SUPPLEMENTARY MATERIALS

^{19}F NMR Diastereotopic Signals in Two *N*-CHF_2 derivatives of (4*S*,7*R*)- 7,8,8-trimethyl-4,5,6,7-tetrahydro-4,7-methano-2*H*-indazole

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NMR

COMPUTATIONAL RESULTS

NMR parameters

NMR spectra were recorded on a Bruker DRX 400 (9.4 Tesla, 400.13 MHz for ^{1}H, 100.61 MHz for ^{13}C and 40.54 MHz for ^{15}N using a 5-mm inverse-detection H-X probe equipped with a *z*-gradient coil, at 300 K. Chemical shifts (δ in ppm) are given from internal solvent, $CDCl_3$ 7.26 for ^{1}H and 77.0 for ^{13}C and for ^{15}N, nitromethane (0.00) was used as external reference. Signals were characterized as s (singlet), d (doublet), and cm (complex multiplet).

Typical parameters for ^{1}H NMR spectra were spectral width 4800 Hz and pulse width 9.5 μs at an attenuation level of 0 dB. Typical parameters for ^{13}C NMR spectra were spectral width 21 kHz, pulse width 12.5 μs at an attenuation level of -6 dB and relaxation delay 2s, WALTZ-16 was used for broadband proton decoupling; the FIDS were multiplied by an exponential weighting (lb=1 Hz) before Fourier transformation.

Inverse proton detected heteronuclear shift correlation spectra, (^{1}H-^{13}C) gs-HMQC and (^{1}H-^{13}C) gs-HMBC, were acquired and processed using standard Bruker NMR software and in nonphase-sensitive mode. Gradient selection was achieved through a 5% sine truncated shaped pulse gradient of 1 ms.

Selected parameters for (^{1}H-^{13}C) gs-HMQC and (^{1}H-^{13}C) gs-HMBC spectra were spectral width 4800 Hz for ^{1}H and 20.5 kHz for ^{13}C, 1024 x 256 data set, number of scans 2 (gs-HMQC) or 4 (gs-HMBC) and relaxation delay 1s. The FIDs were processed using zero filling in the F_1 domain and a sine-bell window function in both dimensions was applied prior to Fourier transformation. In the gs-HMQC experiments, GARP modulation of ^{13}C was used for decoupling. Selected parameters for (^{1}H-^{15}N) gs-HMQC and (^{1}H-^{15}N) gs-HMBC spectra were spectral width 3500 Hz for ^{1}H and 12.5 kHz for ^{15}N, 1024 x 256 data set, number of scans 4, relaxation delay 1s, 37-60 ms delay for evolution of the ^{15}N-^{1}H long-range coupling. The FIDs were processed using zero filling in the F_1 domain and a sine-bell window function in both dimensions was applied prior to Fourier transformation.

^{19}F NMR spectra were recorded on the same spectrometer (376.50 for ^{19}F) using a 5 mm QNP direct-detection probehead equipped with a *z*-gradient coil, at 300 K. Chemical shifts (δ in ppm) are given from $CFCl_3$ as external reference [one drop of $CFCl_3$ in $CDCl_3$ (0.00)]. Typical parameters for ^{19}F NMR spectra were spectral width of 55 kHz, pulse width of 13.75 us at attenuation level of -6 dB and relaxation delay of 1s. WALTZ-16 was used for broadband proton decoupling $^{19}F\{^{1}H\}$, the FIDS were multiplied by an exponential weighting (lb=1 Hz) before Fourier transformation.

Table S1: ^{1}H chemical shifts and spin-spin coupling constants (*J*, Hz) in $CDCl_3$ of compounds **13-14** at 300 K.

Comp.	CHF_2	H3	H4	H5	H6	Others
13	7.14 (dd) $^{2}J_F$ = 59.5 $^{2}J_F$ = 60.5	7.27 (s)	2.81 (d) ^{3}J = 3.8	1.03^{ax} (cm) 2.05^{ec} (cm)	1.18^{ax} (cm) 1.81^{ec} (cm)	CH_3–11 = 0.77 (s) CH_3–10 = 0.92 (s) CH_3–9 = 1.37 (dd) $^{6}J_F$ = $^{6}J_F$ =1.4
14	7.11 (dd) $^{2}J_F$ = $^{2}J_F$ = 60.9	7.28 (s)	2.79 (d) ^{3}J = 4.1	1.22^{ax} (cm) 2.10^{ec} (cm)	1.35^{ax} (cm) 1.88^{ec} (cm)	CH_3–11 = 0.65 (s) CH_3–10 = 0.97 (s) CH_3–9 = 1.29 (s)

Table S2: ^{13}C chemical shifts and spin-spin coupling constants (*J*, Hz) with fluorine in $CDCl_3$ of compounds **13-14** at 300 K.

Comp.	CHF_2	C3	C3a	C4	C5	C6	C7	C7a	C8
13	111.6 (dd) $^{1}J_F$ = 246.0 $^{1}J_F$ = 248.7	134.3 (dd) $^{4}J_F$ = $^{4}J_F$ = 2.3	132.1	47.6	27.4	33.0	53.7	153.6 (dd) $^{3}J_F$ = $^{3}J_F$ = 1.6	63.2
	Others								
	CH_3 –9 = 11.6 (dd) $^{5}J_F$~$^{5}J_F$ = 1.4; CH_3–10 = 19.5; CH_3–11 = 20.1								
14	111.2 (dd) $^{1}J_F$ = 246.4 $^{1}J_F$ = 246.5	117.9	130.2	46.9	27.2	33.3	50.1	169.1 (dd) $^{4}J_F$ = $^{4}J_F$ = 2.2	60.4
	Others								
	CH_3–9 = 10.4; CH_3–10 = 18.9; CH_3–11 = 20.4								

Table S3: ^{15}N and ^{19}F chemical shifts and spin-spin coupling constants (*J*, Hz) in $CDCl_3$ of compounds **13-14** at 300 K.

Comp.	N1	N2	Fa/Fb	Fa/Fb
13	-177.4 (dd) $^{2}J_F$ = $^{2}J_F$ = 27.9	-79.9	-89.16 (ddd) $^{2}J_F$ = 226.6 $^{2}J_H$ = 60.6 $^{6}J_H$ = 1.4	-91.64 (dd) $^{2}J_F$ = 226.6 $^{2}J_H$ = 59.4
14	n.d.	-177.2(dd) $^{2}J_F$ = $^{2}J_F$ = 24.9	-90.80 (dd) $^{2}J_F$ = 225.5 $^{2}J_H$ = 61.3	-92.05(dd) $^{2}J_F$ = 225.4 $^{2}J_H$ = 60.7

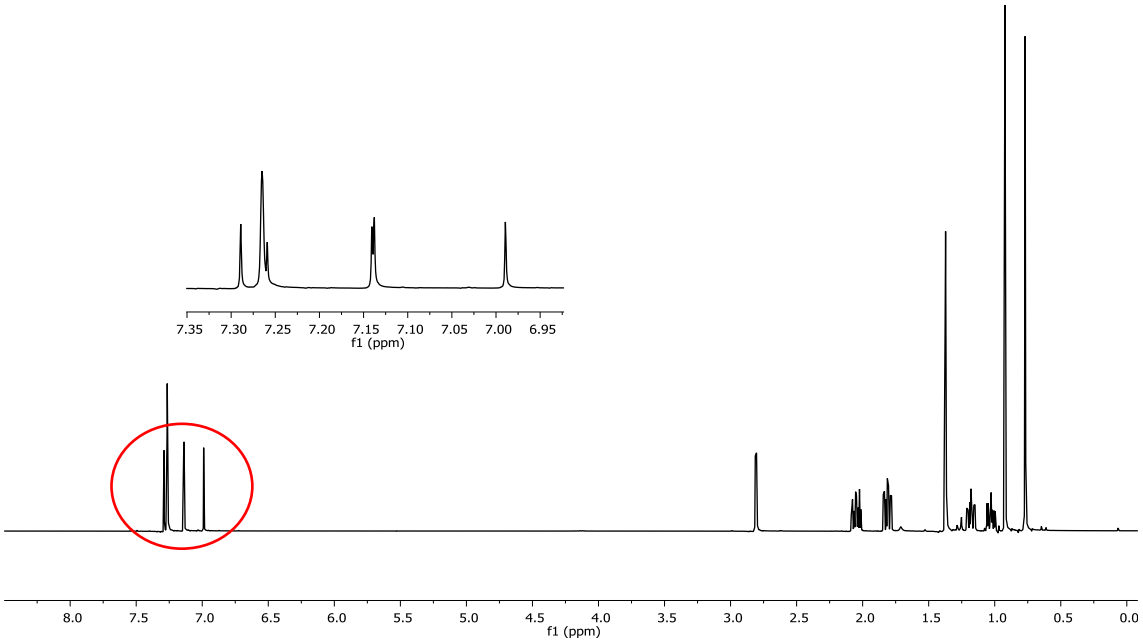

Figure S1: ^{1}H NMR spectrum of **13** in $CDCl_3$ and amplification of circled region.

