Supplementary Materials

CartesianCo−ordinates of optimized geometry at B3LYP/6−31G (d, p) (1)

C	3.19696900	−1.18947100	−0.11479500
C	2.33950900	−0.05164900	−0.16975400
C	0.59856500	−1.50038200	−0.30643000
C	2.78752700	1.36261900	−0.23987600
C	3.95114700	1.73798200	−0.93139500
C	1.98366100	2.36206800	0.33313900
C	4.30492300	3.08110900	−1.03612200
H	4.56977600	0.98124500	−1.39986500
C	2.35039300	3.70227700	0.24078200
H	1.07112200	2.07482100	0.84343500
C	3.51180600	4.06586600	−0.44369400
H	5.20024200	3.35867900	−1.58418000
H	1.72512000	4.46342400	0.69760100
H	3.79455800	5.11168900	−0.52051900
C	4.65206700	−1.17580900	0.18198500
C	5.51081400	−2.04730800	−0.50675000
C	5.18399100	−0.36263000	1.19587700
C	6.87043100	−2.08726300	−0.20393300
H	5.09699000	−2.69340400	−1.27320200
C	6.54296100	−0.40907500	1.50008200
H	4.53038100	0.30052900	1.75305700
C	7.39187600	−1.26729500	0.79846300
H	7.52323800	−2.76132900	−0.75085100
H	6.93771500	0.22158000	2.29121900
H	8.45135200	−1.30013500	1.03501100
N	1.01704000	−0.23682000	−0.21723000
N	1.37988100	−2.58962700	−0.46653400
N	2.67810600	−2.41301700	−0.32840000
H	−1.01266900	−2.74938800	−0.38051600
C	−2.92449600	−1.11360300	−0.12704800
H	−3.21999700	−2.16274300	−0.20490000
N	−0.74499500	−1.77426200	−0.27995700
N	−1.66932600	−0.79652000	−0.15581500
C	−3.95181400	−0.09899800	0.00753500
C	−5.35210500	−0.45602600	0.04782300
C	−3.58936400	1.26055600	0.10290500
C	−5.82548000	−1.79337500	−0.03700100
C	−6.33475600	0.57862900	0.18139000
C	−4.58220800	2.26595800	0.23421300
C	−7.17296400	−2.08695900	0.00646800

H	−5.12749400	−2.61655400	−0.13766400
C	−7.71205400	0.24621700	0.22287800
C	−5.90847400	1.93344700	0.27185300
H	−4.24557500	3.29479900	0.30181700
C	−8.13307600	−1.06173200	0.13743700
H	−7.49598900	−3.12181200	−0.06113300
H	−8.43412800	1.05235700	0.32461200
H	−6.66185100	2.71017300	0.37236400
H	−9.19042000	−1.30519700	0.17036100
O	−2.31975800	1.69150800	0.07643300
H	−1.71834000	0.90999600	−0.02875200

CartesianCo−ordinates of optimized geometry at B3LYP/6−31G (d, p) (2)

C	2.97758400	−1.06480900	−0.09537300
C	2.00152200	−0.02876400	−0.15747600
C	0.42175000	−1.65181800	−0.26638600
C	2.29672100	1.42541900	−0.24219000
C	3.39498300	1.92055700	−0.96353700
C	1.40729700	2.33481900	0.35282600
C	3.60249400	3.29365700	−1.07506400
H	4.07769000	1.23259800	−1.44922900
C	1.62851000	3.70633100	0.25465600
H	0.54415900	1.94850900	0.88354000
C	2.72652200	4.19004900	−0.45948800
H	4.44898800	3.66348100	−1.64586500
H	0.94003500	4.39847000	0.73046800
H	2.89593500	5.25978500	−0.54099400
C	4.42430900	−0.89107000	0.19121200
C	5.36809800	−1.68409600	−0.48115900
C	4.87273500	−0.00090900	1.18046700
C	6.72560600	−1.57267600	−0.18689900
H	5.02178700	−2.39013800	−1.22797300
C	6.23034700	0.10482800	1.47589800
H	4.15529700	0.60311100	1.72605700
C	7.16250200	−0.67647100	0.79044800
H	7.44338600	−2.18826500	−0.72135700
H	6.55915600	0.79412400	2.24814100
H	8.22059700	−0.59109000	1.02007300
N	0.70595200	−0.35014300	−0.19525400
N	1.31879700	−2.65316100	−0.41897300
N	2.59064900	−2.33934600	−0.29159500

H	−1.00728200	−3.08845300	−0.32895800
C	−3.10493300	−1.77478900	−0.13127900
H	−3.23685800	−2.86304800	−0.21367200
N	−0.87856100	−2.08342300	−0.23101400
N	−1.93255400	−1.24324100	−0.12873300
C	−4.31923400	−0.97297700	−0.02781900
C	−5.56954600	−1.60360300	−0.02722200
C	−4.28137000	0.43414800	0.07092300
C	−6.75572300	−0.87470200	0.06817100
C	−5.44944500	1.16741600	0.16610200
C	−6.69875800	0.51990100	0.16571200
H	−5.43100400	2.24966400	0.24124700
H	−5.62205800	−2.68703500	−0.10272300
H	−7.70431700	−1.39760000	0.06539900
O	−7.78448500	1.33702700	0.26308100
C	−9.07539300	0.74585000	0.26445200
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H	−9.26874300	0.19548300	−0.66497600
H	−3.31778200	0.93216900	0.06876700

CartesianCo−ordinates of optimized geometry at B3LYP/6−31G (d, p) (3)

C	3.33597000	−1.04160900	−0.08827100
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C	0.80016200	−1.71692300	−0.25983700
C	2.57097100	1.42248800	−0.25338100
C	3.65237500	1.95027900	−0.97687100
C	1.65039600	2.30506000	0.33439100
C	3.81324200	3.32893800	−1.09734100
H	4.35884400	1.28287600	−1.45728900
C	1.82473800	3.68271400	0.22718200
H	0.79989300	1.89275300	0.86596800
C	2.90651300	4.19913900	−0.48884000
H	4.64748400	3.72348000	−1.66970800
H	1.11226500	4.35403300	0.69761100
H	3.03953500	5.27349900	−0.57725700
C	4.77538500	−0.81768000	0.19963500
C	5.74649700	−1.58419700	−0.46481000
C	5.19299300	0.09463800	1.18220800
C	7.09908400	−1.42553000	−0.16969000
H	5.42491800	−2.30754200	−1.20610500

C	6.54596200	0.24821600	1.47818700
H	4.45504800	0.67834000	1.72253700
C	7.50478000	−0.50718900	0.80053800
H	7.83764900	−2.02151500	−0.69810700
H	6.85036700	0.95445600	2.24517100
H	8.55913100	−0.38479300	1.03075600
N	1.04136600	−0.40508300	−0.19829700
N	1.73349900	−2.68818200	−0.40587700
N	2.99253900	−2.33013900	−0.27862900
H	−0.57574400	−3.20121400	−0.31434900
C	−2.71834100	−1.96866600	−0.12744500
H	−2.80075900	−3.06259800	−0.20588100
N	−0.48193200	−2.19184300	−0.22177800
N	−1.56820100	−1.38797800	−0.12467600
C	−3.96726900	−1.22781300	−0.02975200
C	−5.19222500	−1.91261200	−0.03359300
C	−4.00789300	0.17600800	0.06316900
C	−6.40517500	−1.24306100	0.05462700
H	−5.19693300	−2.99749700	−0.11173100
C	−5.20904300	0.85760700	0.15270600
H	−3.07250400	0.72590800	0.05826400
C	−6.44814800	0.16669100	0.16071700
H	−7.32095900	−1.82030600	0.04008000
H	−5.18830000	1.93847700	0.21469500
C	−7.66726900	2.29774300	0.22333800
H	−8.69242500	2.64662700	0.35304700
H	−7.06629800	2.73069600	1.03152800
H	−7.28869000	2.69497300	−0.73044800
C	−8.90035400	0.12301100	0.12520600
H	−8.99411000	−0.66715200	0.87961400
H	−9.73208300	0.81393600	0.26731800
H	−9.00655500	−0.34191300	−0.86659400
N	−7.64886300	0.84547100	0.27398400

CartesianCo−ordinates of optimized geometry at B3LYP/6−31G (d, p) (4)

C	2.33411600	−1.13082900	−0.11277400
C	1.36791600	−0.08347600	−0.16627100
C	−0.22262500	−1.69677700	−0.27897700
C	1.67422800	1.36742200	−0.24721200
C	2.77808800	1.85213500	−0.96789600
C	0.79149800	2.28521100	0.34571600

C	2.99683500	3.22303000	−1.08155600
H	3.45532100	1.15797800	−1.45226200
C	1.02414100	3.65452500	0.24476400
H	−0.07595600	1.91192400	0.87857200
C	2.12701000	4.12750100	−0.46889500
H	3.84686200	3.58488400	−1.65209400
H	0.33950800	4.35237300	0.71724600
H	2.30478600	5.19563300	−0.55280700
C	3.78292500	−0.97037000	0.17134100
C	4.71860800	−1.76567200	−0.50930400
C	4.23925900	−0.09137300	1.16687100
C	6.07743800	−1.66711100	−0.21656300
H	4.36569100	−2.46282400	−1.26135100
C	5.59804800	0.00076500	1.46107700
H	3.52760000	0.51440800	1.71805900
C	6.52259600	−0.78246900	0.76752400
H	6.78953600	−2.28378400	−0.75718200
H	5.93373200	0.68100700	2.23827000
H	7.58165100	−0.70739300	0.99610800
N	0.06976800	−0.39784000	−0.19972800
N	0.66028600	−2.70480900	−0.43797400
N	1.93645400	−2.40087900	−0.31244800
H	−1.70283300	−3.09955400	−0.34277800
C	−3.76503400	−1.65600200	−0.09715800
H	−3.98847200	−2.72678900	−0.18127500
N	−1.53343800	−2.10242200	−0.24376700
N	−2.54894500	−1.22138200	−0.11910700
C	−4.88434700	−0.74286500	0.04263000
C	−6.19635300	−1.25410500	0.06415800
C	−4.69486100	0.66243100	0.16276200
C	−7.29692600	−0.42086800	0.20037900
C	−5.81341500	1.49637400	0.30085400
C	−7.09554700	0.96083200	0.31944600
H	−5.64343800	2.56404500	0.39049100
H	−7.94826500	1.62501800	0.42690800
O	−3.47823900	1.23777000	0.15006400
H	−2.79512900	0.53595300	0.03285300
H	−6.33549300	−2.32870500	−0.02847200
H	−8.29965400	−0.83485800	0.21487100

