Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Is Energy Transfer Limiting Multiphotochromism ? Answers from *Ab Initio* Quantifications

Electronic Supplementary Information

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Table S1: Cartesian coordinates (in Å) of 1-oc.

Atom	X	Y	Z
C	1.93291100	-0.49035700	-0.70818400
C	2.95251400	0.40878100	-0.44541700
C	4.24184700	-0.16789000	-0.69188700
C	4.17923400	-1.46939000	-1.15791800
C	5.52338900	0.53216800	-0.52162700
C	5.82522800	1.81431600	-1.26036900
C	6.59755600	0.14103400	0.20439300
C	7.36136900	1.88999600	-1.24504400
C	7.72141800	1.13687800	0.04341300
C	6.68741400	-0.97584800	1.15345700
C	7.61503400	-2.07979600	1.06627900
C	5.85562300	-1.04756300	2.25199500
C	7.43123900	-2.95885000	2.09474900
C	5.29331900	-2.37369500	-1.56362800
C	4.79363200	-0.09262400	2.68745300
S	2.55379600	-2.01231900	-1.28043500
S	6.19217800	-2.46122900	3.17732800
H	6.12193300	-1.79029000	-1.97605400
H	5.67714300	-2.94088600	-0.70738000
H	4.96832300	-3.08824000	-2.32530800
H	5.04606600	0.92353000	2.36917400
H	3.81922900	-0.35012800	2.25453000
H	4.68502800	-0.08687000	3.77599100
C	0.55725300	-0.28706500	-0.56078600

C	-0.64631100	-0.12179200	-0.43828300
H	7.97112200	-3.88015100	2.27273800
C	8.64715800	-2.28386400	-0.00383100
H	9.58488000	-1.77772800	0.24526200
H	8.86365900	-3.34860300	-0.12935600
H	8.31848400	-1.88763000	-0.96935500
C	2.68994200	1.79849600	0.03888700
H	2.84789100	2.53158200	-0.75938700
H	1.65666800	1.89297000	0.38189300
H	3.35745500	2.07130700	0.86163900
F	8.94921900	0.58536900	-0.03587400
F	7.73977400	2.00841600	1.08437100
F	7.82727000	3.14427900	-1.27491000
F	7.85037900	1.21144500	-2.30368300
F	5.34343800	2.91298900	-0.61950100
F	5.32857900	1.82566900	-2.51225100
C	-2.01645300	0.10772200	-0.27296200
C	-3.03134600	-0.77213200	-0.57831100
S	-2.52647700	1.65602200	0.39945500
C	-4.32451900	-0.22071900	-0.29037900
C	-2.75344900	-2.13575000	-1.12789500
C	-4.27222700	1.29218900	-0.06484000
C	-5.57157600	-0.78058600	-0.27515500
H	-1.71317300	-2.20555800	-1.45545000
H	-2.92552700	-2.91086700	-0.37430900
H	-3.40341300	-2.36063900	-1.97765300
C	-5.27558700	1.68395000	1.02590600

C	-4.54874100	1.96501800	-1.42465000
C	-5.96949200	-2.17000800	-0.67031900
C	-6.75718900	-0.00628100	0.06005900
C	-6.67460700	1.25362200	0.57858900
S	-5.37211700	3.51180200	1.28832200
C	-4.99893600	1.03853800	2.39651100
H	-3.80737300	1.62009100	-2.15014300
H	-5.54413300	1.69271300	-1.78958700
H	-4.48528800	3.05253300	-1.34744500
C	-7.46818900	-2.26977500	-0.30581400
F	-5.28257200	-3.15177700	-0.03823300
F	-5.83185500	-2.38738400	-2.00756200
C	-7.97865800	-0.81237300	-0.25560900
C	-7.66933700	2.27252200	0.81331200
C	-7.10066800	3.45327100	1.17314900
H	-5.78152600	1.34067400	3.09757900
H	-5.00939700	-0.05233000	2.31174500
H	-4.03075700	1.35085000	2.79429900
F	-7.57993000	-2.80197000	0.92766200
F	-8.15651000	-3.02724200	-1.17041400
F	-8.52230500	-0.49133900	-1.46275300
F	-8.96885400	-0.71734200	0.66127900
C	-9.14675300	2.13382100	0.60653900
H	-7.65684600	4.36366000	1.37292500
H	-9.36774500	1.69930300	-0.37374700
H	-9.60335800	1.48313400	1.35742500
H	-9.62939500	3.11335300	0.66137600

Table S2: Cartesian coordinates (in Å) of 2-oc.

