

Supplementary Materials

Table A.1: Optimized bond distances (in Å) of the chlorophyll a molecule calculated with the M06, M06L, M06-2X and M06-HF density functionals and the MIDIY and DGDZVP basis sets

	M06	M06L	M06-2X	M06-HF
R(2-3)	1.211	1.222	1.214	1.205
R(3-4)	1.460	1.461	1.471	1.468
R(4-6)	1.378	1.389	1.381	1.379
R(4-7)	1.416	1.422	1.423	1.416
R(5-8)	1.511	1.517	1.518	1.527
R(5-9)	1.523	1.528	1.532	1.539
R(5-66)	1.099	1.097	1.097	1.089
R(6-10)	1.487	1.492	1.500	1.511
R(6-11)	1.449	1.455	1.455	1.441
R(7-9)	1.403	1.405	1.412	1.436
R(7-12)	1.333	1.344	1.335	1.323
R(8-13)	1.353	1.366	1.354	1.345
R(8-14)	1.217	1.228	1.222	1.214
R(9-15)	1.368	1.378	1.367	1.351
R(10-67)	1.103	1.101	1.100	1.095
R(10-68)	1.099	1.097	1.097	1.093
R(10-69)	1.103	1.102	1.100	1.095
R(11-12)	1.398	1.405	1.406	1.402
R(11-16)	1.387	1.395	1.390	1.392
R(13-17)	1.441	1.455	1.450	1.452
R(15-18)	1.515	1.519	1.524	1.540
R(15-19)	1.374	1.380	1.384	1.410
R(16-20)	1.397	1.402	1.402	1.390
R(16-70)	1.093	1.091	1.091	1.086
R(17-71)	1.099	1.097	1.097	1.092
R(17-72)	1.098	1.097	1.096	1.091
R(17-73)	1.095	1.093	1.093	1.090
R(18-21)	1.557	1.563	1.563	1.560
R(18-22)	1.552	1.561	1.563	1.555
R(18-74)	1.100	1.100	1.099	1.097
R(19-23)	1.361	1.371	1.363	1.341
R(20-24)	1.381	1.391	1.389	1.393
R(20-25)	1.445	1.452	1.450	1.448
R(21-23)	1.528	1.534	1.538	1.531
R(21-26)	1.529	1.536	1.541	1.561
R(21-75)	1.104	1.101	1.100	1.090
R(22-27)	1.529	1.534	1.539	1.551

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	M06	M06L	M06-2X	M06-HF
R(22-76)	1.098	1.096	1.095	1.092
R(22-77)	1.099	1.099	1.097	1.094
R(23-28)	1.380	1.386	1.385	1.393
R(24-29)	1.367	1.378	1.367	1.346
R(25-30)	1.370	1.376	1.373	1.369
R(25-31)	1.493	1.497	1.503	1.508
R(26-78)	1.100	1.099	1.098	1.094
R(26-79)	1.099	1.098	1.097	1.096
R(26-80)	1.100	1.099	1.099	1.093
R(27-32)	1.520	1.524	1.527	1.537
R(27-81)	1.103	1.103	1.102	1.094
R(27-82)	1.104	1.102	1.099	1.095
R(28-33)	1.403	1.408	1.407	1.394
R(28-83)	1.091	1.089	1.088	1.084
R(29-30)	1.443	1.450	1.448	1.447
R(29-34)	1.403	1.405	1.414	1.433
R(30-35)	1.490	1.495	1.503	1.512
R(31-36)	1.542	1.551	1.555	1.563
R(31-84)	1.102	1.101	1.100	1.094
R(31-85)	1.101	1.100	1.098	1.094
R(32-37)	1.209	1.220	1.212	1.208
R(32-38)	1.366	1.377	1.371	1.360
R(33-39)	1.363	1.377	1.363	1.349
R(33-40)	1.448	1.448	1.462	1.482
R(34-41)	1.381	1.392	1.379	1.359
R(34-86)	1.092	1.091	1.089	1.084
R(35-87)	1.103	1.102	1.101	1.096
R(35-88)	1.099	1.098	1.097	1.093
R(35-89)	1.103	1.101	1.100	1.096
R(36-90)	1.101	1.099	1.098	1.094
R(36-91)	1.101	1.099	1.099	1.095
R(36-92)	1.100	1.099	1.098	1.094
R(38-42)	1.451	1.473	1.459	1.464
R(39-41)	1.384	1.389	1.394	1.396
R(40-43)	1.489	1.492	1.501	1.508
R(40-44)	1.373	1.385	1.370	1.350
R(41-44)	1.454	1.459	1.465	1.479
R(42-45)	1.501	1.503	1.513	1.521
R(42-93)	1.100	1.098	1.098	1.091
R(42-94)	1.105	1.103	1.101	1.094
R(43-95)	1.100	1.101	1.099	1.093
R(43-96)	1.104	1.102	1.101	1.096
R(43-97)	1.101	1.099	1.099	1.096

