Geometric and Energetic Aspects of Aluminum Nitride Cages

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Table S1. Computed Total Electronic Energies (au) for the most stable (AlN)_n ($n = 2-41$) structures.

(AlN) _n /Symmetry	ZPE (NImag) ^a	E _{tot} ^a	E _{tot} ^b	E _{tot}
(AlN) ₁ /C _{∞v}	0.9 (0)	−56.26206 (T)	−56.61607 (T)	(−297.04621) ^{c,d}
	1.0 (0)	−56.15291 (S)	−56.57389 (S)	(−297.00339) ^{c,d}
(AlN) ₂ /D _{2h}	4.5 (0)	−112.63462	−113.48523	
(AlN) ₃ /D _{3h}	9.7 (0)	−168.90204	−170.23156	
(AlN) ₄ /D _{4h}	14.3 (0)	−225.33924	−227.06667	
(AlN) ₅ /D _{5h}	18.6 (0)	−281.75333	−283.87899	
(AlN) ₆ /D _{3d}	24.7 (0)	−338.19299	−340.80278	
(AlN) ₇ /C _{3v}	28.9 (0)	−394.56132	−397.60304	
(AlN) ₈ /S ₄	34.1 (0)	−451.09176	−454.52967	
(AlN) ₉ /C _{3h}	39.1 (0)	−507.56768	−511.41541	
(AlN) ₁₀ /C ₃	43.4 (0)	−563.97873	−568.24845	
(AlN) ₁₁ /C _s	48.5 (0)	−620.49450	−625.16029	(−3269.87013) ^{c,d}
(AlN) ₁₂ /T _h	53.8 (0)	−677.05454	−682.10573	(−3567.24299) ^{c,d}
(AlN) ₁₂ /D _{3h}		−676.59970	−681.71298	
(AlN) ₁₂ /T _h		−676.48020	−681.45933	
(AlN) ₁₃ /C ₁	57.7 (0)	−733.39004	−738.88592	(−3864.44704) ^{c,d}
(AlN) ₁₄ /C _s	62.7 (0)	−789.89827	−795.79336	
(AlN) ₁₅ /C _{3h}	67.8 (0)	−846.42741	−852.71471	
(AlN) ₁₆ /T _d ^a	72.7 (0)	−902.91046	−909.60755	(−4756.58729) ^e
(AlN) ₁₆ /C ₃		−902.72807	−909.47310	(−4756.45839) ^e
(AlN) ₁₆ /C _{3v}		−902.88284	−909.58101	(−4756.56973) ^e
(AlN) ₁₆ /S ₄		−902.62743	−909.39289	(−4756.38750) ^e
(AlN) ₁₇ /C _s	76.9 (0)	−959.30793	−966.42757	
(AlN) ₁₈ /S ₆	81.8 (0)	−1015.80590	−1023.32481	
(AlN) ₁₉ /C ₃	86.2 (0)	−1072.21756	−1080.16487	
(AlN) ₂₀ /C ₂	90.9 (0)	−1128.69036	−1137.04750	
(AlN) ₂₁ /C _{3h}	95.8 (0)	−1185.19505	−1193.94042	
(AlN) ₂₂ /C ₃	100.7 (0)	−1241.67077	−1250.83119	

(AlN) ₂₃ /C ₁	105.2 (0)	−1298.11446	−1307.67118
(AlN) ₂₄ /S ₄	109.9 (0)	−1354.59354	−1364.56658
(AlN) ₂₅ /C ₃	114.7 (0)	−1411.07574	−1421.47327
(AlN) ₂₆ /C _{2h}	119.3 (0)	−1467.52924	−1478.33367
(AlN) ₂₇ /C _{3v}	124.1 (0)	−1524.00271	−1535.23063
(AlN) ₂₈ /T	128.9 (0)	−1580.50662	−1592.10508
(AlN) ₂₉ /C _s		−1636.94095	−1648.98617
(AlN) ₃₀ /C ₂		−1693.38704	−1705.86240
(AlN) ₃₁ /C ₃		−1749.90089	−1762.77067
(AlN) ₃₂ /C ₁		−1806.34569	
(AlN) ₃₃ /C _s		−1862.81416	
(AlN) ₃₄ /C ₃		−1919.31463	
(AlN) ₃₅ /C _s		−1975.78539	
(AlN) ₃₆ /T _d		−2032.25676	
(AlN) ₃₆ /C _{3h}		−2032.26335	
(AlN) ₃₆ /C ₃		−2032.25401	
(AlN) ₃₆ /S ₆		−2032.25308	
(AlN) ₃₆ /C ₂		−2032.25388	
(AlN) ₃₆ /C ₁		−2032.24631	
(AlN) ₃₇ /C _s		−2088.75039	
(AlN) ₃₈ /C ₂		−2145.20383	
(AlN) ₃₉ /C ₁		−2201.67482	
(AlN) ₄₀ /C ₃		−2258.15408	
(AlN) ₄₁ /C ₁		−2314.63355	

(a) At HF/LANL2DZ. (b) At B3LYP/LANL2DZp//LANL2DZ. (c) At B3LYP/6-31G*. (d) At the B3LYP/6-311G*//B3LYP/6-31G* level, −297.07939/(AlN)₁/triplet; −297.03755 /(AlN)₁/singlet; −3270.23039/(AlN)₁₁; −3567.63793/(AlN)₁₂, −3864.87099/(AlN)₁₃ (e) At B3LYP/cc-pvDZ.

HF/LANL2DZ//Fopt

(AlN)₂/D_{2h}

Al	1.97514619	0.00000000	0.00000000
Al	-1.97514619	0.00000000	0.00000000
N	0.00000000	0.64540328	0.00000000
N	0.00000000	-0.64540328	0.00000000

(AlN)₃/D_{3h}

Al	-1.55679933	0.00000000	-0.41714312
N	-1.31974799	0.00000000	1.31974799
Al	0.41714312	0.00000000	1.55679933
N	1.80280927	0.00000000	0.48306129
Al	1.13965620	0.00000000	-1.13965620
N	-0.48306129	0.00000000	-1.80280927

(AlN)₄/D_{4h}

N	-1.84829599	-0.00000002	-1.41824739
Al	-2.11715721	-0.00000000	0.27872904
Al	2.11715721	0.00000000	-0.27872904
N	-1.41824739	0.00000000	1.84829599
N	1.84829599	0.00000002	1.41824739
Al	0.27872904	0.00000002	2.11715721
Al	-0.27872904	-0.00000002	-2.11715721
N	1.41824739	-0.00000000	-1.84829599

(AlN)₅/D_{5h}

Al	1.57204761	2.16373791	0.00000000
Al	2.54362647	-0.82647434	0.00000000
Al	0.00000000	-2.67452715	0.00000000
Al	-2.54362647	-0.82647434	0.00000000
Al	-1.57204761	2.16373791	0.00000000
N	0.00000000	2.82021079	0.00000000
N	2.68217985	0.87149306	0.00000000
N	1.65767831	-2.28159846	0.00000000
N	-1.65767831	-2.28159846	0.00000000
N	-2.68217985	0.87149306	0.00000000

(AlN)₆/D_{3d}

Al	1.78708744	0.00000000	0.94192101
N	1.87368877	0.00000000	-0.99768846
Al	-0.89354372	1.54766313	0.94192101
Al	-0.89354372	-1.54766313	0.94192101
N	-0.93684438	1.62266207	-0.99768846
N	-0.93684438	-1.62266207	-0.99768846
Al	0.89354372	1.54766313	-0.94192101
N	0.93684438	1.62266207	0.99768846
Al	-1.78708744	0.00000000	-0.94192101
Al	0.89354372	-1.54766313	-0.94192101
N	-1.87368877	0.00000000	0.99768846
N	0.93684438	-1.62266207	0.99768846

(AlN)₇/C_{3v}

Al	0.00000000	1.74430188	0.92879762
N	-1.37736702	0.79522322	1.82217384
N	0.00000000	1.79046017	-0.87204433
Al	-1.26183984	0.72852357	-1.78360376
Al	0.00000000	0.00000000	2.80601777
N	0.00000000	0.00000000	-2.95393111
N	1.37736702	0.79522322	1.82217384
Al	1.26183984	0.72852357	-1.78360376
Al	-1.51060974	-0.87215094	0.92879762
Al	1.51060974	-0.87215094	0.92879762
N	0.00000000	-1.59044643	1.82217384
N	-1.55058399	-0.89523008	-0.87204433
N	1.55058399	-0.89523008	-0.87204433
Al	0.00000000	-1.45704714	-1.78360376

(AlN)₈/S₄

N	0.96827175	0.97784734	-2.45642403
Al	0.91971570	1.69277470	-0.75944456
N	1.67646724	1.00712597	0.72748489
Al	0.85338048	0.93791615	2.36280367
N	-0.96827175	-0.97784734	-2.45642403
N	-0.97784734	0.96827175	2.45642403
N	0.97784734	-0.96827175	2.45642403
Al	-0.91971570	-1.69277470	-0.75944456
Al	-1.69277470	0.91971570	0.75944456
Al	1.69277470	-0.91971570	0.75944456
N	-1.67646724	-1.00712597	0.72748489
N	-1.00712597	1.67646724	-0.72748489
N	1.00712597	-1.67646724	-0.72748489
Al	-0.85338048	-0.93791615	2.36280367
Al	-0.93791615	0.85338048	-2.36280367
Al	0.93791615	-0.85338048	-2.36280367

(AlN)₉/C_{3h}

Al	0.01941678	1.85336224	1.56090234
N	1.62905810	0.85669486	1.61484710
N	0.50412600	2.72792255	0.00000000
Al	2.03161309	1.65893911	0.00000000
Al	-1.61476717	-0.90986570	1.56090234
Al	1.59535040	-0.94349655	1.56090234
N	-1.55644856	0.98245827	1.61484710
N	-0.07260954	-1.83915313	1.61484710
N	-2.61451323	-0.92737536	0.00000000
N	2.11038723	-1.80054720	0.00000000
Al	-2.45248996	0.92995900	0.00000000
Al	0.42087686	-2.58889810	0.00000000
Al	0.01941678	1.85336224	-1.56090234
N	1.62905810	0.85669486	-1.61484710
Al	-1.61476717	-0.90986570	-1.56090234
Al	1.59535040	-0.94349655	-1.56090234
N	-1.55644856	0.98245827	-1.61484710

