

1 **Supplementary Material**

2 **P1-C₇N₄O₈: Improved Stability and Energy Density via a**
3 **Covalent Framework with Uniform Single Bonds**

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14 **Table S1.** Crystal structure parameters of $P1-C_7N_4O_8$ at 31 GPa.

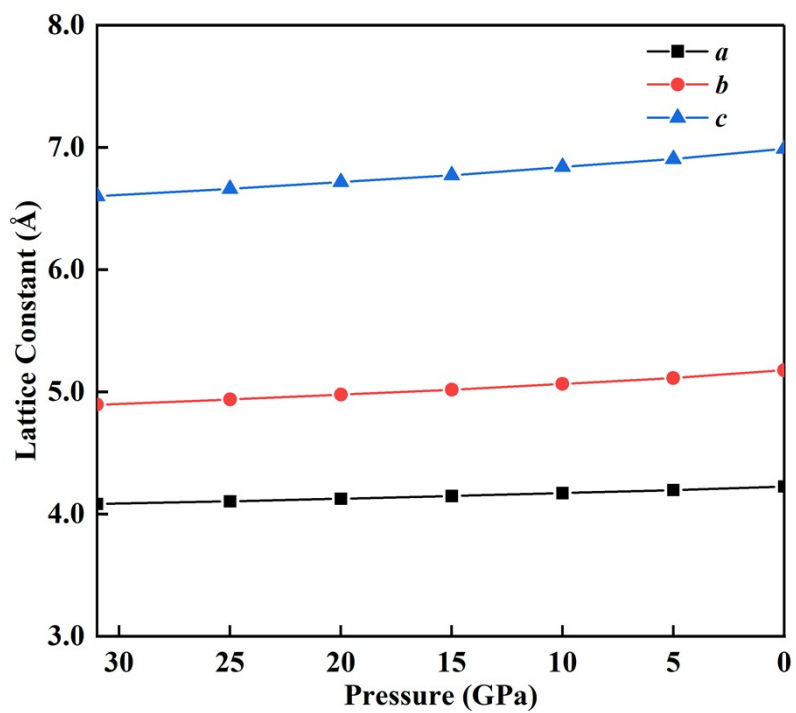
Structure	Lattice parameters	Atomic coordinates
$P1-C_7N_4O_8$	$a=4.083 \text{ \AA};$ $b=4.896 \text{ \AA};$ $c=6.602 \text{ \AA}$ $\alpha=68.430^\circ;$ $\beta=75.908^\circ;$ $\gamma=118.423^\circ$	C1 0.318612 0.448583 0.513528
		C2 0.052831 0.109059 0.185609
		C3 0.513996 0.262853 0.856419
		C4 0.007646 0.503501 0.852760
		C5 0.267220 0.892712 0.655908
		C6 0.806848 0.182061 0.518609
		C7 0.551381 0.864422 0.180721
		N1 0.607084 0.370443 0.605619
		N2 0.117189 0.169214 0.583360
		N3 0.137121 0.639799 0.615371
		N4 0.159805 0.250576 0.947045
		O1 0.338543 0.040007 0.264617
		O2 0.119490 0.744713 0.890543
		O3 0.605325 0.975437 0.948186
		O4 0.401923 0.578454 0.275552
		O5 0.846990 0.849413 0.247330
O6 0.662740 0.452763 0.928385		
O7 0.616580 0.909982 0.600995		
O8 0.886441 0.297441 0.279188		

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16 **Table S2.** Bond length and integrated crystal orbital Hamilton population (-ICOHP) of $P1-C_7N_4O_8$ at 31 GPa and 0
17 GPa.

Chemical Bonds	31 GPa		0 GPa	
	Bond length (Å)	-ICOHP (eV)	Bond length (Å)	-ICOHP (eV)
N10-C1	1.449	-11.348	1.479	-10.793
N10-C4	1.417	-11.397	1.419	-11.416
N10-C5	1.488	-10.070	1.569	-8.262
N11-C2	1.419	-11.878	1.457	-11.065
N11-C3	1.416	-12.057	1.446	-11.393
N11-C4	1.390	-12.454	1.408	-12.091
N8-C1	1.443	-11.306	1.478	-10.738
N8-C3	1.488	-10.531	1.563	-9.125
N8-C6	1.418	-12.072	1.453	-11.461

N9-C1	1.452	-11.279	1.524	-9.909
N9-C5	1.451	-11.370	1.507	-10.365
N9-C6	1.427	-11.770	1.475	-10.945
O12-C2	1.384	-12.286	1.400	-11.930
O12-C7	1.385	-12.136	1.399	-11.901
O13-C4	1.391	-11.404	1.414	-10.730
O13-C5	1.417	-10.804	1.413	-11.038
O14-C3	1.404	-11.821	1.430	-11.233
O14-C7	1.386	-12.267	1.414	-11.609
O15-C1	1.412	-11.479	1.436	-11.005
O15-C7	1.375	-12.534	1.408	-11.729
O16-C2	1.392	-11.895	1.413	-11.433
O16-C7	1.375	-12.573	1.394	-12.167
O17-C3	1.387	-11.981	1.398	-11.898
O17-C4	1.364	-12.545	1.395	-11.687
O18-C5	1.378	-12.677	1.406	-12.028
O18-C6	1.390	-12.091	1.416	-11.516
O19-C2	1.382	-12.484	1.410	-11.867
O19-C6	1.420	-11.163	1.467	-10.148
Average value	1.410	-11.774	1.443	-11.124
Standard deviation	0.032	0.641	0.049	0.894



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20 **Figure S1.** During releasing pressure from 31 GPa to ambient conditions, the change of lattice
 21 constant of of P1-C₇N₄O₈.

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