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Table A.1 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
R(44-46)	1.449	1.447	1.462	1.472
R(45-47)	1.334	1.342	1.335	1.328
R(45-98)	1.093	1.091	1.090	1.085
R(46-48)	1.337	1.348	1.339	1.333
R(46-99)	1.095	1.093	1.092	1.086
R(47-49)	1.506	1.510	1.519	1.528
R(47-50)	1.503	1.508	1.514	1.519
R(48-100)	1.091	1.089	1.089	1.084
R(48-101)	1.091	1.089	1.089	1.086
R(49-102)	1.097	1.096	1.095	1.092
R(49-103)	1.104	1.102	1.102	1.097
R(49-104)	1.101	1.101	1.100	1.095
R(50-51)	1.543	1.549	1.553	1.559
R(50-105)	1.102	1.100	1.099	1.095
R(50-106)	1.106	1.105	1.103	1.098
R(51-52)	1.532	1.539	1.544	1.550
R(51-107)	1.104	1.102	1.101	1.097
R(51-108)	1.102	1.101	1.099	1.094
R(52-53)	1.539	1.546	1.549	1.552
R(52-109)	1.104	1.102	1.102	1.097
R(52-110)	1.106	1.104	1.103	1.098
R(53-54)	1.534	1.541	1.545	1.551
R(53-55)	1.539	1.547	1.549	1.552
R(53-111)	1.105	1.103	1.102	1.097
R(54-112)	1.100	1.098	1.098	1.094
R(54-113)	1.100	1.099	1.098	1.094
R(54-114)	1.104	1.102	1.102	1.098
R(55-56)	1.534	1.540	1.546	1.552
R(55-115)	1.104	1.103	1.102	1.097
R(55-116)	1.106	1.104	1.103	1.098
R(56-57)	1.533	1.541	1.545	1.552
R(56-117)	1.105	1.103	1.102	1.097
R(56-118)	1.101	1.100	1.098	1.093
R(57-58)	1.539	1.546	1.549	1.552
R(57-119)	1.105	1.103	1.102	1.097
R(57-120)	1.106	1.104	1.103	1.098
R(58-59)	1.539	1.546	1.548	1.551
R(58-60)	1.534	1.541	1.545	1.550
R(58-121)	1.105	1.103	1.102	1.096
R(59-61)	1.535	1.541	1.546	1.552
R(59-122)	1.105	1.103	1.102	1.098
R(59-123)	1.106	1.104	1.103	1.098
R(60-124)	1.100	1.099	1.098	1.094

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Table A.1 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
R(60-125)	1.100	1.099	1.098	1.094
R(60-126)	1.104	1.102	1.101	1.097
R(61-62)	1.534	1.541	1.546	1.552
R(61-127)	1.104	1.102	1.101	1.096
R(61-128)	1.102	1.101	1.099	1.093
R(62-63)	1.541	1.548	1.551	1.553
R(62-129)	1.105	1.103	1.102	1.097
R(62-130)	1.105	1.102	1.102	1.098
R(63-64)	1.534	1.542	1.546	1.551
R(63-65)	1.534	1.541	1.545	1.551
R(63-131)	1.103	1.101	1.100	1.094
R(64-132)	1.101	1.100	1.099	1.095
R(64-133)	1.102	1.100	1.100	1.095
R(64-134)	1.101	1.099	1.099	1.095
R(65-135)	1.101	1.100	1.100	1.096
R(65-136)	1.102	1.100	1.100	1.095
R(65-137)	1.101	1.099	1.099	1.095

