Supporting Information

Singlet and triplet excited states of a series of BODIPY dyes as calculated by TDDFT and DLPNO-STEOM-CCSD methods

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Table S1: Singlet excited state properties of BOD-Ph at the S_0 geometry calculated in a vacuum with MN15.

State	Transition	Weight (%)	Energy(eV)	λ (nm)	f
S_1 $\pi_{BOD} \rightarrow \pi_{BOD}*$	108a -> 109a	84	3.02	410	0.736
S_2 $\pi_{BOD} \rightarrow \pi_{BOD}*$	107a -> 109a	93	3.63	341	0.067
S_3 $\pi_{BOD} \rightarrow \pi_{BOD}*$	106a -> 109a	84	3.66	338	0.496
S_4 $\pi_{Ph} \rightarrow \pi_{BOD}*$	103a -> 109a	75	4.15	299	0
S_5 $n_I \rightarrow \pi_{BOD}*$	105a -> 109a	75	4.36	284	0
S_6 $n_I \rightarrow \pi_{BOD}*$	104a -> 109a	98	4.37	283	0
S_7 $\pi_{BOD} \rightarrow \sigma_I*$	108a -> 112a	46	4.43	279	0
S_8 $\pi_{BOD} \rightarrow \sigma_I*$	108a -> 113a	54	4.50	275	0.002
S_9 $\pi_{Ph} \rightarrow \pi_{BOD}*$	102a -> 109a	98	4.57	271	0.008
S_{10} $\pi_{BOD} \rightarrow \pi_{Ph}*$	108a -> 110a	94	4.69	264	0
S_{11} $\pi_{BOD} \rightarrow \pi_{BOD}*$	101a -> 109a	69	4.82	257	0.014
S_{12} $\pi_{BOD} \rightarrow \pi_{Ph}*$	108a -> 111a	75	4.91	252	0.045
S_{13} $\pi_{BOD} \rightarrow \pi_{BOD}*$	100a -> 109a	95	5.09	243	0.005
S_{14} $\pi_{BOD} \rightarrow \sigma_I*$	106a -> 112a	44	5.25	236	0
S_{15} $\pi_{BOD} \rightarrow \sigma_I*$	106a -> 113a	33	5.32	233	0
S_{16}	105a -> 112a	45	5.39	230	0
S_{17}	104a -> 112a	50	5.39	230	0
S_{18}	102a -> 110a	45	5.43	228	0
S_{19}	98a -> 109a	94	5.62	220	0
S_{20} $\pi_{BOD} \rightarrow \pi_{BOD}*$	99a -> 109a	82	5.71	217	0.219
S_{21} $\pi_{BOD} \rightarrow \pi_{Ph}*$	106a -> 110a	88	5.80	213	0.001
S_{22} $\pi_{BOD} \rightarrow \pi_{Ph}*$	107a -> 110a	97	5.88	210	0
S_{23} $\pi_{BOD} \rightarrow \pi_{Ph}*$	106a -> 111a	94	5.93	209	0.011
S_{24} $\pi_{BOD} \rightarrow \pi_{Ph}*$	107a -> 111a	96	6.01	206	0.002
S_{25}	108a -> 114a	63	6.20	200	0.295
S_{26}	97a -> 109a	92	6.22	199	0
S_{27}	96a -> 109a	87	6.25	198	0.005
S_{28} $\pi_{BOD} \rightarrow \sigma_I*$	100a -> 112a	42	6.38	194	0
S_{29} $\pi_{BOD} \rightarrow \sigma_I*$	100a -> 113a	38	6.40	193	0
S_{30}	102a -> 111a	33	6.409	193	0.029

Table S2: Triplet excited state properties of BOD-Ph at the S_0 geometry calculated in a vacuum with MN15.

State	Transition	Weight (%)	Energy(eV)	λ (nm)	f
$T_1\,\pi_{BOD} \rightarrow \pi_{BOD}*$	108a -> 109a	93	1.59	779	0
$T_2\,\pi_{BOD} \rightarrow \pi_{BOD}*$	106a -> 109a	85	2.77	447	0
$T_3\,\pi_{BOD} \rightarrow \pi_{BOD}*$	107a -> 109a	84	2.93	422	0
$T_4\,\pi_{BOD} \rightarrow \pi_{BOD}*$	101a -> 109a	73	3.51	353	0
$T_5\,\pi_{BOD} \rightarrow \sigma_I*$	108a -> 112a	45	3.91	319	0
$T_6\,\pi_{BOD} \rightarrow \sigma_I*$	108a -> 113a	40	3.95	314	0
T_7	103a -> 110a	55	4.10	302	0
$T_8\,\pi_{Ph} \rightarrow \pi_{BOD}*$	103a -> 109a	75	4.13	300	0
T_9	105a -> 109a	76	4.34	286	0
T_{10}	104a -> 109a	98	4.36	285	0
$T_{11}\,\pi_{Ph} \rightarrow \pi_{BOD}*$	102a -> 109a	99	4.55	272	0
T_{12}	105a -> 112a	50	4.60	269	0
T_{13}	104a -> 112a	52	4.61	269	0
$T_{14}\,\pi_{BOD} \rightarrow \pi_{Ph}*$	108a -> 110a	86	4.65	267	0
$T_{15}\,\pi_{BOD} \rightarrow \pi_{Ph}*$	108a -> 111a	47	4.69	264	0
T_{16}	102a -> 110	36	4.73	262	0
T_{17}	101a -> 109a	14	4.74	261	0
T_{18}	100a -> 109a	86	4.90	252	0
$T_{19}\,\pi_{BOD} \rightarrow \sigma_I*$	108a -> 112a	52	5.10	243	0
T_{20}	99a -> 109a	53	5.11	243	0
T_{21}	99a -> 109a	23	5.16	241	0
T_{22}	102a -> 110a	46	5.19	239	0
$T_{23}\,\pi_{BOD} \rightarrow \sigma_I*$	108a -> 113a	48	5.21	238	0
T_{24}	108a -> 115a	80	5.33	232	0
T_{25}	98a -> 109a	45	5.54	224	0
T_{26}	107a -> 115a	17	5.76	215	0
$T_{27}\,\pi_{BOD} \rightarrow \pi_{Ph}*$	106a -> 110a	89	5.80	214	0
$T_{28}\,\pi_{BOD} \rightarrow \pi_{Ph}*$	107a -> 110a	96	5.88	211	0
T_{29}	107a -> 111a	32	5.89	211	0
T_{30}	106a -> 111a	57	5.92	210	0

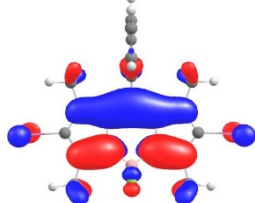**Table S3**: Molecular orbitals of BOD-Ph at the S_0 geometry calculated in a vacuum with MN15.
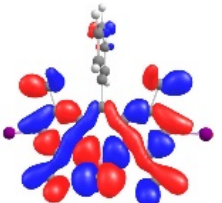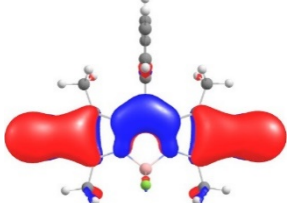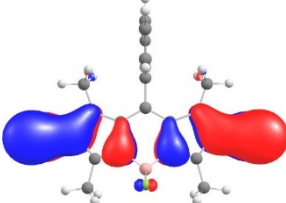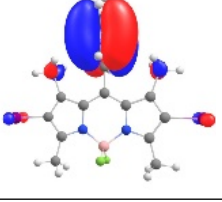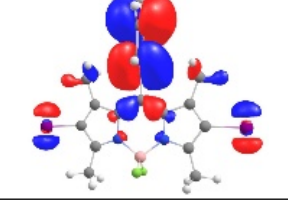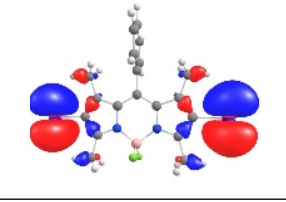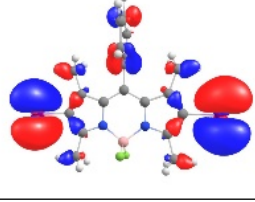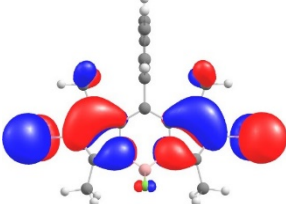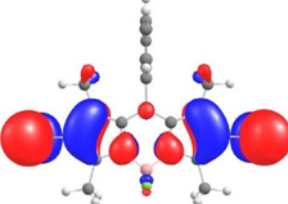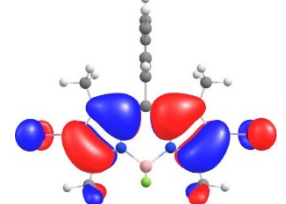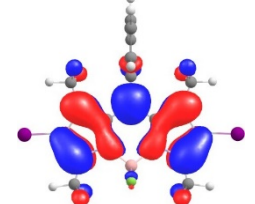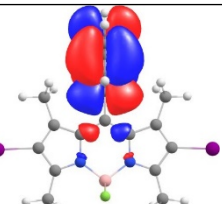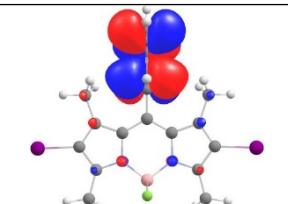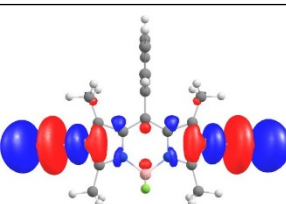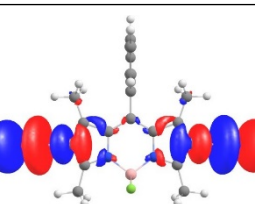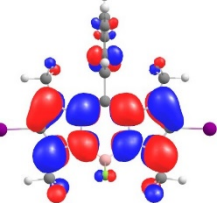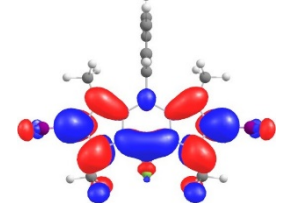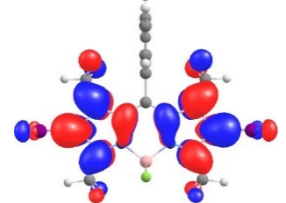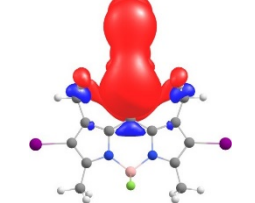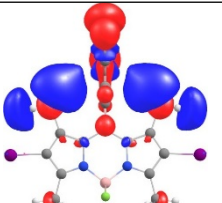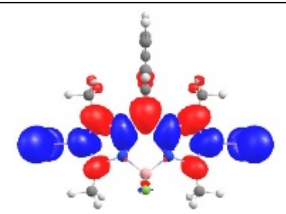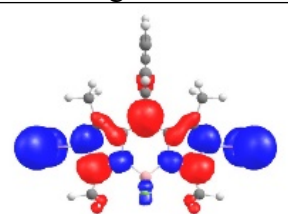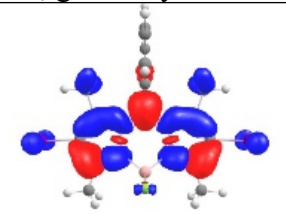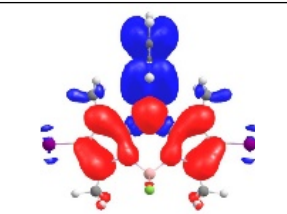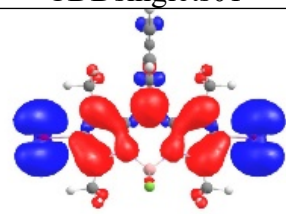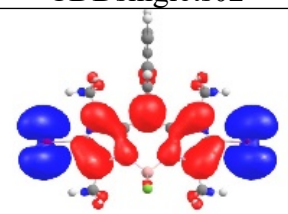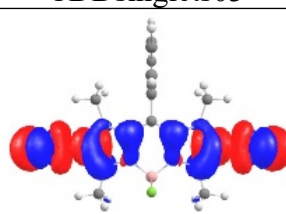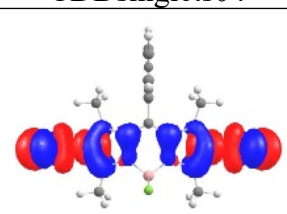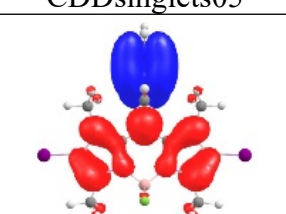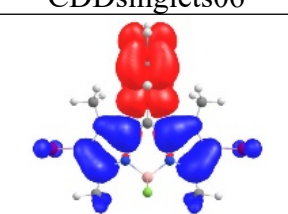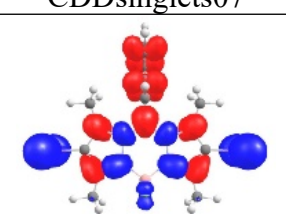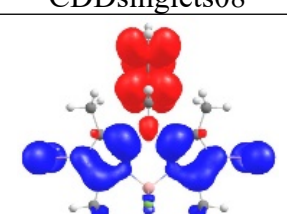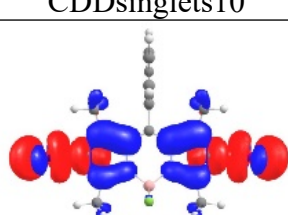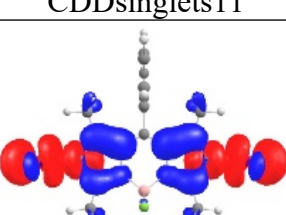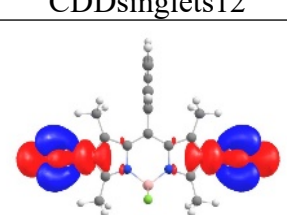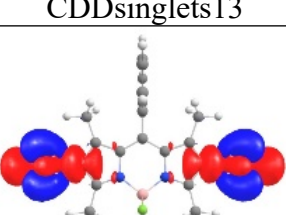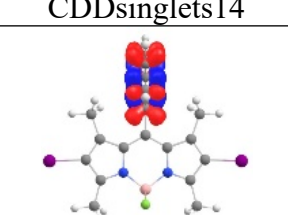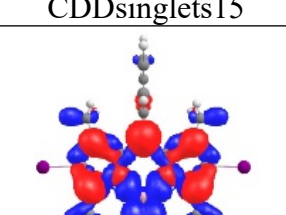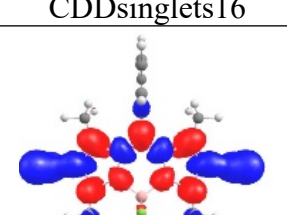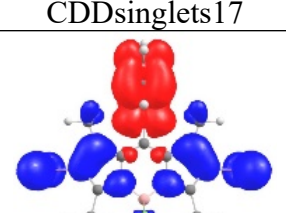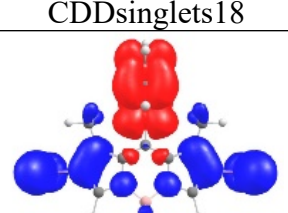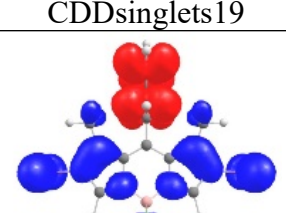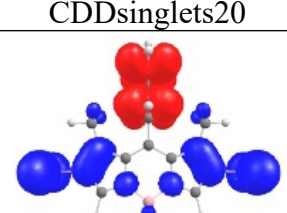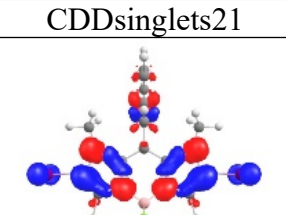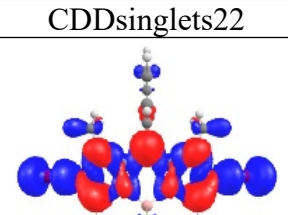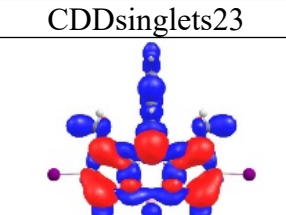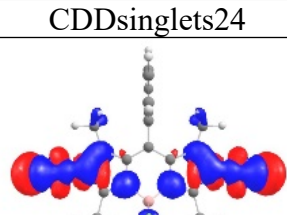
MO 98	MO 99	MO 100	MO 101
MO 102	MO 103	MO 104	MO 105
MO 106	MO 107	MO 108	MO 109
MO 110	MO 111	MO 112	MO 113
MO 114	MO 115	MO 116	MO 117
MO 118			