Atom	X	Y	Z
C	3.15440600	-0.12104500	-1.05177000
C	4.05889100	0.63095000	-0.33748000
C	5.41341600	0.37239500	-0.68978800
C	5.53452800	-0.56421400	-1.70322400
C	6.52866700	1.08538800	-0.07032900
C	6.40778100	2.56739600	0.16642200
C	7.72173900	0.62139600	0.37053600
C	7.85474700	3.03632400	0.41640000
C	8.58457300	1.75414900	0.86787800
C	8.18296800	-0.75982000	0.50400700
C	9.46905100	-1.20682900	0.06594100
C	7.44247000	-1.76458800	1.09637100
C	9.69918400	-2.53664200	0.29320100
C	6.76593200	-1.05482900	-2.38671000
C	6.09348900	-1.70022200	1.73134200
S	3.98926300	-1.14132500	-2.19620200
S	8.32814900	-3.24496100	1.09438200
H	7.54652100	-0.28951400	-2.35175800
H	7.16696000	-1.95249300	-1.90059300
H	6.56909900	-1.29657500	-3.43549200
H	5.88360600	-0.68258600	2.07313300
H	5.29852500	-1.98372500	1.03057000
H	6.03027000	-2.36741100	2.59658900
C	1.76087600	-0.13388100	-0.96001100

C	-2.02822800	-0.25276300	-0.72019400
F	9.84174000	1.71757400	0.36480600
F	8.69140500	1.73385600	2.21582500
F	7.93191400	4.01857700	1.32238300
F	8.38159200	3.46342700	-0.74651000
F	5.64748700	2.82571800	1.26638200
F	5.84811800	3.22319300	-0.86779200
C	-3.41911500	-0.27670100	-0.61267700
C	-4.23228000	-1.35681700	-0.83891400
S	-4.28118600	1.18366200	-0.10286300
C	-5.60920300	-1.08937700	-0.63435700
C	-5.91218400	0.40554700	-0.50190300
C	-6.66993100	-1.94344500	-0.59248600
C	-6.97673900	0.59733900	0.59127100
C	-6.35184700	0.91351500	-1.88750700
C	-6.69901100	-3.40431000	-0.91712900
C	-7.98981700	-1.49190300	-0.24434200
C	-8.20829600	-0.24166100	0.24948500
S	-7.62292200	2.32283000	0.72029500
C	-6.50464600	0.16551100	1.99307100
H	-5.56972400	0.68485400	-2.61614100
H	-7.27555700	0.41599500	-2.20002500
H	-6.51927800	1.99276900	-1.87933600
C	-8.08402200	-3.86829500	-0.40069200
F	-5.69682600	-4.11112700	-0.34632100
F	-6.63388800	-3.62906100	-2.25451200
C	-8.96825100	-2.59865800	-0.46739500

C	-9.41891600	0.41293400	0.60150800
C	-9.28011400	1.74383200	0.87781800
H	-7.33485200	0.26758000	2.69689000
H	-6.18489000	-0.88133800	1.98043600
H	-5.67165300	0.78231800	2.33686900
F	-7.96341700	-4.23762800	0.89077500
F	-8.58459900	-4.88923100	-1.10594200
F	-9.54645400	-2.53950800	-1.69605300
F	-9.96672000	-2.64398100	0.44290700
H	10.17802900	-0.56183100	-0.43820500
H	3.75951300	1.34138000	0.42361100
H	-3.84320600	-2.33375800	-1.10061500
H	-10.36947400	-0.10631300	0.63624100
C	10.88607700	-3.32709800	-0.03805800
C	10.80401800	-4.70637800	-0.27257800
C	12.14056100	-2.70677900	-0.12970400
C	11.93981700	-5.44169600	-0.59005100
H	9.83847300	-5.20423300	-0.22354100
C	13.27195800	-3.44217300	-0.45913700
H	12.22869400	-1.64495600	0.08237800
C	13.17803100	-4.81296100	-0.68900600
H	11.85427000	-6.50992600	-0.76949000
H	14.23521800	-2.94341500	-0.52317800
H	14.06510300	-5.38767700	-0.93992400
C	-10.34241000	2.67525500	1.25072500
C	-10.05318600	3.87862500	1.91139800
C	-11.68270800	2.38114800	0.95013200

C	-11.07180600	4.75198900	2.27189700
H	-9.02371800	4.11859400	2.16342100
C	-12.69701700	3.25567500	1.31180900
H	-11.92612400	1.47162700	0.40925000
C	-12.39668200	4.44426200	1.97572700
H	-10.82845800	5.67573100	2.78922100
H	-13.72727600	3.01327200	1.06673400
H	-13.19236000	5.12894000	2.25557000
C	-0.80756600	-0.20658900	-0.79743000
C	0.54059000	-0.17067000	-0.88442100

Table S3: Cartesian coordinates (in Å) of 3-oc.

