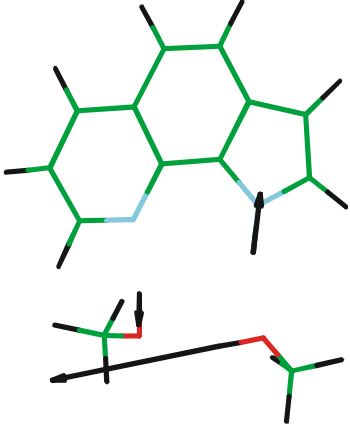
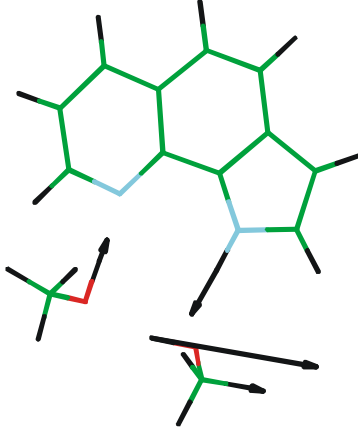
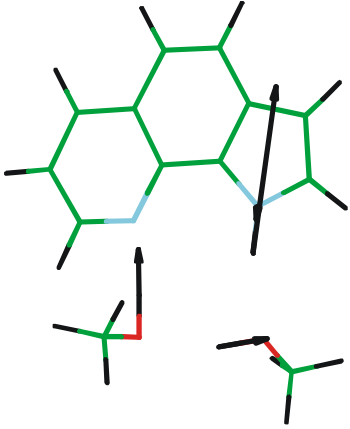
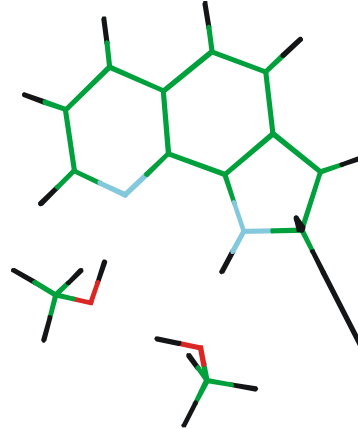
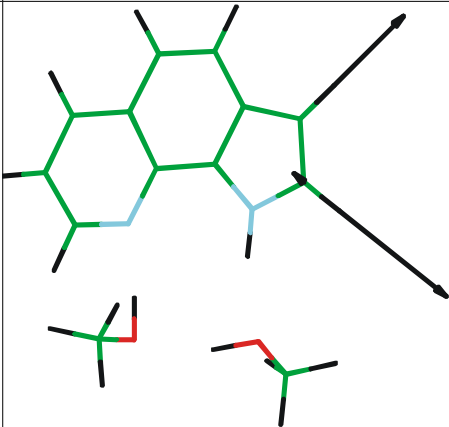
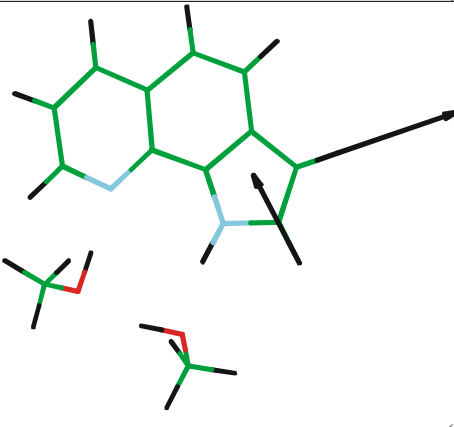
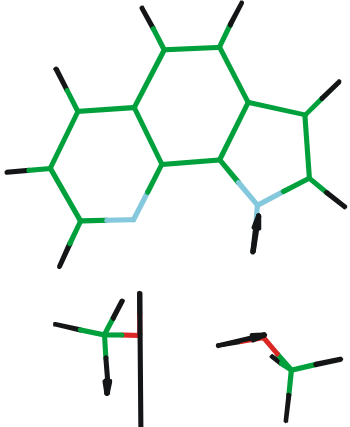
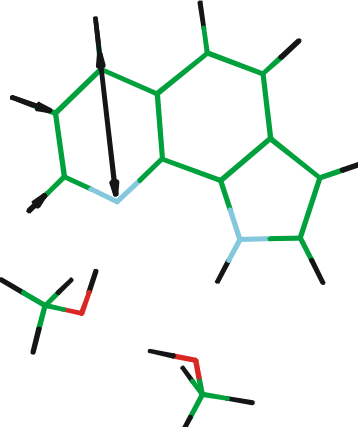
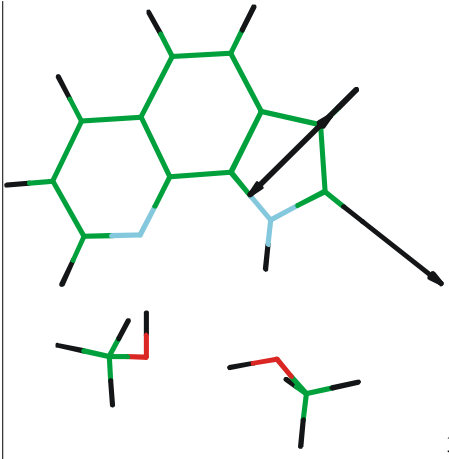
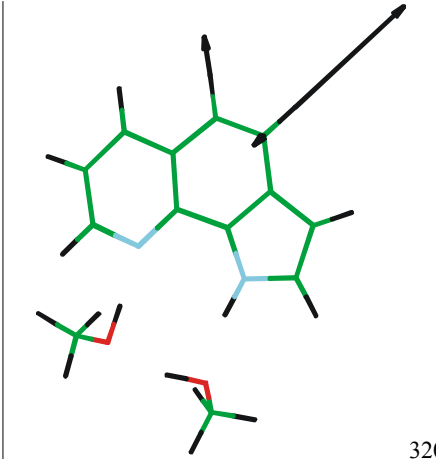
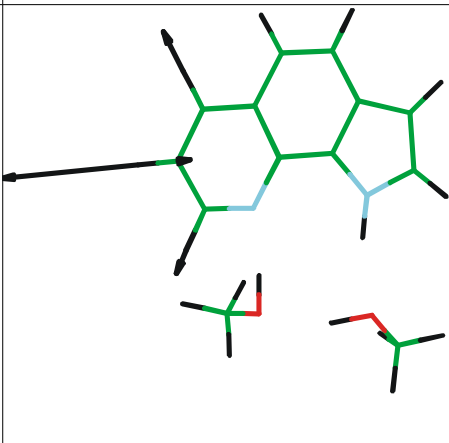
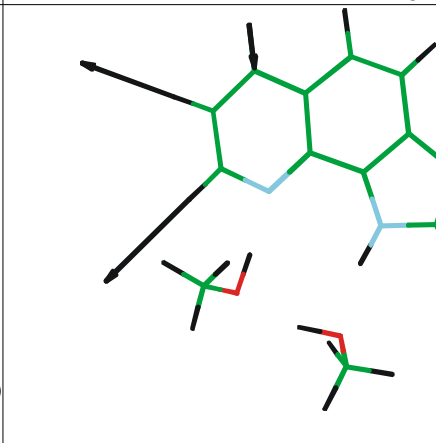
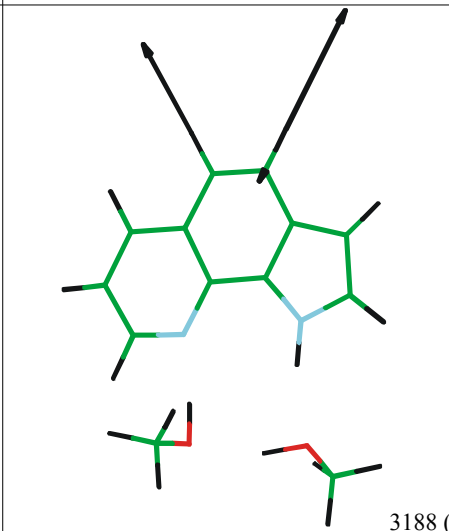
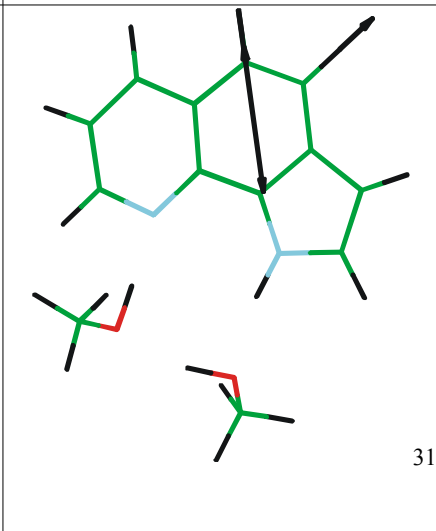
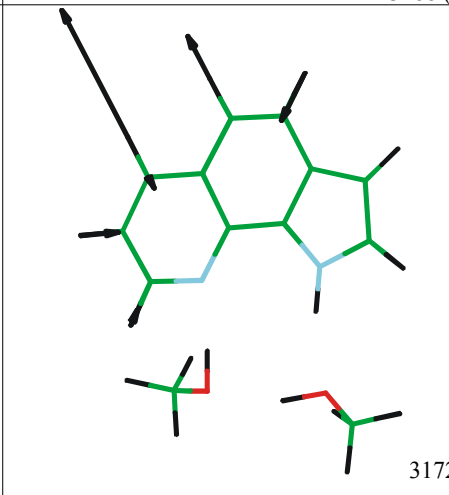
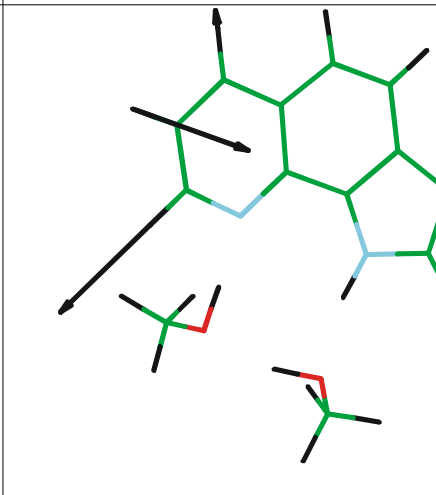
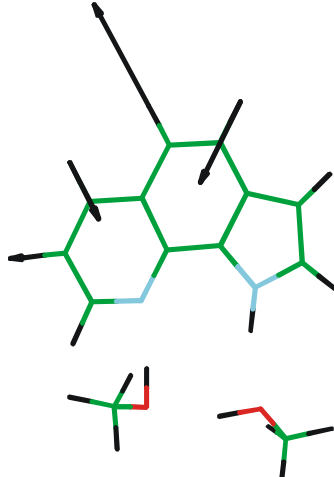
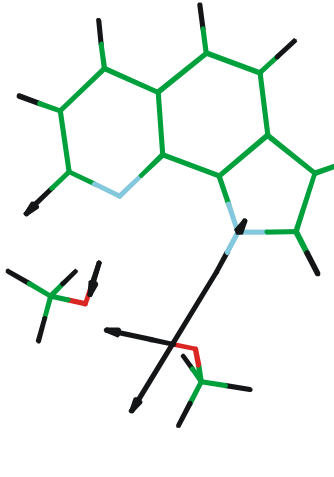
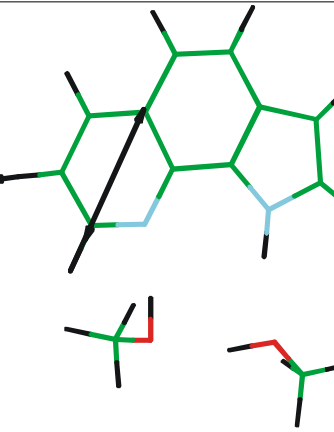
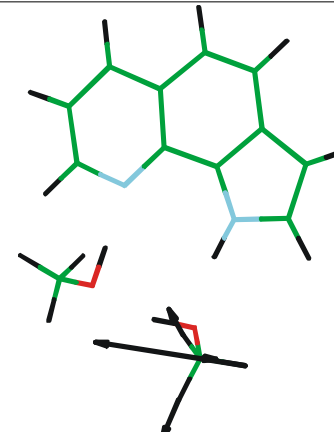
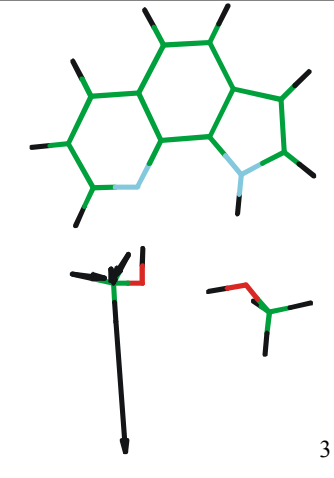
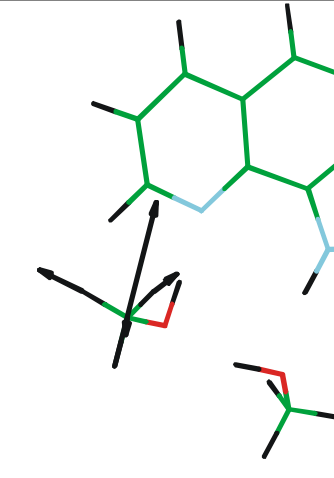
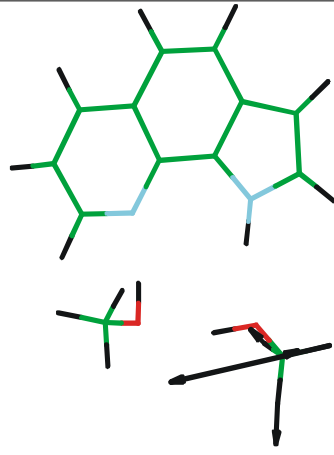
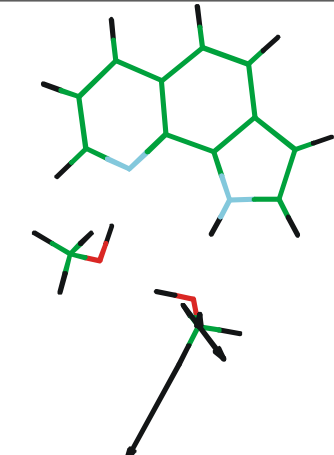
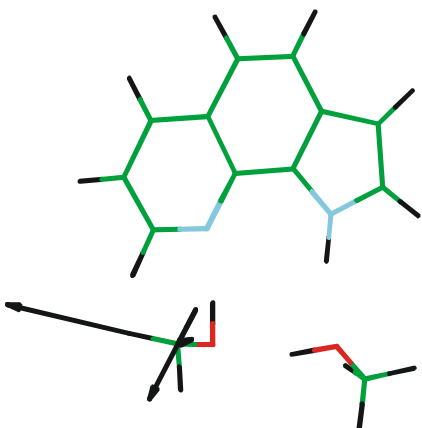
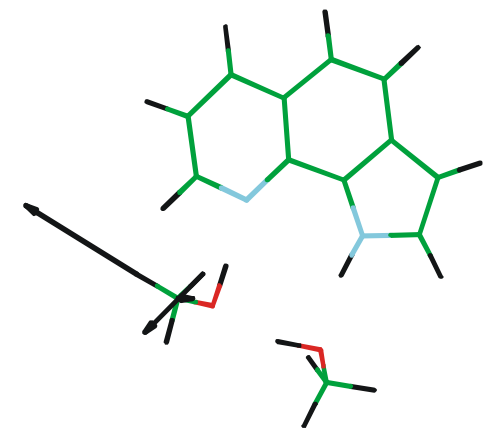
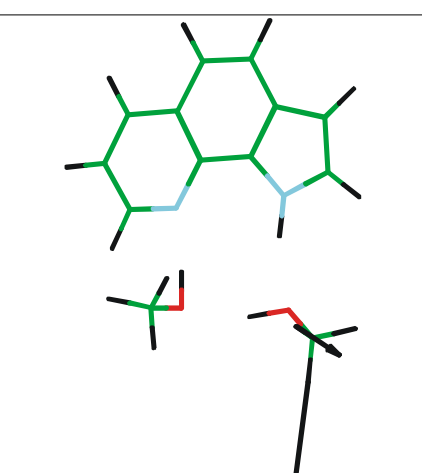
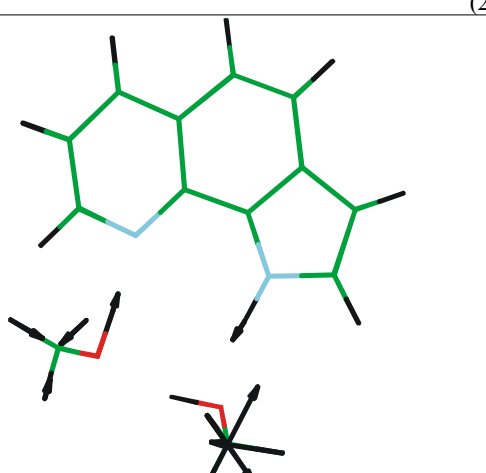
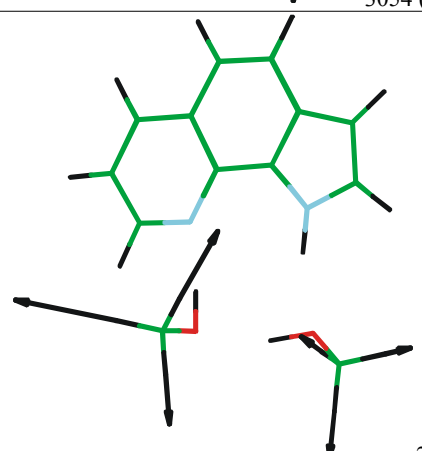
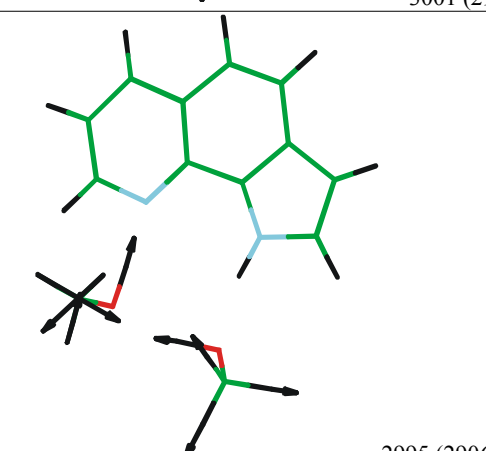
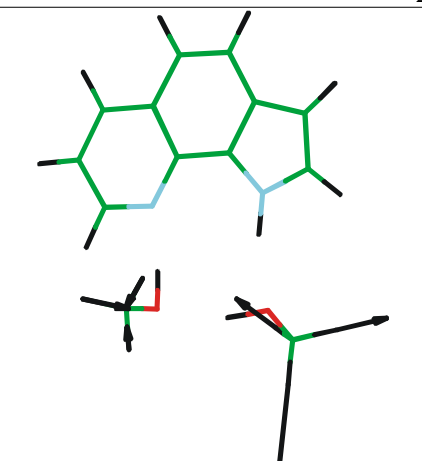
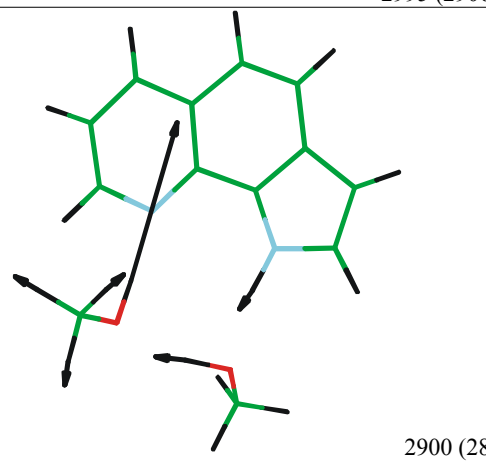