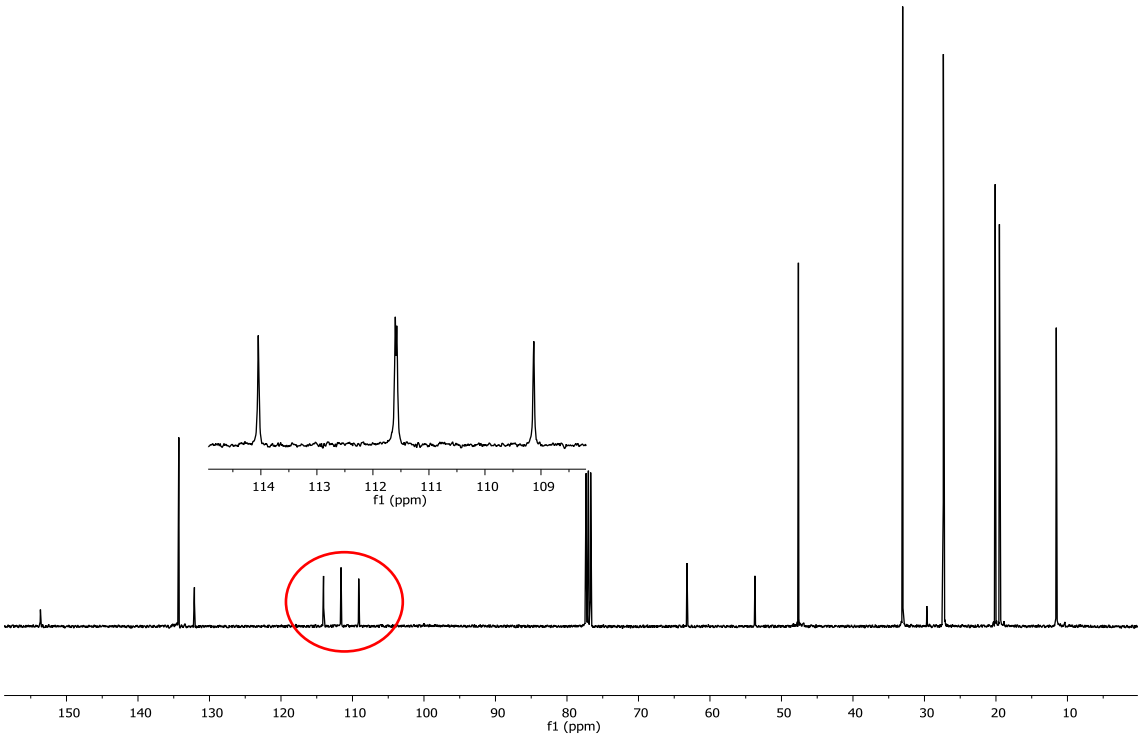

Figure S2: ^{13}C NMR spectrum of **13** in $CDCl_3$ and amplification of circled region.

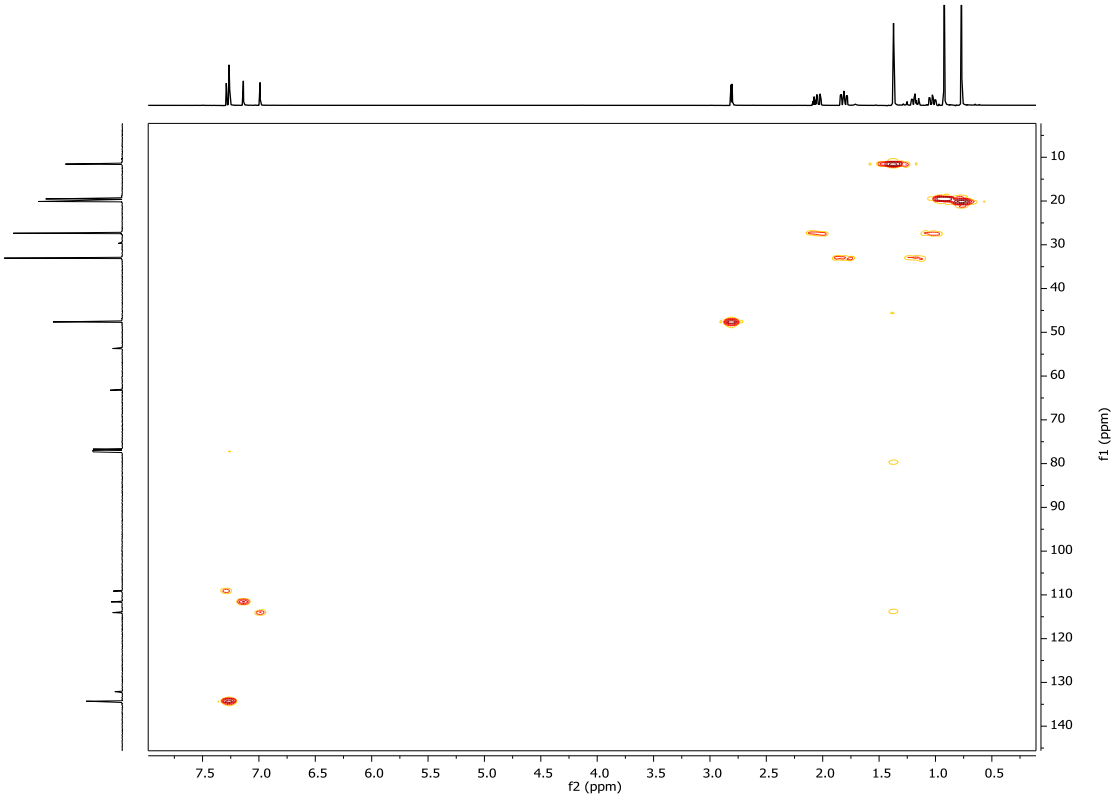

Figure S3: NMR spectrum (^{1}H-^{13}C) gs-HMQC of **13** in $CDCl_3$.

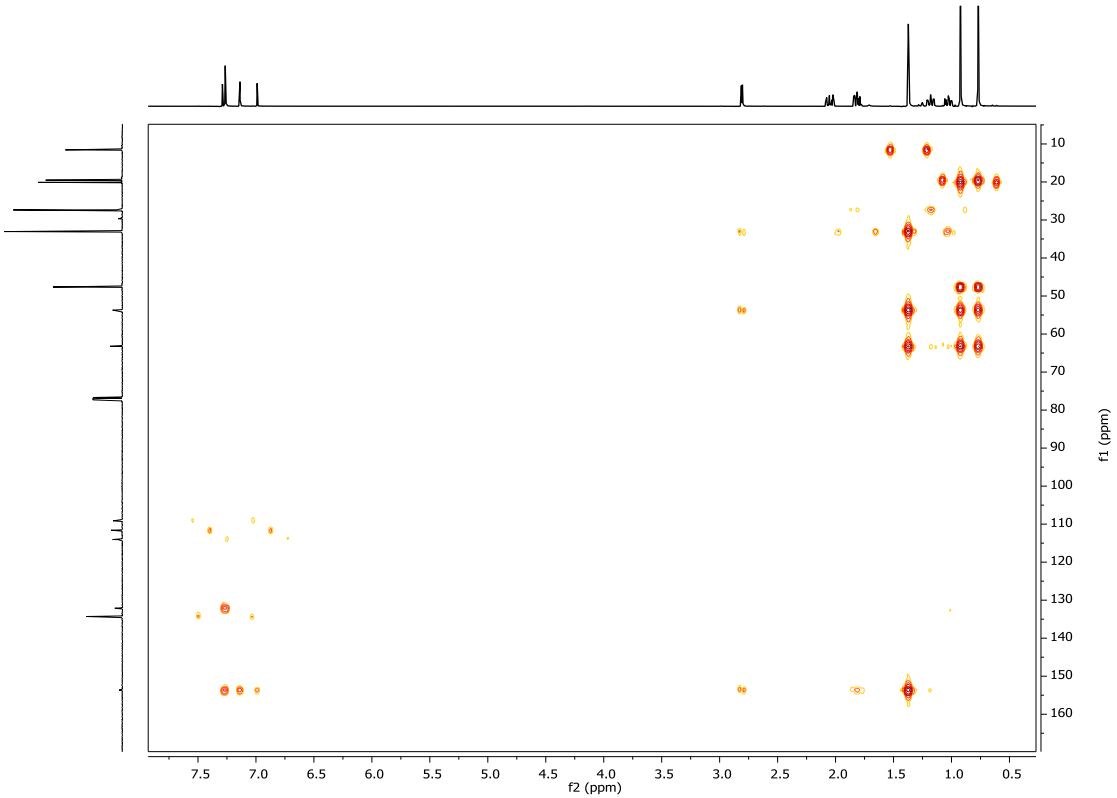

Figure S4: NMR spectrum (^{1}H-^{13}C) gs-HMBC of **13** in $CDCl_3$.

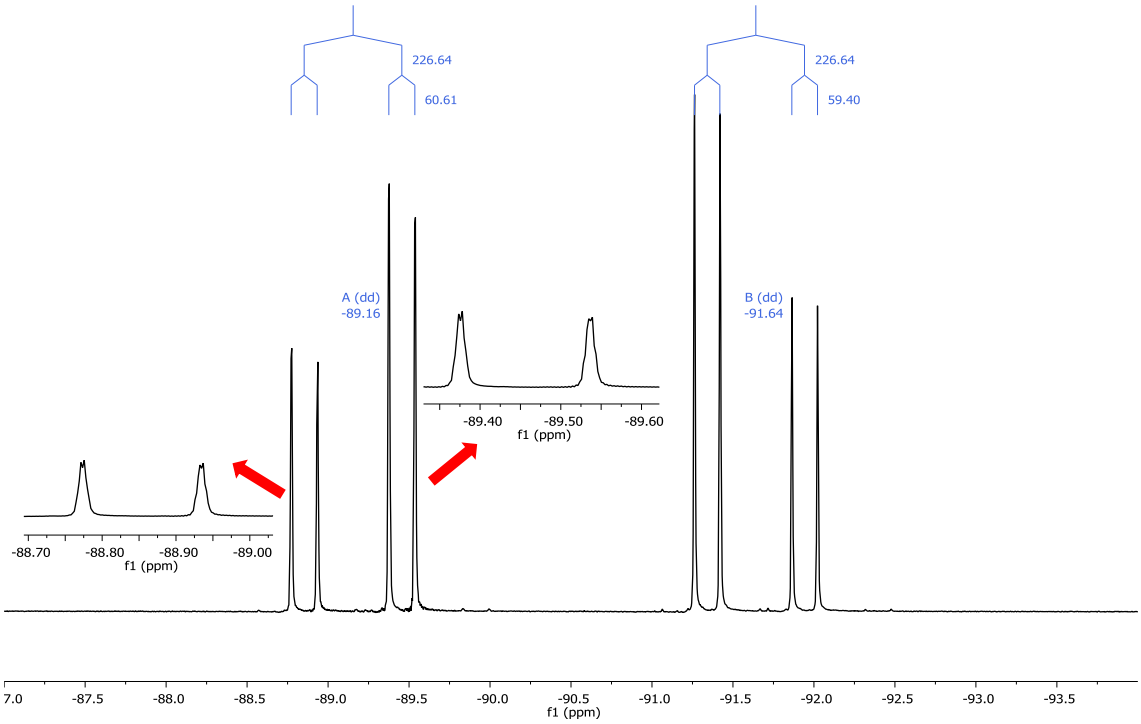

Figure S5: ^{19}F NMR spectrum of **13** in $CDCl_3$.