Atom	X	Y	Z
C	7.44362200	2.13230100	-5.51260100
C	7.78495000	2.23202900	-4.19374000
C	7.09411000	1.25797100	-3.38364500
C	6.26761200	0.43773200	-4.09992500
C	7.25114800	1.12713600	-1.92376000
C	8.56575600	0.69771200	-1.31973200
C	6.31767700	1.28112400	-0.97177500
C	8.20149600	0.27477500	0.11692200
C	6.91923400	1.07386100	0.39388900
C	4.91519000	1.70301400	-1.12712900
C	3.78219200	0.86987200	-0.80898100
C	4.57323200	2.93930300	-1.60002700
C	2.59849500	1.50103500	-1.07142600
C	5.46611100	4.06398500	-2.01438700
S	6.30797200	0.84396600	-5.77190400
S	2.86284900	3.10896000	-1.67506300
H	6.38296200	4.06046500	-1.42492700
H	5.74257900	3.98324500	-3.06824500
H	4.98347400	5.03089800	-1.86927200
C	5.42067900	-0.69618200	-3.61921800
H	5.89257100	-1.19495700	-2.77252700
H	4.43511600	-0.35060800	-3.29909000
H	5.27392600	-1.44199500	-4.40098700
F	9.13394300	-0.31585400	-2.00562300

F	9.48151000	1.70006200	-1.26229100
F	7.91314600	-1.04355800	0.13667400
F	9.17753900	0.51283400	1.00086400
F	6.11581500	0.43511000	1.26965300
F	7.24042600	2.26833400	0.96007900
C	1.22333800	1.00107400	-0.91657700
C	0.26936600	1.20421900	-1.91698400
C	0.83131900	0.31978300	0.23741300
C	-1.02461700	0.73718700	-1.77298400
H	0.54925400	1.72023300	-2.82825100
C	-0.46396300	-0.14557600	0.38373400
H	1.54403000	0.16713100	1.03813300
C	-1.41509400	0.06059300	-0.61607000
H	-1.74456300	0.90923100	-2.56482000
H	-0.73986600	-0.68425800	1.28233600
C	7.90414400	2.93638800	-6.65870800
C	6.99210100	3.45431800	-7.58128500
C	9.26433000	3.18271700	-6.85599900
C	7.42730800	4.20198600	-8.66467600
H	5.93111500	3.28142900	-7.43868600
C	9.69788700	3.93619300	-7.93647800
H	9.98762600	2.76249300	-6.16741200
C	8.78150700	4.44846600	-8.84450300
H	6.70391500	4.59860300	-9.36827800
H	10.75838700	4.11514300	-8.07436100
H	9.12152700	5.03469400	-9.69072100
C	3.89281100	-0.54567400	-0.31747700

H	4.82203000	-1.00867600	-0.64884800
H	3.89041100	-0.59769000	0.77214900
H	3.06520300	-1.15457700	-0.68193200
C	8.72456800	3.26734100	-3.64565500
H	8.40769500	3.60978600	-2.66086600
H	9.73687600	2.87548000	-3.52910400
H	8.77757000	4.13382300	-4.30392700
C	-2.78865900	-0.45112800	-0.46978600
S	-3.44230200	-1.35887000	-1.82909400
C	-3.62077400	-0.29141800	0.58981800
C	-4.95865600	-1.78555400	-0.87655900
C	-4.90933300	-0.92485700	0.38697300
C	-6.25501600	-1.46093100	-1.63188200
C	-4.83290300	-3.26120400	-0.45350100
C	-6.05892300	-0.89040500	1.09879600
S	-6.50638100	-2.49860100	-3.13383100
C	-7.45810800	-1.75525700	-0.73778200
C	-6.36067900	0.01562700	-2.06500000
H	-3.91092900	-3.39466400	0.11172200
H	-5.66913100	-3.55734100	0.17989100
H	-4.80184000	-3.92032500	-1.31897900
C	-7.31744700	-1.43114100	0.56663600
C	-6.31595000	-0.34533200	2.46645200
C	-8.21011500	-2.70644100	-2.73164300
C	-8.57664100	-2.29361200	-1.49515200
H	-5.55923500	0.28435800	-2.74975500
H	-7.31251100	0.17568300	-2.57028600

