552155088000	0.091414845200
C	-1.217179138100	0.859993382000	0.045237855100
C	-0.060674033800	1.592809238100	-0.171809491500
C	-2.450806148600	-1.011883012000	0.306225519700
C	-3.334698539200	0.084223298100	0.432456235100
C	-2.587766789000	1.257212480900	0.268601773000
C	2.524091898200	1.302429428300	-0.183613482900
C	3.388709219500	0.069825553600	-0.276719012700
C	2.535408690900	-1.016428957500	-0.311751372500
C	-3.132501546200	2.649310039900	0.378419721900
C	3.128921733500	2.662103395900	-0.082240343800
C	2.833343648000	-2.480054108900	-0.380679800600
C	-2.743149203200	-2.473678816600	0.348933763500
C	-5.626882404300	0.076795769800	-0.648032599000
C	-4.816311006000	-0.014135247600	0.658456913000

C	5.441742151800	0.014529543300	1.186557834500
C	4.874800473000	0.062673559500	-0.255779015100
C	-0.065597697300	3.071080181200	-0.437241189000
F	-0.121449854100	-2.180331710000	-1.360455101100
F	0.190845975500	-2.357429409400	0.901761303400
H	-2.501112045700	3.290749357700	1.002067675000
H	-4.130207633000	2.637038851700	0.826191691300
H	-3.232296788500	3.143828380000	-0.597624343400
H	2.414498312000	3.428301973900	0.208506952900
H	3.942683097300	2.661610850600	0.653301738400
H	3.580732099300	2.963328840400	-1.037909472500
H	2.261808821700	-2.945565218900	-1.188904513200
H	3.899200350600	-2.647859259600	-0.552366172700
H	2.535198965600	-2.981385573500	0.544651107300
H	-3.805516559900	-2.660840288700	0.513829411300
H	-2.439851665800	-2.946367461600	-0.592759027300
H	-2.160365974400	-2.961893518300	1.137189170600
H	-6.702480492800	0.003744772100	-0.453971861200
H	-5.346656374300	-0.728687663100	-1.334443663000
H	-5.435311486900	1.026666555000	-1.157831453900
H	-5.141384358000	0.782439717000	1.339143425300
H	-5.052765922200	-0.954971424100	1.167825866700
H	6.536058231600	0.015077606200	1.163804205400
H	5.102995085600	-0.889497920500	1.699719588300
H	5.108875327700	0.876668695200	1.772138548900
H	5.249516375400	-0.805179336300	-0.809196117200
H	5.262641968500	0.957163392700	-0.758430233300
H	-1.037584581800	3.413325414200	-0.788093247100
H	0.660690640600	3.323146812200	-1.217629684600
H	0.190423985300	3.674980210100	0.447102414900

Table S4. Cartesian coordinates (Å) for ground and excited states of bifluorene.

S₀

C	0.000000000000	0.000000000000	1.483877284457
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C	0.000000000000	0.000000000000	0.000000000000
C	-0.958454756428	0.742716986792	2.203706168603
C	0.958048667395	-0.739046484538	2.205115316710
C	-1.211845522759	0.003488962230	-0.718224619020
C	1.210919499721	0.000000000000	-0.722609563319
C	-0.949579108794	0.734357949188	3.591079601124
C	0.015890295144	-0.011349753842	4.296199138165
C	-1.881429889300	1.469005507400	4.555759715976
C	-0.212216231360	0.168525084232	5.734317911376
C	0.973680442519	-0.750511361368	3.599099270691
C	-1.316231076322	1.028610564520	5.906469911806
C	0.460825230358	-0.354552870707	6.840968663516
C	-1.747806636603	1.366683204977	7.184277768392
C	-3.346936585423	1.012189896292	4.380983030310
C	-1.781190153040	3.000967908350	4.377817354103
H	-1.685366310062	1.340509872071	1.660367206284
H	1.683063985902	-1.336191396774	1.660378276249
H	1.719023581531	-1.337984641891	4.128474811032
C	0.021754595560	-0.011186030794	8.121717090287
H	1.311696596004	-1.018148795766	6.712571404196
C	-1.073253936739	0.842332445032	8.293802127729
H	0.534927033765	-0.410153106686	8.992138429328
H	-1.402761529619	1.100320113692	9.296251096335
H	-2.597440184167	2.029554715011	7.328600404821
H	-3.718831673361	1.278165227603	3.385708541222
H	-3.993901696285	1.494829609252	5.121252052938
H	-3.438310909026	-0.070904401119	4.502274167112
H	-0.749770946298	3.344218944225	4.497944024780
H	-2.126890807075	3.298919379940	3.382273546974
H	-2.401781448967	3.517597234771	5.117763226706
C	1.195148753549	0.004498887326	-2.110154929868
C	-0.026817252928	0.010199047754	-2.811913681674
C	0.259023374742	0.021158765526	-4.250790403873
C	1.657816534055	0.026842962952	-4.427268852661

