Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

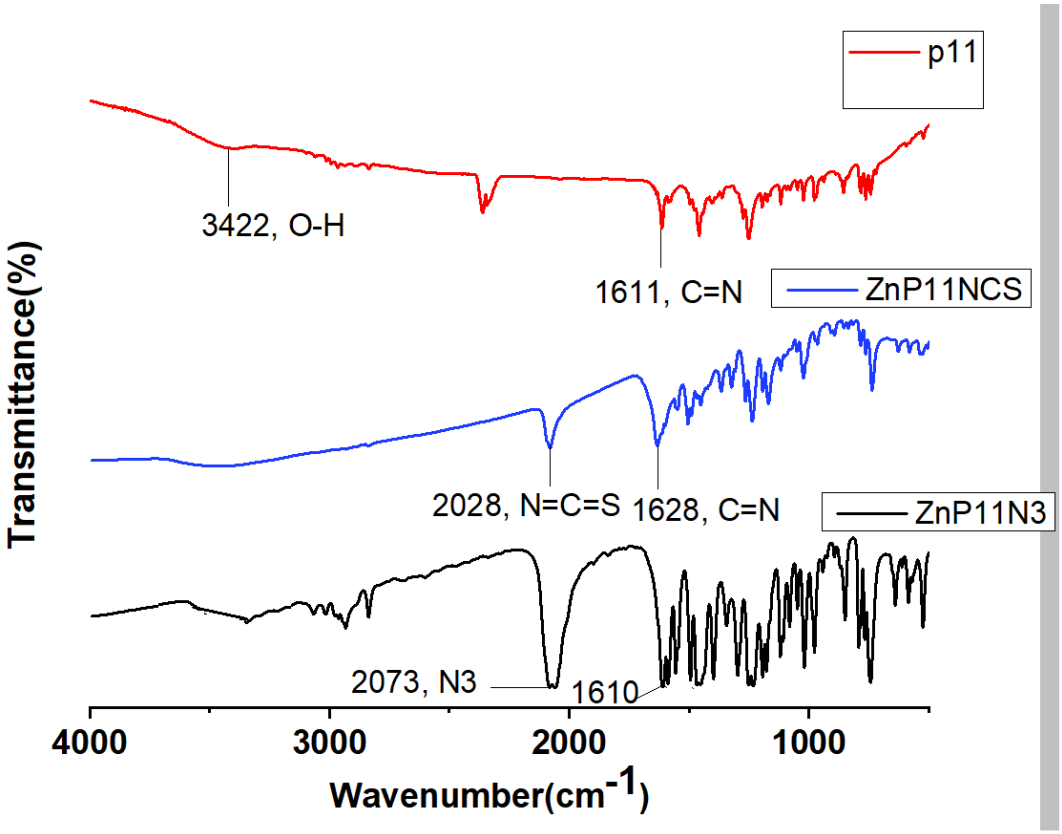

Fig. S1 FT-IR spectra of the zinc complexes

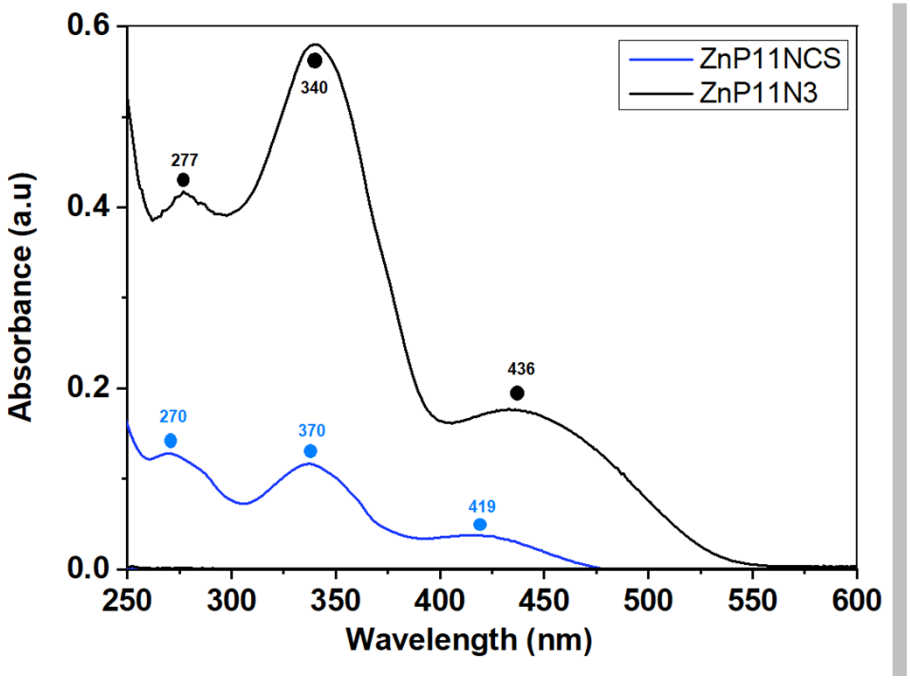

