Electronic Supplemental Information for

BN benzonitrile: an electrondeficient 1,2-dihydro-1,2-azaborine featuring linkage isomerism

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General

All oxygen- and moisture-sensitive manipulations were carried out under an inert atmosphere using either standard Schlenk techniques or a glove box.

THF, Et_2O, CH_2Cl_2, and pentane were purified by passing through a neutral alumina column under argon. Cyclohexene was dried over CaH_2 and distilled under N_2 prior to use.

Trisacetonitrile(tricarbonyl)chromium(0) was purchased from Acros or Aldrich and used as received. All other chemicals and solvents were purchased (Aldrich or Strem) and used as received. Pentacarbonylcyanochromate[1] and 1,2-azaborine precursor **1**[2] were prepared according to literature procedures.

^{11}B NMR spectra were recorded on a Varian Unity/Inova 600 MHz spectrometer at ambient temperature. ^{1}H NMR spectra were recorded on a Varian Unity/Inova 300 MHz or Varian Unity/Inova 600 MHz spectrometer. ^{13}C NMR spectra were recorded on a Varian Unity/Inova 300 MHz spectrometer or Varian Unity/Inova 500 MHz spectrometer. ^{15}N NMR spectra were recorded on a Varian Unity/Inova 500 MHz spectrometer. ^{11}B NMR spectra were externally referenced to $BF_3{\bullet}Et_2O$ (δ 0). ^{15}N NMR spectra were externally referenced to nitromethane (δ 0).

IR spectra were recorded on a Nicolet Magna 550 FT-IR instrument with OMNIC software.

High-resolution mass spectroscopy data were obtained at the Mass Spectroscopy Facilities and Services Core of the Environmental Health Sciences Center at Oregon State University. Financial support for this facility has been furnished in part by the National Institute of Environmental Health Sciences, NIH (P30 ES00210).

Electronic Structure Calculations

The electrostatic potential (ESP) was calculated at the B3LYP/6-311+G** level using Spartan.[3] All other computations were calculated using the Gaussian 03[4] suite of programs at the B3LYP/DGDZVP2 level of theory. All stationary points were confirmed by harmonic frequency analysis ($N_{imag} = 0$). The energies of the stationary points were determined, including zero point energies at the same level of theory. Structure **4** was calculated at 0 K.[5] NICS calculations were carried out using standard GIAO methods with Bq atoms (NICS probes) 1.0 Å above the geometric center of the ring.

Synthesis

Compound 2. In a glovebox, a solution of 2-chloro-1-ethyl-1,2-azaborine **1** (0.150 g, 1.06 mmol in 4.0 mL CH_2Cl_2) was added dropwise to a stirring suspension of AgCN (0.171 g, 1.28 mmol in 10.0 mL CH_2Cl_2). The reaction was protected from light and stirred at rt for 8 h, whereupon pentane (10 mL) was added and solids removed by filtration. Removal of solvents under reduced pressure provided **2** as a clear, colorless liquid (0.138 g, 99%). An identical procedure was followed using $Ag^{13}C^{15}N$ (99 atom%) to confirm atom connectivity. ^{1}H NMR

(600 MHz, CD_2Cl_2): δ 7.76 (app t, $^3J_{HH}$ = 7.1 Hz, 1H), 7.41 (d, $^3J_{HH}$ = 6.6 Hz, 1H), 7.00 (d, $^3J_{HH}$ = 10.7 Hz, 1H), 6.64 (app t, $^3J_{HH}$ = 6.0 Hz, 1H), 4.06 (q, $^3J_{HH}$ = 7.3 Hz, 2H), 1.43 (t, $^3J_{HH}$ = 7.3 Hz, 3H). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 145.3, 139.8, 131 (br), 125.6 (br q, $^1J_{BC}$ = 85 Hz), 115.1, 52.0, 18.7. ^{15}N NMR (50.7 MHz, CD_2Cl_2): δ -105.0 (d, $^1J_{CN}$ = 15 Hz). ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 22.5 (d, $^1J_{BC}$ = 85 Hz). FTIR (thin film) 3076, 3047, 2981, 2937, 2904, 2875, 1602, 1524, 1478, 1454, 1443, 1412, 1382, 1355, 1333, 1244, 1178, 1160, 1123, 1110, 1008, 751, 688, 518, 475 cm^{-1}. HRMS (EI) calcd for $C_7H_9BN_2$ (M+) 132.08589, found 132.08628.