Table A.2: Optimized bond angles (in degrees) of the chlorophyll a molecule calculated with the M06, M06L, M06-2X and M06-HF density functionals and the MIDIY and DGDZVP basis sets

	M06	M06L	M06-2X	M06-HF
A(2-3-4)	131.5	131.6	131.6	131.3
A(3-4-6)	143.7	143.5	143.5	143.9
A(3-4-7)	109.2	109.5	109.5	108.9
A(6-4-7)	107.1	107.0	107.0	107.2
A(4-6-10)	127.2	127.5	127.5	127.3
A(4-6-11)	105.4	105.2	105.3	105.0
A(4-7-9)	114.4	114.4	114.3	114.2
A(4-7-12)	112.1	112.4	112.3	111.7
A(8-5-9)	111.8	112.7	112.3	109.4
A(8-5-66)	107.7	107.9	108.1	111.1
A(5-8-13)	109.4	109.1	109.8	109.9
A(5-8-14)	126.8	127.6	127.0	127.8
A(9-5-66)	114.2	114.3	114.5	117.4
A(5-9-7)	106.8	107.2	107.0	105.6
A(5-9-15)	128.5	128.2	128.6	130.5
A(10-6-11)	127.4	127.2	127.4	128.0
A(6-10-67)	111.9	112.0	111.6	111.0
A(6-10-68)	109.5	109.7	109.0	108.3

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Table A.2 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
A(6-10-69)	111.9	111.9	111.6	111.1
A(6-11-12)	109.5	109.9	109.6	109.5
A(6-11-16)	129.0	128.9	128.9	128.7
A(9-7-12)	133.5	133.2	133.4	134.1
A(7-9-15)	124.7	124.6	124.3	123.8
A(7-12-11)	105.9	105.4	105.7	106.2
A(13-8-14)	123.8	123.3	123.2	122.2
A(8-13-17)	113.4	112.5	112.9	113.7
A(9-15-18)	125.3	124.9	124.9	128.4
A(9-15-19)	122.6	122.4	122.8	121.4
A(67-10-68)	108.3	108.3	108.6	108.8
A(67-10-69)	106.9	106.7	107.5	108.5
A(68-10-69)	108.2	108.1	108.5	109.0
A(12-11-16)	121.5	121.1	121.4	121.8
A(11-16-20)	126.4	126.2	126.2	126.7
A(11-16-70)	116.9	117.2	117.1	116.6
A(13-17-71)	110.8	110.4	110.2	109.8
A(13-17-72)	110.7	110.3	110.2	109.8
A(13-17-73)	105.4	105.1	105.3	105.0
A(18-15-19)	112.1	112.6	112.3	110.2
A(15-18-21)	101.8	102.0	101.9	101.1
A(15-18-22)	110.4	110.7	110.5	114.4
A(15-18-74)	109.8	109.6	109.4	107.9
A(15-19-23)	109.7	109.3	109.5	109.8
A(20-16-70)	116.7	116.6	116.7	116.8
A(16-20-24)	125.0	125.2	125.2	125.2
A(16-20-25)	125.7	125.1	125.4	125.9
A(71-17-72)	108.7	108.8	109.1	109.7
A(71-17-73)	110.6	111.0	111.0	111.2
A(72-17-73)	110.6	111.2	111.1	111.2
A(21-18-22)	116.4	116.6	116.7	114.8
A(21-18-74)	110.4	109.9	110.1	107.9
A(18-21-23)	102.8	102.9	102.8	102.2
A(18-21-26)	117.0	116.7	116.6	113.7
A(18-21-75)	107.5	107.8	107.9	112.0
A(22-18-74)	108.0	107.8	108.0	110.0
A(18-22-27)	111.3	111.1	110.6	113.8
A(18-22-76)	112.0	111.9	112.3	109.6
A(18-22-77)	110.3	110.1	110.2	110.4
A(19-23-21)	111.1	111.6	111.6	111.5
A(19-23-28)	125.6	125.6	125.9	127.8
A(24-20-25)	109.3	109.7	109.4	108.9
A(20-24-29)	106.9	106.4	106.6	106.9

