

Supporting information for: What Does Graphitic Carbon Nitride Really Look Like?

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1 Additional Tables

Table S1: Relative energies (in kJ/mol per tecton) and the contribution of the dispersion corrections (in parenthesis). Note: (a) The thermal correction which needs to be added to ΔE in order to obtain the Gibbs free energy ΔG .

Species	$\Delta E_{\text{therm}}^a$	$\Delta E_{\text{B3LYP-D3}}$	$\Delta E_{\text{B3LYP-dDsC}}$	$\Delta E_{\text{PBE-dDsC}}$	$\Delta E_{\text{PBE-MBD}}$
1D	-4.2	+91 (+30)	+97 (+35)	+92 (+21)	+94 (+23)
2D	0	0	0	0	0
Fina	5.3	-92 (-112)	-96 (-116)	-81 (-90)	-68 (-77)
S1	5.3	-91 (-108)	-87 (-104)	-75 (-84)	-63 (-81)
Lotsch	4.9	-93 (-113)	-88 (-108)	-77 (-88)	-66 (-77)
S2	5.4	-94 (-112)	-95 (-114)	-79 (-89)	-65 (-85)

Table S2: Geometrical parameters of the investigated systems at the B3LYP-D* and PBE-dDsC level of theory and experiment. Lattice vectors are given in Å and angles in degrees.

Species	a/Å	b/Å	c/Å	$\alpha/^\circ$	$\beta/^\circ$	$\gamma/^\circ$
exp						
Fina	12.4	6.49	16.4	90.0	90.0	90.0
S1	16.4	12.4	3.3	90.0	98	90.0
Lotsch	12.4	16.7	3.31	90.0	92-115	90.0
S2	3.95	10.87	16.26	98.5	90.1	96.4
B3LYP-D*						
Fina	12.73	6.43	16.71	90.0	90.0	90.0
S1	16.76	12.73	4.73	90.0	43.2	90.0
Lotsch	12.71	16.74	4.69	90.0	136.7	90.0
S2	4.84	8.68	16.71	99.1	97.8	92.7
PBE-dDsC						
Fina	12.70	6.24	16.58	90.0	90.0	90.0
S1	16.66	12.71	4.66	90.0	42.7	90.0
Lotsch	12.67	16.61	4.61	90.0	137.4	90.0
S2	4.68	8.81	16.37	101.3	95.3	91.7

2 Coordinates

Here, the optimized structures are provided. In the first section, all structures are provided in POSCAR (VASP) format. In the second section, all structures are provided in .gui (Crystal14) format. In the last section, all structures are provided in .cif (Crystallographic) format.

2.1 Structures in POSCAR format

Fina, POSCAR format

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P2₁/a POSCAR format

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S1, POSCAR format

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0.2749080351888011      0.7323685072667985      0.0198218978089812
0.7749080351888011      0.7676314927332015      0.0198218978089812
0.7250919648111989      0.2676314927332015      0.9801781021910188
0.5746459039051004      0.1338506925651970      0.0136364323913227
0.9253540960949209      0.6338506925651970      0.9863635676086773
0.4253540960948996      0.8661493074348030      0.9863635676086773
0.0746459039050791      0.3661493074348030      0.0136364323913227
0.1658875851692017      0.0671957391464773      0.0144081619721277
0.3341124148307983      0.5671957391464986      0.9855918380278723
0.8341124148307983      0.9328042608535227      0.9855918380278723
0.6658875851692017      0.4328042608535014      0.0144081619721277
0.2993310188353036      0.0844841725859808      0.0406297093320802
0.2006689811646964      0.5844841725860022      0.9593702906679198
0.7006689811646964      0.9155158274140192      0.9593702906679198
0.7993310188353036      0.4155158274139978      0.0406297093320802
0.2772945602997012      0.4001118637130006      0.9770854508954088
0.2227054397002988      0.9001118637130006      0.0229145491045912
0.7227054397002988      0.5998881362869994      0.0229145491045912
0.7772945602997012      0.0998881362869994      0.9770854508954088
0.2862888236404970      0.2974134118135012      0.9861806082765483
0.2137111763595030      0.7974134118135012      0.0138193917234517
0.7137111763595030      0.7025865881864988      0.0138193917234517
0.7862888236404970      0.2025865881864988      0.9861806082765483
0.3423998540773994      0.4592016468467008      0.9801661753024220
0.1576001459226006      0.9592016468466582      0.0198338246975780
0.6576001459226006      0.5407983531532992      0.0198338246975780
0.8423998540773994      0.0407983531533418      0.9801661753024220
0.5031124963715996      0.1763114355693034      0.0114818780667605
0.9968875036284359      0.6763114355693034      0.9885181219332395
0.4968875036284004      0.8236885644306966      0.9885181219332395
0.0031124963715641      0.3236885644306966      0.0114818780667605
0.4281283809837007      0.3238540811411994      0.9941608191700482
0.0718716190163278      0.8238540811411994      0.0058391808299518
0.5718716190162993      0.6761459188588006      0.0058391808299589
0.9281283809836722      0.1761459188588006      0.9941608191700482
0.3663535262462005      0.1475923778239974      0.0225111723702298
0.1336464737537995      0.6475923778239974      0.9774888276297702
0.6336464737537995      0.8524076221760026      0.9774888276297702
0.8663535262462005      0.3524076221760026      0.0225111723702298
0.2336465840079995      0.1285466362091015      0.0134518729248825
0.2663534159920005      0.6285466362091015      0.9865481270751175
0.7663534159920005      0.8714533637908985      0.9865481270751175
0.7336465840079995      0.3714533637908985      0.0134518729248825
0.6272506581366031      0.1797448095452978      0.0009505595977544
0.8727493418633969      0.6797448095452978      0.9990494404022456
0.3727493418633969      0.8202551904547022      0.9990494404022456
0.1272506581366031      0.3202551904547022      0.0009505595977544

