Supporting Information for

Quasi-1D Chains of Dinickel Lantern Complexes and their Properties

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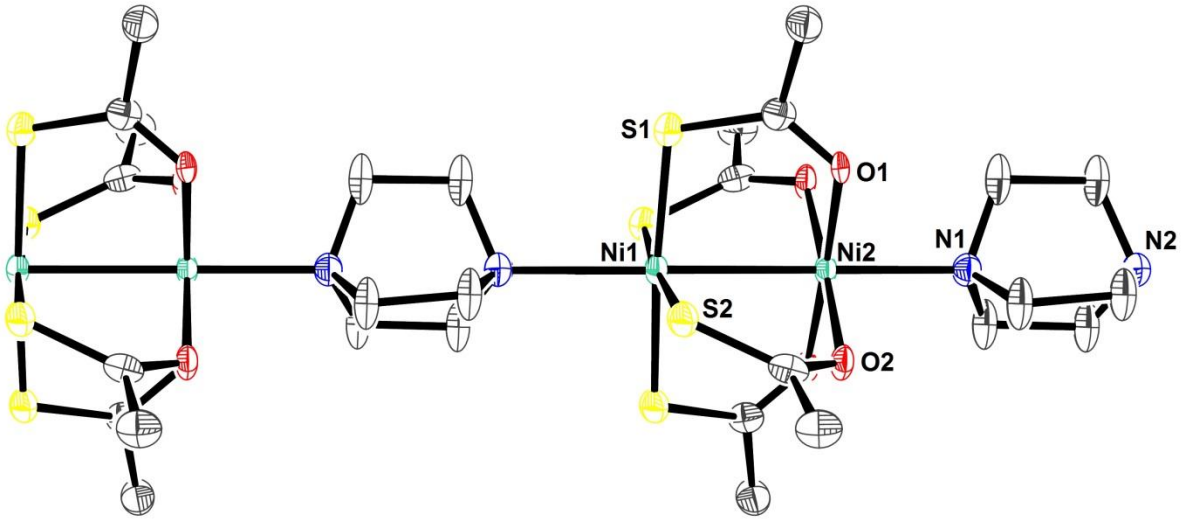

Figure S1. ORTEP with displacement ellipsoids drawn at the 50% probability level of $[Ni_2(SAc)_4(DABCO)]_n$ (**3**). Hydrogen atoms and disordered part are omitted for clarity. Unlabeled atoms are related by (-x+1, y, -z+1/2).

