Supplementary Information

Crystal Structure and ^{1}H NMR Experimental and Theoretical Study of Conformers of 5-Methyl-1-(4'-methylphenylsulfonylamino)-1*H*-[1,2,3]-triazole-4-carboxylic Acid Ethyl Ester and 5-Methyl-1-(phenylsulfonylamino)-1*H*-[1,2,3]-triazole-4-carboxylic Acid Ethyl Ester

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Compound I

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 1A

Total Energy (E / au): -1383.369839

Gibbs free Energy (G / au): -1383.146049

C	-2.18269100	0.87537200	0.30954500
S	-2.81973000	-0.74902600	0.03177300
N	-1.66800300	-1.31718900	-1.12390700
N	-0.41459800	-1.54744300	-0.60718200
N	-0.13205600	-2.65640700	0.12398100
N	1.09564000	-2.55507900	0.48747800
C	1.61525000	-1.38244000	0.01520800
C	0.65057900	-0.71254900	-0.71041400
O	-4.04807200	-0.71385800	-0.74015400
O	-2.72634300	-1.49915900	1.26931300
C	-2.48982000	1.88037300	-0.60251700
C	-1.33450600	1.08550300	1.39232100
C	0.62990000	0.56771000	-1.46146600
H	1.55790800	0.67832200	-2.01979500
H	-0.22674200	0.59463300	-2.13476700
H	0.55397500	1.40937100	-0.76836800
C	4.63188800	0.67826400	0.04885600
H	5.34264700	-0.05559300	-0.33683800
H	4.78378600	0.75686600	1.12788500
C	4.76693700	2.01541800	-0.64017700
H	5.77118700	2.41020100	-0.47608400
H	4.60615500	1.91445400	-1.71530500
H	4.04513600	2.73234000	-0.24410500
O	3.29584300	0.20147100	-0.19351400
O	3.79033900	-1.69082900	0.92552000
C	3.00888100	-1.00625000	0.30749500
H	-2.03219600	-2.14900000	-1.58488400
C	-1.92490400	3.13566800	-0.42091000
H	-2.15387800	3.93367500	-1.11612200
H	-3.15889800	1.67699000	-1.42971700
C	-1.06455200	3.36353600	0.65196300
H	-0.62152700	4.34319300	0.78599300
H	-1.12312300	0.27905200	2.08383700
C	-0.77122100	2.34614600	1.55658500
H	-0.10421700	2.53125100	2.38906400

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 2A

Total Energy (E / au): -1383.370134

Gibbs free Energy (G / au): -1383.14812

C	-2.85595000	-0.00614000	0.36597200
S	-1.99206700	1.52806400	0.20164600
N	-0.93867200	1.38295200	-1.14165500
N	0.04335100	0.43020300	-1.02211000
N	-0.16630100	-0.85568900	-1.40198500
N	0.93563400	-1.48349500	-1.19544600
C	1.85835500	-0.62283500	-0.66875300
C	1.29814400	0.63570400	-0.55416700
O	-1.10780600	1.68522500	1.34072700
O	-2.91673200	2.56117300	-0.22180400
C	-2.24811100	-1.05080000	1.05818900
C	-4.11520800	-0.13429200	-0.21281700
C	1.77102100	1.95575800	-0.06772000
H	2.85540300	1.95376100	0.00328100
H	1.43290500	2.74288100	-0.74399600
H	1.34075400	2.15610600	0.91566500
C	5.29915000	-0.50736400	0.57457300
H	5.81765900	-0.86312700	-0.31814900
H	5.25197400	-1.33238300	1.28869500
C	5.95744000	0.71720700	1.16530400
H	6.98603100	0.48136200	1.44388300
H	5.97685000	1.53206100	0.43922800
H	5.42551200	1.05377400	2.05690000
O	3.95584200	-0.13813100	0.21095600
O	3.60375800	-2.23102300	-0.54038400
C	3.21321000	-1.10412200	-0.34019200
H	-1.44120100	1.28231800	-2.01998600
C	-2.92991200	-2.25482100	1.17315700
H	-2.47690800	-3.07947200	1.70859900
H	-1.26973600	-0.91496600	1.50362200
C	-4.19282400	-2.39938400	0.60401900
H	-4.71943900	-3.34186600	0.69986400
H	-4.56155400	0.70436400	-0.73268000
C	-4.78455700	-1.34507500	-0.08669300
H	-5.76831400	-1.46258300	-0.52408700

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 3B

Total Energy (E / au): -1383.366501

Gibbs free Energy (G / au): -1383.143949

C	3.04307200	-0.11020200	-0.30977600
S	1.84407200	-1.40135400	-0.19390100
N	0.94331300	-0.95188900	1.19304900
N	-0.12843300	-0.12810000	0.97286000
N	0.01959100	1.20476900	1.17275200
N	-1.10713800	1.74806800	0.88241000
C	-1.99724900	0.78164500	0.50034300
C	-1.37645100	-0.44960100	0.54203800
O	2.47821000	-2.64152600	0.21630500
O	0.97056700	-1.33008500	-1.35354300
C	4.31523600	-0.33231300	0.20629100
C	2.67517400	1.09972000	-0.89260600
C	-1.79005300	-1.84387300	0.24298500
H	-2.86495100	-1.87754200	0.08588100
H	-1.27836000	-2.19143200	-0.65681800
H	-1.52535900	-2.51293200	1.06551100
C	-5.48140500	0.34244400	-0.53897600
H	-5.51337700	1.04679500	-1.37286700
H	-5.96426200	0.81571000	0.31820200
C	-6.11636600	-0.98304100	-0.88488800
H	-7.17308600	-0.83152600	-1.11250100
H	-5.63623600	-1.43162500	-1.75622500
H	-6.04224100	-1.67870800	-0.04666300
O	-4.10465500	0.08576600	-0.20529300
O	-3.81186100	2.28338500	0.18645800
C	-3.38224200	1.15344700	0.15094400
H	0.72324200	-1.76449500	1.76219200
C	5.24925200	0.69392400	0.13234200
H	6.24680900	0.54068000	0.52436000
H	4.56181400	-1.28971400	0.64804700
C	4.89977400	1.91267700	-0.44276600
H	5.63129400	2.71071000	-0.49576200
H	1.67641700	1.24128700	-1.28656400
C	3.61922600	2.11647300	-0.95162700
H	3.35592000	3.06639700	-1.39909900

