Structural studies on 4-oxo-*N*-5-methyl-1,3-thiazol-2-yl-4*H*-chromone -3-carboxamide

Supplementary Information

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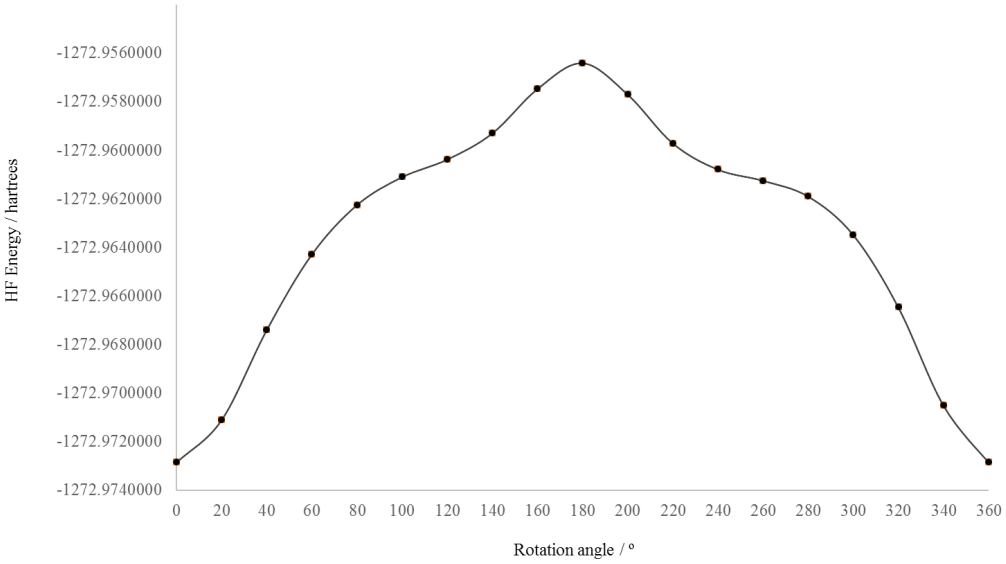
Gaseous phase quantum chemical calculations

Single point geometric energies calculations for **1_P2$_1$/n** at crystal geometry and for of conformers obtained by rotation of the thiazole ring (C) around the C-C bond connecting the B and C fragments were performed using density functional theory. The quantum chemical calculations were performed at the B3LYP exchange correlation functional, which combines the hybrid exchange functional of Becke (Becke, 1997) with the gradient-correlation functional of Lee, (Lee *et al*. 1998) and the split-valence polarised 6-311+G(d, p) basis set (Hehre, 1986) level of theory. The GaussView 3.0 (DenningtonII, program was used to get visual animation. All theoretical calculations were performed with the GAUSSIAN 03 program package (Frisch *et al*., 2003) The bonding characteristics of the compounds studied were investigated using natural population (NPA) analysis of Reed and Weinhold(Reed & Weinhold, 1983, Reed et al., 1998). Figure SI1 gives the graphic representation of the HF energy (with ZPE correction) for the conformers obtained by the rotation above mentioned. The lowest energy calculated corresponds to a rotation angle of 0º, that is when the S atom of the thiazole ring is in a –cis position with respect to the carbonyl oxygen atom of the amide, while the maximum energy computed corresponds to a rotation angle of 180º, when it is in a *trans* position.

The values for the atomic natural total charges have been retrieved at same theory level. Relevant values are presented in figure SI2 at crystal conformation. The inspection of the files for the different geometries obtained from the rotations around the C-C bond connecting the thiazole and the amide moiety revealed

that the change of charges for the S atom was the most sensitive. The lowest energy conformer (at 0º of rotation) showed the highest positive charge for the atom, as depicted in graphic representation of Figure SI3.


HF Energy / hartrees
-1272.9560000
-1272.9580000
-1272.9600000
-1272.9620000
-1272.9640000
-1272.9660000
-1272.9680000
-1272.9700000
-1272.9720000
-1272.9740000
0 20 40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360
Rotation angle / º

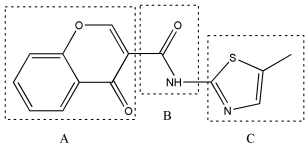

O
O
NH
S
N
O
A
B
C

Figure SI1 - HF energy at the B3LYP/6-311+G(d) level of theory of **1_P21/n** at conformations archived by rotation of the thiazole ring around the C-C bond connecting to the amide.

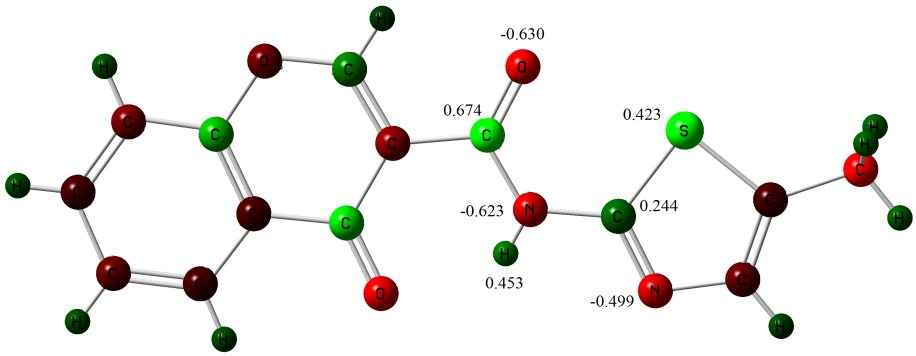


Figure SI2 - Natural atomic charges from population analysis (NBO), at the B3LYP/6-311+G(d) level of theory for **1_P21/n** at crystal geometric conformation. The charge distributions are presented within a relative charge range of -1.000 (green) to +1.000 (light red).