Fig. S2 UV-Vis spectra of the zinc complexes in methanol

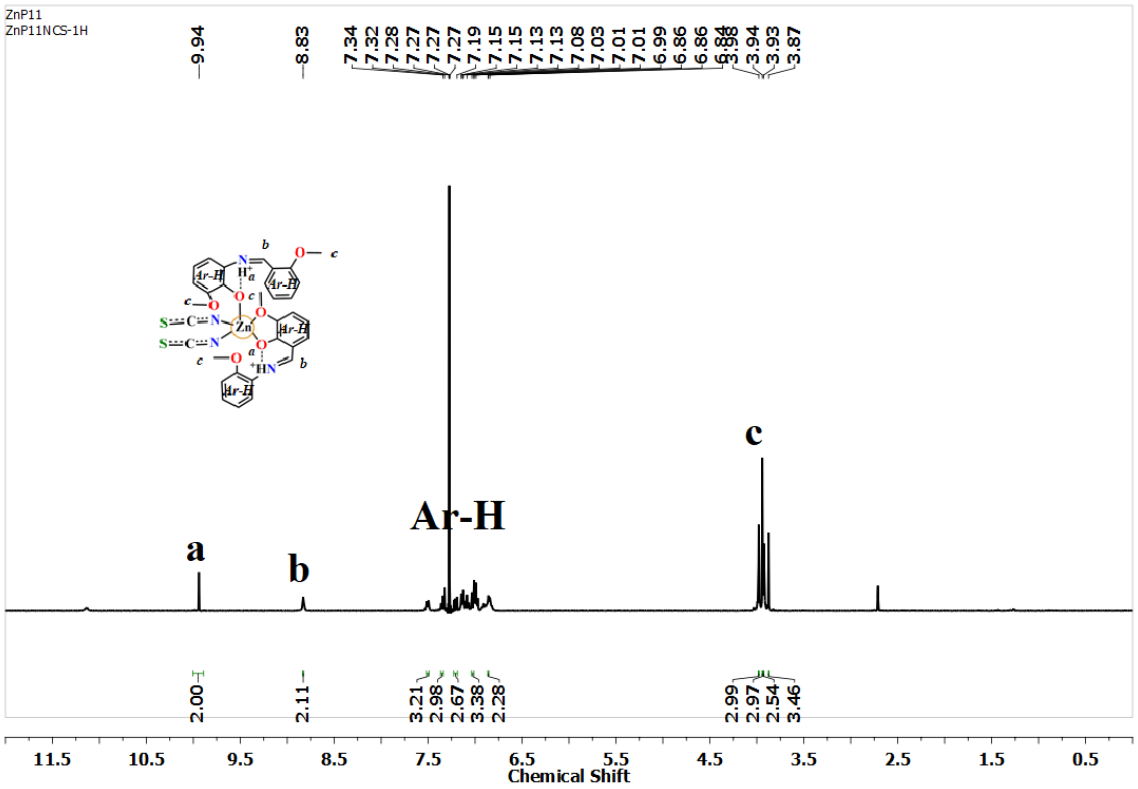

Fig. S3 ^{1}H NMR spectrum of ZnP11^{NCS}

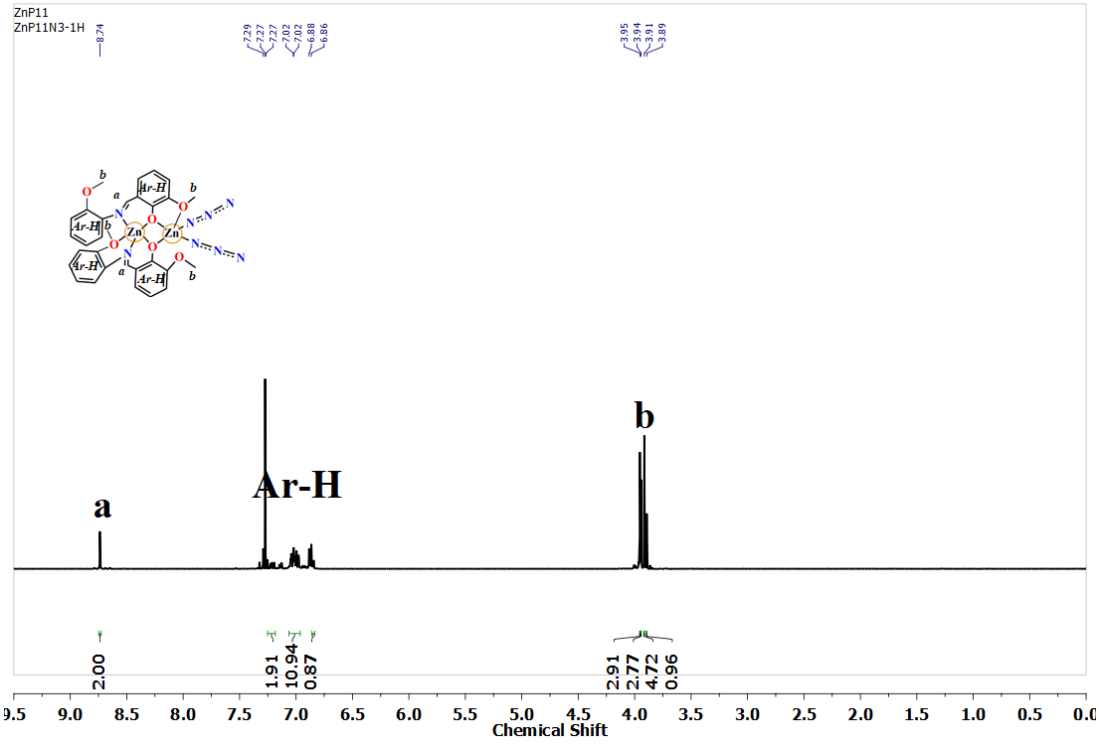