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 4B

Total Energy (E / au): -1383.366305

Gibbs free Energy (G / au): -1383.142897

C	2.17428100	0.88058300	0.30723800
S	2.84508500	-0.72105800	-0.03541600
N	1.69420200	-1.49755700	-1.02580300
N	0.41843400	-1.60688700	-0.54082600
N	0.09467700	-2.70954400	0.18191800
N	-1.12713600	-2.56827100	0.54781300
C	-1.61617900	-1.38882400	0.06032200
C	-0.62809900	-0.74135100	-0.65022700
O	2.88416300	-1.47271800	1.19979800
O	3.98991500	-0.59446900	-0.91711500
C	1.33466700	1.03865300	1.40681200
C	2.44689200	1.92348700	-0.57402300
C	-0.59639900	0.54081200	-1.40160300
H	-1.49407200	0.62766800	-2.01095400
H	-0.58108900	1.38270900	-0.70524300
H	0.28624300	0.60883200	-2.03735600
C	-4.62075300	0.68872600	-0.03005800
H	-4.79365100	0.78713100	1.04405300
H	-5.32731100	-0.04878300	-0.41634700
C	-4.73486800	2.01295800	-0.74659400
H	-5.73738500	2.41989200	-0.60155700
H	-4.01128800	2.73085300	-0.35569200
H	-4.56377700	1.89030500	-1.81797700
O	-3.28271700	0.19862300	-0.23590800
O	-3.80310500	-1.63946900	0.95913800
C	-3.00940900	-0.98741700	0.32173200
H	1.75196700	-1.24080800	-2.00529900
C	0.74496400	2.27993000	1.61755800
H	0.08755300	2.42371200	2.46549200
H	1.15365000	0.20894300	2.07936900
C	1.00256400	3.33290000	0.74273900
H	0.54095500	4.29810400	0.91338300
H	3.11776200	1.76623000	-1.40991700
C	1.85571600	3.15904200	-0.34552100
H	2.06153100	3.98522900	-1.01456400

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 5B

Total Energy (E / au): -1383.370055

Gibbs free Energy (G / au): -1383.148867

C	0.00000000	0.00000000	0.00000000
S	0.00000000	0.00000000	1.76810000
N	1.63788013	0.00000000	2.27287907
N	2.35895204	1.11548234	1.92283420
N	2.98624978	1.20983200	0.72289296
N	3.57997446	2.34924118	0.70854918
C	3.33355098	3.00684437	1.88207519
C	2.54191066	2.21497202	2.69280867
O	-0.48968111	-1.27696839	2.24922803
O	-0.52366017	1.26907374	2.23688817
C	-0.08224686	-1.21500282	-0.67408398
C	0.10042569	1.21583578	-0.67114513
C	1.94047428	2.35892382	4.04192133
H	2.41884383	3.17742298	4.57308853
H	0.87199325	2.56129881	3.94154677
H	2.05026407	1.42642036	4.59828223
C	4.12314506	6.10711834	3.66271901
H	3.71894583	6.85918374	2.98128055
H	5.20529107	6.07311315	3.52267416
C	3.74481384	6.38013406	5.09872942
H	4.15525588	7.34270863	5.40985066
H	2.66043495	6.41215963	5.21718813
H	4.14525237	5.60614656	5.75630165
O	3.57288503	4.82398747	3.31331138
O	4.62965531	4.91974512	1.32696522
C	3.91950965	4.34016779	2.11590858
H	2.12727726	-0.85109278	2.00751041
C	-0.06502619	-1.20509029	-2.06314187
H	-0.13478131	-2.13880167	-2.60778812
H	-0.17452632	-2.13976184	-0.11803160
C	0.03455626	0.00183380	-2.75071175
H	0.04729114	0.00303369	-3.83433625
H	0.15576353	2.14290113	-0.11383626
C	0.11635982	1.20796321	-2.05933137
H	0.19250283	2.14195436	-2.60104396

