Electronic Supplementary Information for

The structure of fluorinated indazoles: the effect of the replacement of an H by a F atom

on the supramolecular structure of NH-indazoles

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- X-ray crystallography, page S-2 - S-8

- NMR, page S-8

- Optimized geometries of the indazoles, page S-9 - S15

X-ray crystallography. Two structures (compounds **7** and **9**) have been recorded at low temperature (180 K) on a Xcalibur Oxford Diffraction diffractometer using a graphite-monochromated Mo-K α radiation ($\lambda = 0.71073$ Å) and equipped with an Oxford Cryosystems Cryostream Cooler Device. The final unit cell parameters have been obtained by means of a least-squares refinement performed on 3500 (for **7**) or 1650 (for **9**) well measured reflections. The structure of compound **6** has been recorded at low temperature (180 K) on a IPDS STOE diffractometer using a graphite-monochromated Mo-K α radiation ($\lambda = 0.71073$ Å) and equipped with an Oxford Cryosystems Cryostream Cooler Device. The final unit cell parameters have been obtained by means of a least-squares refinement performed on 3500 (for **7**) or 1650 (for **9**) well measured reflections. The structure of compound **6** has been recorded at low temperature (180 K) on a IPDS STOE diffractometer using a graphite-monochromated Mo-K α radiation ($\lambda = 0.71073$ Å) and equipped with an Oxford Cryosystems Cryostream Cooler Device. The final unit cell parameters have been obtained by means of a least-squares refinement performed on a set of 8000 well measured reflections, and the crystal decay has been monitored during the data collections, no significant fluctuations of intensities have been observed.

The structures have been solved by Direct Methods using SIR92,^{S1} and refined by means of least-squares procedures on a F² with the aid of the program SHELXL97^{S2} include in the software package WinGX version 1.63.^{S3} The Atomic Scattering Factors were taken from International tables for X-Ray Crystallography.^{S4} All hydrogen atoms were geometrically placed and refined by using a riding model. All non-hydrogen atoms were anisotropically refined, and in the last cycles of refinement a weighting scheme was used, where weights are calculated from the following formula: $w = 1/[\sigma^2(Fo^2)+(aP)^2+bP]$ where $P = (Fo^2+2Fc^2)/3$.

- S1 SIR92 A program for crystal structure solution. A. Altomare, G. Cascarano, C. Giacovazzo and A. Guagliardi, J. Appl. Crystallogr. 1993, 26, 343-350.
- S2 SHELX97 Includes SHELXS97, SHELXL97, CIFTAB Programs for Crystal Structure Analysis (Release 97-2). G. M. Sheldrick, Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.

- WINGX 1.63 Integrated System of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data. L.Farrugia, J. Appl. Crystallogr.1999, 32, 837 838.
- S4 International tables for X-Ray crystallography, 1974, Vol IV, Kynoch Press, Birmingham, England.

Table S1. Bond lengths [Å] and angles [°] for 6.

N(1)-C(7A)	1.3638(16)
N(1)-N(2)	1.3693(15)
N(2)-C(3)	1.3203(16)
C(3A)-C(4)	1.4050(17)
C(3A)-C(7A)	1.4060(17)
C(3A)-C(3)	1.4264(18)
C(6)-C(7)	1.3762(19)
C(6)-C(5)	1.4069(19)
C(7A)-C(7)	1.4041(19)
C(4)-C(5)	1.372(2)
C(8)-C(3)	1.4919(18)
C(7A)-N(1)-N(2)	111.75(10)
C(3)-N(2)-N(1)	106.53(10)
C(4)-C(3A)-C(7A)	119.85(12)
C(4)-C(3A)-C(3)	134.93(12)

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C(7A)-C(3A)-C(3)	105.22(11)		
C(7)-C(6)-C(5)	121.98(13)		
N(1)-C(7A)-C(7)	132.11(12)		
N(1)-C(7A)-C(3A)	105.92(11)		
C(7)-C(7A)-C(3A)	121.97(11)		
C(5)-C(4)-C(3A)	118.18(12)		
C(4)-C(5)-C(6)	121.31(12)		
N(2)-C(3)-C(3A)	110.56(11)		
N(2)-C(3)-C(8)	121.99(11)		
C(3A)-C(3)-C(8)	127.44(11)		
C(6)-C(7)-C(7A)	116.70(12)		

Table S2. Bond lengths [Å] and angles [°] for 7.

