

Supporting Information

Anchoring of palladium nanoparticles on N-doped mesoporous carbon

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Experimental

Table S1. Physicochemical properties of the carbon materials and supported catalysts.

Sample	Pd ^a [wt%]	S_{BET}^b [m ² g ⁻¹]	V_{pore} [cm ³ g ⁻¹]	D_{pore}^c [nm]	D_{particle}^d [nm]
NMC	–	657	0.7	4.9	–
CMC	–	997	1.2	5.0	–
Pd/NMC	0.95	625	0.7	4.7	3.4
Pd/CMC	0.98	971	1.2	4.9	4.2

[a] Pd loading determined by AAS;

[b] Specific surface area (BET method);

[c] Average pore diameter (BJH method);

[d] Mean particle size from TEM.

Table S2. Chemical compositions of NMC, CMC, Pd/NMC, and Pd/CMC.

Sample	N (wt/at %)		O (at %)
	bulk ^a	surf. ^b	surf. ^b
NMC	13.4	10.6	6.3
CMC	–	–	11.0
Pd/NMC	13.3	10.1	8.1
Pd/CMC	–	–	11.5

[a] Bulk composition determined by elemental analysis;

[b] Surface composition determined by XPS.

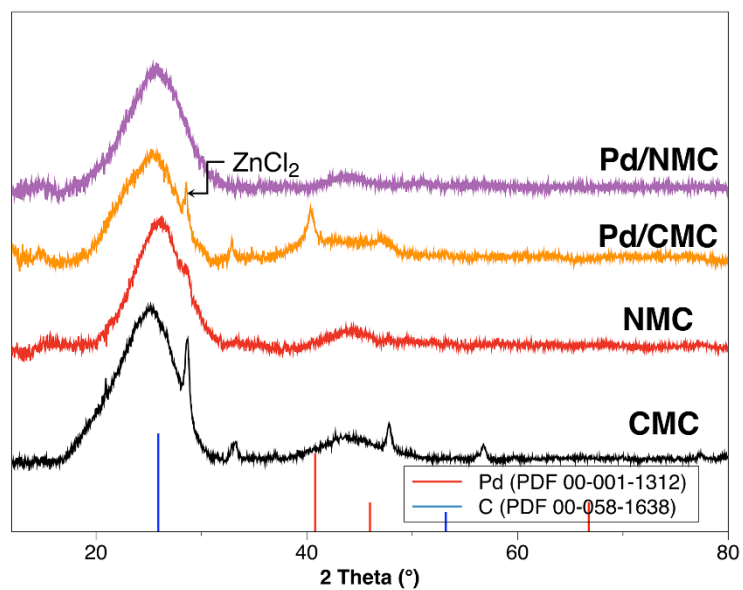


Figure S1. XRD patterns of Pd/NMC, Pd/CMC and the mesoporous carbon supports.

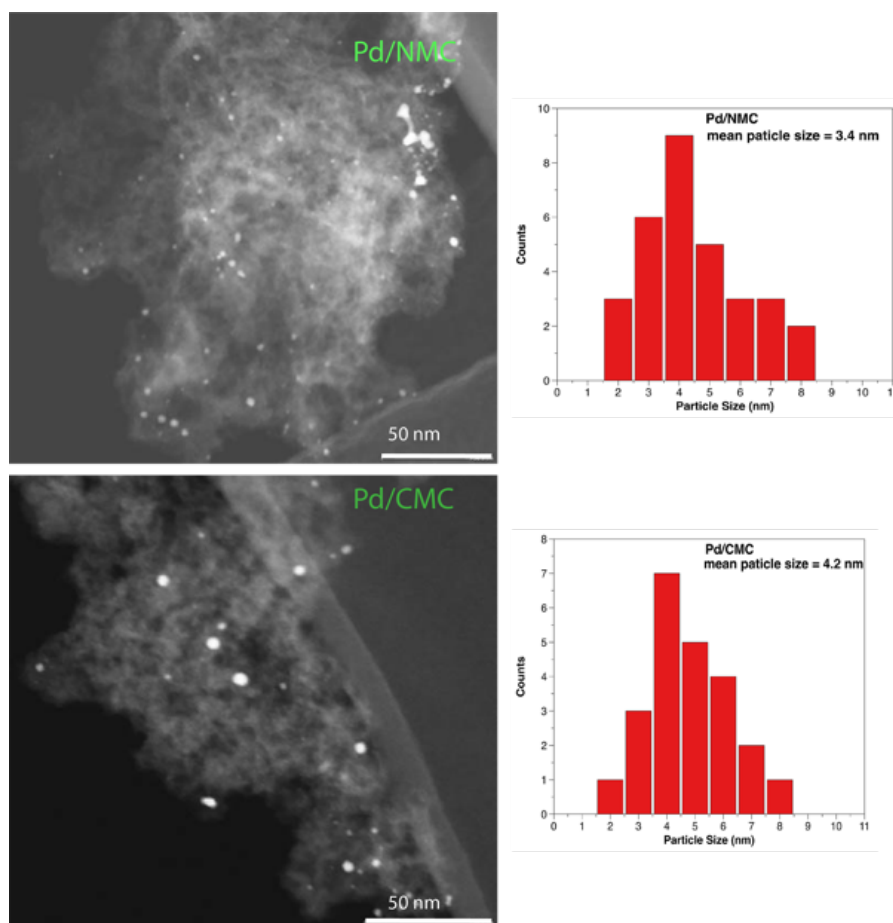


Figure S2. HAADF-STEM images and Pd particle size distributions for Pd/NMC and Pd/CMC.

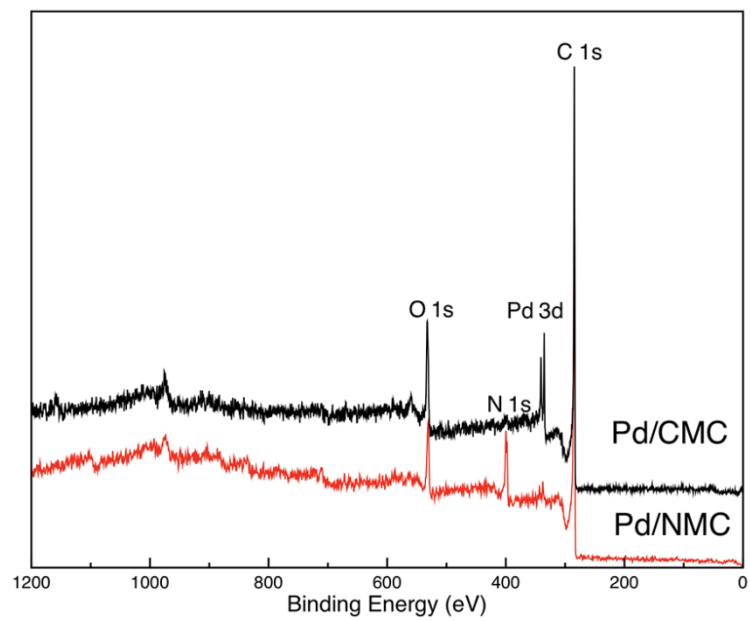


Figure S3. XP survey spectra of Pd/NMC and Pd/CMC.

Computational

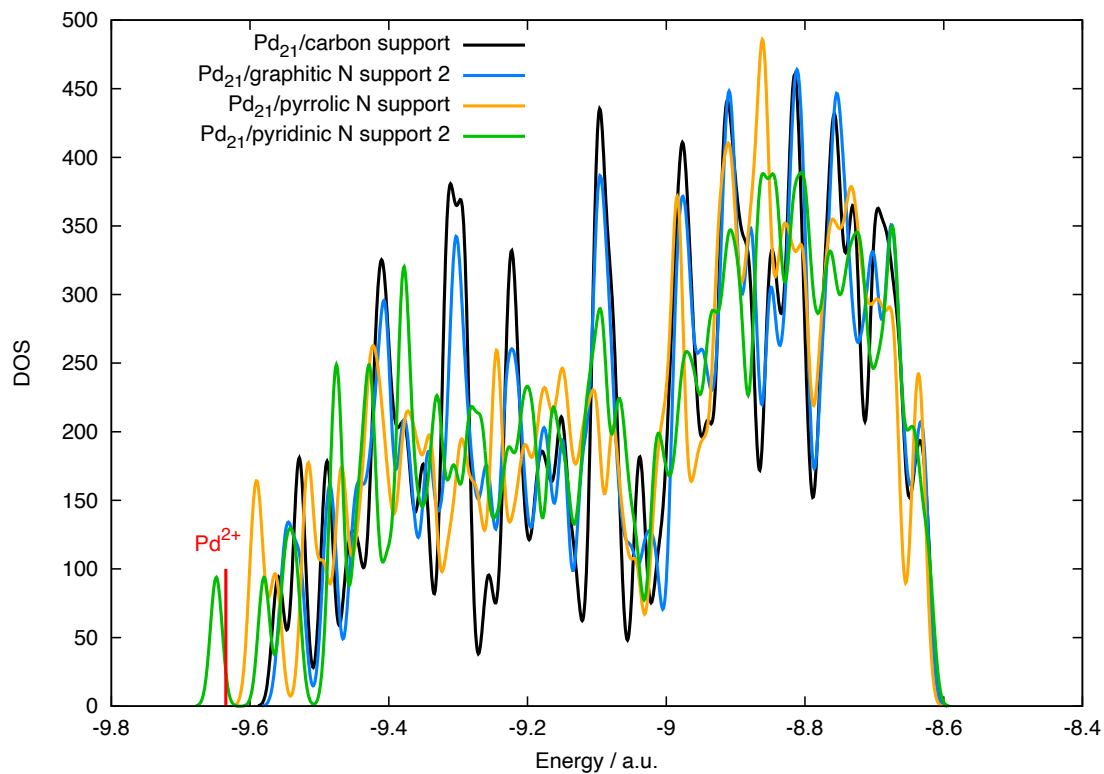


Figure S4. Pd 3d density of states plot for the different Pd₂₁ systems.

Coordinates of the studied structures

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Graphitic N support material

C	11.1286669	0.6897803	0.0769510
C	11.1310353	-0.6788594	0.0747329
C	9.9012069	-1.4390640	0.0727021
C	9.8849673	-2.8352104	0.0704892
C	8.6690148	-3.5796552	0.0684565
C	8.6455055	-4.9925504	0.0662302
C	7.4373606	-5.7216759	0.0642087
C	7.4035693	-7.1482871	0.0620368
C	6.2050660	-7.8627055	0.0600422

C	6.1643253	-9.3080801	0.0578234
C	4.9797686	-9.9930362	0.0559343
C	3.7078441	-9.3056469	0.0559964
C	2.4896215	-9.9857925	0.0540851
C	1.2392073	-9.3014376	0.0541562
C	0.0037781	-9.9866408	0.0522224
C	-1.2285859	-9.3043134	0.0523428
C	-2.4824760	-9.9903636	0.0503888
C	-3.6990802	-9.3132479	0.0505853
C	-4.9695746	-10.0037452	0.0485697
C	-6.1534577	-9.3201533	0.0488651
C	-6.1943737	-7.8746826	0.0510879
C	-7.3923292	-7.1668439	0.0514023
C	-7.4303984	-5.7404130	0.0536230
C	-8.6364548	-5.0195416	0.0539315
C	-8.6639583	-3.6050501	0.0561616
C	-9.8811937	-2.8707714	0.0565210
C	-9.9056171	-1.4731789	0.0587362
C	-11.1375156	-0.7198628	0.0590165
C	-11.1391337	0.6495800	0.0612729
C	-9.9107337	1.4098469	0.0632473
C	-9.8969611	2.8096458	0.0654343
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C	-8.6598919	4.9682951	0.0696575
C	-7.4504424	5.6986467	0.0716441
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C	-4.9975222	9.9736171	0.0801481
C	-6.2192771	7.8413614	0.0758978
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C	-2.5067571	9.9729765	0.0819343
C	-3.7247527	9.2889874	0.0799526
C	-0.0187869	9.9772460	0.0837157
C	-1.2555188	9.2920152	0.0817172
C	2.4683117	9.9811547	0.0855514
C	1.2155383	9.2961727	0.0835426
C	4.9574519	9.9910117	0.0873478
C	6.1429969	9.3084263	0.0871548
C	3.6857364	9.3019388	0.0853616
C	6.1858309	7.8624899	0.0848636
C	7.3845870	7.1506638	0.0845788
C	7.4216157	5.7226869	0.0823030
C	8.6301943	4.9970771	0.0819887

