SUPPORTING INFORMATION

Condensed Fukui Function Predicts Innate C-H Radical Functionalization Sites On Multi-nitrogen Containing Fused Arenes

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Table of Contents

General: Reagents were purchased and used without further purification, unless otherwise stated. Yields refer to chromatographically and spectroscopically (^{1}H-NMR) homogeneous material, unless otherwise stated. Flash chromatography was performed on silica gel (300-400 mesh ASTM), and monitored by thin layer chromatography (TLC) on HSGF-254 (10-40 μm) TLC plates. NMR data were collected on a *Varian* Mercury-300 High Performance Digital FT-NMR, a *Varian* Mercury-400 High Performance Digital FT-NMR, or a *Bruker* Ultrashield 500 NMR. Spectra from solutions in $CDCl_3$ (δC = 77.16 ppm) are calibrated relative to TMS (δH = 0.00 ppm). The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, heptet = heptet, m = multiplet, br = broad. HRMS were carried out on a *Thermo Finnigan* MAT-95 spectrometer (for EI), or on a *Waters*, Q-Tof Ultima Global spectrometer (for ESI). Melting points were measured on an uncorrected SGW X-4 micro melting point apparatus. Unless otherwise mentioned, HPLC analysis was performed on a Gilson HPLC system (306 pump, UV/vis-156 Detector, 215 liquid handle) with a YMC-ODS column (4.6 x 50 mm, 5 μm). HPLC conditions: solvent A = H_2O containing 0.1% (v/v) TFA, solvent B = MeCN containing 0.1% (v/v) TFA; flow rate = 2.5 mL/min; Gradient (B%): 0-0.5 min (4% isostatic), 0.5-4.5 min (4% - 95%); peaks were identified at 254 nm and 214 nm. X-Ray diffraction data were collected at T = 292(2) K using APEXII Bruker-AXS diffractometer. The samples **16** were studied with graphite monochromatized Cu-Kα radiation (λ = 1.54178 Å) and the samples **18**, **20**, and **22** were studied with graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods using the SIR97 program,[1] and then refined with full-matrix least-square methods based on F^2 (SHELX-97)[2] with the aid of the WINGX program.[3] All non-hydrogen atoms were refined

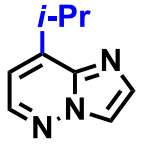
[1] A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Crystallogr.*, 1999, **32**, 115-119.

[2] G. M. Sheldrick, *Acta Crystallogr., Sect. A*, 2008, **A64**, 112-122.

with anisotropic atomic displacement parameters. Hydrogen atoms were finally included in their calculated positions. Molecular diagrams were generated by ORTEP-3 (version 2.02).

General radical alkylation procedure: [4] A solution of a heterocycle (0.625 mmol) and zinc isopropylsulfinate (1.25 mmol, 350 mg, 2 equiv) in DMSO (5 mL) was cooled in ice water and stirred vigorously while TBHP (70% solution in water, 260 μL, 1.875 mmol, 3 equiv) was added dropwise (Do not freeze the DMSO). The solution was stirred while warming to room temperature, then warmed to 50 °C and stirred at this temperature for 12 h. The reaction was cooled to room temperature. The solution was diluted with ethyl acetate (15 mL) and washed with $NaHCO_3$ solution (15 mL). The aqueous layer was extracted with ethyl acetate (15 mL) and the combined organic layers were washed with brine (2x15 mL), dried over $MgSO_4$, and concentrated under reduced pressure, and purified by flash chromatography eluting with ethyl acetate/hexanes or dichloromethane/methanol.

Characterization of new compounds:

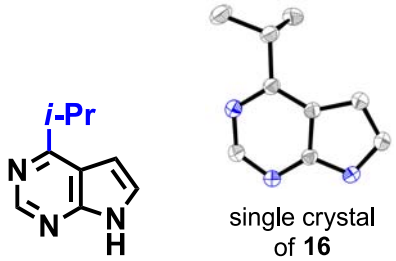


7-isopropyl-imidazo[1,2-b]pyridazine (15). From compound **7** (74mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **15** (brown oil, 31 mg, 0.194 mmol, 31%); R_f 0.4 (1:2, ethyl acetate : 60 – 90 °C petroleum ether); ^{1}H NMR (400 MHz, Chloroform-

[3] L. J. Farrugia, *J. Appl. Crystallogr.*, 2012, **45**, 849-854.

[4] F. O'Hara, D. G. Blackmond, P. S. Baran, *J. Am. Chem. Soc.*, 2013, **135**, 12122-12134.

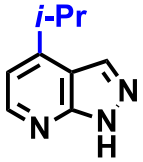
d) δ 8.24 (d, *J* = 4.7 Hz, 1H), 7.96 (d, *J* = 1.2 Hz, 1H), 7.74 (d, *J* = 1.2 Hz, 1H), 6.85 (dd, *J* = 4.8, 0.8 Hz, 1H), 3.71 (hept, *J* = 6.9 Hz, 1H), 1.42 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 147.3 (C), 143.4 (CH), 139.3 (CH), 132.6 (CH), 116.8 (CH), 111.9 (CH), 28.8 (CH_3), 21.7 (CH_3); HRMS (ESI+) calcd for $C_9H_{12}N_3$ 162.1026, found 162.1025.



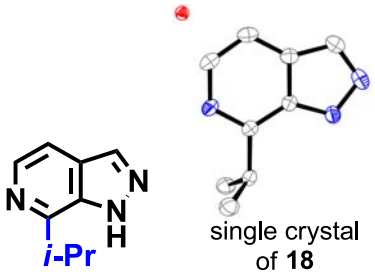
4-isopropyl-1H-pyrrolo[2,3-d]pyrimidine (16). From compound **8** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **16** (white powder, 62 mg, 0.388 mmol, 62%); mp 94-95°C (from dichloromethane/methanol eluent); R_f 0.4 (15:1, dichloromethane: methanol); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.81 (s, 1H), 8.89 (s, 1H), 7.38 (dd, *J* = 3.5, 2.0 Hz, 1H), 6.66 (dd, *J* = 3.4, 1.7 Hz, 1H), 3.49 (hept, *J* = 7.0 Hz, 1H), 1.45 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3 (C), 151.8 (C), 151.1 (CH), 124.9 (CH), 116.4 (C), 99.9 (CH), 34.1 (CH), 21.6 ($2CH_3$); HRMS (ESI+) calcd for $C_9H_{12}N_3$ 162.1026, found 162.1023. A single crystal of **16** was grown from ethyl acetate and *n*-hexane; X-ray crystal structure data for compound **16**: [5] $C_9H_{11}N_3$, *M* = 161.21, monoclinic, *P* $2_1/c$, *a* = 7.9968(2), *b* = 4.75170(10), *c* = 22.7801(6) Å, β = 95.9490(10) °, *V* = 860.95(4) Å^3, *Z* = 4, *d* = 1.244 g cm^{-3}, μ = 0.620 mm^{-1}. A final refinement on F^2 with

[5] CCDC 979233 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

1557 unique intensities and 111 parameters converged at $\omega R(F2) = 0.1246$ ($R(F) = 0.0446$) for 1281 observed reflections with $I > 2\sigma(I)$.