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0.5791588743391003	0.0539661805157579	0.0118582640761176
0.9208411256608784	0.5539661805158005	0.9881417359238824
0.4208411256608997	0.9460338194842421	0.9881417359238824
0.0791588743391216	0.4460338194841995	0.0118582640761176
0.1151464850046011	0.1061299086168006	0.0021299523181852
0.3848535149953989	0.6061299086168006	0.9978700476818148
0.8848535149953989	0.8938700913831994	0.9978700476818148
0.6151464850046011	0.3938700913831994	0.0021299523181852

S2, POSCAR format

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1.0000000000000000
  4.7247995723700003    -0.3300690995270000    -0.1707838361170000
  0.1209360489830000      8.9798520228500003    -0.3397386322170000
 -1.1417356344400000    -2.4690329267000002    16.2825099185000006
N      C      H
36      24      12
Direct
0.2767855142498021    0.4271092770874034    0.4152831334688969
0.7232144857501979    0.5728907229125966    0.5847168665311031
0.0551679054991325    0.0722316688895717    0.9166126195967976
0.9448320945008675    0.9277683311104283    0.0833873804032024
0.0651033591076100    0.2839976800600965    0.4999810231419985
0.9348966408923900    0.7160023199399035    0.5000189768580015
0.4291884346889034    0.2184110787980984    0.0009167036030817
0.5708115653110966    0.7815889212019016    0.9990832963969183
0.6519498023908028    0.1129336684446969    0.4423400931465977
0.3480501976091972    0.8870663315553031    0.5576599068534023
0.7268020918212983    0.3895226466142034    0.9421526009903189
0.2731979081787017    0.6104773533857966    0.0578473990096811
0.8739303177371980    0.2608508117448025    0.3606133943586016
0.1260696822628020    0.7391491882551975    0.6393866056413984
0.3416914843670966    0.2422509862077007    0.8608180800278973
0.6583085156329034    0.7577490137922993    0.1391819199721027
0.6968237841207028    0.2356346820689978    0.2200992442685035
0.3031762158792972    0.7643653179310022    0.7799007557314965
0.2494215865346021    0.2615206739040019    0.7205408251298024
0.7505784134653979    0.7384793260959981    0.2794591748701976
0.8391798713037986    0.1322010659499000    0.5760140167904026
0.1608201286962014    0.8677989340501000    0.4239859832095974
0.8108423538867982    0.3669227008963034    0.0769749815879806
0.1891576461132018    0.6330772991036966    0.9230250184120194
0.3077826668572001    0.0726910853789988    0.1665253299488967
0.6922173331427999    0.9273089146210012    0.8334746700511033
0.5241907714138989    0.4289775567059024    0.6672255410745009
0.4758092285861011    0.5710224432940976    0.3327744589254991
0.4658758533973000    0.0959511649821181    0.3073310141675023
0.5341241466027000    0.9040488350178819    0.6926689858324977
0.6342438391716030    0.4119924217963984    0.8062791189331975
0.3657561608283970    0.5880075782036016    0.1937208810668025
0.0806324484922172    0.4050642477386006    0.2738187466400035
0.9193675515077828    0.5949357522613994    0.7261812533599965
0.9711200519970831    0.0920272956109400    0.7735187925451967
0.0288799480029169    0.9079727043890600    0.2264812074548033
0.8844967202671015    0.3013327627128035    0.2836613560063981
0.1155032797328985    0.6986672372871965    0.7163386439936019
0.1842121558765015    0.1981717778404999    0.7836310933890971
0.8157878441234985    0.8018282221595001    0.2163689066109029
0.2646072521262965    0.4630908215769978    0.3400561565535014
0.7353927478737035    0.5369091784230022    0.6599438434464986
0.9179050727622808    0.0355781493912204    0.8404170847412971
0.0820949272377192    0.9644218506087796    0.1595829152587029
0.8540167071381006    0.1778578067325967    0.5050124407566017
0.1459832928618994    0.8221421932674033    0.4949875592433983
0.6519597447441967    0.3232064790323008    0.0055942078015079
0.3480402552558033    0.6767935209676992    0.9944057921984921
0.0768312876742101    0.3256122151711978    0.4276896984808971
0.9231687123257899    0.6743877848288022    0.5723103015191029
0.2743592826981001    0.1763085908928019    0.9286188837194231
0.7256407173018999    0.8236914091071981    0.0713811162805769
0.6613567447967981    0.1543529744099033    0.3708135111342017
0.3386432552032019    0.8456470255900967    0.6291864888657983
0.5710546554471989    0.3505814872503024    0.8704294004433990
0.4289453445528011    0.6494185127496976    0.1295705995566010
0.4947198956496024    0.1359684136405974    0.2352231321087999
0.5052801043503976    0.8640315863594026    0.7647768678912001
0.4718625876494968    0.3666295417890026    0.7352762888506987
0.5281374123505032    0.6333704582109974    0.2647237111493013
0.9851787673907921    0.1744191025337969    0.6258687545632995
0.0148212326092079    0.8255808974662031    0.3741312454367005
0.7723000981129005    0.3191490157695966    0.1268422102323967

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0.2276999018870995	0.6808509842304034	0.8731577897676033
0.6802065089045968	0.0526987166018031	0.5791215303831976
0.3197934910954032	0.9473012833981969	0.4208784696168024
0.9832656155695005	0.4412694021708035	0.0794645320051117
0.0167343844304995	0.5587305978291965	0.9205354679948883
0.3324734676979020	0.1136011313950007	0.1133874480904993
0.6675265323020980	0.8863988686049993	0.8866125519095007
0.3966941115813967	0.3853407757070997	0.6134360669896992
0.6033058884186033	0.6146592242929003	0.3865639330103008