N	-0.07260954	-1.83915313	-1.61484710
(AlN)₁₀/C₃			
N	0.00027433	-0.00001422	-1.97637119
N	-0.35631466	2.74544782	-0.31475997
Al	0.60100794	1.72897534	-1.60491579
Al	2.65281821	0.59684393	0.29560860
N	2.21315959	2.02719995	-0.74943202
Al	1.15238135	2.61242719	0.69006180
N	1.44543982	1.09129415	1.68895977
Al	-0.00029188	0.00001350	2.10056059
N	-2.19940618	-1.68134026	-0.31498655
N	2.55585201	-1.06411140	-0.31432663
Al	-1.79751381	-0.34420539	-1.60523411
Al	1.19717652	-1.38479694	-1.60480749
Al	-1.84334995	1.99902207	0.29497266
Al	-0.80958835	-2.59585684	0.29514964
N	-2.86203906	0.90295718	-0.75013224
N	0.64918917	-2.93017188	-0.74961374
Al	-2.83876335	-0.30813283	0.68952556
Al	1.68609106	-2.30428221	0.69017304
N	-1.66815037	0.70635621	1.68852547
N	0.22200918	-1.79762091	1.68881088
(AlN)₁₁/C_s			
N	0.00000000	-1.45542636	-1.73327921
Al	0.00000000	0.31224876	-2.27009270
Al	1.56599415	-1.95353900	-0.92713645
N	1.33670464	1.47594368	-1.71622783
Al	2.80674166	0.82196019	-0.93835390
N	3.12902210	-0.98945250	-0.99099883
Al	0.00000000	-1.50331263	1.78283167
N	1.54202672	-2.02635018	0.96102163
Al	0.00000000	2.45506043	-0.87558838
Al	3.01275469	-0.94805014	0.88734158
N	0.00000000	2.52757643	0.92183721
Al	1.29498832	1.44190267	1.71476530
N	0.00000000	0.25287908	2.32949084
N	2.82859358	0.87979928	0.96352697
Al	-1.56599415	-1.95353900	-0.92713645
N	-1.33670464	1.47594368	-1.71622783
Al	-2.80674166	0.82196019	-0.93835390
N	-3.12902210	-0.98945250	-0.99099883
N	-1.54202672	-2.02635018	0.96102163
Al	-3.01275469	-0.94805014	0.88734158
Al	-1.29498832	1.44190267	1.71476530
N	-2.82859358	0.87979928	0.96352697
(AlN)₁₂/T_h			
N	1.33797030	0.00000000	2.60070729
Al	2.55991123	0.00000000	1.29251276
N	2.60070729	1.33797030	0.00000000

N	0.00000000	2.60070729	1.33797030
Al	1.29251276	2.55991123	0.00000000
Al	0.00000000	1.29251276	2.55991123
N	1.33797030	0.00000000	-2.60070729
Al	2.55991123	0.00000000	-1.29251276
N	0.00000000	2.60070729	-1.33797030
Al	0.00000000	1.29251276	-2.55991123
N	2.60070729	-1.33797030	0.00000000
N	0.00000000	-2.60070729	1.33797030
Al	1.29251276	-2.55991123	0.00000000
Al	0.00000000	-1.29251276	2.55991123
N	0.00000000	-2.60070729	-1.33797030
Al	0.00000000	-1.29251276	-2.55991123
N	-1.33797030	0.00000000	2.60070729
Al	-2.55991123	0.00000000	1.29251276
N	-2.60070729	1.33797030	0.00000000
Al	-1.29251276	2.55991123	0.00000000
N	-1.33797030	0.00000000	-2.60070729
Al	-2.55991123	0.00000000	-1.29251276
N	-2.60070729	-1.33797030	0.00000000
Al	-1.29251276	-2.55991123	0.00000000

(AlN)₁₃/C₁

N	0.21241702	1.76297486	2.01544452
Al	-0.38227480	2.58882871	0.46879453
N	0.45891667	2.13761017	-1.07289594
Al	2.24576668	1.94775958	-0.94448974
N	2.98204069	1.38719485	0.70771876
Al	1.79689157	0.88009184	2.01743517
Al	-0.44112673	0.78398235	-2.00965503
N	-2.25592099	0.81484824	-2.00924626
Al	-3.17087106	1.46389380	-0.47568531
N	-2.13611854	2.17144870	0.78562710
N	3.16973959	0.71517109	-1.93009471
Al	2.23253845	-0.87218732	-1.94014476
N	0.41358535	-0.89645804	-1.93011323
Al	-1.48749194	1.06962912	2.13919391
Al	3.87660231	0.12813279	-0.28673737
N	-4.04261351	-0.12813291	-0.18626063
Al	-3.13357472	-0.76519924	-1.70738363
N	3.17861535	-1.55812126	-0.44053401
N	1.57683840	-0.92213884	2.24828470
Al	2.10735542	-2.08712183	0.88880564
Al	-0.12598262	-1.61216415	2.03273586
N	0.39625943	-2.66681194	0.59865214
Al	-2.96406930	-1.29380911	0.75877730
N	-2.25509693	-2.07270423	-0.80855130
Al	-0.46643471	-2.22680093	-0.92760576
N	-1.73608905	-0.74703882	2.01595139

(AlN)₁₄/C_s

Al	0.00000000	-1.31220127	-2.43683734
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N	0.00000000	0.51147401	-2.28967300
N	1.32973535	-2.45308024	-1.80069802
Al	1.61869112	1.29615961	-1.72492444
N	2.79020175	0.15066658	-0.96127436
Al	2.66715398	-1.67210321	-0.92701449
N	1.54849311	2.93536216	-0.94680843
Al	0.00000000	3.88042569	-0.85726781
Al	0.00000000	-3.40190201	-0.92436005
N	0.00000000	-1.33623228	2.48410426
Al	0.00000000	0.46566303	2.33758151
Al	1.28588378	-2.44965748	1.73763395
N	1.58012487	1.26079281	1.71855703
Al	2.71414048	0.10792877	0.88908781
N	2.70743607	-1.73015156	0.94331383
Al	1.47785358	2.90308538	0.94771739
N	0.00000000	3.98158828	1.03564183
N	0.00000000	-3.48521448	0.87912536
N	-1.32973535	-2.45308024	-1.80069802
Al	-1.61869112	1.29615961	-1.72492444
N	-2.79020175	0.15066658	-0.96127436
Al	-2.66715398	-1.67210321	-0.92701449
N	-1.54849311	2.93536216	-0.94680843
Al	-1.28588378	-2.44965748	1.73763395
N	-1.58012487	1.26079281	1.71855703
Al	-2.71414048	0.10792877	0.88908781
N	-2.70743607	-1.73015156	0.94331383
Al	-1.47785358	2.90308538	0.94771739

(AlN)₁₅/C_{3h}

Al	1.88704521	1.84488405	1.52274978
N	0.24758011	2.71039212	1.52808929
N	2.55762736	1.11281684	0.00000000
Al	-0.71107625	2.74336168	0.00000000
N	1.53999013	1.00670341	3.13739500
Al	-0.14370782	1.80353524	3.07955739
Al	-2.54123906	0.71178706	1.52274978
Al	0.65419385	-2.55667112	1.52274978
N	-2.47105849	-1.14078539	1.52808929
N	2.22347838	-1.56960673	1.52808929
N	-2.24254133	1.65856185	0.00000000
N	-0.31508603	-2.77137869	0.00000000
Al	-2.02028278	-1.98749094	0.00000000
Al	2.73135903	-0.75587074	0.00000000
N	-1.64182579	0.83031887	3.13739500
N	0.10183566	-1.83702228	3.13739500
Al	-1.49005343	-1.02622225	3.07955739
Al	1.63376125	-0.77731300	3.07955739
Al	1.88704521	1.84488405	-1.52274978
N	0.24758011	2.71039212	-1.52808929
N	1.53999013	1.00670341	-3.13739500
Al	-0.14370782	1.80353524	-3.07955739
Al	-2.54123906	0.71178706	-1.52274978

Al	0.65419385	-2.55667112	-1.52274978
N	-2.47105849	-1.14078539	-1.52808929
N	2.22347838	-1.56960673	-1.52808929
N	-1.64182579	0.83031887	-3.13739500
N	0.10183566	-1.83702228	-3.13739500
Al	-1.49005343	-1.02622225	-3.07955739
Al	1.63376125	-0.77731300	-3.07955739

(AlN)₁₆/T_d

N	0.94942717	3.10494149	-0.94942717
Al	-0.89412050	3.05231693	-0.89412050
N	-0.94942717	3.10494149	0.94942717
Al	0.89412050	3.05231693	0.89412050
Al	0.89412050	-3.05231693	-0.89412050
N	-0.94942717	-3.10494149	-0.94942717
Al	-0.89412050	-3.05231693	0.89412050
N	0.94942717	-3.10494149	0.94942717
Al	3.05231693	-0.89412050	-0.89412050
N	3.10494149	0.94942717	-0.94942717
Al	3.05231693	0.89412050	0.89412050
N	3.10494149	-0.94942717	0.94942717
N	-3.10494149	-0.94942717	-0.94942717
Al	-3.05231693	0.89412050	-0.89412050
N	-3.10494149	0.94942717	0.94942717
Al	-3.05231693	-0.89412050	0.89412050
N	0.94942717	-0.94942717	3.10494149
Al	0.89412050	0.89412050	3.05231693
N	-0.94942717	0.94942717	3.10494149
Al	-0.89412050	-0.89412050	3.05231693
Al	0.89412050	-0.89412050	-3.05231693
N	0.94942717	0.94942717	-3.10494149
Al	-0.89412050	0.89412050	-3.05231693
N	-0.94942717	-0.94942717	-3.10494149
Al	1.92189118	-1.92189118	1.92189118
N	-1.88443385	-1.88443385	1.88443385
Al	-1.92189118	-1.92189118	-1.92189118
N	1.88443385	-1.88443385	-1.88443385
N	1.88443385	1.88443385	1.88443385
Al	-1.92189118	1.92189118	1.92189118
N	-1.88443385	1.88443385	-1.88443385
Al	1.92189118	1.92189118	-1.92189118

(AlN)₁₇/C_s

N	3.85768981	0.06077619	0.00000000
Al	3.40018564	-1.61720538	0.00000000
N	2.35964194	-2.34144934	-1.33926034
Al	1.26348115	-1.23713554	-2.29275237
N	1.64104947	0.61736710	-2.27617994
Al	3.08274101	1.15688586	-1.26385184
N	2.93942439	2.50255921	0.00000000
Al	1.63134949	-3.39590195	0.00000000
Al	-2.78115933	1.50445604	-1.52959850