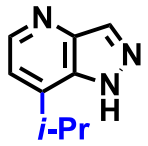


4-isopropyl-1H-pyrazolo[3,4-b]pyridine (17). From compound **9** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide crude compound **17** (pale yellow oil, 41.4 mg, 0.257 mmol, 41%), which contains 33% of starting materials **9** based on NMR analysis and corresponds to a corrected 27% yield of compound **17**; R_f 0.4 (25:1, dichloromethane: methanol); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 13.84 (s, 1H), 8.59 (d, J = 4.9 Hz, 1H), 8.22 (s, 1H), 7.03 (dd, J = 4.8, 0.7 Hz, 1H), 3.39 (hept, J = 6.9 Hz, 1H), 1.44 (d, J = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.6 (C), 152.2 (C), 149.0 (CH), 132.6 (CH), 114.7 (C), 113.5 (CH), 32.3 (CH), 22.9 ($2CH_3$); HRMS (ESI+) calcd for $C_9H_{12}N_3$ 162.1026, found 162.1025.



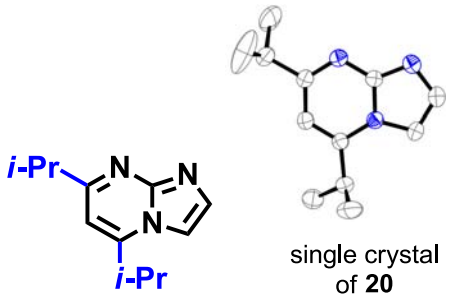
7-isopropyl-1H-pyrazolo[3,4-c]pyridine (18). From compound **10** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **18** (white powder, 59 mg, 0.369 mmol, 59%); mp 93-95 °C (from dichloromethane/methanol eluent); R_f 0.3 (25:1, dichloromethane: methanol); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 11.92 (s, 1H), 8.29 (d, J = 5.6 Hz,

1H), 8.18 (s, 1H), 7.53 (d, J = 5.6 Hz, 1H), 3.57 (hept, J = 7.4 Hz, 1H), 1.49 (d, J = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.1 (C), 138.8 (CH), 135.2 (C), 134.6 (CH), 127.1 (C), 112.7 (CH), 33.3 (CH), 21.4 ($2CH_3$); HRMS (ESI+) calcd for $C_9H_{12}N_3$ 162.1026, found 162.1024. A single crystal of **18** was grown from ethyl acetate and *n*-hexane; X-ray crystal structure data for compound **18**: [6] $C_{18}H_{24}N_6O$, M = 340.43, orthorhombic, $P\ 2_1/c$, a = 10.079(8), b = 11.523(10), c = 15.799(12) Å, β = 90 °, V = 1835.0(3) Å^3, Z = 4, d = 1.232 g cm^{-3}, μ = 0.081 mm^{-1}. A final refinement on F^2 with 1598 unique intensities and 120 parameters converged at ωR(F2) = 0.1358 (R(F) = 0.0506) for 893 observed reflections with $I > 2\sigma(I)$.

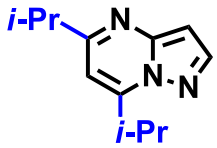


7-isopropyl-1H-pyrazolo[4,3-b]pyridine (19). From compound **11** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **19** (pale white powder, 62 mg, 0.388 mmol, 62%); mp 110-112 °C (from dichloromethane/methanol eluent); R_f 0.35 (15:1, dichloromethane: methanol); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.58 (d, J = 4.6 Hz, 1H), 8.41 (s, 1H), 7.19 (d, J = 4.6 Hz, 1H), 3.45 (hept, J = 6.9 Hz, 1H), 1.45 (d, J = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.6 (CH), 141.0 (C), 140.7 (C), 135.3 (CH), 132.8 (C), 117.5 (CH), 30.2 (CH), 22.1 ($2CH_3$); HRMS (ESI+) calcd for $C_9H_{12}N_3$ 162.1026, found 162.1024.

[6] CCDC number: 979231 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

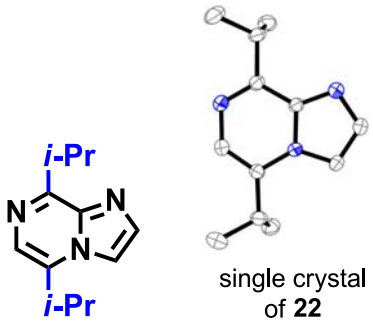


4,6-diisopropyl-imidazo[1,2-a]pyrimidine (20). From compound **12** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **20** (yellow powder, 43 mg, 0.213 mmol, 34%); mp 70-71 °C (from dichloromethane/methanol eluent); R_f 0.3 (25:1, dichloromethane: methanol); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (s, 1H), 7.47 (d, *J* = 1.3 Hz, 1H), 6.62 (s, 1H), 3.23 (hept, *J* = 6.8 Hz, 1H), 3.10 (hept, *J* = 6.7 Hz, 1H), 1.43 (d, *J* = 6.9 Hz, 6H), 1.35 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.5 (C), 152.7 (C), 149.7 (C), 134.7 (CH), 107.3 (CH), 102.6 (CH), 36.8 (CH), 30.2 (CH), 22.0 ($2CH_3$), 19.8 ($2CH_3$); HRMS (ESI+) calcd for $C_{12}H_{18}N_3$ 204.1495, found 204.1503. A single crystal of **20** was grown from ethyl acetate and *n*-hexane; X-ray crystal structure data for compound **20**:[7] $C_{12}H_{17}N_3$, *M* = 203.29, monoclinic, *P* $2_1/c$, *a* = 12.9851(18), *b* = 14.1460(19), *c* = 13.3141(19) Å, β = 95.871(9) °, *V* = 2432.8(6) Å^3, *Z* = 8, *d* = 1.110 g cm^{-3}, μ = 0.068 mm^{-1}. A final refinement on F^2 with 4283 unique intensities and 279 parameters converged at ω*R*(*F*2) = 0.2534 (*R*(*F*) = 0.0801) for 2809 observed reflections with $I > 2\sigma(I)$.



[7] CCDC number:979222 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

5,7-diisopropyl-pyrazolo[1,5-a]pyrimidine (21).[8] From compound **13** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **21** (yellow oil, 15 mg, 0.075 mmol, 12%); R_f 0.45 (1:10, ethyl acetate : 60 – 90 °C petroleum ether); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (d, *J* = 2.3 Hz, 1H), 6.60 (d, *J* = 2.3 Hz, 1H), 6.57 (s, 1H), 3.85 (hept, *J* = 6.9 Hz, 1H), 3.08 (hept, *J* = 6.9 Hz, 1H), 1.44 (d, *J* = 6.9 Hz, 6H), 1.35 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.3 (C), 154.8 (C), 148.8 (C), 144.2 (CH), 102.0 (CH), 95.8 (CH), 36.9 (CH), 28.6 (CH), 22.1 ($2CH_3$), 20.1 ($2CH_3$); HRMS (ESI+) calcd for $C_{12}H_{18}N_3$ 204.1495, found 204.1495.