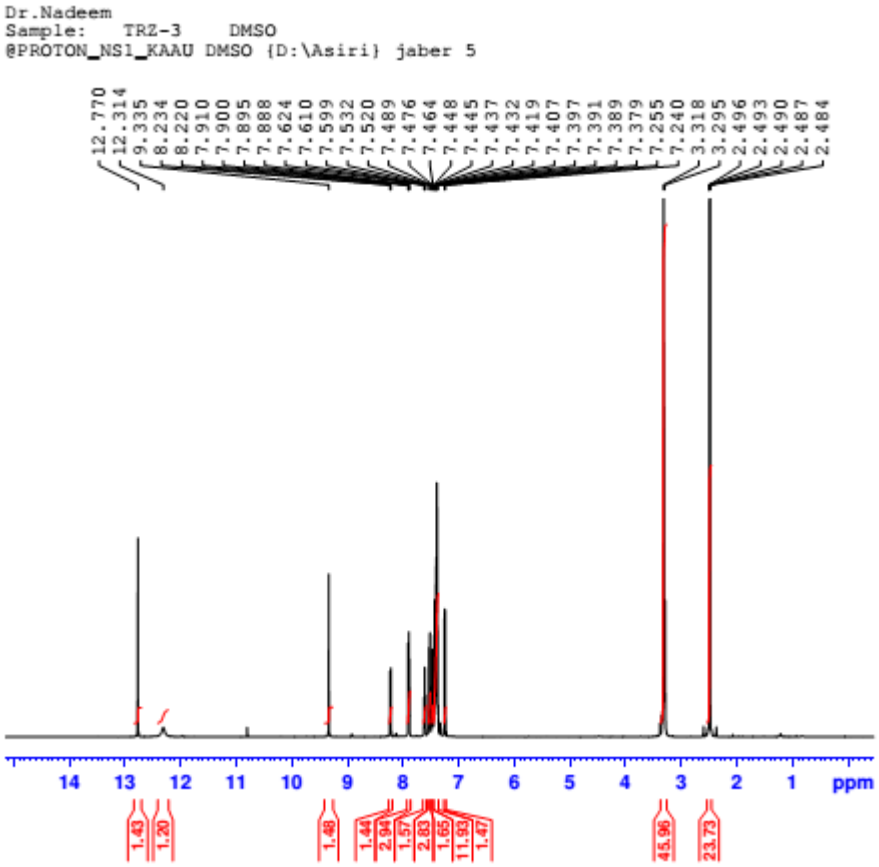

Figure S1. Experimental ^{1}H-NMR spectrum of **1** measured in d_6-DMSO.

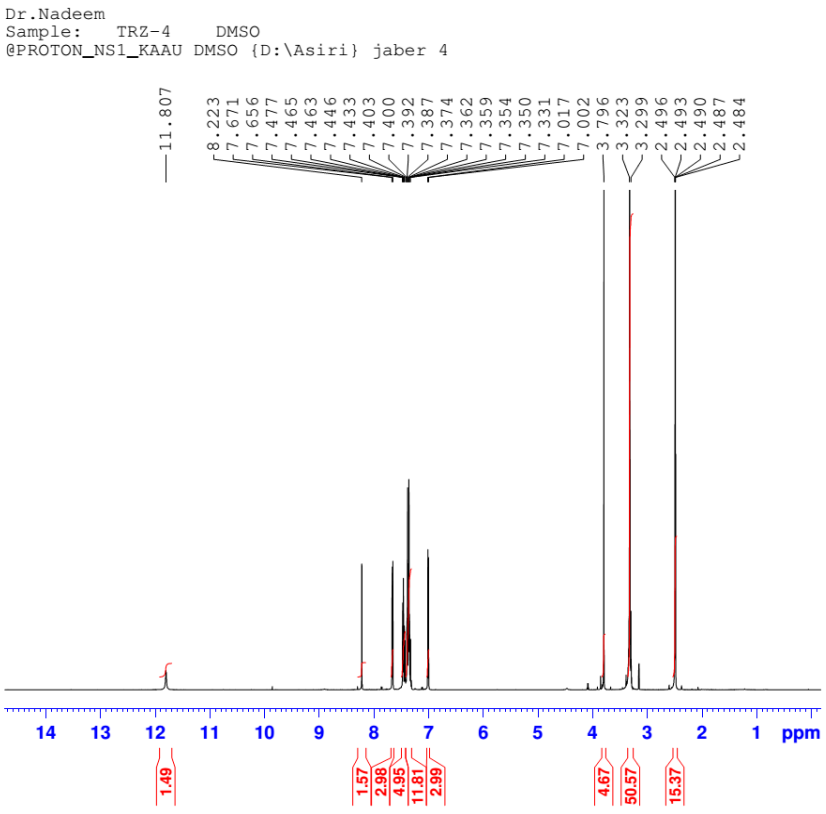

Figure S2. Experimental ^{1}H-NMR spectrum of **2** measured in d_6-DMSO.

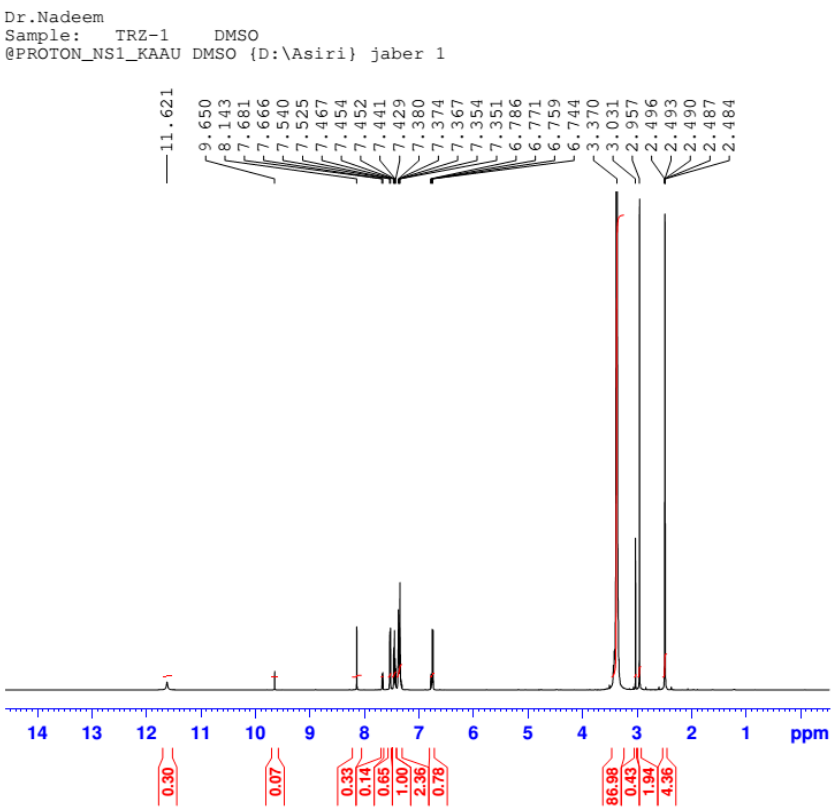

Figure S3. Experimental ^{1}H-NMR spectrum of **3** measured in d_6-DMSO.

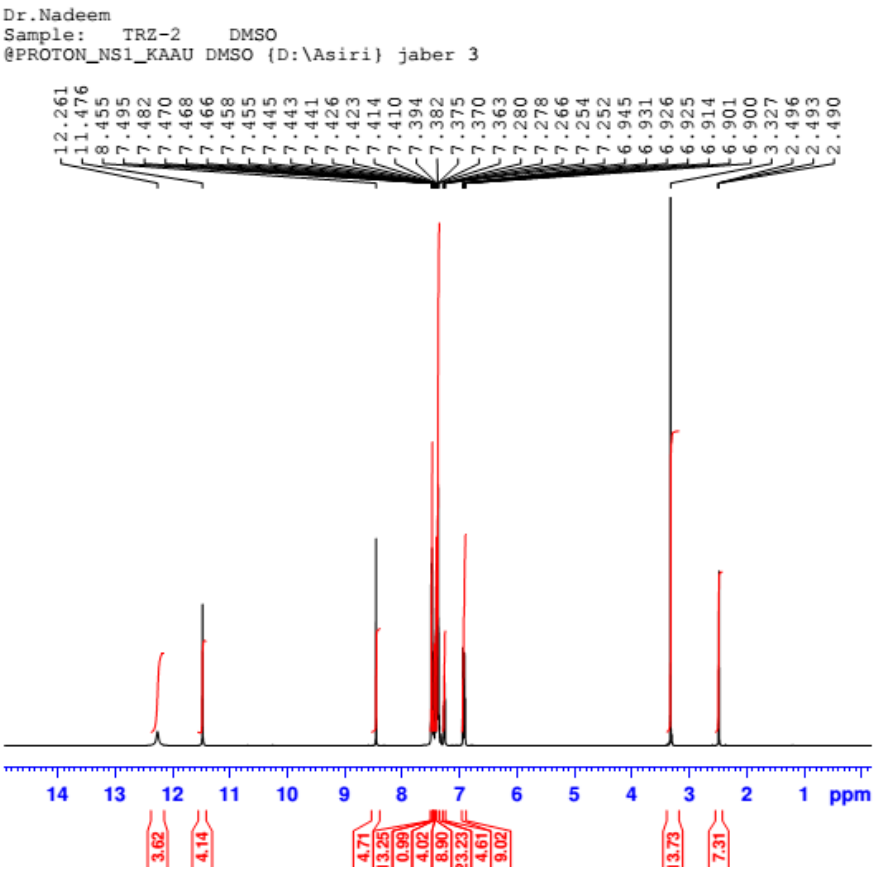

Figure S4. Experimental ^{1}H-NMR spectrum of **4** measured in d_6-DMSO.

