Supplementary Information

Table 1. Selected bond lengths and bond angles in **4** (for atoms numbering see Fig. 1) obtained from the crystallographic data and from the DFT B3LYP/6-31G** calculations.

bonds	Å	DFT	angles	^{0}	DFT
O1-C16	1.218(3)	1.223	N1-C1-C2	122.3(3)	121.8
C16-C8	1.479(3)	1.493	N1-C1-C6	120.9(3)	121.3
O2-C9	1.213(3)	1.228	O1-C16-C15	125.6(2)	126.0
C8-C7	1.351(4)	1.369	O1-C16-C8	126.2(2)	127.2
C8-C9	1.488(4)	1.482	C7-C8-C9	134.3(2)	133.8
C15-C10	1.387(3)	1.399	C8-C7-C4	135.8(3)	134.6
C15-C14	1.375(4)	1.391	C1-N1-C17	120.7(2)	120.5
C12-C13	1.385(5)	1.404	C1-N1-C26	120.9(2)	121.0
N1-C26	1.455(4)	1.459	C17-N1-C26	118.3(2)	118.6
N1-C17	1.449(4)	1.463	O2-C9-C10	125.0(3)	123.7
C1-N1	1.363(3)	1.379	C8-C9-C10	106.4(2)	106.2
C7-C4	1.422(3)	1.436	N1-C26-C25	115.1(3)	115.0
O6-C25	1.412(3)	1.414	O6-C25-C26	109.6(3)	108.4
O6-C24	1.412(5)	1.416	N1-C17-C18	112.3(3)	114.5
O4-C21	1.391(7)	1.416			
O4-C20A	1.511(9)	1.421			
O4-C20B	1.43(1)				
C19-C20A	1.34(1)	1.528			
C19-C20B	1.38(1)				