4,7-diisopropyl-imidazo[1,2-a]pyrazine (22). From compound **14** (74 mg, 0.625 mmol), general procedure was followed with a reaction time of 14 h to provide compound **22** (yellow powder, 48 mg, 0.238 mmol, 38%); mp 63-64 °C (from dichloromethane/methanol eluent); R_f 0.6 (25:1, dichloromethane: methanol); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (d, *J* = 0.9 Hz, 1H), 7.70 (s, 1H), 7.67 (d, *J* = 0.9 Hz, 1H), 3.95 (hept, *J* = 6.9 Hz, 1H), 3.21 (hept, *J* = 6.9 Hz, 1H), 1.45 (t, *J* = 6.9 Hz, 12H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.13 (C), 139.93 (C), 135.13 (C), 134.3 (CH), 124.4 (CH), 111.1 (CH), 31.4 (CH), 28.9 (CH), 21.1 ($2CH_3$), 19.9 ($2CH_3$); HRMS (ESI+) calcd for $C_{12}H_{18}N_3$ 204.1495, found 204.1494. A single crystal of **22** was grown from ethyl acetate and *n*-hexane; X-ray

[8] a) T. Novinson, J. P. Miller, M. Scholten, R. K. Robins, L. N. Simon, D. E. O'Brien, R. B. Meyer, *J. Med. Chem.*, 1975, **18**, 460-464; b) J. P. Miller, C. C. Sigman, H. L. Johnson, T. Novinson, R. H. Springer, K. Senga, D. E. O'Brien, R. K. Robins, *Adv. Cyclic. Nucleotide. Res.*, 1984, **16**, 277-290.

crystal structure data for compound **22**: [9] $C_{12}H_{17}N_3$, M = 203.29, monoclinic, $P\ 2_1/c$, a = 13.087(2), b = 11.462(2), c = 15.654(3) Å, β = 92.333(8) °, V = 2346.2(7) Å^3, Z = 8, d = 1.151 g cm^{-3}, μ = 0.071 mm^{-1}. A final refinement on F^2 with 5370 unique intensities and 279 parameters converged at ωR(F2) = 0.1753 (R(F) = 0.0582) for 2984 observed reflections with $I > 2\sigma(I)$.

Computational Method

All calculations have been performed using geometries optimized for the parent compounds at B3LYP levels of theory using 6-31+G** basis sets with the self consistent reaction field (SCRF) polarizable continuum model (solvent=DMSO). The cations and anions of the selected molecules being open-shell species, their energies and wave functions have been calculated using the single-annihilated (the quartet state is projected out for a doublet state) UHF method. These calculations were performed using the Gaussian 09 program. [10] The condensed Fukui functions (f_A^+, f_A^- and f_A^0) are obtained from

[9] CCDC number: 979230 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

[10] Gaussian 09, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

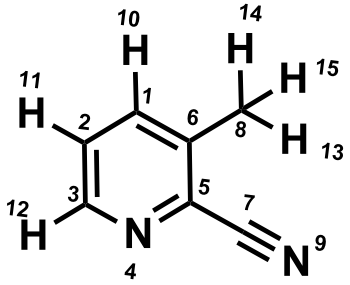
Hirshfeld charges using eq 1. The Hirshfeld recipe for the calculation of atomic charge has been described elsewhere in detail. [11]

$$Nucleophilic\_attack: f_A^+ = q^A{}_N - q^A{}_{N+1}$$
$$Electrophilic\_attack: f_A^- = q^A{}_{N-1} - q^A{}_N$$
$$Radical\_attack: f_A^0 = (q^A{}_{N-1} - q^A{}_{N+1})/2$$

Equation 1. The definition of condensed Fukui functions. The $q^A{}_N$ is the partial charge of atom A in the molecule with N electrons, while $q^A{}_{N-1}$ and $q^A{}_{N+1}$ are partial charges of atom A in the molecule with N-1 electrons and N+1 electrons, respectively.

Computational Results

Compound 1



Cartesian coordinates

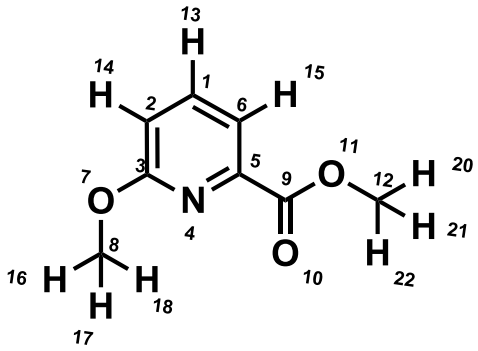
C	-1.43196300	1.09106300	0.00000000
C	-2.27726000	-0.01499600	-0.00001200
C	-1.71349700	-1.29573300	-0.00001000
N	-0.39492000	-1.50687600	0.00000500
C	0.40478900	-0.42272900	0.00006700
C	-0.04169900	0.91382500	0.00002300
C	1.82177900	-0.70581800	-0.00000800
C	0.91421700	2.07771200	-0.00001100
N	2.96464000	-0.92452900	-0.00002400
H	-1.84285100	2.09606000	-0.00002200
H	-3.35531100	0.10560800	-0.00003500
H	-2.34306200	-2.18118300	-0.00005100
H	1.56300300	2.05795600	0.88224000
H	0.36880700	3.02367400	-0.00016400

[11] F. L. Hirshfeld, *Theor. Chem. Acc.*, 1977, **44**, 129-138.

H	1.56318100	2.05777400	-0.88212600

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.008481	0.043393	-0.095591	0.08711	0.051874	0.138984
2	C	-0.018499	0.089580	-0.139207	0.120708	0.108079	0.228787
3	C	0.037537	0.170575	-0.026853	0.06439	0.133038	0.197428
4	N	-0.177993	-0.121456	-0.283421	0.105428	0.056537	0.161965
5	C	0.057555	0.169831	-0.044286	0.101841	0.112276	0.214117
6	C	0.020261	0.126011	-0.035422	0.055683	0.10575	0.161433
7	C	0.081954	0.136468	-0.020786	0.10274	0.054514	0.157254
8	C	-0.069206	-0.034401	-0.089825	0.020619	0.034805	0.055424
9	N	-0.261920	-0.136955	-0.418331	0.156411	0.124965	0.281376
10	H	0.066764	0.098173	0.026216	0.040548	0.031409	0.071957
11	H	0.067005	0.109510	0.014270	0.052735	0.042505	0.09524
12	H	0.056155	0.104497	0.021512	0.034643	0.048342	0.082985
13	H	0.049267	0.085397	0.029414	0.019853	0.03613	0.055983
14	H	0.050425	0.074071	0.033072	0.017353	0.023646	0.040999
15	H	0.049264	0.085390	0.029413	0.019851	0.036126	0.055977

Compound 2



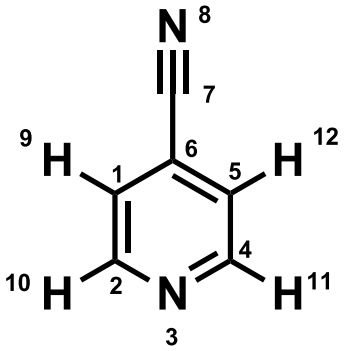
Cartesian coordinates

C	0.87213800	2.33098600	-0.00049300
C	2.03270100	1.57834900	-0.00017100
C	1.90328700	0.17199700	0.00016000
N	0.73881800	-0.45832000	0.00003600
C	-0.38480100	0.29023400	-0.00027400
C	-0.37378200	1.68189300	-0.00049200
O	3.05453300	-0.53856100	0.00050000
C	2.96180500	-1.97441700	0.00073500
C	-1.66923500	-0.49267100	-0.00055800
O	-1.73734100	-1.70969100	-0.00241000
O	-2.74791600	0.30941800	0.00146200
C	-4.03793100	-0.34199500	0.00103700

