Electronic Supplementary Material for CrystEngComm

The conformational polymorphism and weak interactions in solid state structures of ten new monomeric and dimeric substituted dibenzyldimethylammonium chloridopalladate salts

Anssi Peuronen, Manu Lahtinen*, Jussi Valkonen

Department of Chemistry, University of Jyväskylä, P.O.Box 35, FIN-40014 University of Jyväskylä, Finland.

Supplementary material

S1

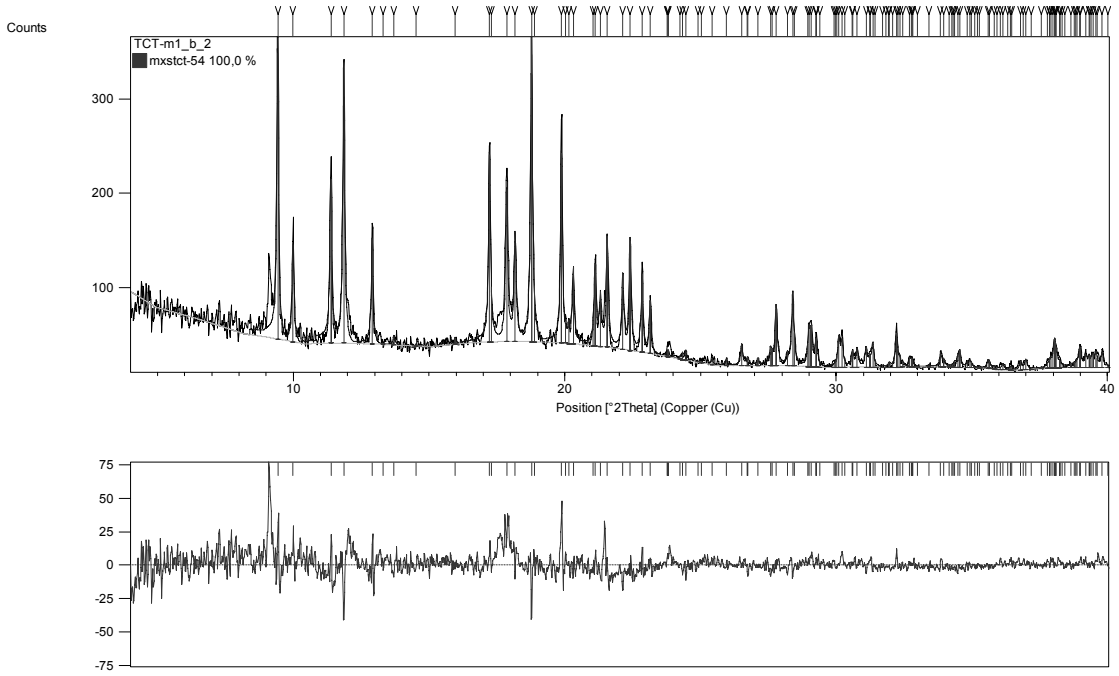
Structures Report: Compound 1

Global Parameters

Zero shift/ °2Theta	0,036(1)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	15,00473
R (profile)/ %	10,08744
R (weighted profile)/ %	13,16005
GOF	0,76923

Relevant parameters

Space group (No.)	$P2_1/c$ (14)
Lattice parameters	
a/ Å	12,239(1)
b/ Å	9,4538(8)
c/ Å	17,875(2)
alpha/ °	90
beta/ °	129,745(4)
gamma/ °	90
V/ 10^6 pm^3	1590,25100
Overall displacement parameter	6,2(3)



S2

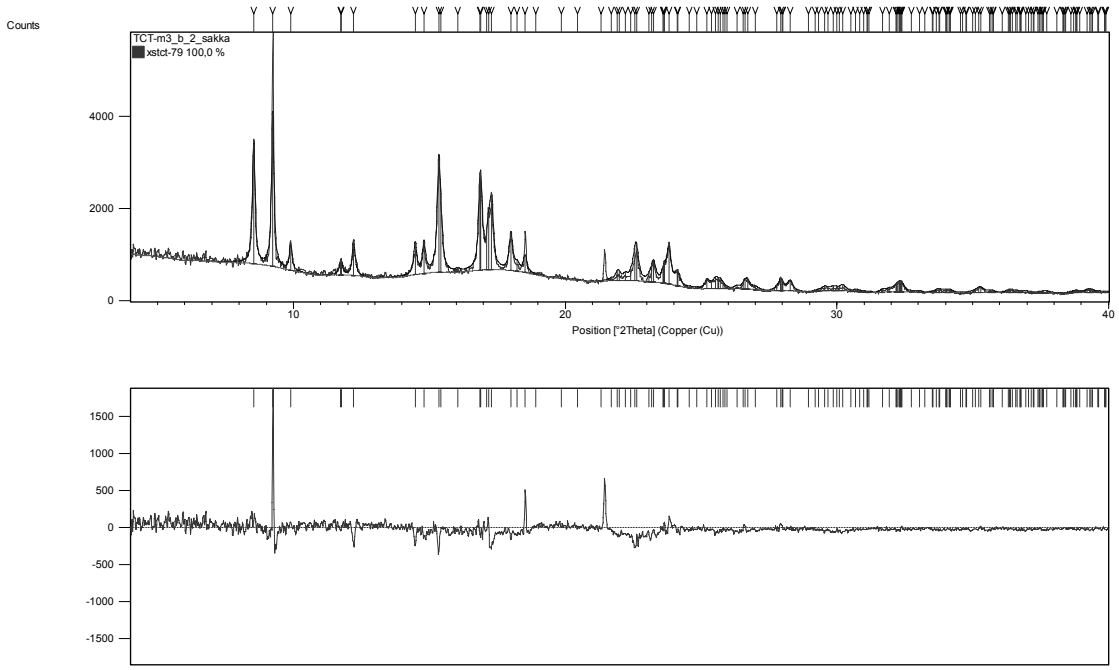
Structures Report: Compound 2

Global Parameters

Zero shift/ °2Theta	0,007(3)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	4,33591
R (profile)/ %	9,52064
R (weighted profile)/ %	12,53146
GOF	8,35300

Relevant parameters

Space group (No.)	P -1 (2)
Lattice parameters	
a/ Å	8,317(2)
b/ Å	10,660(3)
c/ Å	11,634(2)
alpha/ °	107,12(1)
beta/ °	105,60(2)
gamma/ °	103,64(1)
V/ 10^6 pm^3	892,08910
Overall displacement parameter	10,0(4)



