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Synthesis and structure of diamino derivatives of pyrano-[3,4-*c*]pyridines and 5,6,7,8-tetrahydroisoquinolines

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SUPPLEMENTARY INFORMATION

Table. Basic crystallographic characteristics and experimental data

Crystal Data		
Compounds	**2g**	**3g**
Formula	$C_{24}H_{28}N_4O_3$	$C_{22}H_{26}N_4O$
Formula Weight	420.5	362.47
Crystal System	Monoclinic	Triclinic
Space group	P 21/c	P-1
a, b, c [Å]	9.6291(12), 9.9079(10), 23.432(3)	9.3319(19), 10.732(2), 11.149(2)
α, β, γ [deg..]	90, 101.737(10), 90	67.08(3), 85.56(3), 69.66(3)
V [$Å^3$]	2188.8(4)	962.1(4)
Z	4	2
Density [g/cm^3]	1.276	1.251
μ(MoKa) [mm^{-1}]	0.086	0.079
F(000)	896	388
Crystal Size [mm]	0.4x0.36x0.33	0.42x0.35x0.32
Data Collection		
Temperature (K)	293	293
Radiation [Å]	MoKα 0.71073	MoKα 0.71073
$\theta_{min}, \theta_{max}$ [Deg.]	1.8, 30.0	2.0, 30.0
Dataset	$0 \le h \le 13$; $0 \le k \le 13$; $-32 \le l \le 32$	$0 \le h \le 11$; $-14 \le k \le 15$; $-15 \le l \le 15$
Tot., Uniq. Data, R(int)	6713	5713
Observed data	2789 [I > 3.0 σ(I)]	3118 [I > 2.0 σ(I)]
Refinement		
Nref, Npar	6369, 359	5392, 348
R, wR2, S	0.0523, 0.0655, 1.74	0.0550, 0.1568, 1.08
Weight Scheme	$w=1/(\sigma^2(F)+0.0001*F^2)$	$w=1/[\sigma^2(Fo^2)+(0.0620*P)^2+ 0.1380*P]$ where $P=(Fo^2+2Fc^2)/3$