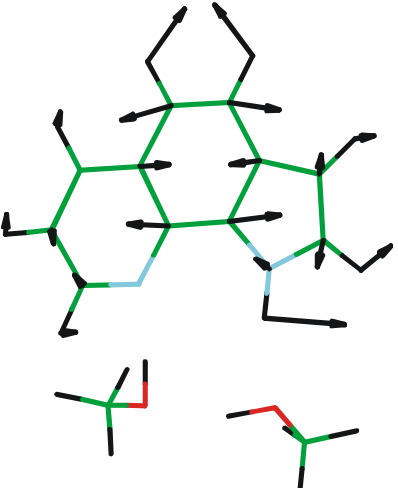
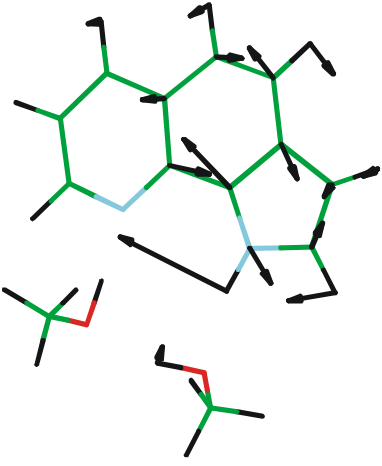
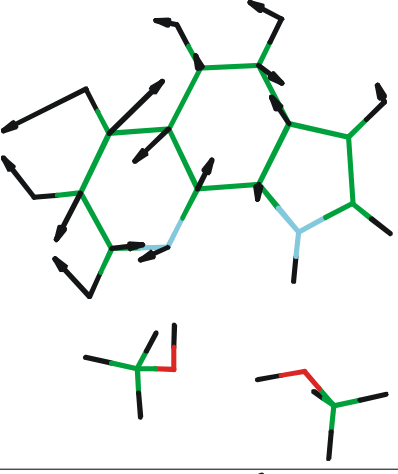
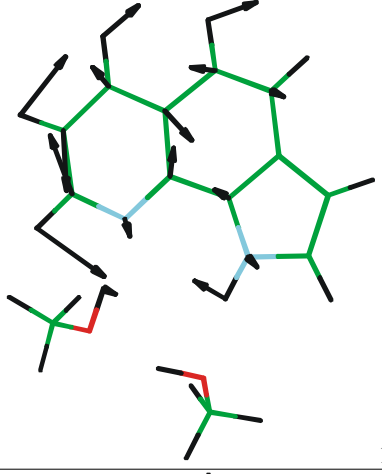
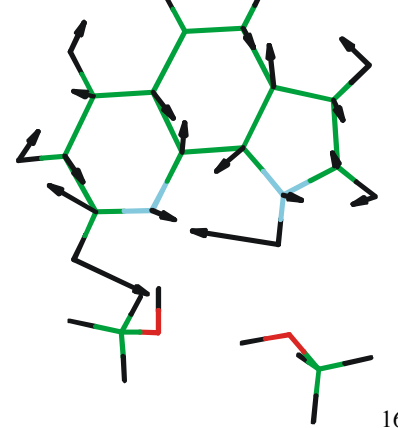
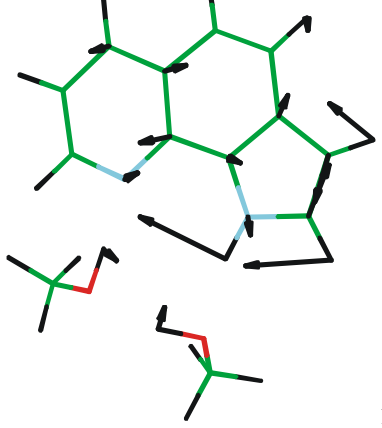
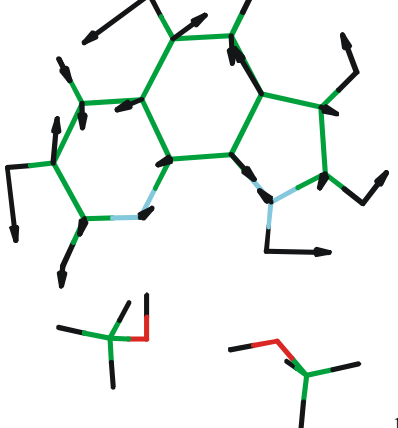
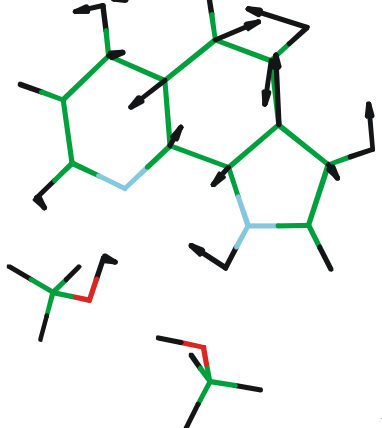
Table S1. Vibrational normal modes of the 1:2 complex of PQ with methanol in the S_0 and S_1 states, calculated at B3LYP/cc-pVDZ level. The normal frequencies are given in cm^{-1} . The frequencies, scaled by 0.9704, are shown in parenthesis.

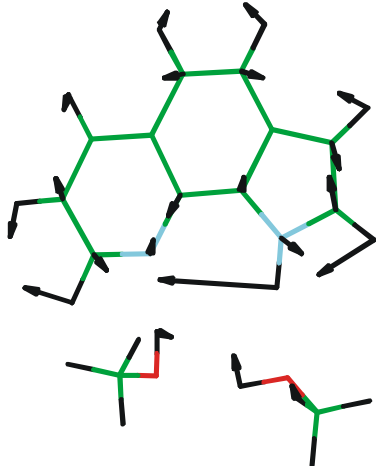
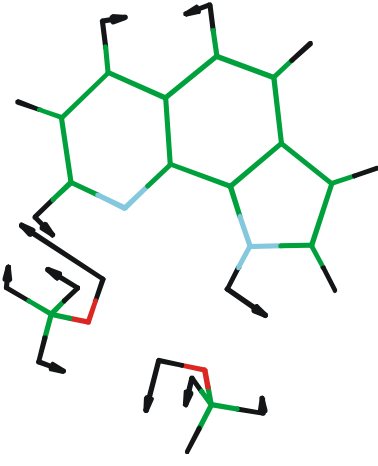
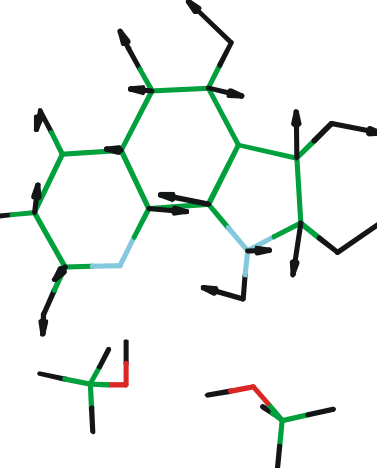
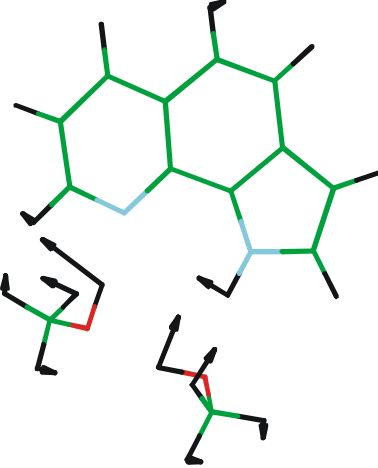
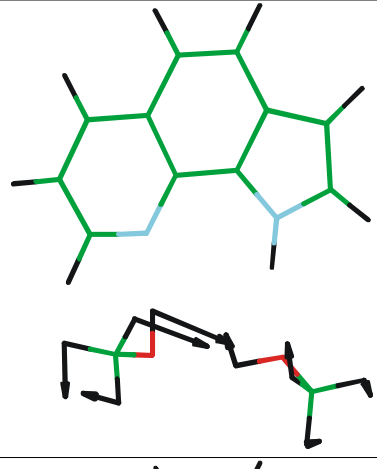
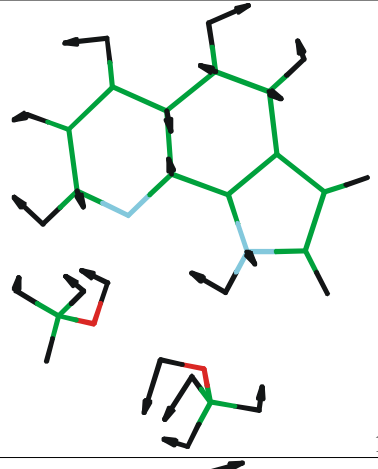
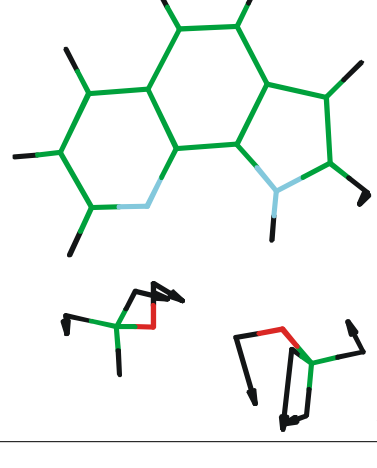
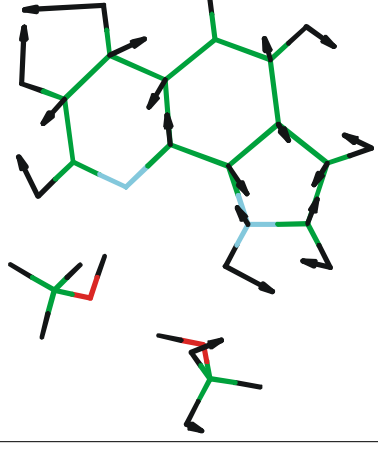
	S_0	S_1
ν_1	 3429 (3328)	 3281 (3183)
ν_2	 3349 (3250)	 3273 (3176)
ν_3	 3262 (3166)	 3253 (3157)
ν_4	 3249 (3153)	 3214 (3119)