H	0.92342800	3.41502800	-0.00075300
H	3.01771900	2.03098000	-0.00016900
H	-1.29895700	2.24277200	-0.00072200
H	3.99316300	-2.32575400	0.00098800
H	2.43846600	-2.32818200	0.89259500
H	2.43879500	-2.32850400	-0.89118900
H	-4.14802700	-0.96066100	0.89392400
H	-4.76734200	0.46610700	0.00185600
H	-4.14827200	-0.95913200	-0.89286600

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.011841	0.041928	-0.093664	0.081823	0.053769	0.135592
2	C	-0.041252	0.067582	-0.155894	0.114642	0.108834	0.223476
3	C	0.145107	0.222195	0.101486	0.043621	0.077088	0.120709
4	N	-0.176681	-0.116895	-0.247528	0.070847	0.059786	0.130633
5	C	0.042637	0.131371	-0.050136	0.092773	0.088734	0.181507
6	C	-0.044505	0.073837	-0.118874	0.074369	0.118342	0.192711
7	O	-0.162649	-0.025357	-0.186191	0.023542	0.137292	0.160834
8	C	0.011740	0.048925	-0.001867	0.013607	0.037185	0.050792
9	C	0.203081	0.223264	0.099593	0.103488	0.020183	0.123671
10	O	-0.323551	-0.282448	-0.438322	0.114771	0.041103	0.155874
11	O	-0.131789	-0.113696	-0.176271	0.044482	0.018093	0.062575
12	C	0.023218	0.034072	0.003063	0.020155	0.010854	0.031009
13	H	0.065309	0.096728	0.026127	0.039182	0.031419	0.070601
14	H	0.061725	0.103924	0.011480	0.050245	0.042199	0.092444
15	H	0.053957	0.095469	0.017447	0.03651	0.041512	0.078022
16	H	0.051071	0.074704	0.041297	0.009774	0.023633	0.033407
17	H	0.039928	0.073344	0.029104	0.010824	0.033416	0.04424
18	H	0.039928	0.073345	0.029104	0.010824	0.033417	0.044241
19	H	0.049198	0.057292	0.033783	0.015415	0.008094	0.023509
20	H	0.056242	0.063176	0.042612	0.01363	0.006934	0.020564
21	H	0.049184	0.057277	0.033773	0.015411	0.008093	0.023504

Compound 3

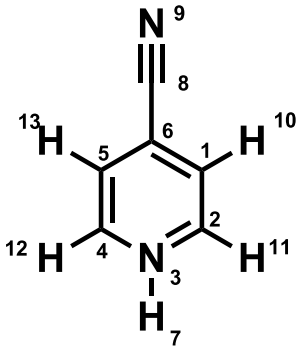


Cartesian coordinates

C	1.21108900	-0.71713700	0.00000000
C	1.18792800	0.66746100	0.00000000
N	0.00000000	1.30890900	0.00000000
C	-1.18791400	0.66747600	0.00000000
C	-1.21109000	-0.71713600	0.00000000
C	-0.00001100	-1.41645800	0.00000000
H	0.00001000	2.32616600	0.00000000
H	2.16279700	-1.23313000	0.00000000
H	2.07486700	1.28665900	0.00000000
H	-2.07486200	1.28666400	0.00000000
H	-2.16281700	-1.23309600	0.00000000
H	-0.00000200	-2.50085800	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.014734	0.128573	-0.102127	0.087393	0.143307	0.2307
2	C	0.042676	0.193330	-0.042313	0.084989	0.150654	0.235643
3	N	-0.183449	-0.120098	-0.308249	0.1248	0.063351	0.188151
4	C	0.042679	0.193328	-0.042310	0.084989	0.150649	0.235638
5	C	-0.014732	0.128574	-0.102131	0.087399	0.143306	0.230705
6	C	0.021274	0.072862	-0.084307	0.105581	0.051588	0.157169
7	C	0.100185	0.123203	-0.000961	0.101146	0.023018	0.124164
8	N	-0.254393	-0.190917	-0.411740	0.157347	0.063476	0.220823
9	H	0.072295	0.123290	0.030062	0.042233	0.050995	0.093228
10	H	0.057987	0.112295	0.017088	0.040899	0.054308	0.095207
11	H	0.057987	0.112294	0.017088	0.040899	0.054307	0.095206
12	H	0.072295	0.123290	0.03006	0.042235	0.050995	0.09323

Protonated compound 3

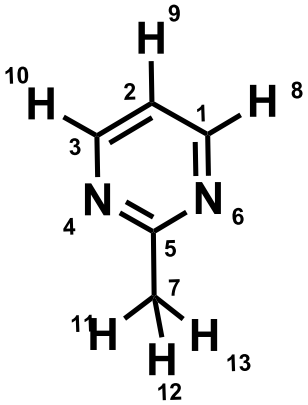


Cartesian coordinates

C	0.06065300	1.21747600	0.00000000
C	1.44434600	1.18715700	0.00000000
N	2.08350300	0.00000700	0.00000000
C	1.44434600	-1.18714500	0.00000000
C	0.06065400	-1.21746700	0.00000000
C	-0.63912700	0.00000500	0.00000000
H	3.10206300	0.00000400	0.00000000
C	-2.07607600	-0.00000900	0.00000000
N	-3.23776000	-0.00002400	0.00000000
H	-0.45504000	2.16877300	0.00000000
H	2.05950600	2.07660600	0.00000000
H	2.05951000	-2.07659100	0.00000000
H	-0.45502600	-2.16877200	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	0.029290	0.167346	-0.050635	0.079925	0.138056	0.217981
2	C	0.131877	0.286448	0.029265	0.102612	0.154571	0.257183
3	N	0.047545	0.089056	-0.047296	0.094841	0.041511	0.136352
4	C	0.131876	0.286448	0.029265	0.102611	0.154572	0.257183
5	C	0.029289	0.167346	-0.050635	0.079924	0.138057	0.217981
6	C	0.070924	0.122117	-0.045797	0.116721	0.051193	0.167914
7	H	0.220290	0.251935	0.176020	0.04427	0.031645	0.075915
8	C	0.120798	0.143923	0.044278	0.07652	0.023125	0.099645
9	N	-0.204708	-0.137164	-0.341881	0.137173	0.067544	0.204717
10	H	0.099341	0.147990	0.060275	0.039066	0.048649	0.087715
11	H	0.112083	0.163284	0.068468	0.043615	0.051201	0.094816
12	H	0.112083	0.163284	0.068467	0.043616	0.051201	0.094817
13	H	0.099341	0.147990	0.060275	0.039066	0.048649	0.087715