C	2.378597023307	0.019643135420	-3.078778574017
C	2.202097507496	0.038342143802	-5.706777617378
C	-0.596902124232	0.026951295959	-5.354704153860
C	-1.234839234420	0.009752845710	-2.111952052002
C	3.240300297719	1.288959420372	-2.894033164624
C	3.256275528881	-1.241749880926	-2.916361979254
C	1.344253482385	0.043671814167	-6.813603057543
H	3.279187696498	0.043349135163	-5.854655723087
C	-0.043550263158	0.037684354732	-6.637116772751
H	1.759539245423	0.052322551787	-7.817338312212
H	-0.696318139430	0.041428070987	-7.505468523649
H	-1.675520467378	0.022540799649	-5.222895041319
H	-2.185319039299	0.004420890304	-2.638645354108
H	-2.149258666678	-0.025909276898	-0.171061114391
H	2.153104454980	0.025810202852	-0.181531434173
H	4.044806517980	1.321526469707	-3.636530327430
H	3.699777264987	1.303225069393	-1.900007317622
H	2.636713572980	2.194216837923	-3.004625136616
H	2.663410004900	-2.152377960923	-3.040679910224
H	4.059679331060	-1.252697161762	-3.660628279131
H	3.718324281334	-1.267152625763	-1.923637977342

S₁

C	0.193355118900	0.543627479700	1.459500895000
C	0.172924546700	0.552506618400	0.023802771800
C	-0.895654320400	1.076758171800	2.239634843600
C	1.305358272400	-0.012583518700	2.191415532400
C	-1.046155853000	0.798013354900	-0.707641089500
C	1.360032315300	0.307129477500	-0.756798650400
C	-0.856046688100	1.042553350000	3.607799745200
C	0.254049278700	0.473078610900	4.307102288700
C	-1.895557884600	1.561545310800	4.600484167300
C	0.016328615400	0.564137588300	5.716817680500
C	1.338872452700	-0.056393875800	3.566840195500

C	-1.243994374000	1.196972159500	5.931179628100
C	0.792532219400	0.145571141000	6.819508890900
C	-1.717413896400	1.405759797300	7.214619314400
C	-3.248975115500	0.842409547500	4.420124192400
C	-2.083875792500	3.088168397300	4.469968122100
H	-1.737794034200	1.545912705400	1.742826291600
H	2.126905064300	-0.455963907300	1.640623778100
H	2.186690157000	-0.503508516700	4.078352942200
C	0.302940126700	0.362188735400	8.102586208500
H	1.753668368100	-0.336887118400	6.666278339000
C	-0.940208913100	0.986501004800	8.308708483700
H	0.887978155800	0.045197586900	8.961575702100
H	-1.300953497700	1.145939445400	9.320614432600
H	-2.677776070700	1.888023483600	7.379132553900
H	-3.669050230000	1.059545099300	3.432016818500
H	-3.966646034500	1.175023456900	5.177619482000
H	-3.129843750100	-0.240708269300	4.511672968100
H	-1.131190615300	3.610496855300	4.593704304700
H	-2.490021424500	3.342242533400	3.484817462000
H	-2.779906521300	3.455985476300	5.231442843400
C	1.308322233600	0.309049776000	-2.125062920500
C	0.082572796200	0.544100573000	-2.823856850600
C	0.326377349100	0.476835136000	-4.233877260600
C	1.709626024100	0.203761219300	-4.449055416000
C	2.448046489300	0.085896743400	-3.118843177000
C	2.211968858900	0.083423716800	-5.732810120900
C	-0.542797681600	0.628655966300	-5.336152330100
C	-1.098973848800	0.789277949700	-2.083039613300
C	3.531989495600	1.176542308800	-2.984295360300
C	3.076862497600	-1.312602098700	-2.946656592800
C	1.341450060000	0.234229281400	-6.826532271000
H	3.266361150600	-0.124100398600	-5.897721545400
C	-0.023043731500	0.504601921400	-6.619660062800
H	1.724209979000	0.142203121400	-7.838718878100