N	-3.25594596	-0.26977721	-1.53618944
Al	-1.78661693	-0.53305813	-2.63832761
N	-1.38626129	1.24335707	-2.71686566
Al	-3.40396918	-1.22409824	0.00000000
N	-2.54491457	2.46448179	0.00000000
Al	1.51620084	3.51947378	0.00000000
Al	0.26412884	1.89570892	-2.43495026
N	0.27280726	3.35499091	-1.34312883
N	-0.04226858	-3.90763793	0.00000000
Al	-1.12425497	-3.11677962	-1.26101522
N	-0.52344157	-1.80686812	-2.39277466
N	-2.41634349	-2.72793294	0.00000000
Al	-1.00207662	3.40677331	0.00000000
N	2.35964194	-2.34144934	1.33926034
Al	1.26348115	-1.23713554	2.29275237
N	1.64104947	0.61736710	2.27617994
Al	3.08274101	1.15688586	1.26385184
Al	-2.78115933	1.50445604	1.52959850
N	-3.25594596	-0.26977721	1.53618944
Al	-1.78661693	-0.53305813	2.63832761
N	-1.38626129	1.24335707	2.71686566
Al	0.26412884	1.89570892	2.43495026
N	0.27280726	3.35499091	1.34312883
Al	-1.12425497	-3.11677962	1.26101522
N	-0.52344157	-1.80686812	2.39277466

(AlN)₁₈/S₆

Al	2.46845399	2.33319975	-0.90449571
N	2.54890077	2.33554091	0.94179018
Al	-0.45091074	2.33319975	2.58999172
N	-2.09006461	2.33554091	1.73651773
Al	-2.01754325	2.33319975	-1.68549601
N	-0.45883616	2.33554091	-2.67830791
Al	2.55037684	-0.79101786	-0.94161328
N	2.54278724	-0.79061355	0.91710710
Al	-0.45972740	-0.79101786	2.67949778
N	-2.06563167	-0.79061355	1.74356480
Al	-2.09064944	-0.79101786	-1.73788449
N	-0.47715557	-0.79061355	-2.66067190
Al	2.09064944	0.79101786	1.73788449
N	0.47715557	0.79061355	2.66067190
Al	-2.55037684	0.79101786	0.94161328
N	-2.54278724	0.79061355	-0.91710710
Al	0.45972740	0.79101786	-2.67949778
N	2.06563167	0.79061355	-1.74356480
Al	2.01754325	-2.33319975	1.68549601
N	0.45883616	-2.33554091	2.67830791
Al	-2.46845399	-2.33319975	0.90449571
N	-2.54890077	-2.33554091	-0.94179018
Al	0.45091074	-2.33319975	-2.58999172
N	2.09006461	-2.33554091	-1.73651773
Al	1.56593922	3.89253663	0.90936294

Al	-1.57050102	3.89253663	0.90146168
N	-1.61337275	3.95387530	-0.88513408
Al	0.00456180	3.89253663	-1.81082462
N	1.57323497	3.95387530	-0.95465475
N	0.04013778	3.95387530	1.83978883
Al	-0.00456180	-3.89253663	1.81082462
Al	-1.56593922	-3.89253663	-0.90936294
N	-0.04013778	-3.95387530	-1.83978883
Al	1.57050102	-3.89253663	-0.90146168
N	1.61337275	-3.95387530	0.88513408
N	-1.57323497	-3.95387530	0.95465475

(AlN)₁₉/C₃

Al	-3.36302272	0.69309139	-1.45479697
Al	-0.57468326	1.78226582	-2.34875655
Al	-1.01261139	2.93133819	1.95986158
Al	-0.00147805	3.94992678	-0.10623582
N	-3.75060498	1.52087800	0.15729570
N	0.00000000	0.00000000	-2.51949783
N	0.56490332	3.04964553	-1.59041774
Al	-2.87714040	2.98412446	-0.51009501
Al	-3.08316020	0.63816946	1.60307946
N	0.68220804	3.43112790	1.52982380
N	-2.33192670	2.07886460	-2.04764219
N	-1.43828917	1.19657825	2.30216104
Al	0.00000000	0.00000000	2.49539848
N	-1.72578137	3.85560190	0.49938792
Al	2.28174611	2.56591742	-1.45479697
Al	1.83082911	-0.39344261	-2.34875655
Al	3.04491904	-0.58872191	1.95986158
Al	3.42147595	-1.97368336	-0.10623582
N	3.19242148	2.48768019	0.15729570
N	2.35861884	-2.01404339	-1.59041774
Al	4.02289779	0.99961445	-0.51009501
Al	2.09425107	2.35101033	1.60307946
N	2.63033990	-2.30637344	1.52982380
N	2.96631290	0.98007546	-2.04764219
N	1.75541175	0.64730584	2.30216104
N	4.20193988	-0.43323044	0.49938792
Al	1.08127661	-3.25900880	-1.45479697
Al	-1.25614584	-1.38882321	-2.34875655
Al	-2.03230765	-2.34261628	1.95986158
Al	-3.41999791	-1.97624341	-0.10623582
N	0.55818350	-4.00855819	0.15729570
N	-2.92352217	-1.03560214	-1.59041774
Al	-1.14575739	-3.98373890	-0.51009501
Al	0.98890914	-2.98917979	1.60307946
N	-3.31254794	-1.12475445	1.52982380
N	-0.63438620	-3.05894006	-2.04764219
N	-0.31712258	-1.84388409	2.30216104
N	-2.47615851	-3.42237146	0.49938792

(AlN)₂₀/C₂

N	0.31098668	-0.89231226	2.48792672
N	2.64578260	-1.83248019	-2.15982789
Al	2.57073856	2.64407066	-0.86356699
N	-3.28885563	0.09125730	-2.19024737
Al	0.91915955	-2.27814259	-2.30324944
N	-1.24499813	3.77192116	0.47275445
N	-2.53020952	-2.60607935	-0.88627846
N	-2.64582713	-1.83242169	2.15979657
Al	-0.91921999	-2.27813454	2.30322594
N	-0.43509626	-3.68292005	1.27075508
N	0.87993371	2.23533084	2.25796417
Al	-0.35363565	0.86595223	2.47902077
N	3.28886191	0.09114554	2.19025918
Al	0.41460894	3.62050404	1.18175235
Al	2.10817421	-1.26500537	2.12424034
Al	-2.10820870	-1.26492920	-2.12425384
Al	2.61014093	1.78180524	2.08461382
N	-2.13542899	1.26779125	2.06597079
N	2.13545883	1.26774737	-2.06595131
Al	-2.57066580	2.64413473	0.86359483
N	1.24510965	3.77190491	-0.47272585
Al	-2.61009197	1.78189858	-2.08458768
Al	-0.41450181	3.62052587	-1.18172369
Al	3.28500425	-0.13092288	-2.08406365
Al	-3.28500942	-0.13085007	2.08405838
N	-0.87987222	2.23537258	-2.25794076
Al	-1.17729643	-3.69278622	-0.43492073
N	0.43499963	-3.68292507	-1.27078959
Al	3.52666430	-2.11453867	-0.55503705
N	4.44207975	-0.53156647	-0.67732168
N	-3.59580002	2.19303355	-0.56447072
Al	-4.35342405	0.53645558	-0.73130749
N	2.53013794	-2.60615420	0.88625091
Al	1.17719753	-3.69282531	0.43488629
Al	-3.52672512	-2.11444462	0.55501111
N	-0.31101081	-0.89228705	-2.48794114
Al	4.35343412	0.53632791	0.73131548
N	3.59585351	2.19292761	0.56449859
Al	0.35365710	0.86596042	-2.47901110
N	-4.44210575	-0.53145253	0.67731931

(AlN)₂₁/C_{3h}

N	-1.59999447	-0.92120471	-2.54034881
Al	-1.60167563	0.92906121	-2.54353529
N	-1.59999447	2.66060896	0.47238773
Al	-1.60167563	1.73823557	2.07635826
N	-1.59999447	-1.73940425	2.06796109
Al	-1.60167563	-2.66729678	0.46717703
N	-3.13838640	1.74790928	-2.10489735

Al	-3.13185642	2.60680126	-0.46865759
N	-3.13838640	0.94893994	2.56618252
Al	-3.13185642	-0.89753125	2.49188491
N	-3.13838640	-2.69684922	-0.46128516
Al	-3.13185642	-1.70927000	-2.02322732
N	1.59999447	-0.92120471	-2.54034881
Al	1.60167563	0.92906121	-2.54353529
N	1.59999447	2.66060896	0.47238773
Al	1.60167563	1.73823557	2.07635826
N	1.59999447	-1.73940425	2.06796109
Al	1.60167563	-2.66729678	0.46717703
N	0.00000000	1.61571804	-2.00671382
Al	0.00000000	2.53448407	-0.40729661
N	0.00000000	0.93000612	2.40260978
Al	0.00000000	-0.91451282	2.39857590
N	0.00000000	-2.54572416	-0.39589596
Al	0.00000000	-1.61997125	-1.99127928
N	3.13838640	1.74790928	-2.10489735
Al	3.13185642	2.60680126	-0.46865759
N	3.13838640	0.94893994	2.56618252
Al	3.13185642	-0.89753125	2.49188491
N	3.13838640	-2.69684922	-0.46128516
Al	3.13185642	-1.70927000	-2.02322732
Al	-4.68442759	0.89767052	-1.57319323
Al	-4.68442759	0.91359004	1.56400209
N	-4.74306594	-0.95094692	1.57606819
Al	-4.68442759	-1.81126056	0.00919114
N	-4.74306594	-0.88944163	-1.61157829
N	-4.74306594	1.84038855	0.03551010
Al	4.68442759	0.89767052	-1.57319323
Al	4.68442759	0.91359004	1.56400209
N	4.74306594	-0.95094692	1.57606819
Al	4.68442759	-1.81126056	0.00919114
N	4.74306594	-0.88944163	-1.61157829
N	4.74306594	1.84038855	0.03551010