C	8.6576202	3.5825403	0.0797437
C	9.8753132	2.8421452	0.0794421
C	9.8963626	1.4456818	0.0772423
C	8.6497597	0.7128868	0.0751960
C	8.6522033	-0.7099274	0.0729670
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C	6.1838126	-3.5755026	0.0665848
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C	4.9500335	-5.7186887	0.0622934
C	4.9470444	-7.1483905	0.0601413
C	3.7166519	-7.8591470	0.0581245
C	2.4759269	-7.1479937	0.0582257
C	1.2385754	-7.8582410	0.0562814
C	0.0000002	-7.1461182	0.0564751
C	-1.2319724	-7.8614928	0.0545200
C	-2.4702130	-7.1508741	0.0547709
C	-3.7122282	-7.8652197	0.0528147
C	-4.9353549	-7.1559606	0.0530801
C	-4.9432387	-5.7222146	0.0553399
C	-6.1767163	-5.0174705	0.0556057
C	-6.1753112	-3.5943723	0.0578719
C	-7.4135583	-2.8797964	0.0581572
C	-7.4240082	-1.4548595	0.0604314
C	-8.6600910	-0.7402656	0.0607631
C	-8.6647419	0.6842768	0.0629582
C	-7.4287426	1.4068355	0.0648787
C	-7.4310412	2.8335021	0.0671046
C	-6.1968073	3.5509203	0.0690518
C	-6.1973327	4.9806448	0.0713155
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C	-4.9650443	5.6981761	0.0732587
C	-4.9620015	7.1292704	0.0755778
C	-1.2550543	7.8475028	0.0793815
C	-2.4902715	7.1339768	0.0773222
C	1.2198299	7.8508340	0.0812532
C	-0.0164181	7.1381651	0.0791842
C	3.6978665	7.8535896	0.0830849
C	4.9275502	7.1459383	0.0828241
C	2.4564663	7.1409601	0.0810750
C	4.9346898	5.7141188	0.0805296
C	6.1696431	5.0005542	0.0802467

C	6.1737428	3.5730094	0.0779567
C	7.4096865	2.8579248	0.0776837
C	7.4131443	1.4299712	0.0754361
C	6.1740959	0.7108180	0.0734492
C	6.1765167	-0.7148989	0.0711816
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C	3.7049337	-3.5745593	0.0646845
C	3.7079064	-5.0045643	0.0624224
C	2.4748148	-5.7174382	0.0603838
C	1.2336599	-5.0039782	0.0606136
C	-0.0020763	-5.7098508	0.0586639
C	-1.2430890	-4.9978382	0.0589291
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C	-4.9516275	1.4065262	0.0664846
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C	-0.0145570	5.7039363	0.0768907
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C	1.2208828	4.9927595	0.0767060
C	3.6981822	3.5667401	0.0762296
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C	3.7013026	-0.7205808	0.0693363
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C	2.4610786	1.4225647	0.0719095
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C	-0.0117519	1.4139923	0.0701209
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H	-0.0204991	11.0732724	0.0854282
H	12.0788459	-1.2287745	0.0744121
H	2.4667260	11.0772964	0.0873099
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H	2.4877456	-11.0818023	0.0524857
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H	-9.5851364	-5.5679474	0.0523758
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H	-7.1336322	9.8282739	0.0784472
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H	-9.6101189	5.5141450	0.0698133
H	-7.1052532	-9.8625502	0.0474847
H	4.9754734	-11.0886348	0.0543040
H	9.5794025	5.5449380	0.0835264
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H	7.0935178	9.8533298	0.0888317
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H	-8.3407288	-7.7160998	0.0499487
H	0.0045150	-11.0824921	0.0505784
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Pyridinic N b support material

C	11.2389295	0.7339786	-0.0186717
C	11.2541223	-0.6333272	-0.0387681
C	10.0289831	-1.4010085	-0.0379923
C	10.0226273	-2.7958189	-0.0638953
C	8.8095079	-3.5475354	-0.0657203
C	8.7867812	-4.9598727	-0.0933919
C	7.5789981	-5.6929892	-0.0950930
C	7.5424712	-7.1195369	-0.1182246
C	6.3415409	-7.8297899	-0.1127000
C	6.2967630	-9.2747606	-0.1289505
C	5.1084982	-9.9516739	-0.1154205
C	3.8386811	-9.2590678	-0.0851505
C	2.6233919	-9.9408978	-0.0625528
C	1.3742637	-9.2547051	-0.0297182
C	0.1423590	-9.9457206	0.0030828
C	-1.0917495	-9.2668215	0.0404401
C	-2.3393262	-9.9606988	0.0793742
C	-3.5615493	-9.2906858	0.1161616
C	-4.8292266	-9.9864481	0.1562746
C	-6.0184681	-9.3103302	0.1892446
C	-6.0683681	-7.8648099	0.1855578
C	-7.2698943	-7.1559493	0.2138590
C	-7.3112578	-5.7285817	0.2063341
C	-8.5216009	-5.0028011	0.2286139
C	-8.5512634	-3.5894476	0.2161788
C	-9.7692207	-2.8480206	0.2314173
C	-9.7883861	-1.4520387	0.2141775
C	-11.0201058	-0.6951105	0.2259223
C	-11.0198417	0.6730700	0.2060565
C	-9.7885237	1.4307256	0.1736793
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C	-8.5552891	3.5683800	0.1223187
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C	-7.3265329	5.7112657	0.0756919
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C	-3.6160907	9.3113574	0.0005088
C	0.0890969	10.0102022	-0.0166399
C	-1.1463331	9.3224752	-0.0095694
C	2.5800058	10.0155746	-0.0130437
C	1.3264825	9.3312693	-0.0092926
C	5.0717039	10.0211911	-0.0063342
C	6.2555741	9.3349033	0.0026977
C	3.7982182	9.3352399	-0.0035251
C	6.2944496	7.8888990	0.0157325
C	7.4894080	7.1703892	0.0218848
C	7.5194141	5.7426230	0.0314875
C	8.7281767	5.0188018	0.0296861
C	8.7527612	3.6062591	0.0304553
C	9.9755854	2.8738371	0.0158187
C	9.9999718	1.4806080	0.0036714
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C	5.0833325	-7.1117667	-0.0876650
C	3.8468870	-7.8120101	-0.0749660
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C	-4.8254401	-5.7141676	0.1445659
C	-6.0615260	-5.0032594	0.1722962
C	-6.0694810	-3.5766999	0.1641554
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C	-7.3053481	-1.4361018	0.1684058
C	-8.5406483	-0.7192134	0.1821035
C	-8.5390500	0.7022641	0.1630481
C	-7.3020047	1.4228807	0.1325784

C	-7.3039000	2.8482653	0.1131170
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C	-6.0733508	4.9943672	0.0690406
C	-3.6187573	7.8642884	0.0145912
C	-4.8422219	5.7128347	0.0466886
C	-4.8449064	7.1446537	0.0313148
C	-1.1440133	7.8785444	0.0027394
C	-2.3764913	7.1597776	0.0139315
C	1.3310778	7.8861619	0.0036814
C	0.0953227	7.1732345	0.0078143
C	3.8090531	7.8873685	0.0102845
C	5.0365939	7.1744854	0.0207351
C	2.5685275	7.1770728	0.0134710
C	5.0404233	5.7417877	0.0345368
C	6.2688611	5.0190453	0.0400377
C	6.2676360	3.5884673	0.0507248
C	7.5069321	2.8801195	0.0413087
C	7.5086123	1.4523476	0.0337944
C	6.2705113	0.7302882	0.0464114
C	6.3012801	-0.6913468	0.0232745
C	5.0767867	-1.4181755	0.0244483
C	5.0878831	-2.8382958	-0.0128014
C	3.8571775	-3.5471866	-0.0250761
C	3.8476395	-4.9704908	-0.0507613
C	2.6046783	-5.6614129	-0.0425945
C	1.3653336	-4.9200609	-0.0305511
C	0.1324547	-5.6647756	-0.0012343
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C	-2.3479245	-5.6966280	0.0765901
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C	-4.8305475	-2.8564766	0.1309823
C	-4.8298654	-1.4287279	0.1234370
C	-6.0655421	-0.7161481	0.1379726
C	-6.0596259	0.7089625	0.1206816
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C	-4.8270195	2.8532455	0.0774367
C	-2.3721862	5.7260432	0.0262141
C	-3.5896050	3.5669506	0.0577063
C	-3.5989486	5.0005380	0.0425885
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C	-1.1336384	5.0190793	0.0252237

C	2.5714985	5.7456814	0.0288802
C	3.8034662	5.0278368	0.0391811
C	1.3348692	5.0360704	0.0352033
C	3.8042192	3.5957106	0.0580727
C	5.0265593	2.8672606	0.0663977
C	5.0049121	1.4260164	0.0778652
C	3.7674649	0.7058469	0.1119990
C	3.8036136	-0.7532612	0.0711277
N	2.6608352	-1.4496751	0.0646196
C	2.6401123	-2.7848898	-0.0029301
C	1.3625840	-3.4888413	-0.0422587
C	0.0877040	-2.7826499	-0.0535915
C	-1.1258708	-3.5499720	0.0257145
C	-2.3638435	-2.8501033	0.0565350
C	-2.3639703	-1.4288701	0.0573256
C	-3.5927700	-0.7120572	0.0919143
C	-3.5777155	0.7128667	0.0750812
C	-1.1278354	3.5896747	0.0374431
C	-2.3201911	1.4149885	0.0564682
C	-2.3493046	2.8554475	0.0538496
C	1.3383467	3.6066569	0.0572635
C	2.5668534	2.8897917	0.0719744
C	2.5156805	1.4542027	0.1309685
C	0.1107994	2.8909586	0.0538487
C	0.1672950	1.4560647	0.0987222
N	1.3363849	0.8128421	0.2002439
N	0.0456036	-1.4411778	-0.1428852
C	-1.0972123	-0.7525635	-0.0154498
C	-1.0789251	0.7029954	0.0432364
H	-4.8932365	11.0879962	-0.0103398
H	0.0849856	11.1061536	-0.0263014
H	12.2060030	-1.1757372	-0.0572762
H	2.5794136	11.1116268	-0.0230893
H	-10.7185660	-3.3953912	0.2556682
H	2.6216473	-11.0369027	-0.0674838
H	-10.7219363	3.3732880	0.1602857
H	-9.4698264	-5.5518614	0.2539705
H	-8.2527439	7.6793363	0.0607755
H	-7.0265800	9.8390888	0.0200147
H	5.0693699	11.1167710	-0.0163373
H	-11.9665950	-1.2466207	0.2507133
H	-11.9662044	1.2252966	0.2147373

H	8.4901352	-7.6699835	-0.1378380
H	7.2452451	-9.8226279	-0.1505619
H	10.9212421	3.4278888	0.0093894
H	12.1792416	1.2965393	-0.0210774
H	-4.8174115	-11.0820117	0.1592654
H	8.4417674	7.7130185	0.0171301
H	9.7377840	-5.5045176	-0.1131848
H	-9.4856429	5.5251549	0.1079511
H	-6.9653742	-9.8606029	0.2185953
H	5.0972242	-11.0471929	-0.1259312
H	9.6778144	5.5658236	0.0224701
H	10.9767838	-3.3349355	-0.0847956
H	7.2075129	9.8772694	-0.0003597
H	-2.3283720	-11.0567461	0.0802634
H	-8.2165613	-7.7077812	0.2408208
H	0.1482434	-11.0416408	0.0020444
H	-2.4077033	11.0957102	-0.0215277