H	-0.679295539700	0.617359401500	-7.478309683100
H	-1.597655493900	0.837375282500	-5.182202649000
H	-2.042494304100	0.958877874900	-2.594200449800
H	-1.967137730200	0.949560639700	-0.156780200400
H	2.312351272800	0.159028522300	-0.259492602900
H	4.306972925600	1.044543337000	-3.746988462100
H	4.009071542700	1.124784333800	-1.999617697600
H	3.098483616500	2.173338766000	-3.103781332200
H	2.318577090500	-2.094900879000	-3.039894496300
H	3.845431007000	-1.485706108000	-3.707576026000
H	3.545420701300	-1.403809477600	-1.960698863300

Table S5. Cartesian coordinates (Å) for ground and excited states of trifluorene.

S₀

C	1.175677298600	-0.490998201500	0.163456125300
C	0.730696476700	0.845466690600	0.137387277900
C	-0.729470164300	0.851964920500	0.242838017600
C	-1.176872044600	-0.480404187400	0.340549892800
C	-0.001988615700	-1.453486411100	0.290128492200
C	2.526521437300	-0.788182348000	0.085802728600
C	3.472669129500	0.250884332000	-0.025960810100
C	3.011452752500	1.581824960600	-0.053310895500
C	1.653839253500	1.886696174300	0.028860262200
C	-1.650106641600	1.901013431400	0.259813710900
C	-3.007773268200	1.608255638300	0.378085327700
C	-3.470555813100	0.281500308500	0.479164755400
C	-2.527546225200	-0.765946741800	0.455686627600
C	0.089028613300	-2.290787554700	1.583055562900
C	-0.095619916300	-2.381612276800	-0.939739732700
C	9.571380792000	0.357398848700	0.593045213500
C	9.120580573900	-0.730723039300	-0.180755999900
C	7.659708611800	-0.658671504000	-0.274537794500
C	7.219349356600	0.471755495400	0.440373027000
C	8.399613358200	1.219653715400	1.054347206900

C	10.927066653700	0.527865709500	0.842963963600
C	11.837422139800	-0.397043610700	0.317013149400
C	11.389106749500	-1.478204068100	-0.449912014400
C	10.027133761100	-1.653232026700	-0.705787956200
C	6.734585964700	-1.485569112700	-0.912831501100
C	5.378412943600	-1.175275766700	-0.828797802300
C	4.920839865000	-0.052287647800	-0.111442400700
C	5.869481826500	0.772883101600	0.525953127900
C	8.504335299700	2.653366657000	0.492541296700
C	8.301259599900	1.258276143700	2.593812612500
C	-7.222277818900	0.463974962300	0.040809828600
C	-7.656345440200	-0.566706658400	0.896591946900
C	-9.120061640600	-0.627124749300	0.849758558600
C	-9.578671597900	0.363640853000	-0.041222972200
C	-8.409104295100	1.139472410500	-0.640662123100
C	-5.872539924800	0.743572094000	-0.101809694100
C	-4.918005118100	-0.007105803200	0.613544080800
C	-5.367981150300	-1.037323331200	1.462656866100
C	-6.724462604400	-1.322512939100	1.608954725900
C	-10.023336553500	-1.458449836600	1.513935922900
C	-11.390120959400	-1.289410534400	1.280677216300
C	-11.845956806900	-0.306097809000	0.395750557200
C	-10.938796816200	0.526309188600	-0.271288212500
C	-8.349408548500	0.962132339000	-2.172851808700
C	-8.483311542700	2.638122542300	-0.281701306200
H	2.865504972700	-1.819092198800	0.137307309000
H	3.731212097200	2.386265137000	-0.168708900900
H	1.323425179700	2.921253600500	-0.001865255300
H	-1.317780744400	2.933314018300	0.195137776300
H	-3.726283998500	2.420984735800	0.423685514000
H	-2.868867693700	-1.796254906700	0.503678209500
H	0.972851875300	-2.936642315300	1.561947773600
H	-0.794901147200	-2.928062264900	1.691190148200
H	0.156815771400	-1.644889445000	2.462787218000