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Table A.2 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
A(20-25-30)	107.0	107.0	106.9	107.0
A(20-25-31)	125.5	125.2	125.0	125.3
A(23-21-26)	114.4	114.0	114.0	106.8
A(23-21-75)	106.7	107.0	106.9	111.7
A(21-23-28)	123.2	122.8	122.5	120.6
A(26-21-75)	107.9	108.0	108.1	110.2
A(21-26-78)	110.7	110.7	110.5	109.3
A(21-26-79)	111.9	111.8	111.6	109.6
A(21-26-80)	111.2	111.1	110.7	111.5
A(27-22-76)	110.2	110.2	110.0	107.2
A(27-22-77)	108.2	108.4	108.4	108.8
A(22-27-32)	110.7	110.9	110.3	109.6
A(22-27-81)	110.9	111.0	111.0	110.7
A(22-27-82)	108.5	109.2	109.3	112.4
A(76-22-77)	104.6	104.9	105.2	106.7
A(23-28-33)	128.2	128.4	127.3	126.1
A(23-28-83)	116.1	115.8	116.5	116.6
A(24-29-30)	110.1	110.3	110.4	110.7
A(24-29-34)	124.3	124.2	124.4	124.7
A(30-25-31)	127.4	127.8	128.0	127.7
A(25-30-29)	106.7	106.7	106.6	106.5
A(25-30-35)	128.0	128.1	128.3	128.5
A(25-31-36)	111.5	112.0	111.5	110.6
A(25-31-84)	110.6	110.3	110.2	110.2
A(25-31-85)	110.0	109.8	109.8	109.8
A(78-26-79)	107.6	107.6	108.0	108.6
A(78-26-80)	106.8	107.2	107.4	108.4
A(79-26-80)	108.5	108.3	108.7	109.3
A(32-27-81)	109.9	109.4	109.1	108.8
A(32-27-82)	110.7	110.7	110.7	107.5
A(27-32-37)	122.8	123.2	122.4	122.0
A(27-32-38)	118.4	118.0	118.3	118.3
A(81-27-82)	106.0	105.6	106.5	107.7
A(33-28-83)	115.7	115.8	116.2	117.3
A(28-33-39)	124.9	124.4	125.2	125.8
A(28-33-40)	125.3	125.4	124.7	124.4
A(30-29-34)	125.6	125.5	125.2	124.5
A(29-30-35)	125.2	125.2	125.0	125.0
A(29-34-41)	128.2	127.9	127.5	126.5
A(29-34-86)	115.6	115.7	115.9	116.3
A(30-35-87)	111.8	111.8	111.5	111.0
A(30-35-88)	111.5	111.4	111.1	110.6
A(30-35-89)	111.9	112.0	111.6	111.2

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Table A.2 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
A(36-31-84)	109.7	109.4	109.6	109.8
A(36-31-85)	109.4	109.2	109.4	109.7
A(31-36-90)	110.4	110.4	110.1	109.6
A(31-36-91)	110.5	110.8	110.4	109.8
A(31-36-92)	111.4	111.3	111.1	110.8
A(84-31-85)	105.6	105.9	106.2	106.6
A(37-32-38)	118.8	118.8	119.3	119.7
A(32-38-42)	119.0	117.9	118.0	116.6
A(39-33-40)	109.9	110.2	110.1	109.8
A(33-39-41)	107.5	106.9	107.3	107.9
A(33-40-43)	125.0	125.3	124.8	124.3
A(33-40-44)	106.9	106.8	106.8	106.7
A(41-34-86)	116.2	116.4	116.6	117.2
A(34-41-39)	125.0	124.6	125.3	126.1
A(34-41-44)	126.1	125.9	125.9	125.7
A(87-35-88)	107.1	107.2	107.4	107.7
A(87-35-89)	106.9	106.8	107.4	108.1
A(88-35-89)	107.3	107.4	107.6	108.0
A(90-36-91)	107.5	107.6	107.8	108.3
A(90-36-92)	108.4	108.3	108.7	109.1
A(91-36-92)	108.5	108.4	108.6	109.2
A(38-42-45)	108.4	107.7	107.8	107.1
A(38-42-93)	110.1	109.6	110.1	108.7
A(38-42-94)	109.4	108.7	109.4	109.4
A(39-41-44)	109.0	109.5	108.8	108.2
A(43-40-44)	128.1	127.8	128.3	128.9
A(40-43-95)	110.8	110.8	110.3	109.7
A(40-43-96)	112.4	112.5	112.1	111.4
A(40-43-97)	111.6	111.8	111.1	110.3
A(40-44-41)	106.9	106.6	107.0	107.4
A(40-44-46)	128.9	129.1	128.6	128.5
A(41-44-46)	124.2	124.2	124.4	124.1
A(45-42-93)	110.2	110.9	110.7	111.8
A(45-42-94)	110.9	111.9	110.7	110.3
A(42-45-47)	124.3	124.1	123.5	122.8
A(42-45-98)	116.5	116.7	116.8	116.9
A(93-42-94)	107.9	108.0	108.2	109.4
A(95-43-96)	107.2	106.8	107.7	108.5
A(95-43-97)	107.6	107.7	108.1	108.7
A(96-43-97)	107.1	107.0	107.5	108.2
A(44-46-48)	126.5	127.2	125.1	123.9
A(44-46-99)	115.7	115.4	116.1	116.3
A(47-45-98)	119.1	119.1	119.7	120.3