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 6B

Total Energy (E / au): -1383.369773

Gibbs free Energy (G / au): -1383.14657

C	2.24005600	0.84465800	0.29549400
S	2.79605300	-0.81193700	0.03798100
N	1.62116800	-1.33978300	-1.11153900
N	0.36526600	-1.54380900	-0.59079100
N	0.05619800	-2.66143900	0.11525700
N	-1.17208700	-2.54393800	0.47172300
C	-1.66569300	-1.35240000	0.01935300
C	-0.68293800	-0.68665700	-0.68568700
O	2.66590800	-1.54223500	1.28503200
O	4.02487400	-0.84515300	-0.73417600
C	1.42677800	1.11168400	1.39203100
C	2.57129600	1.81789700	-0.64299200
C	-0.62855200	0.60552100	-1.41493100
H	-1.56814100	0.76883900	-1.93988900
H	-0.48506300	1.43250400	-0.71426100
H	0.20466000	0.60352500	-2.11778600
C	-4.67364300	0.72398000	0.04111600
H	-4.86237500	0.75148500	1.11655800
H	-5.37038500	0.00973100	-0.40286500
C	-4.78522500	2.09225500	-0.58848500
H	-5.79465000	2.47940300	-0.43816100
H	-4.07746800	2.78850600	-0.13493500
H	-4.59035300	2.04340500	-1.66131000
O	-3.33038800	0.25463500	-0.17789600
O	-3.85700000	-1.65892900	0.88752600
C	-3.05946500	-0.96624100	0.29882400
H	1.96166900	-2.17680400	-1.58124000
C	0.92498300	2.39957400	1.54590800
H	0.28895100	2.63076200	2.39101300
H	1.19794500	0.32597500	2.10159000
C	1.24270300	3.38579900	0.61548700
H	0.84929700	4.38727200	0.74111200
H	3.21079400	1.57110600	-1.48196300
C	2.06677000	3.10000900	-0.47204200
H	2.31489100	3.87504200	-1.18645000

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 7A

Total Energy (E / au): -1383.365308

Gibbs free Energy (G / au): -1383.144931

C	-3.27684800	0.17853900	0.19098300
S	-1.81121000	-0.67031400	0.68876100
N	-0.94728200	-0.57183200	-0.80839500
N	0.38083600	-0.90346800	-0.67067200
N	0.79820700	-2.19267500	-0.72187800
N	2.07423000	-2.17086200	-0.56472400
C	2.48783700	-0.88147500	-0.38617900
C	1.39629300	-0.03596700	-0.45439700
O	-2.14259000	-2.04519400	1.02250800
O	-1.01155800	0.13026700	1.60036300
C	-4.49107400	-0.49590600	0.25215400
C	-3.17973900	1.50337000	-0.23128600
C	1.19585600	1.42686700	-0.31329700
H	2.06969800	1.96061600	-0.67981000
H	0.30101800	1.73395500	-0.85669800
H	1.05038400	1.67268500	0.74046500
C	5.46844400	1.13438000	0.25499100
H	6.05977100	0.87675900	-0.62643400
H	5.86174500	0.56547100	1.09957700
C	5.46463400	2.62056900	0.52255700
H	6.48646200	2.96197200	0.69718200
H	5.05981800	3.16867500	-0.33027200
H	4.86746200	2.85460900	1.40559600
O	4.10504100	0.73275600	0.02655500
O	4.79742600	-1.40174000	-0.16683900
C	3.91290600	-0.57675600	-0.16966600
H	-1.37393700	-1.16755100	-1.51576400
C	-5.64447700	0.17983000	-0.13102800
H	-6.60094300	-0.32711700	-0.09156500
H	-4.52266400	-1.52474200	0.58752200
C	-5.56649300	1.49960300	-0.56445800
H	-6.46800500	2.01950300	-0.86582200
H	-2.21593000	1.99913300	-0.26165500
C	-4.33968500	2.16109600	-0.61580100
H	-4.28993800	3.18929000	-0.95095500

Experimental Structure

Str. X-ray-A

C	8.34272300	3.15498600	-2.92264200
H	8.53991600	3.60333100	-3.76994600
H	8.77168600	2.27382600	-2.91018200
H	7.37265300	3.04626400	-2.82849800
C	10.23440600	6.78109700	-4.94537100
H	11.22084200	6.81319500	-4.86507100
H	9.87970900	7.69539000	-4.80830700
C	9.84575300	6.27683700	-6.30077900
H	10.20968700	6.87325100	-6.98748300
H	10.20555600	5.37393400	-6.42815200
H	8.86894400	6.25302200	-6.37277200
S	6.60636300	2.44363800	0.43265100
O	9.67639300	5.86887400	-3.94162100
N	8.73171000	3.60540200	-0.49841400
O	10.77977300	7.04099200	-2.39238600
N	9.77824700	5.45676900	-0.37242600
C	9.52276500	5.17616500	-1.70014400
N	9.28421800	4.51866000	0.36411900
C	10.05788100	6.11427300	-2.69281800
O	5.89507300	2.95618100	-0.69777900
N	8.20948400	2.40222100	-0.02492100
H	8.67692300	1.98908000	0.63824600
O	6.38995400	1.12138200	0.90960500
C	8.85837500	3.97091200	-1.80121200
C	5.61969100	5.67835300	2.57236800
H	5.24496100	6.53673300	2.41730600
C	5.85141300	4.81997300	1.49939400
H	5.64720300	5.08504600	0.61055700
C	6.38645700	3.57123300	1.76106200
C	5.93131900	5.29006300	3.85163000
H	5.75729600	5.87819300	4.57709900
C	6.71515300	3.18397800	3.05416800
H	7.08944800	2.32663400	3.22030600
C	6.49028100	4.06306700	4.09253000
H	6.72497300	3.81663200	4.97859900

