

**Table 5**  
Topological parameters of bond critical points

	Length[Å]	$\rho_{bcp}[\text{e}\text{\AA}^{-3}]$					$\nabla^2\rho_{bcp}[\text{e}\text{\AA}^{-5}]$				
		APEX	OXFORD	SYN	HUBER	Theo	APEX	OXFORD	SYN	HUBER	Theo
O18-C18	1.4338(6)	2.08(4)	1.93(4)	1.85(6)	2.00(3)	1.73	-19.0(1)	-16.2(2)	-14.3(2)	-16.6(1)	-13.3
O18-C19	1.4319(5)	2.00(4)	1.89(4)	1.82(6)	1.93(3)	1.71	-14.5(1)	-14.9(1)	-13.0(2)	-16.3(1)	-13.1
O21-C21	1.2301(6)	3.28(5)	3.01(5)	3.08(7)	3.21(4)	2.78	-39.3(2)	-34.0(3)	-34.3(3)	-40.5(3)	-15.6
N5-C5	1.4891(5)	1.76(3)	1.72(3)	1.76(5)	1.73(3)	1.70	-9.6(1)	-9.1(1)	-7.3(1)	-8.6(1)	-15.4
N5-C6	1.4156(5)	2.13(4)	2.10(4)	2.13(5)	2.11(3)	1.95	-18.4(1)	-20.7(2)	-15.1(2)	-20.2(1)	-19.9
N5-C21	1.3747(5)	2.39(4)	2.34(4)	2.48(6)	2.37(3)	2.16	-21.0(1)	-23.0(2)	-28.7(2)	-22.7(1)	-23.1
N14-C1	1.4952(5)	1.86(3)	1.79(3)	1.79(5)	1.83(3)	1.72	-13.2(1)	-13.8(1)	-12.4(1)	-12.3(1)	-15.0
N14-C14	1.4766(5)	1.85(4)	1.85(4)	1.82(5)	1.88(3)	1.77	-13.5(1)	-12.1(1)	-11.8(1)	-11.7(1)	-16.2
N14-C15	1.4715(5)	2.01(4)	1.90(4)	1.82(5)	1.92(3)	1.79	-14.7(1)	-11.3(1)	-9.8(2)	-13.0(1)	-16.5
C1-C2	1.5238(5)	1.79(3)	1.73(3)	1.74(5)	1.74(3)	1.70	-14.9(1)	-12.2(1)	-11.2(1)	-12.7(0)	-14.5
C1-C12	1.5477(5)	1.67(3)	1.64(3)	1.59(5)	1.69(3)	1.63	-10.4(1)	-11.1(1)	-9.3(1)	-12.1(0)	-13.2
C2-C3	1.5359(5)	1.66(3)	1.63(3)	1.64(5)	1.73(3)	1.65	-10.9(1)	-8.7(1)	-10.2(1)	-11.8(1)	-13.7
C3-C4	1.5385(5)	1.68(3)	1.64(3)	1.63(5)	1.72(2)	1.63	-11.6(1)	-8.5(1)	-9.4(1)	-11.5(0)	-13.2
C3-C16	1.5238(5)	1.81(3)	1.71(3)	1.71(5)	1.80(3)	1.69	-11.6(1)	-11.1(1)	-9.8(1)	-11.9(1)	-14.3
C4-C5	1.5374(5)	1.70(3)	1.68(3)	1.74(5)	1.72(2)	1.67	-12.4(1)	-10.2(1)	-10.9(1)	-11.5(0)	-13.8
C4-C19	1.5374(5)	1.78(3)	1.74(3)	1.59(5)	1.82(3)	1.68	-16.2(1)	-13.6(1)	-9.7(1)	-16.6(0)	-14.2
C5-C12	1.5579(5)	1.66(3)	1.61(2)	1.58(5)	1.69(2)	1.61	-10.5(0)	-10.0(0)	-10.0(1)	-11.8(0)	-12.8
C6-C7	1.3996(5)	2.23(3)	2.17(3)	2.02(6)	2.19(3)	2.14	-16.4(1)	-17.4(1)	-12.3(2)	-15.3(1)	-22.1
C6-C11	1.4014(5)	2.27(3)	2.21(3)	2.29(5)	2.25(3)	2.13	-21.3(1)	-20.1(1)	-22.6(2)	-21.8(1)	-22.2
C7-C8	1.4036(7)	2.23(4)	2.18(4)	2.29(6)	2.23(3)	2.10	-20.4(1)	-19.2(1)	-22.9(2)	-19.9(1)	-21.5
C8-C9	1.3991(7)	1.94(6)	2.05(6)	2.26(6)	2.21(4)	2.11	-7.6(3)	-13.1(3)	-21.5(2)	-18.9(1)	-21.8
C9-C10	1.4014(6)	2.23(4)	2.16(4)	2.08(6)	2.17(3)	2.11	-14.8(1)	-16.0(1)	-14.4(2)	-13.5(1)	-21.9
C10-C11	1.3896(5)	2.19(4)	2.20(4)	2.27(6)	2.25(3)	2.14	-16.2(1)	-18.8(1)	-24.3(2)	-18.6(1)	-22.3
C11-C12	1.5076(5)	1.84(3)	1.75(3)	1.79(5)	1.80(3)	1.75	-13.3(1)	-12.9(1)	-11.6(1)	-12.7(1)	-15.3
C12-C13	1.5452(5)	1.75(3)	1.63(3)	1.62(5)	1.71(2)	1.61	-11.6(1)	-9.4(1)	-9.6(1)	-10.2(0)	-12.9
C13-C14	1.5288(5)	1.79(3)	1.71(3)	1.76(5)	1.80(3)	1.68	-11.9(1)	-11.8(1)	-15.3(1)	-13.1(1)	-14.3
C15-C16	1.5098(6)	1.83(3)	1.80(3)	1.82(5)	1.84(3)	1.75	-15.1(1)	-13.9(1)	-11.5(1)	-15.0(1)	-15.5
C16-C17	1.3425(6)	2.38(4)	2.41(4)	2.47(6)	2.43(3)	2.35	-19.5(1)	-20.5(1)	-25.0(2)	-21.5(1)	-25.8
C17-C18	1.5083(6)	1.85(3)	1.83(3)	1.89(5)	1.86(3)	1.76	-17.4(1)	-15.3(1)	-14.8(1)	-16.5(1)	-15.9
C19-C20	1.5470(5)	1.78(3)	1.71(3)	1.65(5)	1.74(2)	1.63	-16.4(1)	-12.4(1)	-9.9(1)	-14.0(0)	-13.4
C20-C21	1.5175(6)	1.81(3)	1.77(3)	1.78(5)	1.82(3)	1.74	-13.6(1)	-13.9(1)	-11.4(1)	-13.8(1)	-15.4