(AlN)₂₂/C₃

Al	0.00133980	3.23480517	-0.35414204
N	1.53303200	2.66682229	0.51072247
Al	2.63277741	1.55263063	-0.48184831
N	-0.01522367	1.75772415	-4.27685268
N	0.01640197	3.34043309	-2.12734226
Al	0.00000000	0.00000000	-4.71746627
N	2.54269640	1.48617990	-2.33179295
Al	2.77272595	-0.14097610	-3.10912764
Al	1.25764145	2.47314534	-3.14470082
N	3.22498242	0.02723636	0.36314750
Al	3.25708012	0.04667932	2.14388829
N	2.52232412	1.36360998	3.17726180
Al	1.49241398	2.60131783	2.36075661
N	-0.12359230	2.85713500	3.13526871
Al	1.75738612	0.00318318	4.16658399

N	0.00000000	0.00000000	4.63729194
Al	2.80075355	-1.61856288	-0.35414204
N	1.54301985	-2.66105580	0.51072247
Al	0.02822886	-3.05636744	-0.48184831
N	1.52984560	-0.86567799	-4.27685268
N	2.88469893	-1.68442106	-2.12734226
N	0.01572135	-2.94512962	-2.33179295
Al	-1.50845185	-2.33076306	-3.10912764
Al	1.51298597	-2.32572211	-3.14470082
N	-1.58890383	-2.80653489	0.36314750
Al	-1.58811458	-2.84405378	2.14388829
N	-0.08024117	-2.86620176	3.17726180
Al	1.50660034	-2.59312733	2.36075661
N	2.53614764	-1.32153343	3.13526871
Al	-0.87593635	-1.52353261	4.16658399
Al	-2.80209335	-1.61624228	-0.35414204
N	-3.07605185	-0.00576649	0.51072247
Al	-2.66100628	1.50373681	-0.48184831
N	-1.51462193	-0.89204616	-4.27685268
N	-2.90110090	-1.65601203	-2.12734226
N	-2.55841775	1.45894972	-2.33179295
Al	-1.26427409	2.47173916	-3.10912764
Al	-2.77062742	-0.14742323	-3.14470082
N	-1.63607859	2.77929853	0.36314750
Al	-1.66896554	2.79737446	2.14388829
N	-2.44208295	1.50259178	3.17726180
Al	-2.99901431	-0.00819050	2.36075661
N	-2.41255534	-1.53560157	3.13526871
Al	-0.88144977	1.52034944	4.16658399

(AlN)₂₃/C₁

N	1.95260581	-1.48064161	-2.31685681
N	1.61831068	3.65615642	0.35364508
Al	2.10234852	0.67431597	3.87405949
N	-3.84620080	1.19583039	1.39453915
Al	-0.09158120	3.39313923	-0.09069292
N	-0.13593610	-2.74237188	1.96272798
N	-3.48789689	2.64735318	-0.83896554
Al	-4.63541676	1.30027040	-0.27140273
N	-0.76176269	-1.56815323	-3.94902623
Al	0.94609069	-0.94015240	-3.69319810
N	0.46157482	0.81163203	-3.97056530
Al	-1.25174614	0.21111446	-4.16604335
N	2.16850810	-3.45931822	-0.02311145
Al	1.18268955	-2.85364053	-1.35795927
Al	1.47135636	-3.53579404	1.66821861
Al	2.96293655	-0.24981576	-1.39998719
Al	3.54761005	-2.48447500	0.67791411
N	-0.64118864	-2.90208795	-1.17413296
Al	-1.29495576	-2.63256575	0.53455203
N	3.06643686	-2.96771599	2.41057872
N	1.34826432	-0.98342742	4.10940653

Al	-2.83529395	-0.23148227	1.86445813
Al	-0.15810016	-1.34275085	3.18036553
Al	2.25656500	3.00732305	1.94490546
Al	-1.63975475	-2.47923524	-2.65475165
N	-1.23899356	0.07261762	2.72149128
Al	-2.28542229	2.35583859	-2.16976774
N	-0.51542470	2.74278675	-1.76441442
Al	2.94960429	2.67124977	-0.44281058
N	3.71407826	2.18655342	1.13846527
N	-2.88340810	-1.71825688	0.75579141
Al	-3.98690346	-1.66946008	-0.68125612
N	-4.88728411	-0.14566715	-1.24408975
N	2.46167851	1.50717732	-1.71386236
Al	0.90022161	1.91334966	-2.63261095
Al	-3.90804189	-0.28697793	-2.79532573
N	-2.67852623	0.94850184	-3.33770807
N	3.69705261	-0.01945674	3.23858479
Al	-0.49378863	1.76093294	2.60117161
Al	2.99037000	-1.67575163	3.60463096
N	-3.33411873	-1.98745139	-2.36368947
Al	4.13146241	0.48726875	1.54707636
N	3.83462211	-0.75111085	0.17116758
Al	-2.86105791	2.66096916	0.88692316
N	-1.15931585	2.88052058	1.31767919
N	1.24727054	2.05352810	3.11014435

(AlN)₂₄/S₄

N	3.54947568	-1.97739142	-0.93309025
Al	-1.38586101	2.51692889	1.93050975
Al	-2.25367873	3.27038418	-0.95608025
N	2.64392795	-1.15130990	1.94624975
Al	3.04795196	-1.58790028	-2.64688025
N	2.57959614	0.06260562	-3.22530025
Al	3.44360121	-0.72232048	0.33079975
Al	2.51687531	1.38595497	-1.93057025
Al	-0.14949712	2.62077223	-3.26583025
N	-1.82687076	2.99332380	-2.71184025
Al	1.25473199	0.05353081	-4.44972025
N	-0.03175345	1.33858812	-4.52062025
N	-1.00905788	3.34620390	0.32528975
N	1.33858511	0.03185390	4.52061975
Al	-0.05365122	1.25473038	4.44972975
Al	2.62077223	0.14949712	3.26581975
N	-0.06253858	2.57955136	3.22528975
N	2.99358386	1.82686262	2.71186975
Al	1.58801232	3.04783387	2.64697975
Al	3.27037002	2.25361957	0.95603975
N	1.97729768	3.54928174	0.93314975
N	3.34608929	1.00899572	-0.32535025
Al	0.72229543	3.44367313	-0.33079025
N	1.15133173	2.64409684	-1.94628025
N	-3.54947568	1.97739142	-0.93309025

Al	1.38586101	-2.51692889	1.93050975
Al	2.25367873	-3.27038418	-0.95608025
N	-2.64392795	1.15130990	1.94624975
Al	-3.04795196	1.58790028	-2.64688025
N	-2.57959614	-0.06260562	-3.22530025
Al	-3.44360121	0.72232048	0.33079975
Al	-2.51687531	-1.38595497	-1.93057025
Al	0.14949712	-2.62077223	-3.26583025
N	1.82687076	-2.99332380	-2.71184025
Al	-1.25473199	-0.05353081	-4.44972025
N	0.03175345	-1.33858812	-4.52062025
N	1.00905788	-3.34620390	0.32528975
N	-1.33858511	-0.03185390	4.52061975
Al	0.05365122	-1.25473038	4.44972975
Al	-2.62077223	-0.14949712	3.26581975
N	0.06253858	-2.57955136	3.22528975
N	-2.99358386	-1.82686262	2.71186975
Al	-1.58801232	-3.04783387	2.64697975
Al	-3.27037002	-2.25361957	0.95603975
N	-1.97729768	-3.54928174	0.93314975
N	-3.34608929	-1.00899572	-0.32535025
Al	-0.72229543	-3.44367313	-0.33079025
N	-1.15133173	-2.64409684	-1.94628025

(AlN)₂₅/C₃

N	0.00000000	0.00000000	-3.52336029
Al	0.00000000	0.00000000	3.50796418
N	-1.55618604	0.94668166	3.26028687
Al	1.64790659	2.48542973	2.35290244
Al	-1.37479680	2.71377916	3.03897105
N	0.21898757	3.52120851	2.61521149
N	-3.51238369	0.88883241	0.72444152
Al	-1.33714413	3.94719465	-1.69575361
N	-3.00438356	3.29008521	-1.20816737
Al	1.55706224	3.24938010	-0.71934821
Al	-0.66281443	4.29321812	1.21894189
N	-0.02637059	4.17913357	-0.46782327
N	-2.30328137	3.58513235	1.72177835
Al	-3.27317613	2.71118290	0.47495047
N	-2.95058370	0.31047471	-2.34999280
Al	-2.78923628	2.08052709	-2.55582124
N	-1.20516746	2.81568371	-3.12809576
Al	0.26043934	1.80529106	-3.28049490
N	1.59794338	0.87435581	3.26028687
Al	1.32849199	-2.66984384	2.35290244
Al	3.03760009	-0.16628063	3.03897105
N	2.93996223	-1.95025305	2.61521149
N	2.52594329	2.59739730	0.72444152
Al	4.08694291	-0.81559654	-1.69575361
N	4.35148915	0.95682988	-1.20816737
Al	2.03551460	-2.97314551	-0.71934821
Al	4.04944317	-1.57259493	1.21894189

N	3.63242113	-2.06672919	-0.46782327
N	4.25645637	0.20213400	1.72177835
Al	3.98454133	1.47906223	0.47495047
N	1.74417084	2.40004308	-2.34999280
Al	3.19640745	1.37528593	-2.55582124
N	3.04103735	-0.36413622	-3.12809576
Al	1.43320825	-1.12819261	-3.28049490
N	-0.04175735	-1.82103747	3.26028687
Al	-2.97639858	0.18441410	2.35290244
Al	-1.66280330	-2.54749853	3.03897105
N	-3.15894980	-1.57095545	2.61521149
N	0.98644040	-3.48622971	0.72444152
Al	-2.74979878	-3.13159811	-1.69575361
N	-1.34710559	-4.24691509	-1.20816737
Al	-3.59257684	-0.27623460	-0.71934821
Al	-3.38662874	-2.72062319	1.21894189
N	-3.60605055	-2.11240439	-0.46782327
N	-1.95317501	-3.78726635	1.72177835
Al	-0.71136521	-4.19024513	0.47495047
N	1.20641286	-2.71051779	-2.34999280
Al	-0.40717117	-3.45581302	-2.55582124
N	-1.83586989	-2.45154749	-3.12809576
Al	-1.69364759	-0.67709845	-3.28049490