Fig. S4 ^{1}H NMR spectrum of ZnP11^{N3}

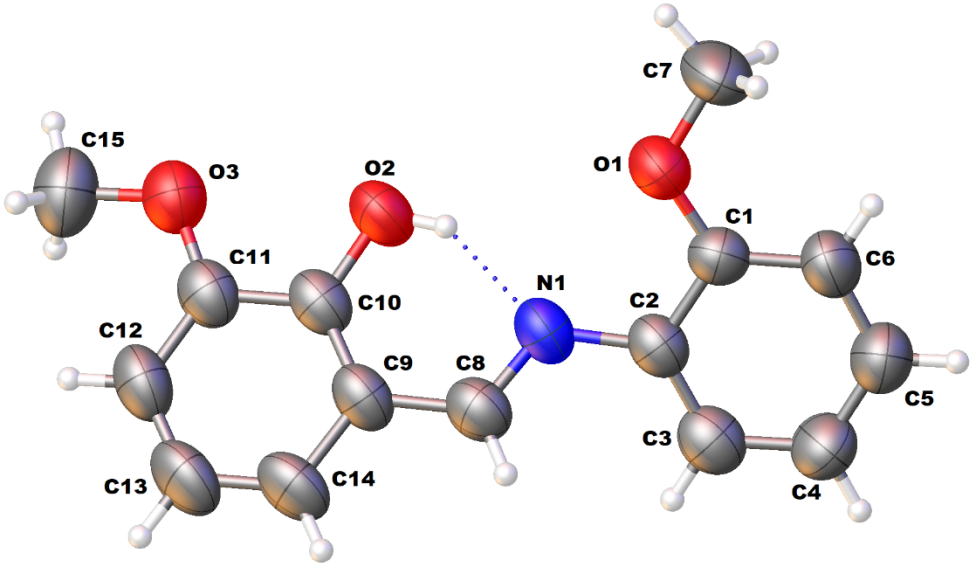

Fig. S5 Molecular structure of the Schiff base complex with 30% ellipsoid probability