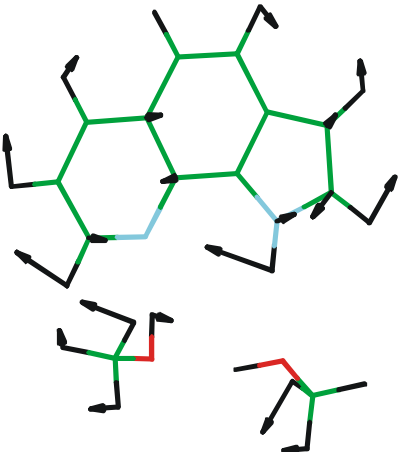
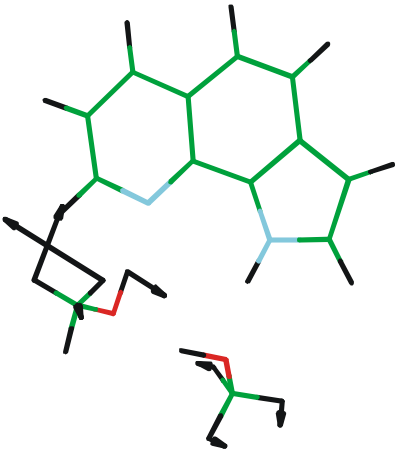
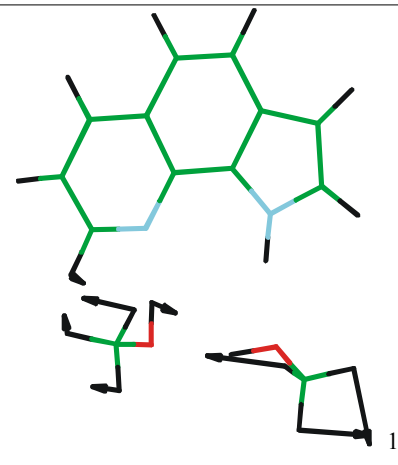
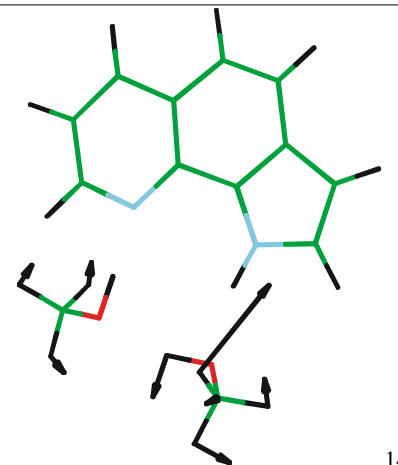
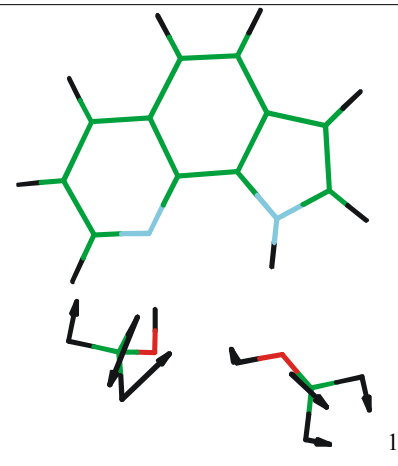
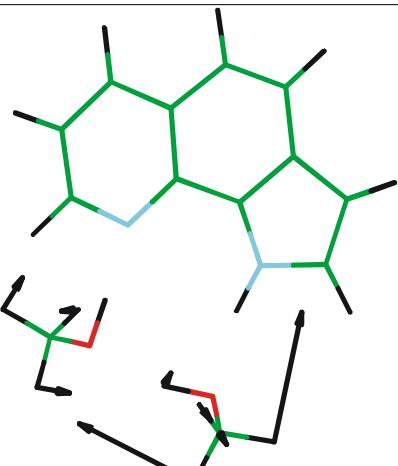
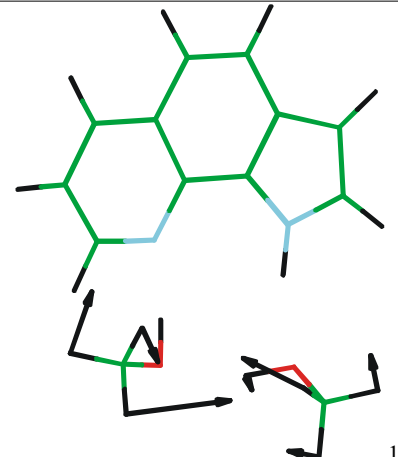
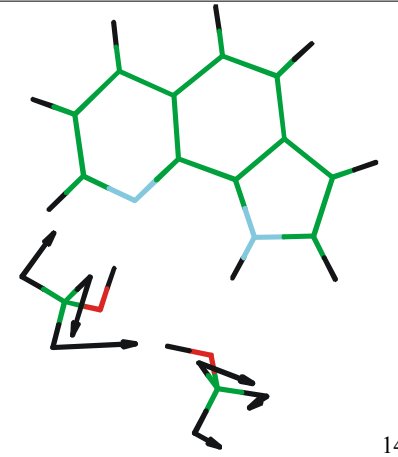
V ₅	 3242 (3146)	 3206 (3111)
V ₆	 3203 (3109)	 3186 (3091)
V ₇	 3188 (3093)	 3171 (3077)
V ₈	 3172 (3078)	 3166 (3073)

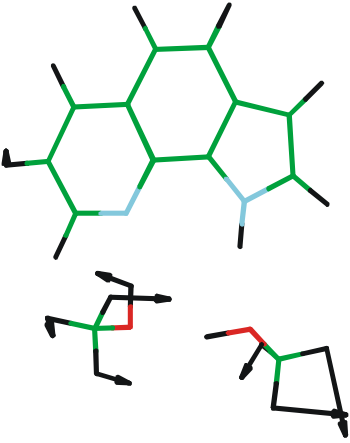
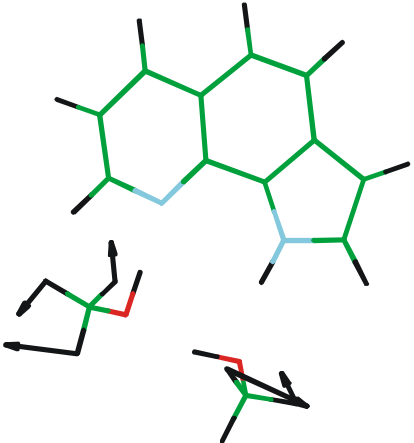
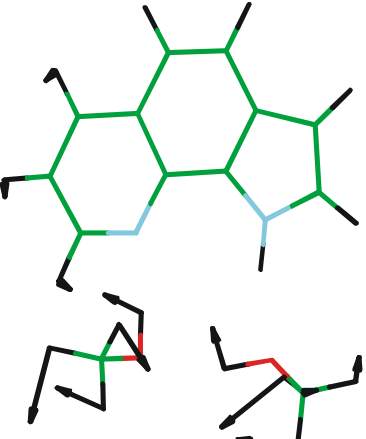
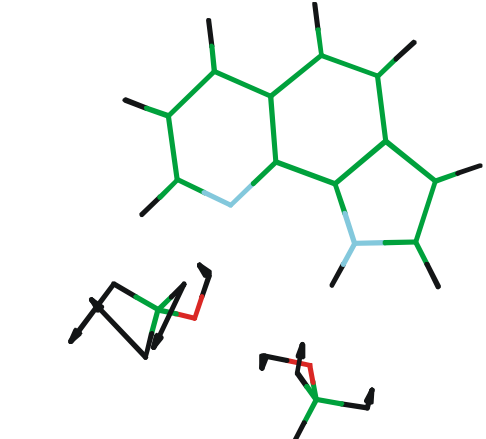
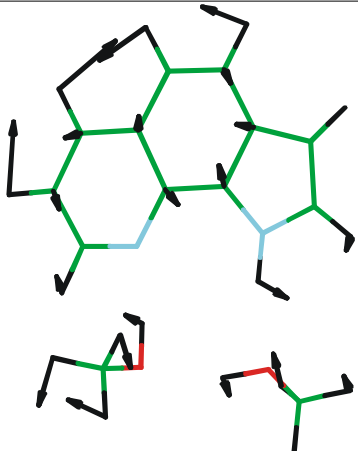
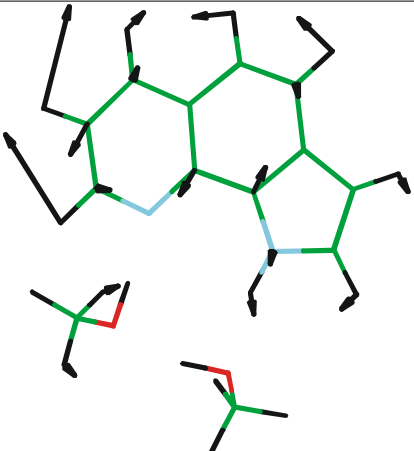
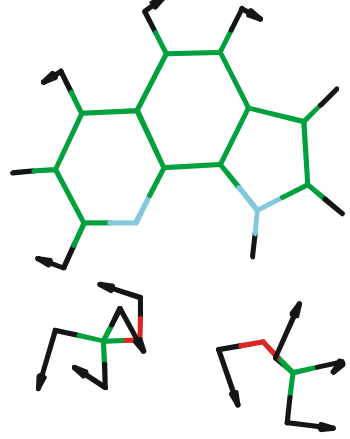
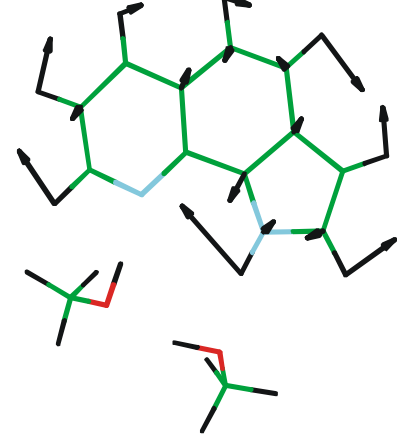
V ₉	 3169 (3075)	 3133 (3040)
V ₁₀	 3151 (3058)	 3103 (3011)
V ₁₁	 3109 (3017)	 3097 (3006)
V ₁₂	 3105 (3013)	 3064 (2973)

