

Table S1. The stiffness matrix of VAN-NIC cocrystal, the unit is GPa.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	21.086	9.331	8.495	2.629	-1.421	-2.837
YY	9.331	14.287	10.720	1.554	2.319	0.329
ZZ	8.495	10.720	34.097	2.695	10.054	-5.290
XY	2.629	1.554	2.695	6.294	1.030	-1.952
YZ	-1.421	2.319	10.054	1.030	8.311	-0.041
ZX	-2.837	0.329	-5.290	-1.952	-0.041	5.846

Table S2. The average properties of VAN-NIC cocrystal, the unit is GPa.

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	14.062	17.609	6.819	0.2913
Reuss	10.924	10.464	3.903	0.3404
Hill	12.493	14.07	5.361	0.3123

Table S3. The stiffness matrix of VAN-INM cocrystal, the unit is GPa.

Direction	XX	YY	ZZ	XY	YZ	ZX
XX	12.366	8.029	13.608	-0.823	-1.244	2.780
YY	8.029	21.540	12.977	-1.408	-1.265	4.460
ZZ	13.608	12.977	32.298	-2.872	-4.951	13.968
XY	-0.823	-1.408	-2.872	4.354	5.480	-2.500
YZ	-1.244	-1.265	-4.951	5.480	10.030	-4.208
ZX	2.780	4.460	13.968	-2.500	-4.208	10.907

Table S4. The average properties of VAN-INM cocrystal, the unit is GPa.

Averaging scheme	Bulk modulus	Young's modulus	Shear modulus	Poisson's ratio
Voigt	15.048	18.549	7.164	0.2946
Reuss	10.137	6.095	2.177	0.3998
Hill	12.593	12.470	4.671	0.3350

