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Pressure-induced Novel Nitrogen-Rich Aluminum Nitrides: AlN<sub>6</sub>, Al<sub>2</sub>N<sub>7</sub> and AlN<sub>7</sub> with Polymeric Nitrogen Chain and Ring

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<sup>&</sup>lt;sup>+</sup>Electronic Supplementary Information (ESI) available: Supplementary material includes structural information, fluctuations of the total energies obtained by molecular dynamics simulation under high temperature, electronic structure and phonon spectrum under high pressure. See DOI: 10.1039/x0xx00000x

structures	lattice parameters(Å)	atomic coordinates
	a = 9.76	Al1(0.098,0.000,0.866)
	b = 3.10	Al2(0.113,0.000,0.360)
Cm-AlN <sub>2</sub>	c = 5.91	A13(0.598,0.500,0.866)
P = 0 GPa	$\alpha = 90.00$	Al4(0.613,0.500,0.360)
	$\beta = 154.08$	N1(0.855,0.500,0.988)
	$\gamma = 90.00$	N2 (0.355,0.000, 0.988)
$\bar{P3m_{1-Al_2N}}$	a = 2.81	Al1 (0.333, 0.667, 0.768)
P = 20  GPa	b = 2.81	Al2 (0.667, 0.333, 0.232)
	c = 8.67	A13(0.000, 0.000, 0.500
	$\alpha = 90.00$	Al4(0.000, 0.000, 0.000)
	$\beta = 90.00$	N1 (0.667, 0.333, 0.632)
	$\gamma = 120.00$	N2(0.333, 0.667, 0.368)
$P^{\bar{3}}m_{1}$ -Al <sub>2</sub> N	a = 2.74	
P = 40  GPa	b = 2.74	All (0.333, 0.667, 0.768)
	c = 4.25	Al2 (0.667, 0.333, 0.232)
	$\alpha = 90.00$	N1 (0.000, 0.000, 0.500)
	$\beta = 90.00$	(,,,,
	$\gamma = 120.00$	
	a = 3.90	
	b = 2.63	Al1 (0.000, 0.000, 0.000)
$\frac{P2/m-Al_2N}{P=0.000}$	c = 2.65	A12 (0.500, 0.500, 0.500)
P = 60 GPa	$\alpha = 90.00$ $\alpha = 06.75$	N1 (0.500, 0.000, 0.000)
	$\beta = 96.75$ $\gamma = 90.00$	
-2m	$\gamma = 30.00$ a = 2.64	
$p\bar{3}m_{1-\mathrm{Al}_2\mathrm{N}}$	a = 2.64 b = 2.64	
P = 80  GPa	c = 4.13	Al1 (0.667, 0.333, 0.768)
	$\alpha = 90.00$	Al2 (0.333, 0.667, 0.232)
	$\beta = 90.00$	N1 (0.000, 0.000, 0.500)
	$\gamma = 120.00$	
	a = 3.12	
	b = 3.12	All (0.333, 0.667, 0.250)
$P6_3mc$ -AlN	c = 4.88	Al2 (0.667, 0.333, 0.750)
P = 0 GPa	$\alpha = 90.00$	N1 (0.333, 0.667, 0.750)
	$\beta = 90.00$	N2 (0.667, 0.333, 0.250)
	$\gamma = 120.00$	
$Fm^{\overline{3}}m$ -AlN		Al1 (0.500, 0.000, 0.000)
P = 20  GPa	a = 3.04	Al2 (0.500, 0.500, 0.500)
	b = 3.04	A13 (0.000, 0.000, 0.500)
	c = 3.75	Al4 (0.000, 0.500, 0.000)
	$\alpha = 90.00$	N1 (0.000, 0.000, 0.000)
	$\beta = 90.00$	N2 (0.000, 0.500, 0.500)
	$\gamma = 120.00$	N3 (0.500, 0.000, 0.500)
		N4 (0.500, 0.500, 0.000)
		All (0.058,0.500, 0.236)
		Al2 (0.942,0.500,0.764)

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$R^3m$ -Al <sub>2</sub> N <sub>3</sub>	a = 7.11	Al3 (0.558,0.000,0.236)
P = 0 GPa	b = 2.75	Al4 (0.442,0.000,0.764)
	c = 6.64	N1 (0.0662,0.000,0.462)
	$\alpha = 90.00$	N2 (0.434, 0.500,0.538)
	$\beta = 132.00$	N3 (0.000,0.000,0.000)
	$\gamma = 90.00$	N4 (0.566,0.500,0.462)
		N5 (0.934,0.000,0.538)
		N6 (0.500,0.500,0.000)
$R^{\overline{3}}m$ -Al <sub>2</sub> N <sub>3</sub>	a = 6.00	Al1(0.733,0.733,0.733)
P = 20 GPa	b = 6.00	Al2(0.267,0.267,0.267)
	c = 6.00	
	$\alpha = 27.04$	N1(0.461,0.461,0.461)
	$\beta = 27.04$	N2(0.000,0.000,0.000)
	$\gamma = 27.04$	N3(0.539,0.539,0.538)
		Al1(0.750,0.250,0.500)
		Al2(0.750,0.750,0.500)
	a = 5.88	Al3(0.250,0.750,0.500)
	b = 4.91	A14(0.250,0.250,0.500)
$Cmmm-Al_2N_3$	c = 2.57	N1(0.118,0.000,0.000)
P = 40  GPa	$\alpha = 90.00$	N2(0.500,0.000,0.500)
	$\beta = 90.00$	N3(0.882,0.000,0.000)
	$\gamma = 90.00$	N4(0.618,0.500,0.000)
	1 20.00	N5(0.000,0.500,0.500)
		N6(0.382,0.500,0.000)
$R^3m$ -Al <sub>2</sub> N <sub>3</sub>	a = 5.85	
P = 60  GPa	b = 5.85	Al1(0.267,0.267,0.267)
P = 60  GPa	c = 5.85	Al2(0.733,0.733,0.733)
	$\alpha = 26.63$	N1(0.461,0.461,0.461)
	$\beta = 26.63$	N2(0.000,0.000,0.000)
	$\gamma = 26.63$	N3(0.539,0.539,0.539)
	a = 5.98	
	b = 5.98	Al1(0.341,0.341,0.341)
R3m-Al <sub>2</sub> N <sub>3</sub>	c = 5.98	Al2(0.477,0.477,0.477)
P = 80  GPa	$\alpha = 25.32$	N1(0.948,0.948,0.948)
1 00 01 4	$\beta = 25.32$ $\beta = 25.32$	N2(0.740,0.740,0.740)
	$\gamma = 25.32$	N3(0.874,0.874,0.874)
$R\overline{3}_{m-AlN_2}$	a = 3.89	
P = 0  GPa	b = 3.89	
1 0 01 4	c = 3.89	All (0.000, 0.000, 0.000)
	$\alpha = 44.04$	N1 (0.564, 0.564, 0.564)
	$\beta = 44.04$	N2 (0.436, 0.436, 0.436)
	$\gamma = 44.04$	
	a = 4.95	Al1 (0.000,0.500, 0.500)
	b = 2.82	Al2 (0.371,0.500,0.730)
C2/m-AlN <sub>2</sub>	c = 9.95	Al3 (0.129,0.000,0.270)
P = 20  GPa	$\alpha = 90.00$	Al4 (0.500,0.000,0.500)
1 20 Gru	$\beta = 95.31$	Al5 (0.871,0.000,0.730)
	$\gamma = 90.00$	Al6 (0.629,0.000,0.730)
	y = 90.00	A10(0.023, 0.000, 0.730)