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Pyridinic N c support material

C	11.1433939	0.6981583	0.0599017
C	11.1449063	-0.6703094	0.0587926
C	9.9144011	-1.4311059	0.0576931
C	9.8969914	-2.8266987	0.0567240
C	8.6794718	-3.5724462	0.0555342
C	8.6536220	-4.9850925	0.0545687
C	7.4440017	-5.7153482	0.0533388
C	7.4080564	-7.1427944	0.0523570
C	6.2088227	-7.8573036	0.0512089
C	6.1658786	-9.3034612	0.0501370
C	4.9805592	-9.9876437	0.0490640
C	3.7069553	-9.3011830	0.0489040
C	2.4883424	-9.9825635	0.0478239
C	1.2338697	-9.2998869	0.0475955
C	-0.0046876	-9.9819208	0.0465688
C	-1.2422267	-9.2980060	0.0463471
C	-2.5007877	-9.9762663	0.0452546
C	-3.7185192	-9.2906210	0.0450475
C	-5.0017318	-9.9620295	0.0439021
C	-6.1840859	-9.2688437	0.0437849
C	-6.2220769	-7.8210043	0.0448755

C	-7.4192925	-7.0935076	0.0448370
C	-7.4407282	-5.6612973	0.0458630
N	-8.6241354	-4.9958284	0.0458437
C	-8.6129050	-3.6383088	0.0469900
C	-9.8446861	-2.9071147	0.0471825
C	-9.8798562	-1.5067064	0.0483967
C	-11.1169204	-0.7532597	0.0485381
C	-11.1300536	0.6172808	0.0497577
C	-9.9092765	1.3964768	0.0509494
C	-9.8982525	2.7939207	0.0522687
C	-8.6837756	3.5483774	0.0533768
C	-8.6613835	4.9621124	0.0547013
C	-7.4535744	5.6973667	0.0557308
C	-7.4216473	7.1251622	0.0570518
C	-5.0027263	9.9773077	0.0604282
C	-6.2243092	7.8434091	0.0581191
C	-6.1860371	9.2896525	0.0593685
C	-2.5105415	9.9798661	0.0614898
C	-3.7268551	9.2949685	0.0603770
C	-0.0192301	9.9869569	0.0625840
C	-1.2543546	9.3008651	0.0613729
C	2.4716070	9.9918228	0.0636296
C	1.2191011	9.3065916	0.0624525
C	4.9629595	10.0017763	0.0645956
C	6.1493373	9.3197739	0.0646212
C	3.6909465	9.3126785	0.0635092
C	6.1938428	7.8738648	0.0633714
C	7.3941174	7.1615815	0.0633396
C	7.4318390	5.7345122	0.0621030
C	8.6428311	5.0068872	0.0621406
C	8.6714137	3.5945132	0.0609259
C	9.8906302	2.8516889	0.0609689
C	9.9112066	1.4562129	0.0598611
C	8.6636072	0.7220866	0.0586772
C	8.6653072	-0.6994899	0.0576262
C	7.4303680	-1.4212286	0.0565036
C	7.4294331	-2.8490168	0.0554351
C	6.1957896	-3.5672400	0.0542296
C	6.1922811	-4.9950329	0.0532145
C	4.9573246	-5.7116903	0.0521046
C	4.9503059	-7.1423603	0.0510974
C	3.7188143	-7.8535438	0.0499535

C	2.4776175	-7.1433683	0.0497861
C	1.2391962	-7.8555405	0.0485988
C	0.0021050	-7.1446757	0.0484399
C	-1.2381438	-7.8540987	0.0473610
C	-2.4737544	-7.1402809	0.0472479
C	-3.7202271	-7.8448162	0.0460845
C	-4.9491748	-7.1289456	0.0459971
C	-4.9394768	-5.7039349	0.0470416
C	-6.1664259	-4.9822108	0.0469458
C	-6.1542367	-3.5650071	0.0480464
C	-7.3898544	-2.8705648	0.0481178
C	-7.4053023	-1.4472620	0.0494093
C	-8.6463269	-0.7466264	0.0495453
C	-8.6558372	0.6755175	0.0508068
C	-7.4246563	1.4065032	0.0519711
C	-7.4290759	2.8333791	0.0532299
C	-6.1967564	3.5565254	0.0542982
C	-6.1978720	4.9832114	0.0555883
C	-3.7329582	7.8477883	0.0591477
C	-4.9640657	5.7033708	0.0567593
C	-4.9625214	7.1332581	0.0580338
C	-1.2523758	7.8569155	0.0601131
C	-2.4883532	7.1419972	0.0590193
C	1.2246465	7.8625507	0.0611975
C	-0.0120193	7.1495323	0.0599984
C	3.7040829	7.8653566	0.0622610
C	4.9364585	7.1565919	0.0621737
C	2.4637257	7.1529555	0.0611294
C	4.9450000	5.7261836	0.0609610
C	6.1812895	5.0120785	0.0608790
C	6.1874189	3.5845552	0.0596651
C	7.4227125	2.8688890	0.0597073
C	7.4269912	1.4412732	0.0586304
C	6.1887131	0.7221955	0.0575235
C	6.1906253	-0.7043013	0.0563986
C	4.9539052	-1.4225881	0.0551626
C	4.9542208	-2.8503246	0.0540924
C	3.7195098	-3.5660976	0.0529774
C	3.7169380	-4.9969158	0.0519536
C	2.4820433	-5.7110937	0.0507948
C	1.2439277	-4.9969567	0.0506504
C	0.0075137	-5.7106060	0.0494431

C	-1.2260823	-4.9963067	0.0493450
C	-2.4661028	-5.7090663	0.0482592
C	-3.6968515	-4.9942251	0.0482271
C	-3.6905014	-3.5658805	0.0493117
C	-4.9192146	-2.8494543	0.0492695
C	-4.9292728	-1.4273225	0.0505023
C	-6.1715512	-0.7221576	0.0505986
C	-6.1792542	0.7009804	0.0518074
C	-4.9441592	1.4222876	0.0528888
C	-4.9499792	2.8476225	0.0541348
C	-2.4855202	5.7105758	0.0577521
C	-3.7158999	3.5653284	0.0553238
C	-3.7193268	4.9944946	0.0566138
C	-0.0079113	5.7160090	0.0587276
C	-1.2429866	5.0008439	0.0576308
C	2.4687501	5.7209960	0.0598733
C	3.7052892	5.0095360	0.0598486
C	1.2305054	5.0053118	0.0586390
C	3.7101405	3.5791030	0.0586140
C	4.9468147	2.8657628	0.0585598
C	4.9502431	1.4382176	0.0574555
C	3.7144155	0.7216060	0.0562632
C	3.7167064	-0.7076864	0.0550980
C	2.4819338	-1.4234808	0.0539714
C	2.4827086	-2.8517059	0.0528859
C	1.2466607	-3.5676420	0.0517184
C	0.0119652	-2.8531494	0.0516366
C	-1.2223700	-3.5677398	0.0504399
C	-2.4562428	-2.8521636	0.0504544
C	-2.4604176	-1.4252238	0.0516094
C	-3.6962121	-0.7115298	0.0516475
C	-3.7030022	0.7146704	0.0528149
C	-1.2386983	3.5727047	0.0563866
C	-2.4691456	1.4300977	0.0540001
C	-2.4745821	2.8564713	0.0552335
C	1.2350278	3.5765619	0.0574127
C	2.4738021	2.8633580	0.0574192
C	2.4775411	1.4354170	0.0562372
C	-0.0000873	2.8613444	0.0562962
C	0.0043220	1.4323996	0.0551122
C	1.2413523	0.7191840	0.0551060
C	1.2445091	-0.7085927	0.0539442

C	0.0102657	-1.4237402	0.0527784
C	-1.2253082	-0.7096248	0.0527914
C	-1.2299707	0.7173330	0.0539551
H	-5.0027127	11.0729491	0.0613678
H	-0.0216587	11.0829562	0.0638636
H	12.0927122	-1.2201854	0.0585781
H	2.4701638	11.0879276	0.0647772
H	-10.7749046	-3.4840690	0.0463905
H	2.4894676	-11.0786856	0.0472298
H	-10.8512800	3.3356685	0.0525668
H	-8.3721529	7.6711231	0.0573204
H	-7.1380703	9.8318640	0.0594717
H	4.9572514	11.0973931	0.0652440
H	-12.0605638	-1.3099510	0.0475809
H	-12.0848584	1.1550984	0.0498017
H	8.3572446	-7.6910031	0.0526203
H	7.1163046	-9.8484800	0.0502040
H	10.8396740	3.4001679	0.0619668
H	12.0899556	1.2501677	0.0609323
H	-5.0102058	-11.0577314	0.0430920
H	8.3424708	7.7112132	0.0643480
H	9.6034126	-5.5320639	0.0549712
H	-9.6124334	5.5070326	0.0551021
H	-7.1364656	-9.8102337	0.0427707
H	4.9772555	-11.0832736	0.0483282
H	9.5914599	5.5558701	0.0632989
H	10.8473563	-3.3728964	0.0569972
H	7.0990724	9.8659736	0.0656655
H	-2.5046743	-11.0724491	0.0446726
H	-8.3829429	-7.6128770	0.0440604
H	-0.0047299	-11.0779832	0.0461123
H	-2.5143299	11.0759698	0.0625948

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Pyrrolic N d support material

C	11.1506130	0.7125900	-0.0194519
C	11.1746853	-0.6514082	-0.0176423
C	9.9545023	-1.4233761	-0.0213964
C	9.9924220	-2.8153726	-0.0222664
C	8.8030558	-3.5930105	-0.0321496
C	8.8254233	-5.0091871	-0.0324998

C 7.6410162 -5.7810781 -0.0451164
C 7.6272144 -7.2181129 -0.0337680
C 6.4428557 -7.9694585 -0.0345567
C 6.3921260 -9.4190158 -0.0100514
C 5.2039093 -10.1092802 0.0027305
C 3.9191666 -9.4355006 -0.0072353
C 2.6802378 -10.0922000 0.0198114
C 1.4249562 -9.3923768 0.0226630
C 0.1682756 -10.0387290 0.0616532
C -1.0507369 -9.3177324 0.0754442
C -2.3149077 -9.9655723 0.1115114
C -3.5052574 -9.2431897 0.1253577
C -4.7798404 -9.9208527 0.1556693
C -5.9528391 -9.2245062 0.1671231
C -5.9663434 -7.7809809 0.1523785
C -7.1625107 -7.0734739 0.1627514
C -7.1881686 -5.6536813 0.1517664
C -8.4075197 -4.9475258 0.1606830
C -8.4504703 -3.5422911 0.1536187
C -9.6861462 -2.8273889 0.1615551
C -9.7400783 -1.4351724 0.1575293
C -10.9869003 -0.7009642 0.1648651
C -11.0165454 0.6673320 0.1616013
C -9.8007073 1.4511255 0.1515234
C -9.8068040 2.8477909 0.1483082
C -8.6018600 3.6165988 0.1391949
C -8.5904511 5.0308964 0.1342127
C -7.3882014 5.7809131 0.1243011
C -7.3582136 7.2105078 0.1164918
C -4.9326649 10.0717753 0.0807085
C -6.1614743 7.9362020 0.1044585
C -6.1177494 9.3833290 0.0944514
C -2.4307272 10.0733281 0.0588162
C -3.6537415 9.3929887 0.0751137
C 0.0730458 10.0643356 0.0329263
C -1.1738298 9.3913292 0.0516581
C 2.5719607 10.0396445 0.0041674
C 1.3073813 9.3736974 0.0237235
C 5.0652578 10.0105419 -0.0245297
C 6.2391748 9.3070453 -0.0335312
C 3.7822472 9.3425290 -0.0059130
C 6.2592954 7.8603617 -0.0257165