S3

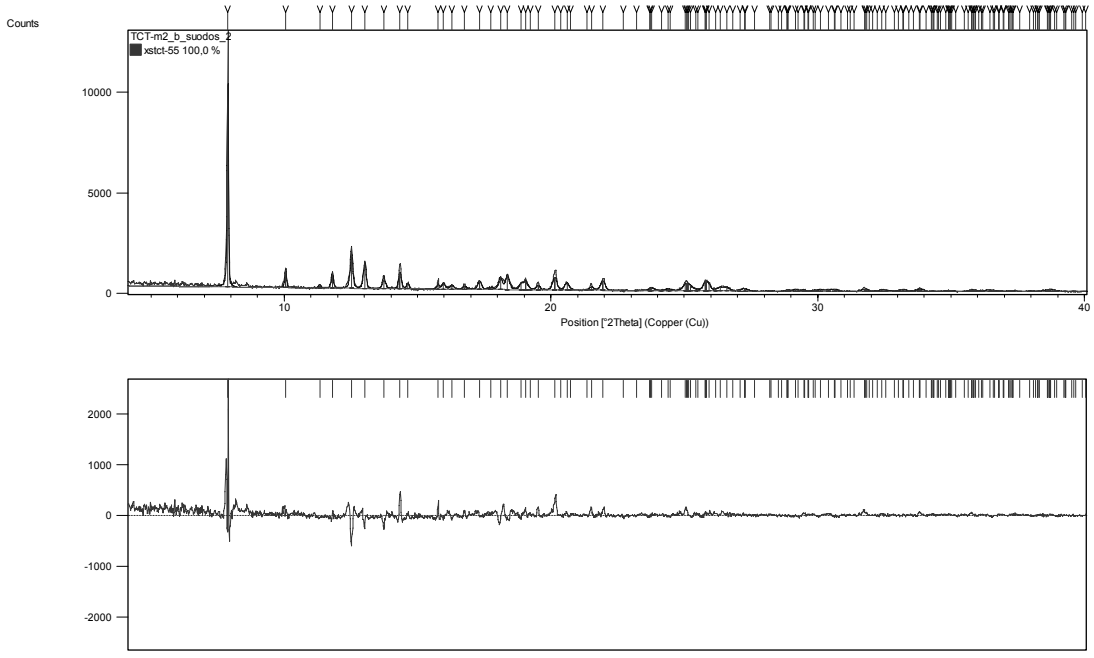
Structures Report: Compound 3

Global Parameters

Zero shift/ °2Theta	0,0391(6)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	9,62352
R (profile)/ %	13,67803
R (weighted profile)/ %	15,96253
GOF	2,75128

Relevant parameters of xstct-55

Space group (No.)	$P2_1/c$ 1 (14)
Lattice parameters	
a/ Å	11,2879(8)
b/ Å	10,901(1)
c/ Å	15,069(2)
alpha/ °	90
beta/ °	93,925(9)
gamma/ °	90
V/ 10^6 pm^3	1849,94700
Overall displacement parameter	5,3(2)



S4

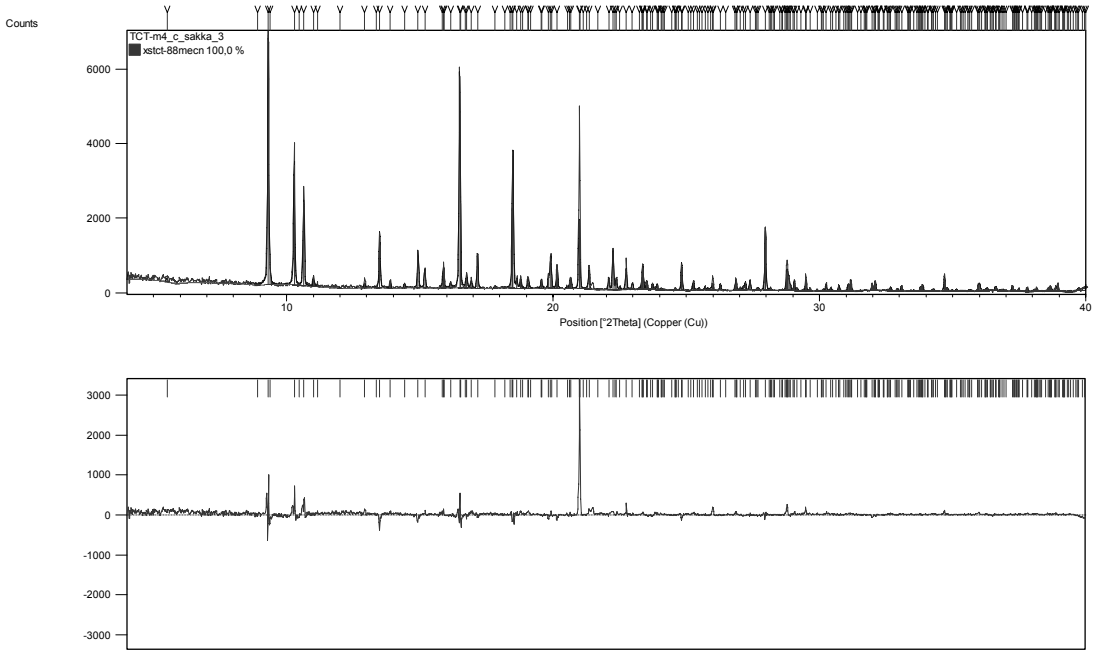
Structures Report: Compound 4

Global Parameters

Zero shift/ °2Theta	0,0245(8)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	10,82287
R (profile)/ %	15,22258
R (weighted profile)/ %	21,72788
GOF	4,03041

Relevant parameters

Space group (No.)	$P2_1/c$ (14)
Lattice parameters	
a/ Å	16,1425(7)
b/ Å	11,6792(7)
c/ Å	19,0958(9)
alpha/ °	90
beta/ °	94,167(3)
gamma/ °	90
V/ 10^6 pm^3	3590,64000
Overall displacement parameter	7,6(4)