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		N1 (0.0618,0.500,0.832)
		N2 (0.900, 0.500,0.036)
		N3 (0.938,0.500,0.168)
		N4 (0.186,0.000,0.615)
		N5 (0.314,0.500,0.385)
		N6 (0.100,0.500,0.964)
		N7 (0.562,0.000,0.832)
		N8 (0.400,0.000,0.036)
		N9 (0.438,0.000,0.168)
		N10 (0.686,0.500,0.615) N11 (0.814,0.000,0.385)
		N11 (0.814,0.000,0.383) N12 (0.600,0.000,0.964)
	a = 2.66	1112 (0.000,0.000,0.904)
	a = 2.60 b = 2.66	
P6/mmm-AlN <sub>2</sub>	c = 4.90	Al1 (0.000, 0.000, 0.000)
P = 40  GPa	$\alpha = 90.00$	N1 (0.000, 0.000, 0.382)
1 +0 01 u	$\beta = 90.00$	N2 (0.000, 0.000, 0.617)
	$\gamma = 120.00$	
	a = 4.45	Al1 (0.000, 0.000, 0.000)
	b = 3.72	A12 (0.500, 0.500, 0.500)
Pnnm-AlN <sub>2</sub>	c = 2.54	N1 (0.596, 0.135, 0.000)
$P = 60 \text{ GPa}^2$	$\alpha = 90.00$	N2 (0.404, 0.865, 0.000)
	$\beta = 90.00$	N3 (0.904, 0.635, 0.500)
	$\gamma = 90.00$	N4 (0.096, 0.365, 0.500)
$R^{\overline{3}}m$ -AlN <sub>2</sub>	a = 4.45	
P = 80  GPa	b = 3.72	A 11 (0.500, 0.500, 0.500)
1 00 01 0	c = 2.54	Al1 (0.500, 0.500, 0.500) N1 (0.064, 0.064, 0.064)
	$\alpha = 90.00$	N1 (0.004, 0.004, 0.004) N2 (0.936, 0.936, 0.936)
	$\beta = 90.00$	N2(0.930, 0.930, 0.930)
	$\gamma = 90.00$	
	a = 4.45	Al1(0.301,0.968,0.521)
	b = 3.72	Al2(0.836,0.318,0.820)
$Pl-Al_2N_5$	c = 2.54	N1(0.146,0.111,0.179)
P = 0 GPa	$\alpha = 90.00$	N2(0.177,0.660,0.818)
	$\beta = 90.00$	N3(0.955,0.278,0.057)
	$\gamma = 90.00$	N4(0.343,0.941,0.302)
	· · · · · ·	N5(0.654,0.308,0.570)
		Al1(0.161,0.500,0.923)
		Al2(0.738,0.500,0.449)
	7.02	Al3(0.661,0.000,0.923)
	a = 7.02 b = 2.77	Al4(0.238,0.000,0.449)
Cm A1 N	b = 2.77 c = 5.73	N1(0.791,0.500,0.111) N2(0.014,0.000,0.762)
$Cm-Al_2N_5$ $P = 20 \text{ GPa}$	$\alpha = 90.00$	N2(0.014,0.000,0.782) N3(0.837,0.000,0.680)
1 - 20 Or a	$\beta = 95.68$	N3(0.837,0.000,0.080) N4(0.979,0.500,0.150)
	$\gamma = 90.00$	N5(0.038,0.500,0.375)
	1 70.00	N6(0.291,0.000,0.111)
		N7(0.514,0.500,0.762)
		N8(0.337,0.500,0.680)
	1	110(0.337,0.300,0.000)

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		NO(0.480.0.000.0.150)
		N9(0.480,0.000,0.150) N10(0.538,0.000,0.375)
	+	
$P^1$ -Al <sub>2</sub> N <sub>5</sub>	a = 2.77	Al1(0.849,0.396,0.650)
P = 40 GPa	b = 2.77	Al2(0.151,0.603,0.350)
	c = 7.59	N1(0.815,0.178,0.046)
	$\alpha = 99.69$	N2(0.185,0.822,0.955)
	$\beta = 96.51$	N3(0.500,0.000,0.501)
	$\gamma = 62.02$	N4(0.211,0.794,0.783)
		N5(0.789,0.206,0.219)
	a = 2.66	Al1(0.599,0.099,0.873)
	b = 2.70	Al2(0.136,0.234,0.408)
P1 -Al <sub>2</sub> N <sub>5</sub>	c = 5.31	N1(0.428,0.839,0.335)
P = 60 GPa	$\alpha = 93.30$	N2(0.241,0.351,0.064)
	$\beta = 92.68$	N3(0.944,0.812,0.706)
	$\gamma = 110.52$	N4(0.407,0.725,0.099)
		N5(0.765,0.455,0.631)
	a = 2.52	Al1(0.367,0.764,0.472)
	b = 3.88	Al2(0.358,0.189,0.102)
P1 -Al <sub>2</sub> N <sub>5</sub>	c = 4.75	N1(0.809,0.832,0.102)
P = 80 GPa	$\alpha = 99.64$	N2(0.934,0.320,0.829)
	$\beta = 77.38$	N3(0.950,0.666,0.833)
	$\gamma = 94.90$	N4(0.829,0.400,0.384)
		N5(0.886,0.143,0.556)
		Al1(0.242,0.247,0.074)
		Al2(0.242,0.753,0.074)
		Al3(0.742,0.747,0.074)
		Al4(0.742,0.253,0.074)
		N1(0.355,0.181,0.636)
	a = 7.10	N2(0.855,0.319,0.636)
	b = 7.01	N3(0.401,0.500,0.121)
Cm-AlN <sub>3</sub>	c = 3.26	N4(0.067,0.000,0.073)
P = 0 GPa	$\alpha = 90.00$	N5(0.527,0.098,0.784)
	$\beta = 103.47$	N6(0.027,0.402,0.784)
	$\gamma = 90.00$	N7(0.855,0.681,0.636)
		N8(0.355,0.819,0.636)
		N9(0.901,0.000,0.121)
		N10(0.567,0.500,0.073)
		N11(0.027,0.598,0.784)
דת.		N12(0.527,0.902,0.784)
$P\bar{1}_{-AlN_3}$	2.00	Al1(0.256,0.226,0.803)
P = 20 GPa	a = 2.80	Al2(0.744,0.774,0.197)
	b = 4.67	N1(0.780,0.197,0.088)
	c = 4.90	N2(0.727,0.215,0.540)
	$\alpha = 79.24$	N3(0.220,0.803,0.912)
	$\beta = 92.58$	N4(0.748,0.348, 0.288)
	$\gamma = 94.22$	N5(0.273,0.785, 0.460)
		N6(0.252,0.652,0.712)
		Al1 (0.244, 0.876, 0.090)

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		Al2 (0.756, 0.124, 0.910)
		Al3 (0.756, 0.376, 0.410)
	a = 11.56	Al4 (0.244, 0.624, 0.590)
$P2_1/c$ -AlN <sub>3</sub>	b = 3.66	N1 (0.258, 0.755, 0.369)
P = 40 GPa	c = 11.22	N2 (0.742, 0.245, 0.631)
	$\alpha = 90.00$	N3 (0.742, 0.255, 0.131)
	$\beta = 165.99$	N4 (0.258, 0.745, 0.869)
	$\gamma = 120.00$	N5 (0.109, 0.656, 0.110)
	,	N6 (0.891, 0.344, 0.890)
		N7 (0.891, 0.156, 0.390)
		N8 (0.109, 0.844, 0.610)
		N9 (0.743, 0.957, 0.055)
		N10 (0.257, 0.043, 0.945)
		N11 (0.257, 0.457, 0.445)
		N12 (0.743, 0.543, 0.555)
		Al1(0.885,0.972,0.248)
		Al2(0.423,0.439,0.120)
	a = 3.16	N1(0.657,0.196,0.687)
	b = 5.24	N2(0.280,0.576,0.527)
P1-Al <sub>2</sub> N <sub>7</sub>	c = 6.98	
P = 0 GPa	$\alpha = 101.35$	N3(0.173,0.693,0.676)
	$\beta = 84.46$	N4(0.806,0.089,0.533)
	$\gamma = 91.46$	N5(0.918,0.617,0.174)
	·	N6(0.506,0.308,0.839)
		N7(0.404,0.114,0.188)
		Al1(0.153,0.500,0.054)
		Al2(0.294,0.500,0.478)
		Al3(0.653,0.000,0.054)
		Al4(0.794,0.000,0.478)
	a = 5.69	N1(0.243,0.202,0.749)
	b = 4.77	N2(0.804,0.274,0.224)
Cm-Al <sub>2</sub> N <sub>7</sub>	c = 5.27	N3(0.304,0.226,0.224)
P = 20 GPa	$\alpha = 90.00$	N4(0.061,0.000,0.792)
	$\beta = 63.26$	N5(0.159,0.000,0.305)
	$\gamma = 90.00$	N6(0.429,0.000,0.704)
		N7(0.243,0.798,0.749)
		N8(0.743,0.702,0.749)
		N9(0.304,0.774,0.224)
		N10(0.804,0.726,0.224)
		Al1(0.153,0.500,0.054)
		Al2(0.294,0.500,0.478)
	a - 5.60	Al3(0.653,0.000,0.054)
	a = 5.69 b = 4.77	Al4(0.794,0.000,0.478)
C A1 N	b = 4.77	N1(0.243,0.201,0.748)
$Cm-Al_2N_7$	c = 5.27	N2(0.804,0.273,0.223)
P = 40  GPa	$\alpha = 90.00$	N3(0.304,0.226,0.223)
	$\beta = 63.26$	N4(0.060,0.000,0.791)
	$\gamma = 90.00$	N5(0.159,0.000,0.304)
		N6(0.429,0.000,0.703)
		N7(0.243,0.798,0.748)
	1	11, (0.213, 0.170, 0.170)