(ALN)₂₆/C_{2h}

Al	1.78127776	0.00000000	2.86946534
N	0.91091959	1.59537466	2.56306638
Al	-0.91698337	1.59787805	2.55073444
N	-1.79208815	0.00000000	2.82236414
Al	-0.91698337	-1.59787805	2.55073444
N	0.91091959	-1.59537466	2.56306638
Al	-3.49190160	2.53034018	0.92094823
N	-4.52465959	1.33293646	1.76425847
Al	-3.58337776	0.00000000	2.62422216
N	-1.87620706	2.92803707	1.69770519
Al	-3.49190160	-2.53034018	0.92094823
N	-1.87620706	-2.92803707	1.69770519
N	-4.52465959	-1.33293646	1.76425847
Al	-0.88319497	-4.18246412	0.88992899
N	0.93193402	-4.25610319	0.96214136
Al	1.87449946	-2.93477754	1.72227638
Al	4.46727023	-1.26113397	1.74125469
N	3.57521778	0.00000000	2.74079275
N	3.48400220	-2.52452754	0.93098987
Al	4.46727023	1.26113397	1.74125469
N	3.48400220	2.52452754	0.93098987
Al	1.87449946	2.93477754	1.72227638
Al	-0.88319497	4.18246412	0.88992899
N	0.93193402	4.25610319	0.96214136
N	5.52405408	0.00000000	0.89392231
Al	-5.44759283	0.00000000	0.88490876
N	1.79208815	0.00000000	-2.82236414

Al	0.91698337	1.59787805	-2.55073444
N	-0.91091959	1.59537466	-2.56306638
Al	-1.78127776	0.00000000	-2.86946534
N	-0.91091959	-1.59537466	-2.56306638
Al	0.91698337	-1.59787805	-2.55073444
N	-3.48400220	2.52452754	-0.93098987
Al	-4.46727023	1.26113397	-1.74125469
N	-3.57521778	0.00000000	-2.74079275
Al	-1.87449946	2.93477754	-1.72227638
N	-3.48400220	-2.52452754	-0.93098987
Al	-1.87449946	-2.93477754	-1.72227638
Al	-4.46727023	-1.26113397	-1.74125469
N	-0.93193402	-4.25610319	-0.96214136
Al	0.88319497	-4.18246412	-0.88992899
N	1.87620706	-2.92803707	-1.69770519
N	4.52465959	-1.33293646	-1.76425847
Al	3.58337776	0.00000000	-2.62422216
Al	3.49190160	-2.53034018	-0.92094823
N	4.52465959	1.33293646	-1.76425847
Al	3.49190160	2.53034018	-0.92094823
N	1.87620706	2.92803707	-1.69770519
N	-0.93193402	4.25610319	-0.96214136
Al	0.88319497	4.18246412	-0.88992899
Al	5.44759283	0.00000000	-0.88490876
N	-5.52405408	0.00000000	-0.89392231

(AlN)₂₇/C_{3v}

Al	-0.83318561	3.18424360	-1.32445501
N	-0.81773430	3.19482898	0.50128893
Al	0.80227122	3.18424353	1.34340635
N	2.22505652	2.43939644	0.47474272
Al	2.20375609	2.43026322	-1.35095018
N	0.58644981	2.43939650	-2.19825692
Al	0.25806365	1.16183843	-3.48286474
N	1.60167002	-0.03069063	-3.89388553
Al	3.30144762	0.46247180	-3.51251952
N	3.59017563	1.70726293	-2.20085543
Al	-2.28085793	2.52774464	1.39821540
N	-2.05063718	1.93420231	3.12767995
Al	-0.63219319	2.57871849	4.04991020
N	0.82097706	3.19705511	3.12293254
N	-3.71762204	1.93420238	0.40838806
Al	-3.89591540	2.57871862	-1.27408138
N	-2.41052749	3.19705524	-2.14850352
Al	3.22084744	1.16183832	1.35021690
N	4.19672957	-0.03069073	0.33934092
Al	4.62807088	0.46247174	-1.34844715
N	2.76822714	0.73782467	3.08563876
Al	1.83126377	1.96711696	4.02841827
N	-1.49381728	0.73782484	-3.86687959
Al	-2.75908171	1.96711714	-3.45964567
N	-4.43220978	1.58603097	-2.74926906

N	0.43910455	1.58603078	5.19712918
N	4.61351821	-0.65974853	-2.82818666
N	-2.26524933	-2.64981703	-0.43676580
Al	-2.14894344	-2.16223142	1.31734885
N	-0.63852869	-2.64981709	2.21684453
Al	0.90954522	-2.92156126	1.29066569
N	0.75546980	-3.39976983	-0.46311944
Al	-0.73751510	-2.92156119	-1.39612402
N	-0.54118334	-2.07370585	-3.01974751
Al	1.16648770	-1.80963196	-3.63740827
N	2.47161836	-2.93281706	-3.09169970
Al	2.26540540	-3.58810149	-1.38874269
N	-3.10060041	-0.69677333	1.90073523
Al	-2.49736780	0.16147382	3.40635885
N	-1.53734760	-0.77604643	4.61554271
Al	-0.48886087	-2.10634269	3.90633789
Al	-4.16865103	0.16147388	0.68005517
N	-4.81065267	-0.77604630	-0.72408102
Al	-3.70294022	-2.10634256	-1.33667308
N	2.44551757	-2.07370596	1.85234926
Al	3.77072513	-1.80963206	0.61078971
N	3.87655913	-2.93281711	-0.79987082
Al	2.33853926	-1.03913501	3.36416897
N	1.07154011	-1.42375400	4.59278201
Al	-1.93698140	-1.03913485	-3.61033269
N	-3.60670573	-1.42375382	-3.03867061
Al	-4.78440129	-0.11973381	-2.45512759
Al	0.01718886	-0.11973400	5.37753212
Al	4.13185322	-2.33336898	-2.53291563

(AlN)₂₈/T

Al	2.30196281	2.30196281	2.30196281
N	2.48680687	3.26199032	0.74126381
Al	1.19477189	4.45612222	0.39259572
N	-2.31196153	2.31196153	2.31196153
Al	-3.27365877	2.50442324	0.75216342
N	-4.52498403	1.27009309	0.41596179
Al	-2.30196281	-2.30196281	2.30196281
N	-2.48680687	-3.26199032	0.74126381
Al	-1.19477189	-4.45612222	0.39259572
N	2.31196153	-2.31196153	2.31196153
Al	3.27365877	-2.50442324	0.75216342
N	4.52498403	-1.27009309	0.41596179
Al	2.30196281	-2.30196281	-2.30196281
N	2.48680687	-3.26199032	-0.74126381
Al	1.19477189	-4.45612222	-0.39259572
N	-2.31196153	-2.31196153	-2.31196153
Al	-3.27365877	-2.50442324	-0.75216342
N	-4.52498403	-1.27009309	-0.41596179
Al	-2.30196281	2.30196281	-2.30196281
N	-2.48680687	3.26199032	-0.74126381
Al	-1.19477189	4.45612222	-0.39259572

N	2.31196153	2.31196153	-2.31196153
Al	3.27365877	2.50442324	-0.75216342
N	4.52498403	1.27009309	-0.41596179
N	0.74126381	2.48680687	3.26199032
N	3.26199032	0.74126381	2.48680687
N	-0.74126381	-2.48680687	3.26199032
N	-3.26199032	-0.74126381	2.48680687
N	0.74126381	-2.48680687	-3.26199032
N	3.26199032	-0.74126381	-2.48680687
N	-0.74126381	2.48680687	-3.26199032
N	-3.26199032	0.74126381	-2.48680687
Al	0.39259572	1.19477189	4.45612222
Al	4.45612222	0.39259572	1.19477189
Al	-0.39259572	-1.19477189	4.45612222
Al	-4.45612222	-0.39259572	1.19477189
Al	0.39259572	-1.19477189	-4.45612222
Al	4.45612222	-0.39259572	-1.19477189
Al	-0.39259572	1.19477189	-4.45612222
Al	-4.45612222	0.39259572	-1.19477189
Al	0.75216342	-3.27365877	2.50442324
Al	2.50442324	0.75216342	-3.27365877
Al	-0.75216342	3.27365877	2.50442324
Al	-2.50442324	-0.75216342	-3.27365877
Al	0.75216342	3.27365877	-2.50442324
Al	2.50442324	-0.75216342	3.27365877
Al	-0.75216342	-3.27365877	-2.50442324
Al	-2.50442324	0.75216342	3.27365877
N	0.41596179	-4.52498403	1.27009309
N	1.27009309	0.41596179	-4.52498403
N	-0.41596179	4.52498403	1.27009309
N	-1.27009309	-0.41596179	-4.52498403
N	0.41596179	4.52498403	-1.27009309
N	1.27009309	-0.41596179	4.52498403
N	-0.41596179	-4.52498403	-1.27009309
N	-1.27009309	0.41596179	4.52498403

(AlN)₂₉/C_s

N	-3.50147209	-2.93327690	0.00000000
N	-0.85948379	-3.26297128	1.59471083
Al	-1.75789708	-3.42242134	0.00000000
N	-4.60751896	-0.47898487	0.00000000
Al	-4.08087547	-1.70779459	1.24984382
N	-3.10538516	-1.30431004	2.67461468
Al	-1.76363015	-2.51591114	3.02271874
Al	-2.87019538	0.48278121	3.03121775
N	-1.83251365	0.87128447	4.51477870
Al	-0.88548490	-0.50566526	5.21898287
N	-0.89814302	-2.21445917	4.55229144
Al	-0.93037656	2.43497373	4.50877290
Al	-3.74099582	1.10148895	0.00000000
N	-3.01758774	1.65938653	1.60628653
Al	-1.85678537	3.08664965	1.57177878

N	-1.01547893	3.55763536	3.07549656
N	-1.00248896	3.43333666	0.00000000
Al	3.58567284	-2.70450629	0.00000000
Al	0.97603839	-3.21491291	1.59876955
N	1.87791278	-3.31979353	0.00000000
Al	4.51646186	-0.36804667	0.00000000
N	4.21511582	-1.58997977	1.32335986
Al	3.16313447	-1.19107603	2.69130726
N	1.84922413	-2.43959424	3.02397857
N	2.85187302	0.58900530	3.06399543
Al	1.83721516	0.95541691	4.56678245
N	0.97464167	-0.45366632	5.30246485
Al	0.92203095	-2.10803417	4.51181323
N	0.91910992	2.50330333	4.59250953
N	3.64513442	1.21504246	0.00000000
Al	2.92872413	1.74742377	1.61748880
N	1.71890413	3.12690939	1.56523127
Al	0.82587315	3.50653371	3.06869154
Al	0.83714138	3.44942344	0.00000000
N	-0.85948379	-3.26297128	-1.59471083
Al	-4.08087547	-1.70779459	-1.24984382
N	-3.10538516	-1.30431004	-2.67461468
Al	-1.76363015	-2.51591114	-3.02271874
Al	-2.87019538	0.48278121	-3.03121775
N	-1.83251365	0.87128447	-4.51477870
Al	-0.88548490	-0.50566526	-5.21898287
N	-0.89814302	-2.21445917	-4.55229144
Al	-0.93037656	2.43497373	-4.50877290
N	-3.01758774	1.65938653	-1.60628653
Al	-1.85678537	3.08664965	-1.57177878
N	-1.01547893	3.55763536	-3.07549656
Al	0.97603839	-3.21491291	-1.59876955
N	4.21511582	-1.58997977	-1.32335986
Al	3.16313447	-1.19107603	-2.69130726
N	1.84922413	-2.43959424	-3.02397857
N	2.85187302	0.58900530	-3.06399543
Al	1.83721516	0.95541691	-4.56678245
N	0.97464167	-0.45366632	-5.30246485
Al	0.92203095	-2.10803417	-4.51181323
N	0.91910992	2.50330333	-4.59250953
Al	2.92872413	1.74742377	-1.61748880
N	1.71890413	3.12690939	-1.56523127
Al	0.82587315	3.50653371	-3.06869154