S5

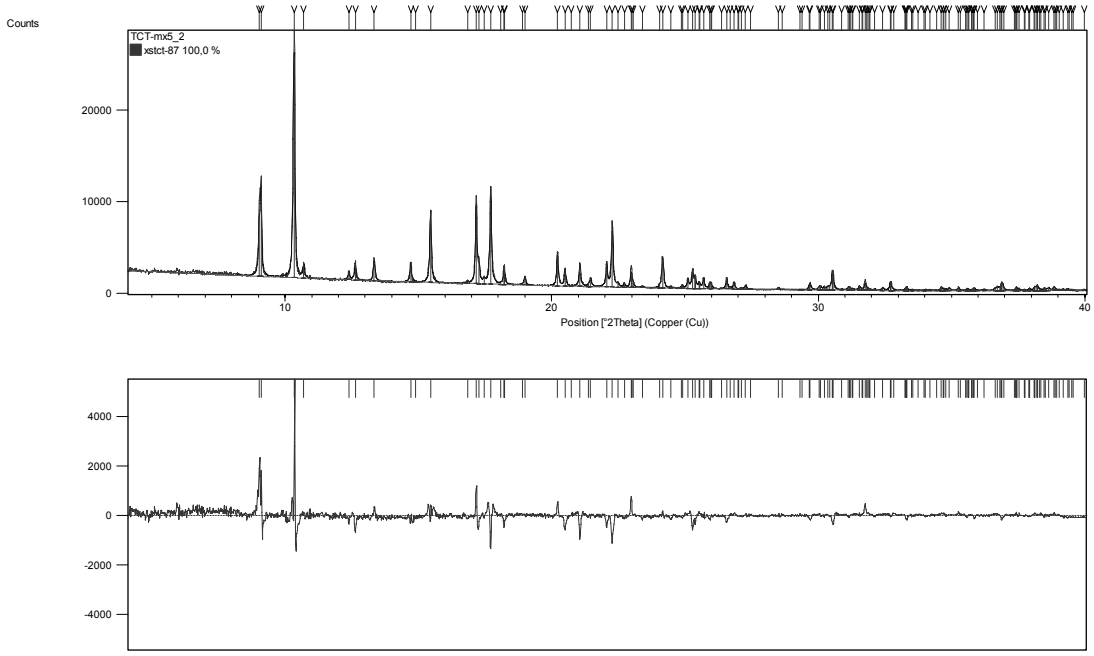
Structures Report: Compound 5

Global Parameters

Zero shift/ °2Theta	0,0288(8)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	4,67977
R (profile)/ %	7,85211
R (weighted profile)/ %	10,84941
GOF	5,37482

Relevant parameters of xstct-87

Space group (No.)	P -1 (2)
Lattice parameters	
a/ Å	8,6549(4)
b/ Å	10,6011(5)
c/ Å	10,8874(7)
alpha/ °	67,486(3)
beta/ °	74,158(4)
gamma/ °	78,919(2)
V/ 10^6 pm^3	883,41890
Overall displacement parameter	10,0(2)



S6

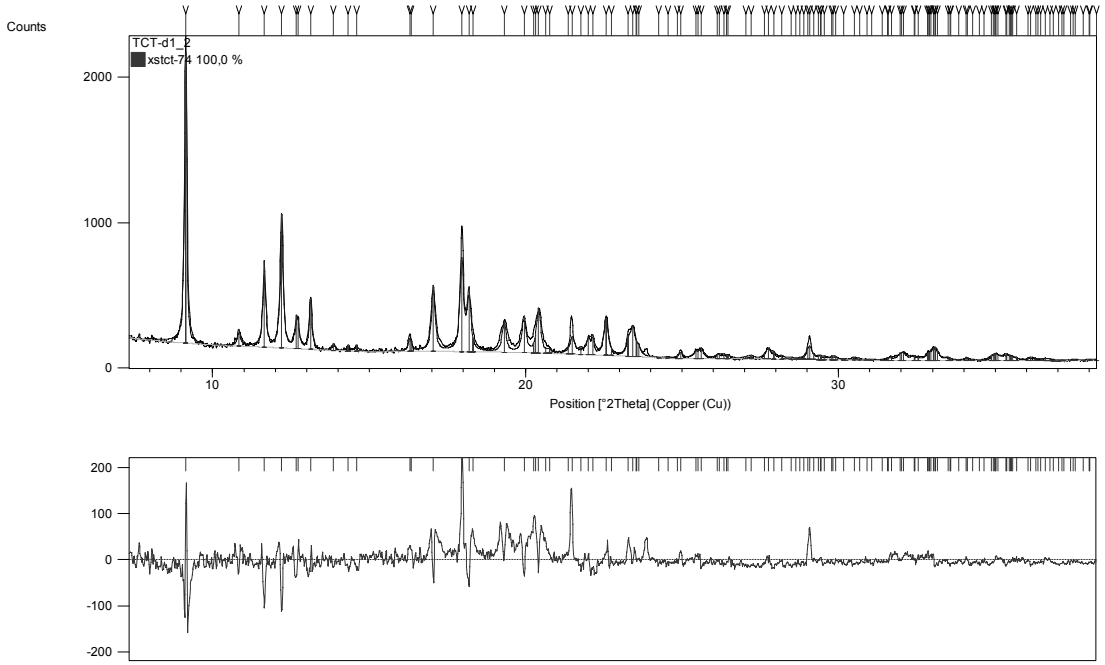
Structures Report: Compound 6

Global Parameters

Zero shift/ °2Theta	0,010(2)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	8,28674
R (profile)/ %	9,69886
R (weighted profile)/ %	12,27171
GOF	2,19302

Relevant parameters

Space group (No.)	$P2_1/c$ (14)
Lattice parameters	
a/ Å	9,265(1)
b/ Å	13,485(2)
c/ Å	15,779(3)
alpha/ °	90
beta/ °	118,23(1)
gamma/ °	90
V/ 10^6 pm^3	1736,90800
Overall displacement parameter	4,2(6)



S7

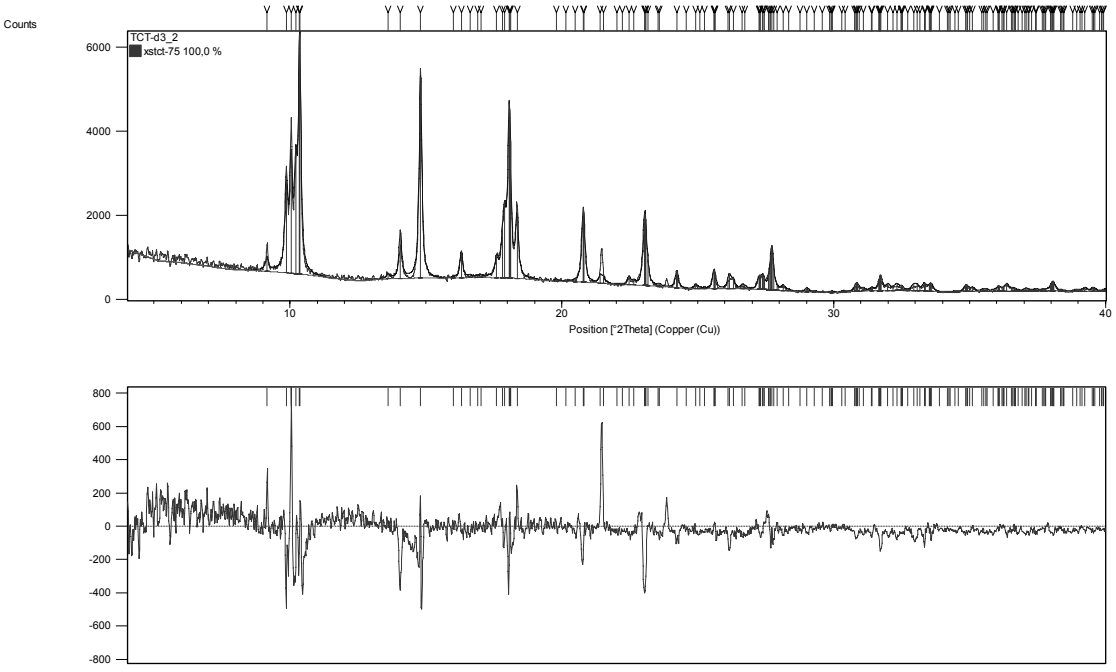
Structures Report: Compound 7

Global Parameters

Zero shift/ °2Theta	0,005(2)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	6,76462
R (profile)/ %	8,34966
R (weighted profile)/ %	11,98932
GOF	3,14124