2D, POSCAR format

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Melon_2D_POSCAR_20A_BOX_631Gdp_with_spec
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-0.0000000000000000    16.7956456289000009    0.000
0.0000000000000000    0.0000000000000000    20.000
N      C      H
36      24      12
Direct
0.4277944259999984    0.41484907200000026    0.9999139648871989
0.9277944255999984    0.08515092849999992    0.0000860351128011
0.5722055740000016    0.58515092799999974    0.0000860351128011
0.0722055744000016    0.91484907150000008    0.9999139648871989
0.2830928970000031    0.49934047299999966    0.9998638540520020
0.7830928970000031    0.0006595274180015    0.0001361459479980
0.7169071029999969    0.50065952700000034    0.0001361459479980
0.2169071029999969    0.9993404725840023    0.9998638540520020
0.1083179920000035    0.4420461340000017    0.9998881472190035
0.6083179920000035    0.05795386629999965    0.0001118527809965
0.8916820079999965    0.5579538659999983    0.0001118527809965
0.3916820079999965    0.94204613370000035    0.9998881472190035
0.2574031739999967    0.3599714079999998    0.9998954550190007
0.7574031739999967    0.14002859200000002    0.0001045449809993
0.7425968260000033    0.64002859200000002    0.0001045449809993
0.2425968260000033    0.8599714079999998    0.9998954550190007
0.2348598040000027    0.22059290499999966    0.9999255585049980
0.7348598040000027    0.27940709500000034    0.0000744414950020
0.7651401959999973    0.77940709500000034    0.0000744414950020
0.2651401959999973    0.72059290499999966    0.9999255585049980
0.1331077780000030    0.57611863000000034    0.9998116310559979
0.6331077780000030    0.92388136990000019    0.0001883689440021
0.8668922219999970    0.42388136999999966    0.0001883689440021
0.3668922219999970    0.07611863009999981    0.9998116310559979
0.0692568282999986    0.1677587100000011    0.9999971001389270
0.5692568280000003    0.33224128999999989    0.0000028998610730
0.9307431717000014    0.83224128999999989    0.0000028998610730
0.4307431719999997    0.6677587100000011    0.9999971001389270
0.0856430814000007    0.30652240999999995    0.9999508521096985
0.5856430810000006    0.19347759000000005    0.0000491478903015
0.9143569185999993    0.69347759000000005    0.0000491478903015
0.4143569189999994    0.80652240999999995    0.9999508521096985
0.4022794270000034    0.27321282199999979    0.9999047065106978
0.9022794270999981    0.22678717800000021    0.0000952934893022
0.5977205729999966    0.72678717800000021    0.0000952934893022
0.0977205729000019    0.77321282199999979    0.9999047065106978
0.2992003960000034    0.28320646699999994    0.9999132048519002
0.7992003960000034    0.21679353300000006    0.0000867951480998
0.7007996039999966    0.71679353300000006    0.0000867951480998
0.2007996039999966    0.78320646699999994    0.9999132048519002
0.4608436359999999    0.33925101399999985    0.9999480514647985
0.9608436358000034    0.16074898600000015    0.0000519485352015
0.5391563640000001    0.66074898600000015    0.0000519485352015
0.0391563641999966    0.8392510139999985    0.9999480514647985
0.1761774240000022    0.50479273300000022    0.9998557197479983
0.6761774240000022    0.9952072669300023    0.0001442802520017
0.8238225759999978    0.4952072669999978    0.0001442802520017
0.3238225759999978    0.0047927330699977    0.9998557197479983
0.3244099700000035    0.42712191500000007    0.9998804481249977
0.8244409970000035    0.07287808520000028    0.0001195518750023
0.675590029999965    0.5728780849999993    0.0001195518750023
0.175590029999965    0.9271219147999972    0.9998804481249977
0.1482879060000002    0.37019833400000012    0.9999085186376035
0.6482879060000002    0.1298016659999988    0.0000914813623965
0.8517120939999998    0.6298016659999988    0.0000914813623965
0.3517120939999998    0.87019833400000012    0.9999085186376035
0.1306728039999996    0.2355217539999970    0.9999607288438028
0.6306728039999996    0.26447824600000030    0.0000392711561972
0.8693271960000004    0.76447824600000030    0.0000392711561972
0.3693271960000004    0.7355217539999970    0.9999607288438028
0.1788118600000033    0.62619469900000027    0.9997961385420027
0.6788118600000033    0.87380530200000009    0.0002038614579973
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0.8211881399999967 0.3738053009999973 0.0002038614579973
0.3211881399999967 0.1261946990000027 0.9997961385420027
0.0531356185000007 0.5800141929999967 0.9998663121710010
0.5531356190000025 0.9199858065000015 0.0001336878289990
0.9468643814999993 0.4199858070000033 0.0001336878289990
0.4468643809999975 0.0800141934999985 0.9998663121710010
0.1086396620000016 0.1145546629999998 0.9999757606757029
0.6086396620000016 0.3854453370000002 0.0000242393242971
0.8913603379999984 0.8854453370000002 0.0000242393242971
0.3913603379999984 0.6145546629999998 0.9999757606757029