(AlN)₃₀/C₂

N	-1.16794100	0.66851754	4.63381992
N	2.05896544	5.08450938	-0.41715148
Al	-2.12942407	1.13252221	3.17297809
Al	2.13131081	1.65351824	-3.64853135
N	4.86973963	1.00004411	-0.05840598
N	3.57907377	3.29163209	1.72283070
N	3.11378089	0.16401327	2.33601339

Al	0.62296554	1.08618371	4.68095640
N	1.03755527	0.82122804	-4.76309650
Al	-0.77970836	0.98457800	-4.56691301
Al	0.30613289	4.89422944	0.08587620
Al	4.50290830	1.45418780	-1.79113835
N	-0.82378835	3.73948254	-0.69749878
N	3.33330594	0.55285284	-2.78608703
N	-1.49865388	2.55200940	2.19005600
Al	2.47522904	4.68398398	1.34417652
N	-1.42074315	1.90490844	-3.14381791
Al	0.03435855	3.37987991	2.79541908
Al	-2.74432554	1.07793569	-2.16998733
Al	-1.88636629	2.70511781	0.39477615
N	1.30427678	2.35147352	3.64641419
Al	4.62160219	2.76985112	0.34872769
N	4.29251143	3.24220262	-1.41513364
Al	2.72691609	4.09128494	-1.75642028
N	-2.96560019	1.45561576	-0.38170796
Al	-0.28669111	3.09203954	-2.32971057
N	1.51127097	3.13519996	-2.75438631
N	0.71606781	4.72953780	1.86027158
Al	2.84943759	1.94367030	2.74930179
Al	-3.84391195	0.25490359	0.70550117
N	1.16794100	-0.66851754	4.63381992
N	-2.05896544	-5.08450938	-0.41715148
Al	2.12942407	-1.13252221	3.17297809
Al	-2.13131081	-1.65351824	-3.64853135
N	-4.86973963	-1.00004411	-0.05840598
N	-3.57907377	-3.29163209	1.72283070
N	-3.11378089	-0.16401327	2.33601339
Al	-0.62296554	-1.08618371	4.68095640
N	-1.03755527	-0.82122804	-4.76309650
Al	0.77970836	-0.98457800	-4.56691301
Al	-0.30613289	-4.89422944	0.08587620
Al	-4.50290830	-1.45418780	-1.79113835
N	0.82378835	-3.73948254	-0.69749878
N	-3.33330594	-0.55285284	-2.78608703
N	1.49865388	-2.55200940	2.19005600
Al	-2.47522904	-4.68398398	1.34417652
N	1.42074315	-1.90490844	-3.14381791
Al	-0.03435855	-3.37987991	2.79541908
Al	2.74432554	-1.07793569	-2.16998733
Al	1.88636629	-2.70511781	0.39477615
N	-1.30427678	-2.35147352	3.64641419
Al	-4.62160219	-2.76985112	0.34872769
N	-4.29251143	-3.24220262	-1.41513364
Al	-2.72691609	-4.09128494	-1.75642028
N	2.96560019	-1.45561576	-0.38170796
Al	0.28669111	-3.09203954	-2.32971057
N	-1.51127097	-3.13519996	-2.75438631
N	-0.71606781	-4.72953780	1.86027158
Al	-2.84943759	-1.94367030	2.74930179

Al	3.84391195	-0.25490359	0.70550117
(AlN)₃₁/C₃			
N	-0.36787050	2.95270004	-3.40712871
N	2.48723323	3.73824224	-2.29465412
N	3.60640347	0.33064616	1.77561921
Al	-1.08231939	3.44147583	-1.77390471
N	2.50385071	2.52335242	3.72527570
al	2.40387322	3.65963086	2.30601670
N	3.80811916	0.98004537	-1.33367138
N	0.65248219	4.13815881	2.63477748
Al	1.83724294	3.93331248	-0.65285729
N	0.00973973	3.97213369	-0.40061357
Al	-0.58711969	3.92625798	1.33828791
N	-0.54864680	1.73504912	4.28261196
N	2.89657028	3.21315104	0.65951228
Al	3.64092767	1.55106662	0.40706048
Al	2.88202651	0.80038563	3.41246577
Al	0.74166916	2.94440418	4.03621045
Al	3.45835260	2.20283988	-2.62107667
Al	1.38999123	3.21365688	-3.64698737
Al	1.81628415	0.16239283	-4.30527414
N	2.47300555	1.81115535	-4.12767458
Al	0.00000000	0.00000000	4.53961382
N	0.00000000	0.00000000	-4.55906452
N	-2.37317799	-1.79493522	-3.40712871
N	-4.48102936	0.28488604	-2.29465412
N	-2.08954971	2.95791395	1.77561921
Al	-2.43924580	-2.65805400	-1.77390471
N	-3.43721265	0.90672211	3.72527570
Al	-4.37126990	0.25199984	2.30601670
N	-2.75280377	2.80790525	-1.33367138
N	-3.90999175	-1.50401325	2.63477748
Al	-4.32497000	-0.37555718	-0.65285729
N	-3.44483855	-1.97763199	-0.40061357
Al	-3.10667931	-2.47158955	1.33828791
N	-1.22827321	-1.34266662	4.28261196
N	-4.23095556	0.90192793	0.65951228
Al	-3.16372693	2.37760254	0.40706048
Al	-2.13416754	2.09571536	3.41246577
Al	-2.92076340	-0.82989776	4.03621045
Al	-3.63689160	1.89360126	-2.62107667
Al	-3.47810411	-0.40306072	-3.64698737
Al	-1.04877839	1.49175180	-4.30527414
N	-2.80500932	1.23610795	-4.12767458
N	2.74104849	-1.15776482	-3.40712871
N	1.99379613	-4.02312828	-2.29465412
N	-1.51685377	-3.28856010	1.77561921
Al	3.52156519	-0.78342183	-1.77390471
N	0.93336195	-3.43007453	3.72527570
Al	1.96739668	-3.91163070	2.30601670
N	-1.05531539	-3.78795062	-1.33367138

N	3.25750955	-2.63414556	2.63477748
Al	2.48772705	-3.55775530	-0.65285729
N	3.43509882	-1.99450170	-0.40061357
Al	3.69379899	-1.45466843	1.33828791
N	1.77692001	-0.39238249	4.28261196
N	1.33438528	-4.11507897	0.65951228
Al	-0.47720074	-3.92866916	0.40706048
Al	-0.74785897	-2.89610099	3.41246577
Al	2.17909424	-2.11450642	4.03621045
Al	0.17853900	-4.09644114	-2.62107667
Al	2.08811288	-2.81059615	-3.64698737
Al	-0.76750576	-1.65414463	-4.30527414
N	0.33200377	-3.04726330	-4.12767458

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Al	4.63934243	1.18668895	-1.21089195
N	4.70375936	-0.18498609	-0.16698711
Al	4.21217841	-1.74651700	-0.87412396
N	3.13502747	-1.72869413	-2.30195711
Al	2.75411012	-0.18590239	-3.10992158
N	3.81792890	1.16654726	-2.81283590
Al	3.02875338	2.69154453	-2.26469297
N	3.93086886	2.76406700	-0.70140951
N	1.10836355	0.21184665	-3.65388277
Al	0.38287022	1.80818050	-3.31564813
N	-1.38158134	2.05891753	-3.32323068
Al	-2.30445293	0.79924752	-4.08717643
N	-1.60946869	-0.82942700	-4.40716045
Al	0.01282177	-1.15623165	-3.87879677
Al	1.93300466	-3.02388581	-2.47042770
N	2.13490887	-4.50199838	-1.56400665
Al	3.18983146	-4.48091702	-0.11592250
N	4.26799045	-3.14957404	0.23068547
Al	0.80294698	-4.90116834	-0.40647979
N	1.87711135	-5.03100846	1.01882671
N	0.27120383	-2.62433798	-2.93171086
Al	-2.97005697	-1.44565053	-3.39432787
N	-2.65773017	-2.40430973	-1.97206471
Al	-1.06710479	-3.17433802	-1.90148817
Al	4.32890307	-2.80786186	1.95448871
N	4.45533412	-1.14814595	2.63785250
Al	4.30426718	0.18597922	1.53609994
Al	1.53987569	-3.99448324	2.39920841
N	2.99703748	-3.30339473	3.09088592
Al	2.92333842	2.76750846	0.73138876
N	3.12611801	1.46853938	1.91920005
Al	2.99076075	-1.58443377	3.59444011
N	1.56431201	-0.60829620	3.56084900
Al	0.03488501	-1.44325746	3.22497938
N	-1.40586143	-0.44456765	3.22859135
Al	-1.27104727	1.32237529	3.39375503
N	0.30180592	2.06027628	3.00703803