Relevant parameters

Space group (No.)	P -1 (2)
Lattice parameters	
a/ Å	10,450(1)
b/ Å	10,420(2)
c/ Å	11,131(2)
alpha/ °	107,898(8)
beta/ °	105,16(1)
gamma/ °	109,942(7)
V/ 10^6 pm^3	989,13430
Overall displacement parameter	10,0(3)



S9

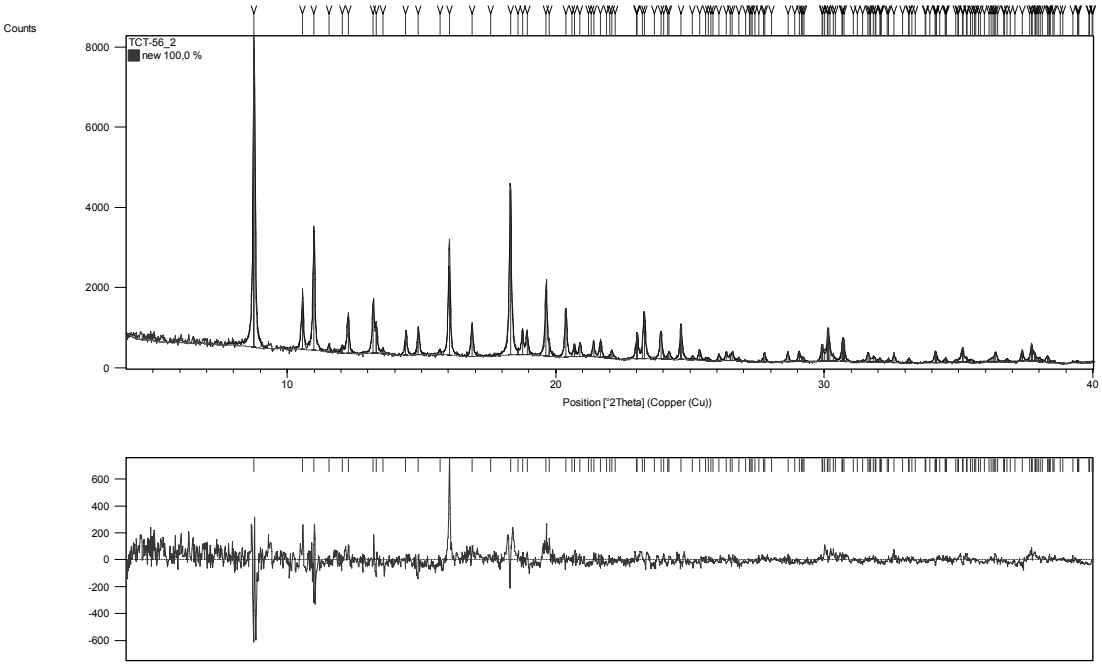
Structures Report: Compound 9

Global Parameters

Zero shift/ °2Theta	0,0040(8)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	7,93833
R (profile)/ %	7,90277
R (weighted profile)/ %	10,30172
GOF	1,68408

Relevant parameters of new

Space group (No.)	$P2_1/c$ (14)
Lattice parameters	
a/ Å	9,5744(5)
b/ Å	15,3043(8)
c/ Å	15,3361(7)
alpha/ °	90
beta/ °	119,049(3)
gamma/ °	90
V/ 10^6 pm^3	1964,50200
Overall displacement parameter	7,4(2)



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S10

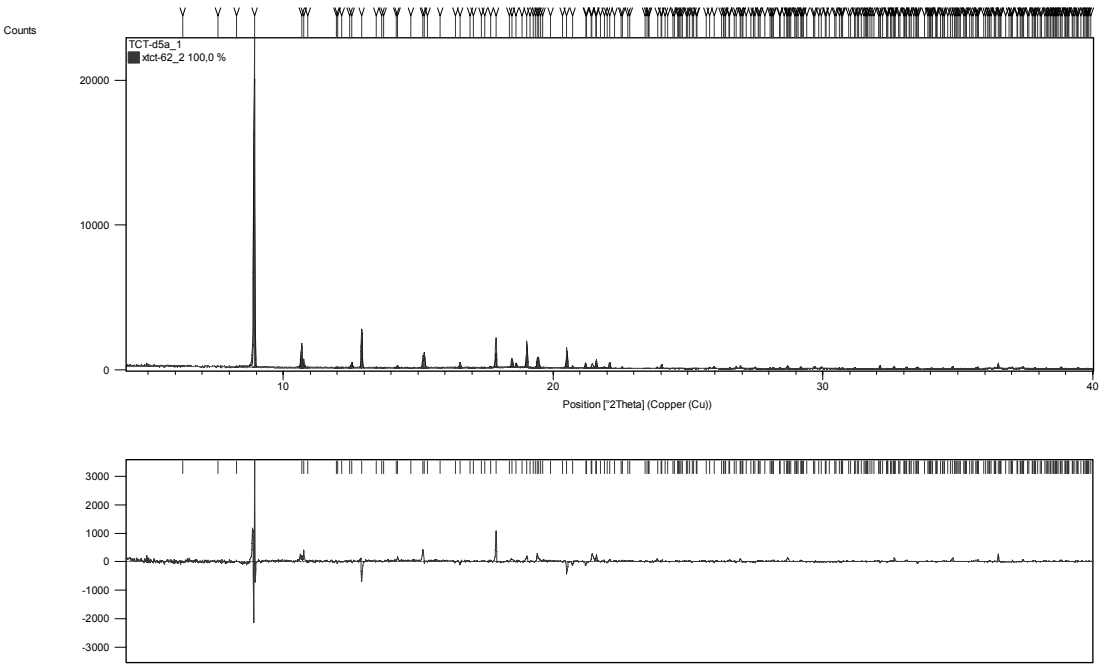
Structures Report: Compound 10

Global Parameters

Zero shift/ °2Theta	0,0233(6)
Profile function	Pseudo Voigt
Background	Polynomial
R (expected)/ %	13,50614
R (profile)/ %	18,75381
R (weighted profile)/ %	24,58805
GOF	3,31425

Relevant parameters

Space group (No.)	$P2_1/c$ (14)
Lattice parameters	
a/ Å	14,6148(7)
b/ Å	16,4540(9)
c/ Å	17,162(1)
alpha/ °	90
beta/ °	104,873(4)
gamma/ °	90
V/ 10^6 pm^3	3988,66700
Overall displacement parameter	7,7(7)



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Optimized atomic coordinates used in DFT calculations