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Table A.2 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
A(45-47-49)	122.5	122.3	122.1	121.7
A(45-47-50)	121.2	121.4	121.6	121.9
A(48-46-99)	117.8	117.4	118.8	119.8
A(46-48-100)	121.1	120.8	121.2	121.3
A(46-48-101)	122.5	122.8	121.9	121.6
A(49-47-50)	116.3	116.3	116.2	116.3
A(47-49-102)	110.9	111.2	110.5	109.8
A(47-49-103)	111.4	111.4	111.1	111.0
A(47-49-104)	110.9	110.9	110.6	110.2
A(47-50-51)	112.6	113.6	112.1	111.2
A(47-50-105)	110.0	110.0	110.0	110.0
A(47-50-106)	109.5	108.8	109.4	109.5
A(100-48-101)	116.4	116.4	116.8	117.2
A(102-49-103)	108.7	108.9	109.1	109.6
A(102-49-104)	107.9	107.7	108.2	108.4
A(103-49-104)	106.9	106.6	107.3	107.9
A(51-50-105)	109.2	109.6	109.4	109.2
A(51-50-106)	108.6	108.0	108.6	109.0
A(50-51-52)	111.6	111.5	111.6	111.3
A(50-51-107)	108.9	109.4	108.9	108.5
A(50-51-108)	109.3	109.1	109.1	109.2
A(105-50-106)	106.9	106.5	107.2	107.9
A(52-51-107)	109.8	110.0	109.8	110.1
A(52-51-108)	110.1	109.9	110.1	109.8
A(51-52-53)	114.7	114.6	114.2	113.8
A(51-52-109)	108.7	109.0	108.8	108.9
A(51-52-110)	109.4	109.1	109.3	109.2
A(107-51-108)	106.9	106.7	107.2	107.9
A(53-52-109)	108.6	108.8	108.6	108.5
A(53-52-110)	108.8	108.7	108.9	109.0
A(52-53-54)	111.1	111.1	111.3	111.0
A(52-53-55)	109.3	109.2	109.3	109.3
A(52-53-111)	108.2	108.4	108.2	108.1
A(109-52-110)	106.3	106.3	106.7	107.3
A(54-53-55)	111.1	111.3	111.2	111.1
A(54-53-111)	108.8	108.7	108.7	108.9
A(53-54-112)	111.8	111.7	111.4	111.4
A(53-54-113)	111.9	111.7	111.6	111.1
A(53-54-114)	110.1	110.4	110.1	109.7
A(55-53-111)	108.2	108.2	108.1	108.3
A(53-55-56)	114.8	114.6	114.4	113.7
A(53-55-115)	108.7	108.6	108.6	108.7
A(53-55-116)	108.8	108.8	108.9	109.0