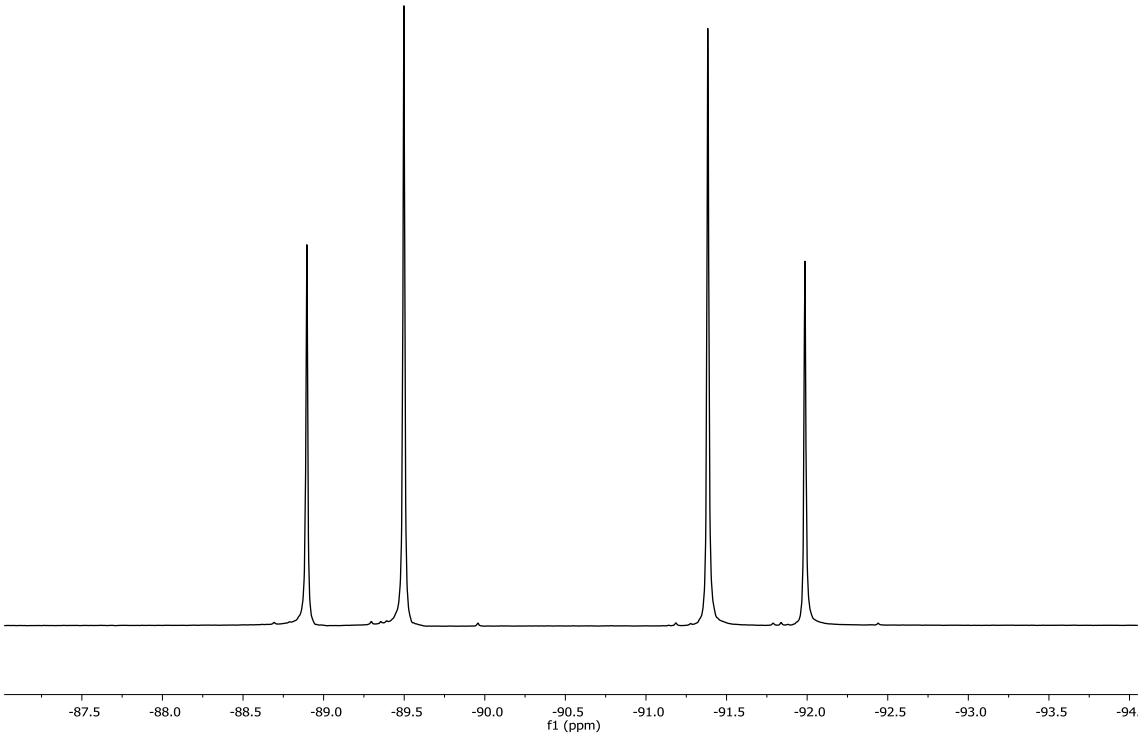

Figure S6: $^{19}F\{^{1}H\}$ NMR spectrum of **13** in $CDCl_3$.

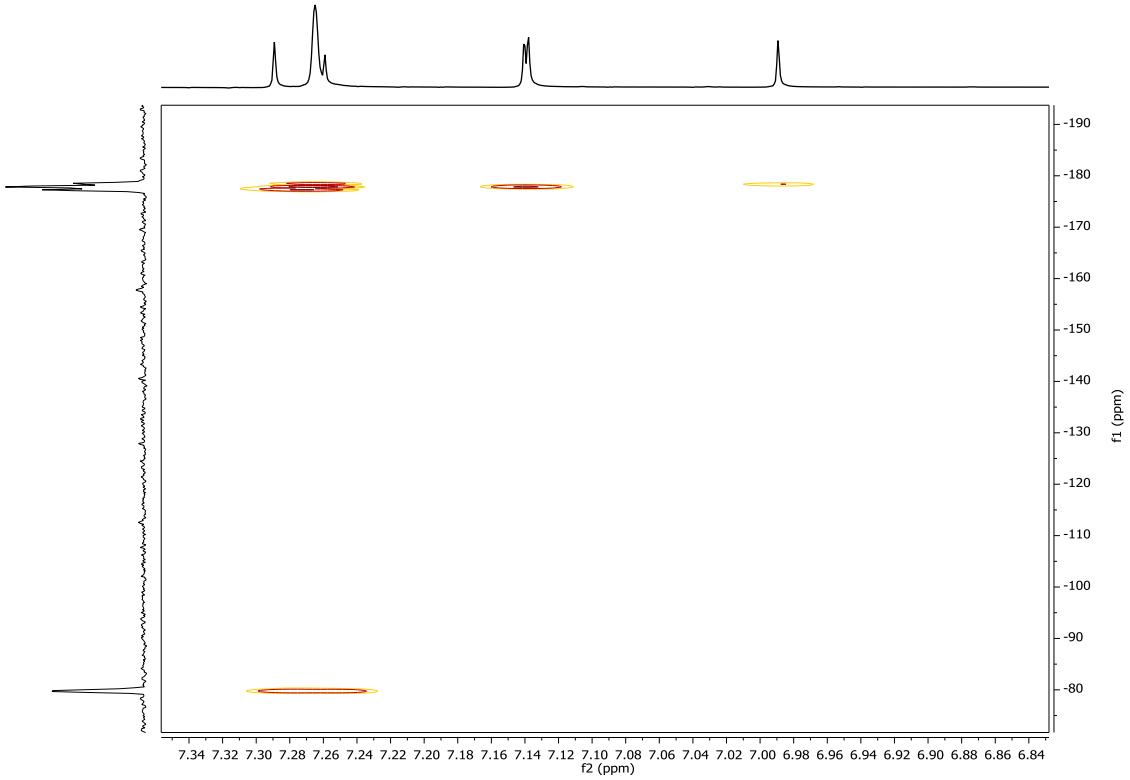

Figure S7: NMR spectrum (^{1}H-^{15}N) gs-HMBC of **13** in $CDCl_3$.

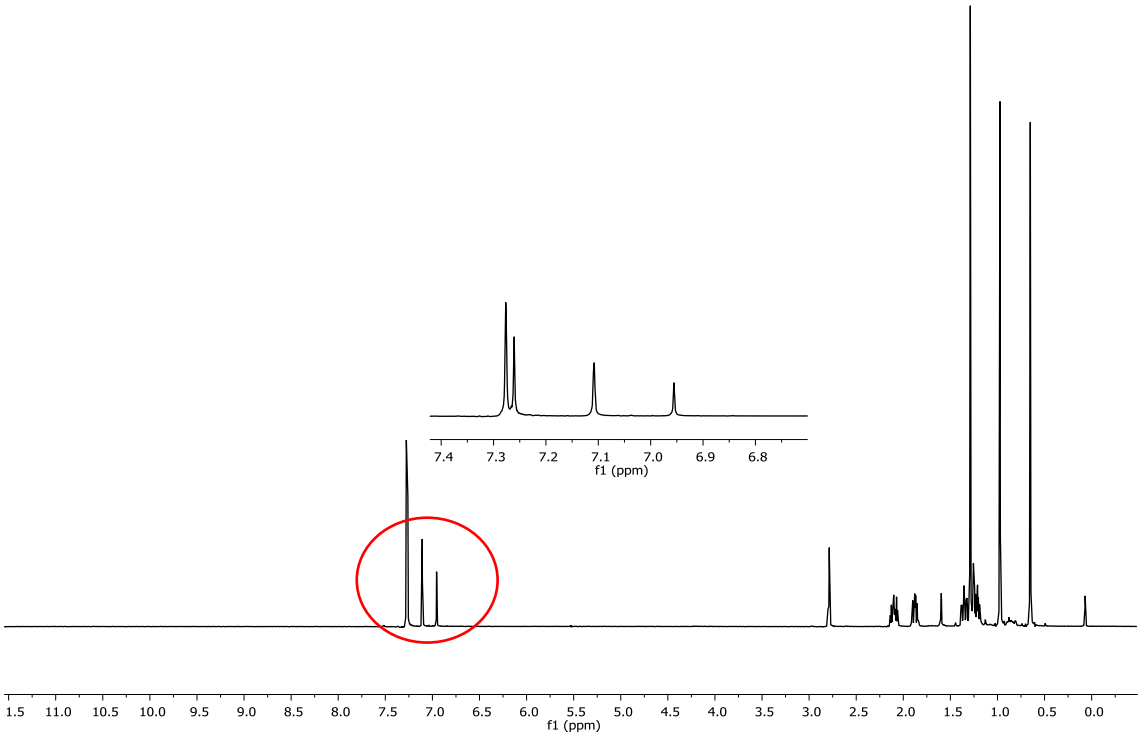

Figure S8: ^{1}H NMR spectrum of **14** in $CDCl_3$ and amplification of circled region.