C	7.4419789	7.1237736	-0.0332592
C	7.4508613	5.6963456	-0.0261949
C	8.6504513	4.9630385	-0.0306074
C	8.6599192	3.5541349	-0.0249491
C	9.8808390	2.8287238	-0.0256266
C	9.9030188	1.4392376	-0.0221580
C	8.6573344	0.6987116	-0.0218515
C	8.6831861	-0.7195467	-0.0246662
C	7.4596617	-1.4597188	-0.0329557
C	7.5394986	-2.8895717	-0.0418823
C	6.3428749	-3.6414691	-0.0626561
C	6.3810186	-5.0809702	-0.0662883
C	5.1806227	-5.8489760	-0.0792063
C	5.1770827	-7.2767894	-0.0558105
C	3.9439284	-7.9933075	-0.0423121
C	2.7014537	-7.2891977	-0.0517494
C	1.4403201	-7.9514660	-0.0116892
C	0.2087981	-7.2050504	0.0055831
C	-1.0363277	-7.8719394	0.0528030
C	-2.2387307	-7.0941255	0.0743644
C	-3.4872010	-7.7904235	0.1091997
C	-4.7064234	-7.0654306	0.1257110
C	-4.6951043	-5.6315830	0.1162709
C	-5.9383181	-4.9288366	0.1317966
C	-5.9514282	-3.5039536	0.1275250
C	-7.2072957	-2.8069902	0.1392057
C	-7.2533976	-1.3836699	0.1373477
C	-8.5059783	-0.6829568	0.1463907
C	-8.5403290	0.7369409	0.1445668
C	-7.3204660	1.4778672	0.1364474
C	-7.3427146	2.9065928	0.1344608
C	-6.1224221	3.6439928	0.1269021
C	-6.1312289	5.0729623	0.1210760
C	-3.6664046	7.9470890	0.0863238
C	-4.9026794	5.8020509	0.1103198
C	-4.8989166	7.2309536	0.1007354
C	-1.1813527	7.9489165	0.0633976
C	-2.4230747	7.2425881	0.0814184
C	1.3005445	7.9283440	0.0340975
C	0.0557482	7.2333758	0.0551481
C	3.7783449	7.8939976	0.0023614
C	4.9947988	7.1607274	-0.0084986

C	2.5307090	7.2011851	0.0225699
C	4.9830037	5.7255625	-0.0023891
C	6.1965610	4.9803458	-0.0127594
C	6.1798672	3.5441942	-0.0093576
C	7.4112706	2.8270588	-0.0175896
C	7.4059417	1.3990472	-0.0185565
C	6.1620336	0.6698724	-0.0166361
C	6.1835145	-0.7603217	-0.0302412
C	4.9480190	-1.5010697	-0.0443394
C	5.0959856	-2.9398135	-0.0740089
C	3.9479761	-3.7444039	-0.1051848
C	3.9450382	-5.1627578	-0.1020989
C	2.7168207	-5.8763810	-0.0882908
C	1.4831345	-5.1762146	-0.0772992
C	0.2165013	-5.7745662	-0.0189710
C	-0.9595062	-4.9328364	0.0221713
C	-2.2142744	-5.6392163	0.0635696
C	-3.4458689	-4.9119758	0.0909748
C	-3.4320463	-3.4674677	0.0932471
C	-4.7093835	-2.7788812	0.1132216
C	-4.7766923	-1.3545161	0.1172176
C	-6.0297731	-0.6525403	0.1280454
C	-6.0722233	0.7746647	0.1300454
C	-4.8590157	1.5139838	0.1258594
C	-4.8776763	2.9387844	0.1241410
C	-2.4271049	5.8137305	0.0932326
C	-3.6545726	3.6708660	0.1162790
C	-3.6592261	5.0977978	0.1075487
C	0.0518928	5.8028884	0.0670941
C	-1.1896648	5.1028296	0.0877501
C	2.5232856	5.7686003	0.0310767
C	3.7420366	5.0246135	0.0162033
C	1.2804181	5.0807639	0.0551273
C	3.7310737	3.5883973	0.0202400
C	4.9349517	2.8241197	0.0040106
C	4.9002686	1.3733744	-0.0007824
C	3.6428405	0.6499377	0.0110568
C	3.6338191	-0.8121053	-0.0223376
C	2.4793234	-1.7181902	-0.0418418
C	2.7284232	-3.0981131	-0.1008180
C	1.5256310	-3.7967662	-0.0870794
C	0.4513459	-2.8960854	-0.0187197

C	-0.9069116	-3.4497626	0.0290380
C	-2.1809526	-2.7332192	0.0769392
C	-2.2850671	-1.2710061	0.1030116
C	-3.5660224	-0.6144071	0.1138738
C	-3.6155927	0.8106328	0.1215381
C	-1.1921229	3.6839611	0.0999595
C	-2.4095561	1.5503107	0.1196211
C	-2.4205901	2.9701776	0.1141422
C	1.2755157	3.6523186	0.0654063
C	2.4888029	2.9031964	0.0447977
C	2.4247304	1.4652702	0.0495173
C	0.0359216	2.9709403	0.0915603
C	0.0718664	1.5506714	0.1047135
N	1.2191773	0.8706077	0.0890227
N	1.0874571	-1.6554895	0.0012683
H	0.5784337	-0.7742474	0.0667987
N	-1.1709752	-0.5181288	0.1158869
C	-1.1934238	0.8155009	0.1191033
H	-4.9365327	11.1675213	0.0730842
H	0.0818878	11.1604166	0.0245363
H	12.1275351	-1.1922014	-0.0147272
H	2.5883772	11.1356437	-0.0030035
H	-10.6200769	-3.4010234	0.1713013
H	2.6606994	-11.1881024	0.0461848
H	-10.7671140	3.3763009	0.1529170
H	-9.3469266	-5.5116391	0.1739048
H	-8.3101677	7.7541615	0.1191883
H	-7.0677862	9.9292522	0.0976037
H	5.0792604	11.1060805	-0.0307975
H	-11.9220158	-1.2720821	0.1731876
H	-11.9752445	1.1979064	0.1670556
H	8.5893828	-7.7437651	-0.0177209
H	7.3390506	-9.9706560	0.0016254
H	10.8259532	3.3833430	-0.0283832
H	12.0830991	1.2876430	-0.0183986
H	-4.7816818	-11.0162382	0.1678285
H	8.4033375	7.6501317	-0.0448791
H	9.7967764	-5.5169609	-0.0203960
H	-9.5471702	5.5658669	0.1373725
H	-6.9140967	-9.7493701	0.1884230
H	5.2145227	-11.2049471	0.0244968
H	9.6063430	5.4988505	-0.0382426

H	10.9630400	-3.3245321	-0.0170246
H	7.1984595	9.8362190	-0.0472399
H	-2.3533076	-11.0607523	0.1268535
H	-8.1128215	-7.6189131	0.1804668
H	0.1283455	-11.1337752	0.0840501
H	-2.4319638	11.1695780	0.0502493

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Pyrrolic N e support material

C	11.1410816	0.7165895	-0.3902491
C	11.1650832	-0.6451233	-0.3021910
C	9.9465326	-1.4129319	-0.1931470
C	9.9796527	-2.8027385	-0.1137118
C	8.7873540	-3.5722059	-0.0340927
C	8.8038549	-4.9858250	0.0282197
C	7.6163232	-5.7479112	0.0767747
C	7.6005653	-7.1814614	0.1308488
C	6.4144481	-7.9250156	0.1590275
C	6.3672231	-9.3729798	0.2061688
C	5.1803433	-10.0625728	0.2200975
C	3.8982131	-9.3869458	0.1886077
C	2.6647433	-10.0494400	0.1889198
C	1.4105981	-9.3536901	0.1498520
C	0.1598934	-10.0083112	0.1300331
C	-1.0610556	-9.2944425	0.0820492
C	-2.3211404	-9.9496970	0.0312259
C	-3.5134249	-9.2333866	-0.0346272
C	-4.7855515	-9.9126045	-0.1146409
C	-5.9580569	-9.2182994	-0.1900337
C	-5.9748518	-7.7745507	-0.1811912
C	-7.1670685	-7.0627771	-0.2538417
C	-7.1917230	-5.6424861	-0.2193306
C	-8.4057656	-4.9298215	-0.2854988
C	-8.4424712	-3.5259910	-0.2293155
C	-9.6710456	-2.8043232	-0.2978662
C	-9.7172697	-1.4147611	-0.2304784
C	-10.9582695	-0.6756586	-0.3030672
C	-10.9825793	0.6901715	-0.2388505
C	-9.7677457	1.4610430	-0.0932438
C	-9.7716050	2.8541023	-0.0388463
C	-8.5684191	3.6108178	0.0925412
C	-8.5588820	5.0211144	0.1117135

C	-7.3582724	5.7629196	0.2028709
C	-7.3330195	7.1890762	0.1769258
C	-4.9167593	10.0443197	0.1429752
C	-6.1383849	7.9118227	0.2131422
C	-6.1003199	9.3565914	0.1537830
C	-2.4231822	10.0421435	0.1304609
C	-3.6418660	9.3624067	0.1897550
C	0.0661238	10.0327374	0.0261339
C	-1.1713006	9.3579865	0.1421912
C	2.5465840	10.0112966	-0.1658333
C	1.2955685	9.3422630	-0.0084704
C	5.0225017	9.9893663	-0.4079645
C	6.1955993	9.2910479	-0.4874909
C	3.7536910	9.3173768	-0.2358931
C	6.2239977	7.8475420	-0.4049394
C	7.4068187	7.1181688	-0.4872153
C	7.4262080	5.6941106	-0.4076451
C	8.6264389	4.9661830	-0.4788503
C	8.6452846	3.5592558	-0.4011892
C	9.8662429	2.8339260	-0.4507652
C	9.8953816	1.4464927	-0.3661185
C	8.6542898	0.7091653	-0.2489766
C	8.6777552	-0.7067269	-0.1724127
C	7.4538089	-1.4407434	-0.0824918
C	7.5254684	-2.8673506	-0.0308509
C	6.3233725	-3.6102287	0.0105219
C	6.3567903	-5.0441857	0.0596372
C	5.1506716	-5.8010936	0.0864600
C	5.1496777	-7.2286079	0.1340511
C	3.9189614	-7.9438077	0.1485356
C	2.6774758	-7.2380960	0.1155029
C	1.4225132	-7.9113560	0.1176621
C	0.1924506	-7.1724874	0.0826669
C	-1.0485795	-7.8492756	0.0701610
C	-2.2533058	-7.0808362	0.0318381
C	-3.4983272	-7.7813896	-0.0292559
C	-4.7180001	-7.0604651	-0.0925809
C	-4.7081035	-5.6290637	-0.0615767
C	-5.9458630	-4.9215525	-0.1055883
C	-5.9548660	-3.4982287	-0.0287753
C	-7.2024931	-2.7972783	-0.0896889
C	-7.2376737	-1.3768230	-0.0107813

C	-8.4845802	-0.6726412	-0.0811749
C	-8.5120302	0.7430392	-0.0091485
C	-7.2932843	1.4730878	0.1464957
C	-7.3149576	2.8978957	0.1951992
C	-6.0965025	3.6253150	0.3231102
C	-6.1064040	5.0526027	0.3076667
C	-3.6495202	7.9192632	0.2835975
C	-4.8790902	5.7773623	0.3648862
C	-4.8794548	7.2044577	0.2955178
C	-1.1725708	7.9196079	0.2577696
C	-2.4088916	7.2126819	0.3400317
C	1.2956928	7.9011155	0.1047335
C	0.0625655	7.2040494	0.2586459
C	3.7567364	7.8715876	-0.1412786
C	4.9714878	7.1457235	-0.2285402
C	2.5216648	7.1759669	0.0408571
C	4.9667086	5.7142851	-0.1466334
C	6.1816380	4.9792015	-0.2404214
C	6.1735832	3.5486818	-0.1672818
C	7.4041248	2.8351123	-0.2594142
C	7.4064793	1.4099174	-0.2026756
C	6.1690584	0.6847402	-0.0888460
C	6.1820257	-0.7406722	-0.0540304
C	4.9405658	-1.4724545	-0.0211913
C	5.0748427	-2.9062322	-0.0113183
C	3.9146615	-3.6914219	-0.0075004
C	3.9151674	-5.1090166	0.0512138
C	2.6872945	-5.8225740	0.0656129
C	1.4549664	-5.1205744	0.0211903
C	0.1986230	-5.7395695	0.0459560
C	-0.9805894	-4.9127240	0.0483468
C	-2.2312392	-5.6291614	0.0448176
C	-3.4636461	-4.9121409	0.0237835
C	-3.4525877	-3.4763168	0.1324220
C	-4.7192334	-2.7791503	0.1189279
C	-4.7691048	-1.3584318	0.2248297
C	-6.0160551	-0.6544368	0.1508474
C	-6.0491826	0.7679989	0.2443242
C	-4.8361822	1.4936952	0.4314926
C	-4.8564289	2.9173530	0.4501526
C	-2.4078539	5.7859010	0.4551244
C	-3.6319912	3.6437661	0.5475047