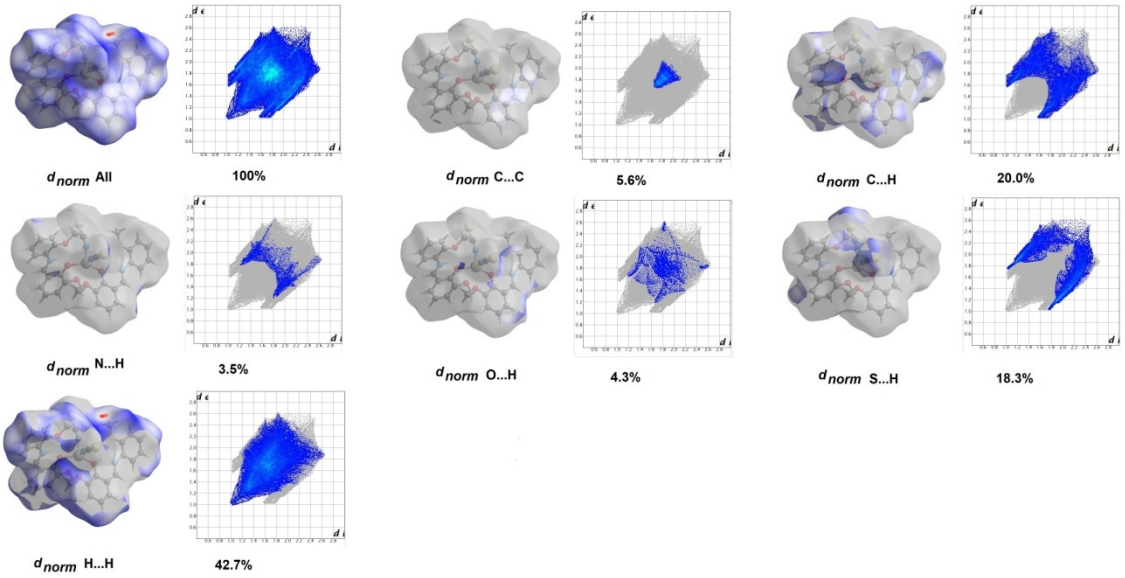

Fig. S6 Hirshfeld surface analysis plots of ZnP11^{NCS}.