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Table A.2 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
A(112-54-113)	106.8	107.1	107.2	107.5
A(112-54-114)	108.0	108.0	108.2	108.4
A(113-54-114)	108.0	107.9	108.2	108.6
A(56-55-115)	108.6	108.9	108.8	108.3
A(56-55-116)	109.4	109.4	109.3	109.6
A(55-56-57)	111.6	111.9	111.6	111.3
A(55-56-117)	109.5	109.5	109.4	109.1
A(55-56-118)	109.7	109.7	109.6	109.8
A(115-55-116)	106.3	106.2	106.7	107.3
A(57-56-117)	109.4	109.4	109.3	109.4
A(57-56-118)	109.7	109.6	109.7	109.5
A(56-57-58)	114.9	114.4	114.5	113.9
A(56-57-119)	108.7	108.9	108.7	108.7
A(56-57-120)	109.3	109.4	109.3	109.3
A(117-56-118)	106.7	106.6	107.1	107.8
A(58-57-119)	108.6	108.6	108.5	108.5
A(58-57-120)	108.7	108.9	108.9	109.0
A(57-58-59)	109.2	109.5	109.2	109.2
A(57-58-60)	111.2	111.2	111.3	111.1
A(57-58-121)	108.3	108.1	108.2	108.2
A(119-57-120)	106.2	106.2	106.6	107.2
A(59-58-60)	111.2	111.2	111.2	111.1
A(59-58-121)	108.1	108.1	108.1	108.3
A(58-59-61)	114.9	114.4	114.5	114.0
A(58-59-122)	108.5	108.6	108.5	108.6
A(58-59-123)	108.8	109.0	108.9	109.0
A(60-58-121)	108.7	108.6	108.7	108.8
A(58-60-124)	111.7	111.6	111.5	111.2
A(58-60-125)	111.7	111.7	111.5	111.2
A(58-60-126)	110.2	110.4	110.1	109.8
A(61-59-122)	108.7	108.8	108.7	108.6
A(61-59-123)	109.3	109.5	109.3	109.2
A(59-61-62)	111.3	111.6	111.2	110.7
A(59-61-127)	109.0	109.0	109.0	108.9
A(59-61-128)	109.7	109.8	109.8	109.6
A(122-59-123)	106.3	106.2	106.7	107.2
A(124-60-125)	107.0	107.2	107.2	107.4
A(124-60-126)	108.1	107.9	108.2	108.5
A(125-60-126)	108.0	107.9	108.2	108.6
A(62-61-127)	110.1	110.0	110.0	110.2
A(62-61-128)	109.7	109.6	109.6	109.4
A(61-62-63)	115.5	114.8	114.8	114.6
A(61-62-129)	108.7	108.9	108.8	108.8

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Table A.2 – Continued from the previous page

	M06	M06L	M06-2X	M06-HF
A(61-62-130)	108.7	108.9	108.8	108.5
A(127-61-128)	106.9	106.7	107.2	108.0
A(63-62-129)	108.6	108.8	108.9	108.7
A(63-62-130)	108.6	108.8	108.7	108.6
A(62-63-64)	112.1	111.7	111.8	112.0
A(62-63-65)	111.9	111.6	111.7	111.8
A(62-63-131)	106.6	106.9	106.9	106.8
A(129-62-130)	106.3	106.3	106.6	107.3
A(64-63-65)	110.5	110.5	110.5	110.3
A(64-63-131)	107.7	107.9	107.8	107.9
A(63-64-132)	111.4	111.4	111.1	110.9
A(63-64-133)	111.4	111.1	111.1	110.9
A(63-64-134)	110.7	111.0	110.6	110.2
A(65-63-131)	107.8	108.0	108.0	107.8
A(63-65-135)	111.4	111.4	111.2	110.8
A(63-65-136)	111.2	111.1	110.9	110.9
A(63-65-137)	110.8	111.0	110.7	110.3
A(132-64-133)	108.0	107.9	108.2	108.6
A(132-64-134)	107.9	107.9	108.1	108.3
A(133-64-134)	107.3	107.4	107.6	107.9
A(135-65-136)	108.0	107.9	108.1	108.5
A(135-65-137)	107.9	107.9	108.1	108.4
A(136-65-137)	107.4	107.4	107.7	107.9

Table A.3: Transition assignments for the TD-DFT calculation of the UV-Vis spectrum of chlorophyll a with the M06 density functional and the MIDIY and DGDZVP basis sets

