Supporting Information for:

Voltage Clustering in Redox-Active Ligand Complexes: Mitigating Electronic Communication Through Choice of Metal Ion

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General Considerations: The complexes described below are air and moisture sensitive, necessitating that manipulations be carried out under an inert atmosphere of argon or nitrogen gas using standard glovebox techniques in an Inert Technologies Pure Lab HE Four Glove Box. Ethereal and halogenated solvents were sparged with nitrogen and then deoxygenated and before passage through Inert Technologies Pure Solv MD-5 system. HPLC grade hexane was purchased from Sigma Aldrich, sparged with nitrogen, and stored over 3 Å sieves. NMR solvents were purchased from Cambridge Isotopes, degassed by three cycles of freeze-pump-thaw and stored over 3 Å sieves prior to use. Gallium metal (99.99% basis), Chromium hexacarbonyl, and di(cyclopenta-2,4-dien-1-yl)cobalt (Cp_2Co) were purchased from Strem chemicals; anhydrous $AlCl_3$ was purchased from Sigma Aldrich and used as received. The ligand (dmp-BIAN^q) and (Ph-BIAN^q) were synthesized according to literature procedures.[i] We were unable to repeat the literature reported preparation of **2**.[ii] A more reproducible route was used to synthesize **2** and is reported below.

For crystal structure determination, crystals of the reported complexes were mounted on a loop and placed in a N_2 stream at 150 K. Data was collected on a SuperNova diffractometer (Oxford Diffraction). The X-ray source was monochromated 0.71073 Å Mo-Kα radiation and the data was integrated and corrected for absorption using the CrysAlisPro software package (Oxford Diffraction, Ltd.). The structures were solved with direct methods[iii] and refined on F-squared with least-squares methods[iv] using the Olex2 software package.[v] All pertinent crystallographic details can be found in Table S1.

Table S-1: Crystal Structure and refinement data for compounds **1**-**3**.

	1	**2**	**3**
Formula	$C_{84}H_{72}N_6Al$	$C_{84}H_{72}N_6Cr$	$C_{84}H_{72}N_6Ga$
FW (g mol^{-1})	1192.45	1217.47	1235.19
Cryst. Sys.	Trigonal	Trigonal	Trigonal
Space Group	R-3*c*	R-3*c*	R-3*c*
a (Å)	13.1342(3)	13.1548(2)	13.1696(2)
b (Å)	13.1342(3)	13.1548(2)	13.1696(2)
c (Å)	72.139(2)	71.8546(12)	72.1013(15)
α (°)	90	90	90
β (°)	90	90	90
γ (°)	120	120	120
Volume (Å^3)	10777.3(5)	10768.4(4)	10829.8(4)
Z	6	6	6
F(000)	5054.0	3852.0	3894.0
Reflns collected	99797	54503	35186
Indep reflns (R_{int})	2122 (0.0781)	2121 (0.0335)	3160 (0.0258)
GOF	1.113	1.117	1.168
R1 [*I*> 2σ(I)][a]	0.0497	0.0413	0.0388
wR2 (all data)[a]	0.1522	0.1350	0.1295
[a] $R1 = \Sigma\|F_o\| - \|Fc\|/\Sigma\|F_o\|$; $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$; $GOF = [\Sigma w(\|F_o\| - \|F_c\|)^2/(n - m)]^{1/2}$.			

Table S-1 (continued): Crystal Structure and refinement data for compounds **4**-**6**.

	4•2(CH_3CN)	**5•2(CH_3CN)**	**6•2(CH_3CN)**
Formula	$C_{88}H_{78}N_8F_{18}P_3Al$	$C_{88}H_{78}N_8F_{24}P_3Cr$	$C_{88}H_{78}N_8F_{18}P_3Ga$
FW (g mol^{-1})	1709.47	1848.49	1752.21
Cryst. Sys.	Monoclinic	Monoclinic	Monoclinic
Space Group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	16.5661(3)	16.5848(3)	16.6140(2)
b (Å)	21.2001(5)	21.1661(4)	21.1569(3)
c (Å)	23.1498(4)	23.1949(4)	23.2187(3)
α (°)	90	90	90
β (°)	91.3886(17)	91.3501(17)	91.3726(12)
γ (°)	90	90	90
Volume ($Å^3$)	8127.9(3)	8140.0(3)	8159.0(2)
Z	4	4	4
F(000)	3528.0	3788.0	3600.0
Reflns collected	238601	285951	247479
Indep reflns (R_{int})	14349 (0.0673)	21878 (0.0741)	19322 (0.0711)
GOF	1.026	1.037	1.047
R1 [$I > 2\sigma(I)$][a]	0.0492	0.0543	0.0530
wR2 (all data)[a]	0.1296	0.1543	0.1438
[a] $R1 = \Sigma\|F_o\| - \|Fc\|/\Sigma\|F_o\|$; $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$; $GOF = [\Sigma w(\|F_o\| - \|F_c\|)^2/(n - m)]^{1/2}$.			

Cyclic voltammetry was carried out using a Bio-Logic SP-200 potentiostat, a glassy carbon working electrode, a platinum wire counter electrode and a silver-wire pseudo reference electrode. Electrochemical experiments were performed at room temperature in a glovebox, under an atmosphere of nitrogen. Electrochemical samples were 1.0 mM analyte solutions in THF or CH_2Cl_2 containing 0.10 M [*n*-Bu_4N][PF_6] as the supporting electrolyte. All potentials were referenced to the $[Cp_2Fe]^{0/+}$ couple as an internal standard.[vi] Ferrocene was purified by sublimation under reduced pressure and [*n*-Bu_4N][PF_6] was recrystallized from hot ethanol three times and dried under vacuum.

NMR spectra were collected on a Varian AS500 spectrometer (500 MHz) in dry, degassed deuterated solvents at 298 K. ^1H NMR spectra were referenced to TMS using the residual proteo impurities of the solvent; ^{13}C NMR spectra were referenced to TMS using the natural-abundance ^{13}C impurities of the solvent. All chemical shifts are reported using the standard δ notation in parts per million; coupling constants are reported in hertz (Hz); integrations are reported in number of protons (H); and positive chemical shifts are to a higher frequency of the given reference. HRMS data was obtained on a Waters LCT Premier XE by direct injection using dichloromethane or acetonitrile in positive mode. UV-vis spectroscopy was performed with a Unico SQ-3802 Scanning UV/visible Spectrophotometer.

Electron Paramagnetic Resonance (EPR) spectra were acquired at X-band with a Varian E-12 spectrometer. The EWWin software and hardware package was used to drive the field sweep and signal average. The magnetic field was calibrated by means of a g-value standard, 2,2-diphenyl-1-picrylhydrazyl (DPPH, g = 2.0037) and Hewlett-Packard model 5245L electronic (frequency) counter. The temperature dependence of the EPR spectra of **1**, **2**, and **3** were measured from 4-150 K using an Oxford Instruments liquid helium cryostat and model ITC-503 temperature controller. EPR intensities were determined by double integration of the first derivative spectra after a suitable background subtraction was performed. To determine the absolute number of spins in **2** the signal intensity of a freshly prepared 2.0 mM toluene solution of **2** was compared to that of a National Bureau of Standards standard reference material (SRM),[vii] a Cr^{3+} doped ruby (SRM 2601). SRM 2601 was oriented with the magnetic field perpendicular to the *c*-axis of the ruby and taped to the outside of the 4 mm o.d. fused silica EPR tube. This orientation of the ruby produces two EPR resonances, one at 1954 G and the other at 5387 G (9.5 GHz). The number of spins in the sample was calculated using equation 1,

$$N = N_0 \left(\frac{A g_0 R_0}{A_0 g R} \right) \times \frac{1}{2.324} \qquad \text{Eq. 1}$$

Where N, A, and g are the number spins, integrated intensity, and g-value of the sample, and N_0, A_0, and g_0 are the number of spins, integrated intensity, and g-value (1.9818) of the SRM. R and R_0 refer to the receiver gain of the instrument; the ratio R_0/R =0.25. All other instrument parameters such as power modulation, amplitude, and time constant were held constant.

Computational Procedures. All DFT and *ab initio* calculations were performed with the ORCA electronic structure package.[viii] The DFT calculations were carried out at the BP86[ix] level of theory, using def2- variants of the all-electron Gaussian basis sets of split-valence (def2-SVP; C, H) and triple-valence (def2-TZVP; N, Al, Cr, Ga) as developed by the Ahlrichs group.[x] The calculations employed the resolution of identity (RI-J) algorithm for the computation of the Coulomb terms.[xi] For the fitting basis in the RI-J treatment, the 'def2' fit basis sets were used.[xii]

The SCF calculations were tightly converged (1×10^{-8} E_h in energy, 1×10^{-7} E_h in the density change, and 5×10^{-7} in the maximum element of the DIIS error vector). In all cases the geometries were considered converged after *i*) the energy change was less than 1×10^{-6} E_h, *ii*) the gradient norm and maximum gradient element were smaller than 3×10^{-4} E_h-Bohr^{-1} and 1×10^{-4} E_h-Bohr^{-1}, respectively, and *iii*) the root-mean square and maximum displacements of all atoms were smaller than 6×10^{-4} Bohr and 1×10^{-3} Bohr, respectively. Geometry optimization calculations on the full molecules were carried out on redundant internal coordinates without imposing symmetry constraints. The crystallographic coordinates were used in conjunction with the Conductor-like Screening Model (COSMO; acetonitrile) as implemented in ORCA for evaluating the electronic structure of $\mathbf{5}^{3+}$. Canonical, natural, and unrestricted corresponding orbital plots (electron density iso-surface threshold = 0.03) as well as spin density plots (electron density iso-surface threshold = 0.003) were generated with the program Chimera.[xiii]

We have used the general abbreviation BS(m,n) to denote a broken-symmetry (BS) DFT calculation with m unpaired or partially paired spin-up electrons and n partially paired spin-down electrons as the two interacting fragments. For predicting the exchange coupling constant *J*, we have employed the BS-DFT method of Noodleman,[xiv] which allows one to treat systems with unpaired electrons within the restriction of a single spin-unrestricted determinant. Having obtained spin-unrestricted solutions for the determinants of maximum spin, using $M_S = S_A + S_B$, and BS spin, using $M_S = |S_A - S_B|$, the following definition of *J* was employed, which is valid over the whole coupling strength regime, as discussed by Yamaguchi and co-workers:[xv] $J = -[(E_{HS} - E_{BS})/(\langle\hat{S}^2\rangle_{HS} - \langle\hat{S}^2\rangle_{BS})$. The final spin energy ladder was computed by direct diagonalization of the HDvV Hamiltonian.

Complete active space self-consistent field calculations were performed on a truncated version of the Al(dmp-BIAN)$_3$ complex, denoted here at **1'**. To obtain the geometry of **1'**, the dimethylphenyl groups of the geometry optimized doublet state of **1** were replaced with hydrogens. The geometry of the non-hydrogen atoms were then frozen while the positions of all hydrogens within the molecule were optimized. The canonical orbital output from this DFT calculation provided the starting point for the wavefunction-based methods. A CAS(3,3) space (3 electrons in three orbitals) was chosen, which included the linear combinations of the three partially occupied BIAN LUMOs.

MRCI calculations were initiated by employing the CASSCF method for the calculation of the zeroth-order wavefunction. In individually selecting MRCI calculations, a test configuration was kept if its perturbation energy $H_{I0}^2/\Delta E$ was larger than a certain threshold T_{sel} (H_{I0} is the CI matrix element between the test configuration and muticonfigurational 0th order wavefunction; ΔE is the energy difference calculated with the Möller-Plesset (MP) 0th order Hamiltonian). The values reported below were obtained with $T_{sel} = 10^{-6}$ E_h. The energetic effects of unselected CSFs were estimated by second-order Rayleigh-Schrödinger theory using Möller-Plesset partitioning. We have employed the difference dedicated CI (MR-DDCI3) approach of Caballol, Malrieu and co-workers in this study.[xvi]

Syntheses

(dmp-BIAN^{isq})$_3$Al, (**1**)**:**

A 50 mL round bottom flask, equipped with a glass coated stir bar, was filled with potassium metal (0.048 g, 1.23 mmol, 3.1 equiv) and 5 mL of THF. Next, an orange solution of dmp-BIAN^q (0.469 g, 1.21 mmol, 3 equiv) in THF (10 mL) was poured into the flask and the solution stirred at room temperature. After 16 hours the dark red solution was treated with a clear colorless solution of $AlCl_3$ (0.054 g, 0.40 mmol, 1 equiv) in toluene (5 mL). The contents were left to stir at room temperature for an additional 18 h. The resulting dark red solution was dried under vacuum and the red residue was

treated with 40 mL of DCM. The resulting red solution was filtered to remove KCl and the filtrate was concentrated down (~10 mL) and treated with 20 mL of diethyl ether. The dark red crystalline solid was isolated by filtration and dried under vacuum. 65% yield (0.331 g). Attempts to acquire accurate elemental analysis failed to give reproducible results. μ_{eff} = 2.71(4) μ_B (CD_2Cl_2, Evan's Method). UV–vis (CH_2Cl_2) λ_{max}/nm (ε/M^{-1} cm^{-1}): 292 (71000), 328 (51000), 478 (5600), 513 (6500), 1003 (4000). HRMS (ESI-TOF; DCM) *m/z*: 1191.56 $[M]^+$, 595.78 $[M]^{2+}$.