C(3)-N(2)	1.329(6)
C(3)-C(3A)	1.413(6)
C(3)-C(8)	1.483(6)
C(8)-F(2)	1.319(5)
C(8)-F(3)	1.325(5)
C(8)-F(1)	1.334(6)
C(7A)-N(1)	1.352(5)
C(7A)-C(7)	1.398(6)
C(7A)-C(3A)	1.410(6)

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C(3A)-C(4)	1.407(6)
C(4)-C(5)	1.365(7)
C(5)-C(6)	1.404(8)
C(6)-C(7)	1.366(7)
N(2)-N(1)	1.355(5)

- N(2)-C(3)-C(3A) 112.1(4)
- N(2)-C(3)-C(8) 119.1(4)
- C(3A)-C(3)-C(8) 128.7(4)
- F(2)-C(8)-F(3)106.8(4)
- F(2)-C(8)-F(1) 106.6(4)
- F(3)-C(8)-F(1)105.7(4)
- F(2)-C(8)-C(3) 112.7(4)
- F(3)-C(8)-C(3)112.9(4)
- F(1)-C(8)-C(3) 111.6(4)
- N(1)-C(7A)-C(7) 131.0(4)
- N(1)-C(7A)-C(3A) 106.9(3)
- C(7)-C(7A)-C(3A)122.1(4)
- C(4)-C(3A)-C(7A) 119.4(4)
- C(4)-C(3A)-C(3) 137.0(4)
- C(7A)-C(3A)-C(3) 103.5(4)
- C(5)-C(4)-C(3A) 117.9(4)
- C(4)-C(5)-C(6) 121.8(5)
- C(7)-C(6)-C(5) 121.8(4)
- C(6)-C(7)-C(7A) 116.9(4)

S	upplementary Material (ESI) for New Journal of Chemistry This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2007
C(3)-N(2)-N(1)	105.3(4)
C(7A)-N(1)-N(2)	112.2(4)

 Table S3.
 Bond lengths [Å] and angles [°] for 9.

C(3)-N(2)	1.334(5)
C(3)-C(3A)	1.405(6)
C(3)-C(8)	1.492(6)
C(3A)-C(4)	1.409(5)
C(3A)-C(7A)	1.415(6)
C(4)-C(5)	1.346(5)
C(4)-F(4)	1.351(5)
C(5)-F(5)	1.342(5)
C(5)-C(6)	1.417(6)
C(6)-C(7)	1.351(5)
C(6)-F(6)	1.352(5)
C(7)-F(7)	1.345(4)
C(7)-C(7A)	1.391(5)
C(7A)-N(1)	1.353(5)
C(8)-F(3)	1.323(5)
C(8)-F(1)	1.331(5)
C(8)-F(2)	1.336(5)
N(1)-N(2)	1.362(5)

- N(2)-C(3)-C(3A) 111.5(4)
- N(2)-C(3)-C(8) 118.5(4)
- C(3A)-C(3)-C(8) 129.8(4)
- C(3)-C(3A)-C(4) 138.0(4)
- C(3)-C(3A)-C(7A) 104.2(3)
- C(4)-C(3A)-C(7A) 117.7(4)
- C(5)-C(4)-F(4) 120.2(3)
- C(5)-C(4)-C(3A) 120.3(4)
- F(4)-C(4)-C(3A) 119.5(4)
- F(5)-C(5)-C(4) 121.9(4)
- F(5)-C(5)-C(6) 117.6(4)
- C(4)-C(5)-C(6) 120.5(4)
- C(7)-C(6)-F(6) 121.3(4)
- C(7)-C(6)-C(5) 121.5(4)
- F(6)-C(6)-C(5) 117.3(4)
- F(7)-C(7)-C(6) 121.5(4)
- F(7)-C(7)-C(7A) 120.3(4)
- C(6)-C(7)-C(7A) 118.1(4)
- N(1)-C(7A)-C(7) 131.3(4)
- N(1)-C(7A)-C(3A) 106.8(3)
- C(7)-C(7A)-C(3A) 121.8(4)
- F(3)-C(8)-F(1) 108.0(3)
- F(3)-C(8)-F(2) 106.7(3)
- F(1)-C(8)-F(2) 106.6(4)

	Supplementary Material (ESI) for New Journal of Chemistry This journal is (c) The Royal Society of Chemistry and The Centre National de la Recherche Scientifique, 2007
F(3)-C(8)-C(3)	111.9(4)
F(1)-C(8)-C(3)	112.0(3)
F(2)-C(8)-C(3)	111.3(3)
C(7A)-N(1)-N(2) 111.6(3)
C(3)-N(2)-N(1)	105.9(3)