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1D, POSCAR format

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Melon_1D_POSCAR_20A_BOX_631Gdp_with_spec
1.000000000000000
  13.7957847100999995 0.0000000000000000 0.0000000000000000
    0.0000000000000000 20.0000000000000000 0.0000000000000000
    0.0000000000000000 0.0000000000000000 20.0000000000000000
  N      C      H
  18     12      6
Direct
0.1667807669999988 0.9678681898000008 0.0469277532000021
0.0825875664000009 0.8712281079999968 0.0115274149000015
0.9959074685899978 0.9694450580999998 0.0466805171000004
0.3376540530000014 0.9694445772000009 0.0466806883000004
0.2509735559999982 0.8712277910000026 0.0115277144999979
0.0792115702000018 0.0613448450000007 0.0867008641000027
0.2543504799999994 0.0613442606000021 0.0867016433000032
0.1667814990000025 0.1497089209999984 0.1263192890000013
0.4167803779999986 0.8769248500000018 0.0040541151600024
0.4959076569999965 0.9692073833000023 0.9609177844000030
0.6667807560000014 0.9676258876000006 0.9606714813999986
0.5825872770000018 0.8711861399999989 0.9966138712499983
0.8376537819999967 0.9692076376000003 0.9609204365999986
0.7509731820000027 0.8711861829999989 0.9966150484999972
0.5792114959999992 0.0608871091000012 0.9203960992999995
0.7543505740000001 0.0608875276999967 0.9203977008999971
0.6667811209999996 0.1490314130000030 0.8802910530000005
0.9167801724999975 0.8769247769999993 0.0040563740500019
0.0785383967999991 0.0006712217319986 0.0603126942000003
0.1667805900000019 0.9014543063000033 0.0235531566000020
0.0027837594800033 0.9083325836000000 0.0209522382000031
0.2550232549999976 0.0006709770350000 0.0603128122999976
0.3307773940000018 0.9083323983999989 0.0209516939999972
0.1667810829999965 0.0883203595000026 0.0988443601999975
0.5027837989999995 0.9082384008999966 0.9869845608999981
0.5785383979999992 0.0003565362329994 0.9471105894999994
0.6667804450000006 0.9013441115999967 0.9844182271000008
0.7550233190000029 0.0003566922639990 0.9471117877999973
0.8307769999999977 0.9082384712000007 0.9869864393999990
0.6667811129999990 0.0877977004000030 0.9081093958999986
0.9167807238999970 0.8263798489999985 0.0041944329599986
0.1031545359999981 0.1724771769999975 0.1356503860000018
0.2304088070000034 0.1724760139999972 0.1356518540000025
0.4167798929999975 0.8263799220000010 0.0041922542200012
0.7304081790000012 0.1717467120000009 0.8708323899999968
0.6031538909999981 0.1717459110000021 0.8708308790000032

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2.2 Structures in .gui format

Fina, .gui format

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3 1 2 E -5.7833181922602E+03 DE-1.6E-08( 28)
0.127337335437E+02 0.776635721440E-15 0.254837198546E-02
-0.130205882973E-17 0.642852794503E+01 0.785097899967E-19
0.332504561112E-02 0.101919047805E-14 0.167106790624E+02
4
0.100000000000E+01 0.000000000000E+00 -0.123259516441E-31
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
-0.100000000000E+01 0.000000000000E+00 0.123259516441E-31

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-0.122464679915E-15	0.100000000000E+01	-0.122464679915E-15
0.000000000000E+00	0.000000000000E+00	-0.100000000000E+01
-0.651029414865E-18	0.321426397251E+01	0.392548949984E-19
-0.100000000000E+01	0.000000000000E+00	0.123259516441E-31
0.000000000000E+00	-0.100000000000E+01	0.000000000000E+00
0.000000000000E+00	0.000000000000E+00	-0.100000000000E+01
0.000000000000E+00	0.000000000000E+00	0.000000000000E+00
0.100000000000E+01	0.000000000000E+00	-0.123259516441E-31
0.122464679915E-15	-0.100000000000E+01	0.122464679915E-15
0.000000000000E+00	0.000000000000E+00	0.100000000000E+01
-0.651029414865E-18	0.321426397251E+01	0.392548949984E-19
72		
6	3.057997331968	1.607131986257
6	1.853020016525	1.607131986257
6	-4.509512648714	1.607131986257
6	-3.305614199772	1.607131986257
6	5.121301967258	1.607131986257
6	-0.201419040267	1.607131986257
6	6.169963658174	1.607131986257
6	-1.244585185908	1.607131986257
6	1.496704062899	1.607131986257
6	3.412963296025	1.607131986257
6	-2.961200866613	1.607131986257
6	-4.875676120004	1.607131986257
6	3.384054852528	1.607131986257
6	1.530455761679	1.607131986257
6	-4.838873373538	1.607131986257
6	-2.982966452094	1.607131986257
6	1.141152210303	1.607131986257
6	3.769469296675	1.607131986257
6	-2.600009170685	1.607131986257
6	-5.224101491768	1.607131986257
6	0.912755449709	1.607131986257
6	4.001915771098	1.607131986257
6	-2.363074521774	1.607131986257
6	-5.452129053294	1.607131986257
1	1.530384606311	1.607131986257
1	3.371278791192	1.607131986257
1	-3.011565480755	1.607131986257
1	-4.840474517706	1.607131986257
1	-0.068283305472	1.607131986257
1	4.980875506586	1.607131986257
1	-1.399560353359	1.607131986257
1	6.296780779176	1.607131986257
1	0.629033070086	1.607131986257
1	4.282728050913	1.607131986257
1	-2.083967702497	1.607131986257
1	-5.732037369061	1.607131986257
7	4.697743073662	1.607131986257
7	0.216496540760	1.607131986257
7	-6.150602683033	1.607131986257
7	-1.669524275571	1.607131986257
7	2.858065298090	1.607131986257
7	2.055917516309	1.607131986257
7	-4.317922276689	1.607131986257
7	-3.509413654851	1.607131986257
7	0.634140397127	1.607131986257
7	4.276383115130	1.607131986257
7	-2.094388070909	1.607131986257
7	-5.734539430600	1.607131986257
7	2.528724874346	1.607131986257
7	2.382874423756	1.607131986257
7	-3.983997383196	1.607131986257
7	-3.835784886664	1.607131986257
7	2.243112422525	1.607131986257
7	2.678381764579	1.607131986257
7	-3.684651827484	1.607131986257
7	-4.126518632935	1.607131986257
7	0.947634073851	1.607131986257
7	3.960676101331	1.607131986257
7	-2.419026870990	1.607131986257
7	-5.419329239058	1.607131986257
7	0.130664456636	1.607131986257
7	4.785840886241	1.607131986257
7	-1.578617401275	1.607131986257
7	-6.235570471596	1.607131986257
7	0.343167936258	1.607131986257
7	4.573562998633	1.607131986257
7	-1.794262885060	1.607131986257
7	-6.023342745771	1.607131986257
7	4.371533776281	1.607131986257
7	0.545207976053	1.607131986257
7	-5.820673835238	1.607131986257
7	-1.993753590009	1.607131986257
		-6.303404523503
		2.065990969036
		3.182438066877
		-5.190711892751
		-7.240881604316
		1.136987638762
		4.118284644187
		-4.252150493662
		6.694962055120
		-1.650763908765
		6.907236667026
		-1.469416415994
		7.996251447563
		-0.341238846610
		5.592610433864
		-2.780284482789
		-7.759000461391
		0.603845925145
		4.647562269468
		-3.729434153034
		-5.499727566820
		2.861062215101
		2.392015374961
		-5.993044836874
		4.660198740480
		-3.691273170773
		-7.760101215975
		0.567516167068
		5.433335251077
		-2.910366067083
		-8.528577636552
		-0.206112035875
		-3.471980785814
		4.895920610999
		0.365680825900
		-8.015053670383
		-8.508980589624
		-0.136418283765
		5.387700974463
		-2.979130959379
		6.783084690256
		-1.558592071001
		6.812786013800
		-1.561968409348
		7.747015492117
		-0.601394269065
		5.860369309563
		-2.524628684504
		-7.588564315073
		0.779864434082
		4.472318492726
		-3.901863546333
		-5.248076068953
		3.117467277452
		2.134217718777
		-6.239933007431
		5.496887075608
		-2.854383268570
		-8.597696384328
		-0.273195230185
		-4.364728272727
		4.002044306546
		1.254943133303
		-7.124653521813
		-6.690517059716
		1.670816748212
		3.587933457031
		-4.795818387979
		-6.130427861806
		2.241835497802
		3.010456506661
		-5.358149958606