(dmp-BIAN^{isq})$_3$Cr (**2**):

A 20 mL scintillation vial, equipped with a stir bar, was filled with chromium hexacarbonyl (0.033 g, 0.15 mmol, 1 equiv) and dmp-BIAN^q (0.188 g, 0.45 mmol, 3 equiv). Next, 15 mL of toluene was added and the vial was sealed and heated to 100°C with constant stirring. After heating for 48 hours the dark purple solution slowly cooled to room temperature and the dark purple solid was isolated by filtration and dried under vacuum. The dark purple crystalline residue was recrystallized from THF layered with acetonitrile (or hexanes). The purple crystalline solid was isolated by filtration and dried under vacuum. 81% yield (0.149 g). Attempts to acquire accurate elemental analysis failed to give reproducible results. ^{1}H NMR (CD_2Cl_2) δ/ppm: 7.37 (br s, 4H, aryl–H), 6.59 (br s, 4H, aryl–H), 6.30 (br s, 2H, aryl-H), 5.06 (br s, 2H, aryl–H), 4.48 (br s, 2H, aryl–H), 2.14 (br s, 18H, CH_3), 1.42 (br s, 18H, CH_3). UV–vis (CH_2Cl_2) λ_{max}/nm (ε/M^{-1} cm^{-1}): shoulder at 350 (31800), 507 (18100), 574 (10100), 808 (3800). HRMS (ESI-TOF; DCM) *m/z*: 608.26 $[M]^{2+}$.

Regarding the EPR spectrum of compound **2**: at room temperature, compound **2** exhibits an isotropic EPR spectrum with hyperfine splitting of 4.3 G and g-value of 1.987 (Figure **S-7**). By comparing the EPR intensity of **2** to a National Bureau of Standards standard reference material, the absolute number of spins in a 2.0 mM toluene solution of **2** was determined. It was found that the EPR signal corresponded to 0.10 % of the expected number of spins based on the concentration and sample volume. Therefore, we conclude that the observed EPR signal of **2** is due to a doublet impurity and that **2** has a singlet ground state.

(dmp-BIAN^{isq})$_3$Ga (**3**):

A 20 mL scintillation vial, equipped with a stir bar, was filled with gallium metal (0.020 g, 0.29 mmol, 1 equiv) and 0.5 grams of mercury. In a separate scintillation vial, dmp-BIAN^q (0.334 g, 0.86 mmol, 3 equiv) was dissolved in 15 mL of THF before it was transferred by pipett into the vial containing the amalgam. The vial was sealed and heated to 65°C temperature with constant stirring. After heating for 16 hours the dark red solution was filtered to remove the excess mercury. The volatiles were removed from the filtrate under vacuum and the dark red crystalline residue was recrystallized from THF layered with acetonitrile (or hexanes). The dark red crystalline solid was isolated by filtration and dried under vacuum. 92% yield (0.326 g). Attempts to acquire accurate elemental analysis failed to give reproducible results. μ_{eff} = 2.76(5) μ_B (CD_2Cl_2, Evan's Method). UV–vis (CH_2Cl_2) λ_{max}/nm (ε/M^{-1} cm^{-1}): 300 (45000), 600 (4000). HRMS (ESI-TOF; DCM) *m/z*: 616.75 $[M]^{2+}$.

[(dmp-BIAN^q)$_3$Al][PF_6]$_3$ (**4**):

A 20 mL scintillation vial, equipped with a stir bar, was filled with a dark red solution of **1** (0.079 g, 0.066 mmol, 1 equiv) in DCM (15 mL). The dark red solution was rapidly stirred as solid $AgPF_6$ (0.054 g, 0.199 mmol, 3 equiv) was poured into the vial. The color changed rapidly to orange with concomitant formation of silver mirror. The reaction continued to stir for 15 minutes, at which point, the mixture was filtered. The volatiles were removed from the filtrate under vacuum and the orange residue was recrystallized from MeCN layered with Et_2O. The orange crystalline solid was isolated by filtration and dried under vacuum. 97% yield (0.105 g). ^{1}H NMR (CD_2Cl_2) δ/ppm: 8.59 (d, J = 8.5 Hz, 6H, aryl–H), 7.88 (t, J = 8 Hz, 6H, aryl–H), 7.28 (s, 6H, aryl–H), 7.20 (d, J = 7.5 Hz, 6H, aryl–H), 6.49 (s, 6H, aryl–H), 4.79 (s, 6H, aryl–H), 2.29 (s, 18H, CH_3), 1.50 (s, 18H, CH_3). ^{13}C{^{1}H} NMR (CD_2Cl_2) δ/ppm: 177.87 (aryl–C), 149.19 (aryl–C), 143.63 (aryl–C), 142.85 (aryl–C), 141.27 (aryl–C), 138.28 (aryl–C), 133.22 (aryl–C), 131.74 (aryl–C), 131.52 (aryl–C), 131.41 (aryl–C), 121.36 (aryl–C), 119.23 (aryl–C), 118.48 (aryl–C), 21.93 (CH_3), 20.72 (CH_3). ^{19}F {^{1}H} δ/ppm: –73.61 (d, $J_{F\text{-}P}$= 709 Hz). ^{31}P {^{1}H} (CD_2Cl_2) δ/ppm: –144.77 (septet, $J_{P\text{-}F}$= 711 Hz). HRMS (MeCN) *m/z*: 1481.49 ([M+2PF_6]$^+$), 668.26 ([M+PF_6]$^{+2}$), 397.19 ([M]$^{+3}$). UV–vis (CH_2Cl_2) λ_{max}/nm (ε/M^{-1} cm^{-1}): 285 (57000).

Reduction of **4**

In a 20 mL scintillation vial, equipped with a stir bar, was filled with an orange solution of **4** (0.041 g, 0.026 mmol, 1 equiv) in 5 mL of DCM. The orange solution was rapidly stirred as brown solution of Cp_2Co (0.014 g, 0.077 mmol, 3 equiv) in DCM (5 mL) was dripped into solution resulting in a slow color change to give a dark red solution. The solution stirred at room temperature for 20 minutes before the volatiles were removed under vacuum. The dark brown solid was washed with acetonitrile to give a dark red solid (**1**, 0.028 g, 92% Yield). The washings were collected and dried under vacuum to give [Cp_2Co][PF_6] (0.025 g, 99% yield). The identity of the **1** was determined by matching its unit cell. The identity of [Cp_2Co][PF_6] was determined by ESI/MS in both positive and negative modes in acetonitrile.

[(dmp-BIAN^q)$_3$Cr][PF_6]$_3$ (**5**):

A 20 mL scintillation vial, equipped with a stir bar, was filled with a dark purple solution of **2** (0.104 g, 0.09 mmol, 1 equiv) in 15 mL of DCM. The dark purple solution was rapidly stirred as solid $AgPF_6$ (0.067 g, 027 mmol, 3 equiv) was poured into the vial. The color changed rapidly to red with concomitant formation of silver mirror. The reaction continued to stir for 15 minutes, at which point, the mixture was filtered. The volatiles were removed from the filtrate under vacuum and the orange residue was recrystallized from MeCN layered with Et_2O. The dark red crystalline solid was isolated by filtration and dried under vacuum. 95% yield (0.135 g). μ_{eff} = 3.75(3) μ_B (CD_2Cl_2, Evan's Method). UV–vis (CH_2Cl_2) λ_{max}/nm (ε/M^{-1} cm^{-1}): 291 (16200), 325 (28400), shoulder 388 (5000), shoulder 517 (900). HRMS (MeCN) *m/z*: 1506.45 ([M+2PF_6]$^+$), 680.74 ([M+PF_6]$^{+2}$), 406.84 ([M+H]$^{+3}$)

Reduction of **5**:

A 20 mL scintillation vial, equipped with a stir bar, was filled with a dark red solution of **5** (0.0534 g, 0.032 mmol, 1 equiv) in 5 mL of DCM. The dark red solution was rapidly stirred as brown solution of Cp_2Co (0.018 g, 0.097 mmol, 3 equiv) in DCM (5 mL) was dripped in solution resulting in a slow color change to give a purple solution. The solution stirred at room temperature for 20 minutes before the

volatiles were removed under vacuum. The dark purple solid was washed with acetonitrile to give a purple solid (**2**, 0.037 g, 95% Yield). The washing were collected and dried under vacuum to give $[Cp_2Co][PF_6]$ (0.031 g, 95% yield). The identity of the **2** was determined by matching its unit cell. The identity of $[Cp_2Co][PF_6]$ was determined by ESI/MS in both positive and negative modes in acetonitrile.

$[(dmp\text{-}BIAN^{isq})_3Ga][PF_6]_3$ (**6**):

A 20 mL scintillation vial, equipped with a stir bar, was filled with a dark red solution of **3** (0.076 g, 0.063 mmol, 1 equiv) in DCM (10 mL). The dark red solution was rapidly stirred as solid $AgPF_6$ (0.047 g, 0.185 mmol, 3 equiv) was poured into the vial. The color changed rapidly to orange with concomitant formation of silver mirror. The reaction continued to stir for 15 minutes, at which point, the mixture was filtered. The volatiles were removed from the filtrate under vacuum and the orange residue was recrystallized from MeCN layered with Et_2O. The orange crystalline solid was isolated by filtration and dried under vacuum. 94% yield (0.097 g). ^{1}H NMR (CD_2Cl_2) δ/ppm: 8.56 (d, J = 8.5 Hz, 6H, aryl–H), 7.86 (t, J = 8 Hz, 6H, aryl–H), 7.28 (s, 6H, aryl–H), 7.23 (d, J = 7.5 Hz, 6H, aryl–H), 6.53 (s, 6H, aryl–H), 4.85 (s, 6H, aryl–H), 2.30 (s, 18H, CH_3), 1.53 (s, 18H, CH_3). ^{13}C{^{1}H} NMR (CD_2Cl_2) δ/ppm: 166.92 (aryl–C), 148.74 (aryl–C), 143.49 (aryl–C), 142.97 (aryl–C), 141.13 (aryl–C), 140.77 (aryl–C), 137.91 (aryl–C), 133.27 (aryl–C), 131.51 (aryl–C), 131.45 (aryl–C), 121.28 (aryl–C), 118.87 (aryl–C), 118.69 (aryl–C), 117.40 (aryl–C), 21.93 (CH_3), 20.69 (CH_3). ^{19}F {^{1}H} δ/ppm: –73.62 (d, $J_{F\text{-}P}$= 711 Hz). ^{31}P {^{1}H} (CD_2Cl_2) δ/ppm: –144.74 (septet, $J_{P\text{-}F}$= 711 Hz). HRMS (MeCN) *m/z*: 1523.44 ($[M+2PF_6]^+$), 689.24 ($[M+PF_6]^{+2}$), 411.50 ($[M+H]^{+3}$). UV–vis (CH_2Cl_2) λ_{max}/nm (ε/M^{-1} cm^{-1}): 276 (27000), 305 (25000).

Reduction of **6**

In a 20 mL scintillation vial equipped with a stir bar, was filled with an orange solution of **6** (0.044 g, 0.027 mmol, 1 equiv) in DCM (5 mL). The orange solution was rapidly stirred as brown solution of Cp_2Co (0.015 g, 0.08 mmol, 3 equiv) in DCM (5 mL) was dripped into solution resulting in a slow color change to give a dark red solution. The solution stirred at room temperature for 20 minutes before the volatiles were removed under vacuum. The dark purple solid was washed with acetonitrile to give a red-brown solid (**3**, 0.032 g, 96% Yield). The washing were collected and dried under vacuum to give $[Cp_2Co][PF_6]$ (0.026 g, 98% yield). The identity of the **3** was determined by matching its unit cell. The identity of $[Cp_2Co][PF_6]$ was determined by ESI/MS in both positive and negative modes in acetonitrile.

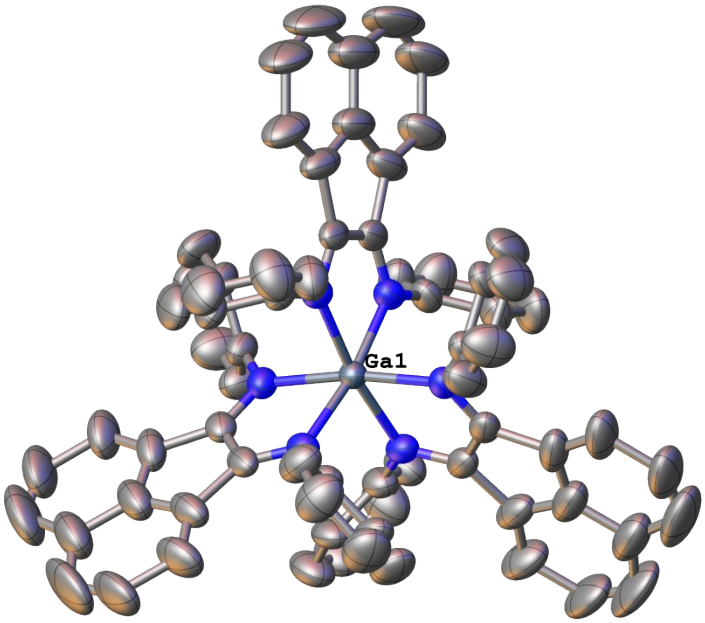


Figure S-1: Connectivity diagram of **3b**. Unit Cell parameters *a* = *b* = 13.4384(4), *c* = 58.5846(10); α = β = 90, γ = 120.