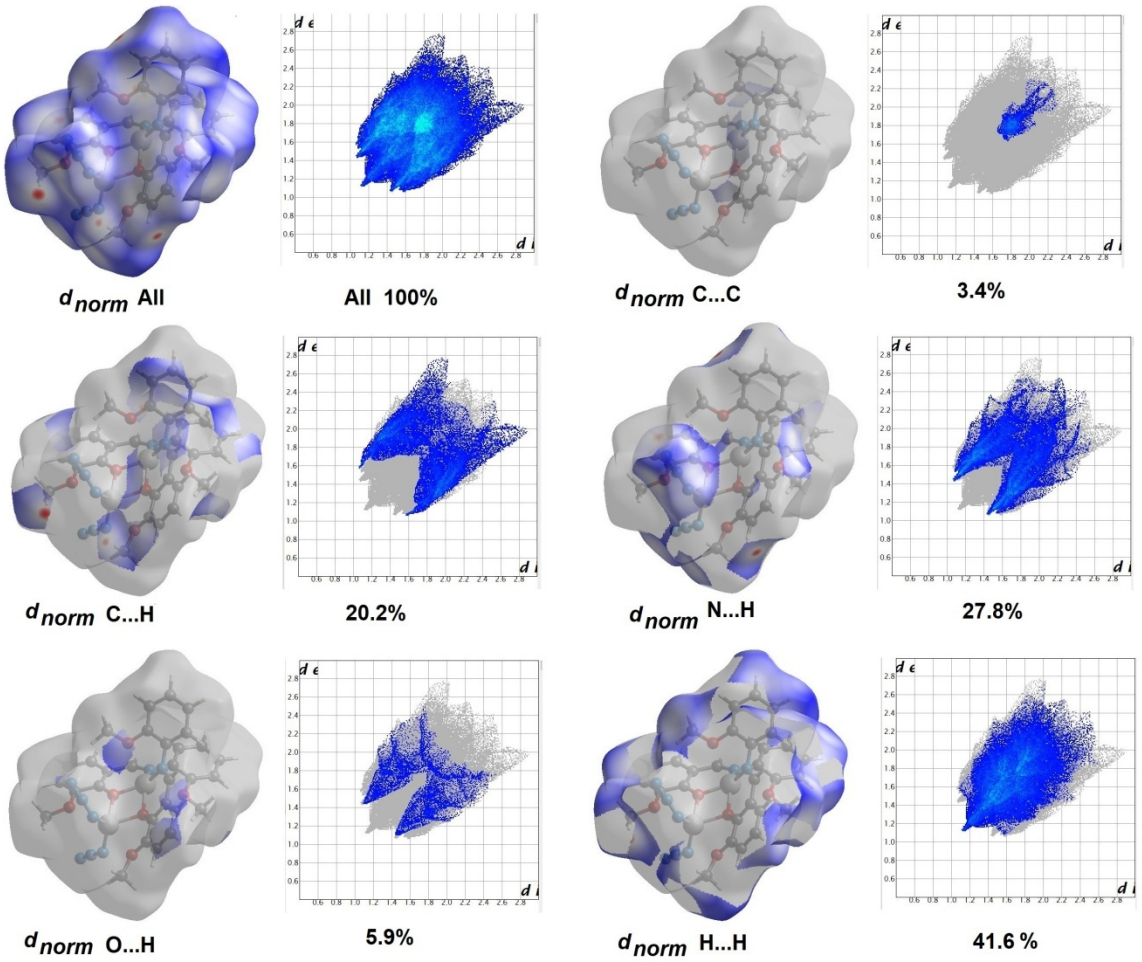

Fig. S7 Hirshfeld surface analysis plots of ZnP11^{N3}.

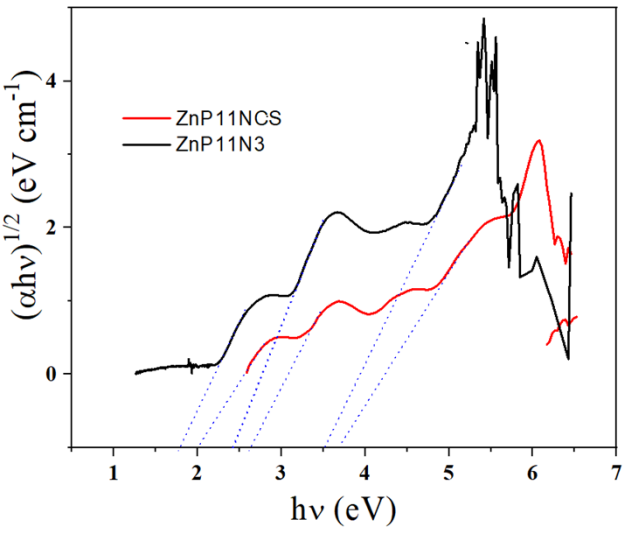

Fig. S8 Tauc plots of the zinc complexes.