P2₁/a, .gui format

```
3 1 2 E -2.8916590116591E+03 DE 1.0E-10( 71)
0.126979868482E+02 0.690566271567E-15 -0.468715797446E+00
-0.120367831600E-15 0.167371449136E+02 -0.353611766341E-16
-0.329236477339E+01 0.290781543338E-15 0.334032352102E+01
4
0.100000000000E+01 0.000000000000E+00 -0.222044604925E-15
0.123259516441E-31 0.100000000000E+01 0.123259516441E-31
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
-0.100000000000E+01 0.000000000000E+00 0.222044604925E-15
-0.122464679915E-15 0.100000000000E+01 -0.298506990459E-15
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01
0.634899342412E+01 0.836857245676E+01 -0.234357898723E+00
-0.100000000000E+01 0.000000000000E+00 0.222044604925E-15
-0.123259516441E-31 -0.100000000000E+01 -0.123259516441E-31
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.100000000000E+01 0.000000000000E+00 -0.222044604925E-15
0.122464679915E-15 -0.100000000000E+01 0.298506990459E-15
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.634899342412E+01 0.836857245676E+01 -0.234357898723E+00
18
6 0.521665369000 4.750502748258 3.306273209870
6 2.578561668334 5.690189463963 3.239583695147
6 2.245381051536 -8.275601547364 -0.034888707435
6 0.838451626440 7.164056351287 3.247407233266
6 1.898917093427 6.205029740639 0.033947985230
6 1.678801547643 3.943628266459 0.070099895064
7 2.157360790131 6.956521618553 3.202100193248
7 0.311611930246 -8.363354001611 3.234560421537
7 1.385049588241 7.408801562068 0.038414745832
7 3.282716367986 6.036488811406 -0.035960751192
7 3.001570209113 3.697427202764 -0.003756706919
7 1.688849054233 -7.079659440515 -0.045724329541
7 0.902062134564 2.801769353712 0.082545913261
7 1.104428774512 5.134753649273 0.119665586402
7 1.834883486644 4.580250263324 3.289623922487
1 2.265112359369 -6.237664803828 -0.118888990046
1 0.671917952906 -7.024172965055 0.009530475265
1 1.409993182503 1.911091045191 0.082423092108
```

S1, .gui format

```
3 1 2 E -2.8916560987187E+03 DE 8.6E-11( 71)
0.167572417171E+02 0.104931238299E-14 0.377158690172E+00
0.214996594033E-16 0.127336342423E+02 0.179189746922E-16
0.337663121126E+01 0.294738444724E-15 0.331878052147E+01
4
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.123259516441E-31
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
-0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
-0.122464679915E-15 0.100000000000E+01 -0.507265313324E-16
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01
0.837862085854E+01 0.636681712114E+01 0.188579345085E+00
-0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 -0.100000000000E+01 -0.123259516441E-31
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.122464679915E-15 -0.100000000000E+01 0.507265313324E-16
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.837862085854E+01 0.636681712114E+01 0.188579345085E+00
18
6 1.373462709733 3.789161887718 -3.256851996808
6 2.295698466527 5.849044150154 -3.255657352212
6 -4.912997760158 2.242957332803 3.169374799393
6 3.777485694027 4.123469311122 -3.177178704584
6 2.835884674998 1.879615758440 -3.105593088666
6 0.581433364005 1.639188634595 -3.185949129453
7 3.568723522324 5.433737745899 -3.225496637806
7 4.997861562051 3.602539545942 -3.124357001620
7 4.045662863338 1.375933403295 -3.058545815289
7 2.660425310947 3.264546659161 -3.181513647372
7 0.326740637349 2.961655722479 -3.300205604089
7 -3.708135165692 1.699999756316 3.203430355043
7 2.825726443085 0.857737851273 0.110418194031
7 1.773432500153 1.077096199934 -3.070237868739
```