Table S4: CDDs of BOD-Ph singlet states at the S_0 geometry calculated in a vacuum with MN15.

CDDsinglets01	CDDsinglets02	CDDsinglets03	CDDsinglets04
CDDsinglets05	CDDsinglets06	CDDsinglets07	CDDsinglets08
CDDsinglets09	CDDsinglets10	CDDsinglets11	CDDsinglets12
CDDsinglets13	CDDsinglets14	CDDsinglets15	CDDsinglets16
CDDsinglets17	CDDsinglets18	CDDsinglets19	CDDsinglets20
CDDsinglets21	CDDsinglets22	CDDsinglets23	CDDsinglets24
CDDsinglets25	CDDsinglets26	CDDsinglets27	CDDsinglets28
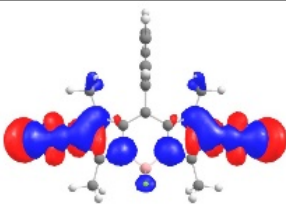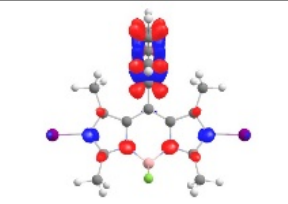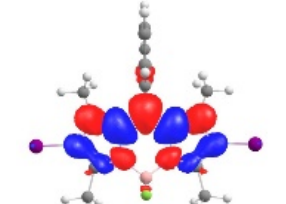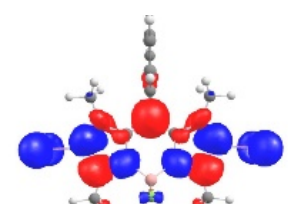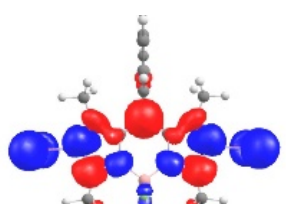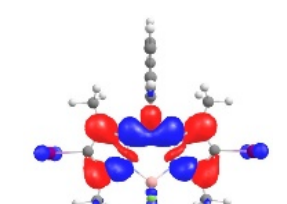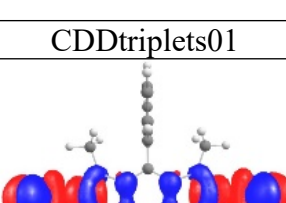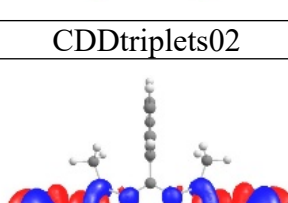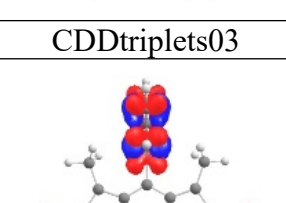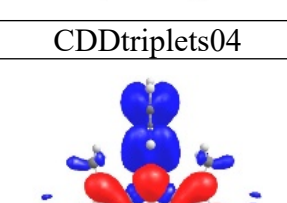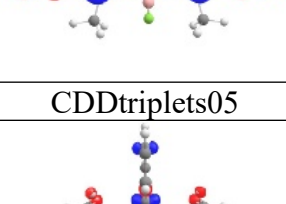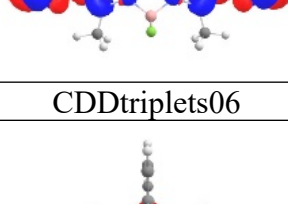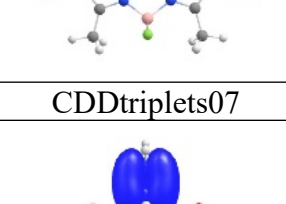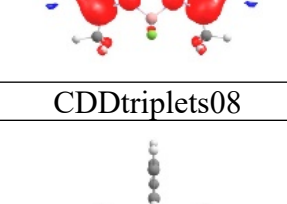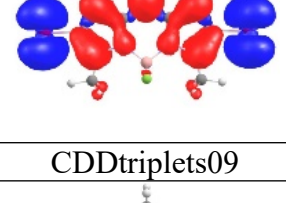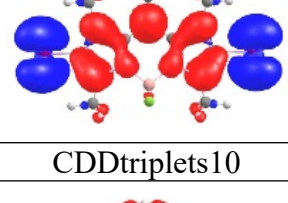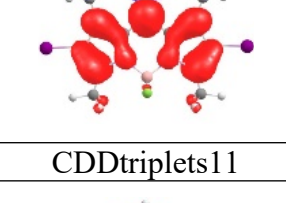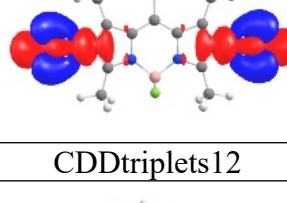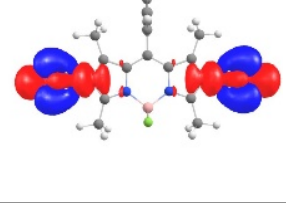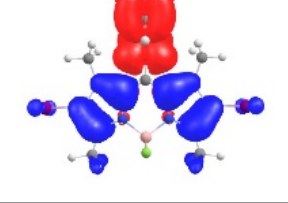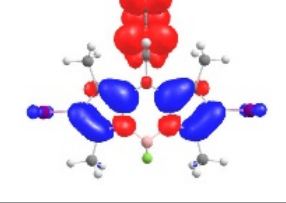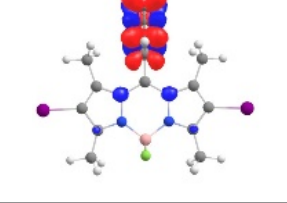
CDDsinglets29	CDDsinglets30		

Table S5: CDDs of BOD-Ph triplet states at the S_0 geometry calculated in a vacuum with MN15.