Experimental Structure

Str. X-ray-B

C	1.75050200	6.01487100	9.58200300
H	2.08758200	6.30893600	10.45422600
H	0.79516000	5.80674800	9.65538000
H	2.23775500	5.21447600	9.29679900
C	3.61438200	9.26304600	12.00761600
H	3.21212800	10.16387900	12.09483800
H	4.58619100	9.36866100	11.84978500
C	3.37904400	8.47714700	13.24395900
H	3.78334500	8.94102400	14.00680800
H	2.41540100	8.38188700	13.39209800
H	3.78450600	7.58977500	13.14981400
S	-0.62556000	5.81358100	6.53240300
O	3.66047400	10.19494200	9.53769900
N	1.57361300	6.96747600	7.29760700
O	2.99721500	8.54030900	10.88756900
N	1.87832000	8.07746700	6.55275500
C	2.49011300	8.34978800	8.62394100
N	2.43140300	8.91203200	7.36821500
N	1.01254900	5.84298800	6.71750900
H	1.53734600	5.59448200	5.93527600
C	3.09618900	9.12222600	9.70799000
O	-1.15833100	6.38245200	7.74617900
C	1.94548100	7.09587000	8.58656000
O	-0.88659000	4.45653400	6.16510000
C	-1.68804700	8.06090000	5.45070700
H	-1.77000600	8.37671000	6.34369800
C	-1.11123400	6.83183300	5.18904000
C	-2.15016200	8.82919700	4.37634900
H	-2.55707000	9.67204500	4.53971800
C	-0.97085900	6.37831000	3.88485800
H	-0.56424300	5.53649800	3.71595100
C	-1.42042600	7.14867800	2.83542000
H	-1.32373600	6.84425800	1.94104400
C	-2.01868000	8.37567400	3.09708700
H	-2.33852300	8.90478400	2.37715600

Compound II

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 1A

Total Energy (E / au): -1422.6785554

Gibbs free Energy (G / au): -1422.431594

C	-2.18363900	0.61784000	0.23214900
S	-2.79881900	-1.02180600	0.03594000
N	-1.62785800	-1.64259800	-1.07506200
N	-0.37401000	-1.81738500	-0.53762900
N	-0.07711900	-2.86901400	0.26836500
N	1.14798700	-2.72472300	0.62668900
C	1.65104200	-1.57908100	0.07682900
C	0.67809600	-0.97459400	-0.69342300
O	-4.01910600	-1.04263300	-0.75058500
O	-2.71352600	-1.70893200	1.31155900
C	-2.49814600	1.57710700	-0.72583700
C	-1.33529800	0.89632400	1.29936100
C	0.63576900	0.25581700	-1.52202900
H	1.56650300	0.35708300	-2.07707600
H	-0.21441800	0.21871500	-2.20290600
H	0.52768500	1.13489900	-0.88111800
C	4.64397700	0.51059200	-0.04657100
H	5.35085500	-0.21964000	-0.44649100
H	4.82864600	0.60196200	1.02595800
C	4.74118600	1.84006200	-0.75617800
H	5.74443700	2.24977300	-0.62411600
H	4.55372300	1.72432800	-1.82549000
H	4.02087400	2.55245300	-0.34916400
O	3.30787500	0.01268500	-0.24188600
O	3.83252300	-1.79248400	1.00007300
C	3.03830700	-1.16244400	0.34057800
H	-1.97257000	-2.51035400	-1.48176900
C	-1.93972500	2.84076600	-0.60879000
H	-2.18031500	3.60110000	-1.34318300
H	-3.16913600	1.33377200	-1.54088000
C	-1.06747200	3.14894900	0.44115500
C	-0.42355600	4.50426600	0.52807100
H	-1.11600200	0.13109100	2.03418200
C	-0.78122500	2.16579700	1.39345400
H	-0.11765300	2.39874800	2.21874200
H	-1.04892300	5.27146500	0.06910700
H	-0.22949900	4.78303200	1.56492700
H	0.53588400	4.49900700	0.00180100

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 2A

Total Energy (E / au): -1422.6791422

Gibbs free Energy (G / au): -1422.430271

C	2.62656800	-0.45859000	0.28300900
S	1.50798200	-1.82279600	0.24070100
N	0.46765200	-1.60767000	-1.10520000
N	-0.40885900	-0.55603800	-1.00883300
N	-0.06304400	0.70295500	-1.37807700
N	-1.09448300	1.44159000	-1.17162400
C	-2.10482700	0.67920200	-0.65356700
C	-1.67855400	-0.63052300	-0.54295100
O	0.62219800	-1.74050300	1.38806400
O	2.24007200	-3.02754600	-0.10059700
C	2.21777000	0.74394700	0.85560800
C	3.90166500	-0.61608700	-0.25199400
C	-2.27944100	-1.89792800	-0.05959700
H	-3.35426600	-1.77948500	0.04862100
H	-2.05329300	-2.70619500	-0.75725600
H	-1.84125700	-2.16043600	0.90563200
C	-5.54592800	0.91376300	0.57284000
H	-6.03758200	1.30558000	-0.31992500
H	-5.40855000	1.74093600	1.27260000
C	-6.31672100	-0.22945200	1.19051400
H	-7.30741700	0.11826600	1.48959700
H	-6.43865900	-1.04715200	0.47762200
H	-5.80208600	-0.60852900	2.07499700
O	-4.25175200	0.40673900	0.19925400
O	-3.66445200	2.46603400	-0.49548900
C	-3.40204500	1.29816900	-0.32180900
H	0.96725100	-1.59582600	-1.99048400
C	3.11389900	1.80125500	0.89013300
H	2.81247000	2.74063200	1.33938500
H	1.22458400	0.84238600	1.27635300
C	4.40367800	1.67390100	0.36502400
C	5.35618200	2.83684900	0.39732800
H	4.19950500	-1.56732200	-0.67560800
C	4.78349000	0.45445700	-0.20236200
H	5.78466200	0.33850500	-0.60160300
H	5.17913500	3.46618000	1.27114900
H	6.39358800	2.49913300	0.41133200
H	5.22240100	3.46063400	-0.49040000