==> 1_TS.xyz <==
37
Structure 1, transition state geometry

C	-0.00670	-0.00050	0.00140
C	-0.00030	0.00100	1.39950
C	1.22440	0.00400	2.07400
C	2.41880	0.03430	1.36440
C	2.40100	0.05300	-0.02720
C	1.18750	0.03010	-0.70850
C	-1.28740	-0.04860	2.16330
N	-1.93340	1.34270	2.54330
C	-2.04420	1.42350	4.03830
C	-3.34330	1.38460	1.89900
C	-4.16310	2.61420	2.16350
C	-4.12370	3.69750	1.27890
C	-4.91630	4.81740	1.49790
C	-5.76610	4.86420	2.59890
C	-5.83110	3.78360	3.47300
C	-5.03920	2.66310	3.25320
C	-1.11600	2.50850	2.06880
H	-3.48590	3.66110	0.40290
H	-4.88090	5.64660	0.80300
H	-6.38900	5.73370	2.76560
H	-6.50910	3.80700	4.31650
H	-5.12250	1.81490	3.92340
H	1.24870	-0.03560	3.15760
H	3.36190	0.02960	1.89560
H	3.33160	0.06930	-0.57980
H	1.17230	0.02190	-1.79080
H	-0.94680	-0.04370	-0.53800
H	-1.04520	1.36320	4.46390
H	-2.50780	2.36640	4.31360
H	-2.64970	0.59420	4.39710
H	-0.12850	2.45670	2.51690
H	-1.02170	2.47170	0.98800
H	-1.62080	3.42090	2.37200
H	-3.84730	0.49420	2.27290
H	-3.16360	1.25750	0.83240
H	-2.05150	-0.57210	1.59450
H	-1.15490	-0.56680	3.10930

==> 1_twisted.xyz <==
37
Structure 1, twisted geometry

C	0.02660	0.00880	0.00670
C	0.03970	0.00380	1.40560
C	1.24290	-0.01200	2.10070
C	2.44810	-0.03560	1.40570
C	2.44760	-0.05640	0.01440
C	1.24420	-0.03980	-0.68040
H	-0.89360	-0.00830	1.95710

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H	1.23960	-0.02090	3.18310
H	3.38530	-0.05560	1.94720
H	3.38280	-0.09990	-0.52880
H	1.25610	-0.08760	-1.76360
C	-1.27600	-0.01890	-0.74150
N	-1.86950	1.35950	-1.11260
C	-3.18320	1.15070	-1.91150
C	-4.29920	0.44710	-1.19480
C	-2.12890	2.17480	0.11860
C	-0.92440	2.11460	-2.00140
C	-5.24680	1.17660	-0.46870
C	-6.30550	0.53200	0.15930
C	-6.43800	-0.84950	0.05790
C	-5.51700	-1.58310	-0.68340
C	-4.45740	-0.93840	-1.31000
H	-5.17320	2.25660	-0.40900
H	-7.03480	1.10870	0.71360
H	-7.26720	-1.35090	0.54050
H	-5.63110	-2.65470	-0.78510
H	-3.76300	-1.51730	-1.90840
H	-1.37720	3.06870	-2.26170
H	0.00950	2.27900	-1.47230
H	-0.74280	1.53500	-2.90370
H	-2.56750	3.12460	-0.17970
H	-2.81560	1.63780	0.76590
H	-1.18660	2.34640	0.63010
H	-1.16940	-0.54180	-1.69130
H	-2.05170	-0.51210	-0.16120
H	-2.88280	0.60290	-2.80350
H	-3.48520	2.15350	-2.21110

==> 1_w.xyz <==
37
Structure 1, w geometry

C	0.00860	0.01840	-0.00330
C	-0.00200	0.00010	1.39560
C	1.21800	-0.01840	2.08030
C	2.41970	0.01850	1.38350
C	2.41670	0.06160	-0.00730
C	1.21020	0.05520	-0.70030
C	-1.29930	-0.08440	2.14700
N	-1.94700	1.26570	2.54750
C	-1.02600	2.04410	3.43770
C	-3.25480	0.91100	3.30030
C	-4.07060	2.07090	3.79410
C	-5.08810	2.61250	3.00100
C	-5.87060	3.65900	3.47340
C	-5.65380	4.16900	4.74980
C	-4.66140	3.62220	5.55740
C	-3.87900	2.57560	5.08480
C	-2.25060	2.08220	1.32780
H	-5.28690	2.20340	2.01690
H	-6.65800	4.06590	2.85210
H	-6.26860	4.97910	5.12080
H	-4.50670	4.00030	6.55980
H	-3.12970	2.13770	5.73450

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H	1.23370	-0.08280	3.16240
H	3.35690	-0.00150	1.92470
H	3.35290	0.08230	-0.55030
H	1.20500	0.06380	-1.78260
H	-0.92400	-0.01730	-0.55490
H	-0.10970	2.25500	2.89470
H	-1.51560	2.97010	3.72380
H	-0.80390	1.45350	4.32380
H	-1.32120	2.29210	0.80700
H	-2.91920	1.51960	0.68000
H	-2.72680	3.00810	1.63600
H	-2.93880	0.27640	4.12720
H	-3.82550	0.30300	2.59960
H	-2.05890	-0.59580	1.55730
H	-1.17240	-0.62340	3.08490

==> 2_TS.xyz <==
43
Structure 2, transition state geometry

C	0.00880	-0.00970	0.00720
C	-0.00190	0.00150	1.40950
C	1.22330	0.01100	2.11030
C	2.40470	0.07530	1.36590
C	2.39900	0.11180	-0.02180
C	1.19260	0.05710	-0.71030
C	-1.32680	-0.10660	2.11180
N	-2.10890	1.21760	2.34630
C	-1.28190	2.16990	3.15660
C	1.33030	-0.08000	3.61480
C	-3.46290	0.83000	3.06380
C	-3.76480	1.51850	4.36220
C	-3.34850	0.89000	5.54310
C	-3.60990	1.44300	6.78710
C	-4.31600	2.63830	6.86110
C	-4.75840	3.25530	5.69800
C	-4.50040	2.71820	4.43420
C	-5.02630	3.44190	3.21790
C	-2.42560	1.87200	1.03330
H	3.35210	0.07900	1.89120
H	3.33520	0.15650	-0.56350
H	1.17520	0.04610	-1.79220
H	-0.92710	-0.09400	-0.53310
H	-5.33060	4.17230	5.76970
H	-4.53890	3.08120	7.82350
H	-3.28330	0.93930	7.68760
H	-2.82580	-0.05900	5.48570
H	-3.01050	2.76710	1.22370
H	-1.49920	2.13290	0.53040
H	-2.99800	1.18170	0.41790
H	-1.83540	3.09360	3.29580
H	-1.06820	1.73190	4.12510
H	-0.36070	2.36210	2.61330
H	-2.01490	-0.72630	1.53810
H	-1.22300	-0.53980	3.10330
H	-3.39400	-0.24150	3.22840
H	-4.23440	1.00470	2.32000