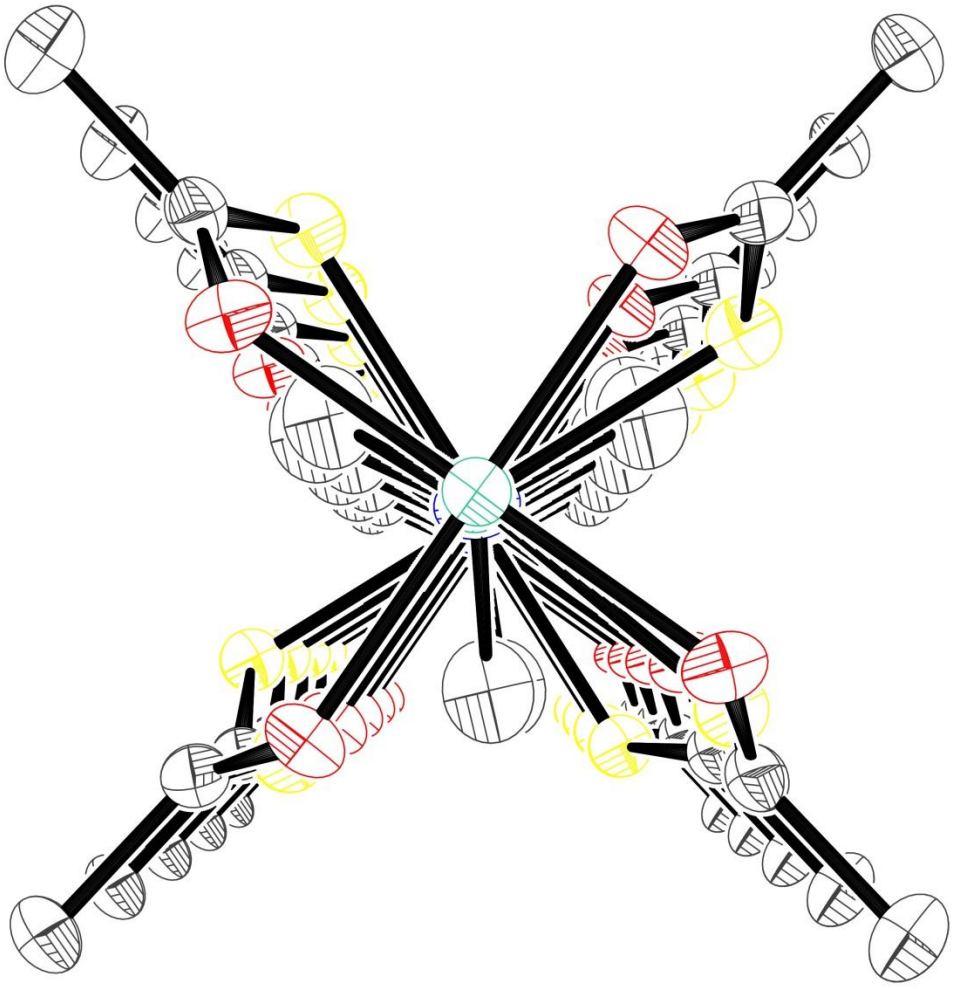

Figure S2. Perspective view of $[Ni_2(SAc)_4(DABCO)]_n$ (**3**) viewed down the *b* direction. Hydrogen atoms and disordered part are omitted for clarity.

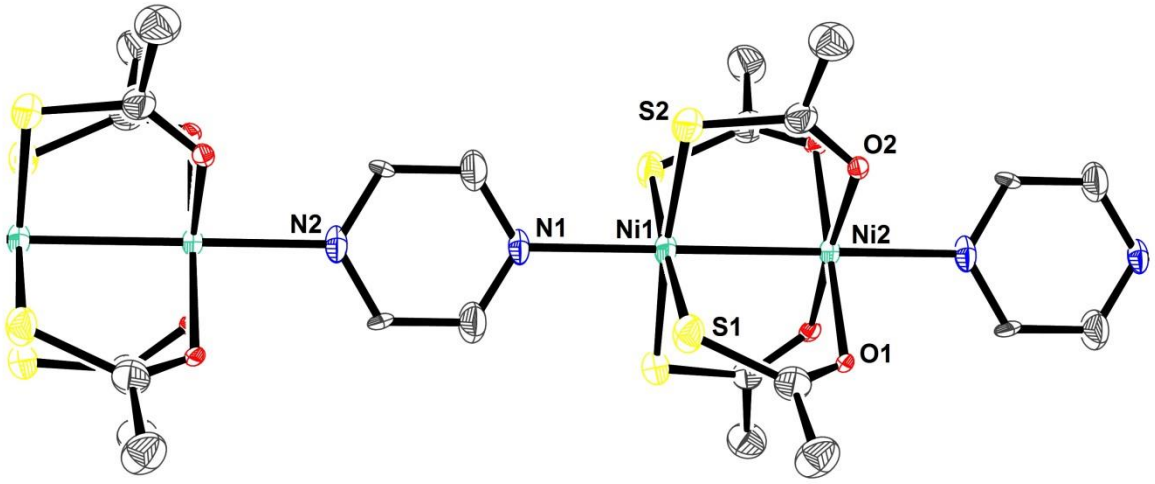

Figure S3. ORTEP with displacement ellipsoids drawn at the 50% probability level of $[Ni_2(SAc)_4(Pyz)]_n$ (**4**). Hydrogen atoms and disordered part are omitted for clarity. Unlabeled atoms are related by (-x+1, y, -z+3/2).

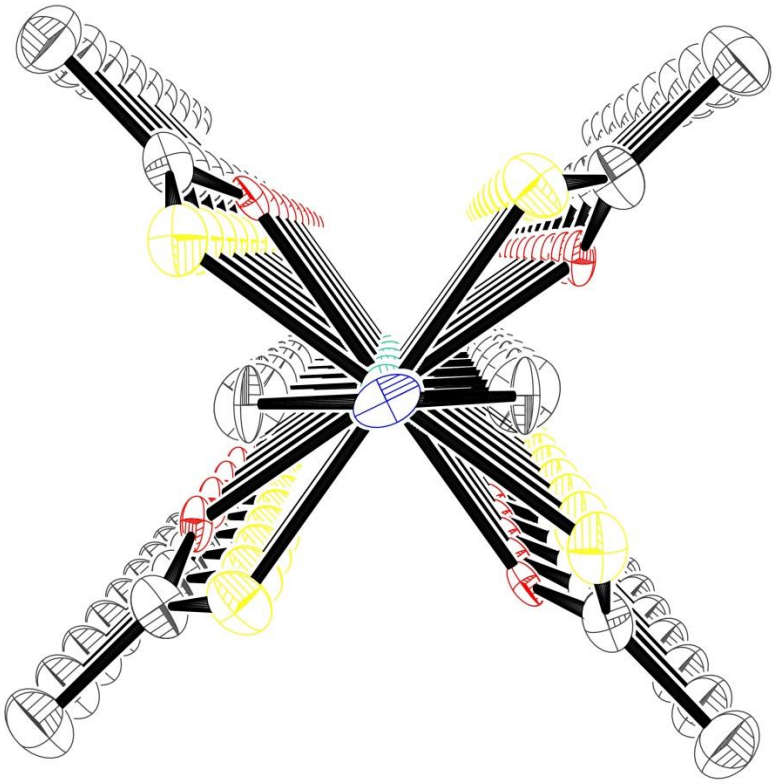

Figure S4. Perspective view of $[Ni_2(SAc)_4(Pyz)]_n$ (**4**) viewed down the *b* direction. Hydrogen atoms and disordered part are omitted for clarity.