H	-6.31867500	0.67727000	-1.19897700
C	-8.35066300	-1.44647500	1.65041200
C	-7.57600600	-1.09845600	2.94051300
F	-5.32048300	-0.53793500	3.36153300
F	-6.58460400	0.99373400	2.45839500
C	-9.06567200	-3.30351600	-3.77723600
F	-8.97866400	-2.63807600	1.81710900
F	-9.32602400	-0.51523000	1.46074500
F	-7.18776600	-2.24300700	3.53881300
F	-8.30875300	-0.39085400	3.80939600
C	-8.77472300	-4.56976400	-4.28510700
C	-10.15273700	-2.59950600	-4.29563300
C	-9.56748100	-5.12793600	-5.27653600
H	-7.93145500	-5.12480300	-3.88955300
C	-10.94030200	-3.15742200	-5.29116000
H	-10.37100600	-1.60469400	-3.92454400
C	-10.65168800	-4.42373500	-5.78162500
H	-9.33636400	-6.11684800	-5.65577900
H	-11.78010500	-2.59840900	-5.68805100
H	-11.26884600	-4.85941600	-6.55914200
C	-3.29330300	0.58563400	1.76382600
H	-4.12753400	1.24898300	1.99324400
H	-3.08809700	0.00923300	2.66622900
H	-2.42578800	1.20739100	1.55231000
C	-9.97019200	-2.42962100	-0.95643700
H	-10.00020700	-3.12505700	-0.11869200
H	-10.35002700	-1.47429700	-0.59106800

H	-10.65052800	-2.79918700	-1.71970700

Table S4: Cartesian coordinates (in Å) of 4-oc.

Atom	X	Y	Z
C	10.76643800	-1.64620900	-0.31572900
C	10.74904200	-0.28033600	-0.31100400
C	9.64924800	0.24120800	0.46345000
C	8.87673400	-0.72828800	1.03911800
C	9.36527200	1.67679000	0.64319000
C	10.31033800	2.56393500	1.41510800
C	8.28318200	2.36314600	0.24580100
C	9.47910400	3.82453200	1.72472400
C	8.41810600	3.81781900	0.61346500
C	7.13614700	1.87959100	-0.54336300
C	5.78945900	1.77574000	-0.03546700
C	7.26373200	1.48729200	-1.84598700
C	4.93131700	1.27934700	-0.97286000
C	8.49157800	1.45644200	-2.69832700
S	9.46796600	-2.29432300	0.63842400
S	5.74695500	0.96819700	-2.47394200
H	9.17041600	2.26234700	-2.41901700
H	9.02721300	0.51056000	-2.58886800
H	8.24778400	1.58084800	-3.75377900
C	7.68138300	-0.57597800	1.92364000
H	7.76477600	0.32594500	2.53023400
H	6.76126600	-0.50358500	1.33918100
H	7.57974800	-1.42242900	2.60360300
F	10.75416200	1.97388200	2.54483800

F	11.40778700	2.92574900	0.69992500
F	8.86896600	3.67726900	2.91936000
F	10.21092000	4.94481400	1.75329900
F	7.27206000	4.40233000	1.01871300
F	8.86829600	4.53815300	-0.44963500
C	-0.72692900	0.18011200	-0.57055400
C	-1.34098900	0.01538800	0.67163200
C	-1.51955100	0.07221000	-1.71394000
C	-2.69531400	-0.25560300	0.76837500
H	-0.75710300	0.12886700	1.57790700
C	-2.87539700	-0.19156000	-1.62094400
H	-1.06555700	0.17361700	-2.69304800
C	-3.48083800	-0.37258300	-0.37780200
H	-3.15497600	-0.35639200	1.74475500
H	-3.46901300	-0.27838100	-2.52373100
C	11.70174700	-2.56460900	-0.98943200
C	11.22833700	-3.64720300	-1.73448200
C	13.08187600	-2.38130900	-0.88302700
C	12.10916000	-4.51628600	-2.35975400
H	10.15947800	-3.79890000	-1.83662800
C	13.96178400	-3.24757900	-1.51427700
H	13.46656300	-1.56469400	-0.28379300
C	13.47904300	-4.31789700	-2.25462400
H	11.72262800	-5.34897200	-2.93671700
H	15.03036400	-3.09042400	-1.41852100
H	14.16767100	-4.99649300	-2.74521100
C	5.37073900	2.20943200	1.34089000