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H 2.34010 -0.37100 3.90000
H 1.12670 0.87430 4.10670
H 0.65310 -0.82330 4.04050
H -5.80480 4.14750 3.50410
H -4.24760 4.02510 2.71610
H -5.46290 2.76530 2.48050

==> 2_twisted.xyz <==
43
Structure 2, twisted geometry
C 0.04070 0.00600 0.04520
C 0.09500 -0.11390 1.45030
C 1.35360 -0.12460 2.05990
C 2.52780 -0.03920 1.32500
C 2.47210 0.03480 -0.06220
C 1.23550 0.04580 -0.68770
C -1.12570 -0.25900 2.32890
H 1.40990 -0.22050 3.13740
H 3.48380 -0.05640 1.83270
H 3.38040 0.06390 -0.64980
H 1.19570 0.06360 -1.77090
C -1.25890 -0.01730 -0.71380
N -1.85060 1.35900 -1.11050
C -3.17350 1.14130 -1.89980
C -4.31560 0.50160 -1.15960
C -2.08800 2.20120 0.10420
C -0.91190 2.09130 -2.02460
C -5.35070 1.25790 -0.56940
C -6.39170 0.56720 0.05940
C -6.43660 -0.81930 0.09910
C -5.43930 -1.56190 -0.52280
C -4.39890 -0.89870 -1.15360
C -5.41820 2.76700 -0.60580
H -7.19480 1.13590 0.51220
H -7.26230 -1.31780 0.59100
H -5.48250 -2.64310 -0.53420
H -3.64480 -1.47900 -1.67250
H -1.36750 3.03840 -2.30490
H 0.02580 2.26990 -1.50770
H -0.73750 1.48980 -2.91380
H -2.45880 3.17230 -0.21240
H -2.81940 1.70980 0.73750
H -1.14660 2.31940 0.63340
H -1.13790 -0.54240 -1.66060
H -2.04720 -0.50460 -0.15040
H -2.87980 0.53100 -2.75290
H -3.43620 2.13010 -2.26750
H -0.84840 -0.70720 3.28210
H -1.58830 0.70470 2.55740
H -1.89340 -0.89590 1.88700
H -6.44090 3.09860 -0.43190
H -4.80210 3.22920 0.16960
H -5.10880 3.18240 -1.56670

==> 2_w.xyz <==
43

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Structure 2, w geometry

C	-0.01090	0.00970	0.00130
C	0.00640	-0.00390	1.41240
C	1.23700	-0.02150	2.08450
C	2.43830	-0.09220	1.39700
C	2.42220	-0.12270	0.00740
C	1.21300	-0.05890	-0.67100
C	-1.24980	0.10290	2.23210
N	-1.84710	-1.22750	2.76700
C	-2.11600	-2.17610	1.63900
C	-1.27210	0.12230	-0.82330
C	-3.16960	-0.84500	3.48670
C	-3.90900	-1.95910	4.17480
C	-4.80780	-2.72480	3.41840
C	-5.54460	-3.75140	3.98790
C	-5.40550	-4.01150	5.34620
C	-4.55400	-3.23070	6.11550
C	-3.79890	-2.19220	5.56230
C	-2.93500	-1.36720	6.48770
C	-0.89820	-1.88540	3.72150
H	-4.48230	-3.41750	7.18010
H	-5.97790	-4.80380	5.81170
H	-6.23300	-4.32780	3.38380
H	-4.94920	-2.49860	2.36780
H	1.21430	-0.04480	-1.75410
H	3.35010	-0.16990	-0.54840
H	3.37560	-0.10330	1.93780
H	1.25530	0.04310	3.16640
H	-1.18190	-2.36640	1.11800
H	-2.51450	-3.10070	2.04540
H	-2.83660	-1.72800	0.96060
H	0.00630	-2.15690	3.18590
H	-0.66070	-1.19140	4.52290
H	-1.37600	-2.77310	4.12640
H	-3.78460	-0.40390	2.70360
H	-2.88810	-0.05720	4.18090
H	-1.07330	0.69790	3.12710
H	-2.05990	0.56410	1.67280
H	-3.27090	-1.48550	7.51680
H	-1.88670	-1.67620	6.46260
H	-2.97180	-0.29970	6.26270
H	-1.03230	0.47100	-1.82680
H	-1.77980	-0.83900	-0.93850
H	-1.99090	0.82920	-0.40510

==> 3_TS.xyz <==
43
Structure 3, transition state geometry

C	0.00370	0.00230	-0.00010
C	0.00160	0.00020	1.39980
C	1.22110	-0.00340	2.08020
C	2.41370	-0.04100	1.36630
C	2.39660	-0.06110	-0.02190
C	1.19050	-0.02960	-0.73050
C	-1.29270	0.08440	2.15540
N	-1.95050	-1.26380	2.55130

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C	-2.23460	-2.07730	1.32310
C	1.18400	-0.00480	-2.23630
C	-3.25900	-0.92220	3.37010
C	-4.55130	-1.42070	2.80140
C	-5.05080	-2.67070	3.18170
C	-6.26060	-3.15470	2.68630
C	-6.97100	-2.34890	1.78940
C	-6.49670	-1.09830	1.41540
C	-5.29080	-0.62750	1.92280
C	-6.80740	-4.48920	3.11950
C	-1.02850	-2.05150	3.43520
H	3.33310	-0.08250	-0.56690
H	3.35840	-0.04070	1.89490
H	1.24690	0.04540	3.16270
H	-7.91630	-2.70100	1.39310
H	-7.07410	-0.48250	0.73760
H	-4.93970	0.36080	1.64720
H	-1.52540	-2.97740	3.71570
H	-0.11240	-2.27050	2.89430
H	-0.80220	-1.46910	4.32560
H	-2.71230	-3.00690	1.61640
H	-2.89950	-1.52460	0.66680
H	-1.29120	-2.27660	0.82330
H	-1.15850	0.61510	3.09700
H	-2.05380	0.60080	1.57240
H	-3.26840	0.16140	3.45260
H	-3.08850	-1.33560	4.36060
H	-0.93780	0.05160	-0.53690
H	-4.49730	-3.27420	3.89440
H	1.76550	-0.83290	-2.64670
H	0.17190	-0.07210	-2.63540
H	1.62970	0.91960	-2.61160
H	-7.08680	-5.09970	2.25860
H	-6.08200	-5.04840	3.71050
H	-7.70520	-4.36080	3.72920

==> 3_twisted.xyz <==
43
Structure 3, twisted geometry

C	0.00000	0.00000	0.00000
C	0.00000	0.00000	1.40000
C	1.22060	0.00000	2.07830
C	2.41210	-0.03630	1.36240
C	2.39280	-0.05970	-0.02560
C	1.18560	-0.03230	-0.73230
C	-1.29480	0.08640	2.15540
N	-1.96950	-1.25920	2.53190
C	-3.25950	-0.93100	3.22480
C	1.17650	-0.01130	-2.23820
C	-1.03560	-2.04790	3.47840
C	-1.56080	-3.36720	3.96960
C	-2.28000	-3.44630	5.16380
C	-2.72100	-4.68070	5.62810
C	-2.44000	-5.83690	4.91290
C	-1.70060	-5.79070	3.72590
C	-1.26680	-4.54550	3.27340