Al	1.74208762	1.05264344	2.95735161
N	-2.75610005	2.31822754	3.29947553
Al	-4.23503846	1.50850139	2.82074094
N	-5.15058670	1.92299846	1.30432343
Al	-4.38050036	3.04240826	0.18460132
N	-3.49236792	4.31479738	0.99390242
Al	-2.62986097	3.89515758	2.54015754
N	-4.33743654	-0.26354374	2.55116071
N	-1.06500822	4.56785657	1.98949657
Al	-1.86700134	4.74276653	0.37552367
N	-3.76854568	2.41817433	-1.36593272
Al	-4.28185308	0.76522223	-1.80056111
N	-4.52017696	-0.47535305	-0.53540326
Al	-5.09082157	0.15953219	0.96791558
N	-3.81199958	0.14895939	-3.34819930
N	0.03222053	-3.04308514	2.43489939
Al	-2.84118326	-1.14484536	2.46003679
Al	-2.20557535	2.97934997	-2.03718385
Al	-1.16439874	-3.24762179	1.12833291
N	-2.60219639	-2.23866001	1.08322347
N	-0.68547482	-4.02214647	-0.39435240
Al	-3.40758132	-1.86814301	-0.45645898
Al	0.33468045	3.53962065	2.03178782
N	1.36302824	3.57688359	0.59479438
N	1.32663104	2.98424085	-2.39055408
Al	0.56674196	3.74130003	-0.98330603
N	-1.17825852	4.05119604	-1.06326160

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N	0.99551893	-3.93452110	0.00000000
Al	-5.56504512	-1.27588154	0.00000000
Al	5.59450705	2.88890386	0.00000000
N	1.85068321	2.11393607	-2.68245843
N	-1.75988666	-3.59323686	-1.56517765
Al	-0.85396826	-3.93650786	0.00000000
Al	-4.46838636	3.17029818	-1.26783936
Al	-0.82972476	-3.64452996	-3.09646809
N	0.99126468	-3.72229732	-3.12215100
Al	1.88513701	-3.58508460	-1.57705856
N	-0.90413662	-2.24188842	-4.29019617
Al	0.84962641	3.16078480	-1.57261504
N	-5.75822531	2.74892029	0.00000000
N	5.67130886	-1.20477192	0.00000000
Al	0.92327249	-2.22255370	-4.19257349
Al	-3.21607016	-2.49058915	-1.55615982
N	-4.14854319	-2.34547487	0.00000000
N	4.40205479	3.33839391	-1.34687028
N	3.30180196	-2.43566832	-1.55077013
Al	4.23841134	-2.25243243	0.00000000
N	-0.94003209	0.78151783	-3.54950216
N	1.85654731	-0.75629929	-3.76817382
Al	3.33499606	-1.01004407	-2.71439284

Al	-1.84146497	-0.80489198	-3.78907338
N	-3.31529202	-1.08473658	-2.74088609
Al	5.84501706	0.11093936	-1.26380360
Al	0.90365189	0.80013250	-3.53699028
N	-5.91277918	-0.06858257	-1.34320639
Al	-1.90616388	2.06756243	-2.66870360
N	4.46807652	0.39884698	-2.40581356
N	6.42395680	1.33620561	0.00000000
Al	3.67332616	2.07075271	-2.42611581
Al	-6.39098915	1.10719938	0.00000000
Al	-4.50122948	0.26603189	-2.42286558
N	-0.94259742	3.14734386	-1.57285051
N	-3.73668421	1.95555876	-2.41498741
N	-3.42452919	3.97976716	0.00000000
Al	3.32298834	3.96604961	0.00000000
Al	-1.67376384	3.72181502	0.00000000
N	1.56682985	3.76011049	0.00000000
N	1.85068321	2.11393607	2.68245843
N	-1.75988666	-3.59323686	1.56517765
Al	-4.46838636	3.17029818	1.26783936
Al	-0.82972476	-3.64452996	3.09646809
N	0.99126468	-3.72229732	3.12215100
Al	1.88513701	-3.58508460	1.57705856
N	-0.90413662	-2.24188842	4.29019617
Al	0.84962641	3.16078480	1.57261504
Al	0.92327249	-2.22255370	4.19257349
Al	-3.21607016	-2.49058915	1.55615982
N	4.40205479	3.33839391	1.34687028
N	3.30180196	-2.43566832	1.55077013
N	-0.94003209	0.78151783	3.54950216
N	1.85654731	-0.75629929	3.76817382
Al	3.33499606	-1.01004407	2.71439284
Al	-1.84146497	-0.80489198	3.78907338
N	-3.31529202	-1.08473658	2.74088609
Al	5.84501706	0.11093936	1.26380360
Al	0.90365189	0.80013250	3.53699028
N	-5.91277918	-0.06858257	1.34320639
Al	-1.90616388	2.06756243	2.66870360
N	4.46807652	0.39884698	2.40581356
Al	3.67332616	2.07075271	2.42611581
Al	-4.50122948	0.26603189	2.42286558
N	-0.94259742	3.14734386	1.57285051
N	-3.73668421	1.95555876	2.41498741

(AlN)₃₄/C₃

Al	-2.84824000	-0.73552000	4.41772000
N	-3.97160000	0.93034000	1.06185000
Al	-4.18664000	0.31731000	2.66717000
N	-3.31319000	0.97964000	4.08827000
Al	-2.94544000	2.36048000	0.83607000
N	-1.97859000	2.95543000	2.21239000
Al	-2.00748000	2.08325000	3.77105000

N	-3.90553000	0.26960000	-1.86638000
Al	-3.04162000	1.78066000	-2.20073000
N	-0.49622000	1.69433000	4.64842000
Al	0.00000000	0.00000000	4.87632000
N	-0.62204000	4.29436000	-2.66323000
Al	-3.86788000	-0.98462000	-3.07319000
Al	-1.17156000	3.90555000	-1.05929000
N	-2.54865000	2.81048000	-0.83177000
N	0.05315000	4.02772000	0.20492000
Al	-3.99343000	-0.30870000	-0.19965000
N	0.71512000	4.05799000	3.10060000
Al	-0.51100000	3.88539000	1.86699000
N	0.61198000	2.91985000	-4.54780000
N	-2.19596000	1.87987000	-3.77320000
Al	-1.08657000	3.18914000	-3.99559000
Al	-1.71499000	0.39684000	-4.65033000
N	0.00000000	0.00000000	-4.91242000
Al	0.78714000	2.83441000	4.41772000
Al	2.06110000	-2.09889000	4.41772000
N	2.79150000	2.97434000	1.06185000
N	1.18010000	-3.90468000	1.06185000
Al	2.36812000	3.46709000	2.66717000
Al	1.81853000	-3.78439000	2.66717000
N	2.50499000	2.37949000	4.08827000
N	0.80820000	-3.35913000	4.08827000
Al	3.51695000	1.37059000	0.83607000
Al	-0.57151000	-3.73107000	0.83607000
N	3.54877000	0.23579000	2.21239000
N	-1.57018000	-3.19122000	2.21239000
Al	2.80789000	0.69691000	3.77105000
Al	-0.80041000	-2.78016000	3.77105000
N	2.18624000	3.24749000	-1.86638000
N	1.71928000	-3.51709000	-1.86638000
Al	3.06290000	1.74380000	-2.20073000
Al	-0.02128000	-3.52445000	-2.20073000
N	1.71544000	-0.41743000	4.64842000
N	-1.21922000	-1.27690000	4.64842000
N	4.03004000	-1.60848000	-2.66323000
N	-3.40800000	-2.68588000	-2.66323000
Al	1.08123000	3.84199000	-3.07319000
Al	2.78665000	-2.85737000	-3.07319000
Al	3.96809000	-0.93817000	-1.05929000
Al	-2.79652000	-2.96738000	-1.05929000
N	3.70827000	0.80195000	-0.83177000
N	-1.15963000	-3.61243000	-0.83177000
N	3.46154000	-2.05989000	0.20492000
N	-3.51469000	-1.96783000	0.20492000
Al	1.72938000	3.61276000	-0.19965000
Al	2.26406000	-3.30407000	-0.19965000
N	3.15677000	-2.64831000	3.10060000
N	-3.87188000	-1.40969000	3.10060000
Al	3.62035000	-1.50016000	1.86699000

Al	-3.10935000	-2.38524000	1.86699000
N	2.22267000	-1.98991000	-4.54780000
N	-2.83465000	-0.92993000	-4.54780000
N	2.72599000	0.96182000	-3.77320000
N	-0.53004000	-2.84169000	-3.77320000
Al	3.30516000	-0.65357000	-3.99559000
Al	-2.21859000	-2.53557000	-3.99559000
Al	1.20117000	1.28680000	-4.65033000
Al	0.51382000	-1.68365000	-4.65033000

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Al	0.91841203	-4.35436299	1.60163617
Al	3.26124240	-2.47675845	2.64604438
N	-0.91642393	-4.37355143	1.59735485
Al	-1.82678262	-3.59050233	3.00268714
N	4.31528528	-3.03493052	1.32816045
Al	-4.24876562	-3.00751708	1.25148786
N	-3.25204429	-2.48969724	2.63003369
N	-3.63501164	0.46581148	1.58537263
al	3.62720240	0.47261664	1.59220425
N	1.82384651	-3.56951990	3.00353665
Al	1.81573832	-0.06934646	4.08594659
N	3.09717486	-0.66731649	2.91966317
N	-1.80235417	-0.08910242	4.05584251
Al	-3.08981380	-0.68120114	2.89484633
N	0.94584309	-1.32564005	5.03070541
Al	-0.89277793	-1.36098199	4.94215070
Al	0.88101851	-3.06580702	4.43341836
N	-0.93820294	-3.14457917	4.48428163
Al	-3.03630115	2.17454844	1.56977163
N	0.92322991	1.47943775	3.70386743
Al	-0.90572910	1.46436195	3.68458992
N	3.04663265	2.18655910	1.56823683
Al	1.72558301	2.76132145	2.69311512
N	-1.72759605	2.76047055	2.70800677
N	-1.80376496	5.55880520	1.34219620
Al	-0.94036886	4.38947789	2.42024246
N	0.90984310	4.38674461	2.40712381
Al	1.74621659	5.51722443	1.26263868
N	0.85978387	6.54558549	0.00000000
N	1.80969754	-4.52499180	0.00000000
Al	-1.80894629	-4.57011162	0.00000000
Al	3.56257905	-4.06648891	0.00000000
N	-3.57492700	-4.18123550	0.00000000
Al	4.82862300	-1.88723427	0.00000000
Al	-4.32183718	-0.17013293	0.00000000
N	4.30379327	-0.16836752	0.00000000
N	-4.93269979	-1.85901641	0.00000000
N	-3.28359997	3.07947806	0.00000000
Al	3.28536018	3.09416158	0.00000000
Al	-2.79686482	4.78815183	0.00000000
Al	0.91841203	-4.35436299	-1.60163617