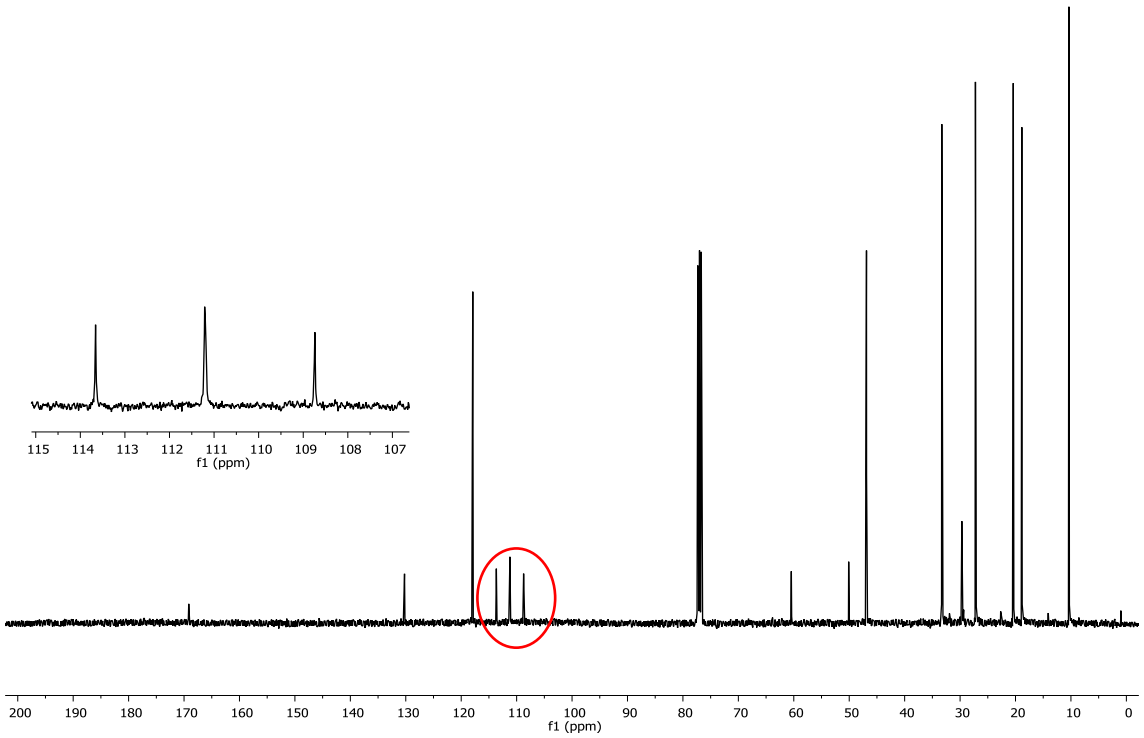

Figure S9: ^{13}C NMR spectrum of **14** in $CDCl_3$ and amplification of circled region.

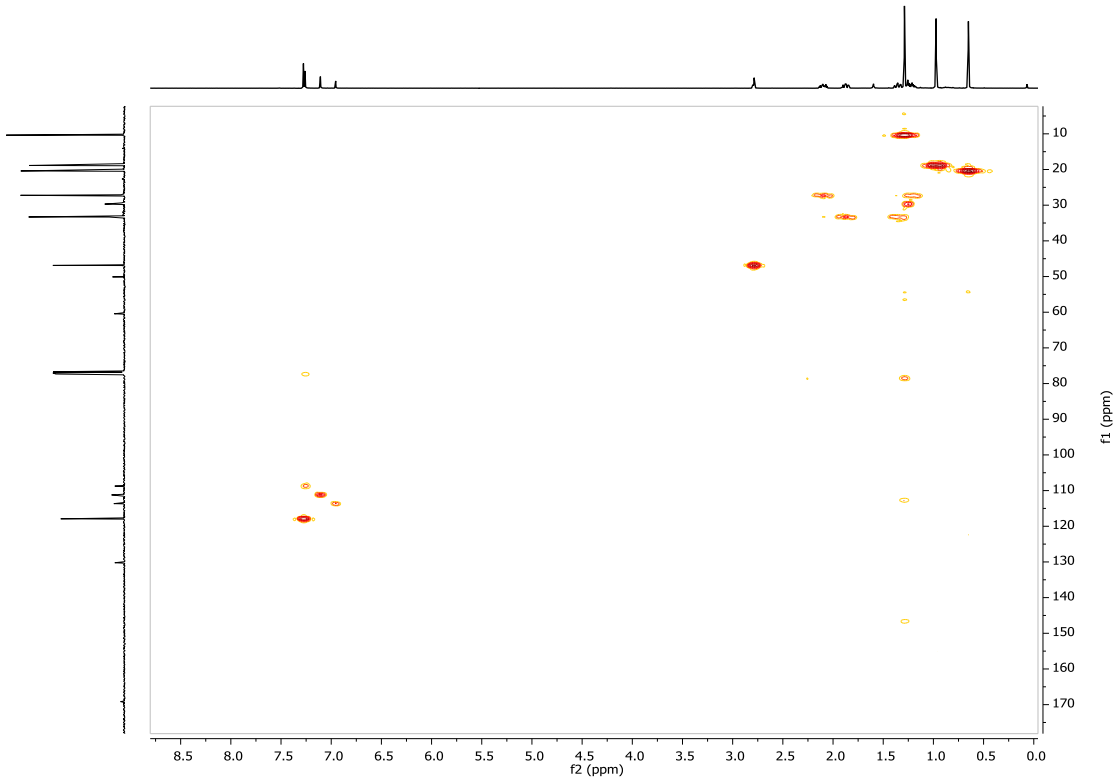

Figure S10: NMR spectrum (^{1}H-^{13}C) gs-HMQC of **14** in $CDCl_3$.

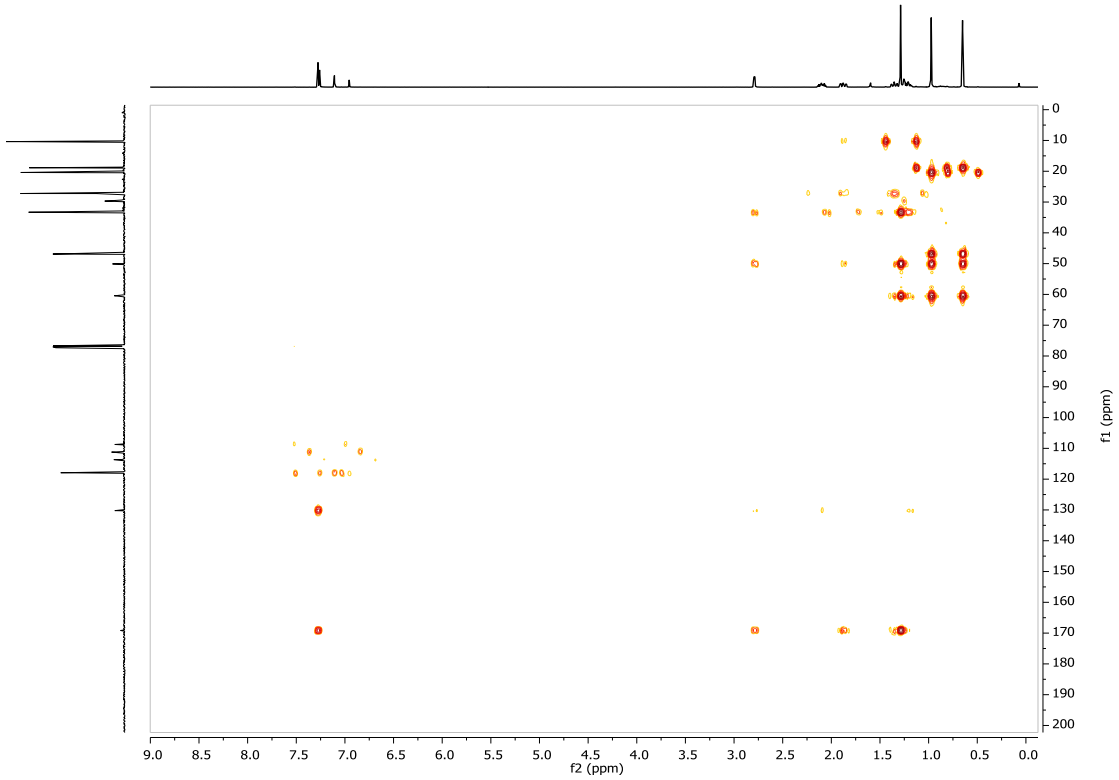

Figure S11: NMR spectrum (^{1}H-^{13}C) gs-HMBC of **14** in $CDCl_3$.

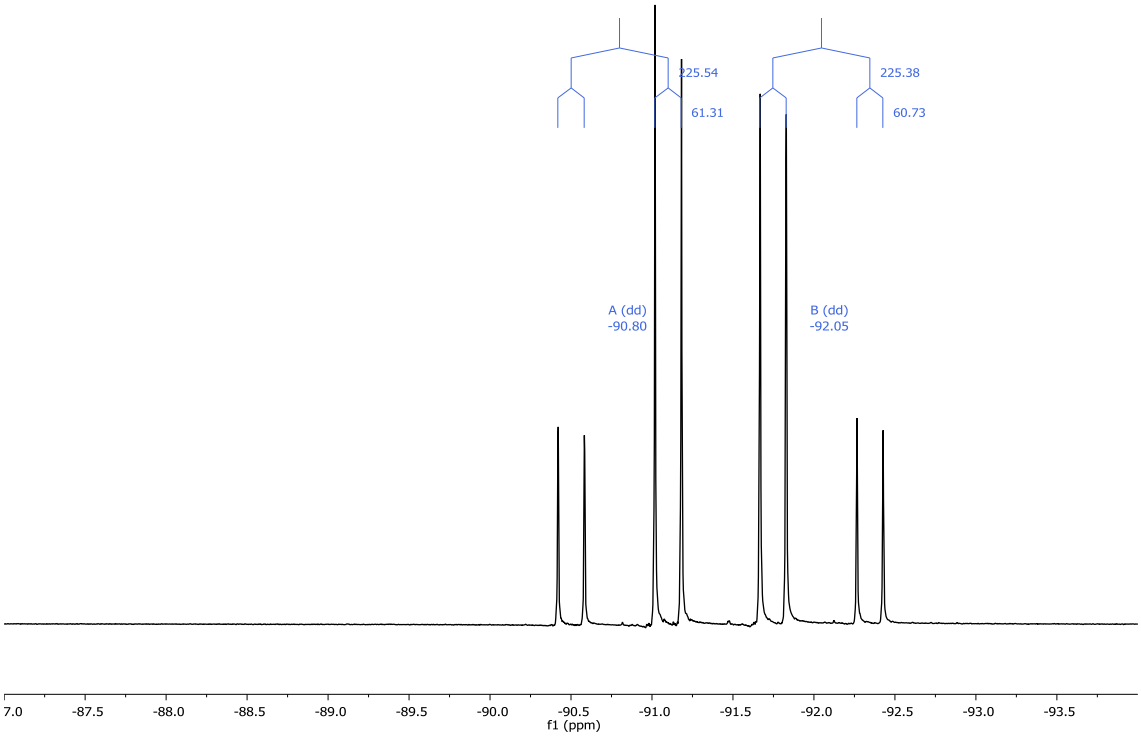

Figure S12: ^{19}F NMR spectrum of **14** in $CDCl_3$.