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 3B

Total Energy (E / au): -1422.675279

Gibbs free Energy (G / au): -1422.428486

C	2.68236900	0.48728300	0.28334100
S	1.43753900	1.73189800	0.22271800
N	0.55597000	1.31547400	-1.18575000
N	-0.42719300	0.37437700	-1.02737600
N	-0.14616100	-0.91536000	-1.33845800
N	-1.20071700	-1.59753900	-1.07398000
C	-2.17696400	-0.76530600	-0.59699900
C	-1.69074400	0.52484100	-0.54780900
O	2.01564200	3.01631200	-0.13078200
O	0.56995600	1.57573100	1.37940400
C	3.93571200	0.75707800	-0.25726700
C	2.37944100	-0.74541800	0.85359200
C	-2.24559200	1.83779200	-0.13104400
H	-3.30909300	1.73475800	0.06809600
H	-1.73354900	2.18180400	0.76967300
H	-2.09799000	2.58504900	-0.91501300
C	-5.62718500	-0.79927600	0.63235400
H	-5.52262400	-1.50618800	1.45863700
H	-6.09101000	-1.32532600	-0.20421800
C	-6.40269200	0.43336900	1.03278000
H	-7.40879800	0.14919700	1.34651100
H	-5.91416200	0.94541800	1.86368000
H	-6.48644800	1.12809600	0.19506300
O	-4.31458700	-0.36437600	0.23256000
O	-3.80187500	-2.48045200	-0.33870400
C	-3.49715500	-1.31500700	-0.23236900
H	0.25778600	2.14440600	-1.69197000
C	4.90446600	-0.23437100	-0.21748700
H	5.88942800	-0.03544200	-0.62503400
H	4.14406000	1.72914800	-0.68654500
C	4.63169100	-1.48574100	0.34396300
C	5.68393400	-2.55874100	0.36410900
H	1.39993200	-0.92877700	1.27775300
C	3.36167100	-1.72446800	0.87561600
H	3.14560200	-2.68760300	1.32317800
H	6.67343300	-2.13425900	0.54235500
H	5.47608600	-3.30197300	1.13536600
H	5.71663000	-3.07725100	-0.59856800

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 4B

Total Energy (E / au): -1422.6754041

Gibbs free Energy (G / au): -1422.426543

DFT ?B97x-D/6-31G(d,p)-PCM-CHCl3 fully optimized geometries.
True minimum energy structure: No imaginary frequencies found.

Str. 4B

C	2.11454500	0.71561600	0.23580000
S	2.86547100	-0.86390100	-0.00226500
N	1.76811900	-1.76567500	-0.95349200
N	0.48754600	-1.87986600	-0.47997800
N	0.19280400	-2.92091100	0.33977600
N	-1.03343600	-2.78064600	0.69265600
C	-1.55230200	-1.66224500	0.10368600
C	-0.58035200	-1.05414600	-0.66182800
O	2.92527900	-1.53813200	1.27643900
O	4.01291500	-0.73508600	-0.88068500
C	1.21600900	0.88803700	1.28613800
C	2.37154900	1.73240000	-0.67923100
C	-0.58817700	0.15354700	-1.52771100
H	-1.43553500	0.10890300	-2.21078500
H	-0.69895000	1.05005200	-0.91334400
H	0.33496800	0.24351100	-2.09943400
C	-4.56674100	0.38603000	-0.12527700
H	-4.75537900	0.49752100	0.94460400
H	-5.27432100	-0.34853100	-0.51588900
C	-4.65523200	1.70393500	-0.85721200
H	-5.65530100	2.12378400	-0.73278900
H	-3.93001200	2.41768800	-0.46079300
H	-4.46796800	1.56979600	-1.92445100
O	-3.23101400	-0.11861200	-0.30490000
O	-3.73770600	-1.86823900	1.02297000
C	-2.94960700	-1.25952600	0.33747500
H	1.82975000	-1.56678400	-1.94685300
C	0.55053100	2.10051800	1.40135000
H	-0.15227800	2.24805100	2.21376600
H	1.04671000	0.08689000	1.99585600
C	0.77730400	3.13726900	0.48942600
C	0.02693700	4.43434200	0.60679500
H	3.08845200	1.57578700	-1.47640100
C	1.70059000	2.93876000	-0.54228300
H	1.89899200	3.74209500	-1.24287400
H	-0.15902900	4.68764900	1.65196500
H	0.57542100	5.25341100	0.13920200
H	-0.94440800	4.35561200	0.10834700

