|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ID | eV (nm) exp | eV (nm) calc | Transition | f | % Contribution |
| 1 | 4.43 (280) | 2.65 (467) -1.78 2.82 (439) -1.61 2.85 (435) -1.58 2.86 (433) -1.57 2.93 (423) -1.5 2.95 (420) -1.48 3.04 (408) -1.39 3.09 (402) -1.34 3.09 (402) -1.34 3.12 (398) -1.31 3.16 (393) -1.27 3.16 (392) -1.27 3.17 (391) -1.26 3.24 (383) -1.19 3.26 (380) -1.17 3.32 (373) -1.11 3.35 (370) -1.08 3.36 (369) -1.06 3.38 (367) -1.05 3.38 (366) -1.04 3.49 (355) -0.94 3.52 (352) -0.91 3.55 (350) -0.88 3.56 (349) -0.87 3.57 (347) -0.86 3.59 (345) -0.83 3.6 (345) -0.83 3.61 (343) -0.82 3.63 (342) -0.8 3.64 (341) -0.79 3.64 (340) -0.79 3.65 (340) -0.78 3.66 (338) -0.77 3.7 (335) -0.73 3.7 (335) -0.73 3.73 (332) -0.7 3.75 (331) -0.68 3.76 (330) -0.67 3.76 (330) -0.67 3.77 (329) -0.65 3.81 (326) -0.62 3.82 (324) -0.61 3.83 (324) -0.6 3.86 (322) -0.57 3.88 (320) -0.55 3.88 (319) -0.55 3.9 (318) -0.53 3.91 (317) -0.52 3.95 (314) -0.48 3.96 (313) -0.47 3.97 (313) -0.46 3.99 (311) -0.44 4.0 (310) -0.43 4.0 (310) -0.43 4.01 (309) -0.42 4.02 (308) -0.41 4.03 (308) -0.4 4.03 (308) -0.4 4.03 (307) -0.4 4.04 (307) -0.39 4.05 (306) -0.38 4.06 (306) -0.37 4.06 (305) -0.36 4.07 (305) -0.36 4.09 (303) -0.34 4.09 (303) -0.33 4.1 (303) -0.33 4.1 (302) -0.33 4.11 (302) -0.32 4.11 (302) -0.32 4.13 (300) -0.3 4.16 (298) -0.27 4.17 (297) -0.26 4.22 (294) -0.21 4.22 (294) -0.21 4.22 (294) -0.21 4.23 (293) -0.2 4.24 (292) -0.19 4.25 (292) -0.18 4.25 (292) -0.18 4.27 (290) -0.16 4.29 (289) -0.14 4.29 (289) -0.14 4.3 (289) -0.13 4.3 (288) -0.13 4.31 (288) -0.12 4.34 (286) -0.09 4.36 (284) -0.06 4.37 (284) -0.06 4.39 (282) -0.04 4.39 (282) -0.04 4.41 (281) -0.02 4.41 (281) -0.02 4.42 (281) -0.01 4.43 (280) -0.0 4.43 (280) 0.0 4.45 (279) 0.02 4.47 (277) 0.04 4.48 (276) 0.06 4.49 (276) 0.06 4.49 (276) 0.06 4.51 (275) 0.08 4.51 (275) 0.09 4.52 (274) 0.09 4.52 (274) 0.1 4.53 (274) 0.1 4.54 (273) 0.11 4.54 (273) 0.11 4.56 (272) 0.14 4.57 (271) 0.14 4.58 (271) 0.15 4.58 (271) 0.15 4.59 (270) 0.16 4.6 (270) 0.17 4.61 (269) 0.18 4.63 (268) 0.2 4.64 (267) 0.21 4.66 (266) 0.23 4.66 (266) 0.23 4.67 (266) 0.24 4.68 (265) 0.25 4.68 (265) 0.25 4.69 (264) 0.26 4.7 (264) 0.27 4.71 (263) 0.29 4.72 (263) 0.29 4.72 (262) 0.3 4.73 (262) 0.3 4.74 (262) 0.31 4.75 (261) 0.32 4.75 (261) 