

Supplementary Information

Theoretical Insight into Joint Photodynamic Action of a Gold(I) complex and a BODIPY chromophore for Singlet Oxygen Generation.

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Table S1

bdp			Ac-bdp			Au-bdp			I-bdp		
C	-0.28245900	0.64431800	-1.33247500	C	-0.28324500	0.64525500	-1.33357900	C	-0.27868000	0.73025200	-1.23029900
C	0.63841700	2.07703300	0.17346900	C	0.63915300	2.07958600	0.16997300	C	0.70226500	2.23251000	0.16656600
C	-0.25112100	0.99733800	0.01309600	C	-0.25128700	0.99778400	0.00949500	C	-0.19353900	1.14797300	0.09450200
N	1.15796000	2.40130300	-1.02980500	H	-0.80978400	0.52878100	0.80935200	H	-0.72125800	0.71918100	0.93685100
C	1.92177900	2.63693100	-3.75268400	N	1.15805400	2.40485500	-1.03127900	N	1.17253100	2.49728900	-1.07116800
C	2.46414700	2.96288700	-5.04036300	C	1.92395000	2.63992400	-3.75578300	C	1.82167000	2.60309900	-3.83458200
C	3.34151300	4.02211500	-4.82947000	C	2.46033800	2.95607700	-5.03708200	C	2.30205400	2.86518500	-5.15323500
C	3.34002200	4.34016100	-3.45775400	C	3.35211000	4.02628500	-4.83123500	C	3.19253500	3.94952600	-5.04175900
N	2.49015000	3.51104800	-2.81493600	C	3.34303200	4.34212400	-3.44655500	C	3.23815500	4.32591200	-3.66838800
B	2.17994900	3.53817700	-1.29486100	N	2.49227400	3.51418400	-2.81681300	N	2.42440700	3.52328000	-2.96186400
F	1.62860900	4.77516500	-0.93680300	B	2.17909800	3.54277100	-1.29318400	B	2.18779200	3.61259000	-1.42812600
F	3.35063500	3.31664100	-0.55906000	F	1.62582300	4.77838000	-0.94182700	F	1.66663100	4.86785200	-1.09645600
C	0.99468900	1.66299200	-3.34541900	F	3.34902600	3.32153000	-0.56035100	F	3.39158000	3.40621400	-0.74209300
C	0.61728000	1.54239100	-1.99751300	C	0.99271000	1.66376600	-3.34500500	C	0.91598100	1.64717700	-3.34031800
C	0.40205700	0.73995800	-4.36183900	C	0.61765300	1.54585900	-2.00082200	C	0.59463600	1.59328300	-1.97387500
C	1.03967600	-0.46773100	-4.67761100	C	0.40058000	0.74056400	-4.36120100	C	0.28452200	0.67341000	-4.28304200
C	-0.79519300	1.07363900	-5.00942300	C	1.04186600	-0.46438300	-4.67982100	C	0.90538400	-0.55404700	-4.55322100
C	0.48672900	-1.32882800	-5.62747600	C	-0.79902800	1.07233700	-5.00534400	C	-0.93463900	0.97793300	-4.90428300
H	1.96808100	-0.73094000	-4.17824600	C	0.48942200	-1.32539800	-5.62996800	C	0.31423600	-1.46362300	-5.43280500
C	-1.34555300	0.21146200	-5.9598200	H	1.97211600	-0.72557600	-4.18290500	H	1.85043800	-0.79455100	-4.07417100
H	-1.29333300	2.00858800	-4.76805300	C	-1.34829500	0.21002900	-5.95635800	C	-1.52346100	0.06695200	-5.78402000
C	-0.70620200	-0.99094200	-6.27067600	H	-1.29954800	2.00532800	-4.76148200	H	-1.41945300	1.92813400	-4.69802700
H	0.98907000	-2.26266000	-5.86409400	C	-0.70570900	-0.98981000	-6.27023400	C	-0.90065300	-1.15517500	-6.04982700
H	-2.27359700	0.48052300	-6.45668300	H	0.99400700	-2.25731900	-5.86906700	H	0.80393600	-2.41212700	-5.63499400
H	-1.13545400	-1.66112300	-7.01014600	H	-2.27807300	0.47704500	-6.45078600	H	-2.46807800	0.31347700	-6.26073900
C	2.19180700	2.34085300	-6.37830600	H	-1.13427100	-1.65994700	-7.01008000	H	-1.15952800	-1.86313500	-6.73422800
H	2.46231200	1.27992700	-6.40182900	C	2.18881100	2.33557700	-6.37347900	C	1.97796400	2.17574300	-6.44314600
H	1.13341600	2.40158600	-6.65265000	H	2.46965200	1.27746000	-6.39777700	H	2.26694200	1.11924200	-6.42714600