#	nm	(f)	Assignments
1	613.6	0.6766	H→L(+95%)
2	546.2	0.2313	H-1→L(+88%) H→L+1(+11%)
3	424.0	1.2232	H→L+1(+87%) H-1→L(10%)
4	409.3	0.3779	H-2→L(+75%) H-1→L+1(+16%)
5	401.6	0.9059	H-1→L+1(+77%) H-2→L(17%)
6	380.1	0.0211	H-3→L(+95%)
7	371.7	0.0036	H-5→L(+83%) H-5→L+2(10%)
8	339.6	0.2017	H-6→L(+96%)
9	326.2	0.0478	H-3→L+1(+67%) H-2→L+1(+27%)
10	322.9	0.0998	H→L+2(+91%)

Table A.4: Transition assignments for the TD-DFT calculation of the UV-Vis spectrum of chlorophyll a with the M06L density functional and the MIDIY and DGDZVP basis sets

#	nm	(f)	Assignments
1	627.5	0.7441	H→L(+95%)
2	592.1	0.1920	H-1→L(+89%) H→L+1(+9%)
3	492.8	0.0167	H-2→L(+97%)
4	461.5	0.0592	H-3→L(+78%) H-4→L(+16%)
5	458.6	0.0011	H-4→L(+81%) H-3→L(18%)
6	448.1	0.7070	H→L+1(+65%) H-1→L+1(19%)
			H-1→L(6%)
7	442.1	0.0021	H-5→L(+100%)
8	437.4	0.9063	H-1→L+1(+68%) H→L+1(+16%)
9	386.6	0.0645	H-7→L(+74%) H-6→L(+24%)
10	382.5	0.1629	H-6→L(+68%) H-7→L(25%)

Table A.5: Transition assignments for the TD-DFT calculation of the UV-Vis spectrum of chlorophyll a with the M06-2X density functional and the MIDIY and DGDZVP basis sets

#	nm	(f)	Assignments
1	597.3	0.6586	H→L(+93%) H-1→L+1(+6%)
2	487.9	0.2538	H-1→L(+85%) H→L+1(13%)
3	399.1	1.6096	H→L+1(+85%) H-1→L(+13%)
4	364.9	1.4395	H-1→L+1(+88%) H→L(6%)
5	343.5	0.0506	H-2→L(+78%) H-3→L(8%) H-2→L+1(+7%)
6	320.8	0.0194	H-3→L(+77%) H-2→L(+10%)
7	318.3	0.0010	H-7→L(+41%) H-7→L+2(+36%)
8	294.9	0.1494	H-5→L(+83%)
9	282.7	0.0926	H→L+2(+75%) H-1→L+2(13%) H-5→L(+5%)
10	279.3	0.0864	H-3→L+1(+59%) H-2→L+1(+29%) H-3→L(+7%)

Table A.6: Transition assignments for the TD-DFT calculation of the UV-Vis spectrum of chlorophyll a with the M06-HF density functional and the MIDIY and DGDZVP basis sets

#	nm	(f)	Assignments
1	564.5	0.5252	H→L(+86%) H-1→L+1(9%)
2	409.0	1.1094	H-1→L(+85%) H-1→L+1(5%)
3	356.6	0.9154	H→L+1(+85%) H-1→L+1(+8%)
4	321.0	1.5282	H-1→L+1(+64%) H→L(+8%) H-1→L(+7%) H→L+1(7%)
5	318.5	0.0730	H-9→L+3(20%) H-10→L+3(13%) H-9→L(+7%) H-9→L+4(+5%) H-10→L(+5%)
6	284.5	0.0931	H-2→L(+45%) H-3→L(25%) H-3→L+1(+18%)
7	276.9	0.1515	H-3→L(+40%) H-2→L(+32%) H-2→L+1(+18%)
8	252.9	0.0946	H-5→L(+49%) H→L+3(+14%) H-5→L+1(+9%) H→L+2(7%)
9	244.6	0.0048	H→L+2(+80%) H→L+3(+9%)
10	239.0	0.0880	H→L+3(+32%) H-5→L(28%) H-1→L+2(+14%) H-8→L(+7%)