0.33 4.76 (260) 0.33 4.77 (260) 0.34 4.77 (260) 0.34 4.77 (260) 0.34 4.79 (259) 0.36 4.79 (259) 0.36 4.8 (258) 0.37 4.81 (258) 0.38 4.81 (258) 0.38 4.82 (257) 0.39 4.82 (257) 0.39 4.82 (257) 0.39 4.83 (257) 0.4 4.83 (256) 0.41 4.84 (256) 0.41 4.84 (256) 0.41 4.85 (256) 0.42 4.85 (255) 0.42 4.88 (254) 0.45 4.89 (254) 0.46 4.89 (254) 0.46 4.89 (253) 0.46 4.91 (253) 0.48 4.92 (252) 0.49 4.92 (252) 0.49 4.93 (252) 0.5 4.95 (251) 0.52 4.95 (250) 0.52 4.95 (250) 0.53 4.97 (250) 0.54 4.98 (249) 0.55 4.98 (249) 0.55 4.99 (248) 0.57 5.0 (248) 0.57 5.02 (247) 0.59 5.02 (247) 0.59 5.03 (247) 0.6 5.04 (246) 0.61 5.04 (246) 0.61 5.05 (246) 0.62 5.05 (245) 0.62 5.08 (244) 0.65 5.08 (244) 0.65 5.09 (244) 0.66 5.09 (244) 0.66 5.11 (243) 0.68 5.11 (243) 0.68 5.12 (242) 0.69 5.13 (242) 0.7 5.14 (241) 0.71 5.14 (241) 0.71 5.15 (241) 0.72 5.16 (240) 0.73 5.16 (240) 0.73 5.16 (240) 0.73 5.17 (240) 0.74 5.18 (240) 0.75 5.18 (239) 0.75 5.19 (239) 0.76 5.19 (239) 0.76 5.2 (239) 0.77 5.2 (238) 0.77 5.21 (238) 0.78 5.23 (237) 0.8 5.23 (237) 0.8 5.23 (237) 0.8 5.24 (237) 0.81 5.24 (236) 0.82 5.25 (236) 0.83 | S\_0->S\_1 S\_0->S\_2 S\_0->S\_3 S\_0->S\_4 S\_0->S\_5 S\_0->S\_6 S\_0->S\_7 S\_0->S\_8 S\_0->S\_9 S\_0->S\_10 S\_0->S\_11 S\_0->S\_12 S\_0->S\_13 S\_0->S\_14 S\_0->S\_15 S\_0->S\_16 S\_0->S\_17 S\_0->S\_18 S\_0->S\_19 S\_0->S\_20 S\_0->S\_21 S\_0->S\_22 S\_0->S\_23 S\_0->S\_24 S\_0->S\_25 S\_0->S\_26 S\_0->S\_27 S\_0->S\_28 S\_0->S\_29 S\_0->S\_30 S\_0->S\_31 S\_0->S\_32 S\_0->S\_33 S\_0->S\_34 S\_0->S\_35 S\_0->S\_36 S\_0->S\_37 S\_0->S\_38 S\_0->S\_39 S\_0->S\_40 S\_0->S\_41 S\_0->S\_42 S\_0->S\_43 S\_0->S\_44 S\_0->S\_45 S\_0->S\_46 S\_0->S\_47 S\_0->S\_48 S\_0->S\_49 S\_0->S\_50 S\_0->S\_51 S\_0->S\_52 S\_0->S\_53 S\_0->S\_54 S\_0->S\_55 S\_0->S\_56 S\_0->S\_57 S\_0->S\_58 S\_0->S\_59 S\_0->S\_60 S\_0->S\_61 S\_0->S\_62 S\_0->S\_63 S\_0->S\_64 S\_0->S\_65 S\_0->S\_66 S\_0->S\_67 S\_0->S\_68 S\_0->S\_69 S\_0->S\_70 S\_0->S\_71 S\_0->S\_72 S\_0->S\_73 S\_0->S\_74 S\_0->S\_75 S\_0->S\_76 S\_0->S\_77 S\_0->S\_78 S\_0->S\_79 S\_0->S\_80 S\_0->S\_81 S\_0->S\_82 S\_0->S\_83 S\_0->S\_84 S\_0->S\_85 S\_0->S\_86 S\_0->S\_87 S\_0->S\_88 S\_0->S\_89 S\_0->S\_90 S\_0->S\_91 S\_0->S\_92 S\_0->S\_93 S\_0->S\_94 S\_0->S\_95 S\_0->S\_96 S\_0->S\_97 S\_0->S\_98 S\_0->S\_99 S\_0->S\_100 S\_0->S\_101 