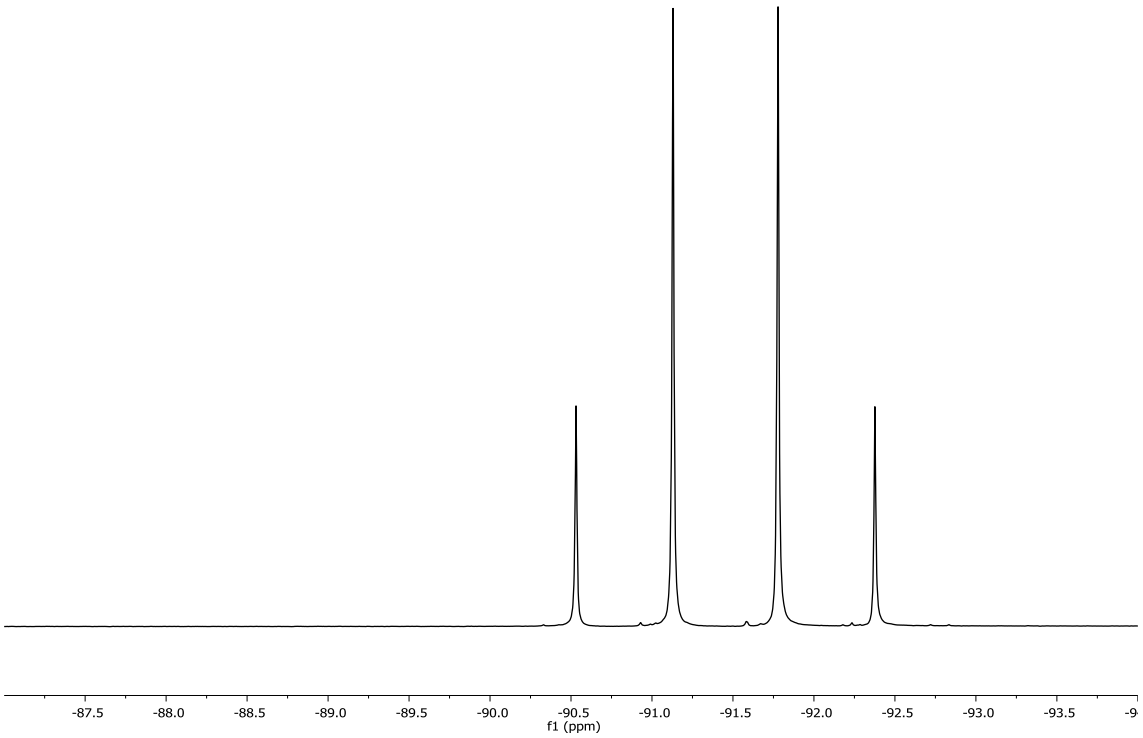

Figure S13: $^{19}F\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$.

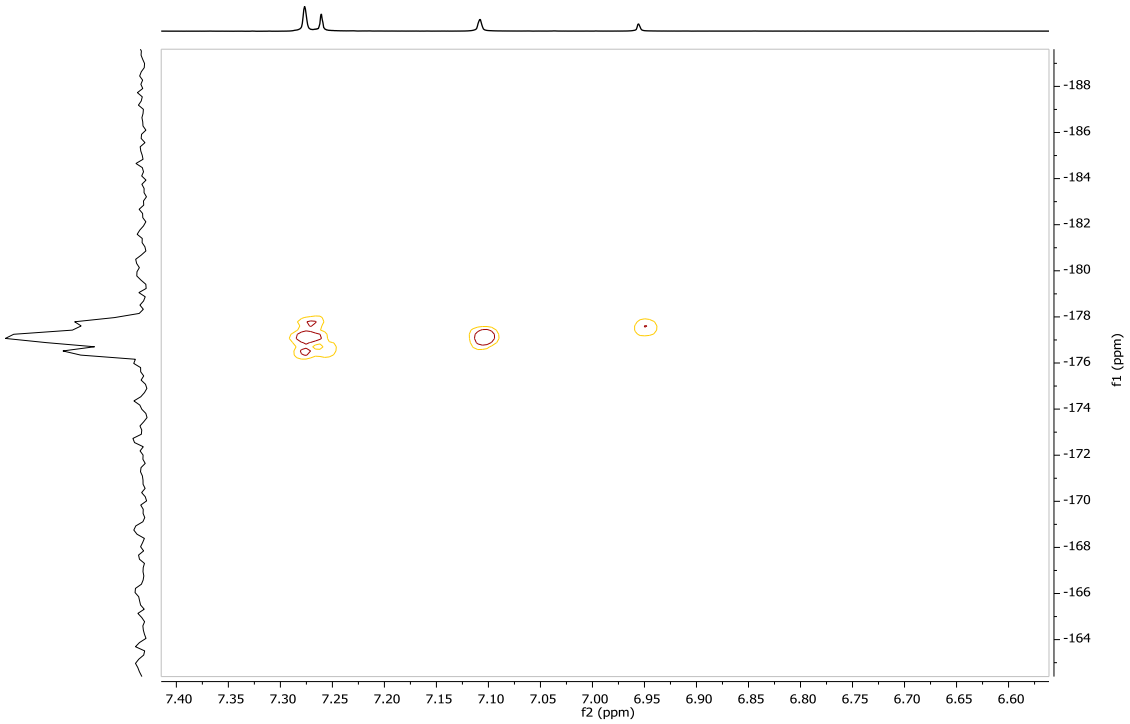

Figure S14: NMR spectrum (^{1}H-^{15}N) gs-HMBC of **14** in $CDCl_3$.

B3LYP/6-311++G(d,p) computational level results in gas phase of the stationary points (minima and TSs).

Optimized geometry and Electronic energy	**Chemical shielding and shift (ppm)**
13 (θ = -3.6°) Electronic Energy= -776.272387310 Hartree NIMAG= 0 H,-1.4648424704,1.7387341004,-2.173598583 H,0.6143232975,3.5439778359,0.4779123323 N,1.8963376686,1.9171782991,0.3069423644 C,0.6889934156,2.4758801072,0.3346208904 H,-0.2637535688,-0.3251623287,-2.4208879591 C,-1.9004184051,0.9283384783,-1.587586778 N,1.6668828505,0.577182361,0.102959539 H,-2.943387123,0.8275397476,-1.8957243407 C,-0.3252283473,1.5051289279,0.1835482123 C,-1.1225830994,-0.4129942197,-1.7533656614 C,0.3300751159,0.3084939424,0.0424208253 C,-1.7900520598,1.2203040768,-0.0543135754 H,-2.5090240149,1.9467778512,0.3253441107 H,-1.7620764281,-1.2035979286,-2.1533155691 C,-0.6602030983,-0.7864972274,-0.2955083467 H,0.5710965822,-2.504622286,-0.769182508 C,-1.8926944263,-0.2306601786,0.5530289229 C,-0.2521856139,-2.2372909569,-0.1022742896 H,-3.4715433751,-0.9967351342,-0.8053114873 H,-0.7536553523,0.1922590526,2.3935427811 C,-3.2249602546,-0.9369451084,0.253920875 H,0.0754487757,-2.4325597194,0.9215351788 H,-4.0422675951,-0.4076221339,0.7537181576 H,-1.0895308084,-2.9031023976,-0.3273405114 C,-1.6811556512,-0.2825911096,2.0745414754 H,-2.5083143437,0.2211347031,2.5843562495 H,-1.669127308,-1.3187974411,2.4250594691 H,-3.2138324624,-1.9564300853,0.649687084 C,2.7908437596,-0.282475772,0.0514805326 H,3.6990148797,0.3105239849,0.1261816241 F,2.7957296346,-1.003085912,-1.1135895155 F,2.7552868261,-1.2076175289,1.0592325008	Atom Abs. Rel. 1H 30.97 0.96 2H 24.70 7.04 3N -84.24 -72.31 4C 44.08 133.25 5H 30.66 1.26 6C 151.74 29.57 7N 23.97 -174.68 8H 29.92 1.98 9C 44.35 132.99 10C 146.11 34.99 11C 22.85 153.70 12C 128.97 51.50 13H 29.21 2.67 14H 30.11 1.80 15C 122.47 57.76 16H 29.95 1.95 17C 111.49 68.34 18C 169.84 12.15 19H 30.94 0.99 20H 31.04 0.89 21C 162.35 19.36 22H 30.47 1.44 23H 31.12 0.82 24H 30.90 1.03 25C 162.17 19.53 26H 31.15 0.79 27H 31.19 0.75 28H 31.01 0.92 29C 62.38 115.63 30H 24.88 6.87 31F 266.19 -93.18 32F 262.59 -89.73
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Atom	Abs.	Rel.
1H	30.73	1.19
2H	24.57	7.17
3N	21.29	-172.14
4C	60.68	117.26
5H	30.55	1.37
6C	150.69	30.58