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$\begin{array}{c cccc} P_{2/m-A} \mathrm{IN}_4 & a = 4.84 \\ P = 0 \ \mathrm{GPa} & a = 4.84 \\ P = 0 \ \mathrm{GPa} & a = 2.84 \\ P = 20 \ \mathrm{GPa} & \mathrm{GPa}$			
$\begin{array}{c cccc} P_{2}(2,-\Lambda _{2}N_{7}) & N11(0.560,0.500,0.791) \\ N12(0.659,0.500,0.703) \\ N13(0.929,0.500,0.703) \\ N14(0.743,0.298,0.748) \\ Al1(0.728,0.832,0.209) \\ Al2(0.771,0.332,0.790) \\ Al3(0.228,0.332,0.209) \\ Al2(0.771,0.332,0.790) \\ Al3(0.228,0.332,0.209) \\ Al4(0.271,0.332,0.790) \\ Al4(0.271,0.332,0.790) \\ N1(0.092,0.224,0.543) \\ N2(0.569,0.197,0.863) \\ N3(0.115,0.539,0.411) \\ N10(0.00,0.452,0.000) \\ c = 4.88 \\ N5(0.884,0.539,0.588) \\ \beta = 127.29 \\ \gamma = 90.00 \\ N6(0.907,0.224,0.543) \\ N9(0.069,0.697,0.136) \\ N8(0.592,0.724,0.543) \\ N9(0.069,0.697,0.136) \\ N8(0.592,0.724,0.543) \\ N9(0.069,0.697,0.863) \\ N10(0.615,0.039,0.411) \\ N11(0.000,0.952,0.000) \\ N12(0.384,0.039,0.588) \\ N13(0.407,0.724,0.456) \\ \hline \\ P_{2}/m-AlN_{4} \\ p = 0 GPa \\ A = 4.84 \\ b = 2.96 \\ N1(0.062,0.000,0.343) \\ N10(0.62,0.000,0.343) \\ N10(0.62,0.000,0.343) \\ N10(0.62,0.000,0.500) \\ N1(0.062,0.000,0.343) \\ N10(0.602,0.000,0.500) \\ N12(0.384,0.039,0.588) \\ N13(0.407,0.724,0.456) \\ \hline \\ P_{2}/m-AlN_{4} \\ p = 0 GPa \\ A = 2.84 \\ N1(0.500,0.000,0.000) \\ Al2(0.000,0.500,0.000) \\ Al2(0.000,0.500$			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			N12(0.659,0.500,0.304)
$\begin{array}{cccc} P_{2/m-AlN_4} & a = 4.84 \\ P = 0 & GPa & a = 4.84 \\ P = 0 & GPa & a = 4.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 0.00 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & a = 0.00 \\ P = 0 & GPa & a = 2.84 \\ P = 0 & GPa & A = 0.00 \\ P = 0 & OPA & A = 0.00 \\ P = 0 & O$			N13(0.929,0.500,0.703)
$\begin{array}{cccc} P2/m-AIN_4 \\ P = 0 \ GPa \\ \begin{array}{c} a = 4.84 \\ b = 2.96 \\ P = 0 \ GPa \\ P = 0 \ GPa \\ \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ rathored p = 0.00 \\ rathored p $			N14(0.743,0.298,0.748)
$\begin{array}{cccc} P2/m-AIN_4 \\ P = 0 \ GPa \\ \begin{array}{c} a = 4.84 \\ b = 2.96 \\ P = 0 \ GPa \\ P = 0 \ GPa \\ \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ p = 90.00 \\ P2/m-AIN_4 \\ P = 0 \ GPa \\ \end{array} \begin{array}{c} a = 4.84 \\ b = 2.96 \\ rathored p = 0.00 \\ rathored p $			Al1(0.728,0.832,0.209)
$\begin{array}{cccc} C2-Al_2N_7 & a = 8.18 & N2(0.528, 0.332, 0.209) & Al4(0.271, 0.832, 0.790) & N1(0.092, 0.224, 0.543) & N2(0.569, 0.197, 0.863) & N2(0.569, 0.197, 0.863) & N2(0.569, 0.197, 0.863) & N3(0.115, 0.539, 0.411) & N4(0.500, 0.452, 0.000) & \beta = 127.29 & N6(0.907, 0.224, 0.456) & \gamma = 90.00 & N5(0.884, 0.539, 0.588) & N5(0.884, 0.592, 0.724, 0.456) & N7(0.930, 0.697, 0.863) & N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & & & & & & & & & \\ P = 0 & GPa & a = 4.84 & A11(0.500, 0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & & & & & & & & & & & \\ P = 0 & GPa & a = 90.00 & N2(0.938, 0.000, 0.677) & & & & & & & & & & & & & & & & & & $			Al2(0.771,0.332,0.790)
$\begin{array}{cccc} C2-Al_2N_7 & a = 8.18 & b = 3.52 & N3(0.115, 0.539, 0.411) \\ C2-Al_2N_7 & c = 4.88 & N2(0.569, 0.197, 0.863) \\ P = 80 GPa & a = 90.00 & N5(0.884, 0.539, 0.588) \\ \alpha = 90.00 & N5(0.884, 0.539, 0.588) & N6(0.907, 0.224, 0.456) \\ \beta = 127.29 & \gamma = 90.00 & N6(0.907, 0.224, 0.456) \\ \gamma = 90.00 & N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) \\ N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) \\ N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) \\ \hline \\ P = 0 GPa & a = 4.84 & b = 2.96 & N1(0.062, 0.000, 0.343) \\ P = 0 GPa & a = 90.00 & N2(0.938, 0.000, 0.657) \\ \gamma = 90.00 & N2(0.938, 0.000, 0.657) \\ \gamma = 90.00 & N2(0.938, 0.000, 0.675) \\ \gamma = 90.00 & N4(0.479, 0.500, 0.675) \\ \gamma = 90.00 & N4(0.479, 0.500, 0.000) \\ A12(0.000, 0.500, 0.325) & b = 4.11 & N2(0.500, 0.398, 0.335) \\ B = 4.11 & N2(0.500, 0.675) & N4(0.479, 0.500, 0.675) \\ \gamma = 90.00 & N5(0.000, 0.895, 0.329) \\ \beta = 90.00 & N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 & N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 & N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 & N5(0.000, 0.65, 0.329) \\ \beta = 40 GPa & a = 2.86 & N1(0.500, 0.000, 0.500) \\ \alpha = 102.88 & N2(0.044, 0.695, 0.634) \\ \beta = 111.13 & N3(0.843, 0.349, 0.996) \\ \gamma = 93.98 & N4(0.157, 0.651, 0.004) \\ \end{array}$			
$\begin{array}{cccc} C2-Al_2N_7 & a = 8.18 & b = 3.52 & N1(0.092, 0.224, 0.543) & N2(0.569, 0.197, 0.863) & N3(0.115, 0.539, 0.411) & N4(0.500, 0.452, 0.000) & N5(0.884, 0.539, 0.588) & N4(0.500, 0.452, 0.000) & N5(0.884, 0.539, 0.588) & N6(0.907, 0.224, 0.456) & N7(0.930, 0.697, 0.136) & N8(0.592, 0.724, 0.543) & N9(0.0697, 0.863) & N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & N10(0.62, 0.000, 0.507) & N10(0.615, 0.039, 0.411) & N11(0.000, 0.520, 0.000) & N12(0.384, 0.039, 0.588) & N12(0.384, 0.039, 0.588) & N12(0.938, 0.000, 0.657) & N2(0.938, 0.000, 0.657) & N2(0.938, 0.000, 0.657) & N2(0.938, 0.000, 0.557) & N2(0.938, 0.000, 0.657) & N2(0.938, 0.000, 0.657) & N2(0.938, 0.000, 0.550) & N1(0.500, 0.602, 0.835) & b = 4.11 & N2(0.500, 0.500, 0.675) & N4(0.479, 0.500, 0.675) & N4(0.479, 0.500, 0.675) & N2(0.900, 0.895, 0.329) & A = 90.00 & N4(0.000, 0.105, 0.829) & A = 90.00 & N4(0.000, 0.105, 0.829) & B = 90.00 & N4(0.000, 0.105, 0.829) & B = 90.00 & N4(0.000, 0.105, 0.671) & N7(0.500, 0.398, 0.165) & N8(0.500, 0.602, 0.665) & R2(0.0044, 0.695, 0.634) & B = 111.13 & N3(0.843, 0.349, 0.996) & \gamma = 93.98 & N4(0.157, 0.651, 0.004) & N4(0.0157, 0.651, 0.004) & N1(0.500, 0.500, 0.500) & N1(0.500, 0.500, 0.500)$			Al4(0.271,0.832,0.790)
$\begin{array}{cccc} C2-Al_2N_7 & a = 8.18 \\ b = 3.52 \\ c = 4.88 \\ a = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ \beta = 0.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ N1(0.907, 0.224, 0.456) \\ N8(0.592, 0.724, 0.543) \\ N9(0.069, 0.697, 0.136) \\ N8(0.592, 0.724, 0.543) \\ N9(0.069, 0.697, 0.136) \\ N8(0.592, 0.724, 0.543) \\ N9(0.069, 0.697, 0.863) \\ N10(0.615, 0.039, 0.411) \\ N11(0.000, 0.952, 0.000) \\ N12(0.384, 0.039, 0.588) \\ N13(0.407, 0.724, 0.456) \\ R = 0.612 \\ P = 0 \ GPa \\ p = 0 \ GPa \\ a = 4.84 \\ b = 2.96 \\ \beta = 71.75 \\ \gamma = 90.00 \\ \beta = 71.75 \\ \gamma = 90.00 \\ Al1(0.000, 0.500, 0.000) \\ Al2(0.000, 0.500, 0.675) \\ N1(0.500, 0.602, 0.835) \\ N1(0.500, 0.602, 0.829) \\ \beta = 90.00 \\ N1(0.500, 0.000, 0.500) \\ Al2(0.000, 0.895, 0.171) \\ \gamma = 90.00 \\ N1(0.500, 0.000, 0.500, 11) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \\ P\overline{1}.AIN_4 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 40 \ GPa \\ A = 2.86 \\ P = 111.13 \\ N3(0.843, 0.349, 0.960) \\ \alpha = 102.88 \\ N2(0.044, 0.695, 0.351, 0.004) \\ \end{array}$			
$\begin{array}{cccc} L = & 1.8 \\ b = 3.52 \\ c = 4.88 \\ a = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ p = 0.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ p = 90.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ p = 0.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ p = 0.00 \\ \beta = 127.29 \\ \gamma = 90.00 \\ p = 0.00 \\ \beta = 17.75 \\ \gamma = 90.00 \\ \beta = 71.75 \\ \gamma = 90.00 \\ \beta = 90.00 \\ \beta = 71.75 \\ \gamma = 90.00 \\ \beta = 71.75 \\ \gamma = 90.00 \\ \beta = 90.00 \\ \beta = 71.75 \\ \gamma = 90.00 \\ \beta = 90.00 \\ \beta = 71.75 \\ \gamma = 90.00 \\ \beta $		0.10	
$\begin{array}{cccc} C2-Al_2N_7 & c = 4.82 & N4(0.500, 0.452, 0.000) \\ c = 4.82 & a = 90.00 & N5(0.884, 0.539, 0.588) \\ \beta = 127.29 & \gamma = 90.00 & N6(0.907, 0.224, 0.456) \\ \gamma = 90.00 & N8(0.592, 0.724, 0.543) & N9(0.069, 0.697, 0.863) \\ N10(0.615, 0.039, 0.411) & N11(0.000, 0.952, 0.000) \\ N12(0.384, 0.039, 0.588) & N13(0.407, 0.724, 0.456) & N10(0.615, 0.039, 0.411) \\ N11(0.000, 0.952, 0.000) & N12(0.384, 0.039, 0.588) \\ N13(0.407, 0.724, 0.456) & N10(0.62, 0.000, 0.000) \\ P2/m-AlN_4 & c = 3.76 & N10(0.62, 0.000, 0.657) \\ P = 0 \text{ GPa} & \alpha = 90.00 & N1(0.062, 0.000, 0.657) \\ \beta = 71.75 & N4(0.479, 0.500, 0.325) \\ Pmcm-AlN_4 & c = 7.24 & N1(0.500, 0.000, 0.000) \\ Al1(0.000, 0.500, 0.675) & N4(0.479, 0.500, 0.675) \\ P = 20 \text{ GPa} & \alpha = 90.00 & Al1(0.500, 0.000, 0.600) \\ Al2(0.000, 0.500, 0.657) & N3(0.000, 0.895, 0.329) \\ \beta = 90.00 & N4(0.000, 0.500, 0.500) \\ P = 20 \text{ GPa} & \alpha = 90.00 & N4(0.000, 0.500, 0.500) \\ P = 20 \text{ GPa} & \alpha = 90.00 & N4(0.000, 0.500, 0.500) \\ P = 40 \text{ GPa} & \alpha = 90.00 & N4(0.000, 0.500, 0.501) \\ \gamma = 90.00 & N5(0.000, 0.895, 0.329) \\ \beta = 90.00 & N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 & N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 & N6(0.000, 0.105, 0.671) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) & N8(0.500, 0.602, 0.665) \\ P\overline{1} -AIN_4 & a = 2.86 \\ P = 40 \text{ GPa} & b = 3.56 \\ A11 (0.500, 0.000, 0.500, 0.500) \\ c = 3.74 & N1 (0.956, 0.305, 0.366) \\ \alpha = 102.88 & N2 (0.044, 0.695, 0.634) \\ \beta = 111.13 & N3 (0.843, 0.349, 0.996) \\ \gamma = 93.98 & N4 (0.157, 0.651, 0.004) \\ \end{array}$			
$\begin{array}{cccc} C2-A1_{2}N7 & C = 4.88 & N5(0.884, 0.539, 0.588) \\ P = 80 \ {\rm GPa} & \alpha = 90.00 \\ \beta = 127.29 & N6(0.907, 0.224, 0.456) \\ \gamma = 90.00 & N8(0.592, 0.724, 0.543) \\ N9(0.0697, 0.136) \\ N8(0.592, 0.724, 0.543) \\ N9(0.0697, 0.136) \\ N8(0.592, 0.724, 0.543) \\ N9(0.0697, 0.863) \\ N10(0.615, 0.039, 0.411) \\ N11(0.000, 0.952, 0.000) \\ N12(0.384, 0.039, 0.588) \\ N13(0.407, 0.724, 0.456) \\ \hline \\ P = 0 \ {\rm GPa} & a = 4.84 \\ b = 2.96 \\ c = 3.76 \\ \beta = 71.75 \\ \gamma = 90.00 & N1(0.062, 0.000, 0.000) \\ N1(0.062, 0.000, 0.343) \\ N2(0.938, 0.000, 0.657) \\ N3(0.521, 0.500, 0.325) \\ \beta = 71.75 \\ \gamma = 90.00 & N4(0.479, 0.500, 0.675) \\ \hline \\ P = 20 \ {\rm GPa} & a = 2.84 \\ b = 4.11 \\ N2(0.000, 0.500, 0.398, 0.35) \\ b = 4.11 \\ N2(0.000, 0.500, 0.398, 0.35) \\ b = 4.11 \\ N2(0.000, 0.895, 0.329) \\ P = 20 \ {\rm GPa} & a = 90.00 \\ \beta = 90.00 \\ N4(0.000, 0.105, 0.829) \\ \beta = 90.00 \\ N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 \\ N5(0.000, 0.895, 0.171) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \\ \hline \\ P = 40 \ {\rm GPa} & a = 2.86 \\ b = 3.56 \\ c = 102.88 \\ N2(0.044, 0.695, 0.305, 0.366) \\ \alpha = 102.88 \\ N2(0.044, 0.695, 0.304) \\ N4(0.157, 0.651, 0.004) \\ \end{array}$			