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 5B

Total Energy (E / au): -1422.67918

Gibbs free Energy (G / au): -1422.43019

C	-2.62673700	-0.45679100	0.28265400
S	-1.51327500	-1.82554900	0.24284100
N	-0.46885900	-1.61303200	-1.09969400
N	0.40763900	-0.56134300	-1.00253100
N	0.06133700	0.69736100	-1.37201600
N	1.09255200	1.43632200	-1.16644700
C	2.10362200	0.67458700	-0.64862200
C	1.67784500	-0.63525700	-0.53722800
O	-2.24843000	-3.02708700	-0.10143700
O	-0.63104300	-1.74721700	1.39266500
C	-3.89761700	-0.60626600	-0.26561400
C	-2.21838600	0.74043600	0.86529500
C	2.27819800	-1.90266900	-0.05265600
H	3.35138400	-1.78090900	0.06758600
H	1.83042300	-2.17010400	0.90668000
H	2.06246900	-2.70857100	-0.75627400
C	5.54825600	0.91979100	0.56592000
H	5.40963200	1.74229800	1.27094500
H	6.03233200	1.31938000	-0.32739900
C	6.32906200	-0.22123500	1.17490200
H	7.31824700	0.13258400	1.47201000
H	5.82076400	-0.60905100	2.05924600
H	6.45452900	-1.03364800	0.45669900
O	4.25507700	0.40715900	0.19628100
O	3.65877900	2.46501100	-0.49441900
C	3.40045200	1.29629500	-0.32072400
H	-0.96610500	-1.60174700	-1.98633600
C	-4.77599700	0.46638400	-0.21654100
H	-5.77335300	0.35698100	-0.62751000
H	-4.19484100	-1.55293900	-0.69962000
C	-4.39665400	1.68106500	0.36246100
C	-5.34976200	2.84374500	0.39128800
H	-1.22843400	0.83277100	1.29514100
C	-3.11147500	1.80118600	0.89908300
H	-2.80994000	2.73684000	1.35633100
H	-5.10644400	3.53518700	1.19928600
H	-5.29700600	3.39865700	-0.54941000
H	-6.37985200	2.50534900	0.51596400

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 6B

Total Energy (E / au): -1422.67878

Gibbs free Energy (G / au): -1422.430427

C	-2.16342700	0.63697900	-0.22182800
S	-2.81985300	-0.98598100	-0.02006500
N	-1.64833800	-1.64656500	1.06795500
N	-0.39948900	-1.82032000	0.51863300
N	-0.11879700	-2.84834000	-0.32298400
N	1.10671300	-2.70744600	-0.68116200
C	1.62666800	-1.58740400	-0.09500200
C	0.66421100	-0.99701500	0.69896600
O	-2.77472700	-1.66876800	-1.29962100
O	-4.02753500	-0.97692600	0.78545500
C	-1.29525800	0.88515800	-1.28193200
C	-2.46622900	1.61256900	0.72195100
C	0.64309000	0.20282300	1.57203000
H	1.58849400	0.28359900	2.10522800
H	0.51998700	1.10521500	0.96673100
H	-0.18737500	0.14162600	2.27541800
C	4.63888000	0.47191100	0.07299600
H	4.82006000	0.57933500	-0.99858000
H	5.34599400	-0.26517100	0.45971500
C	4.74044000	1.79117500	0.80071000
H	5.74137200	2.20581000	0.66630900
H	4.01468400	2.50706800	0.40966800
H	4.56199800	1.65982600	1.86986900
O	3.30219600	-0.02516900	0.26509900
O	3.80125300	-1.79536400	-1.03686400
C	3.01771500	-1.17859300	-0.35276600
H	-1.99982000	-2.52113100	1.45382800
C	-0.71148300	2.13942400	-1.38210100
H	-0.02573900	2.34579900	-2.19594100
H	-1.08058900	0.10698200	-2.00461500
C	-0.99407200	3.14326000	-0.44888400
C	-0.36831300	4.50312200	-0.58716400
H	-3.14814700	1.39069300	1.53387900
C	-1.87980800	2.86393400	0.59657600
H	-2.10971900	3.63543000	1.32250300
H	-0.46177900	5.07757000	0.33520500
H	0.69023600	4.42124200	-0.84179100
H	-0.85661800	5.06625400	-1.38735100

DFT ωB97x-D/6-31g(d)-PCM-$CHCl_3$ fully optimized geometries.
True minimum energy structure: No imaginary frequencies found

Str. 7A

Total Energy (E / au): -1422.674831

Gibbs free Energy (G / au): -1422.428354

C	-2.86158300	-0.20537400	0.22708200
S	-1.44458200	-1.19034600	0.58707800
N	-0.56809900	-1.00077100	-0.89623800
N	0.78947700	-1.13399900	-0.73013400
N	1.38978400	-2.34803300	-0.70047000
N	2.64240000	-2.13264400	-0.50528100
C	2.85892000	-0.78913600	-0.37988300
C	1.65909700	-0.11868800	-0.52365500
O	-1.85979100	-2.57159800	0.76443700
O	-0.59877800	-0.53347000	1.56906800
C	-4.12141600	-0.79459800	0.25155500
C	-2.69421700	1.15551800	-0.01375600
C	1.23090000	1.30082000	-0.46706700
H	2.09319100	1.95283300	-0.57785000
H	0.50029000	1.50294600	-1.25257600
H	0.75713200	1.49562200	0.49918500
C	5.49141400	1.65534500	0.31572500
H	6.15539500	1.48266400	-0.53412600
H	5.92772000	1.16576500	1.18845300
C	5.23988800	3.12514400	0.55571300
H	6.18121400	3.62749200	0.78493200
H	4.80525700	3.59390000	-0.32923400
H	4.55867900	3.26550800	1.39669800
O	4.21679200	1.04950600	0.03636800
O	5.20794500	-0.97058800	-0.05981000
C	4.21821400	-0.27864200	-0.12359200
H	-0.89534800	-1.66036600	-1.59916600
C	-5.23297000	0.00582400	0.03043200
H	-6.22234400	-0.43776800	0.05125700
H	-4.22042000	-1.85536700	0.44725400
C	-5.09965900	1.37576000	-0.21331200
C	-6.32049100	2.22146200	-0.44789500
H	-1.70140300	1.59103800	-0.02505700
C	-3.81850000	1.93665700	-0.23522000
H	-3.70414100	2.99831000	-0.42550400
H	-6.06197000	3.27677900	-0.54049900
H	-6.83056700	1.91224800	-1.36397300
H	-7.03124100	2.11071900	0.37455100