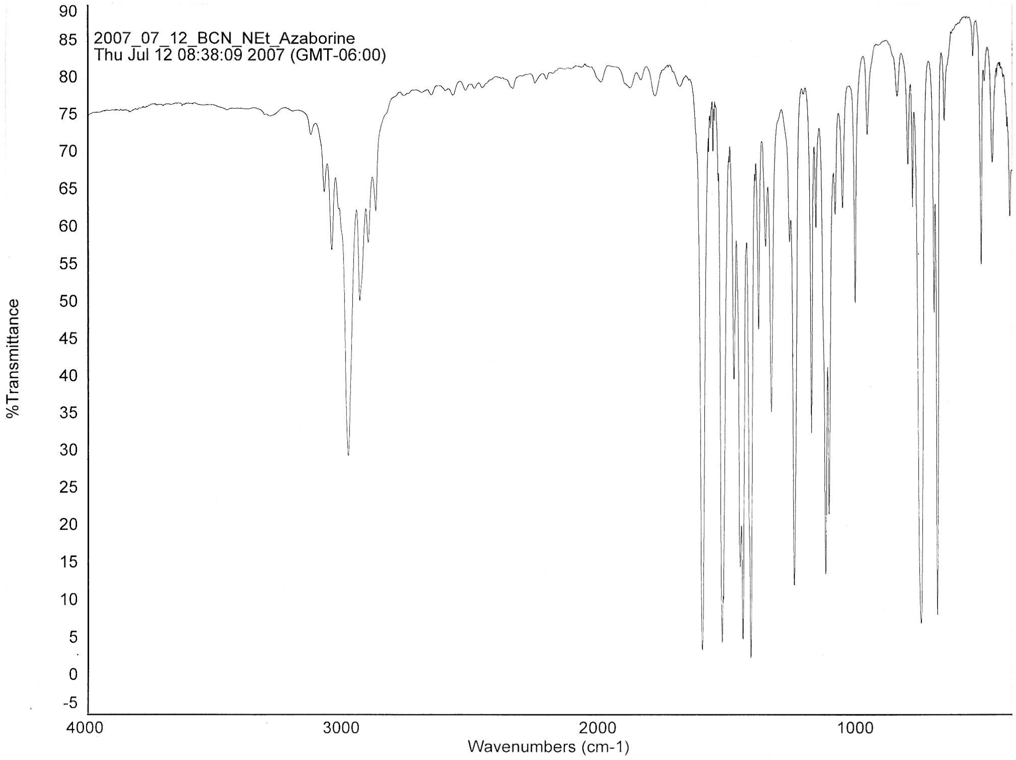

Figure S1. Observed IR spectrum of **2**.

Compound 5 from 1. In a glove box, a solution of **1** (0.300 g, 2.12 mmol in 10.0 mL THF) was added dropwise to a stirred solution of sodium pentacarbonylcyanochromate (0.510 g, 2.12 mmol in 10.0 mL THF). The reaction was stirred for 1 h at rt, whereupon approximately two-thirds of the solvent was removed under reduced pressure. Pentane (10 mL) was added, and solids were removed by filtration. Removal of solvents under reduced pressure provided **5** as a yellow solid (0.680 g, 99%). ^{1}H NMR (600 MHz, CD_2Cl_2): δ 7.76 (app t, $^3J_{HH}$ = 5.9 Hz, 1H), 7.28 (d, $^3J_{HH}$ = 6.1 Hz, 1H), 6.69 (d, $^3J_{HH}$ = 11.0 Hz, 1H), 6.45 (app t, $^3J_{HH}$ = 6.3 Hz, 1H), 3.95 (q, $^3J_{HH}$ = 6.8 Hz, 2H), 1.43 (t, $^3J_{HH}$ = 7.1 Hz, 3H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 217.6, 215.4, 189.2, 147.0, 139.0, 126 (br), 112.8, 49.3, 18.0. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 22.0. FTIR (CH_2Cl_2) 2130, 2051, 1954, 1605, 1521 cm^{-1}.

Compound 5 from reaction of 2 and $Cr(CO)_3(MeCN)_3$ and observation of 4. In a glove box, a Schlenk tube was charged with $Cr(CO)_3(MeCN)_3$ (0.196, 0.758 mmol) and THF (2.0 mL). A solution of **2** (0.100 g, 0.758 mmol in 2 mL THF) was then added to the Schlenk tube, which was then sealed. The flask was heated to 60 °C for 3 h, whereupon the solvent was removed. Crystals of **5** suitable for X-ray crystallography were grown from the resultant dark-brown oil by extraction into hot pentane (10 mL) followed by slow evaporation. Piano-stool complex **4** was identified in the ^{1}H and ^{11}B NMR spectrum of the crude dark-brown oil in 15 mol% abundance relative to **5**.