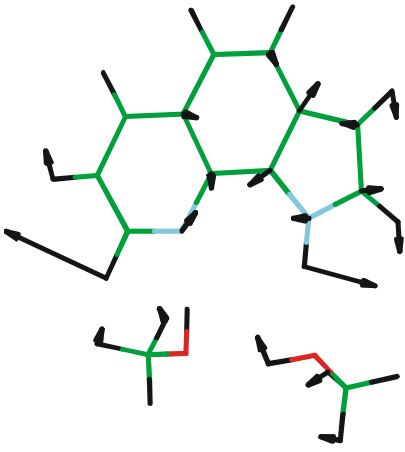
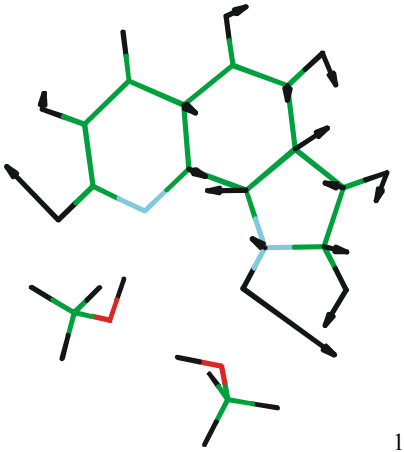
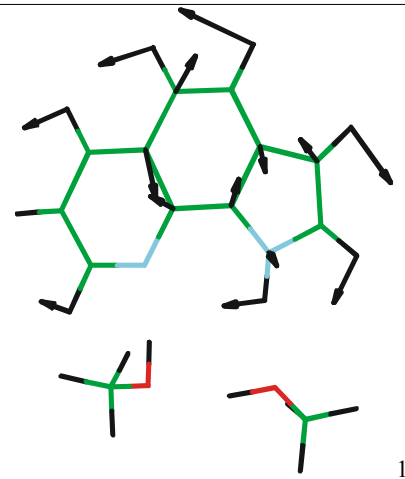
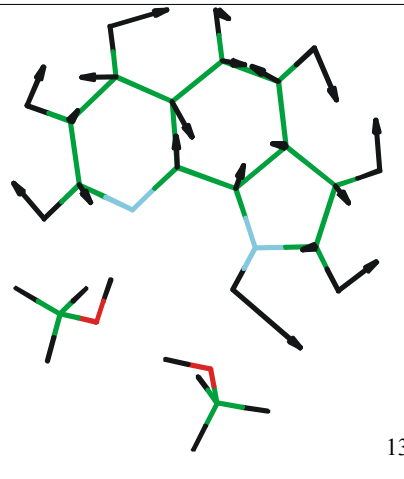
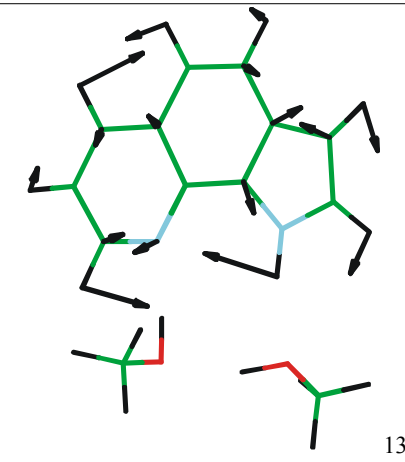
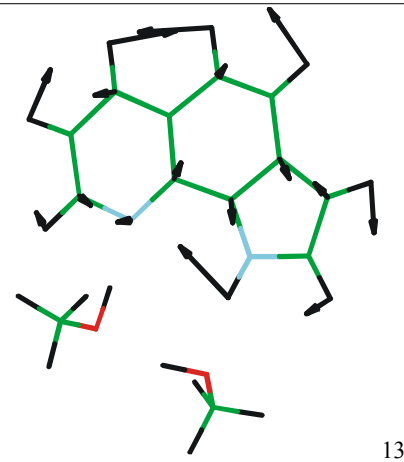
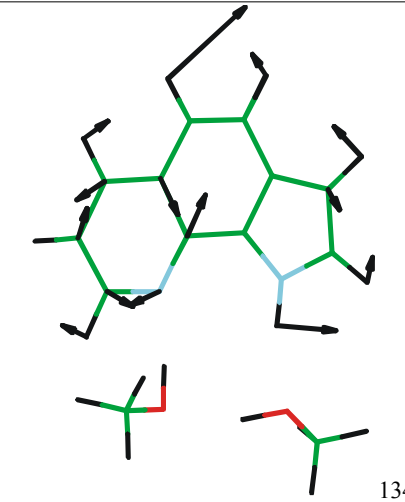
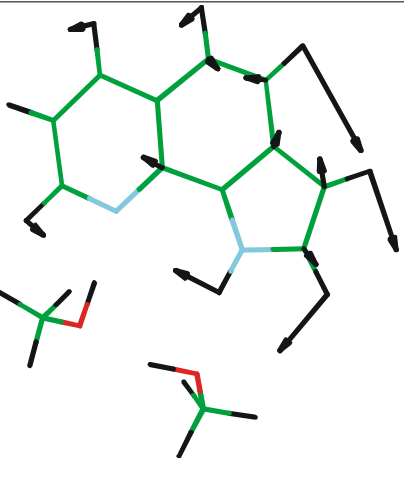
V ₁₃	 3056 (2966)	 3049 (2958)
V ₁₄	 3054 (2963)	 3001 (2912)
V ₁₅	 2997 (2908)	 2995 (2906)
V ₁₆	 2995 (2906)	 2900 (2814)

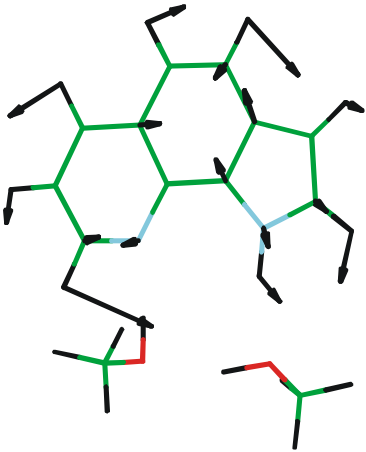
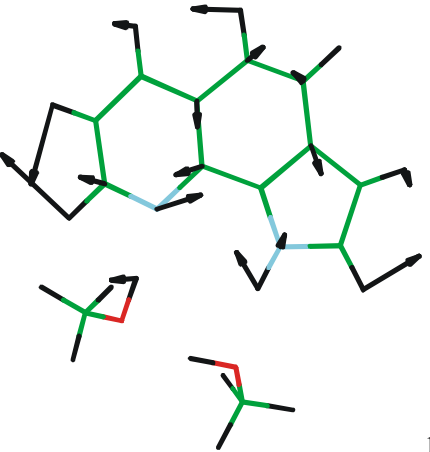
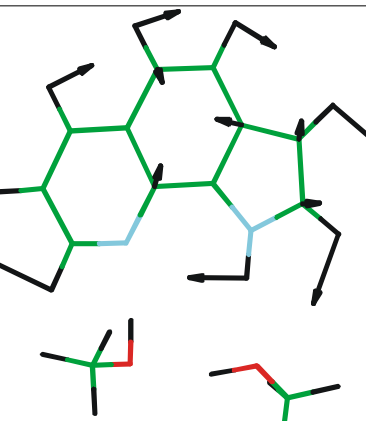
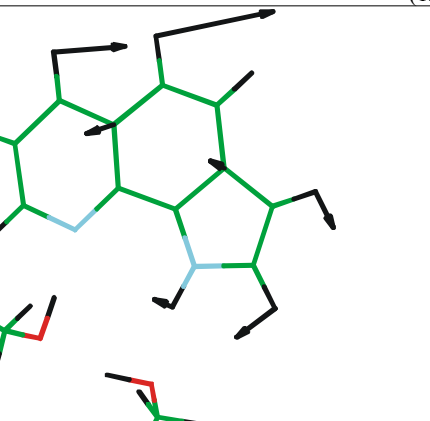
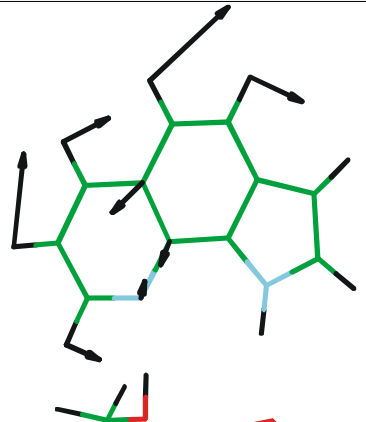
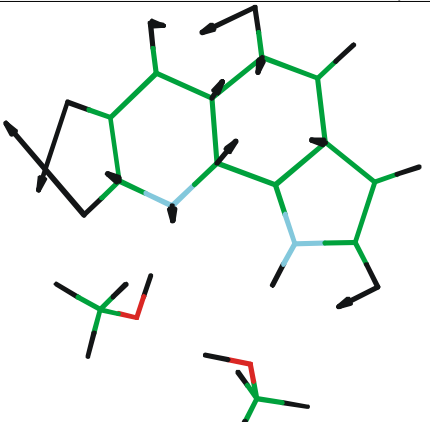
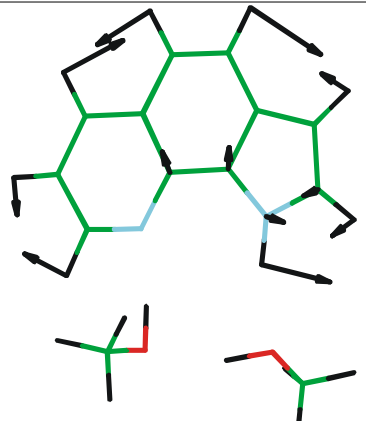
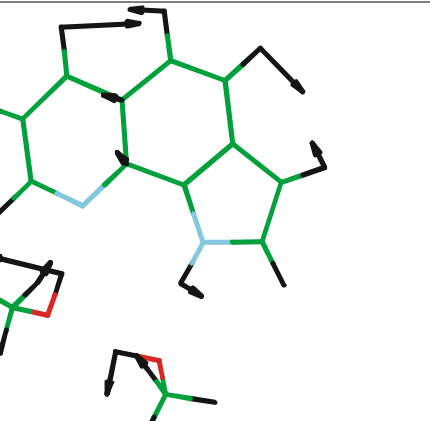
V ₁₇	 1657 (1608)	 1657 (1608)
V ₁₈	 1640 (1592)	 1591 (1544)
V ₁₉	 1605 (1557)	 1572 (1525)
V ₂₀	 1566 (1520)	 1565 (1518)

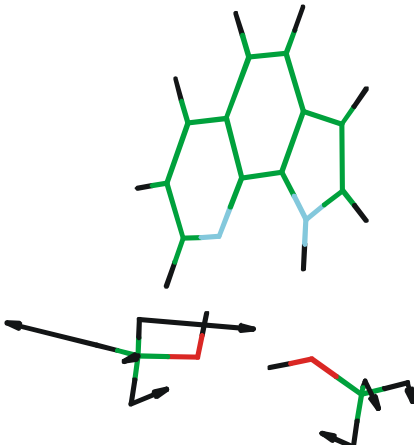
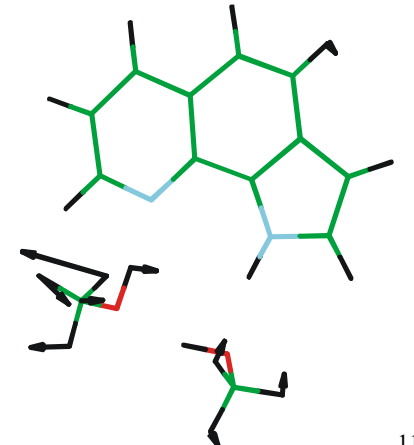
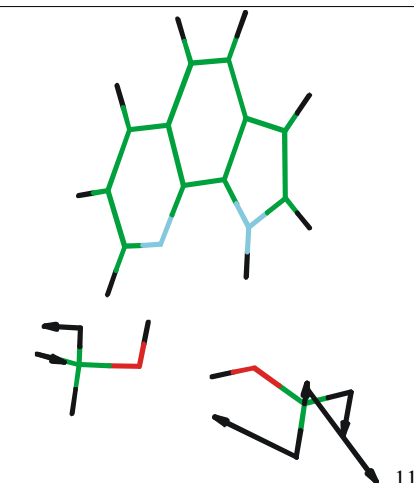
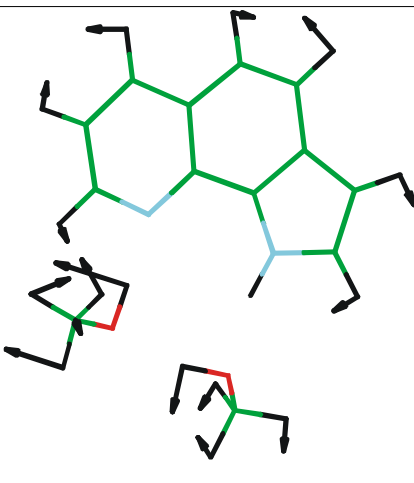
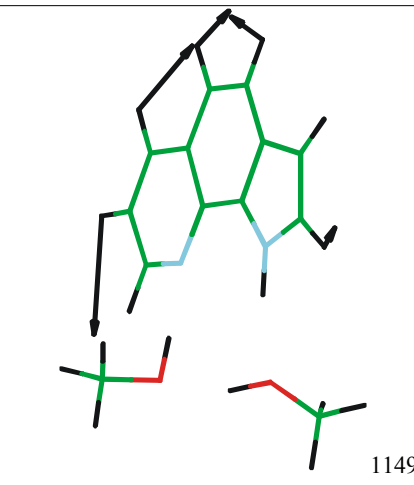
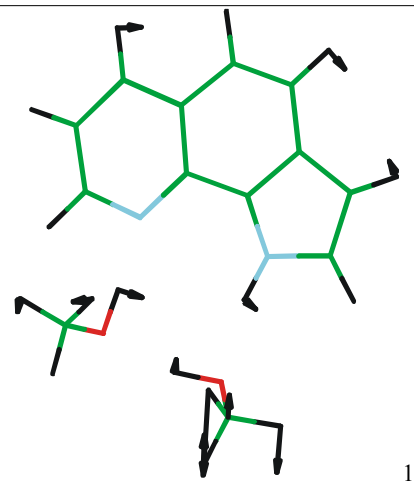
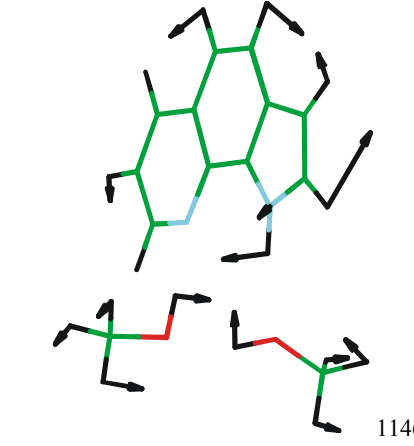
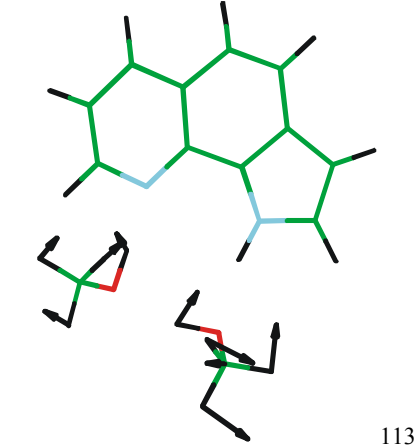
V ₂₁	 1538 (1492)	 1518 (1473)
V ₂₂	 1521 (1476)	 1508 (1463)
V ₂₃	 1494 (1449)	 1498 (1454)
V ₂₄	 1492 (1447)	 1479 (1435)