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C	-1.37240	-7.05460	2.97570
C	-2.27320	-2.05690	1.29980
H	-2.78290	-6.79370	5.28900
H	-3.27360	-4.74100	6.55710
H	-2.47900	-2.55360	5.74560
H	3.32860	-0.08030	-0.57210
H	3.35760	-0.03300	1.88970
H	1.24770	0.04900	3.16060
H	-3.88550	-0.35680	2.54540
H	-3.75970	-1.85380	3.50230
H	-3.04650	-0.34300	4.11480
H	-2.91320	-1.46350	0.65040
H	-1.34490	-2.29240	0.78820
H	-2.78380	-2.96980	1.59150
H	-0.84510	-1.36980	4.30960
H	-0.11240	-2.17520	2.91880
H	-1.16210	0.60470	3.10420
H	-2.04800	0.61930	1.57650
H	-0.66750	-4.49820	2.37020
H	-0.94200	0.04950	-0.53610
H	-2.28170	-7.58420	2.68250
H	-0.79720	-6.84860	2.07300
H	-0.78800	-7.73690	3.59690
H	1.75110	-0.84490	-2.64730
H	0.16330	-0.07210	-2.63560
H	1.62840	0.90870	-2.61670

==> 3_w.xyz <==
43
Structure 3, w geometry

C	-0.00400	-0.00960	-0.00370
C	-0.00180	0.00510	1.39610
C	1.21950	0.01980	2.07280
C	2.41010	-0.01500	1.35520
C	2.38910	-0.05180	-0.03250
C	1.18060	-0.04060	-0.73770
C	-1.29580	0.08340	2.15340
N	-1.93370	-1.26970	2.56070
C	-2.22220	-2.09910	1.34620
C	1.16930	-0.04260	-2.24360
C	-3.24990	-0.92080	3.30190
C	-4.04940	-2.08280	3.81610
C	-3.85580	-2.54850	5.12200
C	-4.60930	-3.59830	5.64460
C	-5.58080	-4.18080	4.82310
C	-5.80130	-3.71680	3.53330
C	-5.04380	-2.66570	3.02820
C	-4.40350	-4.08420	7.05510
C	-1.01090	-2.03160	3.46300
H	3.32420	-0.07060	-0.58000
H	3.35640	0.00060	1.88070
H	1.24790	0.07900	3.15460
H	-6.18360	-4.99530	5.20760
H	-6.57490	-4.16520	2.92300
H	-5.24510	-2.29150	2.03110
H	-1.49620	-2.95670	3.75890

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H	-0.09060	-2.24130	2.92620
H	-0.79690	-1.42860	4.34290
H	-2.68850	-3.02830	1.65960
H	-2.89570	-1.54910	0.69250
H	-1.28840	-2.29940	0.82960
H	-1.16880	0.62450	3.08990
H	-2.06210	0.58750	1.56610
H	-3.82580	-0.33580	2.58620
H	-2.94600	-0.26500	4.11660
H	-0.94770	0.02560	-0.53810
H	-3.11680	-2.07080	5.75680
H	1.69300	-0.91570	-2.63930
H	0.15330	-0.05170	-2.63820
H	1.67350	0.84220	-2.63860
H	-4.15240	-5.14710	7.07180
H	-3.60160	-3.54070	7.55470
H	-5.31250	-3.95820	7.64750

==> 4_TS.xyz <==
43
Structure 4, transition state geometry

C	-0.00070	0.00280	-0.00250
C	0.00090	-0.00120	1.39640
C	1.23360	-0.00410	2.05690
C	2.42220	0.03150	1.34120
C	2.42430	0.05650	-0.05650
C	1.19020	0.03820	-0.71370
C	-1.28430	-0.07880	2.16370
N	-1.93640	1.27380	2.55800
C	-0.99320	2.07050	3.40960
C	3.71380	0.05560	-0.83120
C	-3.29300	0.94030	3.30210
C	-3.42430	1.43860	4.70550
C	-3.02230	0.64760	5.78520
C	-3.15620	1.10750	7.08790
C	-3.70610	2.36440	7.35760
C	-4.12100	3.14510	6.27400
C	-3.98840	2.69010	4.96980
C	-3.88830	2.84440	8.77160
C	-2.25180	2.07450	1.32900
H	1.27050	-0.04960	3.13960
H	3.36450	0.02710	1.87580
H	1.16230	0.03820	-1.79680
H	-0.93840	-0.03970	-0.54570
H	-4.34210	3.31130	4.15370
H	-4.56480	4.11680	6.45540
H	-2.84100	0.47580	7.90980
H	-2.61350	-0.34240	5.61290
H	-2.72680	3.00430	1.63340
H	-1.33130	2.28530	0.79240
H	-2.92770	1.50540	0.69450
H	-1.47540	2.99860	3.70060
H	-0.73990	1.50440	4.30050
H	-0.10010	2.27420	2.82630
H	-2.05020	-0.59770	1.58890
H	-1.14800	-0.60180	3.10930

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H	-3.37520	-0.14290	3.26820
H	-4.07100	1.35900	2.66900
H	-3.15330	2.39920	9.44250
H	-3.80300	3.92930	8.83900
H	-4.87990	2.57090	9.14370
H	3.61620	0.60350	-1.76900
H	4.52580	0.50060	-0.25590
H	4.00990	-0.96750	-1.08010

==> 4_twisted.xyz <==
43
Structure 4, twisted geometry

C	0.03040	0.02200	-0.00860
C	0.04370	0.00020	1.38930
C	1.24340	-0.01310	2.08780
C	2.47010	-0.01980	1.41810
C	2.45240	-0.01820	0.01990
C	1.25580	-0.00480	-0.68260
H	-0.88910	-0.02380	1.94170
H	1.22690	-0.03220	3.17090
C	3.76880	-0.07450	2.17550
H	3.38830	-0.04170	-0.52570
H	1.28050	-0.03480	-1.76630
C	-1.26690	-0.01060	-0.76180
N	-1.86820	1.36490	-1.13690
C	-3.18850	1.14480	-1.92440
C	-4.29740	0.44950	-1.19310
C	-2.12110	2.18560	0.09100
C	-0.93170	2.11610	-2.03620
C	-5.24550	1.18010	-0.46940
C	-6.29730	0.54050	0.17120
C	-6.45120	-0.84730	0.09920
C	-5.51410	-1.57190	-0.64310
C	-4.45940	-0.93680	-1.28390
H	-5.17640	2.26110	-0.41790
H	-7.01940	1.12960	0.72380
C	-7.61540	-1.53340	0.75970
H	-5.61870	-2.64670	-0.73090
H	-3.76760	-1.52850	-1.87300
H	-1.38750	3.06800	-2.29940
H	0.00540	2.28450	-1.51400
H	-0.75530	1.53150	-2.93640
H	-2.56550	3.13220	-0.20910
H	-2.80140	1.64970	0.74590
H	-1.17550	2.36210	0.59460
H	-1.15660	-0.53240	-1.71200
H	-2.04340	-0.50620	-0.18480
H	-2.89170	0.58710	-2.81160
H	-3.49230	2.14420	-2.23400
H	-7.36850	-2.55750	1.04090
H	-7.93890	-0.99940	1.65360
H	-8.46990	-1.57810	0.07820
H	4.55830	0.46730	1.65350
H	3.66630	0.34700	3.17550
H	4.10320	-1.10980	2.28790