Numbering Scheme used for Neutral complexes (**1**-**3**):

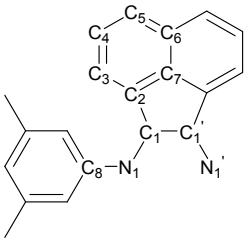


Table S-2: Experimental and calculated bond lengths (Å) for complexes **1**-**3.**

	1		**2**		**3**	
	Expt.	**Calc. (avg., S = ½)**	**Expt.**	**Calc. (avg., S = 0)**	**Expt.**	**Calc. (avg., S = ½)**
C1–N1	1.327(2)	1.339	1.326(2)	1.341	1.3210(17)	1.335
N1–C8	1.434(2)	1.429	1.432(2)	1.428	1.4264(16)	1.424
C1–C1´	1.434(3)	1.448	1.425(3)	1.440	1.438(2)	1.454
M1–N1	2.0111(13)	2.059	2.0300(13)	2.064	2.0645(11)	2.121

Numbering Scheme used for Cationic complexes (**4**-**6**):

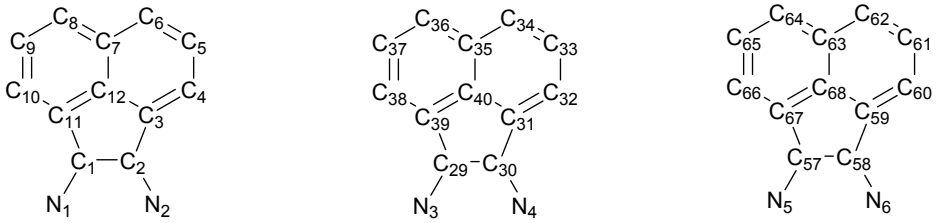


Table S-3: Bond lengths for complexes **4**-**6.**

	4	**5**	**6**
C–N Distances			
C1–N1	1.282(3)	1.292(3)	1.277(3)
C2–N2	1.288(3)	1.290(3)	1.279(3)
C29–N3	1.290(3)	1.290(3)	1.280(3)
C30–N4	1.290(3)	1.288(3)	1.281(3)
C57–N5	1.282(3)	1.288(3)	1.284(3)
C58–N6	1.286(3)	1.291(3)	1.285(3)
C–C Distances			
C1–C2	1.516(3)	1.506(3)	1.516(4)
C29–C30	1.510(3)	1.513(3)	1.524(4)
C57–C58	1.509(3)	1.503(3)	1.512(4)
M–N Distances			
M1–N1	2.0242(19)	2.0673(17)	2.091(2)
M1–N2	2.033(2)	2.0492(17)	2.090(2)
M1–N3	2.0085(19)	2.0720(17)	2.077(2)
M1–N4	2.0257(19)	2.0593(17)	2.093(2)
M1–N5	2.033(2)	2.0708(17)	2.061(2)
M1–N6	2.0297(19)	2.0669(18)	2.078(2)

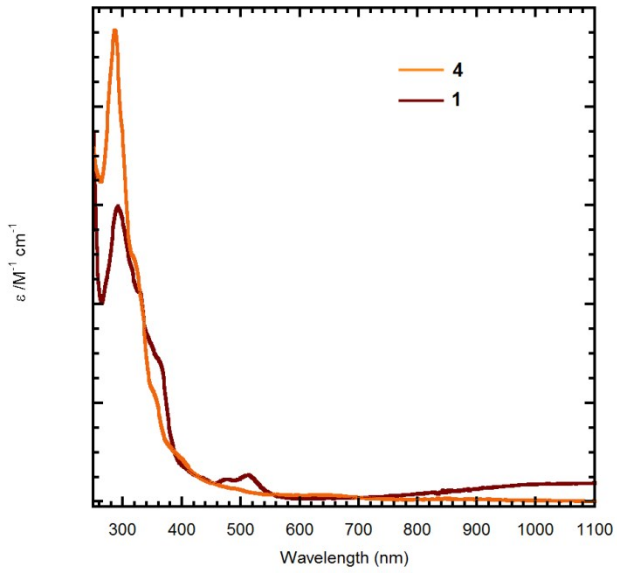


Figure S-2. UV–vis absorption spectra for **1** and **4** in DCM.

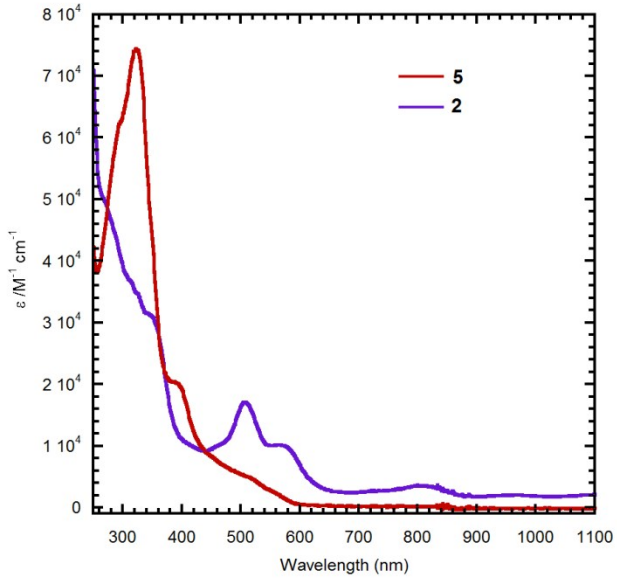


Figure S-3. UV–vis absorption spectra for **2** and **5** in DCM.

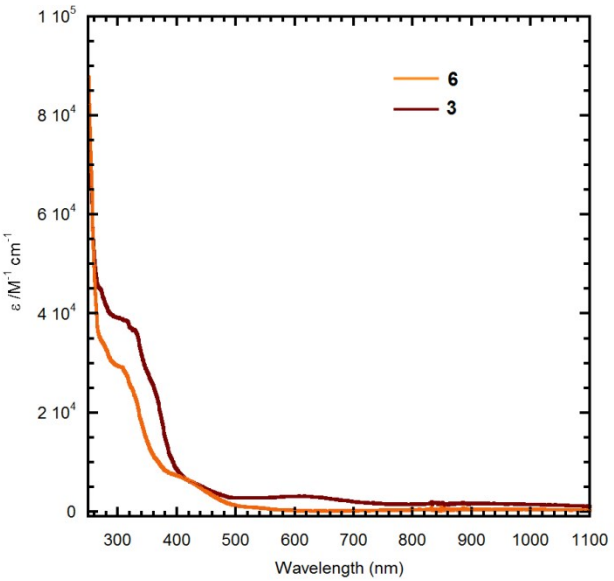


Figure S-4. UV–vis absorption spectra for **3** and **6** in DCM.

EPR Data

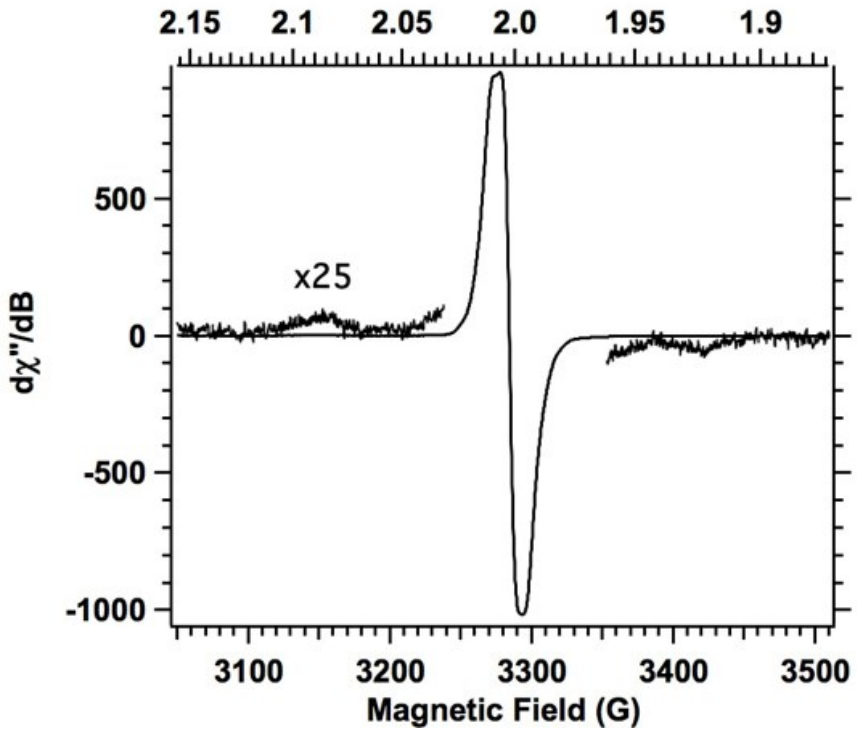


Figure S-5. EPR spectrum of **1** at 5.6 K in toluene.

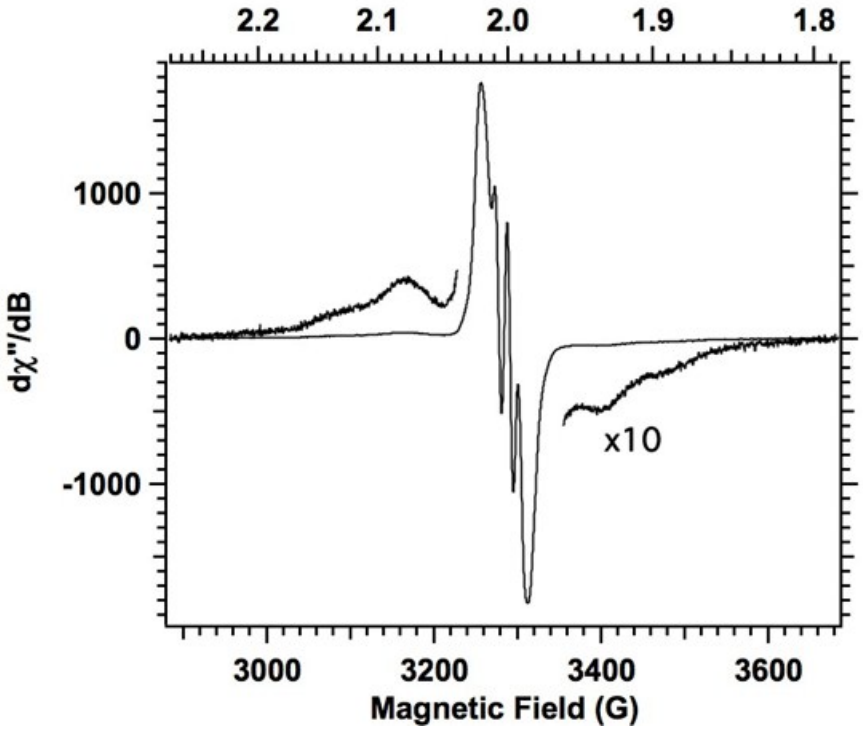


Figure S-6. EPR spectrum of **3** at 4.7 K in toluene.

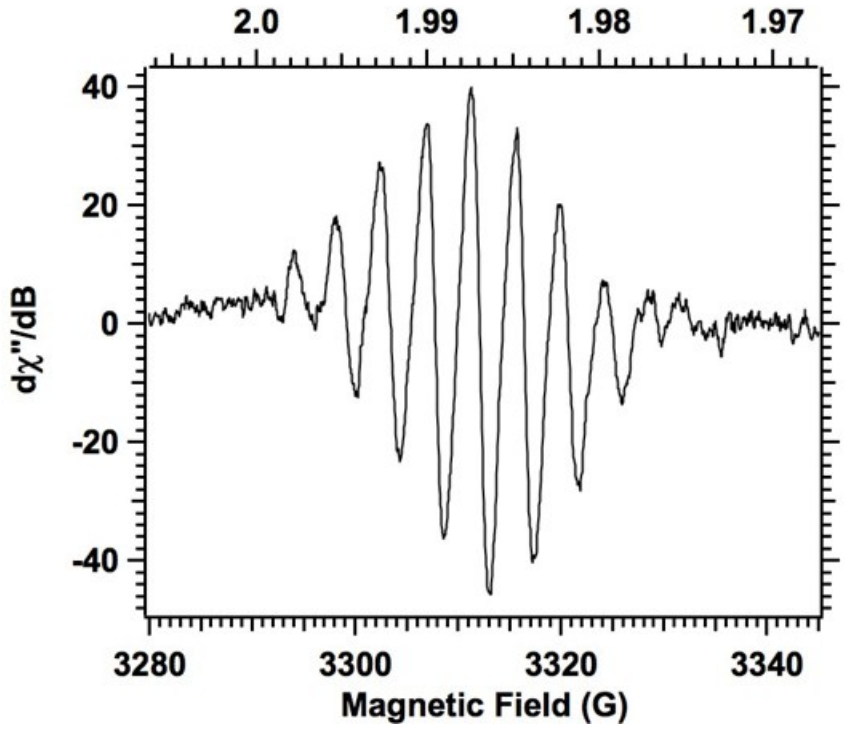


Figure S-7. EPR spectrum of **2** at 298 K in toluene.

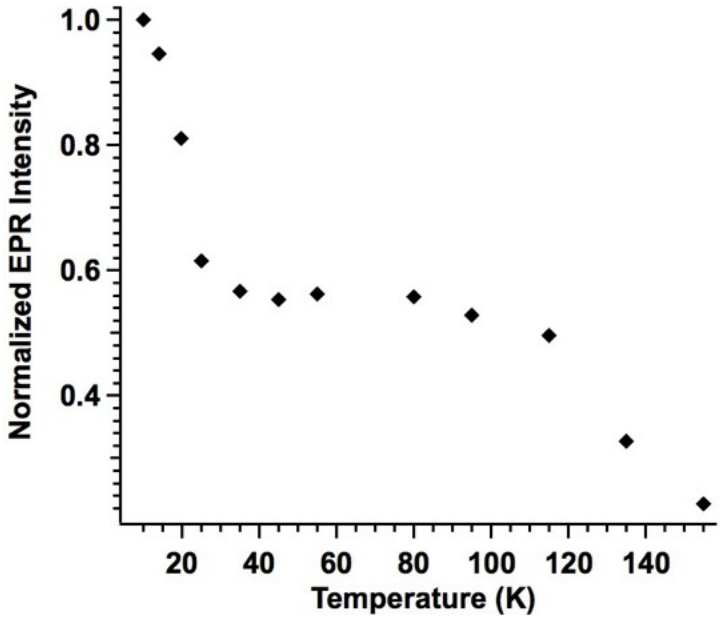


Figure S-8. Normalized EPR signal intensity versus temperature for **2** in Toluene.