N,-0.7860508495,-2.0023553797,-1.0020572638 H,0.3960527114,2.9028254103,-0.7052159183 C,0.8984134408,-0.4577057763,-0.9203501204 C,-1.2214910323,1.4063937949,-0.5407002096 C,-0.3885678642,-0.8639062115,-0.4821513134 C,1.1595872615,0.8814625735,-0.2825049428 H,2.1962421201,1.213906565,-0.2235460898 H,-1.7510653655,2.2006998691,-0.009389407 C,-0.9446886174,0.2025369384,0.4285066142 H,-2.9708256568,-0.4831111354,0.735438152 C,0.4230751283,0.6733239921,1.100828406 C,-2.1039610999,-0.1825324462,1.3303773462 H,-0.1839410145,2.7827938483,1.4165945408 H,1.1994849717,-1.3542365167,1.484009122 C,0.3044521901,1.9582391693,1.9348787575 H,-1.8443979966,-1.023801051,1.9781110969 H,1.3001562529,2.299956301,2.2345613401 H,-2.4070655658,0.6575400759,1.9615191576 C,1.0799732458,-0.395001091,1.9885409558 H,2.0712042414,-0.0600735521,2.3099885067 H,0.485781952,-0.5621528214,2.8917280683 H,-0.2587448584,1.7655038993,2.8525065172 C,0.2431612119,-3.6164739075,-2.4470629291 H,-0.743375117,-4.0594915301,-2.3332943634 F,1.1868242408,-4.4651159677,-1.9216223015 F,0.5605297687,-3.4966921047,-3.7732668776	7N -63.30 -92.12 8H 29.89 2.01 9C 45.04 132.33 10C 145.08 35.99 11C 8.55 167.47 12C 130.25 50.27 13H 29.26 2.62 14H 30.09 1.81 15C 126.23 54.14 16H 30.21 1.69 17C 115.04 64.92 18C 171.39 10.65 19H 30.96 0.97 20H 31.35 0.59 21C 163.05 18.68 22H 30.68 1.24 23H 31.21 0.72 24H 30.95 0.98 25C 161.57 20.11 26H 31.25 0.69 27H 31.18 0.76 28H 31.08 0.85 29C 62.88 115.15 30H 24.87 6.87 31F 258.43 -85.73 32F 270.59 -97.40
14 (θ = 114.9°) TotalEnergy= -776.268491134 Hartree NIMAG= 1 H,0.2540974946,1.8003445468,-2.1034831219 H,2.1886620803,-1.6234019617,-2.3334611793 N,0.2737914987,-2.398588142,-1.7399532497 C,1.2916458289,-1.4567620084,-1.7585999341 H,-1.8981879003,1.0664787105,-1.3380633337 C,0.1525006537,1.8638950114,-1.0191126891 N,-0.7800681072,-2.032218728,-0.9398913714 H,0.3506479902,2.8992173999,-0.7338100399 C,0.8817078646,-0.4590342362,-0.9207059573 C,-1.2502419054,1.3905446335,-0.5216777032 C,-0.3907749796,-0.8727335808,-0.4575969374 C,1.1406708804,0.8892210763,-0.3014304154 H,2.1745371613,1.2333786448,-0.2627867364 H,-1.7757152891,2.1862009422,0.0119188595 C,-0.9443810946,0.1973827113,0.4516131839 H,-2.955484696,-0.5111955197,0.7969591677 C,0.4305396843,0.6875944909,1.0964084995 C,-2.083850632,-0.1933281234,1.3756383805 H,-0.1780940971,2.797383363,1.4015214342 H,1.2272611794,-1.3314486913,1.4850703734 C,0.3140624574,1.9770807564,1.9229012676 H,-1.8033129648,-1.0260115877,2.0254155745 H,1.3104632322,2.3222096531,2.2165299186	

H,-2.3878637893,0.6483129441,2.0043292384 C,1.1128782584,-0.3673870071,1.9814585412 H,2.1085699927,-0.023000677,2.2784414511 H,0.5389971862,-0.5282316183,2.8987188431 H,-0.2451540492,1.7881624739,2.843853124 C,0.2626905684,-3.6144131311,-2.4978484851 H,0.2651060012,-3.445633595,-3.5774545542 F,-0.8056053862,-4.3579680033,-2.1692464363 F,1.3970749778,-4.3365822172,-2.2085806331	
14 (θ = 179.3°) TotalEnergy= -776.272975736 Hartree NIMAG= 0 H,-1.2158240623,2.5905506276,-1.136599604 H,1.7205186828,2.0320845775,1.3805378237 N,2.0143406325,0.2718054959,0.1774778781 C,1.2501721037,1.2461128496,0.8108121535 H,-1.0498615102,0.6139410089,-2.4863440491 C,-1.8903454934,1.8000932056,-0.8045041205 N,1.2516288332,-0.6509856414,-0.4935517801 H,-2.9022605966,2.2107370137,-0.8127924695 C,-0.046900043,0.9334740653,0.5305865116 C,-1.7858120886,0.515461389,-1.6864622045 C,0.0260718245,-0.2350470118,-0.2718188833 C,-1.5066747079,1.2926170525,0.6226972361 H,-1.8106314053,1.948829192,1.4386516868 H,-2.742114912,0.2717037264,-2.1552493754 C,-1.3721410282,-0.6215942013,-0.6861281052 H,-0.9856971702,-2.2204294749,-2.0861284372 C,-2.1437669747,-0.1532995117,0.6293895989 C,-1.5835415835,-2.0382639661,-1.1889780374 H,-4.0448443249,0.3814589185,-0.3773643569 H,-0.7153233058,-1.0447926518,2.0540257621 C,-3.674085857,-0.1552472931,0.4951039216 H,-1.2821419141,-2.7760354222,-0.4411379584 H,-4.1262502623,0.3015251818,1.3811422437 H,-2.6324254202,-2.2136088284,-1.4439652253 C,-1.7894978382,-0.9722088388,1.8807660861 H,-2.2425743785,-0.5193934234,2.7683125095 H,-2.1845121703,-1.9888306252,1.7977729182 H,-4.0482608106,-1.1812893954,0.4356344319 C,3.4190087855,0.1300868368,0.2646395096 H,3.8380059472,0.9677356064,0.8236985183 F,3.9927952136,0.0900160659,-0.9710638762 F,3.773168835,-1.0327275282,0.8888146934	Atom Abs. Rel. 1H 30.84 1.08 2H 25.06 6.69 3N 23.50 -174.23 4C 58.64 119.23 5H 30.59 1.33 6C 150.96 30.33 7N -60.79 -94.49 8H 29.82 2.08 9C 49.30 128.22 10C 145.60 35.49 11C 5.68 170.23 12C 129.57 50.92 13H 29.31 2.57 14H 30.05 1.85 15C 125.87 54.48 16H 30.18 1.73 17C 115.27 64.70 18C 171.35 10.69 19H 30.81 1.11 20H 31.39 0.55 21C 162.76 18.96 22H 30.70 1.23 23H 31.09 0.85 24H 31.02 0.91 25C 161.58 20.09 26H 31.24 0.70 27H 31.17 0.77 28H 30.88 1.05 29C 66.77 111.40 30H 25.29 6.47 31F 265.83 -92.83 32F 261.48 -88.66

14 (θ = 242.9°) TotalEnergy= -776.268646637 Hartree NIMAG= 1 H,0.3548688818,1.8022442739,-2.0876603034 H,2.1927155571,-1.6311087115,-2.3306551722 N,0.2477673648,-2.3695054636,-1.7898837953 C,1.2997915761,-1.466370129,-1.7486189809 H,-1.8335332827,1.1126789955,-1.3873449999 C,0.2237217867,1.8632317012,-1.0064812745 N,-0.8080834167,-1.9977213325,-0.9946878579 H,0.4370026477,2.8923896786,-0.7097800008 C,0.8986161782,-0.4754025328,-0.8988545941 C,-1.2021030667,1.4185517931,-0.5514341867 C,-0.396927988,-0.8617899706,-0.4759436883 C,1.1694011332,0.863855215,-0.2658315441 H,2.2090805027,1.1849356978,-0.1957379822 H,-1.7251071777,2.2224764214,-0.0280980827 C,-0.9508513973,0.2152345584,0.4250840555 H,-2.9827847789,-0.4596811139,0.7065650969 C,0.4150750153,0.6724377415,1.1101402651 C,-2.1262416595,-0.152806048,1.3130163429 H,-0.1618510717,2.7922443269,1.4071334056 H,1.1561952798,-1.3637265622,1.5139447224 C,0.3051618704,1.9627415428,1.9367934747 H,-1.8813557536,-0.9864782856,1.9759213536 H,1.3018671665,2.2898399671,2.2496855245 H,-2.438651164,0.6965633184,1.9272020371 C,1.0476877882,-0.3994770149,2.01131358 H,2.0407877118,-0.0776287368,2.3405813287 H,0.4421628619,-0.5518452312,2.9096236972 H,-0.2743350572,1.7828858294,2.8468687166 C,0.2719700701,-3.6234563793,-2.4815056998 H,1.087254443,-4.2734734494,-2.1546543504 F,0.4624747413,-3.3959139557,-3.8249368179 F,-0.8972664225,-4.2644020241,-2.3267169897	

PCM/($CHCl_3$)//B3LYP/6-311++G(d,p) computational level results of the stationary points (minima and TSs).