Experimental Structure

Str. X-ray-A

O	7.18157400	7.35653500	8.20817100
N	4.94340800	6.81769100	7.38896300
H	4.46089500	6.11667000	7.27047000
O	2.35557300	11.38897500	9.71346500
N	3.40697300	9.83626600	7.69909100
O	3.39312400	10.17003600	11.24070300
N	4.40234700	7.98850000	7.86147000
N	3.91761700	8.90192000	6.98813600
C	3.58272800	9.54225600	9.00982400
C	3.05069100	10.45149100	9.99141100
C	4.22914100	8.33482600	9.14587100
C	2.82969300	11.03637200	12.26910100
H	1.86075600	11.02590900	12.21936400
H	3.13281800	11.94770000	12.14036900
O	6.78875800	5.46273200	6.63119500
C	4.66957100	7.51034100	10.27667100
H	4.44460300	7.94978700	11.09880400
H	4.23290600	6.65656100	10.24009900
H	5.62070700	7.38583200	10.22985900
C	7.80478900	10.40859200	2.42836600
H	8.18508000	11.21947500	2.77360400
H	8.43907900	9.97647000	1.85345800
H	7.00969300	10.61576000	1.93099000
C	3.27489400	10.53414800	13.58568500
H	2.91483400	11.09078000	14.27908600
H	2.96715100	9.63328400	13.70564100
H	4.23405700	10.55193600	13.62664600
S	6.54967400	6.81559800	7.05542800
C	6.83322000	7.88387000	5.69788400
C	7.45475300	9.48994100	3.57525700
C	7.69361400	9.93043300	4.87136100
H	8.06049500	10.77375100	5.01472300
C	7.38776400	9.12059700	5.94218300
H	7.55225500	9.40309800	6.81405400
C	6.89465200	8.25844600	3.38801000
H	6.71768300	7.96548200	2.52345300
C	6.58668000	7.44442400	4.44859200
H	6.21421000	6.60424600	4.30669300

Experimental Structure

Str. X-ray-B

C	1.46415400	6.98091400	13.26239100
H	1.45948400	7.33142400	14.12402200
C	2.00556100	5.20325000	11.76879900
H	2.36967000	4.36097800	11.61519800
C	4.91880600	5.07455500	17.36135600
H	5.26046600	5.38635200	18.20250700
H	3.98723200	4.86215600	17.45351700
H	5.40169700	4.28983000	17.09218800
C	0.95452000	7.21528500	10.95544300
C	0.94926400	7.71332400	12.21936400
H	0.59536200	8.55768800	12.38028000
C	6.73349900	8.34528900	19.69024700
H	7.69262800	8.43213200	19.57468000
H	6.34674800	9.23359800	19.72535600
C	1.46788300	5.96077100	10.73308700
H	1.45708600	5.61026100	9.87145500
C	0.30048900	7.97594500	9.82171800
H	0.39792900	7.48104500	9.00543600
H	-0.63271100	8.09626900	10.01335400
H	0.72004000	8.83391100	9.72809400
C	6.43832300	7.61811000	20.92344800
H	6.80565300	8.09417700	21.67097500
H	5.48738300	7.53963800	21.02877400
H	6.82870500	6.74131100	20.87956200
S	2.51009000	4.77437200	14.39582400
N	4.94807400	7.06880300	14.31419500
C	5.60180100	7.38060000	16.35051200
C	6.22990300	8.17997300	17.40816800
N	4.70202000	5.97541900	15.08220300
C	5.08392000	6.11667000	16.35490100
O	6.75625200	9.23673600	17.21506900
O	6.15795100	7.58672100	18.57700200
O	2.02655400	5.34973200	15.60005900
N	4.13047700	4.87157300	14.52631200
H	4.62508400	4.22600600	14.24544000
C	1.97512500	5.75360400	13.03418300
N	5.51318300	7.92153700	15.10414600
O	2.27103300	3.40884500	14.06111900

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: nhsscl

```
Bond precision:  C-C = 0.0079 A          Wavelength=0.71073

Cell:            a=10.2099(5)    b=10.3544(4)        c=14.5191(8)
                 alpha=90        beta=107.530(5)     gamma=90
Temperature:     150 K

                 Calculated                Reported
Volume           1463.64(13)               1463.64(13)
Space group      P 21                      P 21
Hall group       P 2yb                     P 2yb
Moiety formula   C12 H14 N4 O4 S           C12 H14 N4 O4
Sum formula      C12 H14 N4 O4 S           C24 H28 N8 O8 S2
Mr               310.33                    620.66
Dx,g cm-3        1.408                     1.408
Z                4                         2
Mu (mm-1)        0.242                     0.242
F000             648.0                     648.0
F000'            648.79
h,k,lmax         14,14,20                  14,13,18
Nref             8092[ 4258]               6788
Tmin,Tmax        0.950,0.988
Tmin'            0.950

Correction method= Not given

Data completeness= 1.59/0.84      Theta(max)= 29.419

R(reflections)= 0.0614( 4891)     wR2(reflections)= 0.1328( 6788)

S = 1.031                 Npar= 379
```