Compound 4

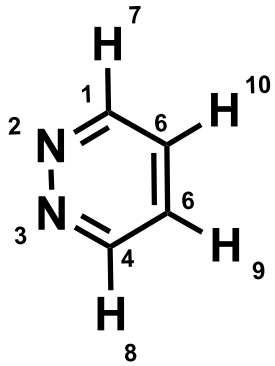


Cartesian coordinates

C	1.11288700	-1.18226700	0.00200200
C	1.84938900	0.00000100	0.00809900
C	1.11288000	1.18227000	0.00200200
N	-0.22769100	1.19367100	-0.00942600
C	-0.84880200	-0.00000400	-0.01323100
N	-0.22768900	-1.19367100	-0.00942600
C	-2.35262100	-0.00000100	0.00622200
H	1.60618800	-2.15154400	0.00397200
H	2.93318600	0.00000600	0.01448800
H	1.60618300	2.15154600	0.00397200
H	-2.71088500	0.00003300	1.04316300
H	-2.74470800	-0.89448100	-0.48207200
H	-2.74470500	0.89445000	-0.48212800

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	0.050480	0.136354	-0.119475	0.169955	0.085874	0.255829
2	C	-0.046351	0.024322	-0.124954	0.078603	0.070673	0.149276
3	C	0.050481	0.136355	-0.119474	0.169955	0.085874	0.255829
4	N	-0.199634	0.009380	-0.321682	0.122048	0.209014	0.331062
5	C	0.133504	0.209208	0.074899	0.058605	0.075704	0.134309
6	N	-0.199634	0.009380	-0.321679	0.122045	0.209014	0.331059
7	C	-0.092378	-0.062050	-0.119042	0.026664	0.030328	0.056992
8	H	0.057820	0.117326	-0.017045	0.074865	0.059506	0.134371
9	H	0.064811	0.103836	0.023633	0.041178	0.039025	0.080203
10	H	0.057820	0.117327	-0.017045	0.074865	0.059507	0.134372
11	H	0.047084	0.072248	0.027050	0.020034	0.025164	0.045198
12	H	0.038035	0.063179	0.017545	0.02049	0.025144	0.045634
13	H	0.038035	0.063180	0.017545	0.02049	0.025145	0.045635

Compound 5

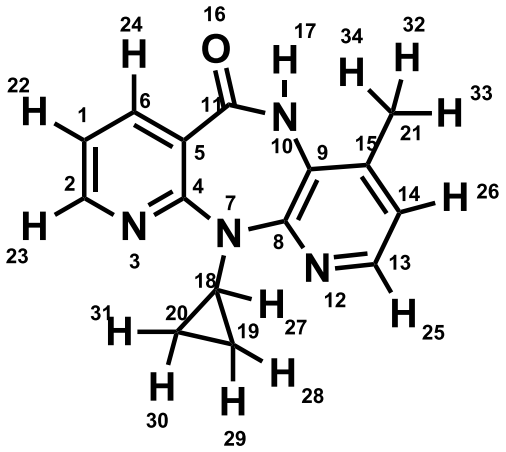


Cartesian coordinates

C	0.00000000	1.32994900	0.00000000
N	-1.19555600	0.73157000	0.00000000
N	-1.26409600	-0.60550900	0.00000000
C	-0.13598600	-1.32302000	0.00000000
C	1.14315000	-0.75148100	0.00000000
C	1.21397600	0.63072000	0.00000000
H	-0.02542000	2.41561800	0.00000000
H	-0.27229100	-2.40038700	0.00000000
H	2.02910100	-1.37733500	0.00000000
H	2.15933000	1.16266400	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	0.028991	0.130688	-0.059668	0.088659	-0.101697	0.190356
2	N	-0.152241	0.079257	-0.310229	0.157988	-0.231498	0.389486
3	N	-0.152255	0.079360	-0.310323	0.158068	-0.231615	0.389683
4	C	0.028939	0.130687	-0.059768	0.088707	-0.101748	0.190455
5	C	-0.008684	0.064985	-0.153096	0.144412	-0.073669	0.218081
6	C	-0.008649	0.065031	-0.153085	0.144436	-0.07368	0.218116
7	H	0.059500	0.107437	0.014814	0.044686	-0.047937	0.092623
8	H	0.059473	0.107395	0.014805	0.044668	-0.047922	0.09259
9	H	0.072500	0.117589	0.008453	0.064047	-0.045089	0.109136
10	H	0.072497	0.117589	0.008440	0.064057	-0.045092	0.109149

Compound 6



Cartesian coordinates

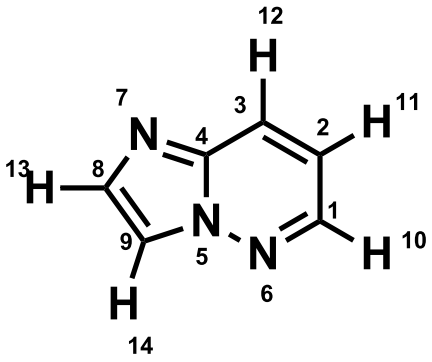
C	3.44099900	-1.48805000	-1.17879900
C	3.41562600	-0.10589700	-1.36440900

N	2.42796100	0.68279600	-0.92392300
C	1.40470500	0.12845500	-0.26101700
C	1.35645800	-1.25678900	0.02334100
C	2.39959500	-2.05831100	-0.45378000
N	0.39197700	1.00837800	0.18873300
C	-0.94113100	0.72836100	-0.22691400
C	-1.55881700	-0.48014300	0.14844400
N	-0.91091300	-1.40490900	0.99725200
C	0.36457700	-1.90199100	0.93170200
N	-1.56360300	1.66055400	-0.94993100
C	-2.83103600	1.43603300	-1.32128600
C	-3.51716400	0.26521900	-1.01573300
C	-2.87960600	-0.73021700	-0.26607200
O	0.67841100	-2.87628600	1.62368100
H	-1.50146200	-1.94599100	1.61883300
C	0.74788900	2.40957300	0.31094600
C	0.14966600	3.16760100	1.46442000
C	1.61698400	2.79762400	1.47624100
C	-3.59336400	-2.00479900	0.10700700
H	4.25843800	-2.08645100	-1.56523700
H	4.22162900	0.39654200	-1.89476500
H	2.38779400	-3.11790000	-0.22220000
H	-3.31119700	2.22768400	-1.89126900
H	-4.53884500	0.12489500	-1.35414400
H	0.89191600	2.94717800	-0.62101900
H	-0.50938000	2.62448400	2.13500700
H	-0.13044200	4.20199000	1.29063000
H	1.92874500	2.00847000	2.15377300
H	2.35683500	3.57475000	1.31076700
H	-3.80405400	-2.05161600	1.18323600
H	-4.55040700	-2.07425700	-0.41410800
H	-2.99709200	-2.88725400	-0.14842500

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.049720	0.004878	-0.102567	0.052847	0.054598	0.107445
2	C	0.044060	0.081468	-0.071709	0.115769	0.037408	0.153177
3	N	-0.174888	-0.144187	-0.229597	0.054709	0.030701	0.08541
4	C	0.121660	0.136027	0.086200	0.03546	0.014367	0.049827
5	C	-0.043176	-0.011598	-0.106407	0.063231	0.031578	0.094809
6	C	-0.009349	0.016896	-0.099491	0.090142	0.026245	0.116387
7	N	-0.080930	0.029780	-0.086530	0.0056	0.11071	0.11631
8	C	0.103381	0.133066	0.094881	0.0085	0.029685	0.038185
9	C	0.027734	0.076474	0.018622	0.009112	0.04874	0.057852