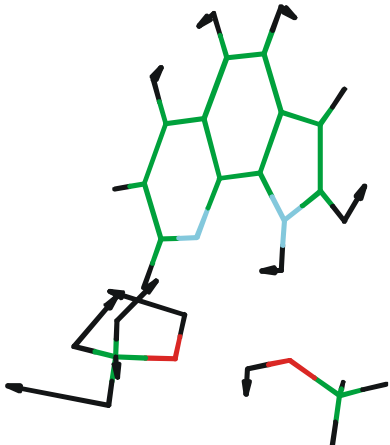
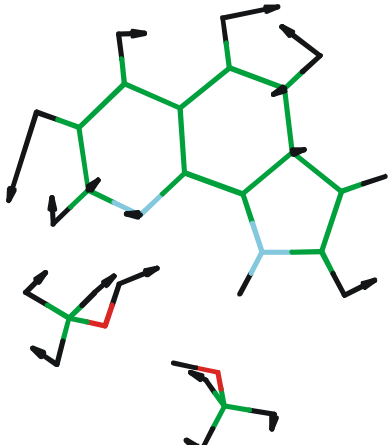
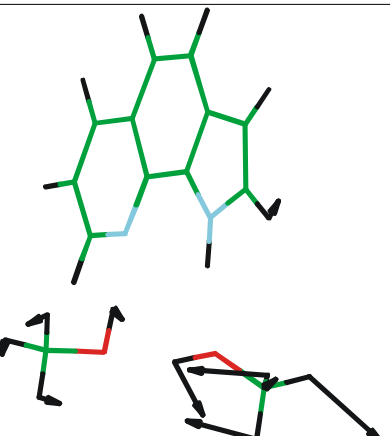
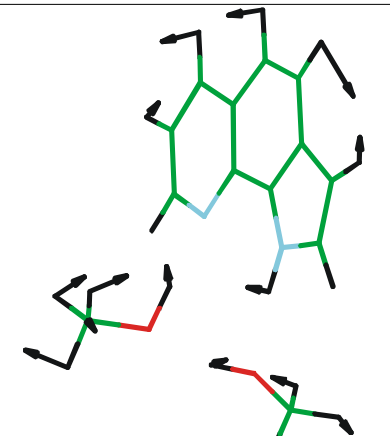
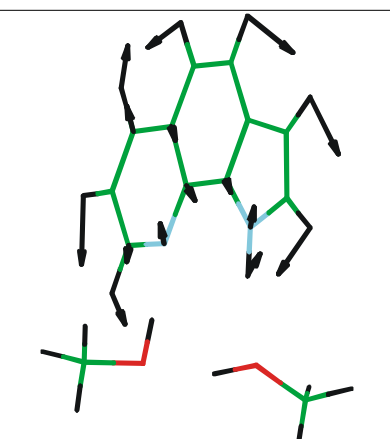
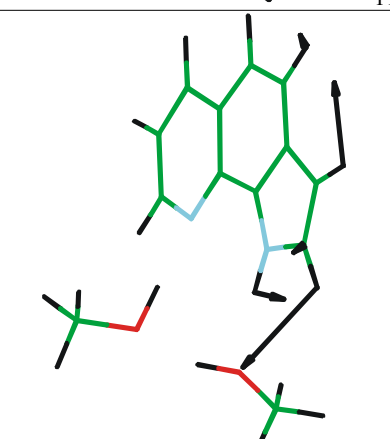
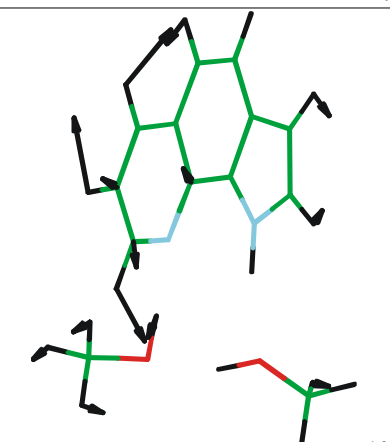
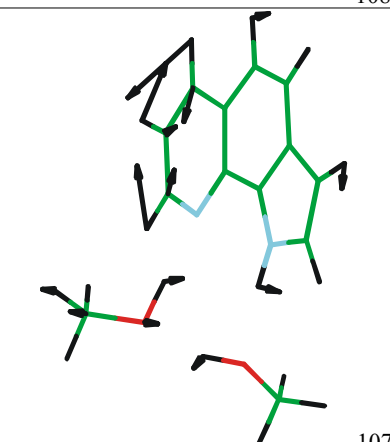
V ₂₅	 1469 (1426)	 1466 (1422)
V ₂₆	 1461 (1417)	 1462 (1419)
V ₂₇	 1459 (1416)	 1459 (1416)
V ₂₈	 1459 (1416)	 1458 (1415)

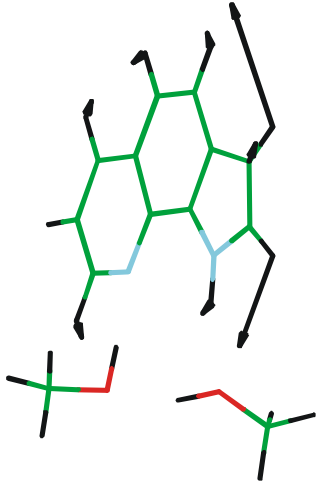
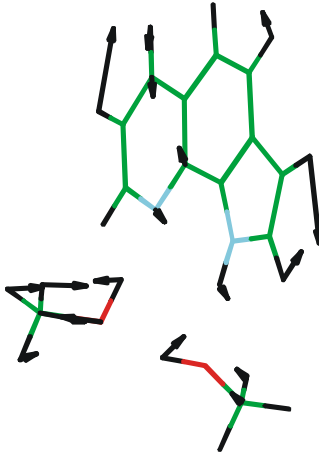
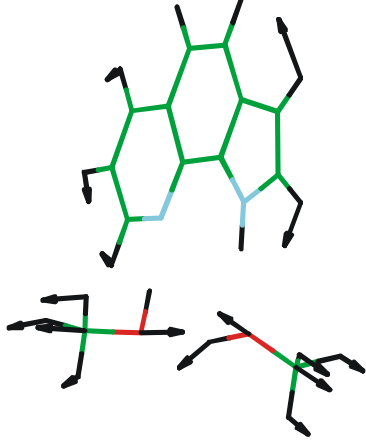
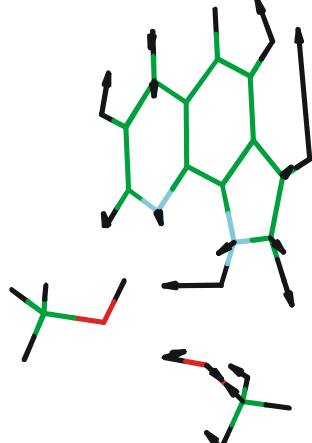
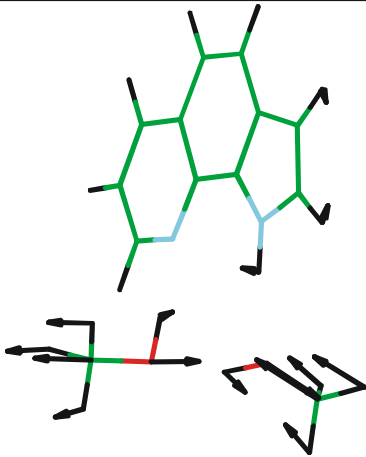
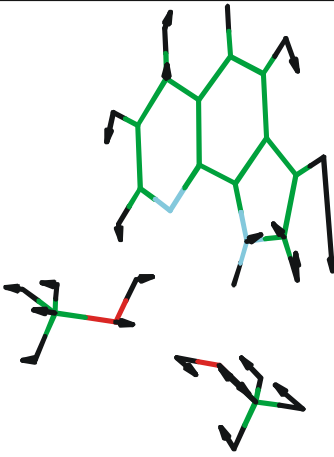
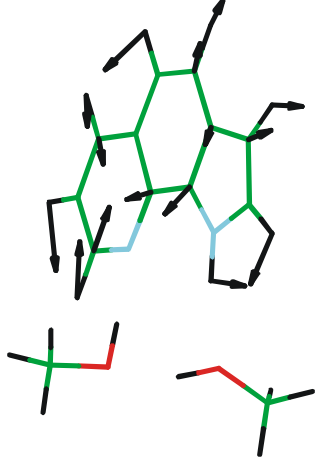
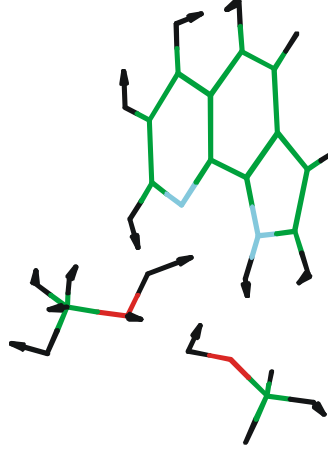
V ₂₉	 1457 (1414)	 1458 (1415)
V ₃₀	 1453 (1410)	 1453 (1410)
V ₃₁	 1450 (1407)	 1440 (1397)
V ₃₂	 1447 (1404)	 1412 (1370)

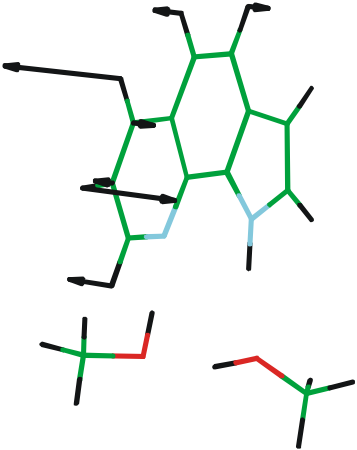
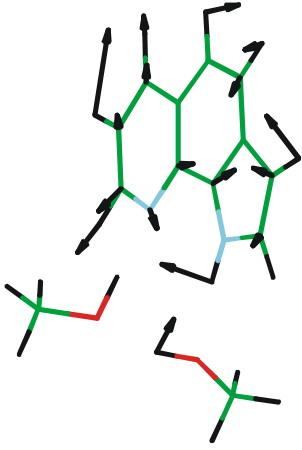
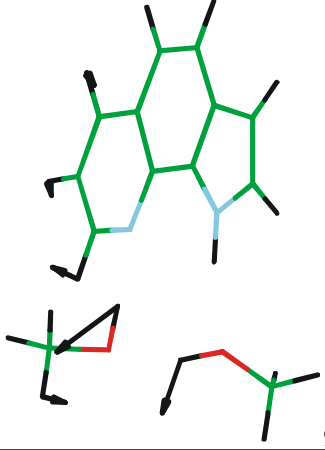
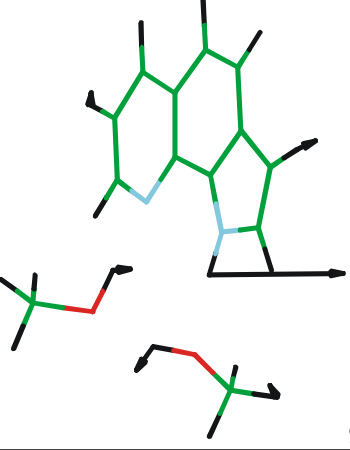
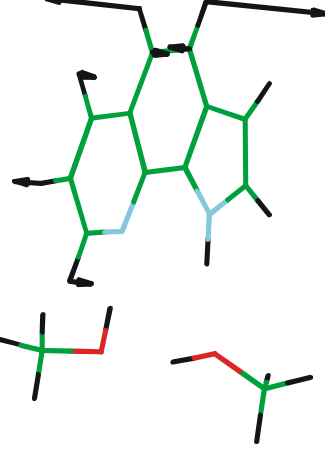
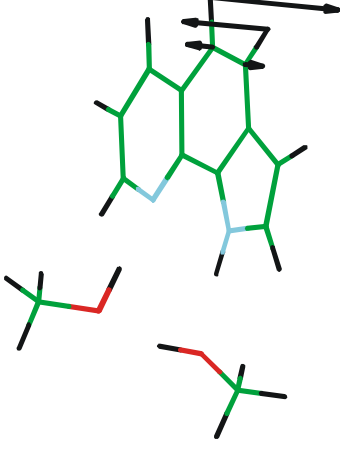
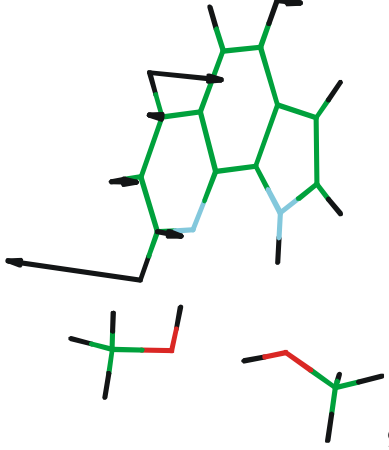
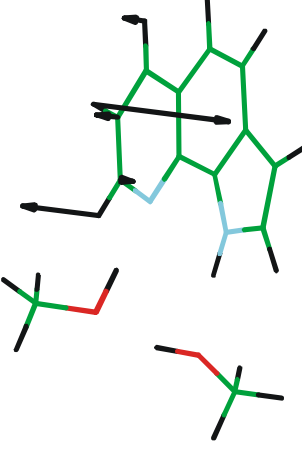
V ₃₃	 1433 (1390)	 1392 (1351)
V ₃₄	 1408 (1367)	 1360 (1320)
V ₃₅	 1366 (1325)	 1338 (1298)
V ₃₆	 1345 (1305)	 1290 (1252)