$\begin{array}{c c} P=80\ {\rm GPa} & a=90.00 \\ \beta=127.29 \\ \gamma=90.00 & N6(0.907,0.224,0.456) \\ N7(0.930,0.697,0.136) \\ N8(0.592,0.724,0.543) \\ N9(0.069,0.697,0.863) \\ N10(0.615,0.039,0.411) \\ N11(0.000,952,0.000) \\ N12(0.384,0.039,0.588) \\ N13(0.407,0.724,0.456) \\ \hline \\ P=0\ {\rm GPa} & a=4.84 \\ b=2.96 \\ c=3.76 \\ n=90.00 \\ \beta=71.75 \\ \gamma=90.00 \\ \beta=71.75 \\ \gamma=90.00 \\ N1(0.062,0.000,0.0325) \\ N4(0.479,0.500,0.675) \\ \gamma=90.00 \\ A11(0.000,0.500,0.000) \\ A12(0.000,0.500,0.000) \\ A12(0.000,0.500,0.000) \\ A12(0.000,0.500,0.500) \\ A11(0.000,0.500,0.000) \\ A12(0.000,0.500,0.500) \\ A11(0.000,0.895,0.329) \\ \beta=90.00 \\ N4(0.000,0.105,0.829) \\ \beta=90.00 \\ N5(0.000,0.895,0.329) \\ \beta=90.00 \\ N5(0.000,0.895,0.171) \\ \gamma=90.00 \\ N6(0.000,0.105,0.671) \\ N7(0.500,0.398,0.165) \\ N8(0.500,0.602,0.665) \\ \hline \\ P=40\ {\rm GPa} & a=2.86 \\ P=111.13 \\ N3(0.843,0.349,0.996) \\ \gamma=93.98 \\ N4(0.157,0.651,0.004) \\ \end{array}$			
$\begin{array}{c c} p = 127.29 \\ \gamma = 90.00 \\ N7(0.930,0.697,0.136) \\ N8(0.592,0.724,0.543) \\ N9(0.069,0.697,0.863) \\ N10(0.615,0.039,0.411) \\ N11(0.000,0.952,0.000) \\ N12(0.384,0.039,0.588) \\ N13(0.407,0.724,0.456) \\ N12(0.384,0.039,0.588) \\ N13(0.407,0.724,0.456) \\ N11(0.062,0.000,0.000) \\ N1(0.062,0.000,0.343) \\ N2(0.938,0.000,0.657) \\ N3(0.521,0.500,0.325) \\ N4(0.479,0.500,0.675) \\ \gamma = 90.00 \\ N1(0.000,0.500,0.000) \\ A12(0.000,0.500,0.000) \\ A12(0.000,0.500,0.000) \\ A12(0.000,0.500,0.500) \\ N1(0.500,0.602,0.835) \\ N4(0.479,0.500,0.675) \\ \gamma = 90.00 \\ N1(0.500,0.622,0.835) \\ N4(0.479,0.500,0.398,0.335) \\ N2(0.500,0.398,0.335) \\ N4(0.000,0.895,0.329) \\ P = 20 \text{ GPa} \\ a = 2.84 \\ N2(0.500,0.398,0.335) \\ B = 4.11 \\ N2(0.500,0.398,0.335) \\ N3(0.000,0.895,0.329) \\ P = 20 \text{ GPa} \\ a = 90.00 \\ A11(0.000,0.105,0.829) \\ \beta = 90.00 \\ N4(0.000,0.105,0.671) \\ N7(0.500,0.398,0.165) \\ N8(0.500,0.602,0.665) \\ N8(0.500,0.602,0.665) \\ N8(0.500,0.602,0.651) \\ N1(0.956,0.305,0.366) \\ \alpha = 102.88 \\ P = 40 \text{ GPa} \\ c = 3.74 \\ N3(0.843,0.349,0.996) \\ \gamma = 93.98 \\ N4(0.157,0.651,0.004) \\ \end{array}$	P = 80  GPa		
$\begin{array}{c cccc} & & & & & & & & & & & & & & & & & $			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		$\gamma = 90.00$	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $			
$\begin{array}{c c} P2/m-AlN_4 \\ P=0 \ GPa \end{array} \begin{array}{ c c c } a=4.84 \\ b=2.96 \\ c=3.76 \\ a=90.00 \\ \beta=71.75 \\ \gamma=90.00 \end{array} \begin{array}{ c c } Al1(0.500,0.000,0.000) \\ N1(0.062,0.000,0.343) \\ N2(0.938,0.000,0.657) \\ N3(0.521,0.500,0.325) \\ N4(0.479,0.500,0.675) \end{array}$			
$\begin{array}{c c} P2/m-AIN_4 \\ P=0 \ GPa \end{array} \begin{array}{ c c c c c } b=2.96 \\ c=3.76 \\ a=90.00 \\ \beta=71.75 \\ \gamma=90.00 \end{array} \begin{array}{ c c c } A11(0.500,0.000,0.000) \\ N1(0.062,0.000,0.343) \\ N2(0.938,0.000,0.657) \\ N3(0.521,0.500,0.325) \\ N4(0.479,0.500,0.675) \end{array}$		a - 4.94	1115(0.407,0.724,0.450)
$\begin{array}{c} P2/m-AlN_4 \\ P=0 \ GPa \end{array} \left( \begin{array}{c} c=3.76 \\ a=90.00 \\ \beta=71.75 \\ \gamma=90.00 \end{array} \right) \\ R=20 \ GPa \end{array} \left( \begin{array}{c} c=3.76 \\ a=90.00 \\ \beta=71.75 \\ \gamma=90.00 \end{array} \right) \\ Al1(0.000,0.500,0.000) \\ Al2(0.000,0.500,0.000) \\ Al2(0.000,0.500,0.000) \\ Al2(0.000,0.500,0.000) \\ Al2(0.000,0.500,0.500) \\ N1(0.500,0.602,0.835) \\ N2(0.500,0.398,0.335) \\ N2(0.500,0.398,0.335) \\ N2(0.500,0.398,0.35) \\ N2(0.000,0.895,0.329) \\ R=20 \ GPa \end{array} \left( \begin{array}{c} a=2.84 \\ b=4.11 \\ N2(0.500,0.398,0.35) \\ N2(0.000,0.895,0.329) \\ R=90.00 \\ N4(0.000,0.105,0.829) \\ N5(0.000,0.895,0.171) \\ N7(0.500,0.398,0.165) \\ N8(0.500,0.602,0.665) \\ R=40 \ GPa \end{array} \left( \begin{array}{c} a=2.86 \\ b=3.56 \\ c=3.74 \\ a=102.88 \\ \beta=111.13 \\ N3(0.843,0.349,0.996) \\ N4(0.157,0.651,0.004) \\ R=93.98 \end{array} \right) \\ R=0.004 \\ R=0.004 \\ R=0.004 \\ R=0.000 $			Al1(0.500,0.000,0.000)
$\begin{array}{c c} P=0 \ \text{GPa} & \alpha=90.00 \\ \beta=71.75 \\ \gamma=90.00 & \text{N}2(0.938,0.000,0.657) \\ \text{N}3(0.521,0.500,0.325) \\ \text{N}4(0.479,0.500,0.675) & \text{N}4(0.479,0.500,0.675) \\ \end{array}$	D2/m AINI		N1(0.062,0.000,0.343)
$ \begin{array}{c c} \beta = 71.75 \\ \gamma = 90.00 \end{array} \begin{array}{c} N3(0.521, 0.500, 0.325) \\ N4(0.479, 0.500, 0.675) \end{array} \\ \hline \\ A11(0.000, 0.500, 0.000) \\ A12(0.000, 0.500, 0.500) \\ A12(0.000, 0.500, 0.500) \\ A12(0.000, 0.500, 0.500) \\ A12(0.000, 0.500, 0.500) \\ N1(0.500, 0.602, 0.835) \\ N2(0.500, 0.398, 0.335) \\ N2(0.500, 0.398, 0.329) \\ \beta = 90.00 \\ \beta = 90.00 \\ \beta = 90.00 \\ \beta = 90.00 \\ N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 \\ N5(0.000, 0.895, 0.171) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \\ \hline \\ P\overline{1} - AIN_4 \\ P = 40 \text{ GPa} \\ \hline \\ P = 3.74 \\ \alpha = 102.88 \\ \beta = 111.13 \\ \gamma = 93.98 \\ \hline \\ N4(0.157, 0.651, 0.004) \\ \hline \\ \end{array} $			N2(0.938,0.000,0.657)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	F – 0 GFa		N3(0.521,0.500,0.325)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		1	N4(0.479,0.500, 0.675)
$\begin{array}{c ccccc} & a = 2.84 & & Al2(0.000, 0.500, 0.500) \\ & a = 2.84 & & N1(0.500, 0.602, 0.835) \\ & b = 4.11 & & N2(0.500, 0.398, 0.335) \\ & b = 4.11 & & N2(0.500, 0.398, 0.335) \\ & p = 20 \text{ GPa} & & \alpha = 90.00 & & N4(0.000, 0.105, 0.829) \\ & \beta = 90.00 & & N5(0.000, 0.895, 0.171) \\ & \gamma = 90.00 & & N5(0.000, 0.895, 0.171) \\ & N7(0.500, 0.398, 0.165) & & N8(0.500, 0.602, 0.665) \\ \hline \\ \hline \\ \hline \\ P = 40 \text{ GPa} & & a = 2.86 & \\ & b = 3.56 & & Al1(0.500, 0.000, 0.500) \\ & c = 3.74 & & N1(0.956, 0.305, 0.366) \\ & \alpha = 102.88 & & N2(0.044, 0.695, 0.634) \\ & \beta = 111.13 & & N3(0.843, 0.349, 0.996) \\ & \gamma = 93.98 & & N4(0.157, 0.651, 0.004) \\ \end{array}$		$\gamma = 90.00$	<u> </u>
$\begin{array}{c cccc} & a = 2.84 & & N1(0.500, 0.602, 0.835) \\ b = 4.11 & & N2(0.500, 0.398, 0.335) \\ c = 7.24 & & N3(0.000, 0.895, 0.329) \\ \beta = 90.00 & & M4(0.000, 0.105, 0.829) \\ \beta = 90.00 & & N5(0.000, 0.895, 0.171) \\ \gamma = 90.00 & & N5(0.000, 0.398, 0.165) \\ N7(0.500, 0.398, 0.165) & \\ N8(0.500, 0.602, 0.665) & \\ \hline \\ P = 40 & GPa & & a = 2.86 \\ b = 3.56 & & A11 & (0.500, 0.000, 0.500) \\ c = 3.74 & & A11 & (0.500, 0.000, 0.500) \\ \alpha = 102.88 & & N2 & (0.044, 0.695, 0.634) \\ \beta = 111.13 & & N3 & (0.843, 0.349, 0.996) \\ \gamma = 93.98 & & N4 & (0.157, 0.651, 0.004) \end{array}$			
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		2.94	
$\begin{array}{c c} Pmcm-AlN_4 \\ P = 20 \ \text{GPa} \end{array} \begin{array}{c} c = 7.24 \\ \alpha = 90.00 \\ \beta = 90.00 \\ \gamma = 90.00 \end{array} \begin{array}{c} N3(0.000, 0.895, 0.329) \\ N4(0.000, 0.105, 0.829) \\ N5(0.000, 0.895, 0.171) \\ N6(0.000, 0.105, 0.671) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \end{array}$			
$\begin{array}{c c} P=20 \ \text{GPa} & \alpha=90.00 & \text{N4}(0.000,0.105,0.829) \\ \beta=90.00 & \text{N5}(0.000,0.895,0.171) \\ \gamma=90.00 & \text{N6}(0.000,0.105,0.671) \\ \text{N7}(0.500,0.398,0.165) \\ \text{N7}(0.500,0.602,0.665) \\ \hline \\ \hline \\ P=40 \ \text{GPa} & a=2.86 \\ b=3.56 & \text{Al1}(0.500,0.000,0.500) \\ c=3.74 & \text{N1}(0.956,0.305,0.366) \\ \alpha=102.88 & \text{N2}(0.044,0.695,0.634) \\ \beta=111.13 & \text{N3}(0.843,0.349,0.996) \\ \gamma=93.98 & \text{N4}(0.157,0.651,0.004) \\ \end{array}$			
$ \begin{array}{c c} \beta = 90.00 \\ \gamma = 90.00 \\ \gamma = 90.00 \\ \hline \\ N5(0.000, 0.895, 0.171) \\ N6(0.000, 0.105, 0.671) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \\ \hline \\ P = 40 \text{ GPa} \\ \hline \\ p = 40 \text{ GPa} \\ \hline \\ \alpha = 102.88 \\ \beta = 111.13 \\ \beta = 111.13 \\ \gamma = 93.98 \\ \hline \\ N4(0.157, 0.651, 0.004) \\ \hline \\ \end{array} $			
$\begin{array}{c c} \gamma = 90.00 & N6(0.000, 0.105, 0.671) \\ N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \\ \hline P = 40 \text{ GPa} & a = 2.86 \\ b = 3.56 \\ c = 3.74 \\ \beta = 111.13 \\ \beta = 111.13 \\ \gamma = 93.98 \\ \hline N1 (0.956, 0.305, 0.366) \\ N2 (0.044, 0.695, 0.634) \\ N3 (0.843, 0.349, 0.996) \\ N4 (0.157, 0.651, 0.004) \\ \hline \end{array}$	P = 20  GPa		
$\begin{array}{c c} p\bar{1}-AlN_4 \\ P=40 \ GPa \end{array} \begin{array}{c} a=2.86 \\ b=3.56 \\ c=3.74 \\ \beta=111.13 \\ \gamma=93.98 \end{array} \begin{array}{c} N7(0.500, 0.398, 0.165) \\ N8(0.500, 0.602, 0.665) \\ Al1(0.500, 0.000, 0.500) \\ N1(0.956, 0.305, 0.366) \\ N2(0.044, 0.695, 0.634) \\ N3(0.843, 0.349, 0.996) \\ N4(0.157, 0.651, 0.004) \end{array}$			
$\begin{array}{c c} p\bar{1}\text{-AlN}_4 \\ P = 40 \text{ GPa} \end{array} \begin{array}{c} a = 2.86 \\ b = 3.56 \\ \alpha = 102.88 \\ \beta = 111.13 \\ \gamma = 93.98 \end{array} \begin{array}{c} \text{All} (0.500, 0.000, 0.500) \\ \text{All} (0.500, 0.500, 0.500) \\ \text{All} (0.500, 0.000, 0.500) \\ \text{All} (0.500, 0.500, 0.500, 0.500) \\ \text{All} (0.500, 0.500, 0.500, 0.500, 0.500) \\ \text{All} (0.500, 0.500, 0.500, 0.500, 0.500, 0.500) \\ \text{All} (0.500, 0.500, 0.500, 0.$		$\gamma = 90.00$	
$ \begin{array}{c c} p\bar{1}\text{-AlN}_4 \\ P = 40 \text{ GPa} \end{array} \begin{array}{c} a = 2.86 \\ b = 3.56 \\ c = 3.74 \\ \beta = 111.13 \\ \gamma = 93.98 \end{array} \begin{array}{c} Al1 \ (0.500, \ 0.000, \ 0.500) \\ N1 \ (0.956, \ 0.305, \ 0.366) \\ N2 \ (0.044, \ 0.695, \ 0.634) \\ N3 \ (0.843, \ 0.349, \ 0.996) \\ N4 \ (0.157, \ 0.651, \ 0.004) \end{array} $			
$ \begin{array}{c} b = 3.56 \\ c = 3.74 \\ \beta = 111.13 \\ \gamma = 93.98 \end{array} \begin{array}{c} Al1 \ (0.500, \ 0.000, \ 0.500) \\ N1 \ (0.956, \ 0.305, \ 0.366) \\ N2 \ (0.044, \ 0.695, \ 0.634) \\ N3 \ (0.843, \ 0.349, \ 0.996) \\ N4 \ (0.157, \ 0.651, \ 0.004) \end{array} $			N8(0.500,0.602,0.665)
$\begin{array}{c} c = 3.74 \\ \alpha = 102.88 \\ \beta = 111.13 \\ \gamma = 93.98 \end{array} \qquad \begin{array}{c} N1 \ (0.956, \ 0.305, \ 0.366) \\ N2 \ (0.044, \ 0.695, \ 0.634) \\ N3 \ (0.843, \ 0.349, \ 0.996) \\ N4 \ (0.157, \ 0.651, \ 0.004) \end{array}$	$P^1$ -AlN <sub>4</sub>		
$\alpha = 102.88$ N2 (0.044, 0.695, 0.634) $\beta = 111.13$ N3 (0.843, 0.349, 0.996) $\gamma = 93.98$ N4 (0.157, 0.651, 0.004)	P = 40  GPa		
$ \begin{array}{ll} \beta = 111.13 \\ \gamma = 93.98 \end{array} \qquad \begin{array}{ll} N3 \; (0.843,  0.349,  0.996) \\ N4 \; (0.157,  0.651,  0.004) \end{array} $			
$\gamma = 93.98$ N4 (0.157, 0.651, 0.004)			
		•	
a = 3.66		•	N4 (0.157, 0.651, 0.004)
		a = 3.66	
$Cc2e-AlN_5$ a = 4.04 Al1(0.000,0.272,0.000)	Cc2e-AlN <sub>5</sub>	a = 4.04	Al1(0.000,0.272,0.000)
P = 0 GPa $b = 3.78$ $A12(0.000, 0.772, 0.500)$			