CDDtriplets01	CDDtriplets02	CDDtriplets03	CDDtriplets04
CDDtriplets05	CDDtriplets06	CDDtriplets07	CDDtriplets08
CDDtriplets09	CDDtriplets10	CDDtriplets11	CDDtriplets12
CDDtriplets13	CDDtriplets14	CDDtriplets15	CDDtriplets16
CDDtriplets17	CDDtriplets18	CDDtriplets19	CDDtriplets20

CDDtriplets21	CDDtriplets22	CDDtriplets23	CDDtriplets24
CDDtriplets25	CDDtriplets26	CDDtriplets27	CDDtriplets28
CDDtriplets29	CDDtriplets30		
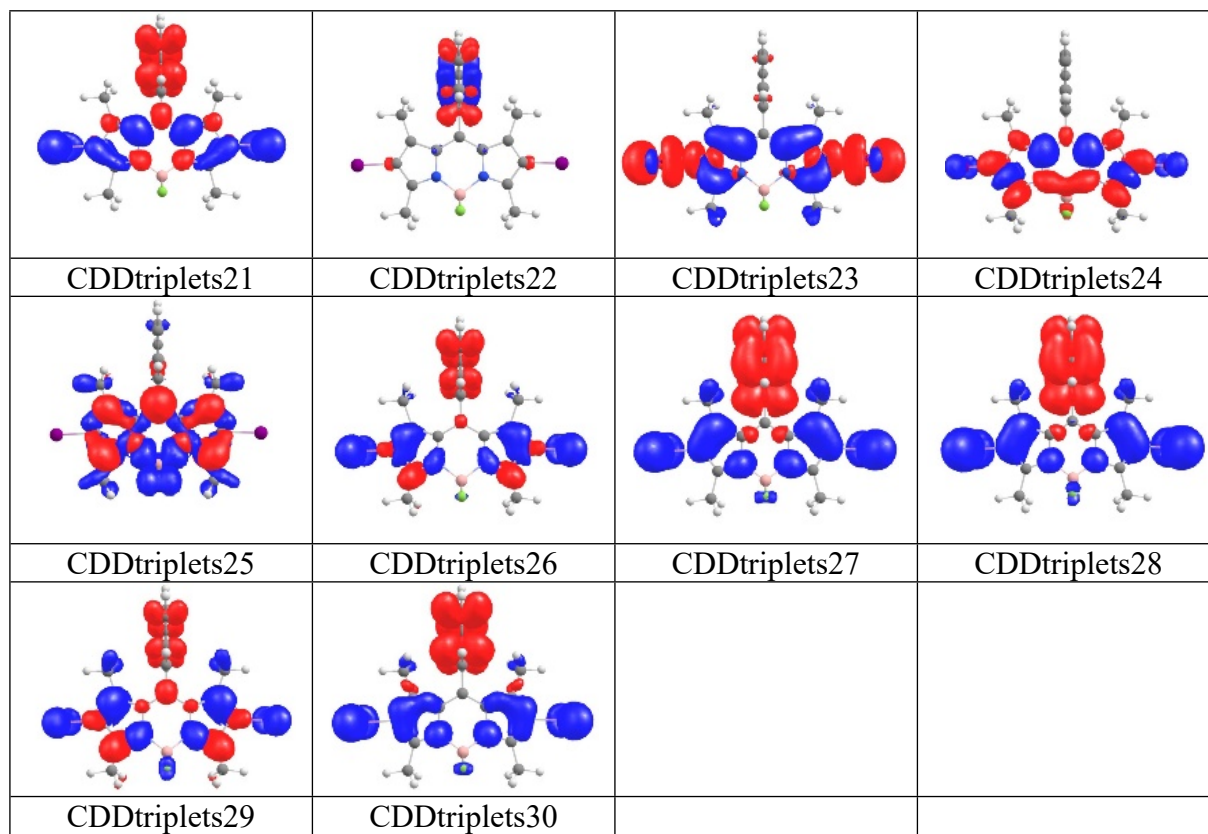
Table S6: Singlet excited state properties of BOD-Ph at the S_0 geometry calculated in a vacuum with DLPNO-STEOM-CCSD/def2-TZVP.

State	Transition	Weight (%)	Energy(eV)	λ (nm)	f	Percentage Active Character
$S_1\ \pi_{BOD} \rightarrow \pi_{BOD}*$	108->109 106->109	89 4	2.09	594	0.543	97.82
$S_2\ \pi_{BOD} \rightarrow \pi_{BOD}*$	106->109 108->109	82 7	3.41	363	0.201	97.82
$S_3\ \pi_{BOD} \rightarrow \pi_{BOD}*$	107->109 101->109	76 15	3.48	356	0.067	98.13
$S_4\ \pi_{Ph} \rightarrow \pi_{BOD}*$	105->109 102->109	95 2	4.34	286	0.000	98.24
$S_5\ \pi_{BOD} \rightarrow \sigma_I*$	108->112 107->113	46 28	4.49	276	0.000	99.22
$S_6\ \pi_{BOD} \rightarrow \sigma_I*$	108->113 107->112	37 36	4.56	272	0.000	99.27
$S_7\ \pi_{BOD} \rightarrow \pi_{BOD}*$	101->109 107->109	77 12	4.66	266	0.146	97.99
S_8	105->111 104->110	47 44	4.68	265	0.000	98.13
$S_9\ \pi_{Ph} \rightarrow \pi_{BOD}*$	104->109	98	4.84	256	0.003	99.30
$S_{10}\ \pi_{BOD} \rightarrow \pi_{Ph}*$	108->110	93	4.93	252	0.000	99.31
$S_{11}\ n_I \rightarrow \pi_{BOD}*$	102->109	96	5.01	248	0.000	99.24
$S_{12}\ n_I \rightarrow \pi_{BOD}*$	103->109	96	5.06	245	0.000	99.47
$S_{13}\ \pi_{BOD} \rightarrow \pi_{Ph}*$	108->111	90	5.08	244	0.106	99.15
S_{14}	102->112 103->113	43 40	5.42	229	0.003	99.27
S_{15}	103->112 102->113	51 45	5.42	229	0.000	99.22
$S_{16}\ \pi_{BOD} \rightarrow \sigma_I*$	108->112 107->113	41 19	5.43	228	0.000	99.09
$S_{17}\ \pi_{BOD} \rightarrow \pi_{BOD}*$	100->109	82	5.52	225	0.025	99.00
$S_{18}\ \pi_{BOD} \rightarrow \sigma_I*$	108->113 107->112	49 18	5.55	223	0.000	99.29
$S_{19}\ \pi_{BOD} \rightarrow \pi_{BOD}*$	99->109	84	5.73	216	0.093	98.63
S_{20}	108->115 108->111	75 5	5.91	210	0.084	98.50
S_{21}	108->114	85	6.08	204	0.000	98.92
S_{22}	108->119 108->117	79 7	6.11	203	0.149	97.74
S_{23}	105->110 104->111	49 24	6.19	200	0.007	98.17
$S_{24}\ \pi_{BOD} \rightarrow \sigma_I*$	100->112 99->113	53 26	6.53	190	0.000	99.06
$S_{25}\ \pi_{BOD} \rightarrow \sigma_I*$	100->113 99->112	46 30	6.56	189	0.000	99.07

State	Transition	Weight	Energy	λ	f	%
S_{26}	104->110 105->111	41 38	6.92	179	0.257	94.85
S_{27}	104->111 105->110	42 17	6.95	178	0.555	96.12
S_{28}	108->118 104->110 105->111	58 9 10	7.02	177	0.119	91.66
S_{29}	108->116 106->114	31 32	7.17	173	0.004	96.85
S_{30}	108->117 101->111	59 8	7.38	168	0.012	88.55

Table S7: Triplet excited state properties of BOD-Ph at the S_0 geometry calculated in a vacuum with DLPNO-STEOM-CCSD/def2-TZVP.

State	Transition	Weight (%)	Energy(eV)	λ (nm)	f	Percentage Active Character
$T_1\,\pi_{BOD} \rightarrow \pi_{BOD}*$	108 -> 109	94	1.38	902	0	99.32
$T_2\,\pi_{BOD} \rightarrow \pi_{BOD}*$	106 -> 109 100 -> 109	77 11	2.56	485	0	99.09
$T_3\,\pi_{BOD} \rightarrow \pi_{BOD}*$	107 -> 109 101 -> 109	54 33	2.74	452	0	98.37
$T_4\,\pi_{BOD} \rightarrow \pi_{BOD}*$	101 -> 109 107 -> 109	46 29	3.27	379	0	98.58
T_5	105 -> 110 104 -> 111	51 41	3.44	360	0	96.39
$T_6\,\pi_{BOD} \rightarrow \sigma_I*$	108 -> 112 107 -> 113	36 33	4.02	308	0	99.25
$T_7\,\pi_{BOD} \rightarrow \sigma_I*$	107 -> 112 108 -> 113	40 30	4.07	304	0	99.34
$T_8\,\pi_{Ph} \rightarrow \pi_{BOD}*$	105 -> 109	94	4.33	287	0	97.85
T_9	108 -> 115 108 -> 111	57 25	4.61	269	0	98.96
T_{10}	104 -> 111 105 -> 110	54 41	4.62	268	0	99.19
T_{11}	104 -> 110 105 -> 111	47 48	4.62	268	0	99.14
T_{12}	102 -> 112 103 -> 113	50 47	4.79	259	0	99.28
T_{13}	102 -> 113 103 -> 112	46 51	4.79	259	0	99.27
$T_{14}\,\pi_{Ph} \rightarrow \pi_{BOD}*$	104 -> 109	98	4.80	259	0	99.56
$T_{15}\,\pi_{BOD} \rightarrow \pi_{Ph}*$	108 -> 110	92	4.88	254	0	99.19
$T_{16}\,n_I \rightarrow \pi_{BOD}*$	102 -> 109	96	4.99	248	0	99.15
T_{17}	108 -> 116 106 -> 116	72 4	5.04	246	0	98.47
T_{18}	103 -> 109	97	5.04	246	0	99.53

T$_{19}$	103 -> 109	97	5.04	246	0	99.52
T$_{20}$ $\pi_{BOD} \to \pi_{Ph}$*	108 -> 111 108 -> 115	67 23	5.31	234	0	99.48
T$_{21}$ $\pi_{BOD} \to \sigma_I$*	108 -> 112 106 -> 112	50 21	5.32	233	0	98.52
T$_{22}$ $\pi_{BOD} \to \sigma_I$*	108 -> 113 106 -> 113	53 14	5.47	227	0	98.92
T$_{23}$	104 -> 110 105 -> 111	49 44	5.53	224	0	99.44
T$_{24}$	108 -> 117 107 -> 116	30 20	5.58	222	0	98.94
T$_{25}$ $\pi_{BOD} \to \pi_{BOD}$*	108 -> 117 106 -> 115	30 12	5.59	222	0	99.07
T$_{26}$	106 -> 116 101 -> 115	33 14	5.83	213	0	97.42
T$_{27}$	108 -> 114 108 -> 119	78 8	5.95	209	0	86.31
T$_{28}$	100 -> 112 99 -> 113	46 24	6.07	204	0	98.34
T$_{29}$	100 -> 113 99 -> 112	41 28	6.10	203	0	98.63
T$_{30}$	97 -> 112 98 -> 113	45 47	6.63	187	0	95.12

Table S8: Singlet excited state properties of BOD-Ph at the S$_0$ geometry calculated in a vacuum with DLPNO-STEOM-CCSD/def2-SVP.

State	Transition	Weight (%)	Energy(eV)	λ (nm)	f	Percentage Active Character
S$_1$	108 -> 109	88	2.10	591	0.536	98.08
S$_2$	106 -> 109	81	3.47	358	0.226	98.30
S$_3$	107 -> 109	78	3.49	356	0.076	98.85
S$_4$	105 -> 109	95	4.44	279	0.000	98.88
S$_5$	104 -> 110	48	4.71	263	0.000	98.59
S$_6$	101 -> 109	79	4.73	262	0.149	98.21
S$_7$	108 -> 112	41	4.75	261	0.000	99.32
S$_8$	107 -> 112	38	4.80	258	0.001	99.33
S$_9$	104 -> 109	98	4.94	251	0.003	99.67
S$_{10}$	103 -> 109	94	4.99	248	0.000	98.51
S$_{11}$	102 -> 109	97	5.02	247	0.000	99.58
S$_{12}$	108 -> 110	97	5.17	240	0.000	99.53
S$_{13}$	108 -> 111	91	5.40	229	0.069	99.38
S$_{14}$	100 -> 109	84	5.47	227	0.035	98.78
S$_{15}$	102 -> 112	33	5.61	221	0.000	99.18
S$_{16}$	103 -> 112	32	5.61	221	0.000	99.11
S$_{17}$	99 -> 109	82	5.71	217	0.090	98.79
S$_{18}$	108 -> 112	45	5.74	216	0.000	99.26

S_{19}	106 -> 113	22	5.86	212	0.001	99.45
S_{20}	108 -> 114	75	6.12	203	0.080	98.75
S_{21}	108 -> 116	82	6.37	195	0.046	98.11
S_{22}	98 -> 109	92	6.59	188	0.000	94.88
S_{23}	107 -> 111	33	6.78	183	0.593	97.48
S_{24}	100 -> 112	51	6.80	182	0.000	99.12
S_{25}	100 -> 113	46	6.82	182	0.000	99.19
S_{26}	104 -> 111	40	7.25	171	0.556	96.67
S_{27}	104 -> 110	45	7.28	170	0.386	95.11

Table S9: Triplet excited state properties of BOD-Ph at the S_0 geometry calculated in a vacuum with DLPNO-STEOM-CCSD/def2-SVP.