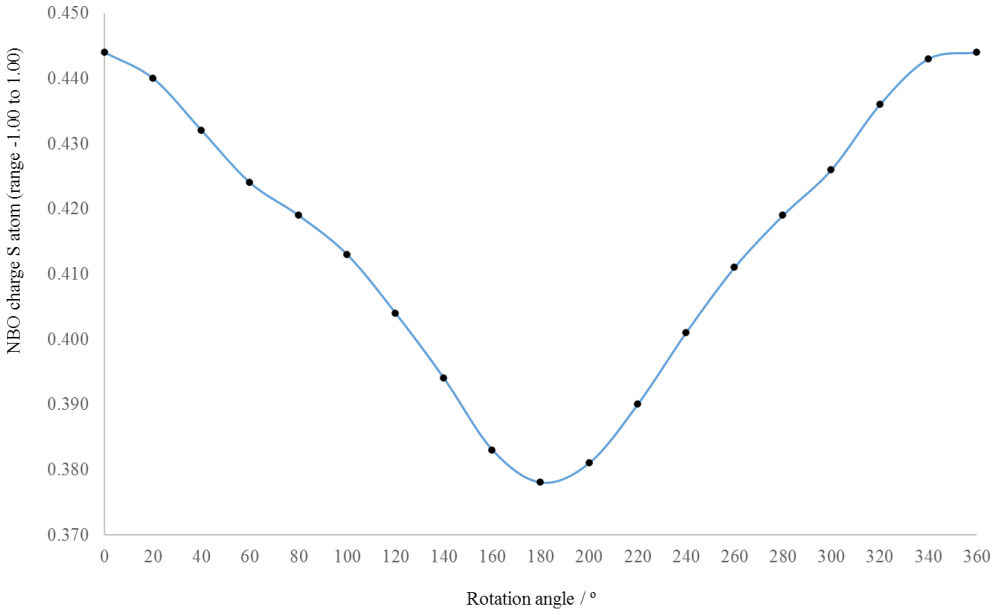

0.450
0.440
0.430
0.420
0.410
0.400
0.390
0.380
0.370
NBO charge S atom (range -1.00 to 1.00)
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
Rotation angle / °

Figure SI3 - Natural atomic charges from population analysis (NBO), at the B3LYP/6-311+G(d) level of theory for the S atom of **1_P21/n** at conformation archived by rotation of the thiazole ring around the C-C bond connecting to the amide. The charge distributions are presented within a relative charge range of -1.000 to +1.000.

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Lee, C., Yang , W. & Parr, W.G. (1998) *Phys Rev* **B37**, 785--789.

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DenningtonII, R., Keith, T. & Millam, J. GaussView, Version 4.1.2, Semichem, Inc., Shawnee

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Datablock: P21/n

Bond precision: C-C = 0.0069 A Wavelength=0.71075
Cell: a=4.8722(4) b=12.0436(10) c=21.9803(16)
alpha=90 beta=96.353(8) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1281.86(18)	1281.86(18)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H10 N2 O3 S	C14 H10 N2 O3 S
Sum formula	C14 H10 N2 O3 S	C14 H10 N2 O3 S
Mr	286.30	286.30
Dx,g cm-3	1.484	1.484
Z	4	4
Mu (mm-1)	0.261	0.261
F000	592.0	592.0
F000'	592.76	
h,k,lmax	6,15,28	6,15,28
Nref	2960	2948
Tmin,Tmax	0.991,0.995	0.814,1.000
Tmin'	0.930	

Correction method= # Reported T Limits: Tmin=0.814
Tmax=1.000 AbsCorr = MULTI-SCAN
Data completeness= 0.996 Theta(max)= 27.544
R(reflections)= 0.0977(1984) wR2(reflections)= 0.2251(2945)
S = 1.141 Npar= 182

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.24
Report
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00692
Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 24.783
Check
And 2 other PLAT906 Alerts
More ...
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 6
Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers 1
Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0
Note

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 1
Report
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 2
Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 8
Note

PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 5 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
4 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: P21/c

Bond precision: C-C = 0.0042 A Wavelength=0.71075
Cell: a=7.4646(5) b=30.626(2) c=11.0869(8)
alpha=90 beta=93.232(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2530.6(3)	2530.6(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H10 N2 O3 S	C14 H10 N2 O3 S
Sum formula	C14 H10 N2 O3 S	C14 H10 N2 O3 S
Mr	286.30	286.30
Dx,g cm-3	1.503	1.503
Z	8	8
Mu (mm-1)	0.264	0.264
F000	1184.0	1184.0
F000'	1185.52	
h,k,lmax	9,39,14	9,39,14
Nref	5834	5716
Tmin,Tmax	0.984,0.997	0.984,0.997
Tmin'	0.984	

Correction method= # Reported T Limits: Tmin=0.984
Tmax=0.997 AbsCorr = MULTI-SCAN
Data completeness= 0.980 Theta(max)= 27.529
R(reflections)= 0.0598(3733) wR2(reflections)= 0.1532(5716)
S = 1.078 Npar= 371

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00421 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H28 .. N133 .. 2.69 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H23B .. S131 .. 3.00 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.647 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 49 Report

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT432_ALERT_2_G Short Inter X...Y Contact O14 .. C22 .. 3.00 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact O24 .. C12 .. 2.96 Ang.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 67 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 7 Note

   0 **ALERT level A** = Most likely a serious problem - resolve or explain
   0 **ALERT level B** = A potentially serious problem, consider carefully
   5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
   6 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check