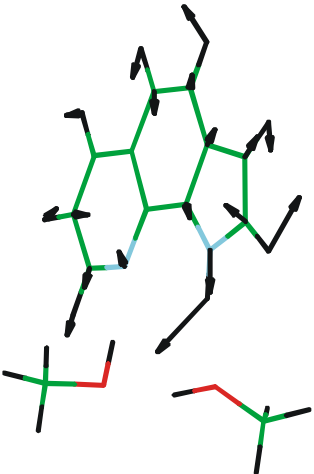
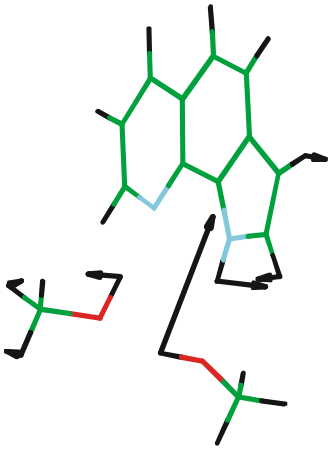
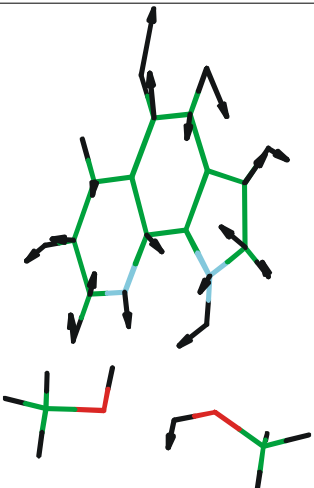
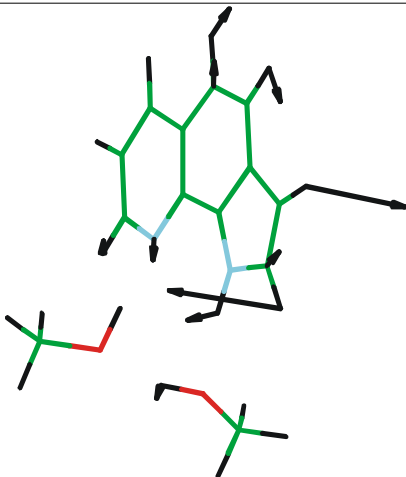
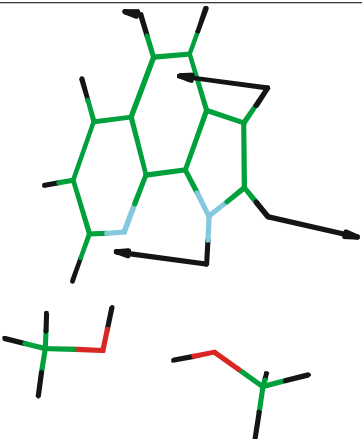
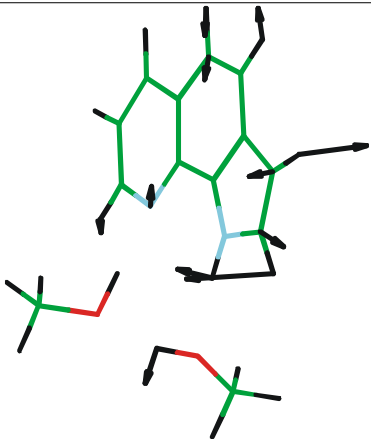
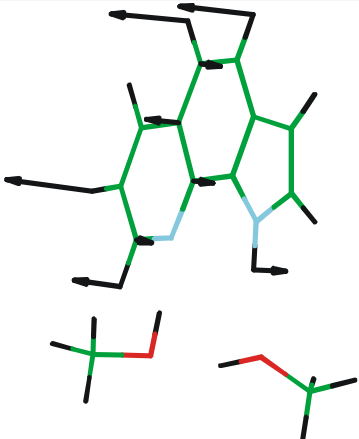
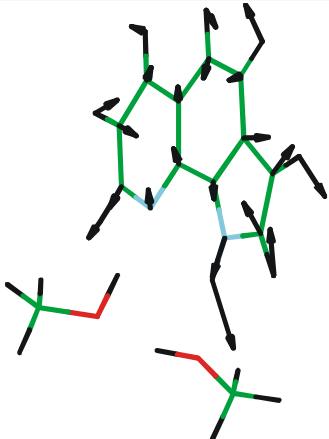
V ₃₇	 1301 (1262)	 1283 (1245)
V ₃₈	 1267 (1229)	 1235 (1199)
V ₃₉	 1236 (1199)	 1217 (1181)
V ₄₀	 1210 (1174)	 1176 (1141)

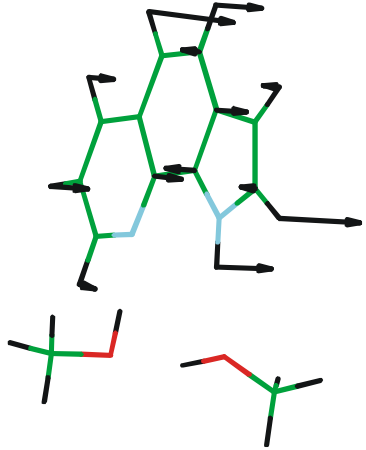
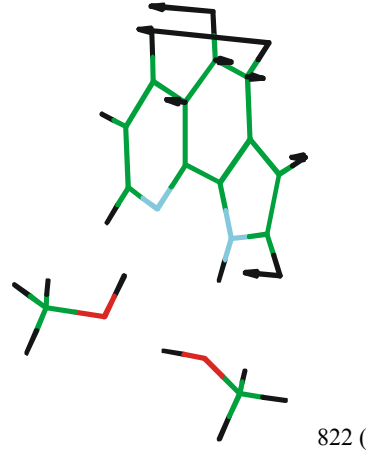
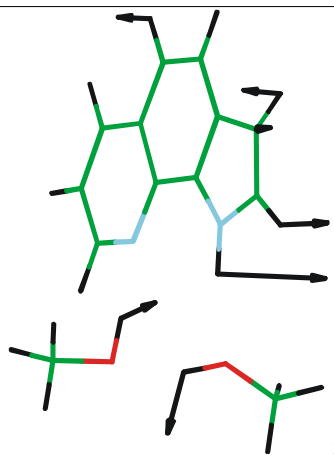
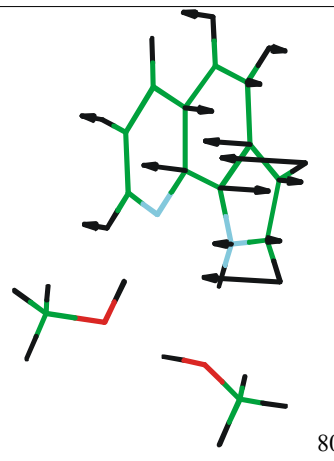
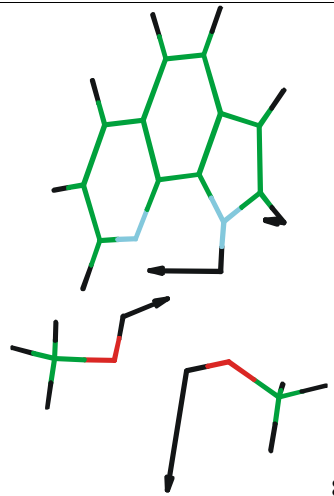
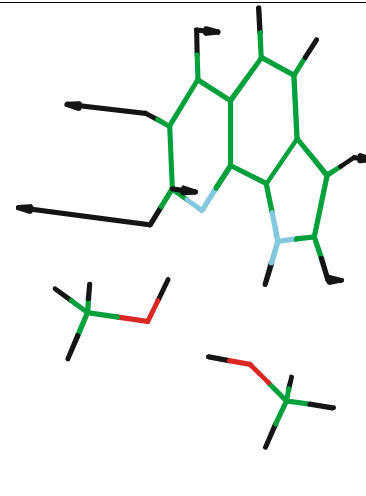
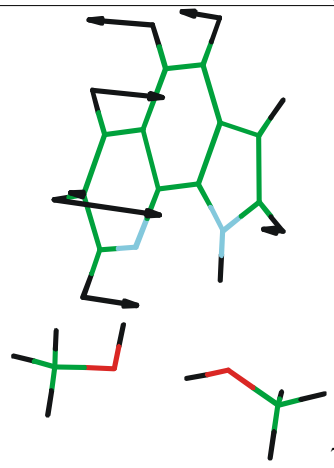
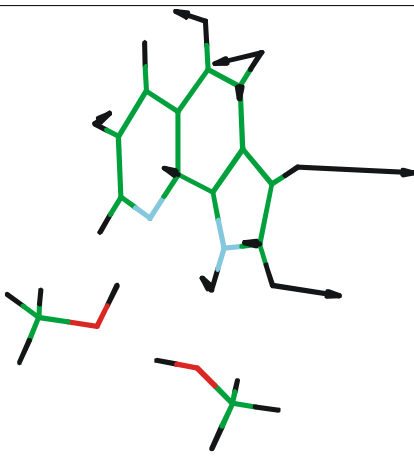
V ₄₁	 1165 (1130)	 1168 (1134)
V ₄₂	 1164 (1129)	 1166(1132)
V ₄₃	 1149 (1115)	 1166 (1131)
V ₄₄	 1146 (1112)	 1137 (1104)

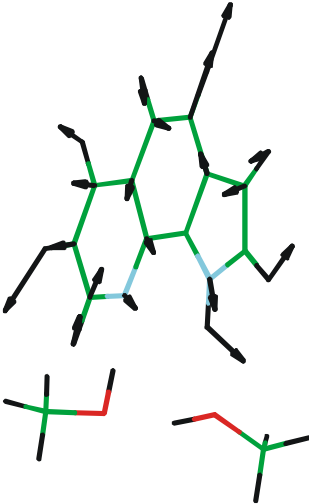
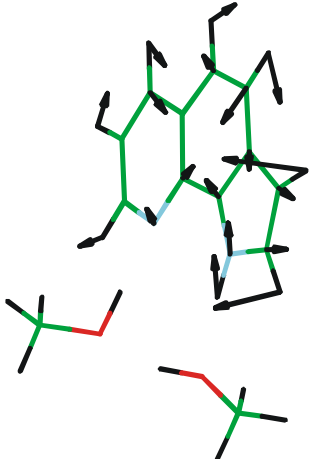
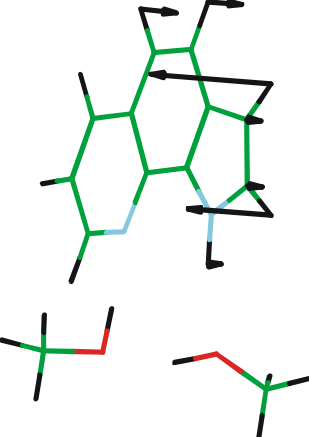
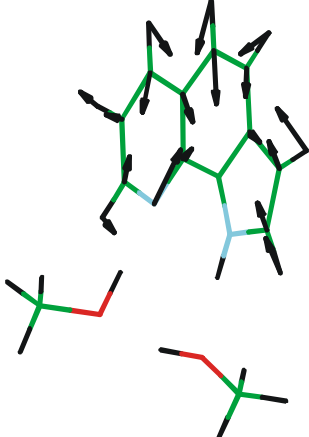
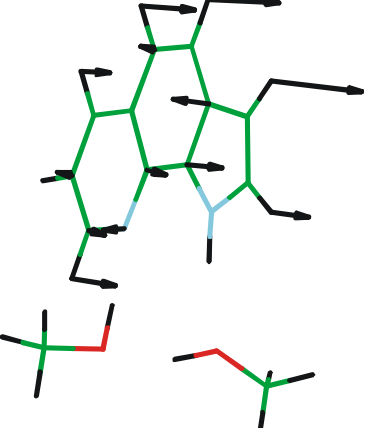
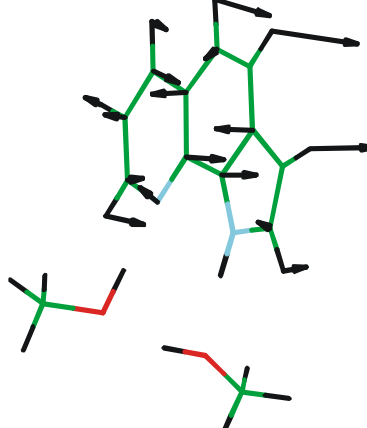
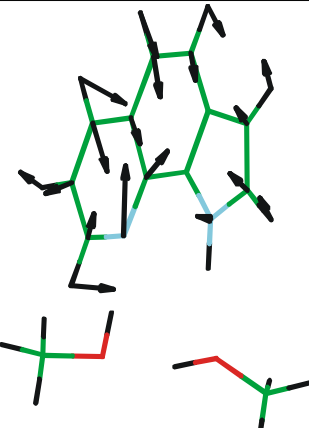
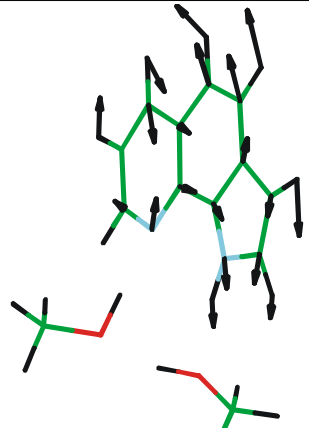
V ₄₅	 1133 (1100)	 1112 (1079)
V ₄₆	 1128 (1094)	 1102 (1070)
V ₄₇	 1102 (1069)	 1082 (1050)
V ₄₈	 1090 (1058)	 1074 (1042)