7	1.193530593011	5.097337335111	-3.290193377398
1	-2.868202618136	2.282462548982	3.181487430844
1	-3.641242635243	0.682016675924	3.198848197734
1	1.933764853731	1.353309557100	0.050304470639

S2, .gui format

```

3 1 1 E -2.8916593606854E+03 DE 1.0E-10( 73)
0.481848877294E+01 -0.313144365534E+00 -0.272739127308E+00
0.145782279636E+00 0.867913772870E+01 -0.230330572336E+00
-0.149404169984E+01 -0.217497080094E+01 0.164965529405E+02
2
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
-0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 -0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
36
6 -0.948432057984 2.055743182214 4.645432187921
6 1.251442368914 2.110396328899 -3.666838776254
6 0.824227214177 3.216872164150 5.433623633766
6 -0.128716752061 0.645919803223 -2.624617640009
6 -1.429902980462 0.497997531787 8.325654945406
6 -1.626102153994 2.887158851459 0.109237706786
6 -0.225201138548 1.886530960385 6.959931212699
6 1.475156803020 1.571673193680 -1.299795385337
6 -2.170007994049 0.657833518810 6.172905655032
6 -1.814978085334 3.446422849480 -2.101814747493
6 2.033455304321 0.545482671895 3.719144725267
6 -2.088011196588 3.905928777469 -4.307890105294
1 0.516206273873 2.328371522637 -6.209975959042
1 -1.233808001975 2.565107876841 2.082417195118
1 -0.898589631779 1.471972870697 -6.876335647488
1 -0.135246057843 3.664431523482 1.214174263485
1 1.425335550723 0.673446135507 1.761729897350
1 -2.411078204521 -4.326388682676 -6.070639641495
7 0.765027324061 2.738249125051 6.680391431049
7 0.429789711929 0.751963889195 -1.417238129046
7 -0.390346992406 1.364712069822 8.162277303594
7 2.118433948462 1.735796220842 -0.158893279683
7 2.496077645296 -0.174784967688 7.090028134422
7 -1.167897992408 3.582517882635 -0.969568621836
7 -1.114936814990 1.536521808609 5.924072899829
7 1.901589230097 2.279415814932 -2.447900055920
7 -1.774100192560 1.688551683851 3.666577312478
7 1.667846585203 2.777951190487 -4.739445901623
7 -0.115129533168 2.117667136715 -6.987231164613
7 -0.963830703902 3.070376315644 1.234350653109
7 1.219887272791 0.209926449930 2.654430164087
7 -1.871688376928 -4.100217762743 -5.229229381279
7 1.788385374393 0.047209503677 4.920257773615
7 -1.409340273325 4.101655536410 -3.189762695087
7 0.026545759426 2.916550354805 4.405017221449
7 0.228598493178 1.271034577035 -3.751955850912

```

2D, .gui format

```

2 1 2 E -2.8915892342465E+03 DE 1.1E-10( 67)
0.127325346371E+02 0.779642889420E-15 0.000000000000E+00
-0.502747107234E-17 0.167944365802E+02 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.500000000000E+03
4
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.100000000000E+01 0.000000000000E+00 -0.122464679915E-15
0.122464679915E-15 -0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01
0.636626731856E+01 0.839721829010E+01 0.000000000000E+00
-0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 -0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 -0.100000000000E+01

```

```

0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
-0.100000000000E+01 0.000000000000E+00 0.122464679915E-15
-0.122464679915E-15 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.636626731856E+01 0.839721829010E+01 0.000000000000E+00
18
6 3.809501911592 4.756387326080 -0.001124276182
6 5.867611093156 5.697759553710 -0.000850153475
6 2.242874895853 -8.316425614532 -0.001569281921
6 4.130750265174 7.173594493673 -0.001338641653
6 1.887940944680 6.217303996404 -0.000914765531
6 1.663771053819 3.955272344272 -0.000418670650
7 5.446715853918 6.967434822135 -0.001171273440
7 3.604237392771 8.386523468794 -0.001607534897
7 1.379030565788 7.424035035418 -0.001076916020
7 3.277243121007 6.045632666798 -0.001169857008
7 2.990304932981 3.704668095038 -0.000959040903
7 1.694144383358 -7.118639646038 -0.001938671289
7 0.881738149920 2.817175740328 0.000181535975
7 1.090351960995 5.147805801682 -0.000387466893
7 5.121941864305 4.588582922793 -0.001110657324
1 2.275275173564 -6.277054172264 -0.001909039610
1 0.675835163141 -7.053838166707 -0.001335436379
1 1.383186083433 1.923569341726 -0.000137111132