State	Transition	Weight (%)	Energy(eV)	λ (nm)	f	Percentage Active Character
T_1	108 -> 109	95	1.44	860	0	99.44
T_2	106 -> 109	75	2.59	480	0	99.16
T_3	107 -> 109 101 -> 109	54 55	2.76	449	0	98.34
T_4	101 -> 109 107 -> 109	44 29	3.33	373	0	98.53
T_5	105 -> 110 104 -> 111	51 41	3.41	364	0	96.54
T_6	107 -> 113 108 -> 112	35 33	4.18	297	0	99.40
T_7	107 -> 112	40	4.22	294	0	99.43
T_8	105 -> 109	95	4.45	279	0	98.08
T_9	104 -> 111 105 -> 110	43 33	4.77	260	0	99.36
T_{10}	104 -> 110 105 -> 111	38 37	4.77	260	0	99.31
T_{11}	108 -> 114	65	4.80	258	0	98.82
T_{12}	102 -> 112 103 -> 112	32 26	4.88	254	0	99.46
T_{13}	102 -> 112 103 -> 112	31 26	4.88	254	0	99.49
T_{14}	104 -> 109	98	4.91	253	0	99.61
T_{15}	103 -> 109	92	4.98	249	0	98.63
T_{16}	102 -> 109	92	5.01	248	0	99.57
T_{17}	108 -> 110	96	5.17	240	0	99.13
T_{18}	108 -> 115 102 -> 109	49 24	5.20	239	0	98.29
T_{19}	100 -> 109 99 -> 109	43 13	5.53	224	0	97.20

T_{20}	108 -> 111 108 -> 116	54 14	5.57	223	0	99.22
T_{21}	99 -> 109 108 -> 116	19 11	5.57	223	0	99.22
T_{22}	108 -> 112 106 -> 112	53 16	5.58	222	0	98.83
T_{23}	99 -> 109	65	5.63	220	0	99.35
T_{24}	108 -> 113	56	5.72	217	0	99.06
T_{25}	104 -> 110 105 -> 111	47 47	5.88	211	0	99.67
T_{26}	100 -> 113 99 -> 112	29 17	6.38	194	0	98.28
T_{27}	97 -> 112 98 -> 112	27 28	6.82	182	0	94.46
T_{28}	98 -> 113 97 -> 112	32 22	6.84	181	0	94.75
T_{29}	108 -> 117	54	6.87	181	0	91.46
T_{30}	108 -> 117	54	6.87	180	0	91.53

Table S10: Molecular orbitals of BOD-Ph at the S_0 geometry calculated in a vacuum with DLPNO-STEOM-CCSD/def2-TZVP.
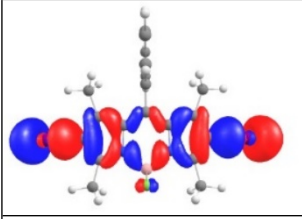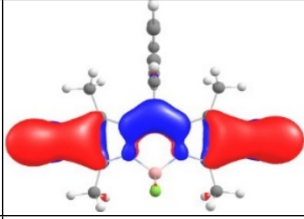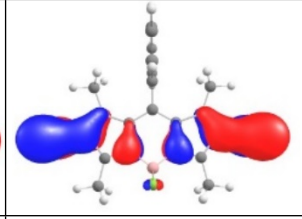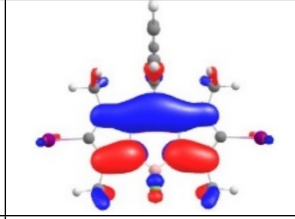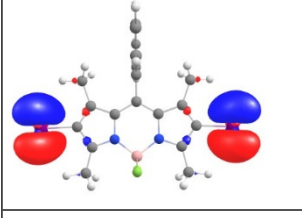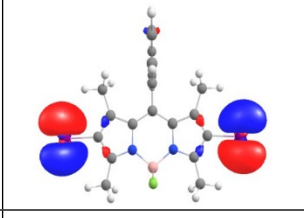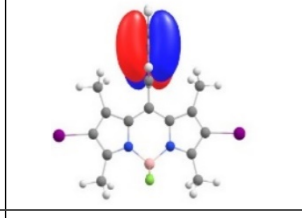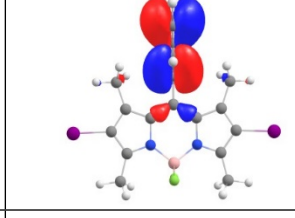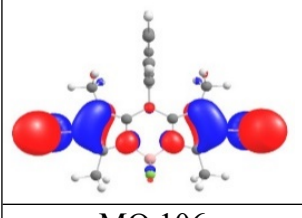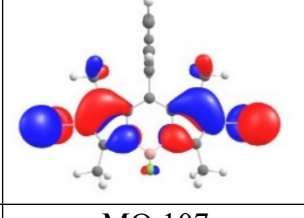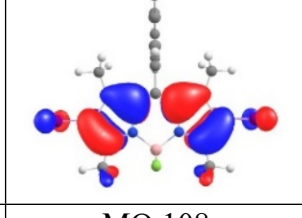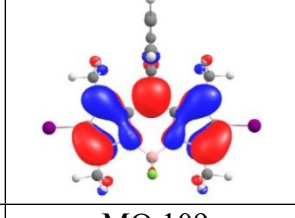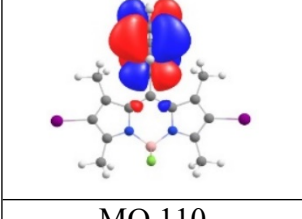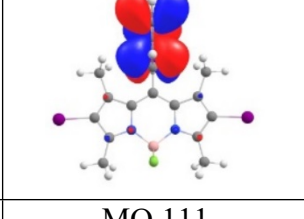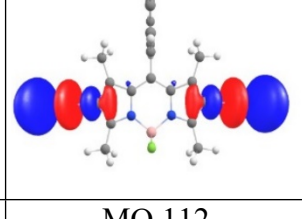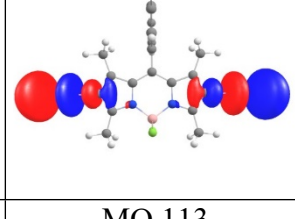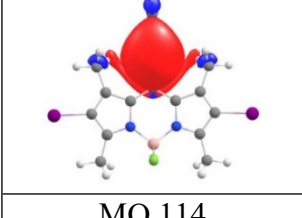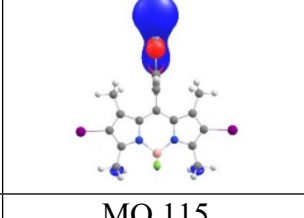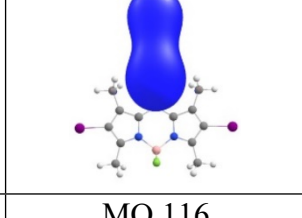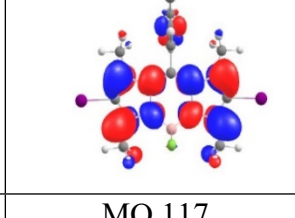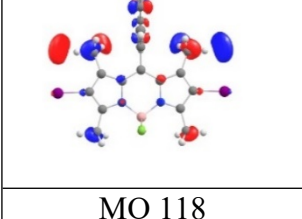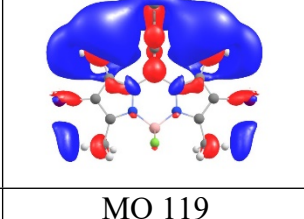
MO 98	MO 99	MO 100	MO 101
MO 102	MO 103	MO 104	MO 105
MO 106	MO 107	MO 108	MO 109
MO 110	MO 111	MO 112	MO 113
MO 114	MO 115	MO 116	MO 117
MO 118	MO 119		

Table S11: Singlet transition energies of BOD-Ph at the S_0 geometry calculated in a vacuum with different methods. All values are in eV.

State	B3LYP	TDA B3LYP	TDA MN15	TDA SOS-PBE-QIDH	TDA SOS-ωPBEPP86[a]	DLPNO-STEOM-CCSD
$\pi_{BOD} \rightarrow \pi_{BOD}*$	2.69	2.88	3.02	2.73	2.65 (2.58)	2.09
	3.15	3.23	3.64	3.49	3.54 (3.48)	3.41
	3.25	3.55	3.66	3.52	3.65 (3.61)	3.48
$\pi_{BOD} \rightarrow \sigma_I*$	4.17	4.20	4.44	4.80	4.85 (4.63)	4.49
	4.30	4.32	4.50	4.89	4.89 (4.69)	4.56
	4.81	4.84	5.25	5.62	5.86 (5.58)	5.43
	4.83	4.85	5.32	5.76	6.01 (5.73)	5.55
$\pi_{BOD} \rightarrow \pi_{Ph}*$	4.15	4.16	4.69	4.91	5.19 (5.03)	4.93
	4.25	4.26	4.91	5.21	5.43 (5.16)	5.08
$\pi_{Ph} \rightarrow \pi_{BOD}*$	3.82	3.82	4.15	4.49	4.60 (4.50)	4.34
	4.00	4.01	4.57	4.77	4.98 (4.87)	4.84

[a] Values given in brackets for SOS-ωPBEPP86 were calculated with the def2-TZVP basis set.

Table S12: Triplet transition energies of BOD-Ph at the S_0 geometry calculated in a vacuum with different methods. All values are in eV.

State	B3LYP	TDA B3LYP	TDA MN15	TDA SOS-PBE-QIDH	TDA SOS-ωPBEPP86[a]	DLPNO-STEOM-CCSD
$\pi_{BOD} \rightarrow \pi_{BOD}*$	1.50	1.62	1.59	1.77	1.69 (1.65)	1.38
	2.43	2.51	2.77	2.89	2.93 (2.90)	2.56
	2.57	2.64	2.93	3.12	3.18 (3.17)	2.74
	3.23	3.36	3.51	3.67	3.63 (3.60)	3.27
$\pi_{BOD} \rightarrow \sigma_I*$	3.79	3.82	3.91	4.28	4.27 (4.15)	4.02
	3.86	3.89	3.95	4.32	4.29 (4.19)	4.07
	4.60	4.59	5.10	5.60	5.86 (5.62)	5.32
	4.58	4.65	5.21	5.74	6.32 (5.79)	5.47
$\pi_{BOD} \rightarrow \pi_{Ph}*$	4.13	4.14	4.65	4.98	5.16 (5.01)	4.88
	4.19	4.20	4.69	5.62	5.78 (5.45)	5.31
$\pi_{Ph} \rightarrow \pi_{BOD}*$	3.80	3.80	4.13	4.46	4.58 (4.48)	4.33
	3.98	3.98	4.55	4.80	4.96 (4.86)	4.80

[a] Values given in brackets for SOS-ωPBEPP86 were calculated with the def2-TZVP basis set.

Table S13: Vertical transition energies of BOD-Ph for the selected excited states calculated with MN15 in a vacuum at the S_0 geometry, optimized with B3LYP and MN15. All values are in eV.