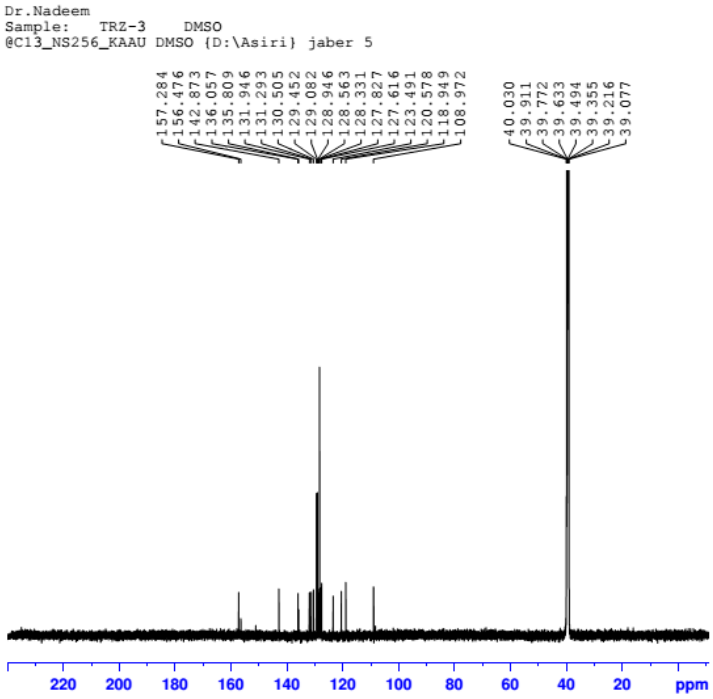

Figure S5. Experimental ^{13}C-NMR spectrum of **1** measured in d_6-DMSO.

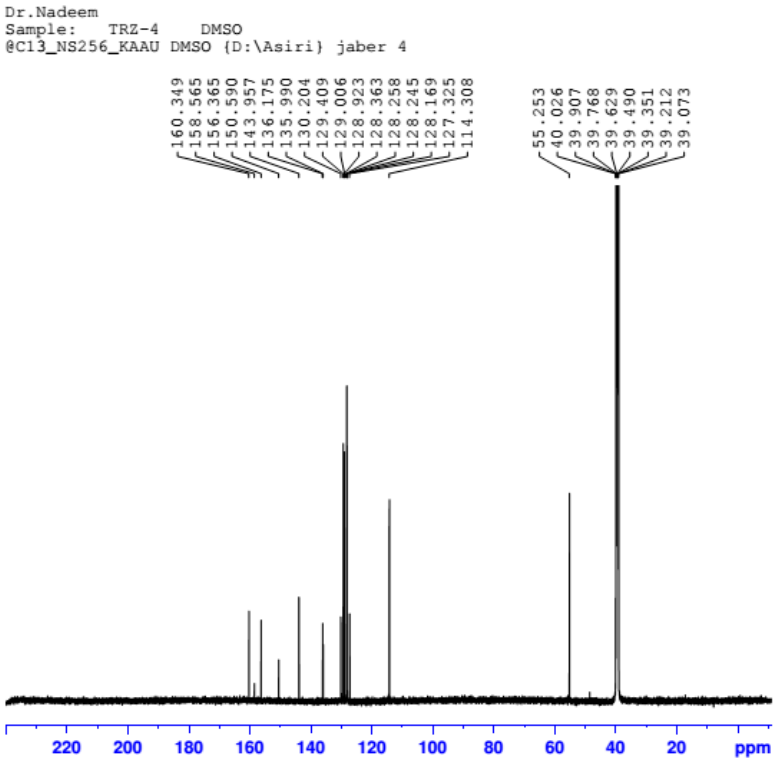

Figure S6. Experimental ^{13}C-NMR spectrum of **2** measured in d_6-DMSO.

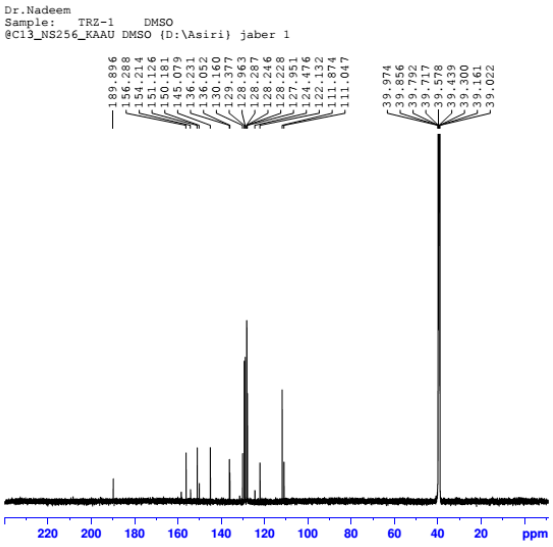

Figure S7. Experimental ^{13}C-NMR spectrum of **3** measured in d_6-DMSO.

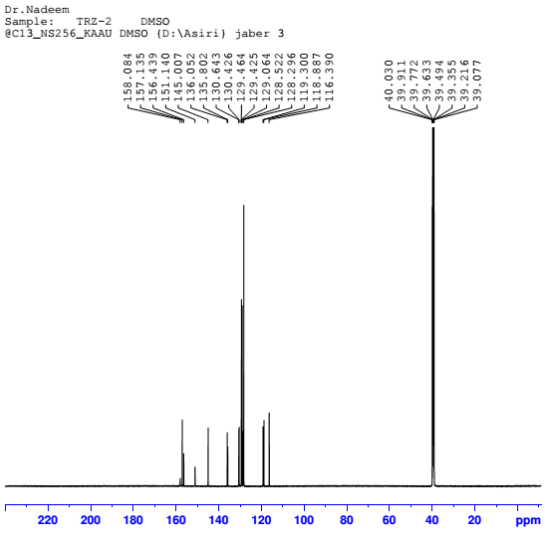

Figure S8. Experimental ^{13}C-NMR spectrum of **4** measured in d_6-DMSO.

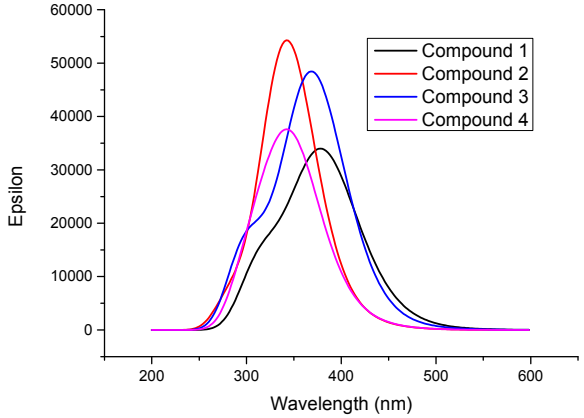

Figure S9. Combined simulated UV–vis. spectra of (**1**–**4**) measured at TD–B3LYP/6–31G (d, p) level in gas phase.

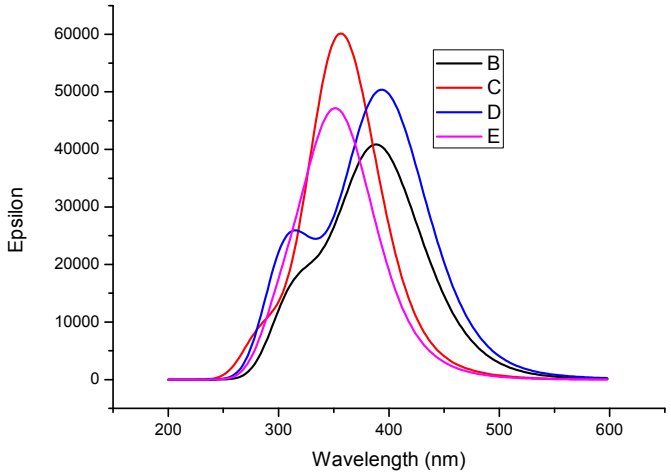

Figure S10. Combined simulated UV–vis. spectra of Compounds (**1**–**4**) measured at TD–B3LYP/6–31G (d, p) level measured in DMSO.