10	N	-0.085183	-0.051511	-0.113525	0.028342	0.033672	0.062014
11	C	0.175893	0.193329	0.088341	0.087552	0.017436	0.104988
12	N	-0.179735	-0.147921	-0.194839	0.015104	0.031814	0.046918
13	C	0.024366	0.082985	-0.006901	0.031267	0.058619	0.089886
14	C	-0.055189	0.003957	-0.075581	0.020392	0.059146	0.079538
15	C	0.005585	0.032402	-0.011335	0.01692	0.026817	0.043737
16	O	-0.348406	-0.302280	-0.450433	0.102027	0.046126	0.148153
17	H	0.143287	0.164734	0.118743	0.024544	0.021447	0.045991
18	C	0.000504	0.013696	-0.001846	0.00235	0.013192	0.015542
19	C	-0.077320	-0.053999	-0.087059	0.009739	0.023321	0.03306
20	C	-0.077037	-0.051577	-0.083618	0.006581	0.02546	0.032041
21	C	-0.072011	-0.060723	-0.079047	0.007036	0.011288	0.018324
22	H	0.056702	0.080676	0.024967	0.031735	0.023974	0.055709
23	H	0.051684	0.072734	-0.000801	0.052485	0.02105	0.073535
24	H	0.057581	0.074988	0.014760	0.042821	0.017407	0.060228
25	H	0.047188	0.075469	0.031007	0.016181	0.028281	0.044462
26	H	0.053035	0.079980	0.040289	0.012746	0.026945	0.039691
27	H	0.031843	0.065178	0.022496	0.009347	0.033335	0.042682
28	H	0.040080	0.052525	0.034774	0.005306	0.012445	0.017751
29	H	0.043200	0.060777	0.034292	0.008908	0.017577	0.026485
30	H	0.040860	0.054175	0.038005	0.002855	0.013315	0.01617
31	H	0.043253	0.061503	0.035907	0.007346	0.01825	0.025596
32	H	0.047623	0.059719	0.039340	0.008283	0.012096	0.020379
33	H	0.048007	0.060518	0.038981	0.009026	0.012511	0.021537
34	H	0.045319	0.055752	0.039675	0.005644	0.010433	0.016077

Compound 7



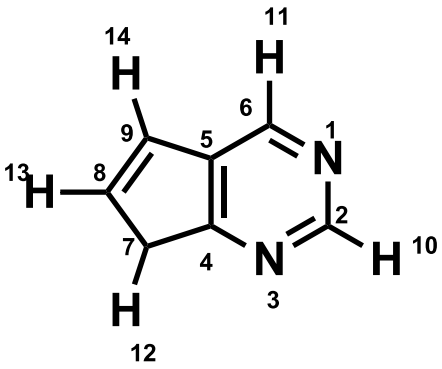
Cartesian coordinates

C	1.97810000	-0.77514600	-0.00000900
C	2.09570700	0.64395800	0.00000700
C	0.95628700	1.41267500	-0.00000100
C	-0.28755800	0.74737600	-0.00000500
N	-0.26528000	-0.65671300	0.00000400
N	0.83903200	-1.43635600	0.00000900
N	-1.54500200	1.19595400	-0.00003000
C	-2.32485300	0.07181600	0.00005000

C	-1.56751100	-1.08598100	-0.00003500
H	2.86307100	-1.40311200	0.00004600
H	3.08131800	1.09432500	0.00001500
H	0.98078000	2.49659200	-0.00000500
H	-3.40436500	0.13733600	0.00008100
H	-1.82308900	-2.13353000	-0.00005800

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	0.034290	0.087176	-0.077538	0.111828	0.052886	0.164714
2	C	-0.040355	0.067949	-0.143228	0.102873	0.108304	0.211177
3	C	-0.018163	0.044541	-0.172891	0.154728	0.062704	0.217432
4	C	0.078869	0.154279	0.040234	0.038635	0.07541	0.114045
5	N	0.047408	0.073283	0.002132	0.045276	0.025875	0.071151
6	N	-0.125251	-0.045898	-0.266087	0.140836	0.079353	0.220189
7	N	-0.258556	-0.139509	-0.316172	0.057616	0.119047	0.176663
8	C	-0.017245	0.085987	-0.085271	0.068026	0.103232	0.171258
9	C	-0.024804	0.149878	-0.080728	0.055924	0.174682	0.230606
10	H	0.063941	0.091868	0.014907	0.049034	0.027927	0.076961
11	H	0.065406	0.104820	0.017122	0.048284	0.039414	0.087698
12	H	0.071163	0.102348	0.005776	0.065387	0.031185	0.096572
13	H	0.056054	0.099622	0.024981	0.031073	0.043568	0.074641
14	H	0.067350	0.123722	0.036986	0.030364	0.056372	0.086736

Compound 8



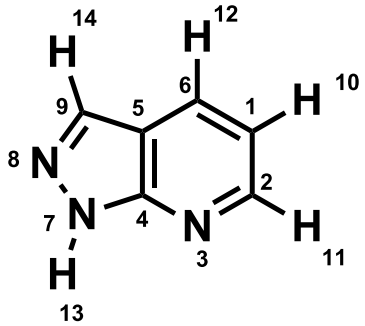
Cartesian coordinates

N	-2.15429700	0.65554900	0.00000100
C	-2.03602100	-0.68853400	-0.00000600
N	-0.90791400	-1.40562700	0.00000400
C	0.19951100	-0.65783100	0.00000400
C	0.22791500	0.76762700	-0.00000200
C	-1.02662700	1.38206800	-0.00000700

N	1.49225500	-1.09879700	-0.00000300
C	2.34122300	-0.00089600	-0.00000700
C	1.60932900	1.16039800	0.00001100
H	-2.96576200	-1.25096800	0.00001700
H	-1.13675400	2.46429100	0.00000100
H	1.78055600	-2.06730100	0.00001200
H	3.41175000	-0.14553300	-0.00001500
H	2.00792400	2.16464700	0.00001600

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	N	-0.226542	-0.175066	-0.301782	0.07524	0.051476	0.126716
2	C	0.072689	0.163728	-0.032552	0.105241	0.091039	0.19628
3	N	-0.219538	-0.155673	-0.343877	0.124339	0.063865	0.188204
4	C	0.101479	0.167227	0.044614	0.056865	0.065748	0.122613
5	C	-0.046488	-0.003566	-0.106232	0.059744	0.042922	0.102666
6	C	0.041186	0.121443	-0.124157	0.165343	0.080257	0.2456
7	N	-0.061791	0.005360	-0.092478	0.030687	0.067151	0.097838
8	C	0.021555	0.174327	-0.079070	0.100625	0.152772	0.253397
9	C	-0.082144	0.084431	-0.140224	0.05808	0.166575	0.224655
10	H	0.042260	0.078713	-0.007078	0.049338	0.036453	0.085791
11	H	0.055533	0.088897	-0.016117	0.07165	0.033364	0.105014
12	H	0.172321	0.210209	0.144554	0.027767	0.037888	0.065655
13	H	0.071443	0.124703	0.025872	0.045571	0.05326	0.098831
14	H	0.058047	0.115250	0.028680	0.029367	0.057203	0.08657