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 ....       2.15 Report
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00785 Ang.
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C24 H28 N8 O8 S2
            Atom count from _chemical_formula_moiety:C12 H14 N4 O4
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       2.00 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C6B Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          8 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ          2 Units
```

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

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

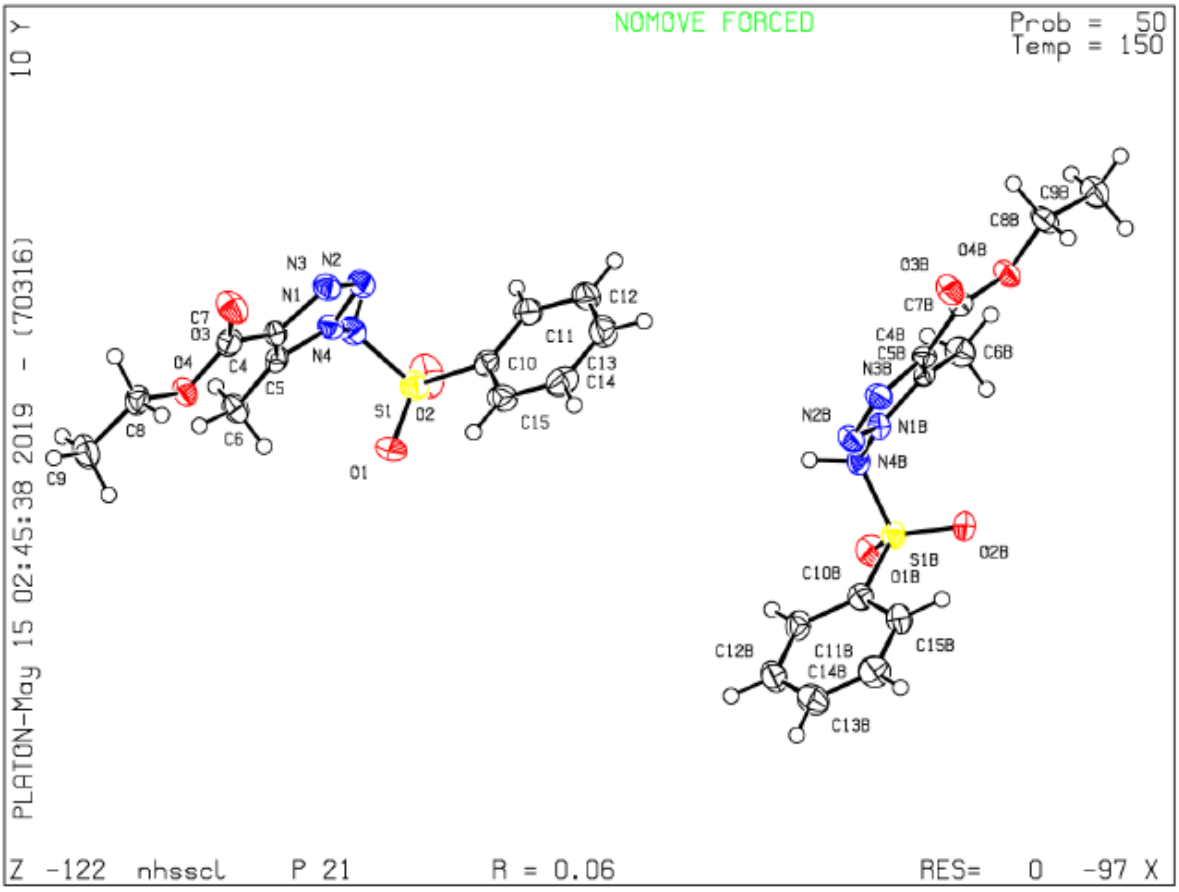
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock nhsscl - ellipsoid plot



checkCIF/PLATON report

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: nhslfch3

```
Bond precision:  C-C = 0.0128 A          Wavelength=0.71073

Cell:            a=10.311(2)     b=10.463(2)         c=15.257(3)
                 alpha=90        beta=106.50(3)      gamma=90
Temperature:     298 K
```

	Calculated	Reported
Volume	1578.2(6)	1578.2(6)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C13 H16 N4 O4 S	C13 H16 N4 O4 S1
Sum formula	C13 H16 N4 O4 S	C26 H32 N8 O8 S2
Mr	324.36	648.71
Dx,g cm-3	1.365	1.365
Z	4	2
Mu (mm-1)	0.228	0.228
F000	680.0	680.0
F000'	680.80	
h,k,lmax	12,12,18	12,12,18
Nref	5577[2957]	5567
Tmin,Tmax	0.973,0.991	
Tmin'	0.969	

```
Correction method= Not given

Data completeness= 1.88/1.00      Theta(max)= 25.026

R(reflections)= 0.0588( 2762)     wR2(reflections)= 0.1228( 5567)

S = 1.017                 Npar= 397
```

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 B

```
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01282 Ang.
```

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
            Rint given   0.158
PLAT234_ALERT_4_C Large Hirshfeld Difference C4       --C7       .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14      --C15      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C12B     --C13B     .       0.18 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C13B Check
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C10      -C15             1.37 Ang.
PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C10B     -C15B            1.37 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H9BA     ..H16D     .       2.10 Ang.
                                              1+x,y,1+z  =      1_656 Check
```

Alert level G

```
FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C26 H32 N8 O8 S2
            Atom count from _chemical_formula_moiety:C13 H16 N4 O4 S1
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.158 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       2.00 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C6B Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C16B Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          8 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
```

```
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PLATON version of 03/05/2019; check.def file version of 29/04/2019

Datablock: nhslfch3 - ellipsoid plot