S\_0->S\_102 S\_0->S\_103 S\_0->S\_104 S\_0->S\_105 S\_0->S\_106 S\_0->S\_107 S\_0->S\_108 S\_0->S\_109 S\_0->S\_110 S\_0->S\_111 S\_0->S\_112 S\_0->S\_113 S\_0->S\_114 S\_0->S\_115 S\_0->S\_116 S\_0->S\_117 S\_0->S\_118 S\_0->S\_119 S\_0->S\_120 S\_0->S\_121 S\_0->S\_122 S\_0->S\_123 S\_0->S\_124 S\_0->S\_125 S\_0->S\_126 S\_0->S\_127 S\_0->S\_128 S\_0->S\_129 S\_0->S\_130 S\_0->S\_131 S\_0->S\_132 S\_0->S\_133 S\_0->S\_134 S\_0->S\_135 S\_0->S\_136 S\_0->S\_137 S\_0->S\_138 S\_0->S\_139 S\_0->S\_140 S\_0->S\_141 S\_0->S\_142 S\_0->S\_143 S\_0->S\_144 S\_0->S\_145 S\_0->S\_146 S\_0->S\_147 S\_0->S\_148 S\_0->S\_149 S\_0->S\_150 S\_0->S\_151 S\_0->S\_152 S\_0->S\_153 S\_0->S\_154 S\_0->S\_155 S\_0->S\_156 S\_0->S\_157 S\_0->S\_158 S\_0->S\_159 S\_0->S\_160 S\_0->S\_161 S\_0->S\_162 S\_0->S\_163 S\_0->S\_164 S\_0->S\_165 S\_0->S\_166 S\_0->S\_167 S\_0->S\_168 S\_0->S\_169 S\_0->S\_170 S\_0->S\_171 S\_0->S\_172 S\_0->S\_173 S\_0->S\_174 S\_0->S\_175 S\_0->S\_176 S\_0->S\_177 S\_0->S\_178 S\_0->S\_179 S\_0->S\_180 S\_0->S\_181 S\_0->S\_182 S\_0->S\_183 S\_0->S\_184 S\_0->S\_185 S\_0->S\_186 S\_0->S\_187 S\_0->S\_188 S\_0->S\_189 S\_0->S\_190 S\_0->S\_191 S\_0->S\_192 S\_0->S\_193 S\_0->S\_194 S\_0->S\_195 S\_0->S\_196 S\_0->S\_197 S\_0->S\_198 S\_0->S\_199 S\_0->S\_200 | 0.0002 0.0076 0.0004 0.0032 0.0047 0.0021 0.0000 0.0000 0.0002 0.0008 0.0008 0.0006 0.0002 0.0133 0.0019 0.0020 0.0006 0.0000 0.0003 0.0006 0.0001 0.0003 0.0043 0.0041 0.0145 0.0132 0.0002 0.0021 0.0006 0.0025 0.0005 0.0043 0.0005 0.0006 0.0005 0.0004 0.0030 0.0099 0.0044 0.0013 0.0017 0.0097 0.0007 0.0033 0.0041 0.0025 0.0013 0.0003 0.0005 0.0014 0.0020 0.0034 0.0067 0.0168 0.0198 0.0043 0.0026 0.0178 0.0137 0.0070 0.0013 0.0070 0.0100 0.0007 0.0016 0.0009 0.0273 0.0037 0.0111 0.0010 0.0001 0.0004 0.0001 0.0006 0.0029 0.0057 0.0016 0.0005 0.0041 0.0021 0.0002 0.0015 0.0004 0.0007 0.0011 0.0002 0.0115 0.0010 0.0034 0.0012 0.0228 0.0006 0.0012 0.0001 0.0001 0.0004 0.0000 0.0091 0.0004 0.0008 0.0016 0.0008 0.0004 0.0027 0.0008 0.0016 0.0124 0.0048 0.0059 0.0030 0.0206 0.0000 0.0118 0.0017 0.0095 0.0053 0.0065 0.1068 0.0340 0.0074 0.0002 0.0003 0.0005 0.0084 0.0038 0.1045 0.0163 0.0339 0.0013 0.0030 0.0010 0.0417 0.0070 0.0089 0.0017 0.0318 0.1968 0.0111 0.0293 0.0188 0.0012 0.0113 0.0142 0.1001 