H	2.77294900	2.85631400	-7.14890600	H	1.12845000	2.38744900	-6.64067300	H	0.90674000	2.20656400	-6.66795200
C	4.12387600	5.40279300	-2.75833300	H	2.76285200	2.85903500	-7.14296900	H	2.51540900	2.66498200	-7.26060300
H	3.45696800	6.09148200	-2.22881400	C	4.12665300	5.40309800	-2.74876300	C	4.03266800	5.43012000	-3.05579500
H	4.78799000	4.96347500	-2.00614900	H	3.45874000	6.08612100	-2.21383300	H	3.37027500	6.20505600	-2.65323400
H	4.72389500	5.96761900	-3.47561100	H	4.79527100	4.96082800	-2.00256300	H	4.63226400	5.05667000	-2.21984400
C	-1.11497800	-0.46849400	-1.89811300	H	4.71940900	5.96912800	-3.47018100	H	4.68963500	5.87853200	-3.80415500
H	-1.84401300	-0.10622700	-2.63087300	C	-1.11409000	-0.46746700	-1.90005700	C	-1.13460500	-0.40588200	-1.70784600
H	-0.50468600	-1.22126100	-2.40777800	H	-1.84454600	-0.10380800	-2.63057400	H	-1.88021200	-0.07963400	-2.44070900
H	-1.66345700	-0.96443900	-1.09155500	H	-0.50230900	-1.21655100	-2.41313000	H	-0.54359200	-1.19195500	-2.18957300
C	0.99590900	2.79566500	1.43379700	H	-1.65980800	-0.96654000	-1.09378700	H	-1.66398500	-0.84989500	-0.85930300
H	2.07254500	2.73324800	1.62449900	C	4.13215000	4.68877600	-5.81405400	C	3.92420600	4.57496200	-6.08469100
H	0.74917700	3.86009500	1.35647500	C	4.79983800	5.25570200	-6.65211700	C	4.56082800	5.12023700	-6.98448300
H	0.45806400	2.36670700	2.28248000	C	5.38810100	5.75537100	-7.38944000	Au	5.60309500	6.02618200	-8.43389300
H	-0.81093600	0.52804000	0.81207900	C	0.99562200	2.79627900	1.43099300	P	6.83920000	7.10546200	-10.12326200
H	3.93118000	4.52603500	-5.58473300	H	2.07209200	2.73191200	1.62178500	C	7.80162800	8.53480500	-9.48750100
				H	0.75057700	3.86098700	1.35281500	C	8.00064400	9.69911100	-10.24502400
				H	0.45631900	2.36772600	2.27868600	C	8.36523000	8.44399200	-8.20345500
								C	8.75735900	10.75256500	-9.72659100
								H	7.56448900	9.78841600	-11.23501700
								C	9.12463900	9.49665900	-7.69217800
								H	8.20677900	7.55226000	-7.60262000
								C	9.32079300	10.65259000	-8.45263600
								H	8.90350300	11.65098800	-10.31941900
								H	9.55483400	9.41657600	-6.69803700
								H	9.90632200	11.47473400	-8.05104500
								C	5.78598600	7.76892900	-11.47454100
								C	6.20999200	7.78670600	-12.81215200
								C	4.51970900	8.28253400	-11.14707700
								C	5.38153800	8.31640400	-13.80410300
								H	7.18124100	7.38498200	-13.08347900
								C	3.69796900	8.81546100	-12.14062100
								H	4.17497200	8.26093900	-10.11658000
								C	4.12734900	8.83213000	-13.47041500
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								H	7.22044900	9.20867700	-11.87667600
								H	3.48384900	9.24053300	-14.24447800
								C	8.05955100	5.99990200	-10.93707700
								C	9.31732200	6.45568200	-11.36007000
								C	7.70694200	4.65629100	-11.14941400
								C	10.20522800	5.58064500	-11.99032900
								H	9.60834100	7.48857900	-11.19658500
								C	8.59467800	3.78776000	-11.78478000
								H	6.74069200	4.28902700	-10.81336700
								C	9.84556800	4.24841100	-12.20472000
								H	11.17798700	5.94221500	-12.31125000
								H	8.31256200	2.75082500	-11.94294500
								H	10.53930600	3.56950200	-12.69241900
								C	1.11131800	3.01135000	1.37455700
								H	2.19924000	2.99155100	1.49710800
								H	0.82238400	4.06361100	1.27520200
								H	0.64251600	2.59866600	2.27097900