Al	3.26124240	-2.47675845	-2.64604438
N	-0.91642393	-4.37355143	-1.59735485
Al	-1.82678262	-3.59050233	-3.00268714
N	4.31528528	-3.03493052	-1.32816045
Al	-4.24876562	-3.00751708	-1.25148786
N	-3.25204429	-2.48969724	-2.63003369
N	-3.63501164	0.46581148	-1.58537263
Al	3.62720240	0.47261664	-1.59220425
N	1.82384651	-3.56951990	-3.00353665
Al	1.81573832	-0.06934646	-4.08594659
N	3.09717486	-0.66731649	-2.91966317
N	-1.80235417	-0.08910242	-4.05584251
Al	-3.08981380	-0.68120114	-2.89484633
N	0.94584309	-1.32564005	-5.03070541
Al	-0.89277793	-1.36098199	-4.94215070
Al	0.88101851	-3.06580702	-4.43341836
N	-0.93820294	-3.14457917	-4.48428163
Al	-3.03630115	2.17454844	-1.56977163
N	0.92322991	1.47943775	-3.70386743
Al	-0.90572910	1.46436195	-3.68458992
N	3.04663265	2.18655910	-1.56823683
Al	1.72558301	2.76132145	-2.69311512
N	-1.72759605	2.76047055	-2.70800677
N	-1.80376496	5.55880520	-1.34219620
Al	-0.94036886	4.38947789	-2.42024246
N	0.90984310	4.38674461	-2.40712381
Al	1.74621659	5.51722443	-1.26263868
Al	-0.90088426	6.45753293	0.00000000
N	2.88027522	4.82498250	0.00000000

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Al	-3.14986949	0.90864858	-3.14986949
N	-4.01364972	1.80208431	-1.80208431
Al	-3.14986949	3.14986949	-0.90864858
N	-1.80208431	4.01364972	-1.80208431
Al	-0.90864858	3.14986949	-3.14986949
N	-1.80208431	1.80208431	-4.01364972
Al	-0.88630616	5.24993273	-0.88630616
Al	-0.88630616	0.88630616	-5.24993273
Al	-5.24993273	0.88630616	-0.88630616
Al	3.14986949	0.90864858	3.14986949
N	4.01364972	1.80208431	1.80208431
Al	3.14986949	3.14986949	0.90864858
N	1.80208431	4.01364972	1.80208431
Al	0.90864858	3.14986949	3.14986949
N	1.80208431	1.80208431	4.01364972
Al	0.88630616	5.24993273	0.88630616
Al	0.88630616	0.88630616	5.24993273
Al	5.24993273	0.88630616	0.88630616
N	-3.16532418	0.93822492	3.16532418
Al	-4.04596607	1.82322966	1.82322966
N	-3.16532418	3.16532418	0.93822492

Al	-1.82322966	4.04596607	1.82322966
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Al	-1.82322966	1.82322966	4.04596607
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N	-0.94472691	0.94472691	5.33141546
N	-5.33141546	0.94472691	0.94472691
N	3.16532418	0.93822492	-3.16532418
Al	4.04596607	1.82322966	-1.82322966
N	3.16532418	3.16532418	-0.93822492
Al	1.82322966	4.04596607	-1.82322966
N	0.93822492	3.16532418	-3.16532418
Al	1.82322966	1.82322966	-4.04596607
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N	-3.16532418	-0.93822492	-3.16532418
Al	-4.04596607	-1.82322966	-1.82322966
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Al	-1.82322966	-4.04596607	-1.82322966
N	-0.93822492	-3.16532418	-3.16532418
Al	-1.82322966	-1.82322966	-4.04596607
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Al	4.04596607	-1.82322966	1.82322966
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Al	1.82322966	-4.04596607	1.82322966
N	0.93822492	-3.16532418	3.16532418
Al	1.82322966	-1.82322966	4.04596607
N	0.94472691	-5.33141546	0.94472691
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Al	-3.14986949	-0.90864858	3.14986949
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N	-1.80208431	-1.80208431	4.01364972
Al	-0.88630616	-5.24993273	0.88630616
Al	-0.88630616	-0.88630616	5.24993273
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Al	3.14986949	-0.90864858	-3.14986949
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Al	-3.14778651	1.82908809	-2.83716085
N	-2.18993065	3.33290890	-2.41201435
Al	1.25000447	4.04077072	-1.59736852
N	-3.85074759	0.87353113	-1.44833424
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N	1.85667284	3.03061364	4.70083517
N	0.00000000	0.00000000	-5.59213120
N	0.01013363	4.05879222	-0.24974862
Al	0.60115320	3.89698803	1.45461345
Al	-1.71416321	3.62188274	-0.66718908
Al	-3.76206559	1.49336038	0.25492912
N	-2.73955255	2.95144916	0.66848700
Al	-4.22506922	1.00077471	3.25874812
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Al	-1.69712629	-3.64677897	2.41149058
Al	3.97489975	-1.05258860	-3.66922939
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Al	3.15793001	1.81151904	-2.83716085
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Al	2.87440786	-3.10292099	-1.59736852
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Al	3.07431403	-2.46910796	1.45461345
Al	-3.67546723	-1.42788007	1.45461345
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Al	3.17432082	2.51136418	0.25492912

Al	0.58774477	-4.00472456	0.25492912
N	3.92580623	0.89679753	0.66848700
N	-1.18625368	-3.84824669	0.66848700
Al	2.97923093	3.15862992	3.25874812
Al	1.24583829	-4.15940464	3.25874812
N	3.40937195	-1.32610902	2.84420821
N	-2.85313007	-2.28954821	2.84420821
Al	2.55259112	-1.57223347	4.45622540
Al	-2.63788969	-1.42449202	4.45622540
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Al	-3.43698920	-0.65865488	-4.63238704
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Al	-0.55941391	-1.73924617	-5.34698957
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Al	2.68845290	1.43340958	5.06466101
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Al	3.34653681	2.99943161	-2.37358055
N	2.80927682	3.77595175	-0.81593986
Al	3.45355450	3.15860922	0.78716609
N	2.62374742	3.59457288	2.35389336
Al	1.44439324	4.95747362	2.29264834
N	0.72476695	5.48301691	0.68284098
Al	1.18427405	4.60709203	-0.80111813
N	-0.20350958	4.89753916	3.11013317
Al	-0.91176721	5.17770897	1.44748743
Al	4.83561725	0.29521570	-3.01747002
N	2.06979602	2.57747530	-3.62244566
Al	0.30283688	3.03046704	-3.36776772
N	-0.15495985	3.91397920	-1.84098598
Al	3.89444584	0.21647046	1.82716462
N	2.99254333	0.58540490	3.36942951
Al	2.34557109	2.29058035	3.61357588
Al	2.42626306	1.11918787	-4.68891962
N	-2.06091204	4.00977534	0.71154162
Al	-1.79033556	3.61435047	-1.06616800
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Al	-0.58609265	3.41827316	4.02014250
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Al	-2.74944789	2.72719473	1.84162487
N	-5.31829307	0.47457835	-1.43009305

Al	-0.55328755	1.12890239	-5.68076949
Al	-2.32641102	0.82857778	4.33780957
Al	-4.19896238	1.67679388	-0.70691141
N	1.18751121	0.59217687	-5.84452503
Al	0.44720380	1.17018168	5.76609926
N	-1.26014610	0.46960714	5.74892319
Al	-2.62191845	1.79373496	-3.48550282
N	-3.45869611	0.24342506	-4.00600995
N	-3.77025714	1.44549659	1.06396604
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Al	-5.28631022	-1.22284930	-0.73082230
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Al	-3.34653681	-2.99943161	-2.37358055
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N	-2.62374742	-3.59457288	2.35389336
Al	-1.44439324	-4.95747362	2.29264834
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Al	-1.18427405	-4.60709203	-0.80111813
N	0.20350958	-4.89753916	3.11013317
Al	0.91176721	-5.17770897	1.44748743
Al	-4.83561725	-0.29521570	-3.01747002
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Al	-0.30283688	-3.03046704	-3.36776772
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Al	-2.42626306	-1.11918787	-4.68891962
N	2.06091204	-4.00977534	0.71154162
Al	1.79033556	-3.61435047	-1.06616800
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Al	0.58609265	-3.41827316	4.02014250
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Al	2.74944789	-2.72719473	1.84162487
N	5.31829307	-0.47457835	-1.43009305
Al	0.55328755	-1.12890239	-5.68076949
Al	2.32641102	-0.82857778	4.33780957
Al	4.19896238	-1.67679388	-0.70691141
N	-1.18751121	-0.59217687	-5.84452503
Al	-0.44720380	-1.17018168	5.76609926
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Al	2.62191845	-1.79373496	-3.48550282
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Al	0.32061487	-5.06789027	1.22758409
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N	1.00247858	5.87507074	0.64822655
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Al	-4.49091990	0.15944182	1.45786244
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Al	-0.74430017	-1.52428509	4.57441648
Al	2.38976351	-1.28658542	4.01800561
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Al	0.95158958	-4.04590062	4.14101683
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N	3.07113809	-2.90590630	-2.02482862
Al	3.82488199	4.21642294	-1.66731645
Al	2.71373251	1.70205222	-3.02584592
Al	0.89548321	4.21326958	-2.66036706
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N	-1.43665963	-2.71516600	-4.53612278
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Al	0.01221845	-4.77766522	-1.87321461
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Al	1.62857912	-0.76970365	-4.59111364
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Al	3.44165433	-1.10972604	-1.97290734
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Al	-2.46139370	-4.17278079	-0.02983888
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Al	2.62676675	-3.76206080	-0.47817251
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Al	0.01032483	1.82557875	-5.85371974
N	0.65288392	3.93011921	-2.91767792
N	-1.38361533	2.64332135	-4.95769351
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Al	1.20462780	3.82142024	-1.17080972
Al	-1.72949950	3.51401570	-0.20226819
Al	0.57065564	3.86985831	1.93382278
N	-2.77654362	2.93351181	1.17671341
Al	0.06294445	2.99891887	4.95888301
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Al	3.18461439	2.57916412	0.85174979
N	2.35163795	3.50907679	2.17278346
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Al	-4.10628341	-0.17437939	-4.18469965
Al	2.20415869	-3.46895605	-4.18469965
N	-3.06599667	0.08119803	-5.68219268
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Al	-2.46939462	-2.66465617	-3.33433637
Al	3.54235724	-0.80623039	-3.33433637
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N	3.07714111	-2.53047366	-2.91767792
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Al	-2.17847712	-3.25479836	-0.20226819
Al	3.90797662	-0.25921735	-0.20226819
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