Molecule 1Cif

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(compiled Jul 11 2012,15:38:31)
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LATT 1
SYMM 0.5−X, 0.5+Y, 0.5−Z
SFACCHN O
UNIT 104 76 20 4
MERG 2
FMAP 2
GRID
PLAN 20
TEMP 23
SIZE 0.48 0.16 0.15
BOND $H
HTAB
CONF
L.S. 15
ACTA 52
WGHT 0.06050 0.31320 0.00000 0.00000 0.00000 0.33330
FVAR 5.19820
N1    3   0.65264   0.03442   0.14503  11.00000   0.05845   0.05648 =
     0.04739  −0.00239   0.01050   0.00118
C2    1   0.68311   0.00284   0.21855  11.00000   0.05185   0.04894 =
     0.04712  −0.00394   0.00665  −0.00510
N2    3   0.94170  −0.02273   0.10197  11.00000   0.06634   0.06351 =
     0.05186   0.00111   0.01592   0.00687
N3    3   0.96464  −0.05728   0.17355  11.00000   0.06178   0.05772 =
     0.05537  −0.00058   0.01294   0.00388
N5    3   0.60803   0.09574  −0.00542  11.00000   0.06318   0.06522 =
     0.05439  −0.00340   0.01108   0.00839
N4    3   0.75933   0.04938   0.01218  11.00000   0.07255   0.07502 =
     0.05289   0.00850   0.01935   0.01977
C16   1   0.60562   0.12956  −0.07406  11.00000   0.05662   0.05982 =
     0.05149  −0.00593   0.00817   0.00423
AFIX 43
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```
H16   2   0.70769   0.12283  −0.10909  11.00000  −1.20000
AFIX 0
C17   1   0.44474   0.17814  −0.09724  11.00000   0.05206   0.05525 =
     0.06199  −0.01641   0.00025   0.00187
O1    4   0.26256   0.14727   0.01996  11.00000   0.07524   0.09976 =
     0.08665  −0.01813   0.02980   0.00230
C3    1   0.83687  −0.04733   0.23186  11.00000   0.05265   0.05078 =
     0.04977  −0.00361   0.00787  −0.00290
C1    1   0.78237   0.01918   0.08875  11.00000   0.06045   0.05600 =
     0.04846  −0.00303   0.01089   0.00130
C10   1   0.87174  −0.09157   0.30699  11.00000   0.06036   0.04663 =
     0.05235  −0.00234   0.00782   0.00138
C4    1   0.55179   0.02649   0.28247  11.00000   0.06050   0.04692 =
     0.05020  −0.00025   0.01421  −0.00241
C22   1   0.45290   0.22129  −0.16932  11.00000   0.06078   0.04820 =
     0.06547  −0.01198  −0.01089   0.00379
C15   1   1.06929  −0.10474   0.34288  11.00000   0.06098   0.07059 =
     0.07676   0.01028   0.00792   0.00616
AFIX 43
H15   2   1.17982  −0.08493   0.32082  11.00000  −1.20000
AFIX 0
C11   1   0.71025  −0.12195   0.34051  11.00000   0.06394   0.05434 =
     0.05893  −0.00102   0.00811  −0.00285
AFIX 43
H11   2   0.57684  −0.11354   0.31706  11.00000  −1.20000
AFIX 0
C21   1   0.28750   0.26597  −0.19321  11.00000   0.06510   0.05507 =
     0.09240  −0.01992  −0.01384   0.00837
C9    1   0.62712   0.03353   0.36682  11.00000   0.08251   0.05689 =
     0.05299  −0.00217   0.00973   0.00318
AFIX 43
H9    2   0.76115   0.02132   0.38527  11.00000  −1.20000
AFIX 0
C23   1   0.61896   0.22284  −0.21813  11.00000   0.06597   0.05851 =
     0.06810  −0.00148  −0.00348   0.00258
AFIX 43
H23   2   0.73035   0.19471  −0.20388  11.00000  −1.20000
AFIX 0
C5    1   0.35235   0.04602   0.25593  11.00000   0.06013   0.06297 =
     0.06367   0.00198   0.01554  −0.00088
AFIX 43
H5    2   0.30247   0.04287   0.19929  11.00000  −1.20000
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AFIX 0
C18   1   0.27932   0.18373  −0.05053  11.00000   0.05927   0.06991 =
     0.07449  −0.02360   0.00956  −0.00230
C19   1   0.11700   0.22897  −0.07540  11.00000   0.05551   0.08524 =
     0.11061  −0.03928   0.01213   0.00461
AFIX 43
H19   2   0.00602   0.23186  −0.04421  11.00000  −1.20000
AFIX 0
C12   1   0.74536  −0.16476   0.40862  11.00000   0.08891   0.05719 =
     0.06847   0.00651   0.02176  −0.00066
AFIX 43
H12   2   0.63565  −0.18523   0.43051  11.00000  −1.20000
AFIX 0
C24   1   0.62003   0.26500  −0.28631  11.00000   0.09234   0.06469 =
     0.07831   0.00716  −0.00299  −0.00408
AFIX 43
H24   2   0.73275   0.26534  −0.31670  11.00000  −1.20000
AFIX 0
C6    1   0.22776   0.07007   0.31319  11.00000   0.06948   0.07181 =
     0.09393   0.00400   0.03362   0.00546
AFIX 43
H6    2   0.09361   0.08245   0.29521  11.00000  −1.20000
AFIX 0
C26   1   0.29389   0.30726  −0.26564  11.00000   0.09873   0.05040 =
     0.10238  −0.00167  −0.03025   0.01510
AFIX 43
H26   2   0.18335   0.33513  −0.28242  11.00000  −1.20000
AFIX 0
C20   1   0.12352   0.26795  −0.14449  11.00000   0.06813   0.06830 =
     0.11506  −0.02553  −0.01397   0.01567
AFIX 43
H20   2   0.01525   0.29704  −0.16007  11.00000  −1.20000
AFIX 0
C14   1   1.10248  −0.14725   0.41141  11.00000   0.07616   0.08202 =
     0.08226   0.01401  −0.00047   0.01825
AFIX 43
H14   2   1.23541  −0.15558   0.43552  11.00000  −1.20000
AFIX 0
C7    1   0.30152   0.07574   0.39652  11.00000   0.10837   0.06968 =
     0.08312  −0.00576   0.04938   0.00348
AFIX 43
H7    2   0.21637   0.09105   0.43519  11.00000  −1.20000
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AFIX 0
C8    1   0.50102   0.05887   0.42313  11.00000   0.12174   0.06718 =
     0.05460  −0.00545   0.02563   0.00032
AFIX 43
H8    2   0.55165   0.06451   0.47938  11.00000  −1.20000
AFIX 0
C13   1   0.94141  −0.17718   0.44405  11.00000   0.10531   0.06408 =
     0.06807   0.01568   0.01221   0.01992
AFIX 43
H13   2   0.96473  −0.20582   0.49008  11.00000  −1.20000
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C25   1   0.45545   0.30703  −0.31044  11.00000   0.11083   0.06160 =
     0.09242   0.00879  −0.01289   0.00479
AFIX 43
H25   2   0.45689   0.33479  −0.35717  11.00000  −1.20000
H2    2   0.86974   0.04137  −0.02193  11.00000   0.08658
H1    2   0.39354   0.11887   0.03188  11.00000   0.12375
HKLF 4
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 Refinement of F^2^ against ALL reflections.  The weighted R−factor wR and
 goodness of fit S are based on F^2^,Conventional R−factors R are based
 on F, with F set to zero forNegative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only forCalculating R−factors(gt) etc. and is
Not relevant to theChoice of reflections for refinement.  R−factors based
 on F^2^ are statistically about twice as large as those based on F, and R−
 factors based on ALL data will be even larger.
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C2C 0.6831(2) 0.00284(7) 0.21855(8) 0.0492(3) Uani 1 1 d . . .
N2N 0.9417(2) −0.02273(7) 0.10197(8) 0.0599(3) Uani 1 1 d . . .
N3N 0.96465(19) −0.05728(6) 0.17355(8) 0.0578(3) Uani 1 1 d . . .
N5N 0.6080(2) 0.09574(7) −0.00542(8) 0.0606(3) Uani 1 1 d . . .
N4N 0.7593(2) 0.04938(7) 0.01218(8) 0.0659(4) Uani 1 1 d . . .
C16C 0.6056(2) 0.12956(8) −0.07406(9) 0.0558(3) Uani 1 1 d . . .
H16H 0.7077 0.1228 −0.1091 0.067 Uiso 1 1Calc R . .
C17C 0.4447(2) 0.17814(8) −0.09724(10) 0.0569(4) Uani 1 1 d . . .
O1 O 0.2626(2) 0.14727(8) 0.01996(9) 0.0857(4) Uani 1 1 d . . .
C3C 0.8369(2) −0.04733(7) 0.23186(9) 0.0509(3) Uani 1 1 d . . .
C1C 0.7824(2) 0.01918(8) 0.08875(9) 0.0546(3) Uani 1 1 d . . .
C10C 0.8717(2) −0.09157(7) 0.30699(9) 0.0530(3) Uani 1 1 d . . .
C4C 0.5518(2) 0.02649(7) 0.28247(9) 0.0519(3) Uani 1 1 d . . .
C22C 0.4529(2) 0.22129(7) −0.16932(10) 0.0595(4) Uani 1 1 d . . .
C15C 1.0693(3) −0.10474(9) 0.34288(11) 0.0694(4) Uani 1 1 d . . .
H15H 1.1798 −0.0849 0.3208 0.083 Uiso 1 1Calc R . .
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C11C 0.7102(2) −0.12195(8) 0.34051(10) 0.0590(4) Uani 1 1 d . . .
H11H 0.5768 −0.1135 0.3171 0.071 Uiso 1 1Calc R . .
C21C 0.2875(3) 0.26597(8) −0.19321(12) 0.0725(5) Uani 1 1 d . . .
C9C 0.6271(3) 0.03353(8) 0.36682(10) 0.0640(4) Uani 1 1 d . . .
H9H 0.7612 0.0213 0.3853 0.077 Uiso 1 1Calc R . .
C23C 0.6190(3) 0.22284(8) −0.21812(10) 0.0650(4) Uani 1 1 d . . .
H23H 0.7303 0.1947 −0.2039 0.078 Uiso 1 1Calc R . .
C5C 0.3524(2) 0.04601(8) 0.25593(11) 0.0616(4) Uani 1 1 d . . .
H5H 0.3025 0.0429 0.1993 0.074 Uiso 1 1Calc R . .
C18C 0.2793(2) 0.18373(9) −0.05053(11) 0.0677(4) Uani 1 1 d . . .
C19C 0.1170(3) 0.22897(11) −0.07540(15) 0.0836(6) Uani 1 1 d . . .
H19H 0.0060 0.2319 −0.0442 0.100 Uiso 1 1Calc R . .
C12C 0.7454(3) −0.16476(9) 0.40862(11) 0.0705(4) Uani 1 1 d . . .
H12H 0.6356 −0.1852 0.4305 0.085 Uiso 1 1Calc R . .
C24C 0.6200(3) 0.26500(9) −0.28631(12) 0.0794(5) Uani 1 1 d . . .
H24H 0.7328 0.2653 −0.3167 0.095 Uiso 1 1Calc R . .
C6C 0.2278(3) 0.07007(9) 0.31319(13) 0.0766(5) Uani 1 1 d . . .
H6H 0.0936 0.0824 0.2952 0.092 Uiso 1 1Calc R . .
C26C 0.2939(4) 0.30726(9) −0.26564(14) 0.0869(6) Uani 1 1 d . . .
H26H 0.1834 0.3351 −0.2824 0.104 Uiso 1 1Calc R . .
C20C 0.1235(3) 0.26795(10) −0.14449(15) 0.0856(6) Uani 1 1 d . . .
H20H 0.0153 0.2970 −0.1601 0.103 Uiso 1 1Calc R . .
C14C 1.1025(3) −0.14725(10) 0.41141(12) 0.0808(5) Uani 1 1 d . . .
H14H 1.2354 −0.1556 0.4355 0.097 Uiso 1 1Calc R . .
C7C 0.3015(4) 0.07574(10) 0.39652(13) 0.0842(6) Uani 1 1 d . . .
H7H 0.2164 0.0911 0.4352 0.101 Uiso 1 1Calc R . .
C8C 0.5010(4) 0.05887(9) 0.42313(11) 0.0800(5) Uani 1 1 d . . .
H8H 0.5517 0.0645 0.4794 0.096 Uiso 1 1Calc R . .
C13C 0.9414(3) −0.17718(9) 0.44406(12) 0.0790(5) Uani 1 1 d . . .
H13H 0.9647 −0.2058 0.4901 0.095 Uiso 1 1Calc R . .
C25C 0.4555(4) 0.30703(10) −0.31044(14) 0.0901(6) Uani 1 1 d . . .
H25H 0.4569 0.3348 −0.3572 0.108 Uiso 1 1Calc R . .
H2H 0.8697 0.0414 −0.0219 0.087(6) Uiso 1 1 d R . .
H1H 0.3935 0.1189 0.0319 0.124(9) Uiso 1 1 d R . .