H	-0.158062225400	-1.799635362900	-1.863443513300
H	0.785369751900	-3.029332599700	-0.999946575700
H	-0.983470905400	-3.018956237900	-0.874785092900
H	11.279791986500	1.365663755900	1.438886302300
H	12.899879569700	-0.274754723600	0.506087857900
H	12.107256943000	-2.188278581200	-0.849539642200
H	9.681413679000	-2.493334084500	-1.301690152800
H	7.061778367900	-2.354963139000	-1.476195058900
H	4.656752746800	-1.797553011600	-1.348930936600
H	5.534448973400	1.627850384800	1.106545173000
H	9.393905429100	3.156565065300	0.885672319200
H	7.626631227600	3.243104501000	0.777099112600
H	8.570901200700	2.640918184700	-0.598873577200
H	8.227460061200	0.248032946800	3.005654443500
H	9.184923309800	1.741603158100	3.023327007000
H	7.417945462400	1.823558297200	2.909123783400
H	-5.541881098600	1.522581312200	-0.783009014100
H	-4.639581157500	-1.602010190700	2.036717445600
H	-7.046554955900	-2.115710378500	2.277821366400
H	-9.670852275100	-2.222398269400	2.201141764500
H	-12.106494783200	-1.926496607700	1.791159624500
H	-12.912115150300	-0.187475416400	0.226205093600
H	-11.297790687600	1.288568696900	-0.957854179800
H	-7.469668663900	1.467050561900	-2.585399831700
H	-9.240125673600	1.390962485500	-2.643769651700
H	-8.295289598100	-0.096700965400	-2.440661210700
H	-8.526109911300	2.777824917400	0.802010278800
H	-9.374327838800	3.096199561100	-0.723474810800
H	-7.604520432300	3.168422764300	-0.663411008400

S₁

C	1.179792422433	-0.671733417634	-0.048333898487
C	0.710641654460	0.680503255272	-0.027743590985
C	-0.710624213466	0.680505402303	0.027788437010

C	-1.179783068431	-0.671729875639	0.048296228475
C	0.000002417017	-1.641863564904	-0.000047973992
C	2.519650747504	-0.958572348450	-0.094846451858
C	3.491670992926	0.093844106803	-0.121178667798
C	2.999067731223	1.439878301270	-0.102582703456
C	1.654203166804	1.737093929829	-0.061436342465
C	-1.654180300844	1.737098877848	0.061546853461
C	-2.999045428254	1.439888502272	0.102677521436
C	-3.491656693922	0.093855984821	0.121192011796
C	-2.519641525532	-0.958564133450	0.094792601881
C	0.049380638603	-2.524232634853	1.264877340602
C	-0.049380542557	-2.524158148816	-1.265024556654
C	9.586797251396	0.482228757930	0.240347508393
C	9.136772780790	-0.778702306416	-0.224275767260
C	7.689738123000	-0.763067630289	-0.275572518951
C	7.227575654538	0.508005580810	0.154069369136
C	8.406405888901	1.407219532923	0.523241368895
C	10.942187362597	0.736583086338	0.383191991737
C	11.863939819317	-0.271806293666	0.062643408523
C	11.421091062271	-1.520700344160	-0.396517015710
C	10.060517883705	-1.785929545340	-0.544035982419
C	6.757760118494	-1.744705674382	-0.655721624505
C	5.406038865551	-1.456123621483	-0.599015495390
C	4.913403965875	-0.184818027381	-0.169344831279
C	5.883437141149	0.795907865632	0.207573639020
C	8.453399376284	2.664097841976	-0.371515257896
C	8.359230605480	1.814405854406	2.011340148663
C	-7.227560295538	0.508055643783	-0.154011178160
C	-7.689728478004	-0.763043148274	0.275549412956
C	-9.136761822800	-0.778666726390	0.224258453269
C	-9.586783071404	0.482296162940	-0.240279474402
C	-8.406388203904	1.407300290927	-0.523116346907
C	-5.883421786172	0.795954352637	-0.207503416035
C	-4.913390997910	-0.184801573408	0.169346067279