4: ^{1}H NMR (600 MHz, CD_2Cl_2): δ 6.05 (1H), 5.92 (1H), 5.23 (1H), 4.62 (1H), N-CH_2CH_3 not resolved from **5** and unreacted **2**. ^{11}B NMR (192.5 MHz, CD_2Cl_2): δ 17.2.

NMR yield of 5 from reaction of 2 and $Cr(CO)_6$. In a glovebox, a Schlenk tube was charged with $Cr(CO)_6$ (0.100 g, 0.450 mmol), **2** (0.030 g, 0.23 mmol), and THF (10.0 mL), which was then sealed. The flask was heated to 60 °C for 3 h, whereupon the solvent was removed under vacuum. The product was extracted into pentane (10 mL) and solids were filtered through an Acrodisc. ^{1}H NMR (CD_2Cl_2) analysis indicated **5** was formed in 23% yield (integrated versus hexamethylbenzene as internal standard).

Calculated IR Stretching Frequencies

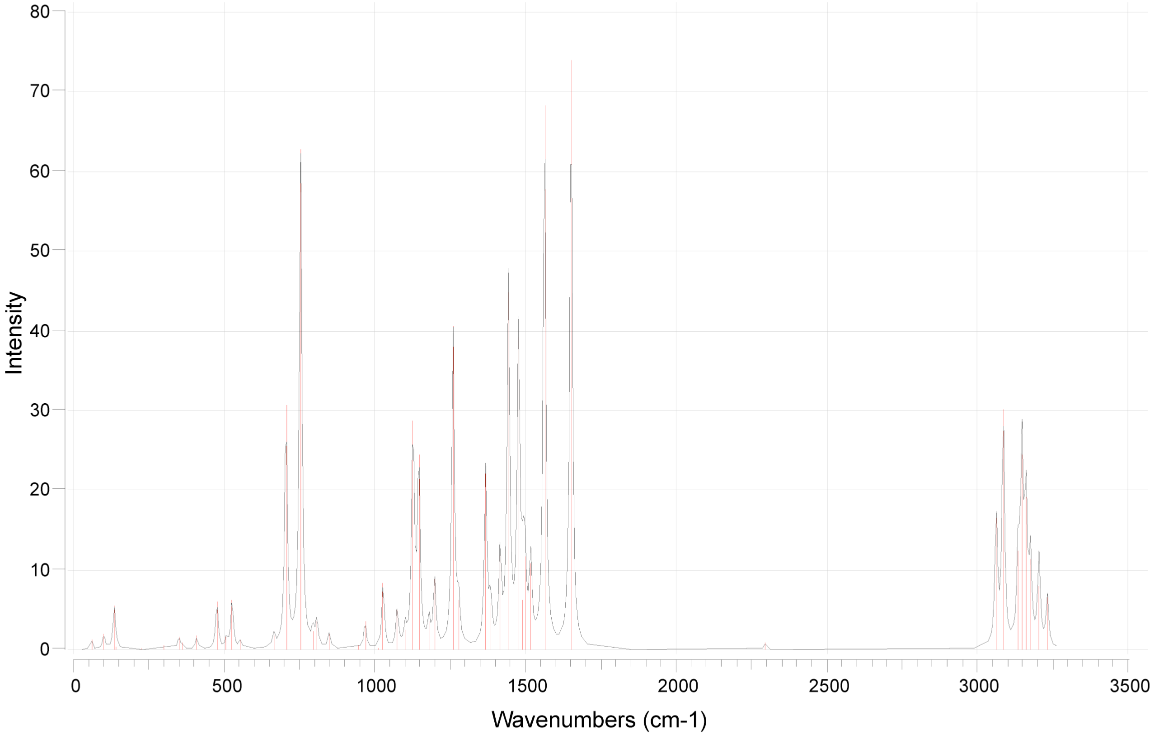

Figure S2. Calculated IR spectrum of **2** at the B3LYP/DGDZVP2 level.