NMR spectroscopy. Solution NMR spectra were recorded on a Bruker DRX 400 (9.4 Tesla, 400.13 MHz for ¹H, 100.62 MHz for ¹³C and 40.56 MHz for ¹⁵N) spectrometer with a 5-mm inverse-detection H-X probe equipped with a z-gradient coil. A Bruker AM 250 (250.13 MHz for ¹H, 62.93 MHz for ¹³C was also used for more routine spectra. Chemical shifts (δ in ppm) are given from internal solvent, CDCl₃ (7.26), DMSO-d₆ (2.49) for ¹H and CDCl₃ (77.0), DMSO-d₆ (39.5) for ¹³C and for ¹⁵N NMR, nitromethane (0.00) were used as external reference. 2D (¹H-¹H) gs-COSY and inverse proton detected heteronuclear shift correlation spectra, (¹H-¹³(C) gs-HMQC, (¹H-¹³(C) gs-HMBC, (¹H-¹⁵N) gs-HMQC and (¹H-¹⁵N) gs-HMBC, were acquired and processed using standard Bruker NMR software and in non-phasesensitive mode. Variable temperature experiments were recorded on the same spectrometer; a Bruker BVT3000 temperature unit was used to control the temperature of the cooling gas stream and an exchanger to achieve low temperatures. ¹⁹F NMR (376.50 MHz) spectra were recorded on the same spectrometer with a 5-mm QNP direct-detection probe equipped with a z-gradient coil. NMR chemical shifts were referenced to CFCl₃ (one drop in CDCl₃) as the external reference which was set at δ 0.00 ppm. Some ¹⁹F NMR experiments were carried out on a Bruker AC200 (4.7 Tesla, 188.30 MHz) and CF₃COOH was used as an external reference. Chemical shifts were converted to the CFCl₃ reference with δ (CF₃COOH) 77.0.

Optimized geometries of the indazoles at the B3LYP/6-311++G computational level.**

3ch3-indazole-1H

N.0.6662083766,1.7565398395,0. N,1.8613191835,1.1035184244,0. C,1.5870993678,-0.1874181752,0. C,-0.395550052,0.8979966885,0. C,0.1672264523,-0.4003208144,0. C,-0.6783791816,-1.5223019279,0. C,-2.047682061,-1.3190978302,0. C,-2.589737454,-0.0143584633,0. C,-1.7814576062,1.1100030278,0. H,-0.2684908144,-2.5260550335,0. H,-2.7196845957,-2.1692102787,0. H,-3.6669204872,0.1081955819,0. H,-2.2054761954,2.1073752581,0. H,0.6625343316,2.7621738806,0. C,2.6763537591,-1.210462552,0. H,3.6483772193,-0.7166088647,0. H,2.614864137,-1.8552590559,0.8822110166 H,2.614864137,-1.8552590559,-0.8822110166

3ch3-indazole-2H

N,-0.3255595904,1.4839181641,-1.2143748894 N,-1.3923886844,0.6715578782,-1.3440206712 C,-1.3831060703,-0.446455613,-0.5796684333 C,0.4319762109,0.8493239178,-0.3005159384 C,-0.1820735129,-0.3731630389,0.1369685446 C,0.4590663917,-1.1905733849,1.1005756439 C,1.6724864839,-0.7786555665,1.5954060838 C,2.2798755034,0.4369315083,1.1583528779 C,1.6849566825,1.250939399,0.2265466669 H,0.0062051987,-2.1159505705,1.4393596145 H,2.1865105943,-1.3834711674,2.333684984 H.3.2387287256.0.7183014885.1.5793085023 H,2.1457617726,2.1734959804,-0.1052546577 C.-2.4818875.-1.456175334.-0.5958518361 H,-2.1120718712,-2.440397928,-0.8981945661 H,-2.9359335884,-1.5645537297,0.3935725238 H,-3.2722379729,-1.1698034485,-1.2940844416 H,-2.1190900697,0.9410157517,-1.9905046918

3cf3-indazole-1H

N,-1.9504700705,0.7899571588,0.4566644358 N,-1.6994480481,-0.529665453,0.5507294549 C,-0.4333851959,-0.6811595026,0.2191972255 C,-0.8532901046,1.5118805038,0.0638501471 C,0.184810281,0.567194736,-0.1083392202 C,1.461106917,0.9981555306,-0.5111605286 C,1.6531007843,2.3494838204,-0.7300237989