State	B3LYP		MN15	
	Singlets	Triplets	Singlets	Triplets
$\pi_{BOD} \rightarrow \pi_{BOD}*$	3.02	1.59	3.02	1.66
	3.64	2.77	3.64	2.81
	3.66	2.94	3.68	2.96
	-	3.51	-	3.52
$\pi_{BOD} \rightarrow \sigma_I*$	4.44	3.91	4.54	4.08
	4.50	3.95	4.60	4.11
	5.25	5.10	5.38	5.24
	5.32	5.21	5.44	5.34
$\pi_{BOD} \rightarrow \pi_{Ph}*$	4.69	4.65	4.76	4.71
	4.91	4.69	4.93	4.75
$\pi_{Ph} \rightarrow \pi_{BOD}*$	4.15	4.13	4.14	4.01
	4.57	4.55	4.57	4.47

Table S14: Singlet transition energies at the S_0 geometry calculated with MN15 in a vacuum and in DCM. All values are in eV.

State	BOD-Ph(Vac)	BOD-Ph(DCM)	BOD-PhOH(Vac)	BOD-PhOH(DCM)	BOD-PhNO₂(Vac)	BOD-PhNO₂(DCM)
$\pi_{BOD} \rightarrow \pi_{BOD}*$	3.02	2.90	3.02	2.90	2.96	2.86
	3.64	3.64	3.66	3.66	3.56	3.58
	3.68	3.62	3.68	3.63	3.66	3.60
$\pi_{BOD} \rightarrow \sigma_I*$	4.54	4.59	4.54	4.59	4.58	4.67
	4.60	4.65	4.60	4.65	4.63	4.67
	5.38	5.42	5.37	5.41	5.43	5.51
	5.44	5.49	5.44	5.49	5.48	5.51
$\pi_{BOD} \rightarrow \pi_{Ph}*$	4.76	5.05	5.11	5.44	3.45	3.51
	4.93	5.22	4.81	5.16	4.51	4.59
$\pi_{Ph} \rightarrow \pi_{BOD}*$	4.14	3.90	3.57	3.29	4.85	4.41
	4.57	4.28	4.67	4.36	5.15	4.66

Table S15: Triplet transition energies at the S_0 geometry calculated with MN15 in a vacuum and in DCM. All values are in eV.

State	BOD-Ph(Vac)	BOD-Ph(DCM)	BOD-PhOH(Vac)	BOD-PhOH(DCM)	BOD-PhNO₂(Vac)	BOD-PhNO₂(DCM)
$\pi_{BOD} \rightarrow \pi_{BOD}*$	1.66	1.69	1.67	1.71	1.61	1.65
	2.81	2.83	2.81	2.84	2.76	2.79
	2.96	3.00	2.97	3.00	2.90	2.95
	3.52	3.50	3.70	3.65	3.54	3.54
$\pi_{BOD} \rightarrow \sigma_I*$	4.08	4.14	4.11	4.13	4.09	4.15
	4.11	4.17	4.17	4.17	4.13	4.18
	5.24	5.29	5.24	5.28	5.29	5.32
	5.34	5.40	5.10	5.30	5.35	5.33
$\pi_{BOD} \rightarrow \pi_{Ph}*$	4.71	5.01	5.06	5.25	3.42	3.50
	4.75	4.86	5.10	5.28	4.46	4.61
$\pi_{Ph} \rightarrow \pi_{BOD}*$	4.01	3.87	3.34	3.13	4.74	4.70
	4.47	4.20	4.61	4.26	5.02	4.75
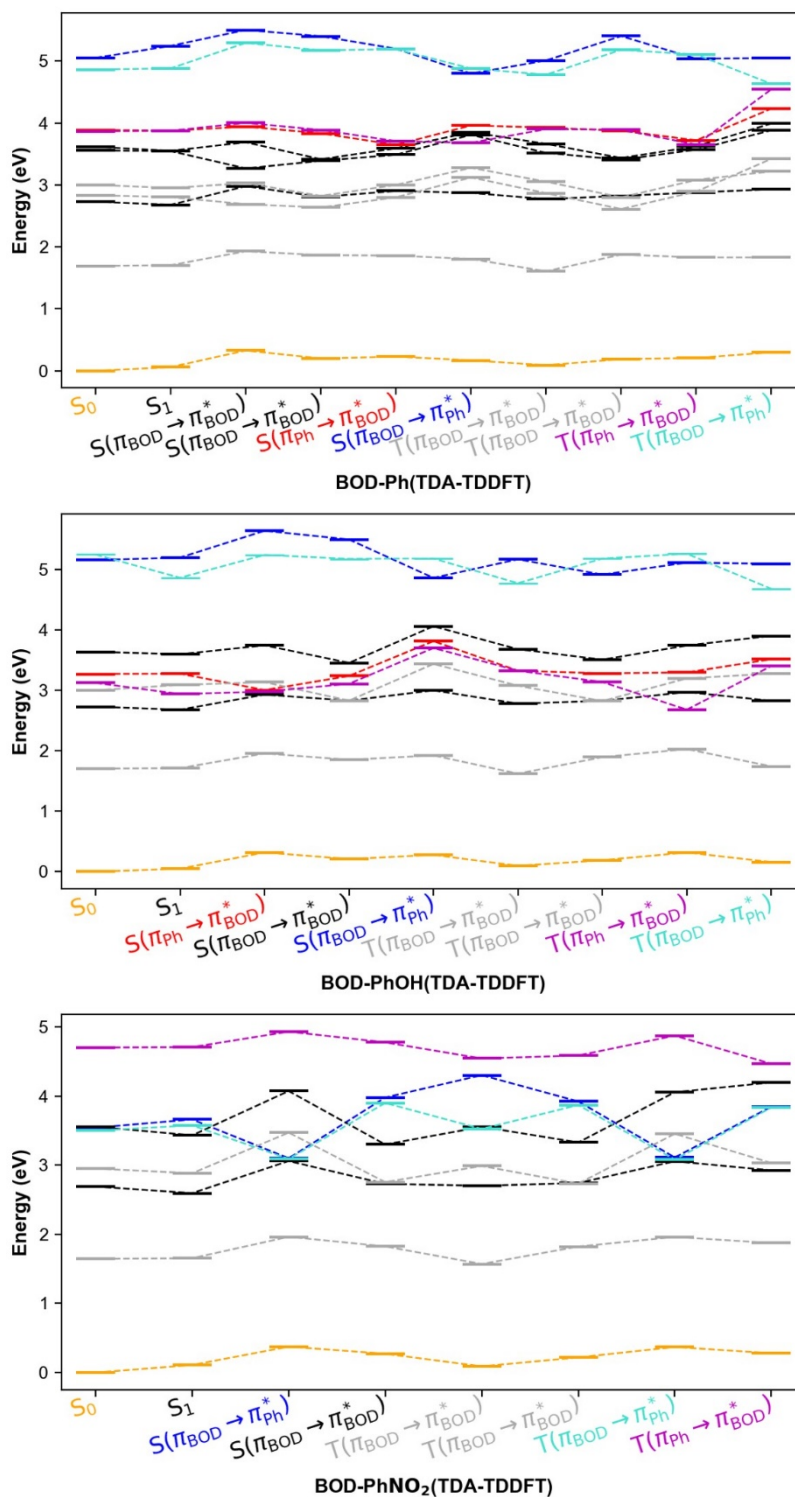
Figure S1: Energy diagrams for selected singlet and triplet states of BOD-Ph, BOD-PhOH and BOD-PhNO$_2$. The calculations were performed at different geometries in DCM with TDA-TDDFT (MN15).

Table S16: Energies (eV) for selected BOD-Ph states at their optimized geometries, calculated with TDA-TDDFT (MN15) in DCM.

State	Geometry					
	S_0	S_1 $(\pi_{BOD}\to\pi_{BOD}*)$	S $(\pi_{Ph}\to\pi_{BOD}*)$	S $(\pi_{BOD}\to\pi_{Ph}*)$	T $(\pi_{Ph}\to\pi_{BOD}*)$	T $(\pi_{BOD}\to\pi_{Ph}*)$
$S_1(\pi_{BOD}\to\pi_{BOD}*)$	2.73	2.68	2.90	2.87	2.88	2.93
$S(\pi_{Ph}\to\pi_{BOD}*)$	3.89	3.88	3.65	3.96	3.72	4.23
$S(\pi_{BOD}\to\pi_{Ph}*)$	5.05	5.24	5.20	4.80	5.04	5.05
$T(\pi_{Ph}\to\pi_{BOD}*)$	3.87	3.87	3.71	3.78	3.65	4.54
$T(\pi_{BOD}\to\pi_{Ph}*)$	4.86	4.88	5.19	4.88	5.10	4.63

Table S17: Energies (eV) for selected BOD-PhNO$_2$ states at their optimized geometries, calculated with TDA-TDDFT (MN15) in DCM.

State	Geometry					
	S_0	S_1 $(\pi_{BOD}\to\pi_{BOD}*)$	S $(\pi_{BOD}\to\pi_{Ph}*)$	S $(\pi_{Ph}\to\pi_{BOD}*)$	T $(\pi_{BOD}\to\pi_{Ph}*)$	T $(\pi_{Ph}\to\pi_{BOD}*)$
$S_1(\pi_{BOD}\to\pi_{BOD}*)$	2.69	2.59	3.06	-	3.06	2.92
$S(\pi_{BOD}\to\pi_{Ph}*)$	3.54	3.66	3.10	-	3.11	3.84
$S(\pi_{Ph}\to\pi_{BOD}*)$	4.40	4.21	4.86	-	4.80	4.15
$T(\pi_{BOD}\to\pi_{Ph}*)$	3.50	3.58	3.09	-	3.08	3.83
$T(\pi_{Ph}\to\pi_{BOD}*)$	4.70	4.71	4.93	-	4.87	4.47

Table S18: Energies (eV) for selected BOD-PhOH states at their optimized geometries, calculated with TDA-TDDFT (MN15) in DCM.

State	Geometry					
	S_0	S_1 $(\pi_{BOD}\to\pi_{BOD}*)$	S $(\pi_{Ph}\to\pi_{BOD}*)$	S $(\pi_{BOD}\to\pi_{Ph}*)$	T $(\pi_{Ph}\to\pi_{BOD}*)$	T $(\pi_{BOD}\to\pi_{Ph}*)$
$S_1(\pi_{BOD}\to\pi_{BOD}*)$	2.73	2.68	2.93	3.00	2.97	2.83
$S(\pi_{Ph}\to\pi_{BOD}*)$	3.27	3.28	3.01	3.82	3.30	3.52
$S(\pi_{BOD}\to\pi_{Ph}*)$	5.16	5.20	5.64	4.86	5.12	5.10
$T(\pi_{Ph}\to\pi_{BOD}*)$	3.13	2.94	2.98	3.70	2.68	3.41
$T(\pi_{BOD}\to\pi_{Ph}*)$	5.25	4.87	5.25	5.19	5.23	4.68

Table S19: Energies (eV) for selected BOD-PhOH states at their optimized TDA-TDDFT geometries, calculated with DLPNO-STEOM-CCSD in DCM.