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А	ĸ		L	LC.

	c = 20.49	Al3(0.500,0.772,0.000)
	$\alpha = 90.00$	Al4(0.500,0.272,0.500)
	$\beta = 90.00$	N1(0.000,0.770,0.000)
	$\gamma = 90.00$	N2(0.000,0.270,0.500)
	·	N3(0.865,0.867,0.808)
		N4(0.135,0.867,0.192)
		N5(0.635,0.867,0.308)
		N6(0.365,0.867,0.692)
		N7(0.881,0.972,0.859)
		N8(0.119,0.972,0.141)
		N9(0.619,0.972,0.359)
		N10(0.381,0.972,0.641)
		N11(0.500,0.270,0.000)
		N12(0.500,0.770,0.500)
		N13(0.365,0.367,0.808)
		N14(0.635,0.367,0.192)
		N15(0.135,0.367,0.308)
		N16(0.866,0.367,0.692)
		N17(0.380,0.472,0.859)
		N18(0.619,0.472,0.141)
		N19(0.119,0.472,0.359)
		N19(0.119,0.472,0.539) N20(0.881,0.472,0.641)
		A11(0.408,0.000,0.532)
		Al2(0.908,0.500,0.532)
	a = 6.46	N1(0.205,0.000,0.866)
	a = 6.46	N2(0.772,0.129,0.267)
	b = 3.10	N3(0.772,0.871,0.267)
$Cm-AlN_5$	c = 20.49	N4(0.112,0.250,0.925)
P = 20 GPa	$\alpha = 90.00$	N5(0.112,0.749,0.925)
	$\beta = 107.36$	N6(0.705,0.500,0.866)
	$\gamma = 90.00$	N7(0.272,0.629,0.267)
		N8(0.272,0.371,0.267)
		N9(0.612,0.751,0.925)
		N10(0.612,0.249,0.925)
$P^1$ -AlN <sub>5</sub>	a = 3.66	Al1(0.010, 0.890, 0.230)
P = 40 GPa	b = 4.41	N1(0.510, 0.770, 0.660)
	c = 6.72	N2(0.880, 0.770, 0.660)
	$\alpha = 85.02$	N3(0.850, 0.520, 0.290)
	$\beta = 81.98$	N4(0.490, 0.530, 0.300)
	$\gamma = 66.28$	N5(0.330, 0.000, 0.000)
$I\overline{4}2d$ -AlN <sub>5</sub>		Al1(0.000, 0.000, 0.500)
P = 60  GPa		Al2(0.500, 0.000, 0.250)
	a = 5.19	Al3(0.500, 0.500, 0.000)
	b = 5.19	Al4(0.000, 0.500, 0.750)
	c = 5.14	N1(0.680, 0.630, 0.650)
	$\alpha = 90.00$	N2(0.320, 0.370, 0.650)
	$\beta = 90.00$	N3(0.630, 0.320, 0.350)
	00.00	
	$\gamma = 90.00$	N4(0.370, 0.680, 0.350)