 $\begin{array}{l} C,0.6030421044,3.2794358254,-0.5531119995\\ C,-0.6611385476,2.8827339468,-0.155006655\\ H,2.2695520838,0.2900165837,-0.6438407568\\ H,2.6264970596,2.7090904885,-1.0417151976\\ H,0.7954247856,4.3307505,-0.7336544211\\ H,-1.4619630677,3.599905311,-0.019739257\\ H,-2.8742551006,1.1229452416,0.6802891105\\ C,0.1897683372,-2.039215046,0.1812274785\\ F,1.3843757276,-2.0412231789,0.82769752\\ F,0.4524820264,-2.4299103039,-1.0933559093\\ F,-0.5779595746,-2.9828452896,0.7397814331\\ \end{array}$

3cf3-indazole-2H

N,-1.9842423773,0.8821008942,0.5025568246 N,-1.6371329333,-0.4034162873,0.5441158893 C,-0.3541843731,-0.6575887568,0.182993139 C,-0.8628073305,1.5098838109,0.0896088772 C,0.210358481,0.5825548264,-0.1306588031 C,1.4765356272,1.0427388116,-0.5684453811 C,1.6308175445,2.3921760784,-0.7698266043 C,0.5627341972,3.3125796014,-0.5503136123 C,-0.6743034215,2.896487516,-0.1264371831 H.2.294959498.0.3537889973.-0.7385172951 H.2.5875420176.2.7760697599.-1.1047573013 H,0.7419282903,4.3672207082,-0.7255318323 H,-1.4887254389.3.5902441703,0.0418640367 C,0.202103604,-2.0336568145,0.1712938671 F,1.2587108643,-2.1718920438,1.0037921127 F,0.6324047125,-2.4076029527,-1.0549091895 F,-0.7369938189,-2.9337349815,0.5600401507 H,-2.3206989867,-1.0900965209,0.830639933

3ch3-4,5,6,7-f-indazole-1H

N.1.3375527877.2.0061407604.0. N.2.5486362969,1.3879495776,0. C,2.3237181457,0.0889043291,0. C.0.3103859874.1.113334358.0. C.0.9083363474,-0.1670220761,0. C,0.0848193924,-1.2994293952,0. C,-1.2845191168,-1.145081365,0. C,-1.8628919224,0.1428757619,0. C,-1.076805661,1.2748553132,0. H,1.2910928866,3.0113507645,0. C,3.4455148302,-0.8982896913,0. H,4.3974198365,-0.3674397635,0. H,3.4024668805,-1.5444550434,0.8807895844 H,3.4024668805,-1.5444550434,-0.8807895844 F.0.612488558,-2.5342323794,0. F,-2.0972457528,-2.2108410103.0. F,-3.1958297195,0.246124928,0.

F,-1.629203985,2.5017799408,0.

3ch3-4,5,6,7-F-indazole-2H

N,-1.3865908266,2.0188083093,0. N,-2.4917487129,1.2499954636,0. C,-2.2872522385,-0.0886753486,0. C,-0.3924479502,1.1218424712,0. C,-0.8945878395,-0.2250737652,0. C.0.0066324986,-1.3111984875.0. C,1.3491254881,-1.061186543,0. C,1.8461886823,0.2762974927,0. C.1.0047916842.1.3540997891.0. C,-3.3954812252,-1.0899629129,0. H,-2.9839382146,-2.0978639409,0. H,-4.0301929448,-0.9852416923,0.8853152091 H,-4.0301929448,-0.9852416923,-0.8853152091 H,-3.388522458,1.7142769693,0. F,-0.4475908749,-2.57985223,0. F,2.2407331456,-2.061750727,0. F.3.1743663754.0.4444075899.0. F,1.4946478807,2.5989273417,0.

3cf3-4,5,6,7-F-indazole

N,2.3190411472,-0.1949067311,0. N.1.951795703,-1.4937797361,0. C,0.6317495375,-1.499308267,0. C,1.2471633691,0.6537634964,0. C,0.098808324,-0.1713663381,0. C,-1.174743561,0.4189790143,0. C,-1.2706537186,1.7973714604,0. C,-0.1101331892,2.6075973545,0. C,1.1539608044,2.0499363973,0. H.3.299923639.0.0408884232.0. C,-0.1446128378,-2.781469216,0. F,0.661697883,-3.8519267467,0. F.-0.9445116443.-2.8553602844.-1.0857286632 F,-0.9445116443,-2.8553602844,1.0857286632 F,-2.2806507913,-0.3312147313,0. F,-2.4645658491,2.4008900784,0. F,-0.2597372159,3.9346856156,0. F,2.2561665995,2.816830068,0.