State	Geometry					
	S_0	S_1 $(\pi_{BOD}\to\pi_{BOD}*)$	S $(\pi_{Ph}\to\pi_{BOD}*)$	S $(\pi_{BOD}\to\pi_{Ph}*)$	T $(\pi_{Ph}\to\pi_{BOD}*)$	T $(\pi_{BOD}\to\pi_{Ph}*)$
$S_1(\pi_{BOD}\to\pi_{BOD}*)$	2.12	2.07	2.45	2.46	2.46	2.31
$S(\pi_{Ph}\to\pi_{BOD}*)$	2.96	2.98	2.72	3.52	2.96	3.20
$S(\pi_{BOD}\to\pi_{Ph}*)$	5.01	5.11	5.84	4.96	5.66	4.99
$T(\pi_{Ph}\to\pi_{BOD}*)$	3.01	2.85	2.74	3.61	2.50	3.65
$T(\pi_{BOD}\to\pi_{Ph}*)$	-	-	-	-	-	-

Cartesian coordinates for the S_0 state of BOD-Ph (MN15/def2-SVP in DCM)

6	0.61346	-0.48889	-0.30262
6	1.209974	-1.66303	-2.10151
6	1.286471	-1.65171	0.188061
7	0.601564	-0.5387	-1.69405
6	0.023367	0.590668	0.376523
6	-0.57973	1.642721	-0.333
5	0.063678	0.569219	-2.64097
7	-0.57782	1.64794	-1.72531
6	-1.29253	2.795703	0.124836
6	-1.2346	2.731972	-2.16434
9	-0.88861	0.045172	-3.50594
9	1.112728	1.122829	-3.3721
6	0.939353	1.421262	2.549752
6	0.024873	0.613715	1.862514
6	-0.8886	-0.17169	2.57648
6	0.942949	1.437079	3.945505
1	1.661177	2.062848	4.479204
6	0.027194	0.657656	4.657334
6	-0.88989	-0.14368	3.971903
1	-1.6072	-0.75232	4.526258
1	1.647567	2.033936	1.986133
1	-1.59791	-0.80156	2.033459
1	0.028149	0.674802	5.749125
6	1.577903	-2.05004	1.598297
1	1.919553	-1.20109	2.2056
1	2.35274	-2.8289	1.612147
1	0.683435	-2.45858	2.093073
6	1.347893	-2.02245	-3.53815
1	0.372436	-2.3187	-3.95275
1	2.052426	-2.85336	-3.66483
1	1.69589	-1.15277	-4.11229
6	-1.58403	3.229885	1.524327
1	-2.36009	4.007426	1.519564
1	-0.68918	3.649854	2.008358
1	-1.92439	2.395844	2.153037
6	-1.42863	3.020102	-3.6105
1	-0.50099	2.81973	-4.16338
1	-1.73052	4.063932	-3.76076
1	-2.2085	2.365334	-4.02856
6	1.640798	-2.37281	-0.95524
53	2.635947	-4.20139	-1.007
6	-1.68704	3.461226	-1.03841
53	-2.77428	5.234034	-1.14717

Cartesian coordinates for the S_0 state of BOD-PhOH (MN15/def2-SVP in DCM)

6	0.600502	-0.48774	-0.30406
6	1.160809	-1.6888	-2.09778
6	1.279844	-1.64511	0.189688
7	0.566454	-0.55492	-1.69439
6	0.031066	0.606444	0.372157
6	-0.5582	1.662997	-0.34469
5	0.052086	0.558786	-2.64695
7	-0.5507	1.663814	-1.73704
6	-1.27037	2.819063	0.105873
6	-1.19775	2.751314	-2.18281
9	-0.92295	0.054969	-3.49923
9	1.110462	1.074103	-3.39299
6	0.892249	1.509679	2.544794
6	0.037087	0.638982	1.854644
6	-0.8144	-0.19812	2.584926
6	0.904379	1.538071	3.93532
1	1.57286	2.205474	4.482046
6	0.042256	0.703902	4.662584
6	-0.82123	-0.16237	3.977543
1	-1.49505	-0.81176	4.542729
1	1.558298	2.1689	1.982078
1	-1.48324	-0.88259	2.056757
6	1.614686	-2.02071	1.596802
1	1.917938	-1.15167	2.195707
1	2.431418	-2.75606	1.59938
1	0.75394	-2.47875	2.108183
6	1.274246	-2.0658	-3.53219
1	0.285154	-2.3269	-3.93767
1	1.946195	-2.9235	-3.65678
1	1.650995	-1.21485	-4.11645
6	-1.58611	3.253345	1.500287
1	-2.40498	3.985915	1.484653
1	-0.71855	3.732787	1.979137
1	-1.87752	2.409372	2.139999
6	-1.38565	3.035486	-3.63067
1	-0.46466	2.806863	-4.18348
1	-1.65979	4.086214	-3.78672
1	-2.184	2.400166	-4.04393
6	1.607551	-2.38502	-0.9503
53	2.59375	-4.21882	-0.99124
6	-1.65135	3.485812	-1.06169
53	-2.72755	5.26476	-1.17954
8	0.08185	0.772768	6.007707
1	-0.55381	0.15742	6.403111

Cartesian coordinates for the S_0 state of BOD-PhNO$_2$ (MN15/def2-SVP in DCM)

6	0.172144	1.211729	-1.05985
6	1.306808	2.953018	-1.86405
6	-0.21928	1.341745	-2.43039
7	1.102648	2.205524	-0.7693
6	-0.22585	0.302264	-0.0667
6	0.304331	0.369526	1.231562
5	1.858189	2.383613	0.577385
7	1.259027	1.330764	1.55146
6	0.016181	-0.39442	2.407492
6	1.589028	1.211759	2.845673
9	1.661375	3.664527	1.074844
9	3.218444	2.148072	0.395676
6	-0.82013	-2.05093	-0.66664
6	-1.23516	-0.74101	-0.39119
6	-2.59668	-0.40983	-0.4202
6	-1.75972	-3.03134	-0.97535
1	-1.46939	-4.05761	-1.19788
6	-3.10578	-2.67537	-0.99323
6	-3.54647	-1.38311	-0.71954
1	-4.61231	-1.1588	-0.74662
1	0.242854	-2.29987	-0.63997
1	-2.91029	0.614013	-0.20541
6	-1.17573	0.510008	-3.22143
1	-1.0257	-0.56529	-3.05476
1	-1.0499	0.716569	-4.29296
1	-2.22021	0.736942	-2.95833
6	2.235859	4.113877	-1.87827
1	1.804168	4.954071	-1.31344
1	2.43063	4.442951	-2.90614
1	3.18274	3.844617	-1.39057
6	-0.94182	-1.52732	2.583218
1	-1.07444	-1.74098	3.652385
1	-0.57279	-2.4451	2.100763
1	-1.92664	-1.30741	2.148673
6	2.573857	2.108373	3.506763
1	3.441391	2.264887	2.851602
1	2.903864	1.684155	4.462913
1	2.123053	3.09451	3.696586
6	0.49718	2.441133	-2.90762
53	0.413602	3.236382	-4.82971
6	0.833478	0.149203	3.400202
53	0.950481	-0.46153	5.386984
7	-4.10441	-3.70801	-1.31471
8	-5.27435	-3.37728	-1.3258
8	-3.69986	-4.83017	-1.54997

Cartesian coordinates for the S_1 state of BOD-Ph (MN15/def2-SVP in DCM)

6	0.585527	-0.51007	-0.29103
6	1.121492	-1.69703	-2.12124
6	1.27972	-1.66137	0.182874
7	0.531241	-0.56583	-1.69682
6	0.010619	0.582008	0.41355
6	-0.57779	1.646796	-0.32132
5	0.015085	0.541007	-2.64138
7	-0.53744	1.656739	-1.72852
6	-1.28316	2.803849	0.121195
6	-1.14999	2.763403	-2.18434
9	-0.99434	0.048138	-3.46984
9	1.057132	1.026322	-3.43549
6	0.824021	1.525744	2.584312
6	0.017556	0.608007	1.893828
6	-0.7842	-0.28304	2.623807
6	0.83122	1.548878	3.979434
1	1.46754	2.262252	4.507645
6	0.026722	0.661032	4.699463
6	-0.78227	-0.25346	4.018742
1	-1.41516	-0.94615	4.577705
1	1.449314	2.219767	2.016291
1	-1.41374	-0.99739	2.086481
1	0.030185	0.681749	5.791307
6	1.652136	-2.03366	1.581384
1	1.96175	-1.15991	2.170943
1	2.483098	-2.75362	1.564992
1	0.817255	-2.50534	2.124646
6	1.240807	-2.04717	-3.55698
1	0.245981	-2.0739	-4.02881
1	1.734887	-3.01747	-3.68627
1	1.813822	-1.27107	-4.08984
6	-1.64468	3.218768	1.510556
1	-2.48082	3.932148	1.479303
1	-0.80755	3.713231	2.029495
1	-1.94206	2.362681	2.131608
6	-1.29549	3.060392	-3.62964
1	-0.32209	2.970519	-4.13583
1	-1.70335	4.066422	-3.78537
1	-1.9624	2.323375	-4.10662
6	1.586943	-2.39809	-0.976
53	2.581198	-4.20765	-1.04422
6	-1.61436	3.495768	-1.05842
53	-2.63734	5.286447	-1.17897

Cartesian coordinates for the S$_1$ state of BOD-PhOH (MN15/def2-SVP in DCM)

6	0.582372	-0.49987	-0.29391
6	1.102546	-1.70591	-2.1166
6	1.279734	-1.64724	0.185561
7	0.517156	-0.56952	-1.69854
6	0.013977	0.599362	0.406232
6	-0.57265	1.660596	-0.33668
5	-0.00069	0.53046	-2.64969
7	-0.53497	1.660549	-1.74402
6	-1.27261	2.823796	0.09867
6	-1.14247	2.767472	-2.20671
9	-1.0228	0.036123	-3.46243
9	1.036364	0.998523	-3.46072
6	0.817213	1.56533	2.577104
6	0.024757	0.635024	1.884475
6	-0.75766	-0.25869	2.629789
6	0.832956	1.601345	3.967513
1	1.453073	2.318218	4.50898
6	0.042123	0.705652	4.701904
6	-0.75586	-0.22509	4.02269
1	-1.376	-0.92227	4.592965
1	1.433829	2.268034	2.010163
1	-1.38163	-0.98895	2.107607
6	1.666997	-2.00456	1.58405
1	1.975076	-1.12322	2.163021
1	2.502723	-2.71909	1.566577
1	0.840738	-2.47749	2.139416
6	1.210969	-2.06977	-3.54984
1	0.214135	-2.08375	-4.01782
1	1.688902	-3.04898	-3.67272
1	1.794919	-1.30795	-4.09152
6	-1.63362	3.248844	1.485189
1	-2.47114	3.96051	1.449048
1	-0.79769	3.74945	2.000212
1	-1.92813	2.39674	2.113026
6	-1.28848	3.055273	-3.65383
1	-0.31419	2.968748	-4.15902
1	-1.70246	4.057797	-3.81581
1	-1.9499	2.310879	-4.12695
6	1.57642	-2.39583	-0.96839
53	2.568781	-4.20737	-1.02673
6	-1.6016	3.509481	-1.08524
53	-2.61609	5.304715	-1.21617
8	0.083863	0.779585	6.048761
1	-0.50076	0.116921	6.445888

Cartesian coordinates for the S_1 state of BOD-PhNO$_2$ (MN15/def2-SVP in DCM)

6	0.100666	1.252768	-1.04308
6	1.153832	3.092405	-1.77671
6	-0.23485	1.366578	-2.42397
7	0.969745	2.305584	-0.70446
6	-0.27552	0.284252	-0.07061
6	0.32348	0.332345	1.219393
5	1.788547	2.43596	0.601477
7	1.348699	1.254254	1.497586
6	0.051047	-0.41518	2.402345
6	1.762179	1.090408	2.764423
9	1.514761	3.645244	1.237993
9	3.151471	2.36205	0.319595
6	-0.92142	-2.11578	-0.33496
6	-1.26822	-0.75064	-0.39386
6	-2.57923	-0.39071	-0.76671
6	-1.85182	-3.09786	-0.64658
1	-1.59925	-4.15746	-0.62395
6	-3.14408	-2.70624	-1.00466
6	-3.52375	-1.36325	-1.06559
1	-4.54673	-1.10681	-1.33907
1	0.09683	-2.39679	-0.05625
1	-2.85321	0.666215	-0.80308
6	-1.01989	0.438496	-3.29193
1	-0.86654	-0.61139	-3.00797
1	-0.70908	0.562812	-4.33936
1	-2.10414	0.630213	-3.24675
6	2.049775	4.273161	-1.76192
1	1.859948	4.88364	-0.86683
1	1.914796	4.8802	-2.66526
1	3.102415	3.949754	-1.70319
6	-1.02017	-1.42217	2.665873
1	-1.2404	-1.45199	3.742808
1	-0.72915	-2.4408	2.362443
1	-1.94756	-1.17921	2.129838
6	2.810511	1.936474	3.382719
1	3.673489	2.027729	2.706822
1	3.131279	1.523111	4.346552
1	2.427922	2.958381	3.542169
6	0.405919	2.541286	-2.85423
53	0.341592	3.341933	-4.75476
6	0.983866	0.050539	3.345001
53	1.186328	-0.60606	5.290524
7	-4.12942	-3.73347	-1.32549
8	-5.24959	-3.37043	-1.64511
8	-3.78064	-4.90069	-1.25704

