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Supporting information for article:

A novel tubular hydrogen-bond pattern in a new diazaphosphole oxide: a combination of X-ray crystallography and theoretical study of hydrogen bonds

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Supporting Information

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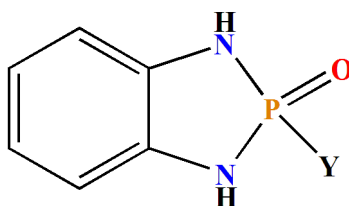


Figure S1

The general chemical structure for 1,3-diazaphosphole-based compounds with the CSD refcodes SAYJIM and JEBFEB for $Y = 4\text{-F-C}_6\text{H}_4\text{C(O)NH}$ and C_6H_5 , respectively.

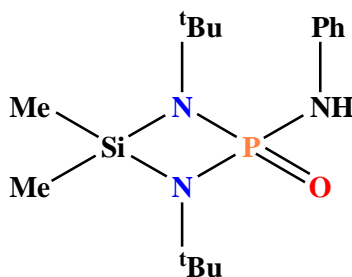


Figure S2

The chemical structure of compound with the CSD refcode ADUTAU.

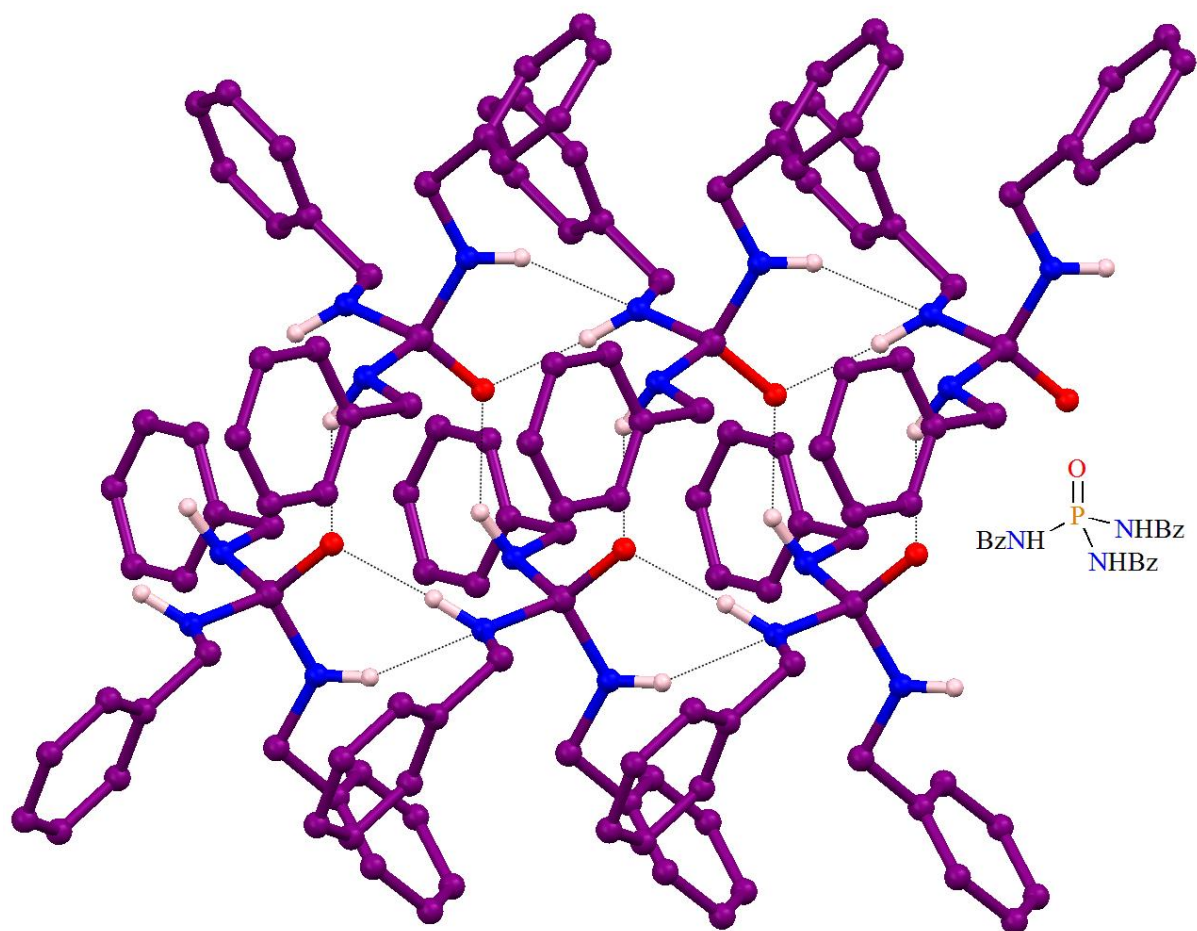


Figure S3

The crystal packing of structure with the CSD refcode TOKXIB showing one of the nitrogen atoms bonded to phosphorous as a hydrogen bond acceptor, redrawn from the Cambridge crystallography data (CCD). Atoms: red oxygen, blue nitrogen, pink hydrogen, purple carbon and phosphorus. The carbon-bound H atoms have been omitted for clarity.