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		N6(0.180, 0.370, 0.100)
		N7(0.870, 0.320, 0.400)
		N8(0.130, 0.680, 0.400)
		N9(0.180, 0.130, 0.150)
		N10(0.820, 0.870, 0.150)
		N11(0.130, 0.820, 0.850)
		N12(0.870, 0.180, 0.850)
		N13(0.320, 0.130, 0.600)
		N14(0.680, 0.870, 0.600)
		N15(0.370, 0.820, 0.900)
		N16(0.630, 0.180, 0.900)
		N17(0.000, 0.500, 0.250)
		N18(0.500, 0.000, 0.750)
		N19(0.500, 0.500, 0.500)
		N20(0.000, 0.000, 0.000)
P1-AlN6	4.00	A11(0.000,0.000,0.500)
P = 0 GPa	a = 4.82	N1(0.824,0.703,0.025)
1 0 01 u	b = 4.84	N2(0.876,0.697,0.765)
	c = 4.11	N3(0.123,0.303,0.235)
	$\alpha = 98.33$	N4(0.595,0.017,0.436)
	$\beta = 107.99$	N5(0.405,0.984,0.564)
	$\gamma = 109.76$	N6(0.176,0.297,0.975)
		A11(0.000,0.000,0.000)
		A12(0.500,0.500,0.000)
		N1(0.839,0.000,0.856)
		N2(0.661,0.500,0.144)
	a = 11.83	N3(0.987,0.500,0.344)
	b = 2.80	N4(0.682,0.500,0.427)
C2/m-AlN <sub>6</sub>	c = 3.72	N5(0.013,0.500,0.656)
P = 20 GPa	$\alpha = 90.00$	N6(0.817,0.000,0.573)
	$\beta = 82.39$	N7(0.339,0.500,0.856)
	$\gamma = 90$	N8(0.161,0.000,0.144)
		N9(0.487,0.000,0.344)
		N10(0.182,0.000,0.427)
		N11(0.513,0.000,0.656)
		N12(0.317,0.500,0.573)
		Al1 (0.000, 0.500, 0.000)
		Al2 (0.500, 0.000, 0.000)
		N1 (0.261, 0.000, 0.775)
	a = 5.11	N2 (0.739, 0.000, 0.225)
	b = 4.96	N3 (0.289, 0.264, 0.334)
C2/m-AlN <sub>6</sub>	c = 4.30	N4 (0.789, 0.236, 0.334)
P = 40  GPa	$\alpha = 90.00$	N5 (0.211, 0.235, 0.666)
1 10 01 0	$\beta = 63.03$	N6 (0.711, 0.264, 0.666)
	$\gamma = 90.00$	N7 (0.761, 0.500, 0.775)
	, , , , , , , , , , , , , , , , , , ,	N8 (0.239, 0.500, 0.225)
		N9 (0.789, 0.764, 0.334)
		N10 (0.289, 0.736, 0.334)
		N11 (0.711, 0.736, 0.666)