```

1D, .gui format

```

1 1 1 E -1.4457186125671E+03 DE 1.3E-10( 59)
0.137948836966E+02 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.500000000000E+03 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.500000000000E+03
1
0.100000000000E+01 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
36
6 1.083272170075 0.014019798038 1.211821559755
6 2.300718157654 -1.968670519954 0.472370367668
6 0.038286029435 -1.830839648319 0.419850643605
6 3.518131938515 0.014064245650 1.211754678801
6 4.563148150377 -1.830793393405 0.419818074031
6 2.300691678914 1.763657385823 1.989682568914
6 -6.859140945050 -1.832685352773 -0.261125929106
6 -5.814131299707 0.007806170251 -1.063160261901
6 -4.596716337180 -1.970883430744 -0.313014293415
6 -3.379273436020 0.007778145502 -1.063190778052
6 -2.334289892213 -1.832722999639 -0.261144588087
6 -4.596692501329 1.753125284955 -1.850631052399
1 -1.148005991519 -3.469671152746 0.083869334178
1 1.422899758283 3.443073516669 2.734043803166
1 3.178464952458 3.443118282402 2.733963803887
1 5.749454687424 -3.469625432404 0.083896321705
1 -3.718898339344 3.428309303175 -2.604467845378
1 -5.474467976781 3.428337112263 -2.604427018878
7 2.300706847501 -0.641462653449 0.942869841381
7 1.139259528458 -2.572735709149 0.230798493386
7 -0.056678075694 -0.609295181765 0.936125446631
7 4.658090217691 -0.609223299957 0.936034172773
7 3.462186728956 -2.572711002362 0.230780400882
7 1.092583689619 1.225567677570 1.743864739308
7 3.508805109129 1.225625878327 1.743766696111
7 2.300685329669 2.988269832191 2.546031266135
7 5.749450756994 -2.458739205170 0.081092908606
7 6.840797049880 -0.613959361692 -0.784022162110
7 -4.596706434265 -0.646260040804 -0.790743630975
7 -5.758183380603 -2.573581160622 -0.068090083490
7 -2.239324797201 -0.614010501785 -0.784070285916
7 -3.435257121491 -2.573601060455 -0.068101326470
7 -5.804805378366 1.216458052684 -1.601751608091
7 -3.388584930468 1.216420361611 -1.601803451344
7 -4.596685864693 2.97462522432 -2.413780134028
7 -1.148005243138 -2.458785162347 0.081089328716

```

2.3 Structures in .cif format

Fina, .cif format

```
# CIF file
# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA

data_findsym-output

_symmetry_space_group_name_H-M 'P 1 21/m 1'
_symmetry_Int_Tables_number 11

_cell_length_a      12.73400
_cell_length_b      6.42900
_cell_length_c      16.71100
_cell_angle_alpha   90.00000
_cell_angle_beta    90.0
_cell_angle_gamma   90.00000

loop_
_space_group_symop_operation_xyz
x,y,z
-x,y+1/2,-z
-x,-y,-z
x,-y+1/2,z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1  N  -0.36905  0.25000  -0.49075  1.00000
N2  N  -0.01700  0.25000  0.00817  1.00000
N3  N   0.48310  0.25000  -0.32248  1.00000
N4  N   0.13106  0.25000  0.17826  1.00000
N5  N  -0.22434  0.25000  -0.40588  1.00000
N6  N  -0.16148  0.25000  0.09329  1.00000
N7  N   0.33920  0.25000  -0.40774  1.00000
N8  N   0.27558  0.25000  0.09343  1.00000
N9  N  -0.04968  0.25000  -0.46359  1.00000
N10 N  -0.33584  0.25000  0.03604  1.00000
N11 N   0.16457  0.25000  -0.35072  1.00000
N12 N   0.45030  0.25000  0.15101  1.00000
N13 N  -0.19870  0.25000  0.45414  1.00000
N14 N  -0.18712  0.25000  -0.04664  1.00000
N15 N   0.31294  0.25000  -0.26768  1.00000
N16 N   0.30117  0.25000  0.23345  1.00000
N17 N  -0.17624  0.25000  0.31408  1.00000
N18 N  -0.21029  0.25000  -0.18652  1.00000
N19 N   0.28939  0.25000  -0.12776  1.00000
N20 N   0.32396  0.25000  0.37336  1.00000
N21 N  -0.07433  0.25000  -0.32893  1.00000
N22 N  -0.31108  0.25000  0.17086  1.00000
N23 N   0.18984  0.25000  -0.48553  1.00000
N24 N   0.42558  0.25000  0.01628  1.00000
N25 N  -0.01033  0.25000  0.26120  1.00000
N26 N  -0.37578  0.25000  -0.23943  1.00000
N27 N   0.12399  0.25000  -0.07512  1.00000
N28 N   0.48958  0.25000  0.42628  1.00000
N29 N  -0.02705  0.25000  0.40038  1.00000
N30 N  -0.35914  0.25000  -0.09993  1.00000
N31 N   0.14096  0.25000  -0.21473  1.00000
N32 N   0.47295  0.25000  0.28692  1.00000
N33 N  -0.34340  0.25000  0.36691  1.00000
N34 N  -0.04278  0.25000  -0.13415  1.00000
N35 N   0.45715  0.25000  -0.18022  1.00000
N36 N   0.15649  0.25000  0.32062  1.00000
C1  C  -0.24025  0.25000  0.37725  1.00000
C2  C  -0.14549  0.25000  -0.12361  1.00000
C3  C   0.35419  0.25000  -0.19050  1.00000
C4  C   0.25951  0.25000  0.31058  1.00000
C5  C  -0.40230  0.25000  0.43337  1.00000
C6  C   0.01584  0.25000  -0.06804  1.00000
C7  C  -0.48447  0.25000  -0.24637  1.00000
C8  C   0.09767  0.25000  0.25444  1.00000
C9  C  -0.11743  0.25000  -0.40062  1.00000
C10 C  -0.26805  0.25000  0.09883  1.00000
C11 C   0.23266  0.25000  -0.41338  1.00000
C12 C   0.38287  0.25000  0.08787  1.00000
C13 C  -0.26563  0.25000  -0.47847  1.00000
C14 C  -0.12019  0.25000  0.02044  1.00000
```