Compound 9



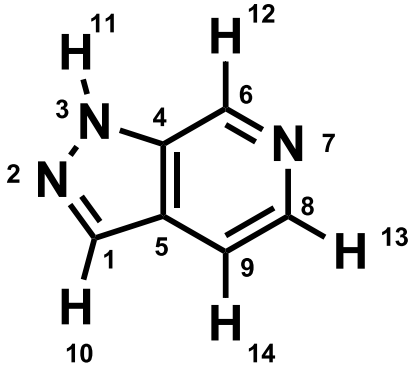
Cartesian coordinates

C	2.13448700	0.63339200	-0.00000300
C	2.01606400	-0.77590100	-0.00000200
N	0.85725000	-1.44240300	0.00000100
C	-0.22570200	-0.65255900	0.00000200
C	-0.24244800	0.76757100	0.00000500

C	0.99602500	1.42975300	-0.00000100
N	-1.53133100	-1.04730000	0.00000700
N	-2.38372800	0.01352800	-0.00002000
C	-1.62993300	1.10390600	0.00001000
H	3.12377800	1.07801100	-0.00000500
H	2.91520900	-1.38700400	-0.00000200
H	1.06388800	2.51319400	0.00000000
H	-1.89598600	-1.98917900	0.00001500
H	-2.09318100	2.08122700	0.00001400

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.054286	0.058085	-0.127297	0.073011	0.112371	0.185382
2	C	0.033789	0.088130	-0.092119	0.125908	0.054341	0.180249
3	N	-0.213564	-0.120088	-0.332885	0.119321	0.093476	0.212797
4	C	0.089989	0.130484	0.047596	0.042393	0.040495	0.082888
5	C	-0.048002	0.001103	-0.101957	0.053955	0.049105	0.10306
6	C	-0.008317	0.078476	-0.146599	0.138282	0.086793	0.225075
7	N	-0.022637	0.115486	-0.060404	0.037767	0.138123	0.17589
8	N	-0.167489	-0.092001	-0.278650	0.111161	0.075488	0.186649
9	C	-0.008418	0.131304	-0.089145	0.080727	0.139722	0.220449
10	H	0.055285	0.096686	0.017074	0.038211	0.041401	0.079612
11	H	0.050107	0.079854	-0.005289	0.055396	0.029747	0.085143
12	H	0.066167	0.102149	0.007021	0.059146	0.035982	0.095128
13	H	0.166003	0.220005	0.135708	0.030295	0.054002	0.084297
14	H	0.061373	0.110320	0.026968	0.034405	0.048947	0.083352

Compound 10



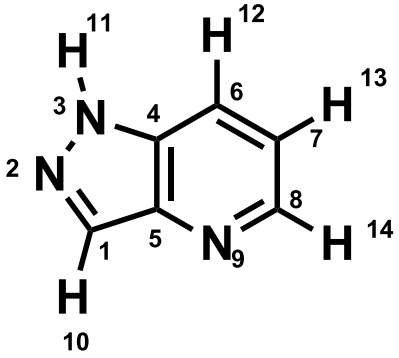
Cartesian coordinates

C	1.91685800	-0.46252300	0.00000000
N	2.25299200	0.82028500	0.00000000

N	1.09559000	1.52541000	0.00000000
C	0.00000000	0.70920000	0.00000000
C	0.49672500	-0.61704800	0.00000000
C	-1.38400200	0.95787600	0.00000000
N	-2.24706600	-0.05293700	0.00000000
C	-1.77625100	-1.33157300	0.00000000
C	-0.43273600	-1.67362000	0.00000000
H	2.68373400	-1.22472300	0.00000000
H	1.12707200	2.53458700	0.00000000
H	-1.78522600	1.96837400	0.00000000
H	-2.53617200	-2.10778300	0.00000000
H	-0.12358300	-2.71362900	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.007423	0.109374	-0.093430	0.086007	0.116797	0.202804
2	N	-0.157243	-0.089953	-0.282608	0.125365	0.06729	0.192655
3	N	-0.010638	0.103090	-0.058282	0.047644	0.113728	0.161372
4	C	0.032996	0.075431	-0.009252	0.042248	0.042435	0.084683
5	C	-0.034093	0.012051	-0.094714	0.060621	0.046144	0.106765
6	C	0.023120	0.127003	-0.119538	0.142658	0.103883	0.246541
7	N	-0.206076	-0.147206	-0.318392	0.112316	0.05887	0.171186
8	C	0.001967	0.125358	-0.061663	0.06363	0.123391	0.187021
9	C	-0.037495	0.072827	-0.145799	0.108304	0.110322	0.218626
10	H	0.062721	0.105303	0.026106	0.036615	0.042582	0.079197
11	H	0.173892	0.219612	0.141840	0.032052	0.04572	0.077772
12	H	0.054038	0.094209	-0.004926	0.058964	0.040171	0.099135
13	H	0.042698	0.088945	0.007808	0.03489	0.046247	0.081137
14	H	0.061419	0.103882	0.012646	0.048773	0.042463	0.091236

Compound 11

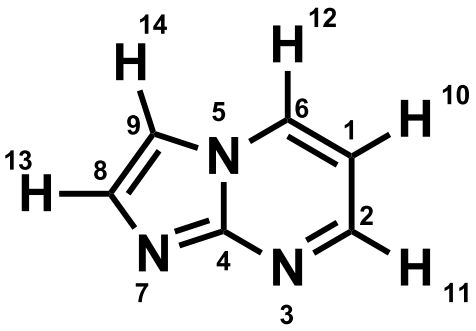


Cartesian coordinates

C	-1.59993400	-1.10922700	0.00002000
N	-2.38347000	-0.04037900	-0.00002200
N	-1.56327300	1.04470500	0.00000500
C	-0.24619200	0.69354300	0.00000200
C	-0.22385200	-0.72618300	-0.00000200
C	0.95394900	1.41968800	0.00000300
C	2.11079600	0.65544900	0.00000100
C	2.04235500	-0.76181000	-0.00000400
N	0.90992400	-1.46130700	-0.00000500
H	-2.02767100	-2.10245500	0.00003000
H	-1.96663800	1.97018700	0.00001000
H	0.97896000	2.50438500	0.00000600
H	3.08448700	1.13390000	0.00000300
H	2.96586700	-1.33591700	-0.00000300

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.021571	0.125417	-0.105056	0.083485	0.146988	0.230473
2	N	-0.164833	-0.089768	-0.276754	0.111921	0.075065	0.186986
3	N	-0.015169	0.129199	-0.053626	0.038457	0.144368	0.182825
4	C	0.034437	0.075603	-0.005395	0.039832	0.041166	0.080998
5	C	0.007170	0.067976	-0.052466	0.059636	0.060806	0.120442
6	C	-0.022293	0.067988	-0.157292	0.134999	0.090281	0.22528
7	C	-0.040764	0.017460	-0.138740	0.097976	0.058224	0.1562
8	C	0.020997	0.105445	-0.074441	0.095438	0.084448	0.179886
9	N	-0.201008	-0.109979	-0.325558	0.12455	0.091029	0.215579
10	H	0.058745	0.110305	0.022299	0.036446	0.05156	0.088006
11	H	0.171956	0.226738	0.143830	0.028126	0.054782	0.082908
12	H	0.067773	0.103189	0.010051	0.057722	0.035416	0.093138
13	H	0.058400	0.088027	0.012142	0.046258	0.029627	0.075885
14	H	0.046115	0.082353	0.001015	0.0451	0.036238	0.081338