Figure S1

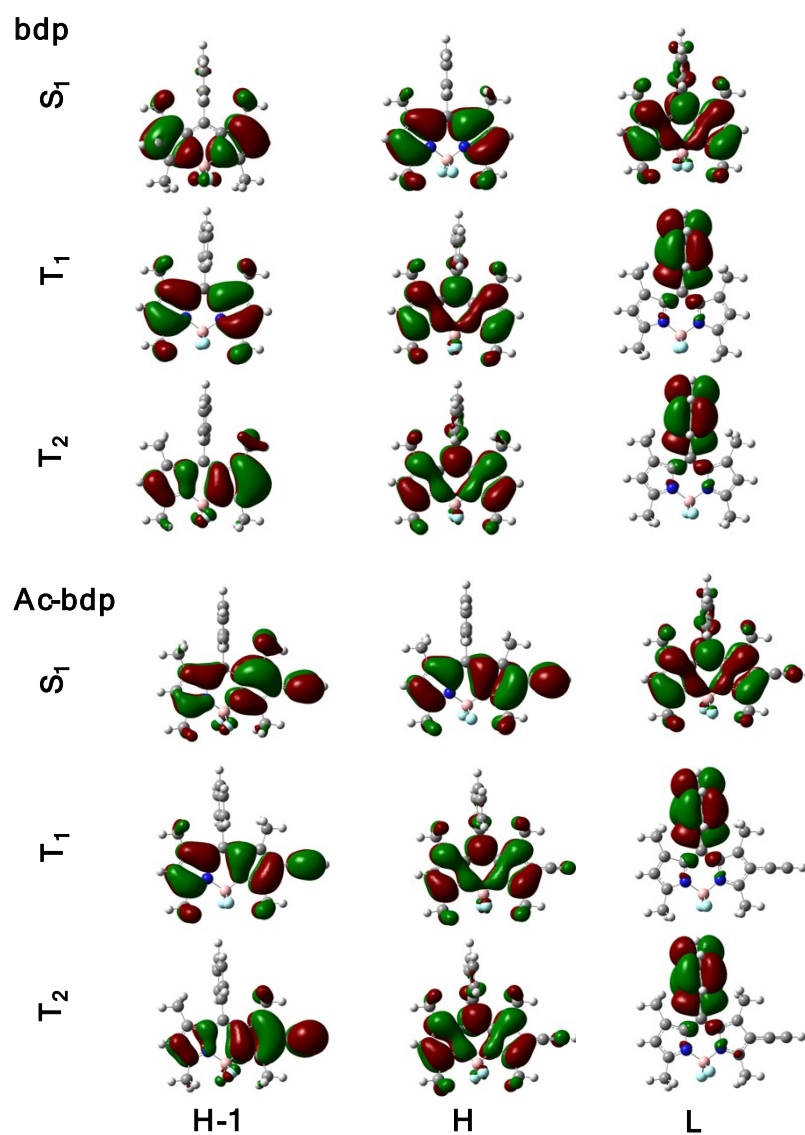


Figure S2