C15	C	0.38009	0.25000	-0.33473	1.00000
C16	C	0.23421	0.25000	0.16634	1.00000
C17	C	-0.08974	0.25000	0.46433	1.00000
C18	C	-0.29601	0.25000	-0.03609	1.00000
C19	C	0.20425	0.25000	-0.27815	1.00000
C20	C	0.41020	0.25000	0.22311	1.00000
C21	C	-0.07177	0.25000	0.32912	1.00000
C22	C	-0.31423	0.25000	-0.17116	1.00000
C23	C	0.18561	0.25000	-0.14317	1.00000
C24	C	0.42807	0.25000	0.35857	1.00000
H1	H	-0.12011	0.25000	-0.27886	1.00000
H2	H	-0.26481	0.25000	0.22093	1.00000
H3	H	0.23638	0.25000	0.46434	1.00000
H4	H	0.38014	0.25000	-0.03402	1.00000
H5	H	0.00545	0.25000	-0.32514	1.00000
H6	H	-0.39120	0.25000	0.17422	1.00000
H7	H	0.10978	0.25000	-0.48965	1.00000
H8	H	-0.49450	0.25000	0.01241	1.00000
H9	H	-0.04945	0.25000	0.20778	1.00000
H10	H	-0.33625	0.25000	-0.29293	1.00000
H11	H	0.16366	0.25000	-0.02191	1.00000
H12	H	0.45002	0.25000	0.47957	1.00000

S1, .cif format

```
# CIF file
# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA

data_findsym-output

_symmetry_space_group_name_H-M 'P 1 21/c 1'
_symmetry_int_tables_number 14

_cell_length_a      11.64133
_cell_length_b      12.73700
_cell_length_c      11.79379
_cell_angle_alpha   90.00000
_cell_angle_beta    23.31663
_cell_angle_gamma    90.00000

loop_
_space_group_symop_operation_xyz
x,y,z
-x,y+1/2,-z+1/2
-x,-y,-z
x,-y+1/2,z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1  N  -0.18268  -0.07329  -0.23560  1.00000
N2  N   0.00079  -0.21695   0.49980  1.00000
N3  N  -0.09673  -0.39186  -0.34062  1.00000
N4  N  -0.27904  -0.24368  -0.08120  1.00000
N5  N   0.43036  -0.26763   0.34455  1.00000
N6  N   0.16293  -0.36615   0.26243  1.00000
N7  N   0.34618  -0.43280   0.48793  1.00000
N8  N  -0.36071  -0.41552   0.06138  1.00000
N9  N  -0.46833  -0.09989   0.19103  1.00000
C1  C  -0.44124  -0.20259   0.15495  1.00000
C2  C  -0.33503  -0.04080  -0.00737  1.00000
C3  C   0.01771  -0.32369   0.47918  1.00000
C4  C  -0.14958  -0.17615  -0.27854  1.00000
C5  C  -0.24478  -0.35241  -0.12157  1.00000
C6  C   0.48075  -0.37145   0.28561  1.00000
H1  H   0.25545  -0.32025   0.11730  1.00000
H2  H   0.17018  -0.44603   0.25066  1.00000
H3  H   0.23242  -0.39387  -0.34757  1.00000

# end_of_file
```

S2, .cif format

```
# CIF file
# This file was generated by FINDSYM
# Harold T. Stokes, Branton J. Campbell, Dorian M. Hatch
# Brigham Young University, Provo, Utah, USA

data_findsym-output

_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2

_cell_length_a      16.50800
_cell_length_b       8.98700
_cell_length_c       4.73900
_cell_angle_alpha    86.85800
_cell_angle_beta     84.60200
_cell_angle_gamma    100.81600

loop_
_space_group_symop_operation_xyz
x,y,z
-x,-y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
N1  N   0.41528  0.42711 -0.27679  1.00000
N2  N   -0.08339  0.07223 -0.05517  1.00000
N3  N    0.49998  0.28400 -0.06510  1.00000
N4  N    0.00092  0.21841 -0.42919  1.00000
N5  N    0.44234  0.11293  0.34805  1.00000
N6  N   -0.05785  0.38952  0.27320  1.00000
N7  N    0.36061  0.26085  0.12607  1.00000
N8  N   -0.13918  0.24225 -0.34169  1.00000
N9  N    0.22010  0.23563  0.30318  1.00000
N10 N   -0.27946  0.26152 -0.24942  1.00000
N11 N   -0.42399  0.13220  0.16082  1.00000
N12 N    0.07698  0.36692  0.18916  1.00000
N13 N    0.16653  0.07269 -0.30778  1.00000
N14 N   -0.33277  0.42898  0.47581  1.00000
N15 N    0.30733  0.09595 -0.46588  1.00000
N16 N   -0.19372  0.41199  0.36576  1.00000
N17 N    0.27382  0.40506 -0.08063  1.00000
N18 N   -0.22648  0.09203  0.02888  1.00000
C1  C    0.28366  0.30133  0.11550  1.00000
C2  C   -0.21637  0.19817 -0.18421  1.00000
C3  C    0.34006  0.46309 -0.26461  1.00000
C4  C   -0.15958  0.03558  0.08210  1.00000
C5  C   -0.49499  0.17786  0.14598  1.00000
C6  C    0.00559  0.32321  0.34804  1.00000
C7  C    0.42769  0.32561 -0.07683  1.00000
C8  C   -0.07138  0.17631 -0.27436  1.00000
C9  C    0.37081  0.15435  0.33864  1.00000
C10 C   -0.12957  0.35058  0.42895  1.00000
C11 C    0.23522  0.13597 -0.49472  1.00000
C12 C   -0.26472  0.36663 -0.47186  1.00000
H1  H   -0.37413  0.17442  0.01482  1.00000
H2  H    0.12684  0.31915  0.22770  1.00000
H3  H   -0.42088  0.05270  0.31979  1.00000
H4  H    0.07946  0.44127  0.01673  1.00000
H5  H    0.11339  0.11360 -0.33247  1.00000
H6  H   -0.38656  0.38534 -0.39669  1.00000

# end_of_file
```