Supplementary data

X-Ray Crystallographic Study of Several 2´-Deoxy-β-D-ribonucleosides with 1-Deazapurine-Derived Aglycones

Jens Müller,[a,*] *Fabian-Alexander Polonius,*[a] *Eva Freisinger,*[b] *Elisa Gil Bardají*[a]

a) University of Dortmund, Department of Chemistry, Otto-Hahn-Straße 6, 44227 Dortmund, Germany

b) University of Zurich, Institute of Inorganic Chemistry, Winterthurerstrasse 190, 8057 Zurich, Switzerland

jens.mueller@uni-dortmund.de, phone: +49 231 755 5034, fax: +49 231 755 3797

Table S1: Hydrogen bond geometries in compound **1** (Å and °).

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O-3b–H···O-5b [a]	0.88(3)	1.85(3)	2.726(3)	175(3)
O-5b–H···N-7a [b]	0.83(3)	1.95(3)	2.770(3)	167(3)
C-2a–H···O-4b [c]	0.93	2.60	3.453(3)	152

Symmetry codes: a: $1 - x, -\frac{1}{2} + y, -z$; b: $1 + x, 1 + y, z$; c: $1 - x, -\frac{1}{2} + y, 1 - z$.

Table S2: Hydrogen bond geometries in compound **2** (Å and °).

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O-3b–H···N-9a [a]	0.82	2.41	2.80(2)	110
O-5b–H···N-3a [b]	0.82	2.42	2.83(1)	112

Symmetry codes: a: $\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z$; b: $-x, y, \frac{1}{2} - z$.

Table S3: Hydrogen bond geometries in compound **3** (Å and °).

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O-3b(II)–H···O-5b(I) [a]	0.78(4)	2.03(4)	2.801(5)	174(5)
O-3b(I)–H···N-3a(II) [b]	0.78(4)	2.02(4)	2.800(4)	170(4)
O-5b(II)–H···N-7a(I) [c]	0.75(4)	2.06(4)	2.793(4)	167(5)
O-5b(I)–H···N-7a(II) [d]	0.89(3)	1.93(4)	2.778(4)	159(4)

Symmetry codes: a: $-\frac{3}{2} + x, \frac{3}{2} - y, -z$; b: $\frac{3}{2} - x, 1 - y, -\frac{1}{2} + z$; c: $-1 + x, y, z$; d: $1 + x, y, z$.

Table S4: Hydrogen bond geometries in compound **4** · CH_3OH (Å and °).

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
N-6a–H···O-1m	0.86	2.20	3.034(5)	165
O-1m–H···N-7a	0.82	2.06	2.783(5)	147
O-5b–H···N-3a	0.92(4)	1.88(4)	2.776(5)	165(4)
O-3b–H···O-5b [a]	0.85(5)	2.01(5)	2.780(5)	150(6)

Symmetry codes: a: $-x, \frac{1}{2} + y, -z$.

Table S5: Hydrogen bond geometries in compound **4** · H_2O (Å and °).

D–H···*A*	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
N-6a–H···O-1w	0.88	2.24	3.113(5)	170
O-1w–H···N-7a	1.12(5)	1.72(4)	2.788(4)	159(4)
O-1w–H···O-4b [a]	0.73(4)	2.32(4)	3.043(4)	173(5)
O-5b–H···N-3a	1.01(3)	1.71(3)	2.713(4)	173(3)
O-3b–H···O-5b [b]	0.83(3)	1.99(3)	2.816(4)	175(4)

Symmetry codes: a: $-\frac{1}{2} + x, \frac{1}{2} - y, -z$; b: $-x, \frac{1}{2} + y, \frac{1}{2} - z$.

The D-H distances reported in Tables S1 – S5 have been determined as follows: For values that are given with their respective error limit, the respective hydrogen atoms were localized in the difference Fourier maps and refined freely. For values without error limits, the hydrogen atoms have been included in the refinement at calculated positions as implemented in the SHELX program.