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N2 0.0663(7) 0.0635(7) 0.0519(7) 0.0011(6) 0.0159(5) 0.0069(6)
N3 0.0618(7) 0.0577(7) 0.0554(7) −0.0006(6) 0.0129(5) 0.0039(6)
N5 0.0632(7) 0.0652(8) 0.0544(7) −0.0034(6) 0.0111(5) 0.0084(6)
N4 0.0725(8) 0.0750(9) 0.0529(7) 0.0085(6) 0.0193(6) 0.0198(7)
C16 0.0566(8) 0.0598(8) 0.0515(8) −0.0059(6) 0.0082(6) 0.0042(7)
C17 0.0521(7) 0.0552(8) 0.0620(8) −0.0164(7) 0.0002(6) 0.0019(6)
O1 0.0752(8) 0.0998(10) 0.0866(9) −0.0181(8) 0.0298(7) 0.0023(7)
C3 0.0526(7) 0.0508(7) 0.0498(7) −0.0036(6) 0.0079(6) −0.0029(6)
C1 0.0605(8) 0.0560(8) 0.0485(7) −0.0030(6) 0.0109(6) 0.0013(7)
C10 0.0604(8) 0.0466(7) 0.0523(8) −0.0023(6) 0.0078(6) 0.0014(6)
C4 0.0605(8) 0.0469(7) 0.0502(7) −0.0003(6) 0.0142(6) −0.0024(6)
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C11 0.0639(8) 0.0543(8) 0.0589(8) −0.0010(7) 0.0081(7) −0.0029(7)
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C19 0.0555(9) 0.0852(13) 0.1106(15) −0.0393(12) 0.0121(9) 0.0046(9)
C12 0.0889(12) 0.0572(9) 0.0685(10) 0.0065(8) 0.0218(9) −0.0007(8)
C24 0.0923(13) 0.0647(10) 0.0783(12) 0.0072(9) −0.0030(9) −0.0041(9)
C6 0.0695(10) 0.0718(11) 0.0939(13) 0.0040(10) 0.0336(9) 0.0055(9)
C26 0.0987(14) 0.0504(9) 0.1024(15) −0.0017(10) −0.0303(12) 0.0151(10)
C20 0.0681(11) 0.0683(11) 0.1151(16) −0.0255(11) −0.0140(11) 0.0157(9)
C14 0.0762(11) 0.0820(12) 0.0823(12) 0.0140(10) −0.0005(9) 0.0182(10)
C7 0.1084(15) 0.0697(11) 0.0831(13) −0.0058(10) 0.0494(12) 0.0035(11)
C8 0.1217(17) 0.0672(10) 0.0546(9) −0.0054(8) 0.0256(10) 0.0003(11)
C13 0.1053(14) 0.0641(10) 0.0681(10) 0.0157(8) 0.0122(10) 0.0199(10)
C25 0.1108(17) 0.0616(11) 0.0924(14) 0.0088(10) −0.0129(13) 0.0048(11)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the fullCovariance matrix. TheCell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles;Correlations between esds inCell parameters are only
used when they are defined byCrystal symmetry. An approximate (isotropic)
treatment ofCell esds is used for estimating esds involving l.s. planes.

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Molecule 2Cif

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CrysAlisPro, Agilent Technologies,
Version 1.171.36.20 (release 27−06−2012CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)
Empirical absorptionCorrection using sphericalHarmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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SYMM −X, 0.5+Y, 0.5−Z
SFACCHN O
UNIT 92 76 20 4
MERG 2
FMAP 2
GRID
PLAN 20
TEMP 23
SIZE 0.05 0.08 0.48
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CONF
L.S. 20
ACTA 52
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FVAR 1.69020
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     0.06466  0.00143 −0.00525 −0.00137
N3    3  0.12818  0.40936  0.46126  11.00000  0.04805  0.05515 =
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N4    3  0.62325  0.44122  0.58888  11.00000  0.05869  0.05261 =
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AFIX 43
H4    2  0.64324  0.47722  0.56601  11.00000 −1.20000
AFIX 0
N5    3  0.77881  0.41939  0.65359  11.00000  0.05624  0.05530 =
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C1    1  0.43856  0.40747  0.56000  11.00000  0.04820  0.05064 =
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     0.04181 −0.00298  0.00426 −0.00114
C3    1  0.08431  0.35113  0.48454  11.00000  0.04319  0.04251 =
     0.04982 −0.00051  0.00565  0.00340
C4    1  0.17969  0.25920  0.58764  11.00000  0.04459  0.04857 =
     0.04099  0.00430 −0.00508 −0.00432
C5    1  0.33970  0.21325  0.58139  11.00000  0.04747  0.05908 =
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AFIX 0
C6    1  0.30303  0.15481  0.61346  11.00000  0.06740  0.05151 =
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AFIX 0
C8 1 −0.04866 0.18733 0.66341 11.00000 0.06669 0.07522 =
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H8 2 −0.17815 0.17881 0.69264 11.00000 −1.20000
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C9 1 −0.01625 0.24557 0.62917 11.00000 0.05326 0.06124 =
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H9 2 −0.12560 0.27588 0.63380 11.00000 −1.20000
AFIX 0
C10 1 −0.10908 0.32283 0.43189 11.00000 0.04671 0.05251 =
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0.05891 0.00293 −0.00613 −0.00107
AFIX 43
H11 2 −0.00533 0.23465 0.43001 11.00000 −1.20000
AFIX 0
C12 1 −0.29937 0.23697 0.35738 11.00000 0.06126 0.06120 =
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H12 2 −0.30288 0.19512 0.34249 11.00000 −1.20000
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H14 2 −0.57878 0.36412 0.32732 11.00000 −1.20000
AFIX 0
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C18   1   1.12508   0.39093   0.79028  11.00000   0.05679   0.05639 =
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AFIX 43
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AFIX 0
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AFIX 0
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C21   1   1.44882   0.48071   0.82603  11.00000   0.06194   0.05952 =
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AFIX 0
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AFIX 43
H22   2   1.27448   0.52606   0.72722  11.00000  −1.20000
AFIX 0
C23   1   1.78566   0.45639   0.96182  11.00000   0.06311   0.10751 =
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H23B  2   1.88034   0.44169   1.01138  11.00000  −1.50000
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 F^2^ > 2sigma(F^2^) is used only forCalculating R−factors(gt) etc. and is
Not relevant to theChoice of reflections for refinement.  R−factors based
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 factors based on ALL data will be even larger.
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N5N 0.7788(4) 0.41939(11) 0.65357(14) 0.0552(7) Uani 1 1 d . . .
C1C 0.4387(4) 0.40749(14) 0.56001(17) 0.0494(8) Uani 1 1 d . . .
C2C 0.2227(4) 0.32186(13) 0.55276(16) 0.0448(7) Uani 1 1 d . . .
C3C 0.0843(4) 0.35112(13) 0.48455(17) 0.0452(7) Uani 1 1 d . . .
C4C 0.1797(4) 0.25920(13) 0.58764(16) 0.0451(7) Uani 1 1 d . . .
C5C 0.3397(5) 0.21324(15) 0.58139(18) 0.0551(8) Uani 1 1 d . . .
H5H 0.4733 0.2221 0.5552 0.066 Uiso 1 1Calc R . .
C6C 0.3030(5) 0.15481(15) 0.6135(2) 0.0638(9) Uani 1 1 d . . .
H6H 0.4098 0.1240 0.6073 0.077 Uiso 1 1Calc R . .
C7C 0.1092(6) 0.14150(16) 0.6548(2) 0.0676(10) Uani 1 1 d . . .
H7H 0.0849 0.1019 0.6767 0.081 Uiso 1 1Calc R . .
C8C −0.0486(5) 0.18732(17) 0.66341(19) 0.0680(9) Uani 1 1 d . . .
H8H −0.1781 0.1788 0.6926 0.082 Uiso 1 1Calc R . .
C9C −0.0163(5) 0.24557(15) 0.62916(18) 0.0588(8) Uani 1 1 d . . .
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C10C −0.1091(4) 0.32283(14) 0.43189(16) 0.0480(7) Uani 1 1 d . . .
C11C −0.1205(5) 0.26100(15) 0.40956(18) 0.0576(8) Uani 1 1 d . . .
H11H −0.0053 0.2347 0.4300 0.069 Uiso 1 1Calc R . .
C12C −0.2993(5) 0.23698(15) 0.35737(19) 0.0654(9) Uani 1 1 d . . .
H12H −0.3028 0.1951 0.3425 0.078 Uiso 1 1Calc R . .
C13C −0.4728(5) 0.27577(17) 0.32758(19) 0.0656(9) Uani 1 1 d . . .
H13H −0.5951 0.2598 0.2937 0.079 Uiso 1 1Calc R . .
C14C −0.4638(5) 0.33782(16) 0.34811(18) 0.0615(9) Uani 1 1 d . . .
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C15C −0.2835(4) 0.36109(14) 0.39973(16) 0.0531(8) Uani 1 1 d . . .
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C19C 1.2915(5) 0.38205(15) 0.85695(19) 0.0648(9) Uani 1 1 d . . .
H19H 1.2951 0.3457 0.8903 0.078 Uiso 1 1Calc R . .
C20C 1.4530(5) 0.42719(15) 0.87436(19) 0.0588(9) Uani 1 1 d . . .
C21C 1.4488(5) 0.48071(15) 0.82602(19) 0.0631(9) Uani 1 1 d . . .
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C8 0.067(2) 0.075(3) 0.0627(19) 0.013(2) 0.0099(17) −0.017(2)
C9 0.0534(19) 0.061(2) 0.0617(18) 0.0046(17) 0.0052(16) −0.0035(17)
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C21 0.062(2) 0.060(2) 0.0659(19) −0.0093(18) −0.0106(17) −0.0094(17)
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C23 0.063(2) 0.107(3) 0.086(2) −0.021(2) −0.0188(19) −0.002(2)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the fullCovariance matrix. TheCell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles;Correlations between esds inCell parameters are only
used when they are defined byCrystal symmetry. An approximate (isotropic)
treatment ofCell esds is used for estimating esds involving l.s. planes.
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C23 O1C20C21 −3.2(4) . . . . ?
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Molecule 3Cif

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Version 1.171.36.20 (release 27−06−2012CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)
Empirical absorptionCorrection using sphericalHarmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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_reflns_threshold_expression     >2sigma(I)
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_computing_cell_refinement     'CrysAlis PRO (Agilent, 2012)'
_computing_data_reduction     'CrysAlis PRO (Agilent, 2012)'
_computing_structure_solution     'SHELXS−97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL−97 (Sheldrick, 1997)'
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_computing_publication_material   ?