Optimized geometry and Electronic energy	Chemical shielding and shift (ppm)		
13 (θ = -4.0°)			
Electronic Energy= -776.276685713 Hartree			
NIMAG= 0	Atom	Abs.	Rel.
H,-1.4671383842,1.7397196637,-2.1740150084	1H	30.97	0.96
H,0.604795361,3.5455346367,0.4770841192	2H	24.59	7.15
N,1.8954164235,1.9215802394,0.3076344288	3N	-77.27	-78.90
C,0.6846316397,2.4775147518,0.334394462	4C	42.92	134.36
H,-0.2640845745,-0.3229077603,-2.4229720414	5H	30.68	1.24
C,-1.9008665622,0.9286406658,-1.5874806313	6C	151.90	29.42
N,1.6686958144,0.5788175446,0.1020880265	7N	24.66	-175.33
H,-2.9440062582,0.8260412485,-1.8932547041	8H	29.85	2.05
C,-0.3256210667,1.5051808895,0.181757324	9C	43.45	133.86
C,-1.1219819039,-0.4117114797,-1.7542723675	10C	146.20	34.91
C,0.3318418087,0.3090605802,0.0403580803	11C	21.27	155.22
C,-1.7903251172,1.2203411199,-0.0543482433	12C	129.10	51.38
H,-2.5081492215,1.9467684571,0.3263178809	13H	29.11	2.77
H,-1.7614142335,-1.2029253403,-2.1522488205	14H	30.02	1.88
C,-0.658798711,-0.786505257,-0.2966741583	15C	122.00	58.21
H,0.5680892938,-2.5077619662,-0.7722750966	16H	30.02	1.88
C,-1.8911259975,-0.2306862796,0.5527330916	17C	111.07	68.74
C,-0.2535334202,-2.2380435961,-0.1041706331	18C	169.95	12.04
H,-3.4694209208,-0.9977833301,-0.8048396596	19H	30.89	1.04
H,-0.749659828,0.1894124002,2.3933346967	20H	31.14	0.79
C,-3.2231926395,-0.9373228661,0.2543223311	21C	162.68	19.04
H,0.071121884,-2.4351887928,0.9202909264	22H	30.49	1.42
H,-4.0390533752,-0.4058671769,0.7539657794	23H	31.07	0.86
H,-1.0931155441,-2.9003662434,-0.3299374226	24H	30.80	1.12
C,-1.6787076662,-0.2830892565,2.07423691	25C	162.44	19.27
H,-2.5048441975,0.222954116,2.5831243469	26H	31.09	0.84
H,-1.6687721906,-1.3195656678,2.423796088	27H	31.15	0.78
H,-3.2112786293,-1.9562847257,0.6511169841	28H	30.98	0.95
C,2.7919559305,-0.2804683922,0.0536459769	29C	62.05	115.94
H,3.7046985381,0.3046035547,0.1246393495	30H	24.78	6.96
F,2.7931642206,-1.0106989217,-1.1071674419	31F	267.12	-94.07
F,2.7538765276,-1.2043268154,1.0668494266	32F	263.12	-90.23
13 (θ = 96.0°)			
Electronic Energy= -776.269387625 Hartree			
NIMAG= 1			
H,-1.4920089009,1.7352195558,-2.1853061422			
H,0.5806467506,3.5562269229,0.4733079093			
N,1.8880894321,1.947990504,0.2800360552			
C,0.670001969,2.4906379658,0.3184921434			
H,-0.2885179417,-0.3262353053,-2.4476508509			
C,-1.9178079945,0.9240098065,-1.5932314968			
N,1.6783234429,0.6134268234,0.0400951977			
H,-2.9637403589,0.8180333757,-1.8883962941			
C,-0.3279612369,1.5109835653,0.1603497029			

C,-1.1366098599,-0.415016615,-1.7666031719 C,0.3429484268,0.3211479072,0.0073334417 C,-1.7915260724,1.2182847052,-0.0623774821 H,-2.5092477477,1.9415568216,0.324763968 H,-1.7797737825,-1.208856282,-2.1532659928 C,-0.6521422094,-0.7823195576,-0.315066581 H,0.5164351125,-2.5403334881,-0.8191600113 C,-1.8764227605,-0.2293379709,0.5491531331 C,-0.2618215485,-2.2379396613,-0.1164383341 H,-3.4630167696,-1.0199489132,-0.7852158713 H,-0.7216500573,0.2166003801,2.3748099383 C,-3.2093380965,-0.9431012546,0.2711412434 H,0.1076038201,-2.4243969578,0.8959453955 H,-4.0220226076,-0.4039269917,0.7676498075 H,-1.1268504286,-2.88513334,-0.2823841841 C,-1.6457353961,-0.2738428414,2.0683483201 H,-2.4740825696,0.2207349988,2.5849716414 H,-1.6154057082,-1.3084496326,2.4228098442 H,-3.1953456112,-1.9555669295,0.6840659966 C,2.7909533739,-0.2966483236,0.0947261096 H,2.9008925489,-0.803351091,1.0541131828 F,3.9342537482,0.3645189485,-0.1862334854 F,2.6128126439,-1.2514478649,-0.8689407123	
13 (θ = 180.5 °) Electronic Energy= -776.273758182 Hartree NIMAG= 0 H,-0.1082715385,1.3933774433,-2.0616038128 H,1.7639732506,-1.9411879274,-2.3029498347 N,-0.0626738255,-2.7990504507,-1.7951183259 C,0.8641407087,-1.8450962944,-1.7123569877 H,-2.2674093249,0.6863923584,-1.2890325184 C,-0.217898193,1.4910284893,-0.9807694383 N,-1.0699986056,-2.3908418867,-0.956149629 H,-0.0207999858,2.5338956816,-0.7242949164 C,0.4840278795,-0.8384513371,-0.799639777 C,-1.6237989962,1.0372651638,-0.4802890677 C,-0.7481960965,-1.2172224616,-0.3328655925 C,0.7587156951,0.5313098709,-0.2254143087 H,1.7965802256,0.8628133339,-0.1993531278 H,-2.1523964931,1.8483677392,0.025811008 C,-1.3260657359,-0.1226934286,0.5420516256 H,-3.3844773266,-0.6912690126,0.9399626726 C,0.0472590664,0.3914073421,1.174666086 C,-2.4697090967,-0.4481357925,1.4893127287 H,-0.5810973618,2.5084066427,1.3905257338 H,0.857324116,-1.6012840968,1.662137166 C,-0.0780148936,1.7164554021,1.9434036812 H,-2.2314818393,-1.2899720756,2.1450623731 H,0.9195688547,2.0804085025,2.2077840526 H,-2.6994548514,0.4144979752,2.1196891747 C,0.7224620862,-0.6191828233,2.1152462611 H,1.7083355789,-0.2491252731,2.4126336033	Atom Abs. Rel. 1H 30.86 1.07 2H 24.42 7.32 3N -68.92 -86.80 4C 40.96 136.25 5H 30.75 1.18 6C 151.28 30.02 7N 26.57 -177.13 8H 29.86 2.03 9C 46.14 131.27 10C 145.56 35.53 11C 18.83 157.57 12C 129.92 50.59 13H 29.16 2.71 14H 30.05 1.85 15C 122.07 58.15 16H 30.41 1.50 17C 111.14 68.67 18C 170.68 11.34 19H 31.02 0.91 20H 31.16 0.77 21C 162.76 18.96 22H 30.64 1.28 23H 31.07 0.86 24H 30.73 1.19 25C 162.56 19.15 26H 31.15 0.78

H,0.1348444138,-0.7444711876,3.0296557365	27H	31.22	0.72
H,-0.6238584367,1.5657222953,2.8791600631	28H	31.00	0.93
C,-2.2037875137,-3.2167881667,-0.7524277689	29C	67.50	110.69
H,-2.9045073405,-2.7409431065,-0.0707011823	30H	24.86	6.89
F,-1.8438070855,-4.4343815733,-0.2394775094	31F	264.93	-91.97
F,-2.8349477646,-3.4801079854,-1.9353189888	32F	272.61	-99.34
13 (θ = 261.7 °) Electronic Energy= -776.268496900 Hartree NIMAG= 1 H,-1.4407805367,1.7462579578,-2.1644190266 H,0.5820081841,3.5507451876,0.5101312471 N,1.8864792052,1.9346806649,0.3723176344 C,0.6699029327,2.4826406143,0.3725289496 H,-0.221824202,-0.3093588318,-2.398673573 C,-1.8775248914,0.9315860275,-1.5851588239 N,1.6739654191,0.5907624266,0.1956552497 H,-2.915953352,0.8219828134,-1.9045372005 C,-0.3284397579,1.5054017204,0.2055262746 C,-1.089444711,-0.4048848173,-1.7428577689 C,0.3412685229,0.3112442878,0.0802888271 C,-1.7877000575,1.2186272149,-0.0512781257 H,-2.5114984181,1.9432429563,0.3217788377 H,-1.7192604291,-1.1966221066,-2.1549962424 C,-0.6487602505,-0.785472312,-0.2787839155 H,0.5479912993,-2.5329827484,-0.7550409166 C,-1.8947591505,-0.2319238054,0.5521167814 C,-0.2733996648,-2.2460680265,-0.0937639911 H,-3.4462274895,-1.0099260315,-0.8301583914 H,-0.7847521578,0.1971951064,2.4080111672 C,-3.2208078842,-0.9410903222,0.2332190711 H,0.0364011632,-2.4602488077,0.9309987747 H,-4.0461372345,-0.4049525625,0.7118960005 H,-1.1263272724,-2.8852469399,-0.3360968186 C,-1.7045296358,-0.2843088477,2.0762908908 H,-2.5425927158,0.2137199008,2.573502448 H,-1.6900646952,-1.3208890189,2.4260636628 H,-3.2183854681,-1.9567264573,0.6386900604 C,2.7988620724,-0.2867245776,0.0084882132 H,2.9953148252,-0.5286469802,-1.0368204413 F,2.5556516086,-1.456426926,0.6729837767 F,3.9060327923,0.2702409006,0.5442174989			