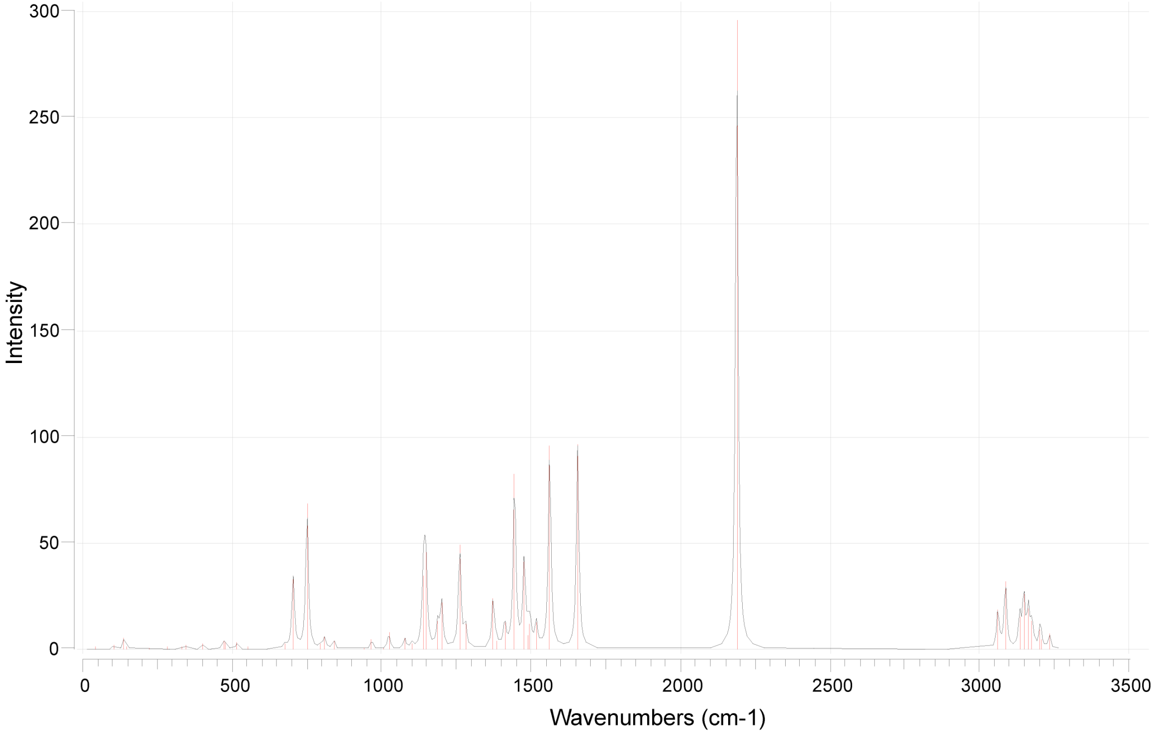

Figure S3. Calculated IR spectrum of **2'** at the B3LYP/DGDZVP2 level.