_iucr_refine_instructions_details
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CELL 0.71073 8.8933 11.1477 11.7484 91.212 106.044 108.519
ZERR 2.0000 0.0010 0.0011 0.0013 0.009 0.010 0.009
LATT 1
SFACCHN
UNIT 48 44 12
MERG 2
FMAP 2
GRID
PLAN 20
TEMP 23
SIZE 0.17 0.26 0.32
BOND $H
HTAB
CONF
L.S. 20
ACTA
EXTI 0.01392
WGHT 0.04620 0.35700 0.00000 0.00000 0.00000 0.33330
FVAR 6.11470
N1    3   0.23539   0.20313   0.27176  11.00000   0.03926   0.04955 =
     0.03608  −0.00672   0.00955   0.01206
N2    3  −0.00809   0.04621   0.14092  11.00000   0.04349   0.05014 =
     0.03287  −0.00682   0.01177   0.01020
N3    3  −0.09474   0.05073   0.21620  11.00000   0.04139   0.04797 =
     0.03569  −0.00442   0.01054   0.01030
N5    3   0.39670   0.17391   0.10685  11.00000   0.04074   0.04991 =
     0.03995  −0.00179   0.01314   0.01242
N4    3   0.23205   0.10501   0.09231  11.00000   0.04079   0.05465 =
     0.03838  −0.00997   0.01361   0.00774
C16   1   0.44741   0.15251   0.01888  11.00000   0.04600   0.04829 =
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    0.03846  −0.00230   0.01396   0.01278
AFIX 43
H16   2   0.37164   0.09580  −0.04639  11.00000  −1.20000
AFIX 0
C2    1   0.14505   0.21107   0.34258  11.00000   0.03809   0.04667 =
    0.03442  −0.00394   0.00779   0.01453
C3    1  −0.02206   0.13014   0.31745  11.00000   0.03967   0.04331 =
    0.03105  −0.00018   0.00855   0.01431
C17   1   0.61704   0.21217   0.01568  11.00000   0.04601   0.04384 =
    0.03697   0.00176   0.01341   0.01382
C10   1  −0.12587   0.12870   0.39699  11.00000   0.04057   0.04051 =
    0.03657  −0.00144   0.01135   0.01074
C18   1   0.66255   0.17611  −0.08029  11.00000   0.04693   0.05321 =
    0.04183  −0.00938   0.01271   0.00835
AFIX 43
H18   2   0.58232   0.11706  −0.14211  11.00000  −1.20000
AFIX 0
C1    1   0.15386   0.11962   0.17231  11.00000   0.04059   0.04192 =
    0.03392  −0.00085   0.01035   0.01365
C22   1   0.74240   0.30237   0.10573  11.00000   0.05630   0.04677 =
    0.03490   0.00149   0.01558   0.01370
AFIX 43
H22   2   0.71625   0.32991   0.17072  11.00000  −1.20000
AFIX 0
N6    3   1.10876   0.36140  −0.00191  11.00000   0.04474   0.06378 =
    0.06240  −0.00211   0.01653   0.00591
C20   1   0.94894   0.31381   0.00399  11.00000   0.04504   0.04397 =
    0.04680   0.00482   0.01239   0.01191
C15   1  −0.28761   0.12828   0.34960  11.00000   0.04376   0.05221 =
    0.04616   0.00501   0.01313   0.01377
AFIX 43
H15   2  −0.33189   0.12517   0.26759  11.00000  −1.20000
AFIX 0
C21   1   0.90269   0.35127   0.10086  11.00000   0.05147   0.04538 =
    0.03587  −0.00006   0.00625   0.00803
AFIX 43
H21   2   0.98247   0.41040   0.16282  11.00000  −1.20000
AFIX 0
C12   1  −0.16206   0.12897   0.59179  11.00000   0.07265   0.07116 =
    0.04001   0.00346   0.02346   0.02361
AFIX 43
H12   2  −0.12095   0.12682   0.67333  11.00000  −1.20000
```

```
AFIX 0
C19   1   0.82241   0.22493  −0.08681  11.00000   0.05053   0.05627 =
     0.04823  −0.00880   0.02124   0.00968
AFIX 43
H19   2   0.84716   0.19842  −0.15291  11.00000  −1.20000
AFIX 0
C11   1  −0.06461   0.12784   0.51938  11.00000   0.05270   0.06139 =
     0.03865   0.00041   0.01337   0.02169
AFIX 43
H11   2   0.04264   0.12651   0.55231  11.00000  −1.20000
AFIX 0
C4    1   0.22613   0.31234   0.44614  11.00000   0.03678   0.06339 =
     0.04295  −0.01709   0.01104   0.00797
C14   1  −0.38289   0.13246   0.42355  11.00000   0.04919   0.07764 =
     0.07051   0.01040   0.02504   0.02592
AFIX 43
H14   2  −0.48985   0.13476   0.39158  11.00000  −1.20000
AFIX 0
C7    1   0.38028   0.50445   0.63536  11.00000   0.06037   0.12292 =
     0.09155  −0.07040   0.01549   0.00185
AFIX 43
H7    2   0.43290   0.56910   0.69886  11.00000  −1.20000
AFIX 0
C9    1   0.16233   0.40864   0.45611  11.00000   0.05965   0.05914 =
     0.06400  −0.01718   0.01526   0.01395
AFIX 43
H9    2   0.06610   0.40881   0.39914  11.00000  −1.20000
AFIX 0
C23   1   1.14903   0.32988  −0.10714  11.00000   0.05250   0.08042 =
     0.08300   0.00093   0.03139   0.01305
AFIX 137
H23A  2   1.12849   0.23988  −0.11804  11.00000  −1.50000
H23B  2   1.26410   0.37522  −0.09776  11.00000  −1.50000
H23C  2   1.08127   0.35360  −0.17555  11.00000  −1.50000
AFIX 0
C13   1  −0.31943   0.13322   0.54484  11.00000   0.07096   0.08269 =
     0.06612   0.00793   0.04227   0.02843
AFIX 43
H13   2  −0.38326   0.13662   0.59478  11.00000  −1.20000
AFIX 0
C24   1   1.24198   0.44671   0.09504  11.00000   0.04708   0.06166 =
     0.06690   0.00930   0.00395   0.00483
```

```
AFIX 137
H24A   2   1.21987   0.52442   0.10560  11.00000  −1.50000
H24B   2   1.34510   0.46525   0.07664  11.00000  −1.50000
H24C   2   1.24925   0.40699   0.16715  11.00000  −1.50000
AFIX 0
C8     1   0.24118   0.50521   0.55081  11.00000   0.07780   0.06850 =
     0.09326  −0.03264   0.03254   0.00996
AFIX 43
H8     2   0.19867   0.57058   0.55637  11.00000  −1.20000
AFIX 0
C6     1   0.44222   0.40916   0.62694  11.00000   0.06213   0.17406 =
     0.08734  −0.07994  −0.01848   0.04084
AFIX 43
H6     2   0.53654   0.40824   0.68561  11.00000  −1.20000
AFIX 0
C5     1   0.36685   0.31337   0.53218  11.00000   0.05765   0.13011 =
     0.07237  −0.05112  −0.01061   0.04415
AFIX 43
H5     2   0.41176   0.24941   0.52679  11.00000  −1.20000
H1     2   0.15930   0.04591   0.02181  11.00000   0.06325
HKLF 4
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 Refinement of F^2^ against ALL reflections.  The weighted R−factor wR and
 goodness of fit S are based on F^2^,Conventional R−factors R are based
 on F, with F set to zero forNegative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only forCalculating R−factors(gt) etc. and is
Not relevant to theChoice of reflections for refinement.  R−factors based
 on F^2^ are statistically about twice as large as those based on F, and R−
 factors based on ALL data will be even larger.
;

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 'calc w=1/[\s^2^(Fo^2^)+(0.0462P)^2^+0.3570P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_wR_factor_gt           0.1218
_refine_ls_goodness_of_fit_ref    1.035
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N3N −0.09474(17) 0.05074(14) 0.21620(12) 0.0432(4) Uani 1 1 d . . .
N5N 0.39670(18) 0.17391(14) 0.10685(13) 0.0441(4) Uani 1 1 d . . .
N4N 0.23205(18) 0.10501(15) 0.09231(13) 0.0465(4) Uani 1 1 d . . .
C16C 0.4474(2) 0.15251(17) 0.01887(16) 0.0448(4) Uani 1 1 d . . .
H16H 0.3716 0.0958 −0.0464 0.054 Uiso 1 1Calc R . .
C2C 0.1450(2) 0.21106(17) 0.34257(15) 0.0404(4) Uani 1 1 d . . .
C3C −0.0221(2) 0.13015(16) 0.31745(14) 0.0384(4) Uani 1 1 d . . .
C17C 0.6170(2) 0.21217(17) 0.01568(15) 0.0424(4) Uani 1 1 d . . .
C10C −0.1259(2) 0.12870(16) 0.39699(15) 0.0401(4) Uani 1 1 d . . .
C18C 0.6626(2) 0.17612(18) −0.08029(17) 0.0498(5) Uani 1 1 d . . .
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H18H 0.5823 0.1171 −0.1421 0.060 Uiso 1 1Calc R . .
C1C 0.1539(2) 0.11962(16) 0.17231(15) 0.0391(4) Uani 1 1 d . . .
C22C 0.7424(2) 0.30237(17) 0.10573(16) 0.0465(4) Uani 1 1 d . . .
H22H 0.7163 0.3299 0.1707 0.056 Uiso 1 1Calc R . .
N6N 1.1088(2) 0.36140(17) −0.00191(16) 0.0601(5) Uani 1 1 d . . .
C20C 0.9489(2) 0.31381(17) 0.00399(17) 0.0463(4) Uani 1 1 d . . .
C15C −0.2876(2) 0.12828(18) 0.34961(17) 0.0480(4) Uani 1 1 d . . .
H15H −0.3319 0.1252 0.2676 0.058 Uiso 1 1Calc R . .
C21C 0.9027(2) 0.35127(17) 0.10085(16) 0.0478(5) Uani 1 1 d . . .
H21H 0.9825 0.4104 0.1628 0.057 Uiso 1 1Calc R . .
C12C −0.1620(3) 0.1290(2) 0.59179(18) 0.0601(6) Uani 1 1 d . . .
H12H −0.1209 0.1268 0.6733 0.072 Uiso 1 1Calc R . .
C19C 0.8224(2) 0.22494(19) −0.08681(17) 0.0526(5) Uani 1 1 d . . .
H19H 0.8472 0.1984 −0.1529 0.063 Uiso 1 1Calc R . .
C11C −0.0646(2) 0.12785(19) 0.51938(16) 0.0504(5) Uani 1 1 d . . .
H11H 0.0426 0.1265 0.5523 0.061 Uiso 1 1Calc R . .
C4C 0.2261(2) 0.31235(19) 0.44614(17) 0.0505(5) Uani 1 1 d . . .
C14C −0.3829(3) 0.1325(2) 0.4236(2) 0.0631(6) Uani 1 1 d . . .
H14H −0.4898 0.1348 0.3916 0.076 Uiso 1 1Calc R . .
C7C 0.3803(3) 0.5044(3) 0.6354(3) 0.1017(11) Uani 1 1 d . . .
H7H 0.4329 0.5691 0.6989 0.122 Uiso 1 1Calc R . .
C9C 0.1623(3) 0.4086(2) 0.4561(2) 0.0635(6) Uani 1 1 d . . .
H9H 0.0661 0.4088 0.3991 0.076 Uiso 1 1Calc R . .
C23C 1.1490(3) 0.3299(2) −0.1071(2) 0.0720(7) Uani 1 1 d . . .
H23AH 1.1285 0.2399 −0.1181 0.108 Uiso 1 1Calc R . .
H23BH 1.2641 0.3752 −0.0978 0.108 Uiso 1 1Calc R . .
H23CH 1.0813 0.3536 −0.1756 0.108 Uiso 1 1Calc R . .
C13C −0.3194(3) 0.1332(2) 0.5448(2) 0.0680(6) Uani 1 1 d . . .
H13H −0.3832 0.1366 0.5948 0.082 Uiso 1 1Calc R . .
C24C 1.2420(2) 0.4467(2) 0.0950(2) 0.0647(6) Uani 1 1 d . . .
H24AH 1.2200 0.5245 0.1055 0.097 Uiso 1 1Calc R . .
H24BH 1.3451 0.4651 0.0767 0.097 Uiso 1 1Calc R . .
H24CH 1.2492 0.4070 0.1672 0.097 Uiso 1 1Calc R . .
C8C 0.2412(3) 0.5052(2) 0.5508(3) 0.0827(8) Uani 1 1 d . . .
H8H 0.1987 0.5706 0.5564 0.099 Uiso 1 1Calc R . .
C6C 0.4422(3) 0.4091(4) 0.6269(3) 0.1178(14) Uani 1 1 d . . .
H6H 0.5365 0.4082 0.6856 0.141 Uiso 1 1Calc R . .
C5C 0.3668(3) 0.3134(3) 0.5322(2) 0.0910(10) Uani 1 1 d . . .
H5H 0.4117 0.2494 0.5268 0.109 Uiso 1 1Calc R . .
H1H 0.1593 0.0459 0.0218 0.063(6) Uiso 1 1 d R . .