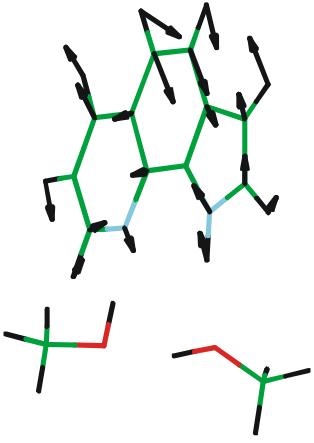
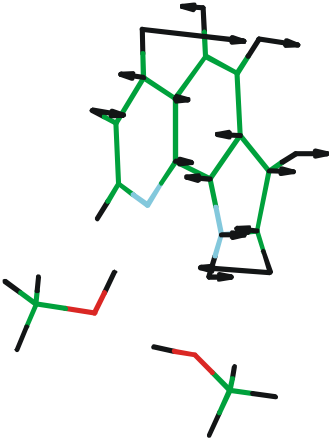
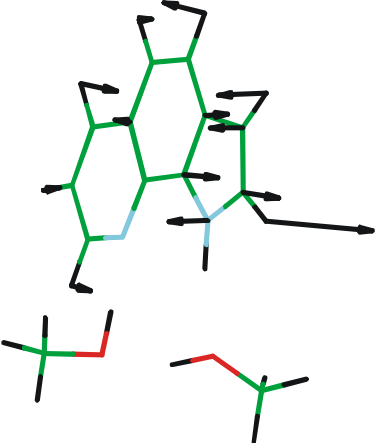
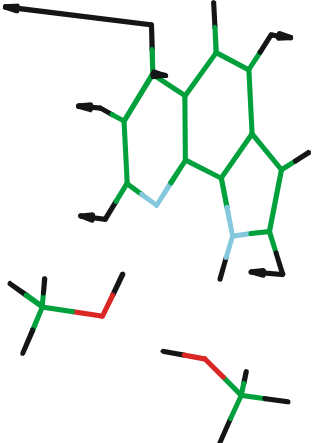
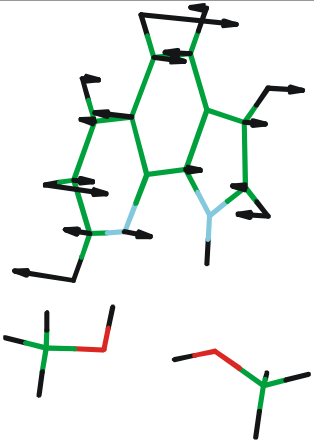
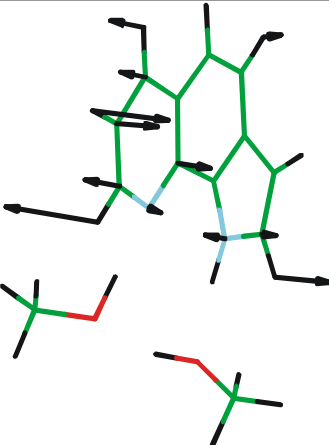
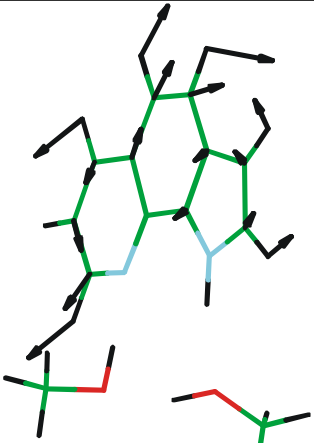
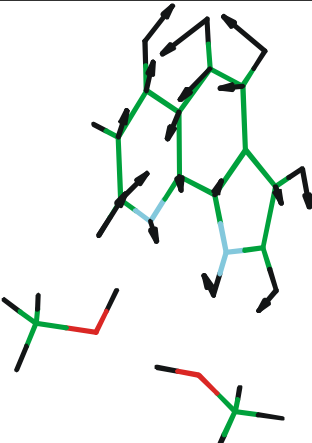
V ₄₉	 1074 (1043)	 1069 (1037)
V ₅₀	 1064 (1032)	 1057 (1026)
V ₅₁	 1055 (1024)	 1054 (1023)
V ₅₂	 1036 (1006)	 1042 (1011)

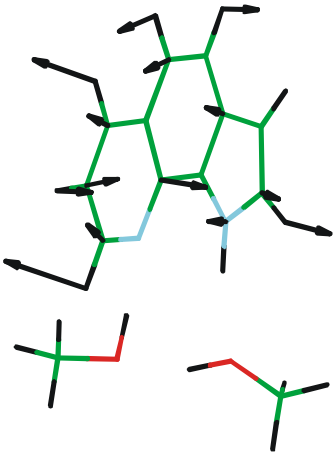
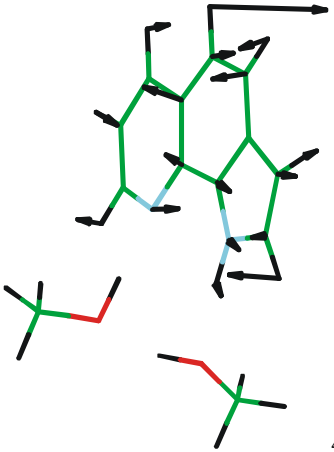
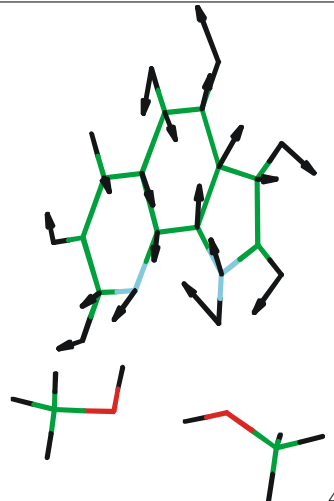
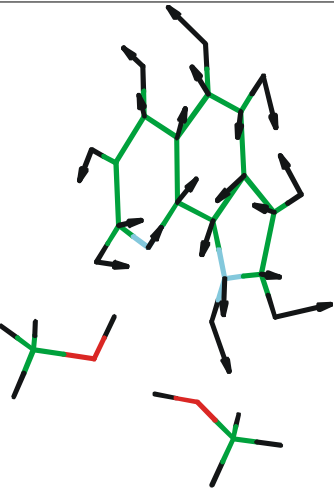
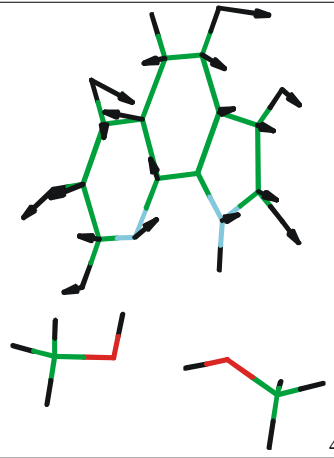
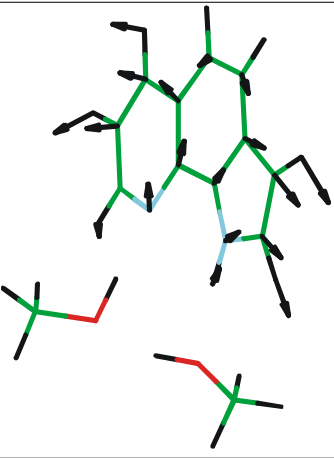
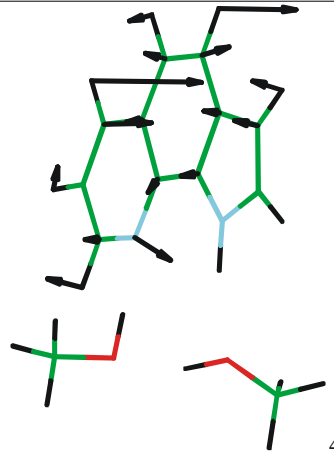
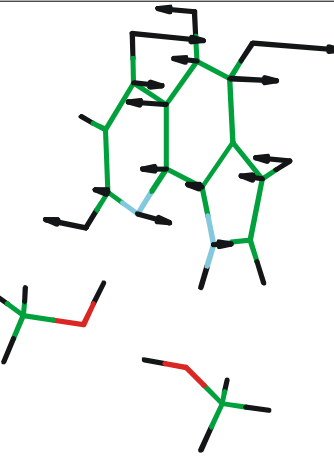
V ₅₃	 995 (966)	 998 (969)
V ₅₄	 982 (953)	 968 (939)
V ₅₅	 975 (946)	 942 (914)
V ₅₆	 965 (936)	 932 (904)

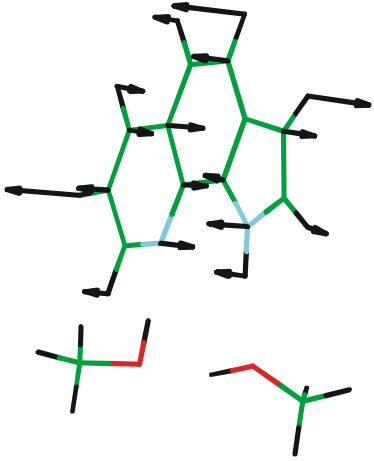
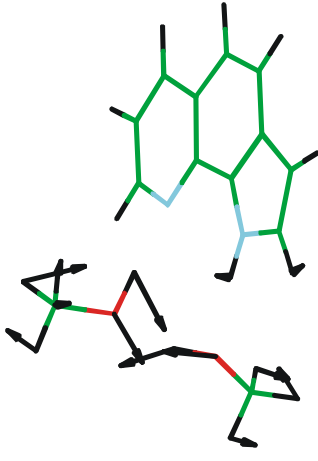
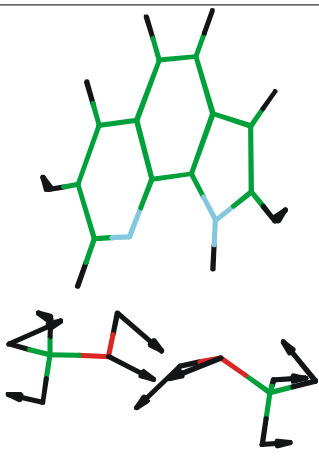
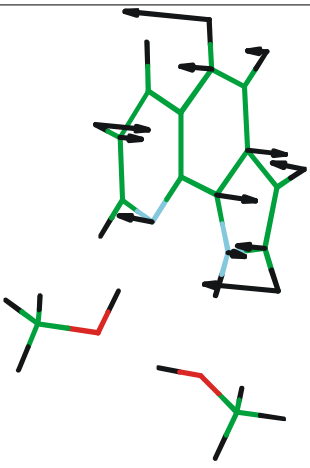
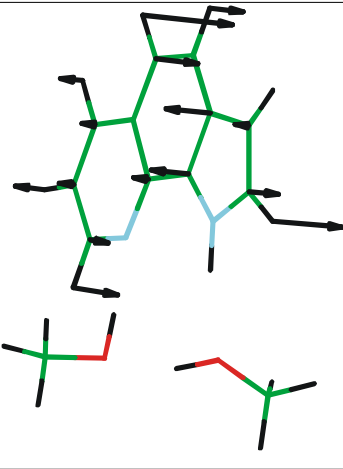
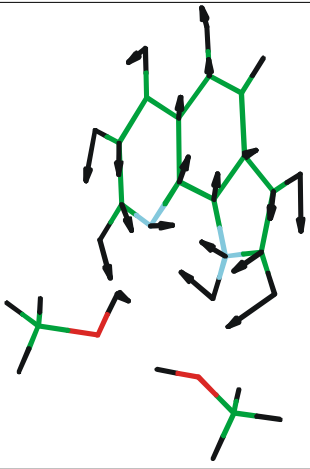
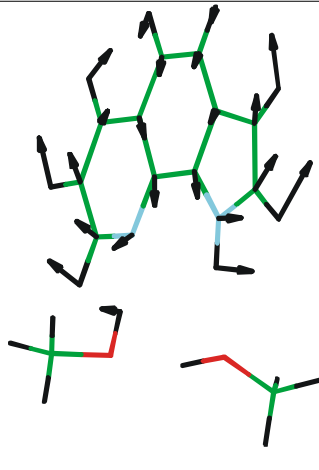
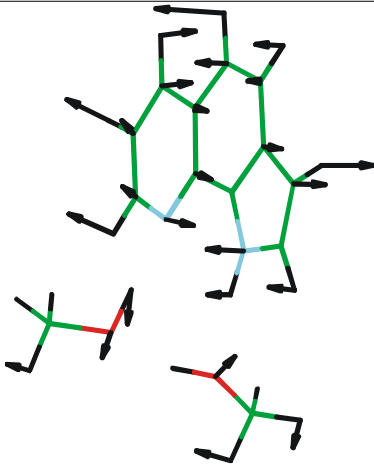
V ₅₇	 906 (879)	 903 (876)
V ₅₈	 892 (866)	 882 (855)
V ₅₉	 879 (853)	 881 (855)
V ₆₀	 851 (826)	 839 (814)