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==> 4_w.xyz <==
43
Structure 4, w geometry

C	-0.00000	-0.00040	0.00020
C	0.00010	-0.00000	1.39880
C	1.23230	0.00040	2.06060
C	2.42160	0.03660	1.34630
C	2.42510	0.05810	-0.05150
C	1.19190	0.03580	-0.70970
C	-1.28480	-0.08020	2.16740
N	-1.93630	1.27330	2.55640
C	-1.00830	2.06970	3.42170
C	3.71610	0.05840	-0.82370
C	-3.23370	0.92460	3.33290
C	-4.04750	2.08640	3.81830
C	-3.84580	2.61900	5.09580
C	-4.62540	3.67000	5.55790
C	-5.64260	4.21660	4.76990
C	-5.85540	3.66730	3.50210
C	-5.07840	2.61630	3.03560
C	-6.51120	5.33010	5.28810
C	-2.26050	2.06840	1.32880
H	1.26870	-0.04500	3.14340
H	3.36330	0.03440	1.88210
H	1.16530	0.03310	-1.79280
H	-0.93680	-0.04630	-0.54410
H	-5.29110	2.19640	2.05870
H	-6.64910	4.05920	2.87730
H	-4.45050	4.06400	6.55190
H	-3.08500	2.20120	5.74590
H	-2.73840	2.99610	1.62890
H	-1.33930	2.27470	0.79220
H	-2.93440	1.49180	0.69910
H	-1.49930	2.99730	3.70020
H	-0.77160	1.49400	4.31370
H	-0.10010	2.27620	2.86340
H	-2.05060	-0.60360	1.59640
H	-1.14380	-0.60290	3.11260
H	-2.90190	0.30410	4.16440
H	-3.80880	0.30230	2.64840
H	-5.97240	5.96050	5.99590
H	-6.87910	5.95970	4.47760
H	-7.38340	4.92460	5.80920
H	3.60450	0.55490	-1.78790
H	4.51220	0.55700	-0.27020
H	4.04560	-0.96610	-1.01930

==> 5_twisted.xyz <==
43
Structure 5, twisted geometry

C	-0.01640	0.01450	0.02270
C	-0.05500	-0.04700	1.42030
C	1.11900	-0.07420	2.16330
C	2.35140	-0.05040	1.51840
C	2.40460	-0.01240	0.12880
C	1.22950	0.01360	-0.61340

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H	-1.00900	-0.09140	1.93340
H	1.07120	-0.12710	3.24340
H	3.26670	-0.07780	2.09570
H	3.36080	-0.01770	-0.37850
H	1.29230	0.01110	-1.69470
C	-1.30040	-0.02010	-0.76270
N	-1.88140	1.34240	-1.21120
C	-3.21590	1.08170	-1.94990
C	-4.30400	0.39260	-1.16990
C	-2.09460	2.20400	0.03080
C	-0.92780	2.06600	-2.15770
C	-5.23170	1.12130	-0.41790
C	-6.26550	0.47610	0.25050
C	-6.39470	-0.90660	0.16730
C	-5.49420	-1.64090	-0.59760
C	-4.46080	-0.99480	-1.26510
H	-5.16630	2.20110	-0.36680
H	-6.97850	1.05470	0.82380
H	-7.20400	-1.40780	0.68260
H	-5.60380	-2.71420	-0.68580
H	-3.78260	-1.57610	-1.87970
H	-1.37540	3.03770	-2.34830
H	-0.01530	2.22320	-1.58530
C	-0.62680	1.38060	-3.48290
C	-2.57840	3.62830	-0.19880
H	-1.13730	2.21510	0.54570
H	-1.18890	-0.60130	-1.67490
H	-2.09030	-0.47480	-0.17160
H	-2.94790	0.48070	-2.81380
H	-3.54250	2.05600	-2.30720
H	-2.81640	4.04790	0.78020
H	-1.81790	4.27000	-0.64110
H	-3.48360	3.69270	-0.80140
H	-2.80010	1.65210	0.64850
H	0.14420	1.97000	-3.98210
H	-0.23520	0.37020	-3.37400
H	-1.48630	1.35210	-4.15100

==> 5_w.xyz <==
43
Structure 5, w geometry

C	-0.05190	-0.33380	0.06230
C	0.00790	0.00650	1.41800
C	1.26430	0.25030	1.98620
C	2.41670	0.19840	1.21110
C	2.33740	-0.11720	-0.14140
C	1.10040	-0.39290	-0.71260
C	-1.25630	-0.00350	2.24060
N	-1.85390	1.37050	2.62810
C	-1.98880	2.27030	1.40080
C	-2.92020	1.79120	0.29990
C	-3.23090	1.07980	3.27190
C	-3.94650	2.24220	3.91360
C	-4.00620	2.32680	5.30870
C	-4.70700	3.35100	5.93460
C	-5.36700	4.30850	5.17290

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C	-5.33810	4.22430	3.78470
C	-4.64270	3.19550	3.16040
C	-0.94640	2.12100	3.60140
C	-0.57640	1.39990	4.88680
H	3.37930	0.38750	1.66890
H	3.23680	-0.16470	-0.74190
H	1.03150	-0.66560	-1.75790
H	-1.00260	-0.58390	-0.39290
H	1.36070	0.46150	3.04290
H	-1.11440	-0.52680	3.18280
H	-2.04710	-0.51690	1.69880
H	-2.61930	0.83860	-0.12880
H	-2.87550	2.52940	-0.50280
H	-3.96110	1.71910	0.61000
H	-0.97740	2.38050	1.01490
H	-2.31030	3.23710	1.78190
H	-0.05420	2.37380	3.03260
H	-1.47350	3.04540	3.82830
H	0.00790	0.49550	4.72680
H	0.04330	2.08240	5.47130
H	-1.43890	1.15150	5.50000
H	-3.04290	0.30570	4.01220
H	-3.82620	0.63410	2.47900
H	-4.66900	3.13420	2.08060
H	-5.87240	4.95050	3.18560
H	-5.91550	5.10600	5.65760
H	-4.74600	3.39290	7.01550
H	-3.52580	1.57170	5.91920