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N2 0.0434(8) 0.0502(9) 0.0329(7) −0.0068(6) 0.0118(6) 0.0102(7)
N3 0.0414(8) 0.0480(8) 0.0357(8) −0.0044(6) 0.0105(6) 0.0103(6)
N5 0.0407(8) 0.0499(9) 0.0399(8) −0.0018(7) 0.0132(6) 0.0124(6)
N4 0.0408(8) 0.0546(9) 0.0384(8) −0.0100(7) 0.0136(7) 0.0077(7)
C16 0.0460(10) 0.0483(10) 0.0384(9) −0.0023(8) 0.0139(8) 0.0128(8)
C2 0.0381(9) 0.0467(10) 0.0344(9) −0.0039(7) 0.0078(7) 0.0145(7)
C3 0.0397(9) 0.0433(9) 0.0310(8) −0.0002(7) 0.0086(7) 0.0143(7)
C17 0.0460(10) 0.0438(10) 0.0370(9) 0.0018(7) 0.0134(8) 0.0138(8)
C10 0.0406(9) 0.0405(9) 0.0366(9) −0.0015(7) 0.0114(7) 0.0108(7)
C18 0.0469(11) 0.0532(11) 0.0418(10) −0.0094(8) 0.0127(8) 0.0084(8)
C1 0.0406(9) 0.0419(9) 0.0339(9) −0.0008(7) 0.0104(7) 0.0136(7)
C22 0.0563(11) 0.0468(10) 0.0349(9) 0.0015(8) 0.0156(8) 0.0137(8)
N6 0.0447(9) 0.0638(11) 0.0624(11) −0.0021(9) 0.0165(8) 0.0059(8)
C20 0.0451(10) 0.0440(10) 0.0468(11) 0.0048(8) 0.0124(8) 0.0119(8)
C15 0.0437(10) 0.0522(11) 0.0461(10) 0.0050(8) 0.0131(8) 0.0137(8)
C21 0.0515(11) 0.0454(10) 0.0359(9) −0.0001(8) 0.0063(8) 0.0080(8)
C12 0.0727(15) 0.0712(14) 0.0400(11) 0.0035(10) 0.0235(10) 0.0237(11)
C19 0.0506(11) 0.0563(12) 0.0482(11) −0.0088(9) 0.0212(9) 0.0097(9)
C11 0.0527(11) 0.0614(12) 0.0387(10) 0.0004(9) 0.0134(8) 0.0217(9)
C4 0.0368(9) 0.0634(12) 0.0429(10) −0.0171(9) 0.0110(8) 0.0080(8)
C14 0.0492(12) 0.0776(15) 0.0705(15) 0.0104(12) 0.0250(11) 0.0259(11)
C7 0.0604(15) 0.123(2) 0.092(2) −0.0704(18) 0.0155(15) 0.0018(15)
C9 0.0596(13) 0.0591(13) 0.0640(14) −0.0172(11) 0.0153(11) 0.0140(10)
C23 0.0525(13) 0.0804(16) 0.0830(17) 0.0009(13) 0.0314(12) 0.0130(11)
C13 0.0709(15) 0.0828(16) 0.0662(15) 0.0080(12) 0.0423(12) 0.0284(12)
C24 0.0471(11) 0.0617(13) 0.0669(14) 0.0093(11) 0.0040(10) 0.0048(9)
C8 0.0777(17) 0.0685(15) 0.093(2) −0.0327(14) 0.0325(15) 0.0100(12)
C6 0.0621(16) 0.174(3) 0.087(2) −0.080(2) −0.0185(14) 0.0409(19)
C5 0.0576(14) 0.130(2) 0.0724(16) −0.0511(16) −0.0106(12) 0.0442(15)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the fullCovariance matrix.  TheCell esds are taken
```

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 into account individually in the estimation of esds in distances, angles
 and torsion angles;Correlations between esds inCell parameters are only
 used when they are defined byCrystal symmetry.  An approximate (isotropic)
 treatment ofCell esds is used for estimating esds involving l.s. planes.
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N1C1 1.347(2) . ?
N2N3 1.3335(19) . ?
N2C1 1.351(2) . ?
N3C3 1.335(2) . ?
N5C16 1.282(2) . ?
N5N4 1.380(2) . ?
N4C1 1.349(2) . ?
N4H1 0.9741 . ?
C16C17 1.454(2) . ?
C16H16 0.9300 . ?
C2C3 1.416(2) . ?
C2C4 1.488(2) . ?
C3C10 1.481(2) . ?
C17C18 1.390(2) . ?
C17C22 1.402(2) . ?
C10C15 1.390(2) . ?
C10C11 1.391(2) . ?
C18C19 1.376(3) . ?
C18H18 0.9300 . ?
C22C21 1.373(3) . ?
C22H22 0.9300 . ?
N6C20 1.372(2) . ?
N6C23 1.444(3) . ?
N6C24 1.449(3) . ?
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C15H15 0.9300 . ?
C21H21 0.9300 . ?
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C12C13 1.372(3) . ?
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C12H12 0.9300 . ?
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C11H11 0.9300 . ?
C4C5 1.371(3) . ?
C4C9 1.381(3) . ?
C14C13 1.379(3) . ?
C14H14 0.9300 . ?
C7C6 1.356(4) . ?
C7C8 1.358(4) . ?
C7H7 0.9300 . ?
C9C8 1.388(3) . ?
C9H9 0.9300 . ?
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C23H23C 0.9600 . ?
C13H13 0.9300 . ?
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C24H24B 0.9600 . ?
C24H24C 0.9600 . ?
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Molecule 4Cif

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CrysAlisPro, Agilent Technologies,
Version 1.171.36.20 (release 27−06−2012CrysAlis171 .NET)
(compiled Jul 11 2012,15:38:31)
Empirical absorptionCorrection using sphericalHarmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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SFACCHN O
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BOND $H
HTAB
CONF
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N2    3  0.30440  0.43955  0.50047 11.00000  0.05052  0.04896 =
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N3    3  0.12818  0.40936  0.46126 11.00000  0.04805  0.05515 =
     0.05971  0.00165 −0.00407  0.00092
N4    3  0.62325  0.44122  0.58888 11.00000  0.05869  0.05261 =
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AFIX 43
H4    2  0.64324  0.47722  0.56601 11.00000 −1.20000
AFIX 0
N5    3  0.77881  0.41939  0.65359 11.00000  0.05624  0.05530 =
     0.05242 −0.00253 −0.00885  0.00159
C1    1  0.43856  0.40747  0.56000 11.00000  0.04820  0.05064 =
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C3    1  0.08431  0.35113  0.48454 11.00000  0.04319  0.04251 =
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C4    1  0.17969  0.25920  0.58764 11.00000  0.04459  0.04857 =
     0.04099  0.00430 −0.00508 −0.00432
C5    1  0.33970  0.21325  0.58139 11.00000  0.04747  0.05908 =
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C6    1  0.30303  0.15481  0.61346 11.00000  0.06740  0.05151 =
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AFIX 0
C7    1  0.10916  0.14150  0.65477 11.00000  0.08041  0.05691 =
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C8    1 −0.04866  0.18733  0.66341 11.00000  0.06669  0.07522 =
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C11   1 −0.12049  0.26099  0.40957 11.00000  0.05002  0.06235 =
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AFIX 0
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C21   1   1.44882   0.48071   0.82603  11.00000   0.06194   0.05952 =
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AFIX 0
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AFIX 0
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 F^2^ > 2sigma(F^2^) is used only forCalculating R−factors(gt) etc. and is
Not relevant to theChoice of reflections for refinement.  R−factors based
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C3C 0.24111(18) 1.2833(4) 0.09301(12) 0.0524(7) Uani 1 1 d . . .
N5N 0.13020(17) 0.6597(4) −0.05376(11) 0.0660(6) Uani 1 1 d . . .
C1C 0.1496(2) 0.9805(5) 0.01395(13) 0.0592(7) Uani 1 1 d . . .
C4C 0.38883(19) 1.1287(4) 0.06992(11) 0.0527(7) Uani 1 1 d . . .
N4N 0.09520(19) 0.8212(4) −0.02047(12) 0.0741(7) Uani 1 1 d . . .
C15C 0.2389(2) 1.6421(4) 0.14746(13) 0.0616(7) Uani 1 1 d . . .
H15H 0.1844 1.6726 0.1166 0.074 Uiso 1 1Calc R . .
C10C 0.28417(18) 1.4457(4) 0.14384(12) 0.0505(6) Uani 1 1 d . . .
C9C 0.4370(2) 1.3147(4) 0.06129(13) 0.0619(7) Uani 1 1 d . . .
H9H 0.4059 1.4465 0.0512 0.074 Uiso 1 1Calc R . .
C16C 0.0711(2) 0.5232(4) −0.08416(13) 0.0645(8) Uani 1 1 d . . .
H16H 0.0104 0.5364 −0.0812 0.077 Uiso 1 1Calc R . .
C11C 0.36520(19) 1.4045(5) 0.19072(12) 0.0624(8) Uani 1 1 d . . .