0.0589 0.0016 0.0027 0.0012 0.0027 0.0120 0.0021 0.0076 0.0022 0.0031 0.0240 0.0049 0.0211 0.0010 0.0057 0.0237 0.0574 0.0114 0.0003 0.0020 0.0190 0.0019 0.0112 0.0012 0.0007 0.0008 0.0287 0.1933 0.0053 0.0014 0.0516 0.0045 0.0001 0.0148 0.0011 0.0012 0.0011 0.0015 0.0004 0.0061 0.0032 0.0115 0.0983 0.0024 0.0072 0.0006 0.0028 0.0006 0.0190 0.0011 0.0085 0.0210 0.0021 0.0153 0.0005 0.0042 | 310->312 (39), 311->312 (46) 301->312 (37), 305->312 (16), 309->312 (21) 310->316 (24), 311->316 (50) 310->313 (25), 311->313 (45) 301->312 (22), 309->312 (48), 310->312 (15) 310->313 (24), 311->312 (22), 311->313 (18) 304->315 (45), 308->315 (20) 310->317 (23), 311->317 (28) 310->312 (20), 311->312 (25), 311->313 (17) 306->312 (36), 308->312 (24), 308->313 (16) 309->319 (35), 310->319 (23) 307->312 (72) 306->312 (28), 308->313 (47) 302->314 (43), 303->314 (23) 306->313 (54) 309->313 (57) 308->312 (49), 308->313 (24) 310->315 (19), 311->315 (47) 310->319 (20), 311->319 (65) 305->312 (66) 310->314 (17), 311->314 (67) 300->317 (38) 307->313 (16), 309->319 (20), 310->319 (20) 307->313 (39) 308->316 (79) 297->312 (67) No trans. over 15% contrib. 296->314 (15), 298->314 (21) 310->314 (23) 306->316 (25) 310->317 (19), 311->317 (24) 303->313 (36) 310->315 (34) 302->313 (44) 304->313 (27), 308->314 (35) 304->313 (30), 308->314 (35) 308->317 (36), 308->319 (18) 292->312 (23) 308->319 (60) 300->312 (28) 300->312 (19), 305->313 (23) 308->315 (26), 308->317 (33) 310->318 (36), 311->318 (40) 303->312 (22) 289->313 (20) 306->315 (15), 306->317 (21) 305->319 (51) 309->314 (66) 309->315 (65) 299->313 (44) 301->318 (33), 305->318 (19), 309->318 (15) 299->313 (17), 306->314 (33) 255->313 (21) 307->319 (41) 299->315 (20), 307->319 (16) 299->315 (18), 310->320 (20), 311->320 (24) 299->315 (16) 260->314 (30) 249->312 (32) 306->319 (34) 304->312 (24), 304->314 (22) 275->316 (34) 277->319 (31), 306->319 (21) 304->312 (39), 304->314 (19) 310->318 (15), 310->320 (15), 311->318 (17), 311->320 (19) 298->313 (16), 300->313 (25) 273->317 (53) 300->313 (18) 262->315 (64) 301->318 (19), 309->318 (38) 298->313 (42) 310->316 (34), 311->316 (25) 302->312 (55), 303->312 (24) 296->313 (17) 302->315 (28), 303->315 (16) 304->317 (29), 307->314 (15) 304->317 (34), 307->314 (42) 309->317 (33) 302->316 (16), 308->318 (17) 302->316 (30) 307->315 (62) 304->316 (59) 306->318 (24), 308->320 (16) 306->318 (17) 307->318 (63) 301->313 (51) No trans. over 15% contrib. 