Compound 12

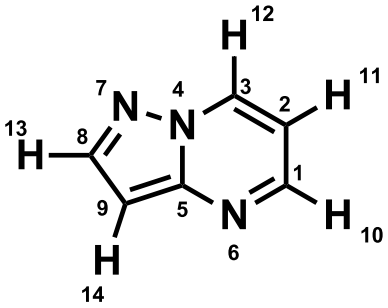


Cartesian coordinates

C	2.17437600	-0.13816100	0.00000000
C	1.59245400	-1.43673200	0.00000000
N	0.28937400	-1.65852000	0.00000000
C	-0.51990000	-0.58042600	0.00000000
N	0.00000000	0.73678600	0.00000000
C	1.34967700	0.95400300	0.00000000
N	-1.84994400	-0.55870300	0.00000000
C	-2.18990100	0.76899600	0.00000000
C	-1.08278000	1.59197300	0.00000000
H	3.24962300	-0.01280600	0.00000000
H	2.23646800	-2.31238500	0.00000000
H	1.68774400	1.98320000	0.00000000
H	-3.22503100	1.08250100	0.00000000
H	-0.96836300	2.66462600	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	-0.052569	0.002870	-0.134463	0.081894	0.055439	0.137333
2	C	0.042131	0.126669	-0.097339	0.13947	0.084538	0.224008
3	N	-0.205741	-0.134881	-0.342170	0.136429	0.07086	0.207289
4	C	0.126737	0.207279	0.083483	0.043254	0.080542	0.123796
5	N	-0.001632	0.023813	-0.046638	0.045006	0.025445	0.070451
6	C	0.065906	0.140333	-0.088168	0.154074	0.074427	0.228501
7	N	-0.274145	-0.143887	-0.330816	0.056671	0.130258	0.186929
8	C	-0.017129	0.087315	-0.085859	0.06873	0.104444	0.173174
9	C	-0.019800	0.159306	-0.069220	0.04942	0.179106	0.228526
10	H	0.068004	0.095791	0.027298	0.040706	0.027787	0.068493
11	H	0.056821	0.091707	-0.003612	0.060433	0.034886	0.095319
12	H	0.084120	0.114844	0.018562	0.065558	0.030724	0.096282
13	H	0.056425	0.100827	0.025106	0.031319	0.044402	0.075721
14	H	0.070982	0.128085	0.044069	0.026913	0.057103	0.084016

Compound 13

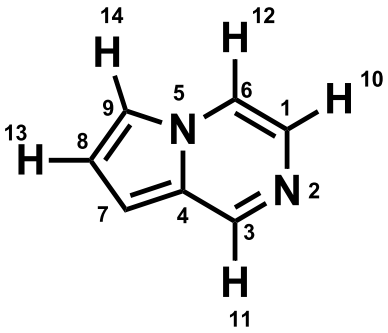


Cartesian coordinates

C	-1.58876900	-1.45703400	0.00000000
C	-2.16992100	-0.15690600	0.00000000
C	-1.34195600	0.93437700	0.00000000
N	0.00000000	0.70807400	0.00000000
C	0.52375000	-0.59771500	0.00000000
N	-0.28715400	-1.68162200	0.00000000
N	0.96714600	1.65458100	0.00000000
C	2.11252600	0.94668600	0.00000000
C	1.91058500	-0.44097000	0.00000000
H	-2.23493100	-2.33120200	0.00000000
H	-3.24482100	-0.02924400	0.00000000
H	-1.66136000	1.96929700	0.00000000
H	3.05388300	1.48008900	0.00000000
H	2.64999700	-1.22680100	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	0.045693	0.116908	-0.095931	0.141624	0.071215	0.212839
2	C	-0.052530	0.024505	-0.134736	0.082206	0.077035	0.159241
3	C	0.059380	0.140636	-0.103681	0.163061	0.081256	0.244317
4	N	0.046510	0.077411	0.001113	0.045397	0.030901	0.076298
5	C	0.082268	0.150889	0.043395	0.038873	0.068621	0.107494
6	N	-0.196406	-0.113386	-0.333221	0.136815	0.08302	0.219835
7	N	-0.192265	-0.054659	-0.243623	0.051358	0.137606	0.188964
8	C	-0.006709	0.072178	-0.066864	0.060155	0.078887	0.139042
9	C	-0.108371	0.067897	-0.160746	0.052375	0.176268	0.228643
10	H	0.057850	0.090575	-0.003411	0.061261	0.032725	0.093986
11	H	0.068158	0.101143	0.027151	0.041007	0.032985	0.073992
12	H	0.078978	0.113178	0.008173	0.070805	0.0342	0.105005
13	H	0.060022	0.097648	0.031982	0.02804	0.037626	0.065666
14	H	0.057361	0.115038	0.030490	0.026871	0.057677	0.084548

Compound 14



Cartesian coordinates

C	-2.15866100	-0.18944600	0.00000000
N	-1.67672600	-1.47512200	0.00000000
C	-0.36884300	-1.64049000	0.00000000
C	0.54011400	-0.55566000	0.00000000
N	0.00000000	0.73821100	0.00000000
C	-1.36313800	0.92236100	0.00000000
N	1.87628100	-0.51771200	0.00000000
C	2.19092000	0.80935100	0.00000000
C	1.05991600	1.61099200	0.00000000
H	-3.23660300	-0.07457100	0.00000000
H	0.02717300	-2.65291800	0.00000000
H	-1.73369000	1.93915500	0.00000000
H	3.21867500	1.14681300	0.00000000
H	0.92570200	2.68122900	0.00000000

Atom index	Atom	Hirshfeld charge of N electrons	Hirshfeld charge of N-1 electrons	Hirshfeld charge of N+1 electrons	f_A^+	f_A^-	$2*f_A^0$
1	C	0.000432	0.087701	-0.067682	0.068114	0.087269	0.155383
2	N	-0.203833	-0.113818	-0.326839	0.123006	0.090015	0.213021
3	C	0.030918	0.103821	-0.135954	0.166872	0.072903	0.239775
4	C	0.078021	0.134639	0.033927	0.044094	0.056618	0.100712
5	N	0.006589	0.036587	-0.044744	0.051333	0.029998	0.081331
6	C	0.034467	0.143312	-0.087957	0.122424	0.108845	0.231269
7	N	-0.251199	-0.124562	-0.319121	0.067922	0.126637	0.194559
8	C	-0.010254	0.068225	-0.081117	0.070863	0.078479	0.149342
9	C	-0.008626	0.142722	-0.071320	0.062694	0.151348	0.214042
10	H	0.055134	0.092468	0.019487	0.035647	0.037334	0.072981
11	H	0.057143	0.091523	-0.011410	0.068553	0.03438	0.102933
12	H	0.078858	0.118478	0.024341	0.054517	0.03962	0.094137
13	H	0.058409	0.095240	0.026098	0.032311	0.036831	0.069142
14	H	0.074092	0.123788	0.042497	0.031595	0.049696	0.081291

-The End-