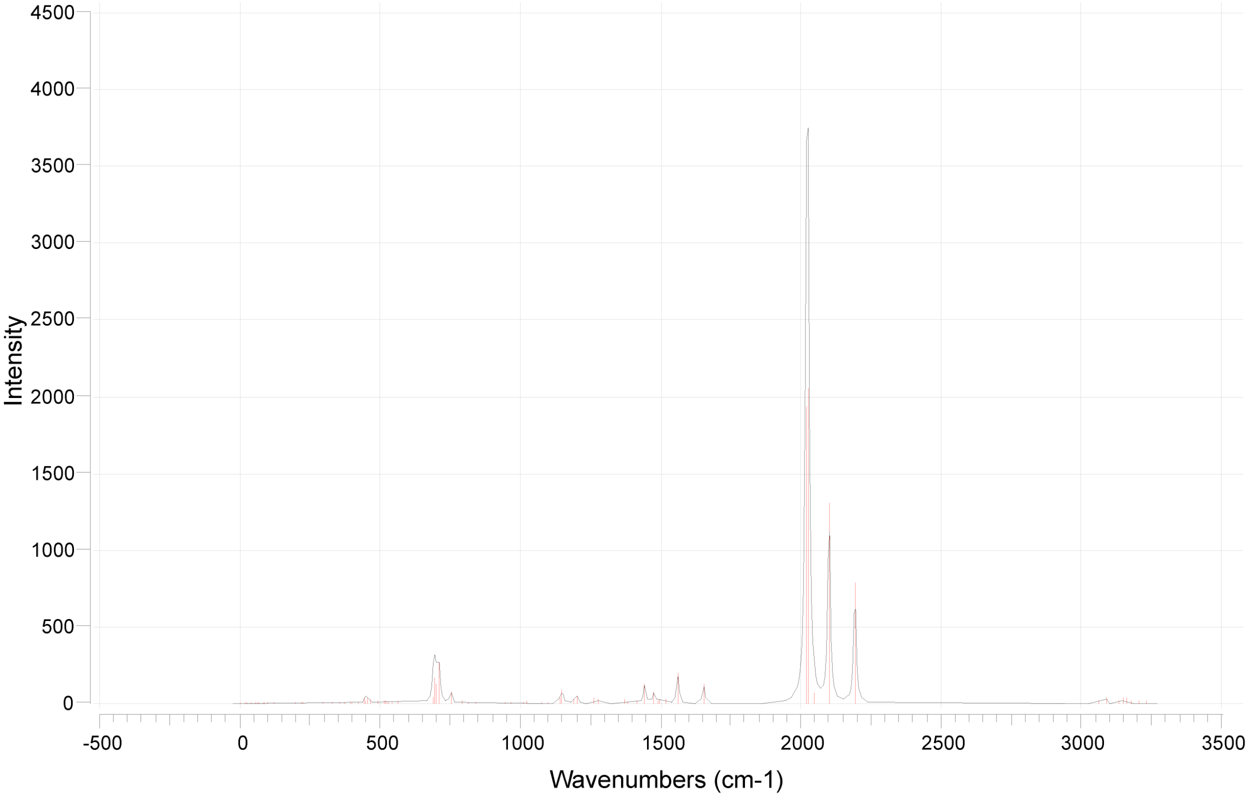

Figure S4. Calculated IR spectrum of **5** at the B3LYP/DGDZVP2 level.

ZPE and NICS Calculations

Table S1. Calculated Zero point energy and relative energy at the B3LYP/DGDZVP2 level

Molecule	Zero Point Energy (kcal/mol)	Relative Energy (kcal/mol)
2 (B-CN)	0.00	0.00
2’ (B-NC)	3.70	3.97

Table S2. NICS at 0, 1, and 2 Å at the B3LYP/DGDZVP2 level of calculation.

Molecule	NICS(0)	NICS(1)	NICS(2)
2 (B-CN)	-5.8267	-7.5537	-4.1374
2’ (B-NC)	-5.7982	-6.9574	-3.7715
5 (gas)	-5.8376	-7.123	-3.864
5 (solid)	-5.0857	-7.2136	-4.0575

Geometrical Parameter Calculations

Table S3. Atomic coordinates for **2**, **2'**, **3**, and **5** calculated at the B3LYP/DGDZVP2 level

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Compound: **2** (B-CN)

B3LYP/DGDZVP2 = -406.650745267 au

B3LYP/DGDZVP2 Zero Point Corrected Energy = -406.496849 au

NIMAG = 0

C	-1.36148600	1.48425500	0.23485400
C	-2.47016900	0.65672300	0.23362800
C	-2.34161300	-0.73671500	-0.02690000
C	-1.10639200	-1.28831000	-0.28076000
H	-1.49756500	2.54376500	0.43514200
H	-3.46469600	1.05405800	0.42859600
H	-3.21342600	-1.38151000	-0.03367800
H	-0.99954700	-2.34951600	-0.48492400
N	0.04103400	-0.54460900	-0.30163100
C	1.30913000	-1.26864000	-0.54378600
H	2.01335700	-0.56789500	-0.99442700
H	1.11609900	-2.05936900	-1.27546600
C	1.90311300	-1.85718800	0.74113400
H	1.21138900	-2.56266300	1.21199800
H	2.83173400	-2.38880900	0.51110200
H	2.13159700	-1.06480800	1.45882300
B	-0.01095600	0.87418700	-0.04557900
C	1.31657500	1.68687800	-0.07355200
N	2.30623700	2.30800700	-0.08936500

Compound: **2’** (B-NC)

B3LYP/DGDZVP2 = -406.644419037 au

B3LYP/DGDZVP2 Zero Point Corrected Energy = -406.490948 au

NIMAG = 0

C	-1.47226600	1.36641700	0.22797400
C	-2.49603000	0.43919400	0.23619300
C	-2.23891200	-0.94060900	-0.01596200
C	-0.96003700	-1.37488200	-0.27094200
H	-1.70309700	2.41077500	0.42138700
H	-3.52291200	0.74261700	0.43232000
H	-3.04712900	-1.66334900	-0.01562600
H	-0.75475000	-2.42258900	-0.46943700
N	0.11573300	-0.52775600	-0.30009300
C	1.44399000	-1.12899100	-0.54688900
H	2.06655900	-0.37981100	-1.03745500
H	1.31570600	-1.96064500	-1.24651600
C	2.11955400	-1.61197000	0.74226200
H	1.51065300	-2.36686700	1.24952000
H	3.09252900	-2.05575300	0.50883200
H	2.28059900	-0.77834600	1.43081800
B	-0.07074100	0.88079300	-0.05093300
C	2.02801500	2.49817700	-0.09465200
N	1.10850500	1.75432600	-0.08377600

Compound: **3** (1-Ethyl-2-H-1,2-azaborine)