Cartesian coordinates for the $S(\pi_{Ph} \rightarrow \pi_{BOD}*)$ state of BOD-Ph (MN15/def2-SVP in DCM)

6	-1.23716	0.23662	0.014135
6	-2.53848	-1.59094	0.001025
6	-2.57365	0.704268	0.020006
7	-1.24429	-1.14206	0.009671
6	-0.00022	0.952038	0.029785
6	1.235775	0.235996	0.029245
5	-0.00123	-2.06057	0.061458
7	1.242341	-1.14297	0.03176
6	2.572333	0.703069	-0.00178
6	2.535784	-1.5921	0.011573
9	0.011012	-2.92659	-1.03543
9	-0.0156	-2.8231	1.237548
6	0.297877	3.148311	1.220055
6	0.000329	2.411855	0.022414
6	-0.29257	3.134074	-1.18568
6	0.299239	4.525565	1.205364
1	0.519755	5.091795	2.110646
6	0.013943	5.209782	0.001659
6	-0.27909	4.511302	-1.19167
1	-0.49372	5.066403	-2.10523
1	0.508098	2.587672	2.132522
1	-0.5087	2.561832	-2.08957
1	0.019552	6.301145	-0.00618
6	-3.06924	2.112087	0.02945
1	-2.59579	2.736128	0.80138
1	-4.15362	2.127733	0.217477
1	-2.91687	2.611633	-0.94469
6	-2.8736	-3.04203	-0.027
1	-2.56719	-3.50047	-0.97972
1	-3.95375	-3.18895	0.102535
1	-2.33819	-3.5745	0.772252
6	3.067815	2.111106	-0.01182
1	4.152121	2.126941	-0.1995
1	2.91374	2.61069	0.961781
1	2.594328	2.735131	-0.78406
6	2.8702	-3.04364	-0.00378
1	2.318202	-3.57182	0.787045
1	3.947125	-3.19159	0.148767
1	2.582263	-3.50583	-0.96045
6	-3.36756	-0.47335	-0.00253
53	-5.45066	-0.53177	-0.01042
6	3.365556	-0.47472	-0.00049
53	5.448203	-0.53718	-0.05262

Cartesian coordinates for the $S(\pi_{Ph} \rightarrow \pi_{BOD}^*)$ state of BOD-PhOH (MN15/def2-SVP in DCM)

6	-1.23097	0.040304	-0.03521
6	-2.51985	-1.78558	0.041652
6	-2.56329	0.508766	-0.06435
7	-1.22586	-1.34433	0.028261
6	-0.00056	0.757238	-0.05393
6	1.242753	0.04717	-0.02703
5	0.012031	-2.26101	0.090543
7	1.254569	-1.34062	0.006662
6	2.568539	0.523376	-0.04892
6	2.54721	-1.77741	-0.0011
9	0.012069	-3.16862	-0.97786
9	0.034505	-2.99225	1.287911
6	0.027293	2.894192	1.263807
6	-0.00748	2.216869	-0.00182
6	-0.0687	3.004007	-1.20664
6	0.003248	4.258511	1.329936
1	0.02735	4.801241	2.274729
6	-0.05676	5.016512	0.115459
6	-0.09234	4.370332	-1.15749
1	-0.14378	4.973653	-2.06574
1	0.075649	2.292971	2.172518
1	-0.09932	2.481865	-2.16378
6	-3.0564	1.920466	-0.16479
1	-2.67774	2.568488	0.641972
1	-4.15343	1.939634	-0.08807
1	-2.79412	2.395812	-1.1231
6	-2.85803	-3.23628	0.099624
1	-2.47656	-3.76288	-0.78729
1	-3.94513	-3.37979	0.158492
1	-2.38566	-3.70791	0.973681
6	3.053684	1.937671	-0.09991
1	4.148426	1.95683	-0.20074
1	2.797667	2.516946	0.800459
1	2.647866	2.487408	-0.96542
6	2.89849	-3.2259	0.038428
1	2.508769	-3.69307	0.955428
1	3.987068	-3.36191	0.003355
1	2.441305	-3.76095	-0.80644
6	-3.34859	-0.66436	-0.01306
53	-5.44277	-0.73312	-0.03899
6	3.370093	-0.65134	-0.03808
53	5.454543	-0.68996	-0.04405
8	-0.07475	6.314117	0.23647
1	-0.11473	6.782071	-0.61804

Cartesian coordinates for the S($\pi_{BOD} \rightarrow \pi_{Ph}$*) state of BOD-Ph (MN15/def2-SVP in DCM)

6	-1.21746	0.204647	0.044224
6	-2.53834	-1.57823	0.02153
6	-2.5774	0.714088	0.0185
7	-1.26295	-1.18976	0.048728
6	-0.00857	0.928772	0.045748
6	1.189713	0.185943	0.043771
5	-0.03136	-2.14797	0.093031
7	1.214378	-1.2088	0.048775
6	2.558372	0.67476	0.017637
6	2.484121	-1.61688	0.021838
9	-0.03805	-2.98587	-1.00429
9	-0.03723	-2.87636	1.269983
6	0.055387	3.144385	1.267542
6	0.005806	2.390046	0.034058
6	0.050675	3.123395	-1.21317
6	0.16905	4.518916	1.236554
1	0.201671	5.065952	2.184387
6	0.238548	5.241251	0.008863
6	0.164487	4.498588	-1.20515
1	0.193648	5.029688	-2.16219
1	0.004283	2.616369	2.224779
1	-0.0042	2.579241	-2.16116
1	0.328746	6.327594	-0.00054
6	-2.99992	2.138476	0.010993
1	-2.59698	2.669328	0.886475
1	-4.09599	2.209419	0.002818
1	-2.5859	2.663488	-0.86312
6	-2.93927	-3.00076	-0.01184
1	-2.79209	-3.39233	-1.03172
1	-3.99406	-3.12057	0.260673
1	-2.29793	-3.5883	0.658731
6	3.003679	2.091383	0.008771
1	4.100421	2.146271	0.000348
1	2.606469	2.630158	0.882746
1	2.595076	2.622393	-0.86501
6	2.862741	-3.04549	-0.01048
1	2.215019	-3.62167	0.66388
1	3.9166	-3.18137	0.258027
1	2.704874	-3.43674	-1.02886
6	-3.38003	-0.40714	0.001346
53	-5.45164	-0.47125	-0.05168
6	3.343343	-0.45938	0.001058
53	5.411735	-0.55535	-0.0521

Cartesian coordinates for the S($\pi_{BOD} \rightarrow \pi_{Ph}$*) state of BOD-PhOH (MN15/def2-SVP in DCM)

6	0.602948	-0.47678	-0.32005
6	1.191128	-1.66941	-2.09884
6	1.292673	-1.65066	0.193163
7	0.583676	-0.54466	-1.71296
6	0.037534	0.606076	0.37277
6	-0.55263	1.648834	-0.35902
5	0.049147	0.556652	-2.68091
7	-0.55863	1.654168	-1.75373
6	-1.28079	2.815925	0.113476
6	-1.21473	2.736623	-2.17798
9	-0.92911	0.036954	-3.5057
9	1.093365	1.081068	-3.42294
6	0.980641	1.448822	2.49594
6	0.044961	0.640309	1.85054
6	-0.89913	-0.13307	2.538532
6	0.969133	1.515254	3.938215
1	1.672518	2.132096	4.497418
6	0.048849	0.715808	4.632836
6	-0.87158	-0.11467	3.987022
1	-1.57567	-0.70738	4.576744
1	1.690862	2.038647	1.911802
1	-1.61121	-0.75539	1.993002
6	1.589085	-1.98183	1.609372
1	1.943077	-1.08982	2.148175
1	2.334928	-2.78602	1.663468
1	0.672895	-2.2988	2.130611
6	1.328083	-2.05214	-3.51965
1	0.337038	-2.3179	-3.92105
1	2.005633	-2.90472	-3.63858
1	1.687319	-1.19201	-4.1025
6	-1.56949	3.190394	1.520214
1	-2.32375	3.987583	1.555297
1	-0.65351	3.529882	2.026926
1	-1.91047	2.310064	2.087628
6	-1.4214	3.033574	-3.61076
1	-0.51182	2.798432	-4.18008
1	-1.71051	4.080233	-3.75931
1	-2.22461	2.38642	-3.99978
6	1.636554	-2.37898	-0.92703
53	2.635045	-4.19003	-0.97863
6	-1.67655	3.477015	-1.03111
53	-2.77287	5.236408	-1.1503
8	0.081453	0.775098	5.996495
1	-0.6019	0.185832	6.346772

Cartesian coordinates for the S($\pi_{BOD} \rightarrow \pi_{Ph}*$) state of BOD-PhNO$_2$ (MN15/def2-SVP in DCM)

6	0.08454	1.245981	-1.03492
6	1.136463	3.121639	-1.81601
6	-0.21977	1.340334	-2.41034
7	0.934352	2.272525	-0.73175
6	-0.27004	0.250082	-0.0452
6	0.35446	0.294714	1.222201
5	1.805058	2.368951	0.575902
7	1.356004	1.220537	1.485361
6	0.097628	-0.43601	2.423986
6	1.775676	1.085203	2.775505
9	1.585286	3.603062	1.170392
9	3.139122	2.242672	0.203081
6	-0.97213	-2.13927	-0.29023
6	-1.27667	-0.76364	-0.37643
6	-2.56868	-0.38037	-0.7976
6	-1.91682	-3.10139	-0.61879
1	-1.69167	-4.16656	-0.57478
6	-3.18539	-2.68317	-1.0287
6	-3.52721	-1.33225	-1.11851
1	-4.53394	-1.05289	-1.42783
1	0.03041	-2.44133	0.020711
1	-2.81971	0.681926	-0.84866
6	-0.92477	0.390152	-3.28993
1	-0.75153	-0.65086	-2.98034
1	-0.62369	0.528165	-4.3376
1	-2.02193	0.535398	-3.24419
6	1.971041	4.348209	-1.72413
1	1.553732	5.054411	-0.99179
1	2.024764	4.840127	-2.70339
1	2.988877	4.097333	-1.39272
6	-0.96678	-1.44373	2.706607
1	-1.1662	-1.47726	3.787441
1	-0.68415	-2.46286	2.395683
1	-1.9045	-1.20095	2.187408
6	2.825821	1.955168	3.369469
1	3.651726	2.10227	2.659524
1	3.215719	1.509075	4.293266
1	2.420932	2.951147	3.609114
6	0.435654	2.580076	-2.86487
53	0.286281	3.341097	-4.75802
6	1.02006	0.064	3.362762
53	1.221818	-0.56807	5.337454
7	-4.18452	-3.68915	-1.37444
8	-5.28097	-3.30213	-1.74319
8	-3.8699	-4.86352	-1.27733

Cartesian coordinates for the T($\pi_{Ph} \rightarrow \pi_{BOD}$*) state of BOD-Ph (MN15/def2-SVP in DCM)