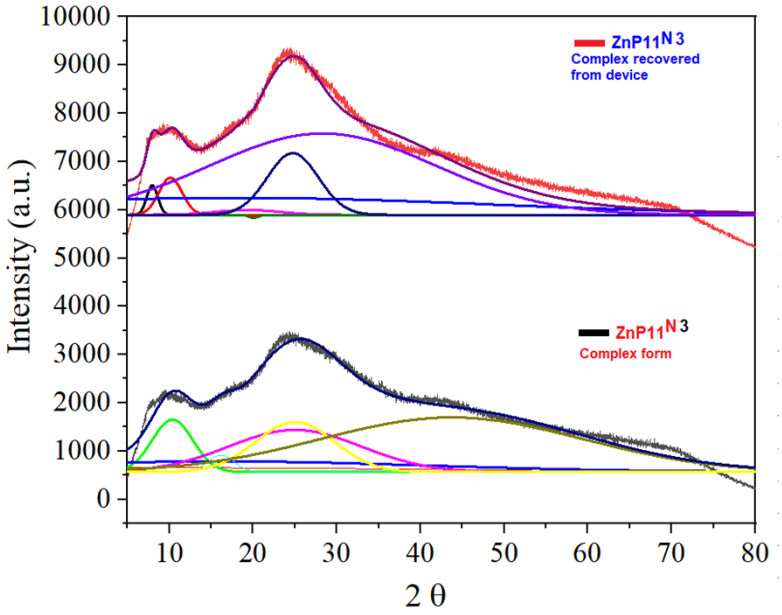

Fig. S9 PXRD plots with de-convoluted peaks of ZnP11^{N3} complex before and after use in device B construction

Table S1. Bond distances and bond angles for the ZnP11^{NCS} complex

Bond lengths (Å)			
Zn1–O1	2.422(2)	Zn1–O2	1.9798(17)
Zn1–O5	1.9975(17)	Zn1–N1	1.993(3)
Zn1–N2	21.988(2)		
Bond angles (°)			
O1–Zn–O2	73.33(7)	O1–Zn1–O5	81.57(7)
O1–Zn–N1	84.18(11)	O1–Zn1–N2	168.92(10)
O2–Zn–O5	138.31(7)	O2–Zn1–N1	103.82(10)
O2–Zn–N2	102.00(9)	O5 –Zn1–N1	106.16(9)
O5–Zn1–N2	96.35(9)	N1–Zn1 –N2	106.80(10)

Table S2. Bond distances and bond angles for the ZnP11^{N3} complex

Bond lengths (Å)			
Zn1–O1	1.9869(15)	Zn1 –O2	2.0094(16)
Zn1–O3	2.3827(17)	Zn1 –O6	2.6041(17)
Zn1–N1	2.0189(18)	Zn1 –N2	2.0440(18)
Zn2 –O1	2.0541(16)	Zn2 –O2	2.0772(16)
Zn2 –O4	2.6605(19)	Zn2 –O5	2.5506(17)
Zn2 –N3	1.962(2)	Zn2 –N6	1.942(3)
Bond angles (°)			
O1 –Zn1 –O2	78.57(7)	O1 –Zn1 –O3	132.49(6)
O1 –Zn1 –O6	88.65(6)	O1 –Zn1 –N1	138.85(7)
O1 –Zn1 –N2	90.15(7)	O2 –Zn1 –O3	90.65(6)
O2 –Zn1 –O6	129.25(6)	O2 –Zn1 –N1	91.27(7)
O2 –Zn1 –N2	143.98(7)	O3 –Zn1–O6	130.47(6)
O3–Zn1 –N1	86.78(6)	O3 –Zn1 –N2	71.97(6)
O6 –Zn1 –N1	67.19(6)	O6 –Zn1 –N2	83.87(6)
N1 –Zn1–N2	118.03(8)	O1 –Zn2 –O2	75.54(6)
O1 –Zn2 –O4	65.32(6)	O1 –Zn2 –O5	141.05(6)
O1 –Zn2 –N3	110.88(9)	O1 –Zn2 –N6	112.36(9)
O2 –Zn2 –O4	139.60(6)	O2 –Zn2 –O5	66.40(6)
O2 –Zn2 –N3	102.39(8)	O2 –Zn2 –N6	118.52(9)
O4 –Zn2 –O5	153.58(6)	O4 –Zn2 –N3	83.29(8)

O4 –Zn2 –N6	86.62(9)	O5 –Zn2 –N3	85.79(8)
O5 –Zn2 –N6	80.47(9)	N3 –Zn2 –N6	125.94(11)

Table S3. Crystallographic data and structure refinement parameters for **HL**

Parameters	**HL**
Empirical formula	$C_{15}H_{15}NO_3$
Formula weight	257.28
Temperature (K)	296
Crystal system	Orthorhombic
Space group	$Pca2_1$
a (Å)	23.723(3)
b (Å)	7.7146(9)
c (Å)	7.3608(5)
Volume ($Å^3$)	1347.1(2)
Z	4
ρ (gcm^{-3})	1.269
μ (mm^{-1})	0.089
F (000)	544
R_{int}	0.040
θ ranges (º)	2.6-32.7
Number of unique reflections	4469
Total number of reflections	10018
Final R indices	0.0601, 0.2106
Largest peak and hole ($eA^{\circ -3}$)	0.17, -0.16