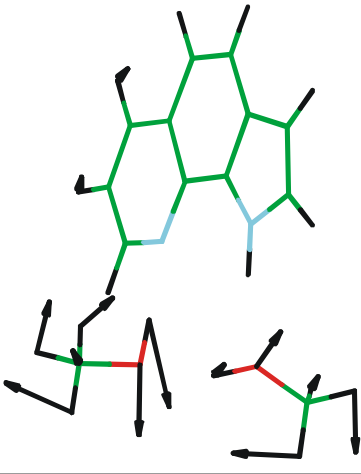
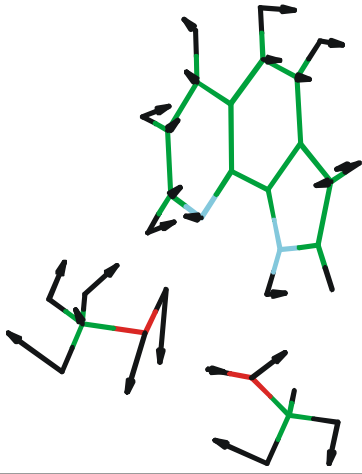
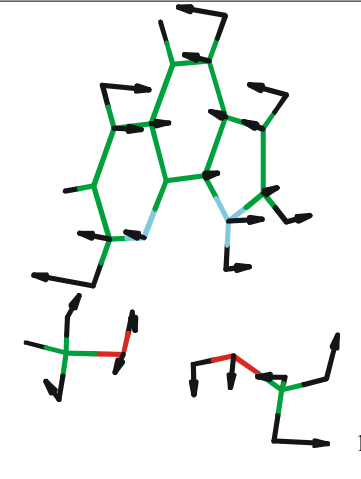
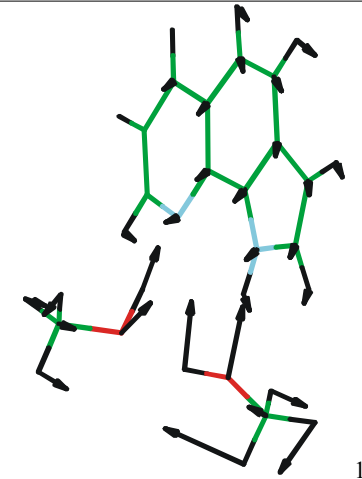
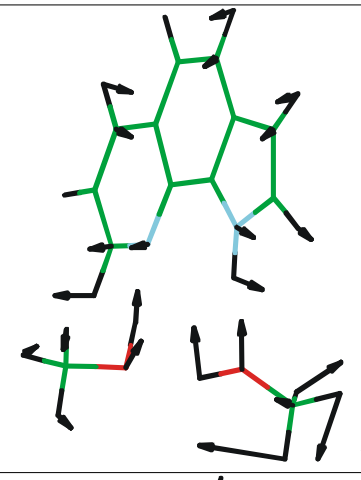
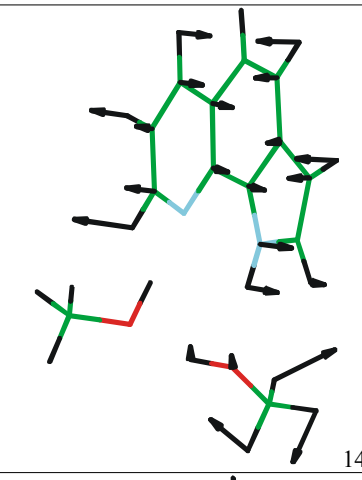
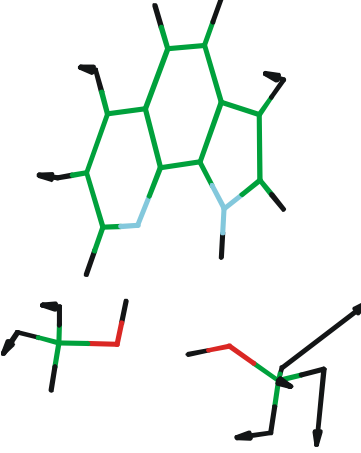
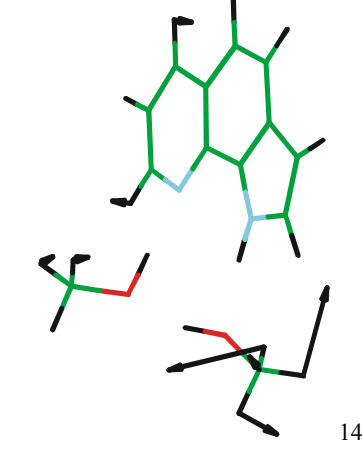
V ₆₁	 835 (810)	 822 (797)
V ₆₂	 831 (807)	 802 (778)
V ₆₃	 817 (793)	 760 (738)
V ₆₄	 791 (767)	 744 (722)

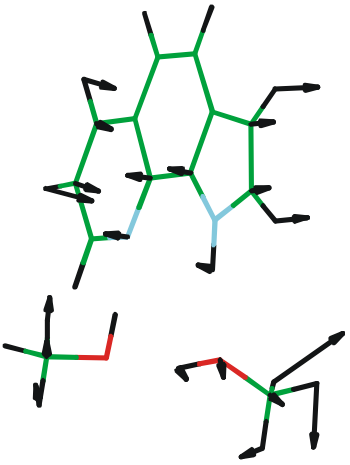
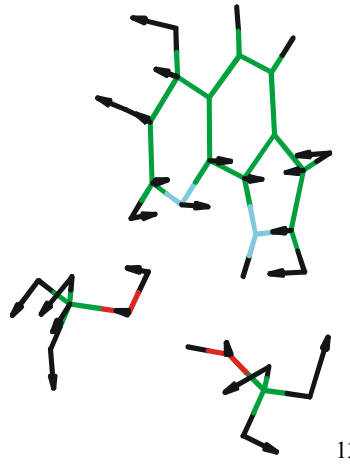
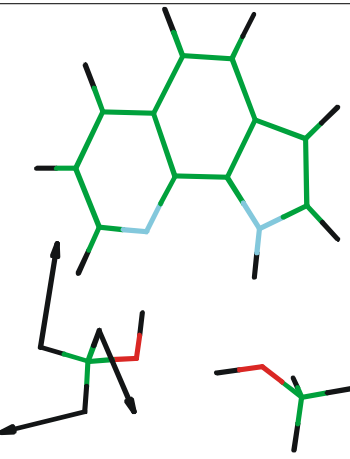
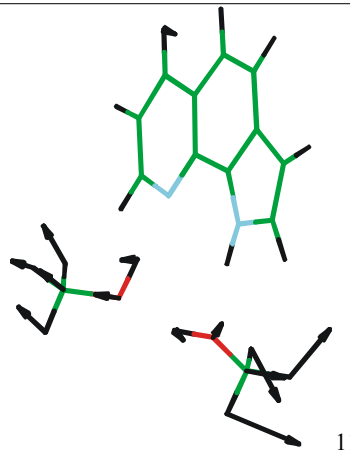
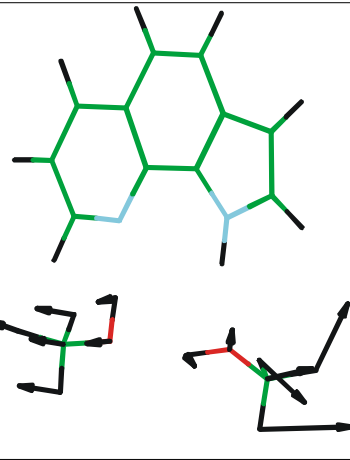
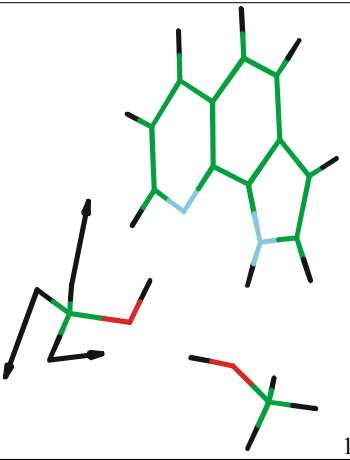
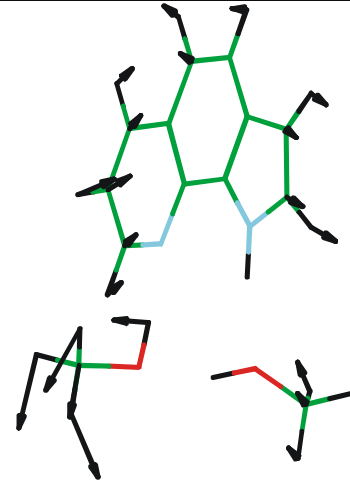
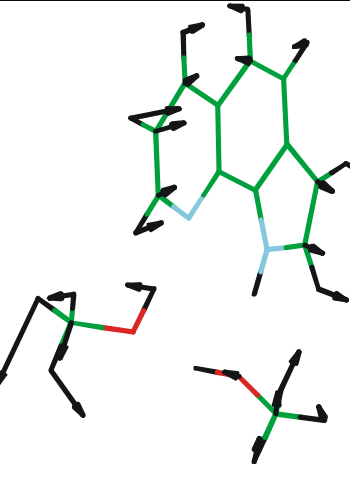
V ₆₅	 771 (748)	 739 (718)
V ₆₆	 754 (732)	 700 (680)
V ₆₇	 721 (699)	 691 (671)
V ₆₈	 700 (679)	 610 (592)

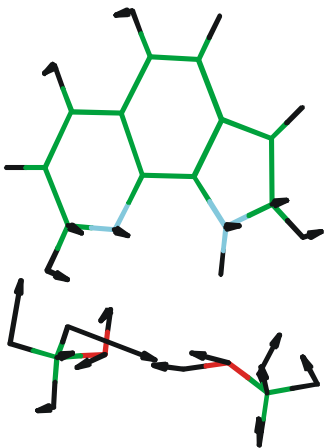
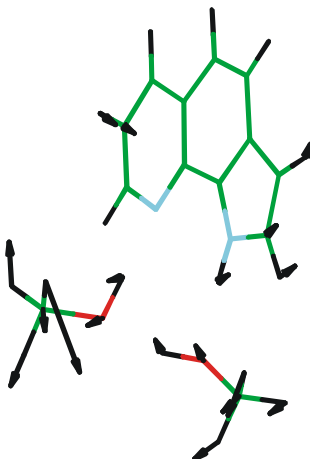
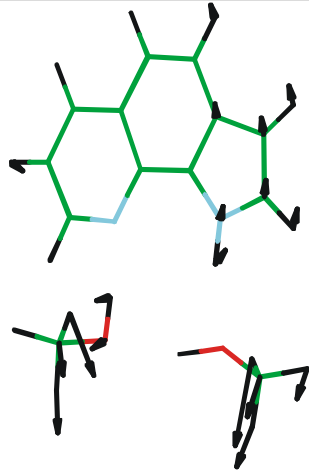
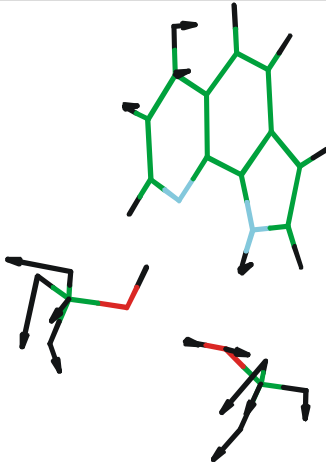
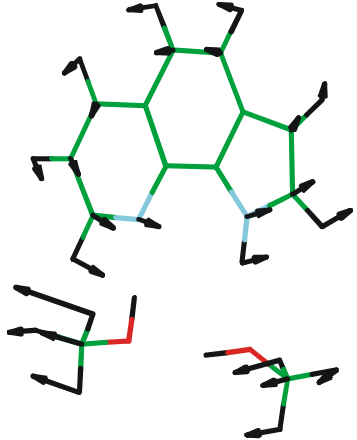
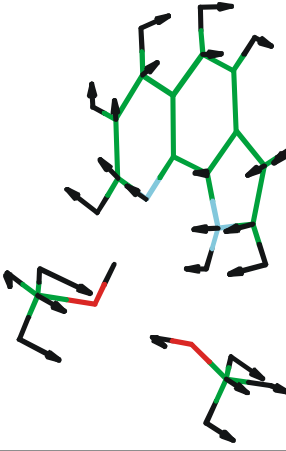
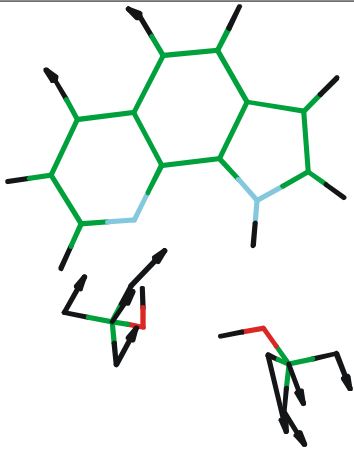
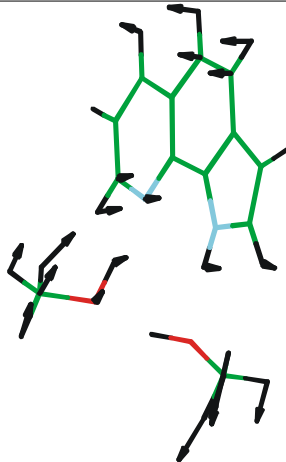
V ₆₉	 627 (608)	 594 (577)
V ₇₀	 619 (600)	 588 (570)
V ₇₁	 592 (574)	 511 (496)
V ₇₂	 532 (516)	 510 (495)

V ₇₃	 529 (514)	 482 (468)
V ₇₄	 481 (467)	 474 (460)
V ₇₅	 444 (431)	 430 (417)
V ₇₆	 440 (427)	 355 (344)

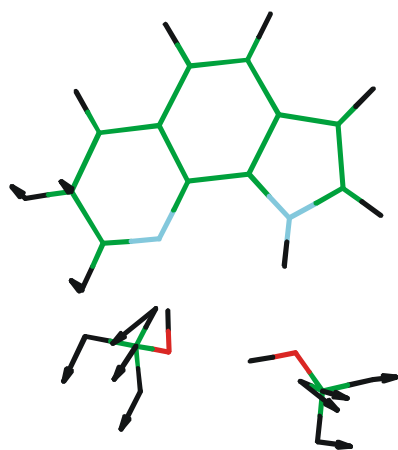
V ₇₇	 294 (285)	 307 (298)
V ₇₈	 275 (267)	 275 (266)
V ₇₉	 263 (255)	 248 (241)
V ₈₀	 252 (244)	 228 (222)

V ₈₁	 195 (189)	 212 (206)
V ₈₂	 168 (163)	 176 (171)
V ₈₃	 155 (151)	 142 (137)
V ₈₄	 137 (133)	 140 (135)

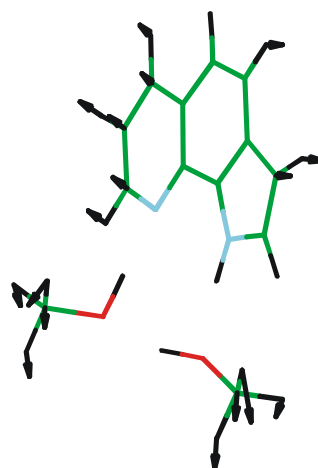
V ₈₅	 132 (128)	 135 (131)
V ₈₆	 122 (118)	 119 (115)
V ₈₇	 110 (107)	 107 (104)
V ₈₈	 96 (93)	 99 (96)

V ₈₉	 78 (75)	 85 (83)
V ₉₀	 72 (70)	 79 (77)
V ₉₁	 51 (49)	 55 (54)
V ₉₂	 39 (38)	 40 (39)

V₉₃



25 (24)



26 (26)