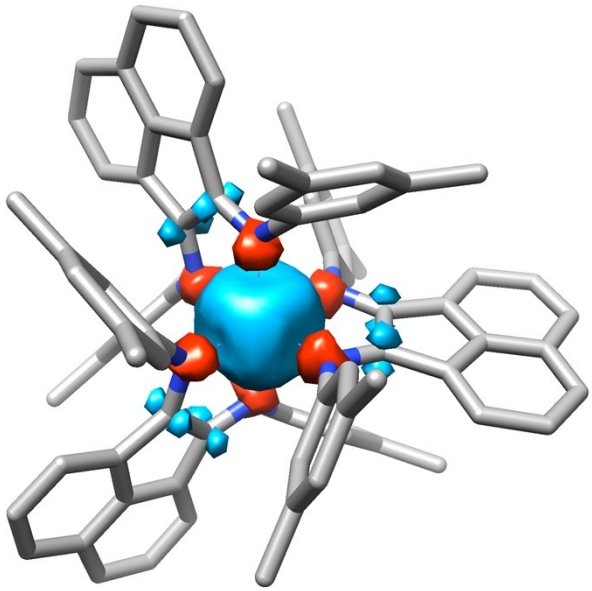
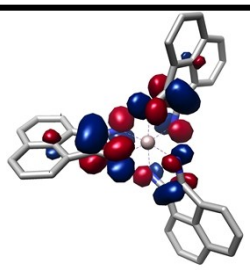
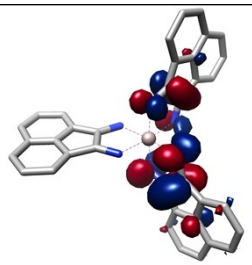
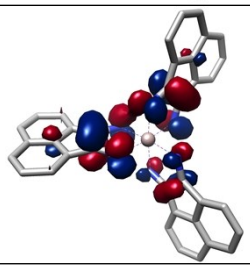


Figure S-9. Spin density plot for S = 3/2 $[Cr(dmp\text{-}BIAN)_3]^{3+}$. Hydrogen atoms removed for clarity. The α-spin density (teal) resides predominantly on the Cr center (+3.29, Mulliken), with residual β-spin density (orange) totally < -0.12/N.

CASSCF computational results: CAS(3,3) S = 1/2

1': E = -1945.0004340582 E_h

Configuration no.	Configuration weight	Representative electron configurations		
		<146> (L_3-1b)	<147> (L_3-1a)	<148> (L_3-2b)
1	0.42105	↑↓	↑	
2	0.36671		↑	↑↓
3	0.18585	↑	↑	↓

Orbital no.	Graphical representation	Orbital description	Natural orbital occupation
148		<L_3-2b>	0.945551
147		<L_3-1a>	1.001307
146		<L_3-1b>	1.053142

MR-DDCI3 computational results: CAS(3,3)/MR-DDCI3 S = 1/2

1': E = -1945.462387844756 E_h, Reference Weight = 0.9248

Configuration no.	Configuration weight	Representative electron configurations		
		<146> (L_3-1b)	<147> (L_3-1a)	<148> (L_3-2b)
1	0.4261	↑↓	↑	
2	0.3312		↑	↑↓
3	0.1558	↑	↑	↓

Coordinates from geometry optimization calculations

Optimized geometry of dmp-BIAN (S = 0):

N	-0.330386	0.757362	-2.106596
N	-0.153442	-1.894324	-1.049383
C	-0.566009	-1.807084	-4.629720
C	-0.314480	-1.690108	-2.303889
C	-0.380486	-0.266642	-2.874686
C	-0.708950	-2.340036	-5.941342
C	-0.539635	-0.408268	-4.348760
C	-0.677897	0.492510	-5.405243
H	-0.666498	1.579801	-5.235883
C	-1.493107	2.874100	-2.431781
H	-2.399995	2.417494	-2.002015
C	-1.492608	4.227288	-2.830085
C	-0.335566	2.080993	-2.578360
C	1.070669	-3.734257	-0.021490
H	2.007146	-3.176478	-0.187649
C	-0.700184	-3.764836	-6.051436
H	-0.807860	-4.235291	-7.043811
C	-0.425469	-4.005859	-3.604764
H	-0.322111	-4.669245	-2.733760
C	0.847085	2.662394	-3.097302
H	1.755190	2.042518	-3.181712
C	1.088009	-4.986949	0.627195
C	-0.556331	-4.560499	-4.912654
H	-0.548138	-5.658364	-5.023468
C	-0.143530	-3.175581	-0.471617
C	-1.358594	-3.864179	-0.236744
H	-2.304369	-3.405385	-0.568226
C	-0.308470	4.780873	-3.355817
H	-0.298556	5.841597	-3.661964
C	0.871279	4.013548	-3.486556
C	-0.131347	-5.660505	0.838294
H	-0.124552	-6.638200	1.350932
C	-0.435794	-2.617796	-3.462785
C	-0.832819	-0.021003	-6.727362
H	-0.942202	0.693163	-7.560769
C	-2.659879	-5.850146	0.667779
H	-2.778539	-6.112381	1.743270
H	-3.542094	-5.246175	0.365781
H	-2.695245	-6.806834	0.098201
C	-1.363004	-5.107547	0.420326
C	-0.845532	-1.390766	-7.000665
H	-0.963450	-1.746230	-8.038654
C	2.133726	4.637510	-4.045669
H	2.993589	3.934611	-3.999848
H	2.001214	4.939487	-5.110168
H	2.415059	5.556456	-3.483763
C	-2.741916	5.067253	-2.661815
H	-3.640869	4.549068	-3.064648
H	-2.944916	5.275575	-1.586011
H	-2.651155	6.045538	-3.179895
C	2.399010	-5.573549	1.108846
H	3.175004	-5.552418	0.310211
H	2.805736	-4.994780	1.969964
H	2.277700	-6.626923	1.440585

Optimized geometry of Al(dmp-BIAN)$_3$ (S = 1/2)

E = -3813.172818416708 E_h

Al	-0.070940	0.078294	0.054726
N	-0.248618	0.747195	-1.884722
N	-0.204239	-1.748323	-0.885649
N	-2.099717	0.251425	0.317211
C	-0.591672	-1.757221	-4.511051
C	-4.310099	4.313314	2.179078
C	-3.366164	3.372979	1.708668
C	-0.331603	-1.613145	-2.212639
C	-0.379737	-0.268982	-2.747295
C	-0.744002	-2.280671	-5.814037
C	-3.711410	2.094837	1.156609
C	-0.582055	-0.356218	-4.203612
C	-0.760149	0.546158	-5.255627
H	-0.768760	1.633550	-5.086097
C	-1.413956	2.884816	-2.235758
H	-2.293506	2.467225	-1.719939
C	-1.453792	4.201549	-2.746668
C	-0.268283	2.082148	-2.393590
C	-5.066905	1.770075	1.054362
H	-5.398521	0.808860	0.635489
C	1.022784	-3.614529	0.141832
H	1.947168	-3.019762	0.071070
C	-0.704139	-3.708401	-5.938184
H	-0.815855	-4.175584	-6.931623
C	-3.563198	-0.847122	-1.326304
H	-3.070257	-0.265489	-2.120819
C	-2.432301	1.444364	0.826508
C	-0.385051	-3.950377	-3.492707
H	-0.252491	-4.622566	-2.632509
C	-3.781627	-1.396713	1.037651
H	-3.446199	-1.254079	2.077090
C	0.855892	2.601062	-3.073682
H	1.748045	1.965830	-3.191658
C	1.061605	-4.919256	0.682292
C	-0.521247	-4.501302	-4.804838
H	-0.485637	-5.598732	-4.917982
C	-0.183060	-3.063624	-0.329931
C	-5.240912	-2.438283	-0.597520
H	-6.073786	-3.124214	-0.834545
C	-1.370061	-3.826646	-0.261694
H	-2.309165	-3.386129	-0.631587
C	-0.322270	4.693194	-3.426327
H	-0.344760	5.718037	-3.837125
C	0.838584	3.905382	-3.601936

C	-0.134412	-5.661653	0.734990
H	-0.113122	-6.684831	1.149783
C	-0.427165	-2.562396	-3.335316
C	-4.838188	-2.283489	0.746482
C	-6.039488	2.713313	1.510631
H	-7.106735	2.446295	1.423184
C	-4.613480	-1.733127	-1.645885
C	-0.931954	0.037871	-6.580875
H	-1.073399	0.759551	-7.403391
C	-3.145529	-0.672913	0.008410
C	-5.508526	-3.066500	1.855795
H	-5.671251	-2.437215	2.758073
H	-6.491910	-3.472108	1.534270
H	-4.879127	-3.929191	2.174952
C	-2.623884	-5.962280	0.313721
H	-2.817749	-6.351995	1.338544
H	-3.509493	-5.369411	0.001020
H	-2.554905	-6.848277	-0.358708
C	-5.691210	3.946254	2.063420
H	-6.473681	4.641935	2.410762
C	-1.357861	-5.131978	0.264262
C	-0.920600	-1.327140	-6.869803
H	-1.051165	-1.677113	-7.908014
C	2.030330	4.452525	-4.360577
H	2.895816	3.757286	-4.310949
H	1.787363	4.612158	-5.436726
H	2.354344	5.437487	-3.955463
C	-2.688102	5.057395	-2.554090
H	-3.616170	4.495865	-2.803034
H	-2.788746	5.385268	-1.494278
H	-2.657425	5.969743	-3.187178
C	-5.044883	-1.922044	-3.085108
H	-5.129114	-0.948924	-3.617381
H	-4.303843	-2.533418	-3.650459
H	-6.026526	-2.438797	-3.152043
C	2.365538	-5.492128	1.196899
H	3.186648	-5.364740	0.455952
H	2.692719	-4.975553	2.127759
H	2.273687	-6.575626	1.426388
N	-0.107379	1.975245	0.864481
C	-1.947205	3.580302	1.728611
C	-1.467563	4.776965	2.268446
H	-0.390030	4.994555	2.319865
C	1.812106	2.627493	2.254110
H	1.620273	1.750364	2.892217
C	-1.357796	2.365993	1.137972
C	1.197219	3.997514	0.335396
H	0.536302	4.173638	-0.528454
C	3.068499	4.637097	1.740799
H	3.885937	5.340552	1.980479
C	2.243712	4.895282	0.623399
C	-2.404198	5.737450	2.761460
H	-2.013511	6.678210	3.185044
C	2.870699	3.508894	2.563430
C	0.972577	2.865205	1.147664
C	2.494058	6.097641	-0.262978
H	1.557751	6.449345	-0.747312
H	2.930043	6.946095	0.309301
H	3.212664	5.851472	-1.079941
C	-3.783667	5.531937	2.720104
H	-4.472336	6.303829	3.103741
C	3.770703	3.236805	3.750484
H	3.182249	2.965365	4.655236
H	4.459079	2.384080	3.547873
H	4.396483	4.120858	4.000839
N	0.251985	-0.734609	1.921836
N	1.982018	-0.011144	-0.007261
C	3.702798	-1.386863	2.896797
C	2.487898	-0.539485	1.114486
C	1.556553	-0.914942	2.159429
C	4.782047	-1.806270	3.706468
C	2.328945	-1.423397	3.306754
C	2.042235	-1.879594	4.596179
H	1.010196	-1.926106	4.974100
C	-1.345460	-0.117193	3.683290
H	-1.115656	0.942719	3.490065
C	-2.272167	-0.468298	4.690253
C	-0.691445	-1.107495	2.926590
C	3.008722	-0.417940	-2.203382
H	2.413387	-1.341060	-2.285184
C	6.089923	-1.718391	3.125629
H	6.970770	-2.035607	3.708985
C	5.138195	-0.801576	1.029275
H	5.317949	-0.420310	0.013742
C	-0.967492	-2.470125	3.177312
H	-0.456477	-3.237626	2.574573
C	3.902460	-0.057435	-3.235731
C	6.243165	-1.235055	1.825876
H	7.255435	-1.177160	1.390397
C	2.879206	0.377416	-1.048912
C	3.652720	1.552019	-0.921984
H	3.543894	2.167238	-0.014880
C	-2.524610	-1.833998	4.925582
H	-3.243333	-2.119164	5.715087
C	-1.879087	-2.847149	4.180863
C	4.665712	1.117644	-3.083767
H	5.373995	1.404569	-3.881873
C	3.849806	-0.870089	1.566850
C	3.119989	-2.296375	5.437313
H	2.881148	-2.653864	6.453082
C	5.369096	3.203691	-1.807363
H	4.876420	4.051753	-2.338215
H	5.487381	3.507357	-0.745389
H	6.381930	3.087797	-2.252255
C	4.554339	1.932956	-1.934309
C	4.451444	-2.273514	5.020524

H	5.252205	-2.612188	5.699559
C	-2.149961	-4.308028	4.474962
H	-1.703662	-4.967421	3.700307
H	-1.720914	-4.608529	5.459024
H	-3.241767	-4.520450	4.523168
C	-2.981023	0.609206	5.483227
H	-2.268994	1.385461	5.841989
H	-3.740132	1.135032	4.859879
H	-3.504763	0.188782	6.368711
C	4.036828	-0.929743	-4.466559
H	4.371665	-1.958143	-4.199835
H	3.062577	-1.037104	-4.995232
H	4.771808	-0.510182	-5.187025