B3LYP/DGDZVP2 = -314.370294000 au

B3LYP/DGDZVP2 Zero Point Corrected Energy = -314.216402 au

NIMAG = 0

C	-1.79049100	1.17930800	0.13933800
C	-2.33267000	-0.08894000	0.23352600
C	-1.52238900	-1.24975900	0.05469900
C	-0.17980400	-1.12362600	-0.21406500
H	-2.44990900	2.03316600	0.28098100
H	-3.39190900	-0.23366100	0.44279700
H	-1.95389700	-2.24252300	0.12188200
H	0.44718000	-1.99965700	-0.35726100
N	0.43094400	0.09752700	-0.32632000
C	1.88487600	0.10279200	-0.57437400
H	2.12937100	1.04485500	-1.06888800
H	2.12660100	-0.70689700	-1.27162700
C	2.70766900	-0.04184800	0.71222400
H	2.48201400	-0.98261700	1.22425400
H	3.77763900	-0.02730200	0.47950600
H	2.49204600	0.78090300	1.39982800
B	-0.31227600	1.32577700	-0.16046400
H	0.28249100	2.35459800	-0.27299900

Compound: **5**

B3LYP/DGDZVP2 = -2017.89581592 au

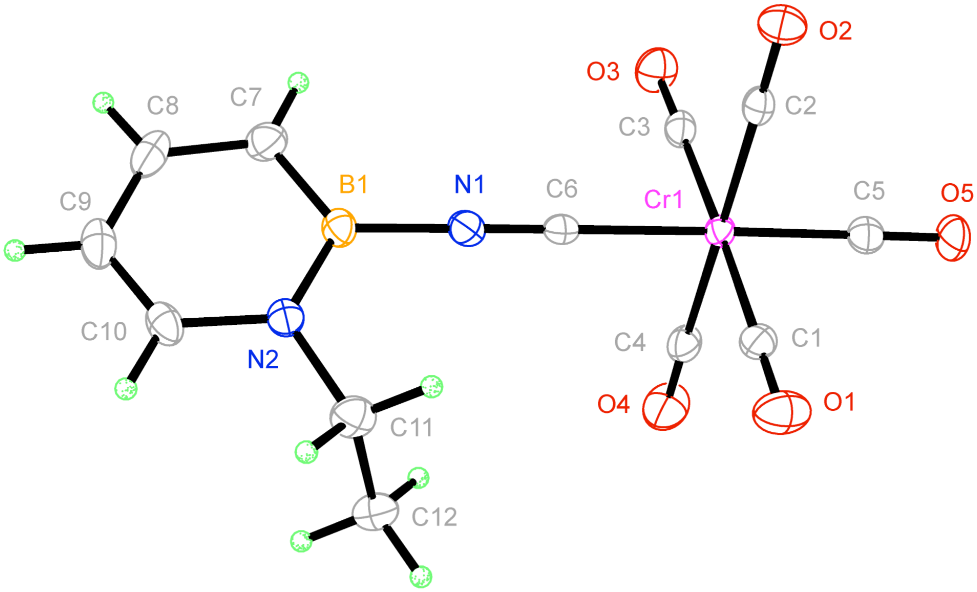
B3LYP/DGDZVP2 Zero Point Corrected Energy = -2017.698074 au

NIMAG = 0

Cr	-1.99984300	-0.07121700	0.00680600
O	-1.66055100	2.82781400	0.96375800
O	-2.12888100	-1.02286700	2.92878400
O	-2.24704100	-2.98440600	-0.94917400
O	-1.82592300	0.87686100	-2.91290800
O	-5.04648000	0.24695300	-0.04706600
N	1.14649200	-0.37873300	0.05912100
N	3.46891900	0.50000400	0.30529300
B	2.59261000	-0.61544700	0.04447900
C	-1.79615000	1.73273700	0.60260400
C	-2.08024500	-0.66488600	1.82694600
C	-2.15484200	-1.88624700	-0.58901700
C	-1.89295800	0.51745500	-1.81210100
C	-3.89145600	0.12587800	-0.02662400
C	-0.03098000	-0.27609300	0.03988100
C	3.21898400	-1.96003100	-0.22896700
H	2.63422000	-2.85398700	-0.42914000
C	4.59782400	-2.04799000	-0.22246500
H	5.09709700	-2.99612100	-0.41359700
C	5.40614700	-0.90305500	0.03797100
H	6.48752200	-0.98035500	0.04751200
C	4.82562400	0.31738300	0.28876600

H	5.43328200	1.19371600	0.49342700
C	2.97264600	1.87153800	0.55010100
H	3.65089400	2.35723300	1.25801800
H	1.99828600	1.79622000	1.03475200
C	2.86016900	2.69671900	-0.73711300
H	2.48621900	3.69860900	-0.50481500
H	2.16741000	2.22847700	-1.44153800
H	3.83279800	2.79849300	-1.22829700

Crystallographic Data for Complex 5 (liu12)



X-ray Crystal Structure Determination. Crystals of **5** suitable for X-ray diffraction were obtained by evaporation of a solution of **5** in pentane.