3cf3-4,5,6,7-F-indazole-2H

N,2.2806616667,-0.1264635976,-0.6076138865 N,1.7700689126,-1.3528548934,-0.6837313114 C,0.4574264192,-1.4505490736,-0.3628200992 C,1.2416992447,0.6300131608,-0.212629022

 $\begin{array}{l} C, 0.0510614864, -0.1532811961, -0.0390075364\\ C, -1.1469555092, 0.4645729927, 0.3734531294\\ C, -1.1437995287, 1.8135381213, 0.6007471614\\ C, 0.0381234492, 2.5917346831, 0.4284994082\\ C, 1.2170531774, 2.0235132058, 0.0293438872\\ C, -0.2646683857, -2.7551979496, -0.3979376109\\ F, 0.5871142343, -3.7400135524, -0.7833619951\\ F, -1.2928761338, -2.7478189269, -1.2661448556\\ F, -0.7607134692, -3.098142821, 0.8050927433\\ F, -2.2669544439, -0.2509690131, 0.540365427\\ F, -2.2537112817, 2.4445160598, 0.9927662979\\ F, -0.0412700151, 3.9027132938, 0.6705916692\\ F, 2.3147864474, 2.7660513029, -0.1272799088\\ H, 2.3678657854, -2.1178613188, -0.9667439218\\ \end{array}$

Dimer of 3ch3-indazole-1H

N,-0.3573178819,1.5534618547,0. N,0.9828633411,1.3082364903,0. C,1.5970567143,2.4828492203,0. C,-0.6261547191,2.8885691207,0. C,0.6332208349,3.542700006,0. C,0.6875974812,4.9495226508,0. C.-0.5029275087.5.6569893339.0. C.-1.7506291062.4.9863635369.0. C,-1.8366475786,3.6038408283,0. H,1.6423430647,5.4688273057,0. H,-0.4868597386,6.7431728561,0. H,-2.664614182,5.5743396421,0. H,-2.7961210043,3.0951766696,0. H,-0.9768407046,0.7415310428,0. C,3.0902539578,2.580647679,0. H,3.5326730177,1.5808027423,0. H,3.4565488053,3.1184799247,-0.8832910446 H.3.4565488053.3.1184799247.0.8832910446 N.0.3573178819,-1.5534618547.0. N,-0.9828633411,-1.3082364903,0. C.-1.5970567143.-2.4828492203.0. C.0.6261547191,-2.8885691207,0. C,-0.6332208349,-3.542700006,0. C,-0.6875974812,-4.9495226508,0. C,0.5029275087,-5.6569893339,0. C,1.7506291062,-4.9863635369,0. C,1.8366475786,-3.6038408283,0. H,-1.6423430647,-5.4688273057,0. H,0.4868597386,-6.7431728561,0. H,2.664614182,-5.5743396421,0. H,2.7961210043,-3.0951766696,0. H,0.9768407046,-0.7415310428,0. C,-3.0902539578,-2.580647679,0. H,-3.5326730177,-1.5808027423,0.

H,-3.4565488053,-3.1184799247,-0.8832910446 H,-3.4565488053,-3.1184799247,0.8832910446

Dimer of 3cf3-indazole-1H

N,-0.4110458072,1.5672949831,0. N,0.9110041925,1.2951694697,0. C,1.5342452334,2.4626483983,0. C,-0.6604915147,2.9113078012,0. C,0.6073025733,3.5468216021,0. C,0.689840002,4.9525178292,0. C,-0.4911384032,5.6727492852,0. C,-1.7504506217,5.0220306912,0. C,-1.8608396315,3.641991855,0. H,1.6549652617,5.4491473872,0. H,-0.4595312526,6.7582809615,0. H,-2.6538915901,5.6253425696,0. H,-2.8271841415,3.1475260741,0. H,-1.039961766,0.7631287482,0. C,3.0250394382,2.5390171073,0. N,0.4110458072,-1.5672949831,0. N,-0.9110041925,-1.2951694697,0. C,-1.5342452334,-2.4626483983,0. C,0.6604915147,-2.9113078012,0. C,-0.6073025733,-3.5468216021,0. C,-0.689840002,-4.9525178292,0. C,0.4911384032,-5.6727492852,0. C,1.7504506217,-5.0220306912,0. C,1.8608396315,-3.641991855,0. H,-1.6549652617,-5.4491473872,0. H,0.4595312526,-6.7582809615,0. H,2.6538915901,-5.6253425696,0. H,2.8271841415,-3.1475260741,0. H.1.039961766.-0.7631287482.0. C,-3.0250394382,-2.5390171073,0. F,3.5953143045,1.321043736,0. F.3.4792895754.3.21081022.-1.0844927465 F,3.4792895754,3.21081022,1.0844927465 F,-3.5953143045,-1.321043736,0. F,-3.4792895754,-3.21081022,1.0844927465 F,-3.4792895754,-3.21081022,-1.0844927465