Optimized geometry of Al(dmp-BIAN)$_3$ (S = 3/2) E = -3813.172086911834 E_h

Al	-0.074749	0.073438	0.040089
N	-0.251109	0.747381	-1.899337
N	-0.206409	-1.756085	-0.897251
N	-2.108177	0.246336	0.301835
C	-0.588851	-1.760487	-4.522867
C	-4.291976	4.289990	2.235023
C	-3.354230	3.352574	1.746589
C	-0.339455	-1.617174	-2.222342
C	-0.371754	-0.270693	-2.759774
C	-0.740071	-2.284235	-5.826273
C	-3.706310	2.077396	1.192735
C	-0.561589	-0.359376	-4.218190
C	-0.720997	0.543313	-5.273034
H	-0.715964	1.630954	-5.105480
C	-1.403495	2.892039	-2.236893
H	-2.281512	2.477968	-1.715728
C	-1.438283	4.210883	-2.742630
C	-0.263765	2.082525	-2.405428
C	-5.062821	1.752093	1.108441
H	-5.399749	0.793161	0.688784
C	1.014900	-3.617884	0.141053
H	1.938648	-3.021744	0.073933
C	-0.719738	-3.712378	-5.947781
H	-0.831652	-4.179562	-6.941189
C	-3.561605	-0.868885	-1.336807
H	-3.065054	-0.293844	-2.133767
C	-2.431481	1.431621	0.833776
C	-0.421873	-3.954814	-3.499911
H	-0.305042	-4.627194	-2.637725
C	-3.796120	-1.393469	1.031199
H	-3.467639	-1.240468	2.071441
C	0.858610	2.597004	-3.092218
H	1.746756	1.957429	-3.217192
C	1.052102	-4.920999	0.685397
C	-0.556879	-4.505986	-4.811861
H	-0.535799	-5.603989	-4.923065
C	-0.189293	-3.069517	-0.338845
C	-5.242720	-2.454298	-0.602787
H	-6.073463	-3.143386	-0.838292
C	-1.375560	-3.834298	-0.275043
H	-2.313615	-3.395527	-0.649735
C	-0.308652	4.697868	-3.428693
H	-0.327263	5.724628	-3.834868
C	0.846226	3.903512	-3.614932
C	-0.143066	-5.665000	0.733283
H	-0.122734	-6.686799	1.151468
C	-0.444750	-2.566018	-3.345052
C	-4.849159	-2.284803	0.742385
C	-6.029539	2.691631	1.584320
H	-7.097707	2.423934	1.511406
C	-4.608980	-1.759372	-1.653936
C	-0.891673	0.035103	-6.598252
H	-1.018660	0.757114	-7.422817
C	-3.152619	-0.679613	-0.001010
C	-5.524549	-3.059703	1.854363
H	-5.662104	-2.433453	2.762718
H	-6.520361	-3.441061	1.541376
H	-4.911734	-3.939209	2.159794
C	-2.630017	-5.969726	0.299590
H	-2.826713	-6.360413	1.323477
H	-3.515170	-5.377449	-0.015556
H	-2.558020	-6.855254	-0.373184
C	-5.674080	3.921942	2.138368
H	-6.451966	4.615034	2.500893
C	-1.364687	-5.138060	0.254660
C	-0.897474	-1.330497	-6.884577
H	-1.026363	-1.680681	-7.922931
C	2.036863	4.446725	-4.378150
H	2.896451	3.743381	-4.341355
H	1.786973	4.618486	-5.450798
H	2.372929	5.424943	-3.966562
C	-2.665162	5.074179	-2.536392
H	-3.598499	4.521999	-2.786791
H	-2.758706	5.392634	-1.473089
H	-2.630432	5.992094	-3.161086
C	-5.030376	-1.963640	-3.094043
H	-5.108460	-0.996443	-3.637889
H	-4.286869	-2.583250	-3.647102
H	-6.012766	-2.478865	-3.162228
C	2.353755	-5.490045	1.209887
H	3.178423	-5.366773	0.472168
H	2.676025	-4.967601	2.139186
H	2.261383	-6.572152	1.445513
N	-0.103992	1.966610	0.849989
C	-1.935512	3.562148	1.744330
C	-1.449225	4.757478	2.281413
H	-0.371428	4.976944	2.316082
C	1.806254	2.626778	2.249516
H	1.608314	1.754843	2.892927
C	-1.353249	2.352767	1.137438

C	1.207765	3.983114	0.316157
H	0.553184	4.154227	-0.553352
C	3.067658	4.632217	1.732306
H	3.883046	5.337390	1.974080
C	2.252054	4.882765	0.606483
C	-2.379384	5.714431	2.793333
H	-1.983339	6.654042	3.214513
C	2.862827	3.509856	2.561185
C	0.975874	2.856809	1.134537
C	2.509491	6.079521	-0.285421
H	1.580081	6.417896	-0.791978
H	2.925676	6.937139	0.288018
H	3.247147	5.832838	-1.085015
C	-3.758992	5.507138	2.773226
H	-4.442682	6.276398	3.170805
C	3.753703	3.245735	3.756848
H	3.159489	2.964549	4.654742
H	4.454614	2.402107	3.558966
H	4.366047	4.136711	4.015794
N	0.241648	-0.736953	1.906182
N	1.983361	-0.018082	-0.023167
C	3.692141	-1.352553	2.907622
C	2.483309	-0.527862	1.109288
C	1.547008	-0.907451	2.149448
C	4.768314	-1.759749	3.727645
C	2.315021	-1.403383	3.304864
C	2.021670	-1.860364	4.592628
H	0.986876	-1.917693	4.961306
C	-1.343789	-0.115552	3.677741
H	-1.106830	0.943472	3.488488
C	-2.267710	-0.464266	4.688144
C	-0.701211	-1.107214	2.912987
C	3.005202	-0.413482	-2.222176
H	2.408685	-1.335435	-2.307657
C	6.080141	-1.659906	3.158224
H	6.958945	-1.966680	3.750232
C	5.137796	-0.758328	1.051342
H	5.322596	-0.378314	0.036287
C	-0.985378	-2.468777	3.159749
H	-0.481852	-3.237435	2.552369
C	3.897315	-0.048469	-3.254661
C	6.240158	-1.178270	1.858665
H	7.255556	-1.111214	1.431913
C	2.880552	0.374528	-1.061704
C	3.658293	1.546472	-0.930284
H	3.552937	2.157047	-0.019606
C	-2.528328	-1.829144	4.919297
H	-3.244515	-2.112571	5.711749
C	-1.893703	-2.843630	4.167176
C	4.663552	1.123692	-3.097896
H	5.370289	1.413852	-3.896231
C	3.845571	-0.838181	1.577798
C	3.096190	-2.264071	5.444295
H	2.851775	-2.622175	6.458542
C	5.376813	3.199243	-1.810537
H	4.916129	4.037469	-2.383843
H	5.451141	3.527520	-0.752009
H	6.407528	3.064292	-2.207272
C	4.557539	1.931845	-1.942517
C	4.431035	-2.227773	5.039852
H	5.229183	-2.556681	5.726708
C	-2.171429	-4.303821	4.458236
H	-1.736764	-4.963004	3.676782
H	-1.734760	-4.611010	5.436881
H	-3.264086	-4.509264	4.516116
C	-2.964577	0.614708	5.489687
H	-2.245653	1.386107	5.845110
H	-3.725682	1.146335	4.873715
H	-3.483754	0.194489	6.377956
C	4.026922	-0.914375	-4.490543
H	4.361568	-1.944494	-4.230167
H	3.051002	-1.017972	-5.016875
H	4.760210	-0.491833	-5.210993

Geometry of $Al(BIAN)_3$ (S = 1/2, see above)

E = -1956.551366920851 E_h

Al	-0.072630	0.082717	0.053190
N	-0.249337	0.752221	-1.886144
N	-0.206058	-1.743591	-0.887757
N	-2.101468	0.256350	0.314896
C	-0.592021	-1.751366	-4.513316
C	-4.311469	4.318324	2.177010
C	-3.367601	3.377863	1.706719
C	-0.332843	-1.608014	-2.214761
C	-0.380391	-0.263680	-2.749053
C	-0.743969	-2.274408	-5.816515
C	-3.712983	2.099974	1.154160
C	-0.582135	-0.350455	-4.205479
C	-0.759556	0.552270	-5.257318
H	-0.770331	1.643212	-5.089193
C	-5.068532	1.775621	1.051270
H	-5.403138	0.812557	0.630815
C	-0.704457	-3.702114	-5.941039
H	-0.814412	-4.170487	-6.933879
C	-2.433921	1.449230	0.824396
C	-0.386426	-3.944869	-3.495508
H	-0.251670	-4.622321	-2.635143
C	-0.522248	-4.495383	-4.807848
H	-0.485734	-5.592681	-4.922772
C	-0.428222	-2.556922	-3.337746
C	-6.041034	2.718994	1.507410
H	-7.108691	2.453412	1.420203
C	-0.930961	0.044400	-6.582770
H	-1.072844	0.765330	-7.405986
C	-5.692634	3.951682	2.060687
H	-6.476276	4.646341	2.407039

C	-0.919875	-1.320532	-6.872078
H	-1.051189	-1.668589	-7.910708
N	-0.108869	1.979450	0.863457
C	-1.948601	3.584781	1.727292
C	-1.468836	4.781155	2.267663
H	-0.388722	4.999117	2.321373
C	-1.359291	2.370472	1.136550
C	-2.405408	5.741768	2.760563
H	-2.016063	6.683008	3.184531
C	-3.784918	5.536655	2.718586
H	-4.471959	6.308931	3.103818
N	0.249316	-0.730797	1.920202
N	1.980330	-0.007268	-0.007993
C	3.699549	-1.384284	2.896378
C	2.485608	-0.536064	1.113813
C	1.553730	-0.911558	2.158270
C	4.778353	-1.804222	3.706367
C	2.325523	-1.420555	3.305760
C	2.038153	-1.877027	4.594946
H	1.003832	-1.923820	4.975450
C	6.086483	-1.716544	3.126082
H	6.967954	-2.034227	3.707921
C	5.135859	-0.798880	1.029594
H	5.318398	-0.418906	0.010668
C	6.240395	-1.232892	1.826530
H	7.253412	-1.175644	1.392566
C	3.847242	-0.867181	1.566632
C	3.115455	-2.294344	5.436396
H	2.877388	-2.652662	6.452174
C	4.447080	-2.271738	5.020152
H	5.246068	-2.610426	5.701079
H	2.642657	0.217482	-0.760783
H	-0.403258	-0.962399	2.678846
H	-0.127213	-2.699154	-0.518082
H	-0.325657	1.704071	-2.265619
H	-2.868879	-0.375663	0.056142
H	0.651774	2.616891	1.128883

Optimized geometry of Cr(dmp-BIAN)$_3$ (S = 0)

E = -4615.343726417783 E_h

Cr	-1.314504	-0.228545	6.807498
N	-1.334784	1.212681	5.334073
N	0.704155	-0.094471	6.394275
N	-1.515457	-1.816788	5.501113
N	-1.113615	-1.816524	8.114991
N	-1.294111	1.213159	8.281737
N	-3.333040	-0.094105	7.221206
C	-0.117285	1.504869	4.853758
C	0.992211	0.790073	5.429020
C	2.229490	1.219731	4.753576
C	3.584466	0.884322	4.808210
H	3.958588	0.113064	5.498241
C	4.499769	1.563168	3.945928
H	5.567343	1.288450	3.996042
C	4.095658	2.556259	3.053165
H	4.836772	3.061765	2.410792
C	2.712076	2.920824	2.965920
C	2.134586	3.914082	2.108760
H	2.780661	4.492150	1.426176
C	0.759761	4.150013	2.143996
H	0.330324	4.923052	1.483646
C	-0.124825	3.425618	3.001754
H	-1.202361	3.649608	2.984126
C	0.403607	2.446174	3.846487
C	1.822041	2.226678	3.816318
C	-2.462195	1.908028	4.801854
C	-2.953324	1.596733	3.519292
H	-2.467744	0.795760	2.939861
C	-4.052768	2.299412	2.980213
C	-4.654334	3.311135	3.755088
H	-5.517918	3.862190	3.341459
C	-4.180566	3.640307	5.045031
C	-3.081101	2.926731	5.559286
H	-2.685700	3.164947	6.558741
C	-4.556610	1.972604	1.589961
H	-5.521424	2.479770	1.373569
H	-4.701804	0.877304	1.458357
H	-3.827336	2.293705	0.810740
C	-4.823889	4.756892	5.840534
H	-4.519439	4.727880	6.908238
H	-5.934920	4.700115	5.799850
H	-4.534753	5.755556	5.436919
C	1.777035	-0.826862	6.986338
C	1.982683	-2.176260	6.637192
H	1.301109	-2.651158	5.913205
C	3.051002	-2.911498	7.193173
C	3.911739	-2.263235	8.102753
H	4.753858	-2.828693	8.540171
C	3.726987	-0.910954	8.466149
C	2.647087	-0.201510	7.903976
H	2.474092	0.852525	8.171033
C	3.250921	-4.365914	6.823420
H	2.451492	-5.006608	7.261243
H	4.227316	-4.749852	7.189805
H	3.213547	-4.515551	5.721105
C	4.689556	-0.223035	9.411444
H	4.180051	0.564085	10.008059
H	5.515433	0.276941	8.852506
H	5.163631	-0.943758	10.113772
C	-1.424302	-3.014038	6.096613
C	-1.468504	-4.410758	5.628816
C	-1.602403	-5.066605	4.402650
H	-1.716131	-4.508375	3.461189
C	-1.593359	-6.495757	4.378597
H	-1.699826	-7.003062	3.404482
C	-1.461139	-7.266416	5.534161