Diffraction intensity data were collected with a Bruker Smart Apex CCD diffractometer at 173(2) K using MoKα - radiation (0.71073 Å). The structure was solved using direct methods, completed by subsequent difference Fourier syntheses, and refined by full matrix least-squares procedures on F^2. All non-H atoms were refined with anisotropic thermal parameters. H atoms were found on the residual density map and refined with isotropic thermal parameters. All software and sources scattering factors are contained in the SHELXTL (6.10) program package (G.Sheldrick, Bruker XRD, Madison, WI). Crystallographic data and some details of data collection and crystal structure refinement for $C_{12}H_9BCrN_2O_5$ are given in the following tables.

Table S4. Crystal data and structure refinement for **5** (liu12a).

Identification code	liu12a	
Empirical formula	$C_{12} H_9 B Cr N_2 O_5$	
Formula weight	324.02	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2(1)	
Unit cell dimensions	a = 12.965(2) Å	α= 90°.
	b = 5.9808(9) Å	β= 90°.
	c = 19.254(3) Å	γ = 90°.
Volume	1493.0(4) $Å^3$	
Z	4	
Density (calculated)	1.441 Mg/m^3	
Absorption coefficient	0.785 mm^{-1}	
F(000)	656	
Crystal size	0.23 x 0.14 x 0.06 mm^3	
Theta range for data collection	2.12 to 27.00°.	
Index ranges	-16<=h<=12, -7<=k<=7, -24<=l<=24	
Reflections collected	9061	
Independent reflections	3243 [R(int) = 0.0425]	
Completeness to theta = 27.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9544 and 0.8400	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3243 / 1 / 191	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.0778	
R indices (all data)	R1 = 0.0538, wR2 = 0.0864	
Absolute structure parameter	0.20(3)	
Largest diff. peak and hole	0.301 and -0.206 $e.Å^{-3}$	

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for liu12a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	6657(1)	7430(1)	9776(1)	26(1)
O(1)	7486(2)	3932(4)	8775(1)	55(1)
O(2)	4623(2)	4941(4)	9940(1)	45(1)
O(3)	5789(2)	11017(4)	10726(1)	48(1)
O(4)	8662(2)	10056(4)	9693(2)	63(1)
O(5)	7561(2)	4899(4)	10990(1)	52(1)
N(1)	5758(2)	10066(4)	8506(1)	35(1)
N(2)	5727(2)	11203(4)	7264(1)	30(1)
B(1)	5390(3)	11603(6)	7950(2)	31(1)
C(1)	7175(3)	5237(5)	9153(2)	33(1)
C(2)	5388(2)	5846(5)	9869(2)	30(1)
C(3)	6121(3)	9656(5)	10371(2)	32(1)
C(4)	7910(2)	9078(5)	9713(2)	38(1)
C(5)	7216(3)	5855(6)	10530(2)	34(1)
C(6)	6086(2)	9084(5)	8972(2)	29(1)
C(7)	4700(3)	13536(6)	8088(2)	41(1)
C(8)	4463(3)	14870(6)	7534(2)	47(1)
C(9)	4837(3)	14417(6)	6867(2)	43(1)
C(10)	5449(3)	12648(5)	6749(2)	36(1)
C(11)	6445(3)	9368(6)	7074(2)	40(1)
C(12)	7559(3)	10065(6)	7169(2)	45(1)

Table S6. Bond lengths [Å] and angles [°] for liu12a.

Cr(1)-C(5)	1.875(4)
Cr(1)-C(3)	1.889(4)
Cr(1)-C(1)	1.900(4)
Cr(1)-C(4)	1.904(3)
Cr(1)-C(2)	1.908(3)
Cr(1)-C(6)	1.981(3)
O(1)-C(1)	1.141(4)
O(2)-C(2)	1.138(3)
O(3)-C(3)	1.147(4)
O(4)-C(4)	1.138(3)
O(5)-C(5)	1.146(4)
N(1)-C(6)	1.153(4)
N(1)-B(1)	1.489(4)
N(2)-C(10)	1.365(4)
N(2)-B(1)	1.412(4)
N(2)-C(11)	1.484(4)
B(1)-C(7)	1.486(5)
C(7)-C(8)	1.368(5)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.399(5)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.342(5)
C(9)-H(9A)	0.9500
C(10)-H(10A)	0.9500
C(11)-C(12)	1.514(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(5)-Cr(1)-C(3)	91.55(15)
C(5)-Cr(1)-C(1)	90.33(14)
C(3)-Cr(1)-C(1)	178.11(16)
C(5)-Cr(1)-C(4)	88.83(16)