Table S4. Contribution of different energy components to the stabilisation of molecular frameworks for ZnP11^{NCS}

Information **ZnP11^{NCS}**

Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	2	x, y, z	10.83	B3LYP/6-31G(d,p)	-9.5	-2.9	-26.1	22.6	-21.0
	1	-x, -y, -z	16.25	B3LYP/6-31G(d,p)	1.3	-0.3	-1.3	0.0	0.0
	1	-x, -y, -z	8.40	B3LYP/6-31G(d,p)	-85.4	-1.0	-130.9	107.9	-138.4
	2	x, -y, z+1/2	9.89	B3LYP/6-31G(d,p)	-23.9	0.0	-25.0	11.7	-39.8
	1	-x+1/2, -y+1/2, -z	8.78	B3LYP/6-31G(d,p)	-82.6	-0.5	-133.1	100.9	-141.3
	2	x, -y, z+1/2	11.79	B3LYP/6-31G(d,p)	-2.4	-6.1	-11.5	11.0	-10.3
	1	-x, y, -z+1/2	11.81	B3LYP/6-31G(d,p)	-20.5	0.0	-91.0	61.0	-63.2
	2	x+1/2, -y+1/2, z+1/2	18.83	B3LYP/6-31G(d,p)	0.8	-0.6	-6.3	2.8	-3.4
	1	-x+1/2, -y+1/2, -z	12.38	B3LYP/6-31G(d,p)	7.5	-1.1	-20.0	5.7	-6.8
	2	-x+1/2, y+1/2, -z+1/2	13.99	B3LYP/6-31G(d,p)	1.2	-2.5	-24.1	10.0	-15.4
	1	-x, -y, -z	10.57	B3LYP/6-31G(d,p)	-21.2	-9.4	-29.2	15.9	-45.0

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618

Table S5. Contribution of different energy components to the stabilisation of molecular frameworks for ZnP11^{N3}

Information **ZnP11^{N3}**

Crystal | Atoms | Surface | Energies

Interaction Energies (kJ/mol)
R is the distance between molecular centroids (mean atomic position) in Å.

Total energies, only reported for two benchmarked energy models, are the sum of the four energy components, scaled appropriately (see the scale factor table below)

	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	x+1/2, y, -z+1/2	7.99	B3LYP/6-31G(d,p)	-63.7	-21.8	-119.9	84.3	-135.8
	1	x, -y+1/2, z+1/2	12.10	B3LYP/6-31G(d,p)	-19.4	-4.1	-33.3	23.5	-38.0
	0	-x, y+1/2, -z+1/2	8.44	B3LYP/6-31G(d,p)	-36.2	0.0	-71.8	49.0	-70.5
	2	-x+1/2, y+1/2, z	11.30	B3LYP/6-31G(d,p)	-3.9	-7.0	-15.2	11.0	-15.7
	1	-x, -y, -z	12.13	B3LYP/6-31G(d,p)	3.1	0.0	-33.7	18.9	-14.4
	1	x+1/2, -y+1/2, -z	14.33	B3LYP/6-31G(d,p)	2.4	-8.9	-8.5	3.0	-9.6
	0	-x+1/2, -y, z+1/2	14.94	B3LYP/6-31G(d,p)	-8.5	0.0	-4.4	1.6	-11.8
	2	-x+1/2, -y, z+1/2	14.45	B3LYP/6-31G(d,p)	-1.1	-8.8	-2.9	0.0	-10.2
	1	-x, -y, -z	12.54	B3LYP/6-31G(d,p)	0.5	0.0	-15.1	6.2	-8.7

Scale factors for benchmarked energy models
See Mackenzie et al. IUCrJ (2017)

Energy Model	k_ele	k_pol	k_disp	k_rep
CE-HF ... HF/3-21G electron densities	1.019	0.651	0.901	0.811
CE-B3LYP ... B3LYP/6-31G(d,p) electron densities	1.057	0.740	0.871	0.618