C	-3.6383887	5.0707466	0.4679582
C	0.0654994	5.7772238	0.3971384
C	-1.1701807	5.0741667	0.5210417
C	2.5195836	5.7467446	0.1501421
C	3.7370489	5.0124541	0.0420096
C	1.2917178	5.0541633	0.3639782
C	3.7321913	3.5810793	0.1283179
C	4.9396886	2.8328820	0.0082240
C	4.9181275	1.3872727	0.0352497
C	3.6764684	0.6716658	0.2001798
C	3.6338220	-0.7756366	0.0103426
C	2.4591882	-1.6519016	-0.1354755
C	2.6925276	-3.0310782	-0.0863792
C	1.4849111	-3.7328099	-0.0723400
C	0.4014342	-2.8476284	-0.1115413
C	-0.9385147	-3.4322272	0.0636772
C	-2.2134849	-2.7504112	0.2685926
C	-2.3172680	-1.3376011	0.6106357
C	-3.5627272	-0.6371135	0.4621159
C	-3.5980907	0.7860482	0.5818510
C	-1.1670404	3.6586853	0.6792632
C	-2.3919893	1.5178367	0.7816853
C	-2.4014099	2.9413494	0.6930090
C	1.2958111	3.6293792	0.5266616
C	2.5123668	2.8925502	0.3929142
C	2.5066828	1.4648957	0.5547411
C	0.0662363	2.9461176	0.7537021
C	0.0879474	1.5433208	1.0455849
C	1.3277944	0.8865240	1.0682345
H	1.3771823	-0.1379458	1.4279402
N	1.0351109	-1.5720490	-0.2395703
H	0.5283097	-0.7026633	-0.3850322
C	-1.2224602	-0.5953350	1.0982353
H	-0.3512378	-1.1426945	1.4485969
C	-1.1794509	0.8068839	1.0605440
H	-4.9161607	11.1385642	0.0874124
H	0.0685363	11.1253333	-0.0598400
H	12.1168422	-1.1876421	-0.3176005
H	2.5519354	11.1045818	-0.2435611
H	-10.6040026	-3.3690942	-0.4065976
H	2.6488295	-11.1453208	0.2153404
H	-10.7250365	3.3902910	-0.1091750

H	-9.3448918	-5.4865749	-0.3792954
H	-8.2839430	7.7298313	0.1072868
H	-7.0520640	9.8973282	0.1068448
H	5.0240528	11.0828867	-0.4755717
H	-11.8903521	-1.2406996	-0.4146282
H	-11.9341057	1.2301172	-0.2993411
H	8.5610025	-7.7100000	0.1456945
H	7.3155813	-9.9215908	0.2286323
H	10.8065616	3.3880164	-0.5493133
H	12.0726228	1.2864846	-0.4779250
H	-4.7858616	-11.0081098	-0.1180693
H	8.3580781	7.6468836	-0.6167393
H	9.7717664	-5.5001278	0.0301459
H	-9.5105386	5.5591653	0.0333261
H	-6.9158736	-9.7458004	-0.2555795
H	5.1879894	-11.1578899	0.2535448
H	9.5740365	5.5043303	-0.5937288
H	10.9469629	-3.3180144	-0.1243038
H	7.1462684	9.8194841	-0.6187956
H	-2.3528430	-11.0452195	0.0327569
H	-8.1161015	-7.6052530	-0.3312044
H	0.1274096	-11.1037393	0.1439681
H	-2.4236167	11.1354801	0.0527499

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Pyrrolic N f support material

C	11.1484066	0.7037482	-0.1095013
C	11.1505226	-0.6648561	-0.1097149
C	9.9221142	-1.4264880	-0.0463485
C	9.9038604	-2.8220852	-0.0672519
C	8.6875387	-3.5681990	-0.0186653
C	8.6593142	-4.9801910	-0.0660323
C	7.4498975	-5.7099670	-0.0381150
C	7.4106435	-7.1355591	-0.1120792
C	6.2106760	-7.8484512	-0.1088171
C	6.1639077	-9.2914140	-0.2044073
C	4.9770974	-9.9726275	-0.2236210
C	3.7055611	-9.2865861	-0.1456513
C	2.4853153	-9.9630506	-0.1891827
C	1.2323305	-9.2802597	-0.1218449
C	-0.0075256	-9.9541047	-0.2014480
C	-1.2435969	-9.2683616	-0.1506318

C	-2.5026165	-9.9336052	-0.2724913
C	-3.7178242	-9.2431315	-0.2454837
C	-4.9992149	-9.8981786	-0.4054901
C	-6.1778931	-9.1983918	-0.4047880
C	-6.2138880	-7.7619962	-0.2291026
C	-7.4071543	-7.0251741	-0.2531359
C	-7.4391418	-5.6065402	-0.0714982
C	-8.6401307	-4.8327432	-0.1487892
C	-8.6625099	-3.4258182	0.0343893
C	-9.8551489	-2.5797052	-0.1487532
C	-9.7495003	-1.1921703	0.0235873
N	-10.5370423	-0.0145099	-0.1746482
H	-11.4957832	-0.0158521	-0.5098131
C	-9.7532905	1.1654669	0.0246628
C	-9.8633560	2.5528238	-0.1464807
C	-8.6733833	3.4025648	0.0372453
C	-8.6554318	4.8097138	-0.1449690
C	-7.4568433	5.5872501	-0.0673478
C	-7.4293141	7.0060905	-0.2482562
C	-5.0303002	9.8865446	-0.4004211
C	-6.2383051	7.7465952	-0.2242448
C	-6.2068199	9.1831506	-0.3994497
C	-2.5338434	9.9296279	-0.2683931
C	-3.7468497	9.2353970	-0.2410908
C	-0.0389284	9.9578900	-0.1981621
C	-1.2727672	9.2682747	-0.1471341
C	2.4537614	9.9747278	-0.1864086
C	1.2030033	9.2879532	-0.1189890
C	4.9454579	9.9922760	-0.2210382
C	6.1344529	9.3148743	-0.2019803
C	3.6761226	9.3021610	-0.1431150
C	6.1858154	7.8720484	-0.1066368
C	7.3880807	7.1629446	-0.1100379
C	7.4318804	5.7374228	-0.0363938
C	8.6436429	5.0114242	-0.0645024
C	8.6763304	3.5994476	-0.0175243
C	9.8950096	2.8571176	-0.0663453
C	9.9176307	1.4615306	-0.0458721
C	8.6731776	0.7265056	0.0334027
C	8.6754038	-0.6953940	0.0331750
C	7.4427952	-1.4180281	0.1013097
C	7.4106435	-7.1355591	-0.1120792

C	6.2106760	-7.8484512	-0.1088171
C	6.1639077	-9.2914140	-0.2044073
C	4.9770974	-9.9726275	-0.2236210
C	3.7055611	-9.2865861	-0.1456513
C	2.4853153	-9.9630506	-0.1891827
C	1.2323305	-9.2802597	-0.1218449
C	-0.0075256	-9.9541047	-0.2014480
C	-1.2435969	-9.2683616	-0.1506318
C	-2.5026165	-9.9336052	-0.2724913
C	-3.7178242	-9.2431315	-0.2454837
C	-4.9992149	-9.8981786	-0.4054901
C	-6.1778931	-9.1983918	-0.4047880
C	-6.2138880	-7.7619962	-0.2291026
C	-7.4071543	-7.0251741	-0.2531359
C	-7.4391418	-5.6065402	-0.0714982
C	-8.6401307	-4.8327432	-0.1487892
C	-8.6625099	-3.4258182	0.0343893
C	-9.8551489	-2.5797052	-0.1487532
C	-9.7495003	-1.1921703	0.0235873
N	-10.5370423	-0.0145099	-0.1746482
H	-11.4957832	-0.0158521	-0.5098131
C	-9.7532905	1.1654669	0.0246628
C	-9.8633560	2.5528238	-0.1464807
C	-8.6733833	3.4025648	0.0372453
C	-8.6554318	4.8097138	-0.1449690
C	-7.4568433	5.5872501	-0.0673478
C	-7.4293141	7.0060905	-0.2482562
C	-5.0303002	9.8865446	-0.4004211
C	-6.2383051	7.7465952	-0.2242448
C	-6.2068199	9.1831506	-0.3994497
C	-2.5338434	9.9296279	-0.2683931
C	-3.7468497	9.2353970	-0.2410908
C	-0.0389284	9.9578900	-0.1981621
C	-1.2727672	9.2682747	-0.1471341
C	2.4537614	9.9747278	-0.1864086
C	1.2030033	9.2879532	-0.1189890
C	4.9454579	9.9922760	-0.2210382
C	6.1344529	9.3148743	-0.2019803
C	3.6761226	9.3021610	-0.1431150
C	6.1858154	7.8720484	-0.1066368
C	7.3880807	7.1629446	-0.1100379
C	7.4318804	5.7374228	-0.0363938

C	8.6436429	5.0114242	-0.0645024
C	8.6763304	3.5994476	-0.0175243
C	9.8950096	2.8571176	-0.0663453
C	9.9176307	1.4615306	-0.0458721
C	8.6731776	0.7265056	0.0334027
C	8.6754038	-0.6953940	0.0331750
C	7.4427952	-1.4180281	0.1013097
C	7.4403729	-2.8457734	0.0725247
C	6.2075656	-3.5645482	0.1204706
C	6.2009906	-4.9911564	0.0586541
C	4.9654739	-5.7071564	0.0778888
C	4.9545587	-7.1349957	-0.0153910
C	3.7218053	-7.8434716	-0.0289837
C	2.4826971	-7.1349716	0.0623319
C	1.2420514	-7.8424904	0.0197422
C	0.0066569	-7.1327648	0.1020350
C	-1.2361514	-7.8337887	0.0166732
C	-2.4708453	-7.1192479	0.0775615
C	-3.7179596	-7.8091605	-0.0614065
C	-4.9458848	-7.0886159	-0.0379076
C	-4.9401336	-5.6775335	0.1634896
C	-6.1714294	-4.9537534	0.1708381
C	-6.1569230	-3.5540713	0.3919081
C	-7.3798494	-2.8286411	0.3609190
C	-7.3126058	-1.4391174	0.5694975
C	-8.4822399	-0.7008136	0.4310495
C	-8.4844416	0.6778106	0.4316796
C	-7.3171450	1.4197267	0.5707125
C	-7.3887853	2.8092094	0.3632326
C	-6.1681293	3.5384977	0.3945984
C	-6.1870296	4.9382788	0.1743950
C	-3.7424969	7.8014173	-0.0573797
C	-4.9579906	5.6659274	0.1671367
C	-4.9681632	7.0770621	-0.0336954
C	-1.2608179	7.8337464	0.0198626
C	-2.4932289	7.1153420	0.0809657
C	1.2172674	7.8502414	0.0223242
C	-0.0158422	7.1366036	0.1047193
C	3.6969499	7.8591059	-0.0267149
C	4.9319514	7.1545474	-0.0133344
C	2.4601134	7.1466412	0.0645686
C	4.9474099	5.7267085	0.0796103

