

Table S1. Some bond and conformational parameters of compounds **1a-3a**, **5a-8a** (10-membered ansa-dioxy rings)

	1a[ref 13]	2a	3a	5a	6a	7a	8a	9a
P1-N1	1.57	1.5888(17)	1.5879(16)	1.5851(14)	1.5755(16)	1.576(2)	1.5796(19)	1.5878(12)
P1-N3	1.59	1.5753(17)	1.5726(17)	1.5697(15)	1.5756(17)	1.572(2)	1.574(2)	1.5807(13)
P2-N1	1.58	1.5855(17)	1.5825(17)	1.5819(14)	1.5865(16)	1.595(2)	1.5966(19)	1.5877(13)
P2-N2	1.59	1.5764(16)	1.5700(18)	1.5726(15)	1.5823(17)	1.577(2)	1.577(2)	1.5781(13)
P3-N2	1.57	1.5927(16)	1.5812(18)	1.5922(15)	1.5706(17)	1.575(2)	1.592(2)	1.5857(12)
P3-N3	1.58	1.5777(17)	1.5887(16)	1.5899(15)	1.5828(17)	1.589(2)	1.598(2)	1.5907(13)
N1-P1-N3	119.7	118.71(9)	118.87(9)	119.20(7)	118.77(9)	119.21(12)	119.09(10)	117.23(7)
N1-P2-N2	118.4	119.11(8)	118.86(9)	119.28(7)	117.14(9)	116.68(13)	116.91(10)	117.37(6)
N2-P3-N3	118.8	117.19(9)	118.61(9)	116.92(8)	119.21(9)	118.83(12)	122.23(12)	117.33(7)
P1-N1-P2	119.0	118.06(10)	118.89(10)	118.02(9)	120.95(10)	118.64(14)	117.57(12)	118.60(8)
P2-N2-P3	119.9	120.86(10)	121.29(11)	120.89(8)	121.31(10)	121.43(14)	122.23(12)	121.57(8)
P1-N3-P3	120.6	122.28(10)	120.00(10)	121.16(9)	119.98(10)	119.36(15)	121.86(12)	120.41(7)
P1-O1	1.574	1.5803(13)	1.5857(15)	1.5885(12)	1.5809(15)	1.589(2)	1.5831(18)	1.5957(11)
P2-O2	1.580	1.5884(12)	1.5831(15)	1.5865(12)	1.5832(14)	1.586(2)	1.5911(16)	1.5877(10)
P1-O1-C1	122.3	122.42(12)	120.88(12)	120.48(11)	121.18(12)	120.57(18)	120.81(15)	118.74(9)
P2-O2-C5	120	120.64(12)	121.81(13)	122.05(10)	121.28(12)	120.68(18)	119.35(14)	121.01(9)
O1-C1-C2	109	108.78(16)	109.26(17)	109.13(13)	109.05(16)	108.9(2)	109.11(19)	109.66(12)
O2-C5-C4	111	109.52(16)	108.53(17)	109.24(14)	108.96(16)	108.9(2)	108.75(19)	109.06(12)
P1-O1-C1-C2	-126	129.93(14)	131.29(15)	130.82(12)	-125.12(16)	136.5(2)	134.42(18)	139.65(11)
P2-O2-C5-C4	130	-131.70(14)	-128.21(16)	-130.47(12)	126.73(15)	-136.5(2)	-138.64(16)	-135.16(10)
P1...P2	2.735	2.722	2.730	2.715	2.751	2.727	2.716	2.730
O...O	4.068	3.986	4.024	3.995	4.130	3.850	3.838	3.835
Puckering amplitude, Q for P₃N₃	0.179(10)	0.2015(13)	0.1727(13)	0.2370(11)	0.1781(14)	0.2133(19)	0.2615(14)	0.2972(10)
Max.Deviation for P₃N₃ ring	0.125(5) (P2)	0.1342(17) (N1)	0.1125(17) (N1)	0.1517(15) (N1)	0.1143(18) (N1)	0.144(2) (N1)	0.1698(19) (N1)	0.1869(14) (N1)
Puckering amplitude, Q for ansa ring	1.475(14)	1.4490(19)	1.4586(19)	1.4529(16)	1.4479(19)	1.450(3)	1.456(2)	1.4465(15)

Table S2. Some bond and conformational parameters of compounds **1b**, **3b**, **5b**, **8b** and **9b** (11-membered ansa-dioxy rings)

	1b [ref 14]	3b	5b	8b	9b
P1-N1	1.576	1.5820(17)	1.5827(13)	1.584(3)	1.583(3)
P1-N3	1.575	1.5787(18)	1.5702(15)	1.571(3)	1.581(3)
P2-N1	1.588	1.5763(17)	1.5864(13)	1.570(3)	1.586(3)
P2-N2	1.570	1.5729(17)	1.5687(13)	1.576(3)	1.582(3)
P3-N2	1.584	1.5832(17)	1.5890(13)	1.586(3)	1.586(3)
P3-N3	1.584	1.5759(17)	1.5767(14)	1.585(3)	1.582(3)
N1-P1-N3	119.1	116.74(9)	117.67(7)	118.75(15)	116.61(15)
N1-P2-N2	118.5	119.06(9)	118.88(7)	117.19(15)	117.50(15)
N2-P3-N3	118.2	118.90(9)	117.24(7)	116.83(15)	118.67(15)
P1-N1-P2	121.0	122.41(11)	121.21(8)	121.98(17)	122.53(18)
P2-N2-P3	121.8	120.31(10)	121.63(8)	122.98(18)	120.66(17)
P1-N3-P3	121.3	122.46(11)	123.15(9)	121.41(17)	121.81(18)
P1-O1	1.578	1.5764(15)	1.5817(12)	1.575(2)	1.585(2)
P2-O2	1.572	1.5834(14)	1.5758(11)	1.593(2)	1.591(2)
P1-O1-C1	120.7	121.83(13)	120.89(10)	122.7(2)	121.9(2)
P2-O2-C6	123.1	121.40(13)	122.69(10)	121.5(2)	119.5(2)
O1-C1-C2	111.0	109.95(17)	110.10(13)	108.7(3)	111.5(3)
O2-C6-C5	109.5	109.14(16)	108.52(12)	110.5(3)	109.2(3)
P1-O1-C1-C2	122.1	-124.81(16)	-124.78(12)	127.3(2)	129.5(3)
P2-O2-C6-C5	124.9	-122.80(15)	-128.40(11)	125.6(3)	-129.4(3)
P1...P2	2.756	2.768	2.761	2.758	2.779
O...O	4.474	4.609	4.548	4.548	4.292
Puckering amplitude, Q for P₃N₃ ring	Planar	Planar	Planar	0.090(3)	0.165(2)
Max.Deviation for P₃N₃ ring (P3)	0.0238(17) (P3)	0.0218(8) (P1)	0.0304(6) (P2)	0.0635(14) (P3)	0.096(3) (N1)
Puckering amplitude, Q for ansa ring	1.390(5)	1.439(2)	System didn't give	1.464(3)	1.415(4)