

Electronic supplementary materials for:

**Recent Advances in Versatile Pyridazine-Cored Materials: Principles,
Applications, and Challenges**

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Table S1. The basic parameters of melting points, pKa values, and theoretical aromaticity of

PD, pyrimidine, pyrazine

Names	b.p./ °C	Aromaticity multicenter indices (MCI/ I_{ring}) [3]	pKa(CH ₃ CN) [1]	pKa(H ₂ O) [1]	Atomic heats [2] of PD (N-N bond/N=N bond) kcal/mol
Pyridazine	208	0.044/0.0304	10.07	2.33	1038.8/1014.6
Pyrimidine	123-124	0.042/0.042	8.72	1.3	-
Pyrazine	115-118	0.0304/0.0291	7.74	0.6	-

[1] A. Albert, J. N. Philli. *J. Chem. Soc.*, 1956, 1294-1304.

[2] J. Tjebbes. *Acta Chem. Scand.*, 1962, **16**, 916.

[3] J. Cioslowski, E. Matito, M. Solà, *J. Phys. Chem. A*, 2007, **111**, 6521-6525. [Lit. 133] in the context.