H11H 0.3964 1.2737 0.1896 0.075 Uiso 1 1Calc R . .
C17C 0.0950(2) 0.3477(4) −0.12331(13) 0.0605(7) Uani 1 1 d . . .
C22C 0.0277(2) 0.1973(5) −0.15222(14) 0.0733(9) Uani 1 1 d . . .
H22H −0.0308 0.2092 −0.1448 0.088 Uiso 1 1Calc R . .
C7C 0.5771(2) 1.1122(6) 0.08330(14) 0.0748(9) Uani 1 1 d . . .
H7H 0.6403 1.1065 0.0874 0.090 Uiso 1 1Calc R . .
C14C 0.2736(2) 1.7923(5) 0.19612(15) 0.0711(9) Uani 1 1 d . . .
H14H 0.2425 1.9226 0.1980 0.085 Uiso 1 1Calc R . .
C12C 0.3999(2) 1.5565(6) 0.23906(13) 0.0764(9) Uani 1 1 d . . .
H12H 0.4546 1.5282 0.2699 0.092 Uiso 1 1Calc R . .
O1 O 0.25154(16) 0.4654(4) −0.10809(15) 0.1261(10) Uani 1 1 d . . .
H1H 0.2336 0.5543 −0.0848 0.151 Uiso 1 1Calc R . .
C5C 0.4365(2) 0.9344(5) 0.08544(13) 0.0644(8) Uani 1 1 d . . .
H5H 0.4049 0.8076 0.0909 0.077 Uiso 1 1Calc R . .
C8C 0.5308(2) 1.3060(6) 0.06764(14) 0.0721(9) Uani 1 1 d . . .
H8H 0.5627 1.4313 0.0613 0.086 Uiso 1 1Calc R . .
C13C 0.3538(3) 1.7491(6) 0.24151(15) 0.0804(10) Uani 1 1 d . . .
H13H 0.3772 1.8506 0.2742 0.096 Uiso 1 1Calc R . .
C18C 0.1816(2) 0.3283(6) −0.13547(17) 0.0848(10) Uani 1 1 d . . .
C6C 0.5308(2) 0.9282(5) 0.09282(14) 0.0731(8) Uani 1 1 d . . .
H6H 0.5627 0.7981 0.1043 0.088 Uiso 1 1Calc R . .
C21C 0.0456(3) 0.0312(5) −0.19158(17) 0.0931(11) Uani 1 1 d . . .
H21H 0.0001 −0.0690 −0.2102 0.112 Uiso 1 1Calc R . .
C19C 0.1992(3) 0.1626(7) −0.1761(2) 0.1140(13) Uani 1 1 d . . .
H19H 0.2568 0.1512 −0.1850 0.137 Uiso 1 1Calc R . .
C20C 0.1315(3) 0.0167(7) −0.20273(19) 0.1083(13) Uani 1 1 d . . .
H20H 0.1442 −0.0952 −0.2291 0.130 Uiso 1 1Calc R . .
H10H 0.019(3) 0.810(5) −0.0309(15) 0.107(11) Uiso 1 1 d . . .

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C2 0.0500(18) 0.0617(16) 0.0418(13) 0.0004(13) 0.0069(13) −0.0089(14)
N2 0.0454(15) 0.0769(16) 0.0698(15) −0.0158(14) 0.0047(12) −0.0136(13)
C3 0.0393(17) 0.0662(17) 0.0489(15) −0.0003(13) 0.0054(12) −0.0095(14)
N5 0.0576(16) 0.0661(14) 0.0672(15) −0.0087(13) 0.0016(13) −0.0039(13)
C1 0.0496(19) 0.0700(19) 0.0517(15) −0.0033(14) 0.0003(14) −0.0093(17)
C4 0.0485(18) 0.0649(17) 0.0447(14) −0.0089(13) 0.0110(12) −0.0094(15)
N4 0.0562(18) 0.0772(16) 0.0805(17) −0.0267(14) 0.0001(14) −0.0171(15)
C15 0.0598(19) 0.0673(18) 0.0581(17) −0.0003(15) 0.0147(15) −0.0107(16)
C10 0.0487(17) 0.0616(16) 0.0431(14) −0.0012(13) 0.0147(13) −0.0106(15)
C9 0.059(2) 0.0693(18) 0.0593(16) −0.0039(14) 0.0190(15) −0.0092(16)
C16 0.0554(19) 0.0680(18) 0.0627(17) −0.0115(15) 0.0000(15) −0.0068(16)
C11 0.0519(18) 0.087(2) 0.0456(15) −0.0058(15) 0.0072(13) −0.0060(16)
C17 0.0529(19) 0.0639(17) 0.0611(17) −0.0006(15) 0.0069(14) 0.0039(15)
C22 0.070(2) 0.0732(19) 0.0729(19) −0.0166(17) 0.0089(17) −0.0055(18)
C7 0.055(2) 0.106(3) 0.0648(19) −0.0170(19) 0.0160(16) −0.005(2)
C14 0.082(3) 0.0650(19) 0.071(2) −0.0086(17) 0.029(2) −0.0128(18)
C12 0.066(2) 0.105(2) 0.0530(18) −0.0089(18) 0.0038(15) −0.017(2)
O1 0.0523(16) 0.144(2) 0.179(3) −0.044(2) 0.0222(16) −0.0111(16)
C5 0.059(2) 0.0665(19) 0.0653(18) −0.0097(15) 0.0098(15) −0.0061(16)
C8 0.061(2) 0.090(2) 0.070(2) −0.0072(17) 0.0259(16) −0.0183(19)
C13 0.098(3) 0.088(2) 0.0569(19) −0.0215(18) 0.022(2) −0.030(2)
C18 0.054(2) 0.096(2) 0.097(2) −0.010(2) 0.0039(19) 0.007(2)
C6 0.060(2) 0.083(2) 0.074(2) −0.0125(17) 0.0105(16) 0.0058(18)
C21 0.098(3) 0.081(2) 0.096(3) −0.027(2) 0.015(2) 0.004(2)
C19 0.080(3) 0.130(3) 0.133(3) −0.028(3) 0.028(3) 0.027(3)
C20 0.103(4) 0.111(3) 0.107(3) −0.029(2) 0.018(3) 0.031(3)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the fullCovariance matrix.  TheCell esds are taken
 into account individually in the estimation of esds in distances, angles
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 and torsion angles;Correlations between esds inCell parameters are only
 used when they are defined byCrystal symmetry.  An approximate (isotropic)
 treatment ofCell esds is used for estimating esds involving l.s. planes.
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C2C3 1.424(3) . ?
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N2C1 1.337(3) . ?
C3C10 1.488(3) . ?
N5C16 1.271(3) . ?
N5N4 1.386(3) . ?
C1N4 1.362(3) . ?
C4C9 1.383(3) . ?
C4C5 1.385(4) . ?
N4H10 1.11(4) . ?
C15C14 1.381(4) . ?
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C15H15 0.9300 . ?
C10C11 1.389(4) . ?
C9C8 1.380(4) . ?
C9H9 0.9300 . ?
C16C17 1.450(4) . ?
C16H16 0.9300 . ?
C11C12 1.384(4) . ?
C11H11 0.9300 . ?
C17C18 1.386(4) . ?
C17C22 1.392(4) . ?
C22C21 1.378(4) . ?
C22H22 0.9300 . ?
C7C6 1.362(4) . ?
C7C8 1.373(4) . ?
C7H7 0.9300 . ?
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C14C13 1.367(4) . ?
C14H14 0.9300 . ?
C12C13 1.374(4) . ?
C12H12 0.9300 . ?
O1C18 1.357(4) . ?
O1H1 0.8200 . ?
C5C6 1.384(4) . ?
C5H5 0.9300 . ?
C8H8 0.9300 . ?
C13H13 0.9300 . ?
C18C19 1.392(5) . ?
C6H6 0.9300 . ?
C21C20 1.365(5) . ?
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C19C20 1.366(5) . ?
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C1N2N3 118.0(2) . . ?
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C16N5N4 114.9(2) . . ?
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N2C1N4 112.9(3) . . ?
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C9C4C2 121.9(3) . . ?
C5C4C2 119.2(2) . . ?

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C14C15C10 121.0(3) . . ?
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N2N3C3C2 3.5(3) . . . . ?
N2N3C3C10 −174.5(2) . . . . ?
N1C2C3N3 −5.8(3) . . . . ?
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N1C2C3C10 171.9(2) . . . . ?
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N1C2C4C9 129.3(2) . . . . ?

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N1C2C4C5 −49.3(3) . . . . ?
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N1C1N4N5 −6.6(4) . . . . ?
N2C1N4N5 174.1(2) . . . . ?
C16N5N4C1 −179.4(2) . . . . ?
C14C15C10C11 0.2(4) . . . . ?
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N3C3C10C11 143.3(2) . . . . ?
C2C3C10C11 −34.6(4) . . . . ?
N3C3C10C15 −32.6(3) . . . . ?
C2C3C10C15 149.5(2) . . . . ?
C5C4C9C8 0.4(4) . . . . ?
C2C4C9C8 −178.2(2) . . . . ?
N4N5C16C17 178.0(2) . . . . ?
C15C10C11C12 −0.7(4) . . . . ?
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N5C16C17C18 −6.3(4) . . . . ?
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C16C17C22C21 178.0(3) . . . . ?
C10C15C14C13 0.2(4) . . . . ?
C10C11C12C13 0.7(4) . . . . ?
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C4C9C8C7 −0.7(4) . . . . ?
C15C14C13C12 −0.2(4) . . . . ?
C11C12C13C14 −0.2(4) . . . . ?
C22C17C18 O1 −178.6(3) . . . . ?
C16C17C18 O1 4.1(5) . . . . ?
C22C17C18C19 0.5(5) . . . . ?
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C8C7C6C5 1.3(4) . . . . ?
C4C5C6C7 −1.6(4) . . . . ?
C17C22C21C20 −0.7(5) . . . . ?
O1C18C19C20 177.7(4) . . . . ?
C17C18C19C20 −1.4(6) . . . . ?
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