H	-1.464585	-8.368434	5.470999
C	-1.316677	-6.626549	6.808792
C	-1.316065	-5.213305	6.808589
C	-1.714517	-1.767659	4.088331
C	-2.978464	-2.060763	3.533479
H	-3.811691	-2.314343	4.207191
C	-3.173333	-2.031744	2.138113
C	-2.082142	-1.691028	1.309037
H	-2.227584	-1.658426	0.213878
C	-0.810623	-1.392469	1.840547
C	-0.638910	-1.437371	3.240087
H	0.345051	-1.220797	3.684811
C	-4.520233	-2.388187	1.543807
H	-4.637624	-3.492981	1.444381
H	-4.649940	-1.952295	0.529358
H	-5.354555	-2.031884	2.186556
C	0.350867	-1.023973	0.942210
H	0.680783	0.024923	1.119524
H	0.084273	-1.118337	-0.132955
H	1.234443	-1.674126	1.133095
C	-1.205987	-3.013897	7.519888
C	-1.162920	-4.410534	7.988109
C	-1.029299	-5.066145	9.214435
H	-0.915018	-4.507741	10.155724
C	-1.039768	-6.495273	9.238929
H	-0.933484	-7.002395	10.213165
C	-1.172898	-7.266163	8.083619
H	-1.170389	-8.368162	8.147112
C	-0.914840	-1.767479	9.527806
C	0.348890	-2.060942	10.082933
H	1.182173	-2.314915	9.409420
C	0.543444	-2.032091	11.478349
C	-0.547768	-1.690942	12.307200
H	-0.402507	-1.658282	13.402378
C	-1.819028	-1.391734	11.775401
C	-1.990464	-1.436666	10.375837
H	-2.974192	-1.219543	9.930860
C	1.890212	-2.388618	12.072917
H	2.007613	-3.493427	12.172150
H	2.019653	-1.952921	13.087483
H	2.724678	-2.032149	11.430439
C	-2.980670	-1.023172	12.673516
H	-3.310435	0.025773	12.496211
H	-2.714330	-1.117669	13.748731
H	-3.864279	-1.673204	12.482389
C	-2.511589	1.505045	8.762023
C	-3.621062	0.790253	8.186664
C	-4.858361	1.219786	8.862175
C	-6.213354	0.884429	8.807421
H	-6.587469	0.113349	8.117195
C	-7.128662	1.563042	9.669893
H	-8.196231	1.288326	9.619694
C	-6.724596	2.555911	10.562900
H	-7.465720	3.061262	11.205383
C	-5.341017	2.920492	10.650218
C	-4.763535	3.913567	11.507592
H	-5.409611	4.491456	12.190325
C	-3.388734	4.149605	11.472342
H	-2.959305	4.922520	12.132845
C	-2.504139	3.425445	10.614399
H	-1.426615	3.649500	10.632084
C	-3.032554	2.446142	9.769509
C	-4.450956	2.226532	9.799697
C	-0.166617	1.908492	8.813651
C	0.324732	1.597627	10.096239
H	-0.160899	0.796985	10.676092
C	1.424150	2.300605	10.634996
C	2.025567	3.312129	9.859736
H	2.889236	3.863289	10.273040
C	1.551641	3.640823	8.569723
C	0.452216	2.926953	8.055803
H	0.056587	3.164892	7.056358
C	1.928586	1.973756	12.025026
H	2.892358	2.482721	12.241856
H	2.076079	0.878648	12.155757
H	1.198593	2.292654	12.804467
C	2.194733	4.757237	7.773789
H	1.890638	4.727493	6.706000
H	3.305776	4.700990	7.814879
H	1.905014	5.756005	8.176730
C	-4.405935	-0.826587	6.629316
C	-4.611113	-2.176149	6.978181
H	-3.929322	-2.650968	7.702015
C	-5.679400	-2.911521	6.422354
C	-6.540424	-2.263328	5.512974
H	-7.382377	-2.828956	5.075463
C	-6.356025	-0.910977	5.149728
C	-5.276277	-0.201303	5.711929
H	-5.103530	0.852780	5.444939
C	-5.878459	-4.366280	6.791236
H	-5.080054	-5.006546	6.350924
H	-6.855693	-4.749902	6.426741
H	-5.838508	-4.516949	7.893316
C	-7.318894	-0.223078	4.204726
H	-6.809296	0.563116	3.606950
H	-8.143821	0.278120	4.763969
H	-7.794192	-0.944022	3.503454

Optimized geometry of Cr(dmp-BIAN)$_3$ (S = 1)

E = -4615.336529874753 E_h

Cr	-1.317208	-0.163322	6.809911
N	-1.297306	1.256067	5.330871
N	0.688303	-0.090676	6.396605
N	-1.543319	-1.773035	5.479623
N	-1.088482	-1.773975	8.136484
N	-1.335336	1.256966	8.286300

N	-3.321355	-0.088281	7.222310
C	-0.087086	1.473476	4.801315
C	1.000412	0.732091	5.385262
C	2.245420	1.091664	4.685821
C	3.588103	0.709684	4.742348
H	3.939598	-0.053604	5.453020
C	4.520307	1.330019	3.854407
H	5.577662	1.019001	3.905781
C	4.145017	2.310873	2.935789
H	4.898861	2.771026	2.274508
C	2.774847	2.723277	2.847882
C	2.228330	3.716207	1.970974
H	2.890015	4.250687	1.268098
C	0.864476	4.008550	2.012709
H	0.459837	4.781817	1.337094
C	-0.039138	3.342337	2.896921
H	-1.106540	3.610032	2.885173
C	0.458264	2.363370	3.760416
C	1.866313	2.085755	3.722934
C	-2.420956	1.969952	4.818343
C	-2.910108	1.692635	3.524069
H	-2.421607	0.907850	2.924389
C	-4.009637	2.405060	3.005597
C	-4.619265	3.390295	3.812565
H	-5.484840	3.950244	3.415907
C	-4.154223	3.677182	5.112692
C	-3.047511	2.956009	5.606732
H	-2.655824	3.164539	6.614408
C	-4.504245	2.132602	1.600520
H	-5.553739	2.471436	1.461060
H	-4.450368	1.049450	1.355064
H	-3.883583	2.667290	0.844415
C	-4.829729	4.723180	5.974027
H	-5.377191	4.254210	6.823879
H	-5.561335	5.322795	5.390692
H	-4.089335	5.424315	6.420594
C	1.760281	-0.812169	7.011218
C	1.990783	-2.157407	6.659533
H	1.320679	-2.642433	5.931513
C	3.068013	-2.873376	7.219736
C	3.914507	-2.208484	8.133443
H	4.768497	-2.756378	8.569695
C	3.703701	-0.862124	8.497749
C	2.612018	-0.171169	7.931156
H	2.422314	0.881234	8.193158
C	3.295184	-4.325794	6.859079
H	2.606500	-4.992451	7.427273
H	4.334352	-4.646392	7.089446
H	3.105649	-4.513626	5.779157
C	4.638126	-0.155254	9.457097
H	4.074529	0.379622	10.252967
H	5.252966	0.611330	8.930593
H	5.338649	-0.866063	9.946885
C	-1.427871	-2.959601	6.094214
C	-1.465953	-4.356741	5.628234
C	-1.601055	-5.011718	4.400998
H	-1.716665	-4.453046	3.460103
C	-1.589899	-6.441089	4.374895
H	-1.697031	-6.946839	3.399940
C	-1.454422	-7.213488	5.528759
H	-1.455813	-8.315446	5.464134
C	-1.308551	-6.574243	6.804280
C	-1.310677	-5.162107	6.805510
C	-1.737768	-1.736033	4.069070
C	-3.004351	-2.017284	3.510891
H	-3.841004	-2.259957	4.184052
C	-3.198144	-1.993706	2.115618
C	-2.103354	-1.668064	1.284544
H	-2.247800	-1.639219	0.189125
C	-0.828839	-1.383686	1.815938
C	-0.658400	-1.426276	3.215969
H	0.330478	-1.226779	3.658018
C	-4.546736	-2.343200	1.520638
H	-4.648290	-3.443895	1.371098
H	-4.694674	-1.864241	0.528141
H	-5.378833	-2.029196	2.187701
C	0.338290	-1.034419	0.917092
H	0.674570	0.014756	1.081455
H	0.075112	-1.141080	-0.157863
H	1.217080	-1.687408	1.119819
C	-1.200191	-2.960343	7.520475
C	-1.157701	-4.358108	7.984140
C	-1.020955	-5.015024	9.210211
H	-0.907211	-4.457691	10.152148
C	-1.028444	-6.444450	9.233895
H	-0.919795	-6.951501	10.208002
C	-1.161478	-7.215340	8.078748
H	-1.156999	-8.317395	8.141470
C	-0.893484	-1.736633	9.546814
C	0.371964	-2.023131	10.105108
H	1.207253	-2.270751	9.432072
C	0.566424	-1.998208	11.500264
C	-0.526394	-1.665757	12.331231
H	-0.381378	-1.635796	13.426536
C	-1.799596	-1.375603	11.799734
C	-1.970818	-1.419653	10.399905
H	-2.958618	-1.214977	9.957845
C	1.913654	-2.353086	12.095169
H	2.010887	-3.454190	12.244629
H	2.063518	-1.874727	13.087676
H	2.746969	-2.042354	11.428083
C	-2.964770	-1.019584	12.698508
H	-3.295674	0.031184	12.533410
H	-2.701993	-1.126821	13.773506
H	-3.846924	-1.668209	12.496429
C	-2.545357	1.477025	8.815459

C	-3.633576	0.736281	8.232402
C	-4.878175	1.098019	8.931311
C	-6.221277	0.717387	8.875606
H	-6.573766	-0.046282	8.165833
C	-7.152549	1.339436	9.763317
H	-8.210241	1.029433	9.712494
C	-6.776056	2.320829	10.680844
H	-7.529216	2.782278	11.342006
C	-5.405466	2.732032	10.767898
C	-4.857505	3.724749	11.644161
H	-5.518374	4.260401	12.346924
C	-3.493337	4.015545	11.601919
H	-3.087677	4.788641	12.277120
C	-2.590664	3.347705	10.717995
H	-1.522812	3.613699	10.729591
C	-3.089467	2.368746	9.855322
C	-4.497815	2.092649	9.893265
C	-0.210903	1.969855	8.798696
C	0.277809	1.691877	10.092951
H	-0.211535	0.907501	10.692487
C	1.378010	2.403195	10.611573
C	1.988917	3.387600	9.804570
H	2.854994	3.946692	10.201346
C	1.524626	3.674640	8.504188
C	0.416976	2.954911	8.010159
H	0.026145	3.163147	7.002072
C	1.871607	2.130826	12.017020
H	2.922396	2.465859	12.155990
H	1.813560	1.048239	12.263975
H	1.252999	2.668937	12.772369
C	2.202056	4.719208	7.642633
H	2.754323	4.248507	6.796820
H	2.929991	5.321937	8.227331
H	1.462452	5.417502	7.190377
C	-4.392682	-0.810570	6.607615
C	-4.619674	-2.157123	6.956354
H	-3.947901	-2.642070	7.682936
C	-5.695947	-2.874155	6.395656
C	-6.544473	-2.209246	5.483880
H	-7.397027	-2.758409	5.046413
C	-6.336302	-0.861949	5.121378
C	-5.246028	-0.169676	5.689003
H	-5.057985	0.883324	5.428015
C	-5.918654	-4.328303	6.752109
H	-5.227892	-4.991221	6.182047
H	-6.956821	-4.651461	6.520846
H	-5.728553	-4.518626	7.831491
C	-7.273037	-0.155150	4.164244
H	-6.711090	0.385406	3.371044
H	-7.891669	0.606516	4.693523
H	-7.970254	-0.866853	3.671036

Optimized geometry of Cr(dmp-BIAN)$_3$ (S = 2)

E = -4615.323440772416 E_h

Cr	-1.313868	-0.295527	6.809746
N	-1.375792	1.234550	5.332401
N	0.735134	-0.115164	6.406546
N	-1.478270	-1.845223	5.499905
N	-1.150619	-1.846828	8.116367
N	-1.254805	1.237461	8.282841
N	-3.364756	-0.115433	7.212839
C	-0.148568	1.493679	4.863617
C	0.974045	0.764837	5.423775
C	2.196458	1.177612	4.714141
C	3.548294	0.822237	4.738141
H	3.927338	0.045541	5.418946
C	4.454201	1.487968	3.855980
H	5.518298	1.196908	3.883143
C	4.046596	2.489092	2.973973
H	4.780917	2.985366	2.316773
C	2.666388	2.873918	2.918062
C	2.083925	3.877428	2.076153
H	2.722911	4.447514	1.380236
C	0.713951	4.133606	2.143526
H	0.280679	4.915040	1.495689
C	-0.161539	3.418856	3.018340
H	-1.235274	3.659225	3.025242
C	0.371969	2.428174	3.847679
C	1.785168	2.190612	3.785680
C	-2.493507	1.935573	4.801496
C	-2.984465	1.630793	3.516122
H	-2.497349	0.831888	2.934296
C	-4.081402	2.337022	2.976279
C	-4.684228	3.346246	3.753093
H	-5.544312	3.901644	3.337918
C	-4.215007	3.667327	5.047276
C	-3.117814	2.950902	5.561104
H	-2.724402	3.185304	6.562512
C	-4.586788	2.010175	1.586414
H	-5.489148	2.605350	1.328082
H	-4.847958	0.932345	1.493846
H	-3.811493	2.218723	0.813847
C	-4.862175	4.779313	5.846347
H	-4.528851	4.770038	6.905606
H	-5.972374	4.696643	5.837214
H	-4.608033	5.779399	5.423189
C	1.816953	-0.819368	7.001875
C	2.012600	-2.187449	6.720023
H	1.319122	-2.694825	6.030053
C	3.086619	-2.899754	7.294561
C	3.966527	-2.211927	8.155451
H	4.813890	-2.759083	8.605785
C	3.793585	-0.841719	8.453350
C	2.707364	-0.156126	7.875189
H	2.540501	0.909708	8.097051
C	3.273561	-4.372430	6.996498