C	6.1852033	5.0145951	0.0601693
C	6.1963055	3.5879573	0.1215830
C	7.4313848	2.8730461	0.0734219
C	7.4383131	1.4452713	0.1017664
C	6.2035530	0.7251379	0.1873331
C	6.2058027	-0.7018003	0.1871038
C	4.9716334	-1.4214204	0.2576623
C	4.9691566	-2.8490854	0.2190345
C	3.7348613	-3.5655705	0.2605821
C	3.7279795	-4.9944463	0.1792328
C	2.4914241	-5.7072576	0.1801622
C	1.2556060	-4.9958037	0.2829385
C	0.0162117	-5.7060109	0.2510581
C	-1.2164492	-4.9947997	0.3452198
C	-2.4611302	-5.6992464	0.2594184
C	-3.6927900	-4.9860506	0.3254879
C	-3.6788960	-3.5695900	0.5142841
C	-4.9089526	-2.8569357	0.5752391
C	-4.8773115	-1.4391696	0.7271254
C	-6.0970387	-0.7195291	0.7355504
C	-6.0992897	0.7038752	0.7361262
C	-4.8818283	1.4273932	0.7281911
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C	-2.4790502	5.6953338	0.2623715
C	-3.6901144	3.5617431	0.5165729
C	-3.7084598	4.9782557	0.3284929
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C	-1.2321712	4.9947498	0.3475917
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C	3.7121687	5.0100336	0.1808185
C	1.2398258	5.0035488	0.2847857
C	3.7235832	3.5811464	0.2617487
C	4.9601382	2.8685506	0.2199464
C	4.9671283	1.4408686	0.2581305
C	3.7357577	0.7228464	0.3500021
C	3.7380192	-0.7073081	0.3497608
C	2.5058174	-1.4251833	0.4182162
C	2.5014691	-2.8532744	0.3658441
C	1.2643653	-3.5699063	0.3909162
C	0.0330450	-2.8581922	0.4977812
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C	-2.4369382	-2.8602340	0.5862681

C	-2.4212217	-1.4348576	0.6903757
C	-3.6477548	-0.7194979	0.7591321
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C	-2.4257271	1.4308657	0.6912667
C	-2.4459272	2.8562486	0.5879603
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C	2.5013058	1.4368233	0.4187292
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C	0.0366646	1.4328916	0.5713191
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H	-0.0455474	11.0475765	-0.3155080
H	12.0971234	-1.2141916	-0.1635520
H	2.4481080	11.0665102	-0.2836313
H	-10.7834874	-3.0665058	-0.4652846
H	2.4831753	-11.0549015	-0.2866011
H	-10.7932693	3.0369698	-0.4625563
H	-8.3750115	7.5346118	-0.4173855
H	-7.1585373	9.7090985	-0.5350123
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H	12.0933277	1.2560452	-0.1631905
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H	-9.5909782	5.3330339	-0.3764036
H	-7.1279170	-9.7272209	-0.5408690
H	4.9705844	-11.0653886	-0.3034423
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180

N-O-like support material

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C 7.4130945 -7.1411616 0.0523506
C 6.2147152 -7.8565322 0.0512523
C 6.1736332 -9.3025940 0.0502003
C 4.9890450 -9.9877511 0.0491097
C 3.7151003 -9.3020935 0.0489821
C 2.4976276 -9.9846294 0.0478842
C 1.2426794 -9.3030407 0.0476933
C 0.0062440 -9.9866898 0.0465041
C -1.2321800 -9.3038795 0.0463097
C -2.4873883 -9.9844407 0.0450844
C -3.7066983 -9.3000940 0.0449138
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C	-0.0207807	9.9845057	0.0624235
C	-1.2554593	9.2983220	0.0613930
C	2.4693372	9.9897846	0.0634290
C	1.2173704	9.3041321	0.0623529
C	4.9603412	10.0004535	0.0643954
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C	8.6410263	5.0071529	0.0619239
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C	9.8893055	2.8527753	0.0607824
C	9.9103787	1.4573883	0.0596980
C	8.6630998	0.7228941	0.0586387
C	8.6654035	-0.6985377	0.0575836
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C	6.1950429	-4.9945356	0.0533297
C	4.9608188	-5.7118438	0.0522206
C	4.9555137	-7.1425114	0.0511706
C	3.7251743	-7.8545324	0.0500552
C	2.4830820	-7.1452751	0.0499593
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C	0.0080514	-7.1483992	0.0486435
C	-1.2308324	-7.8595816	0.0474086
C	-2.4673195	-7.1471385	0.0472564
C	-3.7107836	-7.8550225	0.0460291
C	-4.9422478	-7.1414872	0.0458902
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C	-3.7052675	0.7101472	0.0530840
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C	-2.4710562	1.4260363	0.0542442
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C	0.0093133	-1.4272631	0.0530108
C	-1.2272778	-0.7139492	0.0529889
C	-1.2317386	0.7134990	0.0541890
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H	-0.0233226	11.0805001	0.0632556
H	12.0931098	-1.2178880	0.0585061
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H	2.4994462	-11.0807210	0.0471990
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H	-12.0857749	1.1673276	0.0496382

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H	10.8380968	3.4016725	0.0617066
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H	-9.6121041	5.5090981	0.0547372
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H	4.9863279	-11.0833744	0.0483001
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H	10.8487992	-3.3707382	0.0566244
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Pd₂₁/carbon support

Pd	1.3343183	-2.2870989	5.5362042
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Pd	0.0047613	0.0001066	5.7139339
Pd	-0.6310673	1.0891022	3.1777930
Pd	-1.2159387	-2.2295213	4.7818120
Pd	-2.5322751	0.0394780	4.7881736
Pd	-0.5556067	-3.3631808	2.3328889
Pd	-2.0664408	-1.2065933	2.4286304
Pd	3.2058936	-1.1677826	2.3377730
Pd	2.5414681	-0.0385520	4.7869065
Pd	2.0736866	1.2115474	2.4286534
Pd	1.2246439	2.2304959	4.7828084
Pd	1.9812057	-3.3896349	3.0632050
Pd	0.2182840	-4.4605055	4.6446880
Pd	3.7768519	-2.3858219	4.6519220
Pd	-1.3242038	2.2882715	5.5401050
Pd	-3.7679997	2.3859608	4.6579214
Pd	-0.2089369	4.4619776	4.6477344
Pd	-3.2003765	1.1714703	2.3407528
Pd	0.5600145	3.3669536	2.3340909
Pd	-1.9752210	3.3929695	3.0684702

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C	9.9234361	-1.4321144	0.0878384
C	9.9070408	-2.8265824	0.0186441
C	8.6906757	-3.5742703	-0.0238840
C	8.6653632	-4.9851265	-0.1008128
C	7.4558150	-5.7169995	-0.1411884
C	7.4200833	-7.1424632	-0.2036655
C	6.2201813	-7.8578951	-0.2241476
C	6.1789602	-9.3030790	-0.2724625
C	4.9944400	-9.9891021	-0.2706182
C	3.7203619	-9.3056312	-0.2216773
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C	1.2485954	-9.3121551	-0.1372965
C	0.0122580	-9.9973618	-0.0920994
C	-1.2240572	-9.3174291	-0.0124286
C	-2.4773691	-10.0006856	0.0377582
C	-3.6951298	-9.3211653	0.1082005
C	-4.9678073	-10.0078521	0.1505302
C	-6.1522477	-9.3240907	0.2055747
C	-6.1954675	-7.8779834	0.2231170
C	-7.3948119	-7.1637990	0.2589000
C	-7.4323142	-5.7361157	0.2614175
C	-8.6431605	-5.0066839	0.2732857
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C	-9.8933918	-2.8507433	0.2495458
C	-9.9161020	-1.4552128	0.2106772
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C	-11.1529499	0.6693964	0.1330280
C	-9.9240884	1.4319376	0.0929116
C	-9.9077021	2.8262505	0.0207208
C	-8.6913414	3.5737967	-0.0242289
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C	-7.4564806	5.7164029	-0.1439317
C	-7.4207639	7.1418205	-0.2076883
C	-4.9952394	9.9886621	-0.2705163
C	-6.2208840	7.8573112	-0.2276038
C	-6.1796692	9.3024941	-0.2761279
C	-2.5039387	9.9903876	-0.1900551
C	-3.7212424	9.3053715	-0.2170303
C	-0.0137045	9.9974159	-0.0723398
C	-1.2497943	9.3121573	-0.1233365

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C	8.6741047	-0.7018704	0.1220319
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C	0.0107341	-7.1619510	-0.0357862
C	-1.2278070	-7.8735714	0.0201604
C	-2.4651668	-7.1651010	0.1034992
C	-3.7070045	-7.8742467	0.1385332
C	-4.9374642	-7.1632460	0.1947711
C	-4.9452734	-5.7316643	0.2166218
C	-6.1818827	-5.0150277	0.2431363
C	-6.1902318	-3.5857763	0.2413426
C	-7.4259875	-2.8673864	0.2402537
C	-7.4323816	-1.4383080	0.2110372
C	-8.6703472	-0.7192732	0.1846267
C	-8.6747561	0.7016658	0.1266347
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C	-2.4872737	7.1534078	-0.1360106
C	1.2265975	7.8734351	0.0333270
C	-0.0117556	7.1618277	-0.0270150
C	3.7057507	7.8740048	0.1531403
C	4.9362500	7.1629686	0.2084026
C	2.4640534	7.1648354	0.1140859
C	4.9443123	5.7313140	0.2228497
C	6.1809955	5.0147334	0.2467384
C	6.1894858	3.5855019	0.2402009
C	7.4252681	2.8671829	0.2364019
C	7.4317135	1.4381316	0.2058664
C	6.1963943	0.7173236	0.1959247
C	6.2016137	-0.7110522	0.1424639
C	4.9726983	-1.4389705	0.1165906
C	4.9660655	-2.8620522	-0.0028725
C	3.7290725	-3.5787819	-0.0555242
C	3.7249330	-5.0042344	-0.1127135
C	2.4868733	-5.7214793	-0.1124381
C	1.2483969	-5.0157307	-0.0543751
C	0.0111069	-5.7322506	0.0000336
C	-1.2264762	-5.0298594	0.1209464
C	-2.4690946	-5.7338761	0.1501847
C	-3.7055223	-5.0183528	0.2041842
C	-3.7157802	-3.5869012	0.2303127
C	-4.9519360	-2.8682896	0.2352147
C	-4.9604422	-1.4386953	0.2287083
C	-6.1970430	-0.7175437	0.2004358
C	-6.2022221	0.7107846	0.1456110
C	-4.9733220	1.4387142	0.1204436
C	-4.9667254	2.8617041	-0.0000356
C	-2.4876196	5.7212098	-0.1098339
C	-3.7297315	3.5784662	-0.0532266
C	-3.7256259	5.0038737	-0.1117480
C	-0.0120080	5.7320201	0.0039682
C	-1.2491499	5.0154697	-0.0524473
C	2.4681818	5.7334839	0.1551579
C	3.7046529	5.0179206	0.2068284
C	1.2255612	5.0294532	0.1246723
C	3.7150391	3.5864722	0.2296476
C	4.9512304	2.8679734	0.2325846
C	4.9598175	1.4384232	0.2251540