14 (θ = 11.2 °) Electronic Energy= -776.282012844 Hartree NIMAG= 0 H,0.3136468322,1.8223250426,-2.0899951395 H,2.1999523801,-1.5865052276,-2.3628502789 N,0.2676625514,-2.3555916287,-1.8183566215 C,1.3053098752,-1.4334687964,-1.7811462691 H,-1.8582965763,1.0973455079,-1.3723915406 C,0.1929672819,1.8727250441,-1.0069637304	Atom	Abs.	Rel.
	1H	30.73	1.19
	2H	24.44	7.29
	3N	23.34	-174.08
	4C	59.74	118.17
	5H	30.57	1.35
	6C	150.89	30.40

N,-0.7895460017,-2.0034518051,-1.0020135785 H,0.3960667333,2.901420317,-0.7033029893 C,0.8944976716,-0.4576979878,-0.9215088705 C,-1.2224952305,1.4071179039,-0.5410163861 C,-0.3926745106,-0.8638873601,-0.4822518939 C,1.1582404589,0.8805814768,-0.2834496314 H,2.1953089369,1.210513479,-0.2260811399 H,-1.7504334217,2.2008750411,-0.0079258568 C,-0.9470853624,0.2031377375,0.4290287411 H,-2.978322347,-0.468987552,0.7415387214 C,0.4224022423,0.6720949406,1.0999634069 C,-2.1060823922,-0.1772759803,1.3334069222 H,-0.183846557,2.781033189,1.4179768865 H,1.1992156718,-1.3564359159,1.4817562455 C,0.3057090292,1.9565125962,1.9349503295 H,-1.8493668224,-1.0197762527,1.9808973493 H,1.3029936682,2.2966168967,2.230722254 H,-2.4003131432,0.6643296022,1.9662882038 C,1.0787404328,-0.3973231313,1.9870269581 H,2.0694884971,-0.0614671985,2.3084515449 H,0.4833549523,-0.5653069573,2.8891942609 H,-0.2551566036,1.7625842424,2.8536589838 C,0.2456146641,-3.6166003109,-2.4461643914 H,-0.735516324,-4.0707019394,-2.3373948101 F,1.198108592,-4.4635457693,-1.9201398112 F,0.5700657214,-3.5002150439,-3.7741342891	7N -57.80 -97.32 8H 29.82 2.07 9C 43.71 133.60 10C 145.20 35.87 11C 6.68 169.27 12C 130.44 50.08 13H 29.16 2.71 14H 30.01 1.89 15C 125.94 54.42 16H 30.27 1.64 17C 114.77 65.18 18C 171.63 10.42 19H 30.91 1.02 20H 31.45 0.49 21C 163.39 18.35 22H 30.69 1.23 23H 31.17 0.77 24H 30.86 1.06 25C 161.82 19.87 26H 31.19 0.74 27H 31.14 0.80 28H 31.06 0.88 29C 62.31 115.69 30H 24.76 6.98 31F 259.07 -86.35 32F 271.21 -97.99
14 (θ = 110.0 °) Electronic Energy= -776.274458669 Hartree NIMAG= 1 H,0.2616859748,1.7866807943,-2.1055231055 H,2.1965885129,-1.6278054648,-2.3217746289 N,0.2892089618,-2.4141049699,-1.7218443286 C,1.3010173547,-1.4663139532,-1.7433945792 H,-1.8932100132,1.0555278405,-1.3436759259 C,0.1566775049,1.8544126701,-1.0217069207 N,-0.7739306373,-2.0428037888,-0.9306762662 H,0.3534212589,2.8903756958,-0.7389721194 C,0.8850975903,-0.4670295463,-0.9106391918 C,-1.2472736586,1.382605536,-0.5267204191 C,-0.388266677,-0.8797858106,-0.4496165311 C,1.1430377291,0.88373734,-0.2966065637 H,2.1767474366,1.2268635308,-0.2574369564 H,-1.7738899888,2.1794212886,0.0033538341 C,-0.9443120259,0.194279051,0.4541596855 H,-2.9615387125,-0.5000819921,0.8028717529 C,0.4292362669,0.688365617,1.0997937732 C,-2.0860408269,-0.1878425404,1.3792842915 H,-0.1829087444,2.7982793906,1.3922410542 H,1.2289043978,-1.3277961452,1.5005107225 C,0.3094674615,1.9819572243,1.9193717988 H,-1.8097147016,-1.0180722445,2.0342835351 H,1.3057735746,2.3288119906,2.2108167037	

H,-2.3835937075,0.6584831416,2.0043075578 C,1.1100368556,-0.3614816364,1.9922060232 H,2.1037067981,-0.0126140752,2.2902079592 H,0.5325877928,-0.5192326157,2.9077266811 H,-0.2506717866,1.7967581382,2.8404710044 C,0.2578878058,-3.6033488569,-2.5182878157 H,0.2024918746,-3.412954305,-3.5910481496 F,-0.7841836161,-4.3765399456,-2.1509293998 F,1.4131300447,-4.319282829,-2.295678396	
14 (θ = 179.4 °) Electronic Energy= -776.280081248 Hartree NIMAG= 0 H,-1.2134719292,2.5898893096,-1.1363180992 H,1.7158630913,2.0343924919,1.3869886414 N,2.0171668363,0.2748517642,0.1861465099 C,1.2480748879,1.2482615291,0.8155289834 H,-1.0450507845,0.6129910572,-2.4861423037 C,-1.887684404,1.7988442928,-0.8049445549 N,1.2554741219,-0.6526628483,-0.4884556002 H,-2.8999918538,2.2076617564,-0.8138366947 C,-0.0466055473,0.9318936998,0.5313397058 C,-1.7815094819,0.514376986,-1.6865464408 C,0.0276335597,-0.237725944,-0.2700443811 C,-1.5061056884,1.2917666378,0.6225942091 H,-1.8087871837,1.9481466276,1.4382129457 H,-2.7370925688,0.2692378585,-2.1553897345 C,-1.3705732476,-0.6237575503,-0.6855475059 H,-1.000827936,-2.2227112586,-2.0925992274 C,-2.1432662062,-0.1536953065,0.6291562771 C,-1.5879296388,-2.0396398231,-1.1882521472 H,-4.0420460663,0.3785263261,-0.3825008575 H,-0.717785912,-1.0426761454,2.0596473944 C,-3.6733547959,-0.1555222798,0.4923395116 H,-1.2851854214,-2.7795358337,-0.4428492718 H,-4.1245076324,0.3056200253,1.376457348 H,-2.6395116621,-2.2102478738,-1.4338321717 C,-1.7916722571,-0.9724145575,1.8815632711 H,-2.2491586681,-0.5193478822,2.7665124013 H,-2.1845014868,-1.9896691192,1.7963080492 H,-4.0475740503,-1.1817037912,0.4362819369 C,3.418214687,0.1400223542,0.266705122 H,3.8470388728,0.9692248048,0.8265061269 F,3.9858443345,0.0982552074,-0.9794119756 F,3.7791070311,-1.0381735151,0.8723575325	Atom Abs. Rel. 1H 30.83 1.10 2H 24.81 6.93 3N 25.38 -176.00 4C 56.36 121.42 5H 30.61 1.31 6C 151.15 30.15 7N -50.50 -104.23 8H 29.76 2.14 9C 48.25 129.24 10C 145.65 35.44 11C 3.70 172.13 12C 129.88 50.63 13H 29.21 2.67 14H 29.97 1.93 15C 125.65 54.70 16H 30.26 1.65 17C 115.00 64.95 18C 171.54 10.50 19H 30.78 1.14 20H 31.49 0.46 21C 163.09 18.64 22H 30.71 1.21 23H 31.04 0.89 24H 30.93 1.00 25C 161.86 19.83 26H 31.17 0.77 27H 31.13 0.80 28H 30.86 1.07 29C 65.81 112.32 30H 25.06 6.69 31F 267.26 -94.21 32F 263.58 -90.68
14 (θ = 247.1 °) Electronic Energy= -776.274682675 Hartree NIMAG= 1 H,0.3495323237,1.8089741177,-2.0867270607 H,2.1896896935,-1.6227185402,-2.337684058 N,0.242090844,-2.3612226801,-1.8081778793 C,1.2942920046,-1.458701689,-1.7593323709	

H,-1.8385395425,1.1169524097,-1.3847613853 C,0.2199846505,1.8661181,-1.0050756152 N,-0.8120114183,-1.9958788345,-1.0017921884 H,0.4333500611,2.8937260969,-0.7042915589 C,0.8931655697,-0.4724604329,-0.9042801848 C,-1.2050962307,1.4201534408,-0.5491753002 C,-0.4007495203,-0.8603498944,-0.4787911382 C,1.166691819,0.8650986936,-0.268741719 H,2.2066213506,1.1842476621,-0.200850914 H,-1.7266558012,2.2221076425,-0.0220486871 C,-0.9526306892,0.2149923806,0.4256024918 H,-2.9890930853,-0.4481249826,0.7143774975 C,0.4154134453,0.6708181558,1.1080941142 C,-2.1262115105,-0.1507082697,1.3170389972 H,-0.1637724202,2.7892718358,1.4115381132 H,1.1628844179,-1.3651120788,1.50652313 C,0.3064413881,1.9593122334,1.9376039624 H,-1.8828695848,-0.9864592335,1.9782181468 H,1.3046739038,2.2857207059,2.245790004 H,-2.4297306042,0.6988735103,1.9348667515 C,1.0504943156,-0.4022425215,2.0063421585 H,2.0423038685,-0.0771427402,2.3357643607 H,0.4446161794,-0.5583787973,2.9037167653 H,-0.2692369694,1.7759006879,2.8493325699 C,0.2813993287,-3.6291236306,-2.4714569973 H,1.0661330033,-4.2915046501,-2.1034619692 F,0.5236799533,-3.4247994923,-3.8126894143 F,-0.9123504039,-4.2458150853,-2.3604233421	