H	2.498104	-4.989174	7.506068
H	4.267244	-4.735368	7.337308
H	3.185784	-4.582469	5.907189
C	4.775174	-0.112577	9.347096
H	4.286919	0.728316	9.885075
H	5.612936	0.323899	8.753590
H	5.231379	-0.792475	10.100131
C	-1.402016	-3.045368	6.093090
C	-1.438241	-4.440615	5.623310
C	-1.548258	-5.094205	4.394025
H	-1.643369	-4.534380	3.451306
C	-1.539344	-6.523347	4.369293
H	-1.627023	-7.030092	3.393098
C	-1.429949	-7.294656	5.527005
H	-1.432727	-8.396582	5.462801
C	-1.311574	-6.656351	6.805019
C	-1.311809	-5.243300	6.805876
C	-1.664876	-1.788238	4.083589
C	-2.934488	-2.045477	3.525180
H	-3.777577	-2.272497	4.196383
C	-3.121135	-2.011186	2.128965
C	-2.015864	-1.701629	1.306114
H	-2.154826	-1.664333	0.210313
C	-0.739184	-1.437685	1.843437
C	-0.575582	-1.487304	3.244136
H	0.411128	-1.295726	3.695093
C	-4.474073	-2.329033	1.527062
H	-4.597841	-3.426255	1.369312
H	-4.608164	-1.839620	0.537867
H	-5.301253	-2.002536	2.194089
C	0.435331	-1.098175	0.950944
H	0.782152	-0.053650	1.121700
H	0.175019	-1.196851	-0.125369
H	1.305919	-1.761776	1.154521
C	-1.224705	-3.046297	7.521632
C	-1.186728	-4.442035	7.989577
C	-1.076555	-5.097136	9.218054
H	-0.982091	-4.538462	10.161532
C	-1.083844	-6.526324	9.240897
H	-0.996045	-7.034206	10.216486
C	-1.192484	-7.296220	8.082177
H	-1.188596	-8.398224	8.144914
C	-0.965570	-1.789978	9.532880
C	0.303565	-2.046450	10.092749
H	1.147488	-2.273282	9.422539
C	0.488707	-2.011186	11.489128
C	-0.617607	-1.701808	12.310641
H	-0.479760	-1.663677	13.406558
C	-1.893818	-1.438618	11.771865
C	-2.055897	-1.488942	10.370998
H	-3.042179	-1.297976	9.918856
C	1.841368	-2.327174	12.092668
H	1.965742	-3.424071	12.252147
H	1.974265	-1.836215	13.081257
H	2.668906	-2.001084	11.425884
C	-3.069429	-1.099335	12.662987
H	-3.415594	-0.054534	12.492560
H	-2.810651	-1.198920	13.739592
H	-3.939985	-1.762433	12.457697
C	-2.481878	1.497376	8.751585
C	-3.604432	0.767583	8.192624
C	-4.826870	1.181793	8.901440
C	-6.178659	0.826148	8.878543
H	-6.557687	0.047889	8.199527
C	-7.084524	1.493762	9.759333
H	-8.148599	1.202536	9.732936
C	-6.676911	2.496904	10.639046
H	-7.411211	2.994654	11.295151
C	-5.296711	2.881913	10.693966
C	-4.714246	3.887452	11.533459
H	-5.353241	4.459129	12.228066
C	-3.344239	4.143437	11.465592
H	-2.911007	4.926404	12.111595
C	-2.468745	3.426538	10.592556
H	-1.394993	3.666885	10.584993
C	-3.002308	2.434023	9.765433
C	-4.415590	2.196911	9.827604
C	-0.136569	1.936705	8.815025
C	0.352909	1.630727	10.100669
H	-0.135752	0.832136	10.681673
C	1.450315	2.335240	10.641768
C	2.055255	3.343914	9.865823
H	2.915708	3.898015	10.281962
C	1.587875	3.665846	8.571169
C	0.490070	2.951185	8.056171
H	0.098179	3.185988	7.054261
C	1.954171	2.007049	12.031874
H	2.855715	2.602621	12.292116
H	2.216102	0.929308	12.123400
H	1.177713	2.213961	12.803695
C	2.237401	4.777106	7.772999
H	1.903826	4.769575	6.713798
H	3.347419	4.691841	7.781803
H	1.985686	5.777373	8.197176
C	-4.445977	-0.819828	6.617087
C	-4.640106	-2.188601	6.896768
H	-3.945815	-2.696341	7.585653
C	-5.713744	-2.901023	6.321754
C	-6.594787	-2.212770	5.462315
H	-7.441778	-2.760086	5.011477
C	-6.423214	-0.841987	5.166303
C	-5.337430	-0.156217	5.745049
H	-5.171467	0.910064	5.524424
C	-5.898995	-4.374381	6.617505
H	-5.123267	-4.989526	6.106414
H	-6.892539	-4.737794	6.276768

H	-5.810308	-4.586094	7.706414
C	-7.405742	-0.112412	4.273935
H	-6.918047	0.728785	3.735903
H	-8.242908	0.323747	4.868511
H	-7.862664	-0.791920	3.520983

Optimized geometry of Cr(dmp-BIAN)$_3$ (S = 3)

E = -4615.310348008484 E_h

Cr	-1.313140	-0.224801	6.805164
N	-1.361040	1.275738	5.332675
N	0.744298	-0.137706	6.378611
N	-1.488180	-1.818828	5.446025
N	-1.139746	-1.817639	8.167482
N	-1.264166	1.273441	8.281791
N	-3.369494	-0.139013	7.232423
C	-0.127502	1.517667	4.867363
C	0.986410	0.763979	5.417200
C	2.215847	1.183728	4.721645
C	3.564097	0.816220	4.746619
H	3.932886	0.025743	5.417126
C	4.479259	1.488337	3.879186
H	5.540895	1.188763	3.906078
C	4.082950	2.506350	3.011224
H	4.824551	3.007066	2.365683
C	2.706491	2.903220	2.954611
C	2.135663	3.924610	2.126234
H	2.781644	4.500515	1.441754
C	0.767333	4.190227	2.192205
H	0.343124	4.985065	1.554853
C	-0.117532	3.468524	3.051687
H	-1.189770	3.715839	3.057048
C	0.404848	2.461227	3.868123
C	1.816488	2.213912	3.808322
C	-2.479894	1.961362	4.786909
C	-2.944956	1.655675	3.491454
H	-2.435617	0.867650	2.913634
C	-4.049021	2.341545	2.941143
C	-4.686601	3.330245	3.717607
H	-5.554656	3.867632	3.295437
C	-4.243627	3.651763	5.020558
C	-3.137868	2.956081	5.545242
H	-2.764551	3.190464	6.554434
C	-4.519666	2.023762	1.537063
H	-5.517669	2.466313	1.328498
H	-4.583426	0.925681	1.370249
H	-3.812149	2.424045	0.774455
C	-4.928363	4.741177	5.819530
H	-4.615641	4.725861	6.885095
H	-6.036370	4.636712	5.786766
H	-4.685559	5.750957	5.413001
C	1.821014	-0.850773	6.973369
C	2.025565	-2.211293	6.665892
H	1.342012	-2.706435	5.957043
C	3.094787	-2.930834	7.240363
C	3.959224	-2.257259	8.127876
H	4.802097	-2.810544	8.579187
C	3.775136	-0.894975	8.453753
C	2.694231	-0.202110	7.874323
H	2.517782	0.857782	8.117058
C	3.292817	-4.395988	6.913569
H	2.502824	-5.024590	7.384818
H	4.276247	-4.765889	7.275731
H	3.238039	-4.580473	5.817425
C	4.738446	-0.181846	9.379695
H	4.237013	0.644350	9.928081
H	5.584211	0.270866	8.810260
H	5.184695	-0.876763	10.124959
C	-1.405952	-2.992955	6.086530
C	-1.438026	-4.392622	5.627480
C	-1.536539	-5.048303	4.397058
H	-1.622353	-4.490523	3.452528
C	-1.528359	-6.477296	4.373447
H	-1.606733	-6.984284	3.396510
C	-1.432209	-7.248466	5.532324
H	-1.436853	-8.350447	5.469094
C	-1.323994	-6.608468	6.810752
C	-1.321089	-5.195777	6.809490
C	-1.694831	-1.781709	4.039575
C	-2.964159	-2.079975	3.496357
H	-3.789854	-2.332518	4.180275
C	-3.174385	-2.053189	2.103559
C	-2.093568	-1.707944	1.262350
H	-2.250584	-1.677654	0.168731
C	-0.818533	-1.400468	1.780322
C	-0.631677	-1.442926	3.178011
H	0.355878	-1.219720	3.612406
C	-4.526067	-2.415399	1.523623
H	-4.626220	-3.518640	1.393158
H	-4.681981	-1.952140	0.525015
H	-5.353607	-2.091948	2.191872
C	0.331160	-1.026909	0.868602
H	0.654447	0.025528	1.037068
H	0.054570	-1.128731	-0.203358
H	1.221848	-1.668926	1.053672
C	-1.227435	-2.992069	7.528666
C	-1.200806	-4.391214	7.990105
C	-1.104520	-5.044884	9.221718
H	-1.015799	-4.485702	10.165131
C	-1.118854	-6.473812	9.247876
H	-1.042246	-6.979449	10.225655
C	-1.218594	-7.246533	8.090340
H	-1.219108	-8.348412	8.155558
C	-0.933600	-1.780340	9.574180
C	0.336415	-2.075319	10.117431
H	1.163008	-2.325046	9.433624
C	0.545943	-2.049212	11.510383

C	-0.536135	-1.707573	12.351406
H	-0.379618	-1.677710	13.445119
C	-1.811844	-1.403235	11.833312
C	-1.998109	-1.445361	10.435497
H	-2.986087	-1.224373	10.000900
C	1.898297	-2.408340	12.090634
H	2.001238	-3.511417	12.220301
H	2.052615	-1.945463	13.089671
H	2.725295	-2.082342	11.422953
C	-2.962721	-1.033075	12.744878
H	-3.288397	0.018724	12.576990
H	-2.686238	-1.134863	13.816870
H	-3.851863	-1.677032	12.559074
C	-2.497911	1.513202	8.747868
C	-3.611276	0.759543	8.196871
C	-4.841017	1.176863	8.893370
C	-6.189061	0.808680	8.867105
H	-6.557209	0.019242	8.195019
C	-7.104876	1.478744	9.735441
H	-8.166366	1.178757	9.707564
C	-6.709331	2.495289	10.605486
H	-7.451431	2.994514	11.251609
C	-5.333131	2.892875	10.663257
C	-4.763320	3.913588	11.493158
H	-5.409854	4.487960	12.178404
C	-3.395186	4.180365	11.427726
H	-2.971682	4.974637	12.066259
C	-2.509660	3.460749	10.567181
H	-1.437702	3.709246	10.562105
C	-3.031036	2.454261	9.749096
C	-4.442471	2.205693	9.808518
C	-0.146254	1.960139	8.827776
C	0.319163	1.654950	10.123264
H	-0.189591	0.866687	10.701235
C	1.422250	2.342108	10.673844
C	2.058972	3.331486	9.897534
H	2.926399	3.869764	10.319865
C	1.616214	3.652080	8.594296
C	0.511205	2.955320	8.069498
H	0.138297	3.189007	7.060014
C	1.893594	2.024067	12.077638
H	2.888454	2.472690	12.288190
H	1.964669	0.925999	12.241773
H	1.182623	2.417485	12.840589
C	2.299535	4.742609	7.795616
H	1.987507	4.726654	6.729851
H	3.407717	4.640172	7.829122
H	2.054679	5.752003	8.201867
C	-4.447124	-0.852897	6.639550
C	-4.656229	-2.210930	6.954677
H	-3.975325	-2.704074	7.667501
C	-5.726504	-2.930746	6.382435
C	-6.587193	-2.259799	5.489306
H	-7.430818	-2.813240	5.039577
C	-6.398421	-0.900048	5.155769
C	-5.316516	-0.206939	5.733145
H	-5.136630	0.850996	5.484798
C	-5.929353	-4.393413	6.717217
H	-5.139956	-5.026906	6.251551
H	-6.912925	-4.762617	6.354782
H	-5.877712	-4.571741	7.814558
C	-7.358095	-0.189422	4.224190
H	-6.853156	0.631595	3.671264
H	-8.202954	0.269764	4.789751
H	-7.805884	-0.887489	3.482789

Optimized geometry of Ga(dmp-BIAN)$_3$ (S = 1/2)

E = -5495.762178002255 E_h

Ga	-0.096070	0.100942	-0.000644
N	-0.020325	-0.022039	2.117679
N	2.004308	0.028224	0.281556
N	-0.221542	2.212493	0.095965
C	3.260676	-0.246439	3.687909
C	-4.505276	4.751463	-0.001776
C	-3.533502	3.726051	-0.001179
C	2.315062	-0.083783	1.575359
C	1.240760	-0.091244	2.553366
C	4.211336	-0.347122	4.727864
C	-2.124075	3.953698	0.130559
C	1.844665	-0.158171	3.896959
C	1.379229	-0.141429	5.214607
H	0.306049	-0.063996	5.445663
C	-1.852267	1.101888	3.299495
H	-1.584465	2.035349	2.779671
C	-2.922271	1.084035	4.220468
C	-1.101542	-0.061750	3.042179
C	-1.686784	5.270619	0.297471
H	-0.619723	5.513342	0.412421
C	3.318171	-1.054188	-1.487467
H	2.730403	-1.973435	-1.331687
C	5.585263	-0.448497	4.329984
H	6.373288	-0.534304	5.097636
C	1.523269	3.335169	1.405229
H	1.226630	2.731058	2.277421
C	-1.491216	2.624647	0.055760
C	4.942555	-0.323280	1.940331
H	5.264063	-0.314744	0.888302
C	1.200547	3.934726	-0.935978
H	0.664358	3.780128	-1.886045
C	-1.429147	-1.264319	3.708428
H	-0.844426	-2.171613	3.487909
C	4.350892	-1.027091	-2.449582
C	5.920804	-0.442035	2.975575
H	6.981921	-0.525753	2.684822
C	3.037120	0.078013	-0.698012
C	2.895876	5.056195	0.388255