C(3)-Cr(1)-C(4)	89.27(15)
C(1)-Cr(1)-C(4)	90.92(15)
C(5)-Cr(1)-C(2)	90.62(14)
C(3)-Cr(1)-C(2)	88.58(14)
C(1)-Cr(1)-C(2)	91.24(14)
C(4)-Cr(1)-C(2)	177.77(17)
C(5)-Cr(1)-C(6)	179.16(16)
C(3)-Cr(1)-C(6)	89.07(13)
C(1)-Cr(1)-C(6)	89.04(14)
C(4)-Cr(1)-C(6)	90.62(14)
C(2)-Cr(1)-C(6)	89.95(13)
C(6)-N(1)-B(1)	172.4(3)
C(10)-N(2)-B(1)	119.4(3)
C(10)-N(2)-C(11)	117.0(3)
B(1)-N(2)-C(11)	123.3(3)
N(2)-B(1)-N(1)	117.9(3)
N(2)-B(1)-C(7)	119.0(3)
N(1)-B(1)-C(7)	123.0(3)
O(1)-C(1)-Cr(1)	179.5(3)
O(2)-C(2)-Cr(1)	178.1(3)
O(3)-C(3)-Cr(1)	179.2(3)
O(4)-C(4)-Cr(1)	178.3(4)
O(5)-C(5)-Cr(1)	179.7(4)
N(1)-C(6)-Cr(1)	179.3(3)
C(8)-C(7)-B(1)	116.7(3)
C(8)-C(7)-H(7A)	121.6
B(1)-C(7)-H(7A)	121.6
C(7)-C(8)-C(9)	121.7(3)
C(7)-C(8)-H(8A)	119.2
C(9)-C(8)-H(8A)	119.2
C(10)-C(9)-C(8)	120.9(3)
C(10)-C(9)-H(9A)	119.5
C(8)-C(9)-H(9A)	119.5
C(9)-C(10)-N(2)	122.1(3)
C(9)-C(10)-H(10A)	118.9
N(2)-C(10)-H(10A)	118.9

N(2)-C(11)-C(12)	111.4(3)
N(2)-C(11)-H(11A)	109.3
C(12)-C(11)-H(11A)	109.3
N(2)-C(11)-H(11B)	109.3
C(12)-C(11)-H(11B)	109.3
H(11A)-C(11)-H(11B)	108.0
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters (Å^{2}x 10^3)for liu12a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	22(1)	25(1)	29(1)	4(1)	-2(1)	-1(1)
O(1)	49(2)	46(2)	71(2)	-16(1)	15(2)	-4(1)
O(2)	30(1)	48(1)	56(2)	2(1)	0(1)	-11(1)
O(3)	58(2)	38(1)	49(2)	-8(1)	0(1)	6(1)
O(4)	34(1)	51(1)	105(2)	14(2)	-6(2)	-13(1)
O(5)	42(2)	62(2)	52(2)	26(1)	-12(1)	5(1)
N(1)	31(2)	43(2)	31(1)	5(1)	2(1)	0(1)
N(2)	27(2)	32(2)	31(1)	2(1)	-3(1)	-4(1)
B(1)	30(2)	35(2)	29(2)	4(2)	-5(2)	-3(2)
C(1)	26(2)	28(2)	45(2)	4(2)	3(2)	-3(2)
C(2)	33(2)	29(2)	26(2)	2(1)	-5(2)	3(1)
C(3)	30(2)	30(2)	35(2)	7(2)	-6(2)	-2(2)
C(4)	30(2)	30(2)	53(2)	8(2)	-1(2)	-1(1)
C(5)	29(2)	35(2)	39(2)	3(2)	-3(2)	-6(2)
C(6)	22(2)	34(2)	31(2)	2(1)	4(2)	-1(1)
C(7)	36(2)	53(2)	35(2)	-4(2)	-2(2)	7(2)
C(8)	40(2)	40(2)	61(2)	6(2)	-11(2)	10(2)
C(9)	43(2)	42(2)	44(2)	14(2)	-14(2)	-10(2)
C(10)	36(2)	46(2)	27(2)	7(1)	-6(1)	-11(2)
C(11)	44(2)	34(2)	42(2)	-6(2)	5(2)	2(2)
C(12)	33(2)	51(2)	52(2)	2(2)	7(2)	5(2)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for liu12a.

	x	y	z	U(eq)
H(7A)	4436	13831	8539	49
H(8A)	4033	16137	7603	57
H(9A)	4655	15374	6493	51
H(10A)	5697	12393	6291	44
H(11A)	6328	8938	6584	48
H(11B)	6301	8046	7368	48
H(12A)	8013	8818	7043	68
H(12B)	7678	10477	7655	68
H(12C)	7708	11350	6870	68

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