C	3.7293224	0.7216790	0.2228754
C	3.7283387	-0.7194178	0.1967735
C	2.4765004	-1.4383616	0.1063640
C	2.4877055	-2.8717356	0.0032091
C	1.2528467	-3.5873435	0.0033812
C	0.0150527	-2.8642937	0.1094407
C	-1.2316099	-3.5924475	0.2003228
C	-2.4822085	-2.8753940	0.2271277
C	-2.4788583	-1.4351764	0.2380750
C	-3.7300003	-0.7219907	0.2262421
C	-3.7289682	0.7191496	0.2008545
C	-1.2535132	3.5869425	0.0039774
C	-2.4771266	1.4381321	0.1091936
C	-2.4883968	2.8714718	0.0045928
C	1.2307332	3.5918175	0.2007325
C	2.4814526	2.8748343	0.2265492
C	2.4780377	1.4346242	0.2352621
C	-0.0158156	2.8638661	0.1088091
C	-0.0069542	1.4264775	0.0306145
C	1.2278681	0.7113359	0.0807675
C	1.2340961	-0.7153845	0.0303585
C	0.0062262	-1.4268158	0.0314876
C	-1.2286625	-0.7116799	0.0832084
C	-1.2348656	0.7151317	0.0317845
H	-4.9935009	11.0838380	-0.3022414
H	-0.0150840	11.0932238	-0.0904762
H	12.1013816	-1.2166673	0.1040332
H	2.4762363	11.0966806	0.0482258
H	-10.8419760	-3.3996742	0.2672646
H	2.5064857	-11.0863618	-0.2222539
H	-10.8589366	3.3703247	-0.0047629
H	-9.5916700	-5.5556362	0.2879371
H	-8.3697633	7.6897522	-0.2328158
H	-7.1304306	9.8457063	-0.3124066
H	4.9629691	11.1033357	0.1703658
H	-12.0950626	-1.2505571	0.2154383
H	-12.1020154	1.2167896	0.1150469
H	8.3690741	-7.6904431	-0.2280818
H	7.1297666	-9.8463859	-0.3060677
H	10.8412371	3.3995851	0.2623393
H	12.0944028	1.2507234	0.2029979
H	-4.9649567	-11.1033693	0.1347288

H	8.3420592	7.7126410	0.2919197
H	9.6154905	-5.5308628	-0.1255246
H	-9.6161566	5.5302780	-0.1278868
H	-7.1019603	-9.8695817	0.2340622
H	4.9926434	-11.0842663	-0.3027407
H	9.5907616	5.5554516	0.2909345
H	10.8582766	-3.3706716	-0.0065215
H	7.1001379	9.8694580	0.2640731
H	-2.4781630	-11.0965828	0.0164343
H	-8.3432902	-7.7128324	0.2780164
H	0.0134796	-11.0930987	-0.1141554
H	-2.5075999	11.0862575	-0.2121149

201

Pd₂₁/graphitic N support 1

Pd	1.3774922	-2.1917790	5.4397412
Pd	0.6853569	-1.0086645	3.0687411
Pd	0.0471045	0.0768907	5.6052649
Pd	-0.5913119	1.1878607	3.0801510
Pd	-1.1830390	-2.1591303	4.6583653
Pd	-2.4800534	0.1243577	4.6829453
Pd	-0.4548565	-3.2849044	2.2069638
Pd	-1.9904314	-1.0735308	2.3130869
Pd	3.2386189	-1.1426467	2.2243548
Pd	2.5869470	0.0460328	4.6721319
Pd	2.1174462	1.2623403	2.3056349
Pd	1.2878405	2.3111095	4.6506865
Pd	2.0596675	-3.3479010	3.0108264
Pd	0.2380226	-4.3762284	4.5544578
Pd	3.8416712	-2.2825762	4.5734045
Pd	-1.2514338	2.3733051	5.4753561
Pd	-3.6966196	2.4747412	4.5733112
Pd	-0.1236204	4.5282340	4.5187142
Pd	-3.1875042	1.2828609	2.2346023
Pd	0.5756767	3.4316383	2.1817589
Pd	-1.9287884	3.4933793	2.9768098
C	11.1296860	0.6816862	0.3611094
C	11.1341854	-0.6860252	0.3072334
C	9.9066045	-1.4474288	0.2260937
C	9.8908106	-2.8421665	0.1627412
C	8.6758514	-3.5882160	0.0769418

C	8.6527362	-4.9998103	0.0091608
C	7.4454038	-5.7306181	-0.0703830
C	7.4112646	-7.1569364	-0.1195493
C	6.2125059	-7.8711153	-0.1694577
C	6.1709977	-9.3167610	-0.2008167
C	4.9862502	-10.0015223	-0.2207866
C	3.7124359	-9.3156710	-0.2098144
C	2.4944725	-9.9975442	-0.1961032
C	1.2410881	-9.3154367	-0.1593257
C	0.0061448	-10.0002956	-0.1087578
C	-1.2274469	-9.3165157	-0.0437305
C	-2.4806389	-9.9977830	0.0223345
C	-3.6971684	-9.3183321	0.0939311
C	-4.9672115	-10.0057868	0.1646878
C	-6.1485941	-9.3199200	0.2359678
C	-6.1891050	-7.8740526	0.2435897
C	-7.3871265	-7.1638838	0.3091588
C	-7.4243511	-5.7376975	0.3086959
C	-8.6311660	-5.0113481	0.3632736
C	-8.6570727	-3.5983217	0.3491940
C	-9.8757264	-2.8581898	0.3856061
C	-9.9004993	-1.4629203	0.3490095
C	-11.1335937	-0.7072789	0.3718760
C	-11.1390296	0.6602111	0.3178537
C	-9.9119516	1.4213461	0.2352800
C	-9.8985523	2.8170301	0.1670532
C	-8.6866729	3.5633759	0.0759346
C	-8.6660315	4.9755656	0.0019072
C	-7.4604679	5.7061744	-0.0828193
C	-7.4283213	7.1330079	-0.1322672
C	-5.0080976	9.9816869	-0.2116823
C	-6.2310323	7.8490328	-0.1805881
C	-6.1918843	9.2950862	-0.2034207
C	-2.5169193	9.9824817	-0.1702067
C	-3.7331222	9.2980118	-0.1995807
C	-0.0272746	9.9863652	-0.0601555
C	-1.2614890	9.3027058	-0.1314533
C	2.4606050	9.9872418	0.0959450
C	1.2098029	9.3042812	0.0093098
C	4.9486450	9.9933966	0.2550841
C	6.1324812	9.3094250	0.3212168
C	3.6781791	9.3069459	0.1690955

C	6.1770415	7.8634040	0.3083588
C	7.3760164	7.1493545	0.3644027
C	7.4148026	5.7220664	0.3432675
C	8.6251383	4.9921568	0.3854549
C	8.6557992	3.5795049	0.3539212
C	9.8746548	2.8352219	0.3840122
C	9.8974657	1.4399000	0.3400634
C	8.6528936	0.7050766	0.2668624
C	8.6577794	-0.7160982	0.2103428
C	7.4259885	-1.4393233	0.1336390
C	7.4256218	-2.8659978	0.0594419
C	6.1941359	-3.5856155	-0.0357135
C	6.1927212	-5.0125003	-0.0947550
C	4.9585880	-5.7281946	-0.1557218
C	4.9534655	-7.1576465	-0.1806676
C	3.7221484	-7.8693130	-0.1994240
C	2.4795499	-7.1605257	-0.1895973
C	1.2419024	-7.8714262	-0.1605047
C	0.0026165	-7.1601325	-0.1066877
C	-1.2305598	-7.8738330	-0.0376402
C	-2.4670024	-7.1632569	0.0384171
C	-3.7082118	-7.8712082	0.1023620
C	-4.9323715	-7.1577180	0.1772804
C	-4.9390735	-5.7246516	0.1835223
C	-6.1736994	-5.0164629	0.2454838
C	-6.1732561	-3.5925582	0.2425266
C	-7.4090858	-2.8738589	0.2882819
C	-7.4198659	-1.4462885	0.2600399
C	-8.6563755	-0.7294082	0.2794727
C	-8.6627736	0.6935282	0.2221997
C	-7.4329074	1.4174214	0.1443747
C	-7.4360992	2.8423768	0.0598688
C	-6.2057829	3.5609954	-0.0448225
C	-6.2066589	4.9884934	-0.1102869
C	-3.7414371	7.8506587	-0.2047255
C	-4.9747820	5.7063285	-0.1761951
C	-4.9708893	7.1374376	-0.1945705
C	-1.2620425	7.8586420	-0.1521997
C	-2.4973029	7.1437311	-0.1985271
C	1.2141996	7.8610459	-0.0029411
C	-0.0228598	7.1507999	-0.0971750
C	3.6908709	7.8601514	0.1609934

C	4.9212980	7.1488483	0.2304966
C	2.4513954	7.1510487	0.0799105
C	4.9298994	5.7179315	0.2196675
C	6.1660074	5.0013812	0.2717112
C	6.1750152	3.5727222	0.2472503
C	7.4094290	2.8540084	0.2840823
C	7.4159513	1.4248879	0.2457130
C	6.1813409	0.7051455	0.1824330
C	6.1871755	-0.7230304	0.1305049
C	4.9584199	-1.4504529	0.0587916
C	4.9528411	-2.8744258	-0.0545051
C	3.7167044	-3.5887427	-0.1437025
C	3.7159419	-5.0148368	-0.1749985
C	2.4794376	-5.7295158	-0.1884902
C	1.2392945	-5.0210916	-0.1580416
C	0.0017999	-5.7282094	-0.0958545
C	-1.2381156	-5.0227060	0.0224232
C	-2.4691558	-5.7364283	0.0621316
C	-3.6968315	-5.0112300	0.1245053
C	-3.7030240	-3.5841009	0.1232597
C	-4.9323113	-2.8729078	0.1891498
C	-4.9511041	-1.4431661	0.1971332
C	-6.1843760	-0.7255538	0.2071651
C	-6.1913938	0.7027938	0.1508286
C	-4.9640091	1.4237624	0.0736817
C	-4.9649361	2.8495071	-0.0619515
C	-2.4963029	5.7116901	-0.2157107
C	-3.7346855	3.5669574	-0.1658753
C	-3.7328836	4.9937221	-0.2024878
C	-0.0234393	5.7207564	-0.1117182
C	-1.2571547	5.0046384	-0.1964075
C	2.4562122	5.7198704	0.0862334
C	3.6914894	5.0045092	0.1532517
C	1.2141262	5.0149978	0.0120254
C	3.7025415	3.5736084	0.1492338
C	4.9377926	2.8556896	0.1847493
C	4.9458922	1.4271574	0.1651211
C	3.7141306	0.7111286	0.1159875
C	3.7123652	-0.7310318	0.0826952
C	2.4657696	-1.4485486	-0.0389326
C	2.4737643	-2.8809397	-0.1237020
C	1.2382185	-3.5971049	-0.1143462

C	-0.0027105	-2.8678080	0.0070970
C	-1.2478927	-3.5884781	0.1267560
N	-2.4892961	-2.8843723	0.0596340
C	-2.4693345	-1.4635348	0.1937520
C	-3.7181447	-0.7432677	0.1742916
C	-3.7154778	0.7034160	0.1283776
C	-1.2599137	3.5739838	-0.1701754
C	-2.4768810	1.4256370	-0.0334987
C	-2.4923319	2.8579443	-0.1507060
C	1.2177577	3.5760754	0.0493315
C	2.4694215	2.8604436	0.0988603
C	2.4637115	1.4223807	0.0837527
C	-0.0254987	2.8487844	-0.0731717
C	-0.0158397	1.4108267	-0.1474174
C	1.2193057	0.7012824	-0.0961706
C	1.2268006	-0.7247091	-0.1321877
C	0.0018466	-1.4332597	-0.1065629
C	-1.2338584	-0.7336041	-0.0406034
C	-1.2446451	0.6969160	-0.1218815
H	-5.0070381	11.0773091	-0.2195023
H	-0.0288257	11.0822643	-0.0472963
H	12.0826920	-1.2344413	0.3235864
H	2.4601136	11.0833146	0.1052792
H	-10.8219678	-3.4087552	0.4365181
H	2.4949540	-11.0935587	-0.1993372
H	-10.8503580	3.3605370	0.1805829
H	-9.5792375	-5.5585451	0.4117519
H	-8.3783112	7.6795166	-0.1168965
H	-7.1436286	9.8378109	-0.2045265
H	4.9446152	11.0889911	0.2654107
H	-12.0776388	-1.2602180	0.4313097
H	-12.0875841	1.2084674	0.3342544
H	8.3602334	-7.7053226	-0.1064250
H	7.1218238	-9.8611074	-0.2017964
H	10.8224800	3.3829855	0.4391616
H	12.0747201	1.2331055	0.4205775
H	-4.9640168	-11.1012905	0.1603136
H	8.3227604	7.6985920	0.4227500
H	9.6026761	-5.5461875	0.0254538
H	-9.6168174	5.5203498	0.0188309
H	-7.0989641	-9.8622314	0.2885973
H	4.9833453	-11.0970067	-0.2376108