H	6.17995300	2.09788200	2.06273000
H	5.08492800	3.26241100	1.34568900
H	4.51807000	1.63657400	1.70064300
C	11.72714900	0.57485100	-1.06414200
H	11.24967000	1.47163000	-1.45793300
H	12.54633600	0.91178800	-0.42590100
H	12.16116800	0.02773000	-1.90040700
C	-4.92958100	-0.64303900	-0.27887100
S	-5.99520900	0.57220500	-0.97025600
C	-5.53793700	-1.70261000	0.30630000
C	-7.47669900	-0.46617300	-0.63107900
C	-6.98823200	-1.60093700	0.27329400
C	-8.57675700	0.30821400	0.10738900
C	-7.93285000	-1.08557500	-1.96466000
C	-7.96657000	-2.31134700	0.87911900
S	-9.33615000	1.64605900	-0.90627500
C	-9.72695900	-0.63347400	0.45504100
C	-8.10081300	0.94278600	1.43103000
H	-7.10943100	-1.65438900	-2.39611600
H	-8.77402600	-1.76240300	-1.81306800
H	-8.22887800	-0.31786000	-2.67700700
C	-9.37134600	-1.87337000	0.85836000
C	-7.87799000	-3.56837200	1.68619800
C	-10.94178700	1.19406300	-0.33860100
C	-11.01874600	0.02459500	0.34038800
H	-7.31318700	1.67292000	1.25942900
H	-8.93942600	1.44705100	1.91000900

H	-7.72791700	0.17800200	2.11347400
C	-10.23962400	-2.94271100	1.44476900
C	-9.30378400	-4.15545600	1.63592900
F	-7.00884100	-4.49905100	1.23135100
F	-7.54563000	-3.32506600	2.98755200
C	-12.03945400	2.13050500	-0.65481600
F	-11.29011800	-3.31041200	0.66766400
F	-10.75536800	-2.59312700	2.65592300
F	-9.39632700	-4.95372400	0.55306300
F	-9.60592400	-4.87607900	2.72335900
C	-12.32259800	2.45932900	-1.98062300
C	-12.78426900	2.72499700	0.36396000
C	-13.34336400	3.34850000	-2.28108500
H	-11.74890000	2.00359300	-2.77987400
C	-13.80030900	3.61859400	0.06109700
H	-12.55463500	2.49465000	1.39795800
C	-14.08444700	3.92994800	-1.26165400
H	-13.55957300	3.58804400	-3.31600800
H	-14.36911900	4.07656900	0.86233700
H	-14.87986300	4.62780600	-1.49732300
C	-4.78121000	-2.82935400	0.94551900
H	-5.06095900	-2.95542700	1.99333700
H	-4.98596500	-3.77457400	0.44539000
H	-3.70951500	-2.65174600	0.90176700
C	-12.30620800	-0.54654100	0.85715400
H	-12.54747800	-1.48368700	0.35738900
H	-12.24652900	-0.76124100	1.92515400

H	-13.13248600	0.14047200	0.69204000
C	0.72364900	0.46556700	-0.67185900
C	1.21261300	1.38518000	-1.59958100
C	1.64174400	-0.18261000	0.15560300
C	2.56855900	1.65232500	-1.69322900
H	0.52107400	1.92226700	-2.23885700
C	2.99794400	0.07794400	0.05766400
H	1.29390100	-0.92708900	0.86293300
C	3.48424200	1.00627000	-0.86320100
H	2.92246800	2.38730900	-2.40741800
H	3.69455300	-0.46326000	0.68800700