C	-5.406031452572	-1.456132818478	0.598936331373
C	-6.757752302493	-1.744711526394	0.655630302482
C	-10.060511849708	-1.785912003379	0.543957165384
C	-11.421083699246	-1.520665575151	0.396460760728
C	-11.863928563347	-0.271740208688	-0.062615958512
C	-10.942172473560	0.736666739365	-0.383102253753
C	-8.359218303485	1.814590035447	-2.011186993654
C	-8.453371905317	2.664117254950	0.371727324938
H	2.845179796063	-1.993432652388	-0.069642055036
H	3.707306944521	2.258491011604	-0.165868672016
H	1.321302159726	2.771067168705	-0.067045470860
H	-1.321273191717	2.771070495695	0.067218405879
H	-3.707280319550	2.258501693576	0.166015305021
H	-2.845177005076	-1.993421497385	0.069525329013
H	0.935072303752	-3.168378079513	1.250564071608
H	-0.837856288673	-3.164001991154	1.321751998753
H	0.087287310328	-1.908645262275	2.167953774018
H	-0.087285456303	-1.908518149244	-2.168065166041
H	0.837854064700	-3.163927762192	-1.321937402776
H	-0.935074581754	-3.168300991512	-1.250747835604
H	11.289719180739	1.703175490390	0.738849543499
H	12.928215181436	-0.084621936125	0.171016783414
H	12.148635088976	-2.290066765899	-0.639691921319
H	9.721444892132	-2.754655227510	-0.900139805178
H	7.092186640709	-2.718526356915	-1.002554049608
H	4.701471595562	-2.209857990068	-0.932988991555
H	5.559663931701	1.762782415669	0.578462730897
H	9.340089115551	3.265261019530	-0.143742527404
H	7.567626649171	3.286654203063	-0.206382565968
H	8.487348133769	2.388377398987	-1.429258640524
H	8.322114458788	0.931768852491	2.655945061365
H	9.246206943706	2.398716112757	2.278355825036
H	7.474389206406	2.426718051779	2.215353347470
H	-5.559645092726	1.762851602684	-0.578330752874

H	-4.701466053542	-2.209892678060	0.932856844566
H	-7.092183017697	-2.718552613897	1.002400997631
H	-9.721441368129	-2.754661673524	0.899996110166
H	-12.148630269971	-2.290044955859	0.639588372338
H	-12.928203249441	-0.084543427124	-0.170973360399
H	-11.289701013766	1.703283511394	-0.738695066500
H	-7.474374098396	2.426911045791	-2.215161832456
H	-9.246192433719	2.398925340763	-2.278156816025
H	-8.322111515822	0.931998343487	-2.655854102358
H	-8.487316957768	2.388325041978	1.429451665546
H	-9.340060830551	3.265299551519	0.143999191441
H	-7.567597544157	3.286681703082	0.206632727951

Table S6. Cartesian coordinates (Å) for ground and excited states of tetrafluorene.

S₀

C	5.357668352200	0.611980135900	-0.356912143100
C	4.948151705700	-0.656318101800	-0.814574945300
C	3.487635615400	-0.666032836500	-0.913334248400
C	3.003521772800	0.596296421700	-0.515970655600
C	4.153058001800	1.518316672200	-0.118090144700
C	6.700704233000	0.895955454200	-0.168553273800
C	7.673933904600	-0.087916247400	-0.438032143700
C	7.248558212200	-1.350869631600	-0.896076051600
C	5.898510659900	-1.642614920700	-1.084596352700
C	2.595340303200	-1.664513582300	-1.308028146200
C	1.228475770800	-1.390844694800	-1.303218972000
C	0.728619353900	-0.134004781000	-0.907534082700
C	1.643742075000	0.862347610000	-0.510261719300
C	4.049806295400	1.934626275100	1.364576378500
C	4.205698086700	2.770207968000	-1.019047306400
C	-3.003519591000	-0.596215329800	-0.515988517300
C	-3.487643910100	0.666140751000	-0.913243789600
C	-4.948162127900	0.656399166600	-0.814502763400
C	-5.357669149900	-0.611947238300	-0.356968728800

C	-4.153043892200	-1.518256110800	-0.118114137300
C	-1.643737776800	-0.862258953900	-0.510316092300
C	-0.728626440000	0.134131660000	-0.907511558300
C	-1.228493463100	1.391006797900	-1.303078373400
C	-2.595359101600	1.664666032000	-1.307851855700
C	-5.898527735100	1.642709893500	-1.084450386100
C	-7.248574501100	1.350924544000	-0.895991112600
C	-7.673943062100	0.087917670400	-0.438086983300
C	-6.700705965200	-0.895967466400	-0.168682804900
C	-4.205629869200	-2.770230430300	-1.018945876600
C	-4.049804480100	-1.934402186200	1.364613511300
C	-11.324713663800	0.499422909700	0.455659749400
C	-11.841600165500	-0.767685863100	0.122238547500
C	-13.277414463000	-0.778435782900	0.417030067400
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