H	9.5724346	5.5406099	0.4401533
H	10.8413448	-3.3878577	0.1773896
H	7.0805394	9.8548928	0.3844245
H	-2.4815489	-11.0938692	0.0187859
H	-8.3339924	-7.7133217	0.3594539
H	0.0062581	-11.0961146	-0.1098517
H	-2.5207634	11.0785385	-0.1609769

201

Pd₂₁/graphitic N support 2

Pd	1.2458595	-2.5328421	5.3325420
Pd	0.4205627	-1.5168255	2.9165017
Pd	-0.1736112	-0.3576801	5.3986904
Pd	-0.9115059	0.6641826	2.9027967
Pd	-1.3540387	-2.6743707	4.6090521
Pd	-2.7852848	-0.4766266	4.5454728
Pd	-0.7435233	-3.9732295	2.2269609
Pd	-2.1957168	-1.7137014	2.2000411
Pd	2.9698599	-1.4231768	1.9755718
Pd	2.3679382	-0.2823734	4.4047562
Pd	1.6382254	0.8368965	2.0442216
Pd	0.9465617	1.9173340	4.4655243
Pd	1.8415921	-3.7036776	2.8242557
Pd	0.2390972	-4.8024770	4.5507378
Pd	3.6532868	-2.5790790	4.3069490
Pd	-1.6143362	1.7997195	5.3035735
Pd	-4.0552878	1.8526215	4.4072866
Pd	-0.6392605	4.0487966	4.4346328
Pd	-3.5399432	0.6041127	2.1179624
Pd	0.2879254	3.0867350	2.1076262
Pd	-2.2885276	2.8827894	2.7880356
C	11.1525484	0.7162914	0.2670158
C	11.1583023	-0.6475198	0.1542959
C	9.9312597	-1.4048183	0.0389131
C	9.9176574	-2.7965577	-0.0663386
C	8.7034243	-3.5404676	-0.1643575
C	8.6814620	-4.9516179	-0.2312428
C	7.4735355	-5.6825434	-0.2812320
C	7.4393368	-7.1089353	-0.2798730
C	6.2398604	-7.8228741	-0.2527191
C	6.1992078	-9.2675863	-0.1992660
C	5.0156096	-9.9485979	-0.1113482

C	3.7443933	-9.2595761	-0.0709149
C	2.5321991	-9.9374520	0.0691789
C	1.2832668	-9.2509467	0.1354989
C	0.0537668	-9.9242057	0.3096989
C	-1.1786395	-9.2364264	0.3859605
C	-2.4253124	-9.9145524	0.5400760
C	-3.6416971	-9.2313147	0.5845419
C	-4.9107408	-9.9137946	0.7095052
C	-6.0948096	-9.2284140	0.7259565
C	-6.1395076	-7.7865655	0.6191664
C	-7.3401821	-7.0756748	0.6102946
C	-7.3796391	-5.6543391	0.4922007
C	-8.5920290	-4.9301733	0.4676207
C	-8.6248795	-3.5236603	0.3457966
C	-9.8463824	-2.7857761	0.3210138
C	-9.8720508	-1.3948132	0.2103086
C	-11.1069127	-0.6412695	0.1952363
C	-11.1152686	0.7243177	0.1058588
C	-9.8884693	1.4864391	0.0249314
C	-9.8751143	2.8809524	-0.0397533
C	-8.6596810	3.6279740	-0.1020574
C	-8.6350291	5.0401904	-0.1367043
C	-7.4266984	5.7726346	-0.1740500
C	-7.3914831	7.1988442	-0.1742054
C	-4.9647196	10.0423181	-0.1207057
C	-6.1909588	7.9121586	-0.1759595
C	-6.1493459	9.3578146	-0.1536294
C	-2.4744498	10.0363750	-0.0325402
C	-3.6917869	9.3556533	-0.1041328
C	0.0118326	10.0313253	0.1207343
C	-1.2227103	9.3525628	0.0081692
C	2.4947019	10.0216346	0.3179245
C	1.2446722	9.3446239	0.1871887
C	4.9771909	10.0173381	0.5263907
C	6.1583679	9.3293869	0.5901951
C	3.7083413	9.3362687	0.3902481
C	6.2006001	7.8851453	0.5195491
C	7.3971836	7.1680562	0.5629938
C	7.4343884	5.7435525	0.4754192
C	8.6440361	5.0138062	0.4905008
C	8.6749652	3.6049071	0.3882528
C	9.8946607	2.8632462	0.3861638

C	9.9191314	1.4720654	0.2752915
C	8.6752651	0.7413356	0.1611583
C	8.6812137	-0.6753152	0.0423774
C	7.4501416	-1.3949862	-0.0729452
C	7.4531040	-2.8182912	-0.1780300
C	6.2216547	-3.5363874	-0.2795562
C	6.2205888	-4.9639983	-0.3093125
C	4.9863188	-5.6799794	-0.3173335
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C	3.7514336	-7.8154058	-0.1646851
C	2.5106731	-7.1031470	-0.1362458
C	1.2826231	-7.8108399	0.0276142
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C	-1.1826270	-7.7961972	0.2957859
C	-2.4174515	-7.0808730	0.3707204
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C	-2.4600527	7.2004849	-0.1473050
C	1.2474246	7.9018873	0.1254474
C	0.0121593	7.1971157	-0.0093429
C	3.7186191	7.8900631	0.3296852
C	4.9456802	7.1754862	0.3930582
C	2.4800305	7.1858991	0.2011760
C	4.9521042	5.7457013	0.3259310
C	6.1862180	5.0271382	0.3598350
C	6.1940480	3.6011511	0.2688005
C	7.4294127	2.8832992	0.2765651

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C	6.2031685	0.7425447	0.0571845
C	6.2087104	-0.6800586	-0.0650526
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C	-3.6667286	-3.5017751	0.2371336
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C	1.2427531	5.0519899	0.0315508
C	3.7219401	3.6062774	0.1463010
C	4.9575557	2.8876774	0.1628780
C	4.9653516	1.4614254	0.0644634
C	3.7373007	0.7497003	-0.0328336
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C	-2.4178666	-2.7819593	0.1913619
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C	-3.6749582	-0.6388195	0.0681404
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H	9.6317031	-5.4974587	-0.2169213
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H	-7.0435055	-9.7688402	0.8161809
H	5.0119108	-11.0429265	-0.0584611
H	9.5907915	5.5589261	0.5776337
H	10.8685093	-3.3418457	-0.0629489
H	7.1059580	9.8695400	0.6929206
H	-2.4227888	-11.0082216	0.6111655
H	-8.2868826	-7.6220287	0.6907897
H	0.0552927	-11.0174083	0.3873603

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200

Pd₂₁/pyridnic N support 1

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Pd 2.7664300 -1.1085506 3.1326668
Pd 2.0820339 -0.0302029 5.6220304
Pd 1.2916100 1.0172247 3.1608658
Pd 0.9555347 -2.3864062 4.6691573
Pd -0.4873341 -0.2347627 4.6741892
Pd 1.5481328 -3.5351962 2.3014523
Pd 0.3024498 -1.2268445 2.2437137
Pd 5.3955132 -0.9682763 2.2830455
Pd 4.6202254 0.1043908 4.6245380
Pd 3.7941792 1.1420341 2.1194160
Pd 3.1428960 2.2778942 4.5279634
Pd 4.1747329 -3.2648600 2.9471313
Pd 2.5916921 -4.4705301 4.6026261
Pd 5.9242749 -2.2143969 4.5838449
Pd 0.5936197 2.1118744 5.5918764
Pd -1.8987492 1.9740617 4.7095882
Pd 1.5271904 4.3420609 4.5261951
Pd -1.3676132 0.8257008 2.2977094
Pd 2.1965501 3.3305807 2.1246111
Pd -0.2541867 3.1105805 3.0835084
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C 11.1463444 -0.6601577 0.2371314
C 9.9210362 -1.4285591 0.2315608
C 9.9113594 -2.8247719 0.2763668
C 8.6982730 -3.5797837 0.2504918
C 8.6702457 -4.9938424 0.2955616
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C	6.1669819	9.3314045	-0.1969551
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C	6.2074572	7.8847568	-0.1910009
C	7.4022590	7.1633114	-0.1822707
C	7.4329844	5.7343065	-0.1459229
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C	9.8984249	1.4572501	0.1074939
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C	-3.7114629	-7.8554027	-0.0997407
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C	-4.9420724	5.7178308	0.2803344
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C	1.2365322	7.8909412	-0.0210930
C	0.0002690	7.1796412	0.0518777
C	3.7188994	7.8895110	-0.1457834
C	4.9467306	7.1748524	-0.1784898
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C	4.9517952	5.7422109	-0.1748460
C	6.1805484	5.0148817	-0.1468102
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C	-3.6993608	3.5724116	0.1995890
C	-3.7002821	5.0056970	0.2293817
C	0.0007569	5.7474086	0.0436222
C	-1.2335995	5.0227932	0.1182787
C	2.4765388	5.7561646	-0.1215241
C	3.7128845	5.0353713	-0.1628890
C	1.2362188	5.0534565	-0.0350607
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C	3.6494649	0.6845152	-0.0716423
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N	2.5509898	-1.4850003	-0.1848193
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H	2.4917199	11.1133877	-0.0471120
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H	2.4830195	-11.0709538	0.3116374
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H	-8.3458408	7.6875701	0.4217313
H	-7.1121575	9.8455162	0.4595123
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H	-12.0809590	1.2413276	0.1133018
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H	7.1100883	-9.8588883	0.4536283
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H	9.6193958	-5.5385719	0.3557586
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200

Pd₂₁/pyridinic N support 2

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Pd	-3.5029076	-2.4965238	4.4935732
Pd	-5.0329651	-0.3901539	4.7076363
Pd	-2.9943639	-3.5066016	1.9614044
Pd	-4.6659794	-1.4178553	2.2163397
Pd	0.8742558	-0.6360772	1.6380224
Pd	0.0080119	0.1855314	4.1578696
Pd	-1.0647522	1.1221753	1.8664752
Pd	-1.5363843	2.2518774	4.2576903
Pd	-0.3780968	-3.0820410	2.3725395
Pd	-1.7834148	-4.4682498	4.1254808
Pd	1.4521369	-1.9665771	3.8232894
Pd	-3.9522266	1.9934996	5.4899243
Pd	-6.4969593	1.7791504	4.8799190
Pd	-3.1547088	4.2748544	4.4118021
Pd	-6.1917575	0.8148294	2.4045569
Pd	-2.6963657	3.2740106	1.9312679
Pd	-5.0514729	3.0635511	3.1340409
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C	11.0545193	-0.6644945	0.6244010
C	9.8267432	-1.4235484	0.5408279
C	9.8159658	-2.8167200	0.4862414
C	8.6020089	-3.5603092	0.3954672
C	8.5798579	-4.9697949	0.3233690
C	7.3748306	-5.7000657	0.2244861
C	7.3464272	-7.1234133	0.1448625
C	6.1500179	-7.8351619	0.0530093
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201

Pd₂₁/pyrrolic N support

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Pd	3.3864225	-6.6384952	4.3198638
Pd	7.3660290	-5.2264822	2.3436028
Pd	4.8219665	-6.2949409	2.0362053

Pd	5.3413031	-1.2067993	1.9192050
Pd	3.9084865	-1.6666220	4.2553718
Pd	2.7878353	-2.0071298	1.8349427
Pd	1.5346265	-2.7371102	4.1506396
Pd	7.3155847	-2.6203673	2.9570028
Pd	8.0546853	-4.3570497	4.7454259
Pd	6.3432287	-0.6247759	4.3196915
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Pd	-0.8164791	-3.9286884	4.0417499
Pd	2.3079935	-7.2480803	1.8918488
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