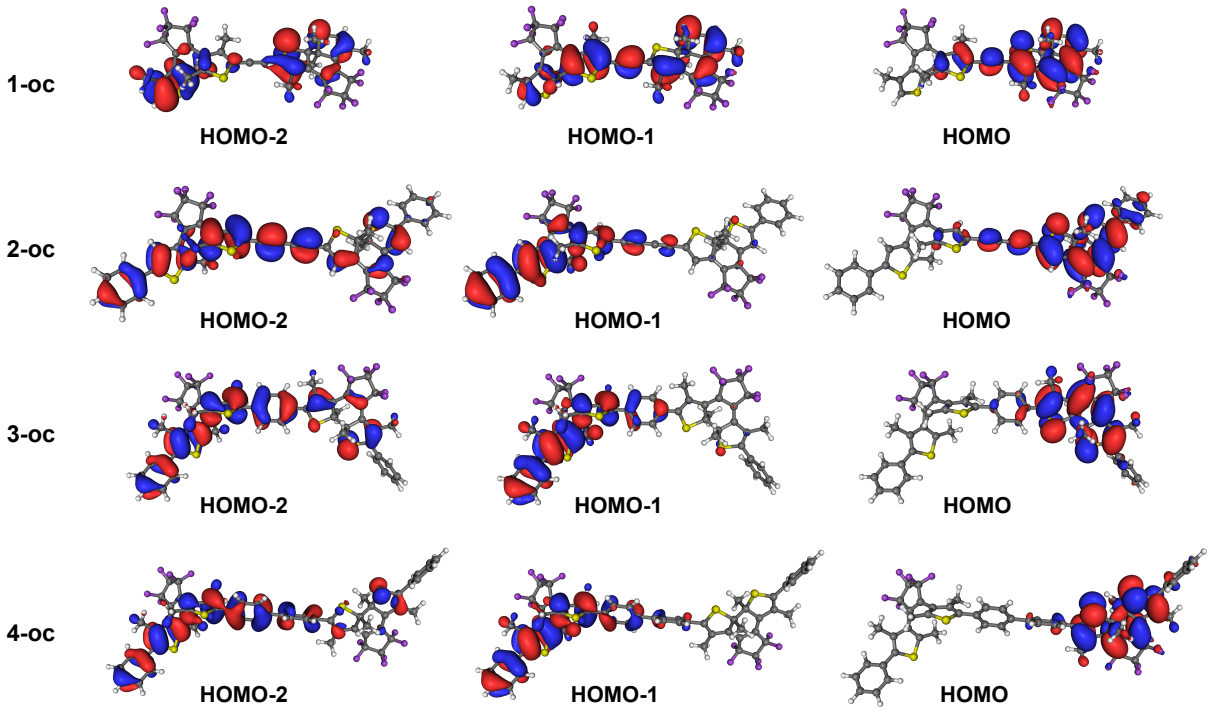

Figure S1: Occupied frontier molecular orbitals for the open-closed dimers (isocontour: 0.02 au). See the main text for the representation of the virtual frontier orbitals for the same compounds.

Table S5: Most relevant electronic transitions in the open-closed dimers: transition wavelengths (in nm), associated oscillator strength (f) and involved molecular orbitals (with contributions are larger than 10%).

Compound	Wavelength (f)	Orbitalar composition
1-oc	533 (0.65)	HOMO→LUMO (93%)
	347 (0.39)	HOMO-1→LUMO (69%)
		HOMO-2→LUMO (18%)
	323 (0.78)	HOMO-3→LUMO (32%)
		HOMO-2→LUMO (21%)
		HOMO-1→LUMO (15%)
		HOMO→LUMO+2 (16%)
	302 (0.16)	HOMO→LUMO+2 (56%)
2-oc	566 (1.06)	HOMO→LUMO (93%)
	365 (0.57)	HOMO-2→LUMO (47%)
		HOMO-1→LUMO (16%)
	327 (0.22)	HOMO-7→LUMO (22%)
		HOMO→LUMO+1 (17%)
		HOMO→LUMO+2 (15%)
		HOMO→LUMO+3 (10%)
	313 (0.22)	HOMO-7→LUMO (43%)
		HOMO→LUMO+1 (14%)
3-oc	480 (0.46)	HOMO→LUMO (94%)
	327 (0.28)	HOMO-3→LUMO (65%)
		HOMO-2→LUMO (25%)
	296 (0.30)	HOMO→LUMO+2 (45%)
		HOMO→LUMO+4 (17%)
		HOMO→LUMO+9 (10%)
	289 (0.70)	HOMO-1→LUMO (21%)
		HOMO-2→LUMO (15%)
		HOMO-3→LUMO (14%)
		HOMO-1→LUMO+1 (14%)
4-oc	471 (0.42)	HOMO→LUMO (95%)
	326 (0.24)	HOMO-3→LUMO (79%)
		HOMO-2→LUMO (12%)
	279 (0.84)	HOMO→LUMO+2 (40%)
		HOMO→LUMO+1 (10%)