295->313 (23) 299->314 (18) No trans. over 15% contrib. 303->317 (16) 306->320 (29) 289->312 (28), 295->312 (16) 310->326 (19), 311->326 (39) 309->316 (71) 299->312 (65) 306->320 (19), 310->320 (26), 311->318 (15) 307->317 (15) 269->319 (30) 303->314 (25) 243->312 (27) 305->314 (25) 305->314 (23), 305->318 (19) 265->316 (33) 305->315 (15), 309->320 (15) 302->321 (29), 303->321 (17) 303->319 (17) 303->319 (20) No trans. over 15% contrib. 305->315 (18) 299->317 (39) No trans. over 15% contrib. 297->318 (16) 298->312 (71) 266->317 (15), 307->317 (18) 298->321 (21) 297->313 (33) 299->316 (29) 291->313 (23) 300->329 (19) 308->318 (48), 308->320 (34) 309->327 (24), 310->327 (36), 311->327 (18) 294->313 (23) 304->324 (18) 298->315 (18), 304->324 (17) 285->315 (38) No trans. over 15% contrib. No trans. over 15% contrib. 300->315 (16) 296->312 (19), 307->320 (15) 296->312 (20) 248->314 (21), 295->314 (15) 252->315 (16) No trans. over 15% contrib. 307->316 (65) No trans. over 15% contrib. 293->319 (36) 295->314 (22) No trans. over 15% contrib. 309->327 (25), 311->327 (26) 304->320 (17) 304->320 (26) No trans. over 15% contrib. No trans. over 15% contrib. 293->312 (27) 300->314 (20) 300->314 (35) 292->318 (24) 291->312 (28) 308->326 (31) 311->322 (19) 298->316 (33), 299->316 (15), 308->326 (25) 300->318 (42) 296->315 (52) No trans. over 15% contrib. 288->312 (19), 293->312 (22) 310->327 (29), 311->327 (16) 310->321 (18), 311->321 (31) 300->319 (17) No trans. over 15% contrib. No trans. over 15% contrib. 295->312 (38) 301->314 (78) 310->323 (15) 311->330 (20) 305->320 (22) 276->312 (15) 296->316 (17) 299->320 (30) 304->319 (68) 305->317 (29) No trans. over 15% contrib. 305->316 (21) 305->316 (54) 292->313 (37) 295->317 (24) 301->315 (84) 293->313 (68) 311->323 (18) 308->321 (40) No trans. over 15% contrib. 302->317 (30) 303->318 (18) 309->322 (52) 296->316 (15) 296->316 (17) 274->315 (27) No trans. over 15% contrib. 304->328 (21) 308->327 (23) 308->327 (30) 302->319 (49), 303->319 (24) 284->317 (31) 311->324 (22) 305->327 (15) No trans. over 15% contrib. 287->312 (38) 310->321 (19) 307->327 (43) No trans. over 15% contrib. |