6	0.613258	-0.50976	-0.31161
6	1.17137	-1.70526	-2.1103
6	1.309567	-1.64391	0.178431
7	0.541175	-0.5725	-1.68713
6	0.002424	0.579082	0.392621
6	-0.61622	1.642966	-0.34228
5	-0.01388	0.526708	-2.62965
7	-0.55903	1.65797	-1.71985
6	-1.30743	2.79353	0.115652
6	-1.19403	2.775468	-2.17519
9	-1.04309	0.018293	-3.4219
9	1.006728	1.007228	-3.44997
6	0.937398	1.450204	2.567691
6	0.01036	0.604503	1.858627
6	-0.90879	-0.21594	2.606572
6	0.920161	1.488415	3.947075
1	1.60572	2.144843	4.485214
6	0.025631	0.653369	4.678011
6	-0.87661	-0.20633	3.986184
1	-1.55618	-0.84359	4.554141
1	1.631984	2.066465	1.993623
1	-1.60944	-0.85159	2.06176
1	0.031536	0.672258	5.76785
6	1.630819	-1.99593	1.593756
1	1.940428	-1.11485	2.175642
1	2.449452	-2.72918	1.625211
1	0.767544	-2.43942	2.116723
6	1.324251	-2.03692	-3.55035
1	0.366306	-1.91124	-4.07451
1	1.681389	-3.06691	-3.6749
1	2.043339	-1.35423	-4.03029
6	-1.61343	3.194459	1.521315
1	-2.43181	3.928513	1.536184
1	-0.74463	3.655652	2.019228
1	-1.91656	2.334137	2.136709
6	-1.3626	3.057005	-3.62414
1	-0.41047	2.912619	-4.15405
1	-1.72085	4.082262	-3.78047
1	-2.08706	2.35851	-4.07219
6	1.643056	-2.38213	-0.97147
53	2.694204	-4.17652	-1.01252
6	-1.65352	3.491485	-1.05548
53	-2.70547	5.283519	-1.14735

Cartesian coordinates for the T($\pi_{Ph} \rightarrow \pi_{BOD}*$) state of BOD-PhOH (MN15/def2-SVP in DCM)

6	0.487904	-0.5624	-0.2651
6	0.935757	-1.79738	-2.08318
6	1.235729	-1.68967	0.18576
7	0.367502	-0.63493	-1.63567
6	-0.00037	0.600179	0.441907
6	-0.49882	1.724913	-0.31721
5	-0.01879	0.523157	-2.58304
7	-0.3949	1.727659	-1.69139
6	-1.24173	2.873438	0.084775
6	-0.96895	2.86558	-2.19034
9	-1.10971	0.165285	-3.38137
9	1.06324	0.839449	-3.41044
6	0.499649	1.790552	2.589901
6	0.010142	0.637587	1.872789
6	-0.46935	-0.47765	2.655423
6	0.53231	1.81502	3.957303
1	0.937497	2.665729	4.507096
6	0.03403	0.706373	4.703014
6	-0.47748	-0.43536	4.024727
1	-0.87733	-1.26877	4.607396
1	0.891875	2.628568	2.011945
1	-0.87222	-1.34319	2.127657
6	1.805029	-1.99149	1.534971
1	2.083433	-1.08003	2.081
1	2.714254	-2.59975	1.41627
1	1.119779	-2.56746	2.178362
6	0.958664	-2.16969	-3.52224
1	-0.03373	-2.02475	-3.9725
1	1.268424	-3.21513	-3.64541
1	1.656679	-1.52446	-4.07811
6	-1.79507	3.24455	1.423495
1	-2.7089	3.841446	1.284342
1	-1.10449	3.856762	2.026252
1	-2.06144	2.36229	2.020942
6	-1.01	3.164263	-3.6461
1	-0.02428	2.99239	-4.10145
1	-1.31766	4.203406	-3.81822
1	-1.71788	2.494743	-4.15915
6	1.460964	-2.46231	-0.97195
53	2.45035	-4.29422	-1.04071
6	-1.48118	3.586226	-1.10794
53	-2.47233	5.412224	-1.25795
8	0.071498	0.792396	6.025531
1	-0.28992	-0.00164	6.454132

Cartesian coordinates for the T($\pi_{Ph} \rightarrow \pi_{BOD}$*) state of BOD-PhNO$_2$ (MN15/def2-SVP in DCM)

6	0.17341	1.224896	-1.0702
6	1.366653	2.919787	-1.90326
6	-0.23387	1.358726	-2.41345
7	1.133777	2.172802	-0.78231
6	-0.26555	0.314702	-0.06037
6	0.25883	0.414222	1.264771
5	1.870222	2.346344	0.566856
7	1.219601	1.358354	1.5635
6	-0.05684	-0.32133	2.425559
6	1.541946	1.256288	2.888043
9	1.734917	3.659673	1.027786
9	3.235017	2.062586	0.418404
6	-0.7619	-2.01907	-0.85248
6	-1.22419	-0.72662	-0.38684
6	-2.64472	-0.50011	-0.25624
6	-1.66094	-3.0135	-1.16485
1	-1.35229	-3.99662	-1.51747
6	-3.02746	-2.72648	-1.01522
6	-3.54131	-1.49556	-0.56906
1	-4.6191	-1.36425	-0.48404
1	0.313448	-2.17558	-0.94614
1	-2.98136	0.476121	0.095018
6	-1.27405	0.572086	-3.1409
1	-1.11753	-0.51782	-3.06794
1	-1.24602	0.809596	-4.21674
1	-2.29726	0.796572	-2.79561
6	2.35682	4.032514	-1.92166
1	2.035365	4.860051	-1.27174
1	2.484563	4.413869	-2.94332
1	3.330007	3.686862	-1.54321
6	-1.0649	-1.41273	2.575901
1	-0.96143	-1.89148	3.563184
1	-0.93817	-2.21974	1.834022
1	-2.10312	-1.04594	2.51127
6	2.556147	2.140931	3.52658
1	3.494482	2.125874	2.952914
1	2.758898	1.810839	4.553948
1	2.21179	3.185612	3.551097
6	0.536347	2.436995	-2.9135
53	0.441019	3.190015	-4.85769
6	0.768573	0.233165	3.434109
53	0.81733	-0.38114	5.428163
7	-3.99942	-3.79832	-1.35179
8	-5.17344	-3.53283	-1.2167
8	-3.53985	-4.85151	-1.73424

Cartesian coordinates for the T($\pi_{BOD} \rightarrow \pi_{Ph}*$) state of BOD-Ph (MN15/def2-SVP in DCM)

6	0.711005	-0.40469	-0.31384
6	1.115741	-1.71972	-2.08992
6	1.518902	-1.52318	0.178839
7	0.491678	-0.56401	-1.69767
6	0.049785	0.658086	0.391341
6	-0.53314	1.69349	-0.34193
5	0.053385	0.557203	-2.6487
7	-0.48641	1.708875	-1.74269
6	-1.28143	2.874173	0.100755
6	-1.14172	2.797129	-2.18867
9	-0.96033	0.121835	-3.50163
9	1.130748	1.017996	-3.41075
6	0.859408	1.356982	2.664328
6	-0.02939	0.606375	1.869029
6	-0.96732	-0.23552	2.484954
6	0.792392	1.261792	4.062847
1	1.485071	1.843846	4.6749
6	-0.15057	0.43474	4.669504
6	-1.03951	-0.31556	3.878443
1	-1.78335	-0.96209	4.348202
1	1.596589	2.007812	2.186825
1	-1.64629	-0.82584	1.863209
1	-0.2006	0.367564	5.758288
6	2.000809	-1.7209	1.570058
1	2.497013	-0.80751	1.938606
1	2.699241	-2.56667	1.620174
1	1.170151	-1.90979	2.267786
6	1.011395	-2.23244	-3.46666
1	-0.03578	-2.48711	-3.71396
1	1.636969	-3.12078	-3.61486
1	1.303315	-1.44812	-4.18681
6	-1.58462	3.259499	1.500491
1	-2.21536	4.157749	1.525517
1	-0.65909	3.456475	2.067437
1	-2.09272	2.443026	2.038082
6	-1.33315	3.071536	-3.62978
1	-0.40447	2.861912	-4.17973
1	-1.65367	4.106583	-3.79764
1	-2.09837	2.392164	-4.04075
6	1.760386	-2.30656	-0.92161
53	2.773008	-4.11594	-0.97582
6	-1.62466	3.536079	-1.06079
53	-2.71804	5.296754	-1.21279

Cartesian coordinates for the T($\pi_{BOD} \to \pi_{Ph}*$) state of BOD-PhOH (MN15/def2-SVP in DCM)

6	-1.22138	0.032452	0.029514
6	-2.52554	-1.79368	-0.05337
6	-2.6059	0.510442	0.065645
7	-1.23287	-1.37742	-0.01574
6	-0.00045	0.741204	0.047967
6	1.223434	0.038194	0.061892
5	0.003966	-2.30091	0.099193
7	1.241877	-1.37185	0.106305
6	2.605562	0.520501	-0.01665
6	2.535465	-1.78407	0.090028
9	0.064831	-3.1753	-0.98293
9	-0.05828	-3.0381	1.284513
6	0.24733	2.934264	1.221109
6	-0.00445	2.219586	0.039674
6	-0.25997	2.915859	-1.14949
6	0.245889	4.334568	1.216267
1	0.434671	4.905389	2.126872
6	-0.00909	5.02745	0.022255
6	-0.26312	4.317883	-1.16194
1	-0.45721	4.862929	-2.08938
1	0.446937	2.3916	2.148679
1	-0.45894	2.362095	-2.07059
6	-3.08684	1.914801	0.172014
1	-2.4616	2.50826	0.854567
1	-4.12591	1.92943	0.530209
1	-3.05709	2.425442	-0.80536
6	-2.89765	-3.22017	-0.1428
1	-2.62976	-3.62995	-1.13288
1	-3.97371	-3.36028	0.017598
1	-2.33008	-3.8039	0.598503
6	3.078222	1.926857	-0.12599
1	4.115612	1.947754	-0.48835
1	3.047205	2.438524	0.850648
1	2.446072	2.516144	-0.80639
6	2.916473	-3.21126	0.098149
1	2.279453	-3.76653	0.802281
1	3.973022	-3.33642	0.367454
1	2.75676	-3.6631	-0.89753
6	-3.37719	-0.62556	-0.00638
53	-5.44853	-0.71118	-0.03923
6	3.381454	-0.61449	0.009876
53	5.451299	-0.70242	-0.07467
8	-0.00012	6.376386	0.061828
1	-0.18645	6.743148	-0.81545

Cartesian coordinates for the $T(\pi_{BOD} \rightarrow \pi_{Ph}^*)$ state of BOD-PhNO$_2$ (MN15/def2-SVP in DCM)

6	0.220583	1.192652	-1.05171
6	1.372322	2.900645	-1.87849
6	-0.18134	1.30733	-2.44152
7	1.164239	2.182366	-0.77578
6	-0.21474	0.293888	-0.06389
6	0.306912	0.40204	1.235525
5	1.882873	2.417806	0.591059
7	1.252602	1.372889	1.566197
6	0.00219	-0.37425	2.423139
6	1.550905	1.26267	2.860024
9	1.639161	3.697909	1.042724
9	3.239527	2.186115	0.459791
6	-0.823	-2.01462	-0.84301
6	-1.22269	-0.73901	-0.38417
6	-2.6006	-0.45992	-0.2396
6	-1.76182	-2.98069	-1.15158
1	-1.475	-3.96916	-1.50738
6	-3.14347	-2.69248	-1.00809
6	-3.55113	-1.41536	-0.54422
1	-4.61738	-1.22024	-0.44061
1	0.241572	-2.23737	-0.95571
1	-2.91585	0.524851	0.11638
6	-1.15955	0.466538	-3.184
1	-0.87138	-0.59405	-3.15962
1	-1.22443	0.797557	-4.22845
1	-2.15851	0.523258	-2.72798
6	2.296555	4.052589	-1.92117
1	1.814213	4.918996	-1.43943
1	2.546619	4.320334	-2.95404
1	3.206842	3.827101	-1.34954
6	-0.94321	-1.51639	2.551711
1	-0.93118	-1.90168	3.579371
1	-0.68105	-2.32906	1.859401
1	-1.96864	-1.21364	2.295017
6	2.502199	2.16423	3.542102
1	3.36547	2.362722	2.892847
1	2.828938	1.74241	4.499389
1	2.00773	3.130792	3.733575
6	0.541563	2.374081	-2.93559
53	0.490872	3.148616	-4.85045
6	0.781119	0.176995	3.420075
53	0.87711	-0.39608	5.402874
7	-4.09517	-3.65618	-1.32306
8	-5.32337	-3.37777	-1.19108
8	-3.71416	-4.79056	-1.73687