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		N12 (0.211, 0.764, 0.666)
	1	Al1(0.235,0.500,0.365)
	a = 6.11	N1(0.915,0.500,0.453)
	a = 0.11 b = 8.07	
		N2(0.738,0.500,0.330)
Pm-AlN <sub>7</sub>	c = 2.85	N3(0.562,0.500,0.210)
P = 0 GPa	$\alpha = 90.00$	N4(0.452,0.814,0.432)
	$\beta = 81.98$	N5(0.452,0.186,0.432)
	$\gamma = 90.00$	N6(0.631,0.838,0.441)
		N7(0.631,0.162,0.441)
		Al1(0.000,0.000,0.672)
	a = 5.19	N1(0.000,0.000,0.166)
	b = 5.19	N2(0.500,0.000,0.666)
P6mm-AlN <sub>7</sub>	c = 3.49	N3(0.000,0.500,0.666)
P = 20 GPa	$\alpha = 90.00$	N4(0.500,0.500,0.666)
	$\beta = 90.00$	N5(0.500,0.000,0.345)
	$\gamma = 120.00$	N6(0.000,0.500,0.345)
		N7(0.500,0.500,0.345)
		Al1(0.934, 0.460, 0.523)
	a = 2.77	N1(0.348, 0.252, 0.968)
	b = 4.58	N2(0.967, 0.046, 0.523)
$P1-AlN_7$	c = 4.72	N3(0.388, 0.300, 0.251)
P = 40  GPa	$\alpha = 112.39$	N4(0.467, 0.492, 0.851)
	$\beta = 94.50$	N5(0.840, 0.767, 0.313)
	$\gamma = 92.125$	N6(0.132, 0.992, 0.766)
		N7(0.622, 0.772, 0.068)
		Al1(0.311, 0.267, 0.965)
	a = 3.47	N1(0.587, 0.355, 0.385)
	b = 3.84	N2(0.967, 0.046, 0.523)
$P1-AIN_7$	c = 4.12	N3(0.179, 0.719, 0.290)
P = 80  GPa	$\alpha = 114.75$	N4(0.796, 0.176, 0.782)
	$\beta = 91.28$	N5(0.965, 0.920, 0.201)
	$\gamma = 101.68$	N6(0.429, 0.547, 0.671)
		N7(0.773, 0.121, 0.460)
		10, (0.775, 0.121, 0.400)

Table S2. Calculated enthalpies of the predicted  $Al_xN_y$  compounds at different pressures.

Structure	Pressure (GPa)	Enthalpy (eV/atom)	Formation enthalpy(eV/atom)
Cm-Al <sub>2</sub> N	0	-5.897	-0.628
$P\bar{3}m_{1}-Al_{2}N$	20	-4.639	0.051
$P\bar{3}m_{1}-Al_{2}N$	40	-3.323	-1.393
P2/m-Al <sub>2</sub> N	60	-1.770	-1.203
$p\bar{3}m_{1}-Al_{2}N$	80	-0.843	-1.820
$P6_3mc$ -AlN	0	-7.445	-1.412
$Fm^{\overline{3}}m$ -AlN	20	-6.263	-2.036
$Fm^{\overline{3}}m$ -AlN	40	-5.304	-2.524
$Fm^{\overline{3}}m$ -AlN	60	-4.398	-2.913