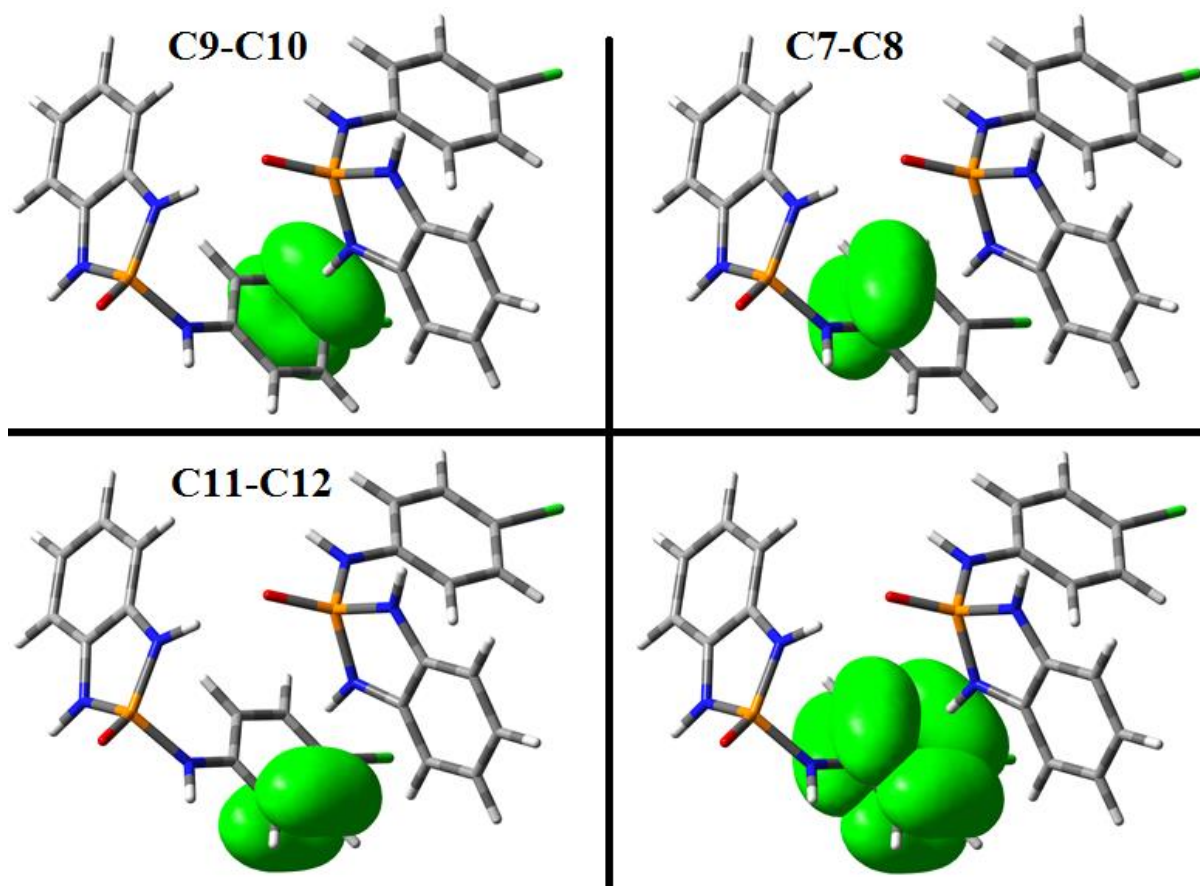


Figure S4

Contour diagrams of the total π system (bottom-right) and π_{C7-C8} , π_{C9-C10} and $\pi_{C11-C12}$ orbitals in a two-molecule assembly of cyclic phosphoric triamide (I). The numbering is according to the X-ray analysis.

Table S1

The NBO analysis of two N—H...O hydrogen bonds in a six-molecule assembly of cyclic phosphoric triamide (I). The numbering is according to the X-ray analysis.

Donor			Acceptor			$E^{(2)}$ (kcal.mol ⁻¹)
MOs	Occupancy (e)	E (a.u.)	MOs	Occupancy (e)	E (a.u.)	
LP(1)O1	1.9572	-0.84739				6.81
LP(2)O1	1.8871	-0.31266	$\sigma^*(1)N1-H1A$	0.03728	0.44599	2.03
LP(3)O1	1.8303	-0.31055				6.02
LP(1)O1	1.9572	-0.84739	$\sigma^*(1)N2-H2A$	0.035213	0.40853	5.83
LP(3)O1	1.8303	-0.31055				6.46

Table S2

The NBO analysis of N3-H3A... π interaction in a six-molecule assembly of cyclic phosphoric triamide (I). The numbering is according to the X-ray analysis.

Donor			Acceptor			$E^{(2)}$ (kcal.mol ⁻¹)
MOs	Occupancy (e)	E (a.u.)	MO	Occupancy (e)	E (a.u.)	
π C9-C10	1.71331	– 0.28722	$\sigma^*(1)$ N3-H3A	0.01108	0.41161	0.47
π C11-C12	1.69322	– 0.29019				0.73

Table S3

The NBO analysis of N3-H3A... π interaction in a two-molecule assembly of cyclic phosphoric triamide (I). The numbering is according to the X-ray analysis.

Donor			Acceptor			$E^{(2)}$ (kcal.mol ⁻¹)
MOs	Occupancy (e)	E (a.u.)	MOs	Occupancy (e)	E (a.u.)	
π C9-C10	1.62737	–0.28722	σ^* N3-H3A	0.01517	0.41640	1.53
π C11-C12	1.71084	–0.29047				0.86
π C7-C8	1.69519	–0.30024				1.36