H	3.702161	5.807603	0.469758
C	3.793973	1.256888	-0.874063
H	3.562474	2.136121	-0.251741
C	-3.222788	-0.124698	4.879017
H	-4.057278	-0.148688	5.603230
C	-2.484542	-1.305937	4.638277
C	5.097343	0.158862	-2.601181
H	5.915375	0.187581	-3.343799
C	3.595015	-0.217929	2.294476
C	2.228521	4.891213	-0.847487
C	-2.653989	6.322794	0.315884
H	-2.296491	7.357872	0.450539
C	2.560895	4.287050	1.519644
C	2.324206	-0.228450	6.283429
H	1.943597	-0.213665	7.319043
C	0.836599	3.160518	0.188988
C	2.627561	5.716963	-2.052767
H	1.886723	5.620809	-2.875656
H	2.724765	6.796128	-1.796423
H	3.615343	5.390884	-2.453877
C	5.631947	2.578949	-2.024870
H	5.181670	3.214688	-2.823815
H	5.661236	3.193659	-1.099140
H	6.678715	2.361714	-2.332408
C	-4.021464	6.090782	0.165243
H	-4.733191	6.933813	0.176287
C	4.832659	1.308369	-1.823264
C	3.698199	-0.336176	6.066535
H	4.392272	-0.411023	6.920850
C	-2.804909	-2.581379	5.389361
H	-2.417110	-3.474829	4.854329
H	-2.340785	-2.579455	6.403147
H	-3.900353	-2.708990	5.535210
C	-3.721253	2.342785	4.485105
H	-3.063310	3.179470	4.812953
H	-4.245773	2.691271	3.566577
H	-4.487285	2.182735	5.274375
C	3.283750	4.471276	2.837369
H	2.575627	4.735313	3.655191
H	3.798541	3.535249	3.151677
H	4.048339	5.275858	2.775255
C	4.646520	-2.254335	-3.285911
H	4.878830	-3.135737	-2.645974
H	3.771313	-2.537011	-3.913930
H	5.511514	-2.088669	-3.963847
N	-2.200967	0.338723	-0.103187
C	-3.836991	2.331535	-0.133736
C	-5.174902	1.964503	-0.301304
H	-5.473320	0.912109	-0.417429
C	-3.412150	-1.351381	-1.402958
H	-2.793679	-1.089619	-2.276277
C	-2.542821	1.628270	-0.064436
C	-3.994155	-0.987001	0.936683
H	-3.812603	-0.454441	1.883945
C	-5.200806	-2.629304	-0.379739
H	-5.994420	-3.394521	-0.458278
C	-5.001939	-1.965406	0.852684
C	-6.173754	2.986601	-0.320430
H	-7.226536	2.685602	-0.456304
C	-4.415209	-2.339677	-1.512640
C	-3.202774	-0.668445	-0.189599
C	-5.843818	-2.317668	2.061232
H	-5.770602	-1.538518	2.850646
H	-6.916672	-2.442323	1.792183
H	-5.510350	-3.280311	2.515000
C	-5.868237	4.339688	-0.169780
H	-6.671909	5.095732	-0.181438
C	-4.633328	-3.061167	-2.825900
H	-4.822444	-2.344597	-3.656755
H	-3.737038	-3.656146	-3.114663
H	-5.498803	-3.756678	-2.771304
N	0.022994	0.021161	-2.122045
N	-0.144201	-1.998504	-0.284118
C	0.070222	-3.267083	-3.690744
C	-0.050876	-2.314496	-1.578134
C	0.025229	-1.241478	-2.556262
C	0.119598	-4.221835	-4.730924
C	0.069144	-1.848653	-3.899765
C	0.091312	-1.382359	-5.216936
H	0.081580	-0.306273	-5.447285
C	-0.999314	1.909245	-3.305496
H	-1.947591	1.688155	-2.790288
C	-0.923280	2.978498	-4.224152
C	0.123814	1.099803	-3.044581
C	0.872793	-3.376527	1.474824
H	1.824059	-2.844753	1.311353
C	0.132851	-5.599595	-4.333676
H	0.175420	-6.391043	-5.101422
C	0.029758	-4.951376	-1.944323
H	-0.007081	-5.272594	-0.892806
C	1.344403	1.367718	-3.704382
H	2.219906	0.737469	-3.480894
C	0.793593	-4.409141	2.434324
C	0.094871	-5.934543	-2.979632
H	0.109600	-6.999019	-2.689230
C	-0.247561	-3.027495	0.695639
C	-1.468506	-3.711620	0.883273
H	-2.337912	-3.427321	0.269502
C	0.301964	3.218308	-4.877230
H	0.371749	4.051577	-5.599884
C	1.443240	2.421128	-4.632383
C	-0.433147	-5.084158	2.595592
H	-0.502924	-5.901913	3.335647
C	0.010946	-3.599516	-2.297677
C	0.129093	-2.330268	-6.285855
H	0.146411	-1.949184	-7.321234

C	-2.885989	-5.472298	2.042613
H	-3.464164	-5.018931	2.882368
H	-3.530464	-5.420443	1.138454
H	-2.727558	-6.543570	2.297691
C	-1.572923	-4.747846	1.830894
C	0.150111	-3.708391	-6.069009
H	0.187668	-4.405446	-6.923376
C	2.736716	2.677378	-5.377305
H	3.608409	2.254099	-4.833189
H	2.720455	2.205227	-6.387297
H	2.914547	3.764633	-5.531118
C	-2.138044	3.842924	-4.489325
H	-3.015940	3.227803	-4.790883
H	-2.441767	4.406257	-3.577645
H	-1.946186	4.582308	-5.296631
C	2.006747	-4.775406	3.263075
H	2.896312	-4.964730	2.621007
H	2.283960	-3.951486	3.959663
H	1.825587	-5.686818	3.872908

Optimized geometry of Ga(dmp-BIAN)$_3$ (S = 3/2)

E = -5495.761854804779 E_h

Ga	-0.085307	0.095917	0.007534
N	-0.013434	-0.025041	2.126186
N	2.015483	0.024880	0.287905
N	-0.211118	2.210633	0.105477
C	3.267690	-0.243699	3.696443
C	-4.499635	4.739928	-0.034516
C	-3.525655	3.716645	-0.022971
C	2.323977	-0.078282	1.582508
C	1.247384	-0.097737	2.560217
C	4.217752	-0.342938	4.737355
C	-2.117170	3.948368	0.110291
C	1.850798	-0.170393	3.904040
C	1.383204	-0.167282	5.221053
H	0.308942	-0.102484	5.450802
C	-1.847220	1.100440	3.301413
H	-1.577165	2.032722	2.780658
C	-2.919616	1.084793	4.219514
C	-1.096504	-0.064415	3.048034
C	-1.683042	5.267558	0.266571
H	-0.616869	5.513415	0.382594
C	3.322811	-1.044356	-1.492313
H	2.734116	-1.963761	-1.341474
C	5.593068	-0.428692	4.341111
H	6.380600	-0.512228	5.109525
C	1.541241	3.330949	1.404701
H	1.250298	2.724740	2.277321
C	-1.481189	2.619308	0.052933
C	4.953198	-0.291775	1.951457
H	5.276247	-0.272822	0.900106
C	1.201776	3.938626	-0.931951
H	0.659407	3.786914	-1.878991
C	-1.427245	-1.265639	3.715111
H	-0.843689	-2.174124	3.496644
C	4.353916	-1.011800	-2.455901
C	5.930810	-0.408709	2.987385
H	6.993090	-0.481078	2.697798
C	3.046179	0.082097	-0.692597
C	2.906975	5.055196	0.383731
H	3.714157	5.806004	0.461841
C	3.803497	1.261606	-0.863314
H	3.574170	2.137192	-0.234978
C	-3.222734	-0.122567	4.879426
H	-4.059186	-0.144678	5.601426
C	-2.485221	-1.304919	4.642176
C	5.102090	0.173924	-2.600454
H	5.918295	0.206906	-3.344902
C	3.604060	-0.201816	2.303962
C	2.229662	4.895202	-0.847517
C	-2.652276	6.318003	0.272387
H	-2.297257	7.355004	0.398592
C	2.579719	4.282643	1.514761
C	2.327305	-0.252169	6.290724
H	1.944989	-0.248960	7.325802
C	0.846277	3.159180	0.192517
C	2.616494	5.730142	-2.050510
H	1.906866	5.582833	-2.892814
H	2.641872	6.816249	-1.804321
H	3.633839	5.460457	-2.417804
C	5.640097	2.589820	-2.009014
H	5.183429	3.235702	-2.796057
H	5.679384	3.193839	-1.076657
H	6.683438	2.374047	-2.328921
C	-4.018916	6.081634	0.120943
H	-4.732388	6.923282	0.121953
C	4.840122	1.318555	-1.814435
C	3.702550	-0.345582	6.075171
H	4.396127	-0.418525	6.930051
C	-2.808087	-2.578748	5.394956
H	-2.421243	-3.473488	4.861318
H	-2.344611	-2.576142	6.409054
H	-3.903810	-2.704499	5.540216
C	-3.718708	2.344441	4.479493
H	-3.060457	3.183306	4.800928
H	-4.245792	2.687459	3.560337
H	-4.482753	2.188065	5.271411
C	3.309298	4.464669	2.829077
H	2.606037	4.733553	3.649604
H	3.820753	3.526499	3.142283
H	4.077656	5.265350	2.762866
C	4.644899	-2.233067	-3.302619
H	4.868373	-3.122064	-2.670140
H	3.770580	-2.503681	-3.937236
H	5.513901	-2.066901	-3.975297
N	-2.188379	0.330400	-0.096708

C	-3.826029	2.320299	-0.143038
C	-5.163015	1.948987	-0.308897
H	-5.459249	0.894875	-0.414883
C	-3.406531	-1.349394	-1.404434
H	-2.791616	-1.081685	-2.278444
C	-2.531059	1.620037	-0.063695
C	-3.979589	-1.000680	0.939594
H	-3.794775	-0.474247	1.889540
C	-5.192665	-2.632793	-0.383651
H	-5.987563	-3.396434	-0.464690
C	-4.989051	-1.977111	0.852430
C	-6.163991	2.968785	-0.338926
H	-7.215931	2.664232	-0.473349
C	-4.410747	-2.336179	-1.517329
C	-3.190647	-0.676442	-0.186644
C	-5.826513	-2.337281	2.061683
H	-5.749914	-1.563509	2.856028
H	-6.900426	-2.459599	1.795823
H	-5.491539	-3.303032	2.507483
C	-5.861556	4.323889	-0.201113
H	-6.666742	5.078131	-0.221058
C	-4.634117	-3.048439	-2.834697
H	-4.809515	-2.325710	-3.663174
H	-3.745381	-3.655378	-3.122275
H	-5.509691	-3.731700	-2.786704
N	0.031126	0.020488	-2.111718
N	-0.132828	-2.006396	-0.276286
C	0.038877	-3.263409	-3.690035
C	-0.057796	-2.317495	-1.572495
C	0.023074	-1.241533	-2.547802
C	0.073879	-4.214526	-4.734166
C	0.053492	-1.844310	-3.893480
C	0.076027	-1.373103	-5.208928
H	0.078674	-0.296070	-5.435061
C	-0.996409	1.903161	-3.300361
H	-1.945355	1.678262	-2.788050
C	-0.922471	2.971519	-4.220234
C	0.129729	1.099516	-3.034662
C	0.869432	-3.377117	1.495030
H	1.820513	-2.842588	1.340001
C	0.073941	-5.593769	-4.342333
H	0.103853	-6.382614	-5.113375
C	-0.012008	-4.953869	-1.950184
H	-0.047016	-5.278762	-0.899784
C	1.350858	1.371496	-3.691505
H	2.228206	0.745103	-3.464920
C	0.783479	-4.407100	2.457278
C	0.037967	-5.933676	-2.989494
H	0.043257	-6.999372	-2.703222
C	-0.243621	-3.034233	0.702653
C	-1.463391	-3.724898	0.878299
H	-2.327548	-3.446004	0.254742
C	0.303668	3.215814	-4.870009
H	0.371718	4.048128	-5.593940
C	1.447630	2.423861	-4.621044
C	-0.441792	-5.086396	2.607543
H	-0.516666	-5.901358	3.350220
C	-0.017943	-3.600533	-2.298156
C	0.097691	-2.317176	-6.281725
H	0.115398	-1.932138	-7.315640
C	-2.884800	-5.490857	2.026812
H	-3.430941	-5.104521	2.919970
H	-3.558087	-5.365640	1.151443
H	-2.725126	-6.579932	2.191770
C	-1.574323	-4.757850	1.828053
C	0.103850	-3.696245	-6.070462
H	0.128878	-4.390322	-6.927695
C	2.741484	2.683409	-5.364141
H	3.613934	2.266410	-4.816442
H	2.729553	2.207189	-6.372257
H	2.914497	3.770886	-5.521817
C	-2.141224	3.827999	-4.492703
H	-3.009023	3.208267	-4.813904
H	-2.463104	4.377764	-3.579110
H	-1.944922	4.578007	-5.289039
C	1.989214	-4.765176	3.300424
H	2.886674	-4.951735	2.668602
H	2.254730	-3.938091	3.997824
H	1.805904	-5.675915	3.910622

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