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$Fm^{\overline{3}}m$ -AlN 80		-3.528	-3.238		
$R^{\overline{3}}m$ -Al <sub>2</sub> N <sub>3</sub>	0	-7.033	-0.542		
$R^{\overline{3}}m-Al_2N_3$	20	-6.153	-1.454		
<i>Cmmm</i> -Al <sub>2</sub> N <sub>3</sub>	40	-4.978	-1.688		
$R^3m$ -Al <sub>2</sub> N <sub>3</sub>	60	-4.260	-2.224		
$\frac{R^{2}m^{2}H_{2}N_{3}}{R^{3}m^{2}Al_{2}N_{3}}$	80	-3.154	-2.272		
$R3_{m-AlN_2}$	0	-7.203	-0.407		
$\frac{C2/m-AlN_2}{C2}$	20	-6.156	-0.519		
P6/mmm-AlN <sub>2</sub>	40	-5.160	-1.530		
Pnnm-AlN <sub>2</sub>	60	-4.295	-1.892		
$R^{\overline{3}}m$ -AlN <sub>2</sub>	80	-3.350	-2.073		
P1-Al <sub>2</sub> N <sub>5</sub>	0	-7.233	-0.218		
<i>Cm</i> -Al <sub>2</sub> N <sub>5</sub>	20	-6.089	-0.852		
$P^{\overline{1}}$ -Al <sub>2</sub> N <sub>5</sub>	40	-5.175	-1.302		
$\frac{PI - Al_2N_5}{PI - Al_2N_5}$	60	-4.124	-1.458		
$\frac{P1 - Al_2N_5}{P1 - Al_2N_5}$	80	-3.322	-1.7631		
$\frac{11 - Al_2 N_5}{Cm - AlN_3}$	0	-6.970	0.209		
PĪ-AIN <sub>3</sub>	20	-6.151	-0.277		
$\frac{P2_1/c-AlN_3}{P2_1/c-AlN_3}$	40	-5.372	-0.277		
$\frac{P2_1/c\text{-AlN}_3}{P2_1/c\text{-AlN}_3}$	60	-3.572	-1.637		
$\frac{P2_1/c\text{-AlN}_3}{P2_1/c\text{-AlN}_3}$	80	-3.668	-1.898		
$\frac{Pl-Al_2N_7}{Pl-Al_2N_7}$	0	-7.403	-0.097		
$Cm-Al_2N_7$	20	-6.010	-0.474		
$Cm-Al_2N_7$	40	-6.035	-1.838		
$Cm-Al_2N_7$	60	-4.198	-1.182		
$\frac{C2-Al_2N_7}{C2-Al_2N_7}$	80	-3.452	-1.517		
$P2/m-AlN_4$	0	-7.436	-0.029		
<i>Pmcm</i> -AlN <sub>4</sub>	20	-6.259	-0.242		
$P^{\overline{1}}$ -AlN <sub>4</sub>	40	-5.300	-0.990		
$P^{\bar{1}}$ -AlN <sub>4</sub>	60	-4.464	-1.326		
$P^{\bar{1}}$ -AlN <sub>4</sub>	80	-3.430	-1.364		
Cc2e-AlN <sub>5</sub>	0	-7.582	-0.022		
Cm-AlN <sub>5</sub>	20	-6.124	-0.013		
$P^{\bar{1}}$ -AlN <sub>5</sub>	40	-5.247	-0.767		
$\bar{I^4}2d$ -AlN <sub>5</sub>	60	-4.224	-0.903		
-	80	-3.623	2.398		
$I^{4}2d$ -AlN <sub>5</sub>					
$P\bar{1}_{-\mathrm{AlN}_6}$	0 20	-7.511	0.158		
$\frac{C2/m\text{-AlN}_6}{C2/m\text{-AlN}_6}$	<u> </u>	-6.243 -5.370	-0.065 -0.493		
$C2/m-AIN_6$	60	-5.570	-0.493		
$C2/m-AIN_6$	80	-4.509	-1.288		
Pm-AlN <sub>7</sub>	0	-7.282	0.469		
P6mm-AlN <sub>7</sub>	20	-5.757	0.472		
P1-AlN <sub>7</sub>	40	-5.185	-1.317		

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$P1-AlN_7$	60	-4.246	-0.695
P1-AlN <sub>7</sub>	80	-3.615	-1.105



Fig. S1 Phonon dispersion curves of C2/m-AlN<sub>6</sub> at 30 GPa.



Fig. S2 Fluctuations of the total energies obtained by molecular dynamics simulation under the NPT ensemble at ambient pressure at 1500 K and for C2/m-AlN<sub>6</sub> phase.



Fig. S3 Enthalpy difference between  $Cm-Al_2N_7$  and other phases of  $Al_2N_7$ .



Fig. S4 (a) Crystal structure and (b) phonon dispersion relation of P1-AlN<sub>7</sub> at 40 GPa.



**Fig. S5** Enthalpy difference between P1-AlN<sub>7</sub> and other phases of AlN<sub>7</sub>. The black line represents the metastable P1-AlN<sub>7</sub> searched under 80 GPa, and the pink line represents the structure searched under 40 GPa.



Fig. S6 Band structure and density of states (DOS) of C2/m-AlN<sub>6</sub> at 30 GPa.



Fig. S7 Three-dimensional partial charge density distribution of an energy band crossing Fermi energy for C2/m-AlN<sub>6</sub> at ambient condition. The value of isosurface is 0.01.



Fig. S8 Two-dimensional ELF distribution diagram on (010) crystal plane.



Fig. S9 The Lewis crystal structure with VSEPR notation for C2/m-AlN<sub>6</sub>.



Fig. S10 COHPs between Al-N4, N2-N3 and N3-N4 pairs for C2/m-AlN<sub>6</sub> phase at 30 GPa. Fermi levels are set at zero energy and marked by dotted lines.



**Fig. S11** COHPs between N1-N2, N4-N7 and N4-N5 pairs for C2m-Al<sub>2</sub>N<sub>7</sub> phase at 40 GPa. Fermi levels are set at zero energy and marked by dotted lines.



**Fig. S12** COHPs between N3-N4, N2-N3, N7-N1 and N5-N6 pairs for C2-Al<sub>2</sub>N<sub>7</sub> phase at 80 GPa. Fermi levels are set at zero energy and marked by dotted lines.



**Fig. S13** COHPs between N1-N2, N2-N3, N3-N4, N4-N5 and N1-N7 pairs for *P*1-AlN<sub>7</sub> phase at 80 GPa. Fermi levels are set at zero energy and marked by dotted lines.

Table S3. The calculated bond	parameters and hardness of C2/m-AlN <sub>6</sub>	$_{5}$ , Cm-Al <sub>2</sub> N <sub>7</sub> , Cm-Al <sub>2</sub> N <sub>7</sub> and P1-AlN <sub>7</sub> .
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Structure	V(Å <sup>3</sup> )	bond	n <sup>µ</sup>	d <sup>µ</sup> (Å)	$\mathbf{P}^{\mu}$	$V^{\mu}_{h}$	$H^{\mu}_{\mu}$	H <sub>v</sub> (GPa)
C2/m-AlN <sub>6</sub>		N-N	4	1.34	0.70	1.91	176.19	
	99.79	N-N	8	1.37	0.69	2.04	155.51	43.86
		Al-N	4	1.99	0.32	6.25	11.15	
		Al-N	8	2.00	0.36	6.35	12.24	
		N-N	4	1.30	0.77	1.29	374.43	
		N-N	4	1.36	0.67	1.47	260.00	
		Al-N	4	1.86	0.41	3.77	33.25	
		Al-N	2	1.86	0.48	3.77	38.93	
$C_{\rm m}$ A1 N		Al-N	2	1.87	0.35	3.83	27.63	
Cm-Al <sub>2</sub> N <sub>7</sub>	127.65	Al-N	2	1.94	0.34	4.28	22.34	39.32
		Al-N	2	1.94	0.35	4.28	23.00	
		Al-N	4	1.98	0.40	4.55	23.73	
		Al-N	4	2.03	0.23	4.90	12.05	
		Al-N	4	2.07	0.34	5.19	16.15	
		Al-N	2	2.09	0.23	5.35	10.41	
	111.78	N-N	4	1.30	0.77	1.07	507.27	
		N-N	4	1.36	0.67	1.23	352.25	
		N-N	4	1.37	0.61	1.25	309.17	
		Al-N	4	1.86	0.41	3.14	45.05	
		Al-N	2	1.86	0.48	3.14	52.74	
$C2-Al_2N_7$		Al-N	2	1.87	0.35	3.19	37.44	63.96
		Al-N	4	1.94	0.35	3.56	31.16	
		Al-N	4	1.98	0.4	3.79	32.15	
		Al-N	4	2.04	0.23	4.14	15.92	
		Al-N	2	2.10	0.23	4.52	13.78	
		Al-N	4	2.07	0.34	4.33	21.88	
P1-AlN <sub>7</sub>	48.49	N-N	1	1.25	0.98	2.79	131.08	
		N-N	1	1.28	0.76	3.00	90.29	
		N-N	1	1.30	0.80	3.14	87.95	
		N-N	1	1.30	0.77	3.14	84.65	
		N-N	1	1.31	0.75	3.21	79.35	22 50
		N-N	1	1.32	0.71	3.29	72.32	33.58
		N-N	1	1.33	0.70	3.36	68.66	
		Al-N	1	1.83	0.17	8.76	3.38	
		Al-N	1	1.83	0.69	8.76	13.72	
		Al-N	1	1.85	0.06	9.05	1.13	