Dimer of 3ch3-4,5,6,7-f-indazole-1H

N,-0.2184413063,1.5716245383,0. N,1.0926740794,1.2022211438,0. C,1.8209469698,2.3082769486,0. C,-0.3526709791,2.9234491546,0. C,0.960475117,3.453955996,0. C,1.1408052846,4.8457149967,0.

C.0.0336640635.5.6696185584.0. C,-1.2721470675,5.1219771164,0. C,-1.4796899204,3.756691763,0. H,-0.9187698649,0.8277744296,0. C,3.3162650358,2.2752448637,0. H.3.6675758897,1.240503163,0. H,3.7232919879,2.7831256189,-0.8816463627 H,3.7232919879,2.7831256189,0.8816463627 N.0.2184413063,-1.5716245383.0. N,-1.0926740794,-1.2022211438,0. C,-1.8209469698,-2.3082769486,0. C.0.3526709791,-2.9234491546,0. C,-0.960475117,-3.453955996,0. C,-1.1408052846,-4.8457149967,0. C,-0.0336640635,-5.6696185584,0. C,1.2721470675,-5.1219771164,0. C,1.4796899204,-3.756691763,0. H,0.9187698649,-0.8277744296,0. C,-3.3162650358,-2.2752448637,0. H,-3.6675758897,-1.240503163,0. H,-3.7232919879,-2.7831256189,-0.8816463627 H,-3.7232919879,-2.7831256189,0.8816463627 F.2.3747893206,5.3752700941,0. F.0.1654527584.7.0039533358.0. F,-2.3137047031,5.9615924236,0. F,-2.7216152636,3.2437548346,0. F,-2.3747893206,-5.3752700941,0. F,-0.1654527584,-7.0039533358,0. F.2.3137047031,-5.9615924236,0. F,2.7216152636,-3.2437548346,0.

Dimer of 3cf3-4,5,6,7-f-indazole-1H

N.-0.5236871628.1.5453715635.0. N.0.8090592452,1.3371616116,0. C,1.3837838331,2.5273995138,0. C.-0.82788517.2.8743114525.0. C,0.4073323584,3.5675216332,0. C,0.413957618,4.9720396781,0. C,-0.7928297286,5.6416373743,0. C,-2.0199592331,4.9335326519,0. C,-2.0538104494,3.5530140774,0. H,-1.1217874771,0.7186417976,0. C,2.8754643642,2.6652296432,0. N,0.5236871628,-1.5453715635,0. N,-0.8090592452,-1.3371616116,0. C,-1.3837838331,-2.5273995138,0. C.0.82788517,-2.8743114525,0. C,-0.4073323584,-3.5675216332,0. C,-0.413957618,-4.9720396781,0.

C,0.7928297286,-5.6416373743,0. C,2.0199592331,-4.9335326519,0. C,2.0538104494,-3.5530140774,0. H,1.1217874771,-0.7186417976,0. C,-2.8754643642,-2.6652296432,0. F,1.5642771759,5.6529456861,0. F,-0.8338547242,6.9784452118,0. F,-3.1556722771,5.6353298353,0. F,-3.2148020169,2.8830936034,0. F,-1.5642771759,-5.6529456861,0. F,0.8338547242,-6.9784452118,0. F,3.1556722771,-5.6353298353,0. F,3.2148020169,-2.8830936034,0. F,3.2982527481,3.3446900034,1.0856931401 F,3.2982527481,3.3446900034,-1.0856931401 F,3.4756463482,1.4617747854,0. F,-3.2982527481,-3.3446900034,1.0856931401 F,-3.2982527481,-3.3446900034,-1.0856931401 F,-3.4756463482,-1.4617747854,0.