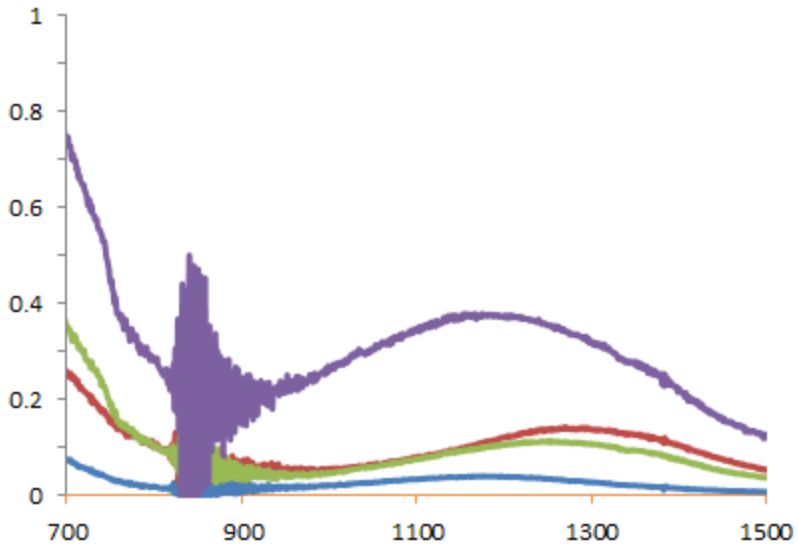

Figure S5. Diffuse reflectance spectra of complexes **1**-**4**.

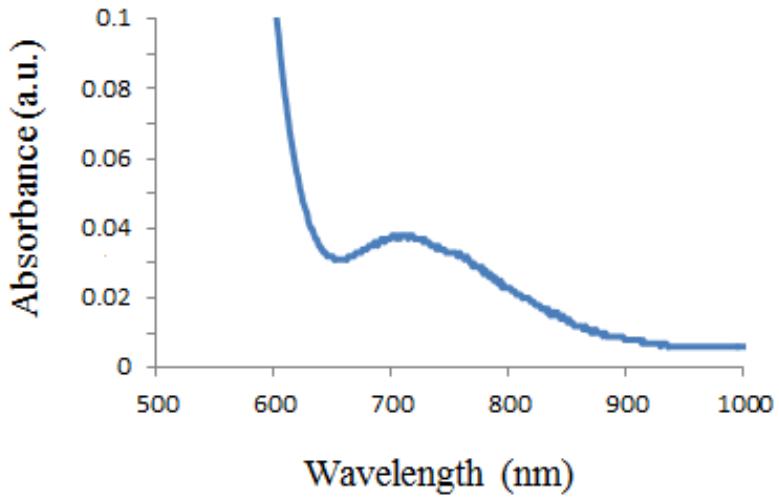

Figure S6. Electronic spectrum of compound **5**.

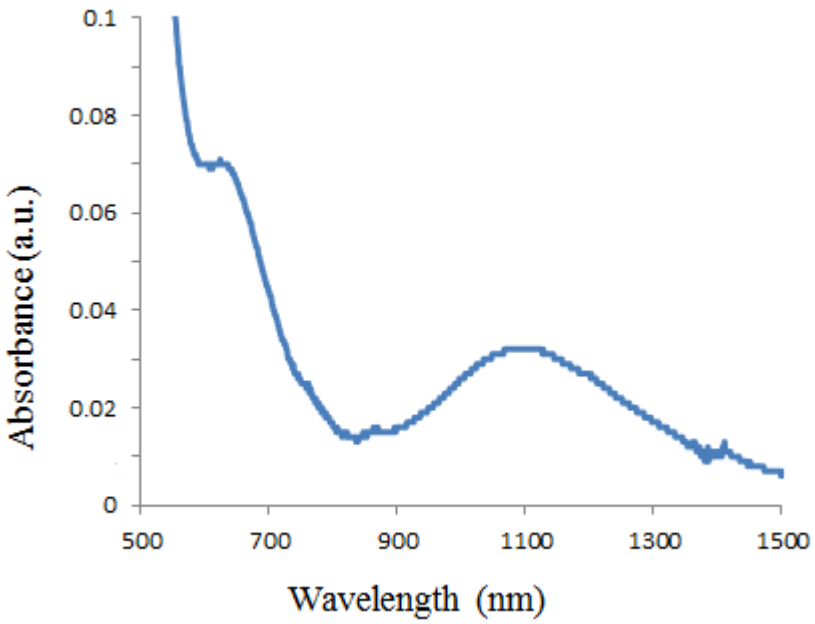

Figure S7. UV-vis spectrum of compound **6** in acetone.

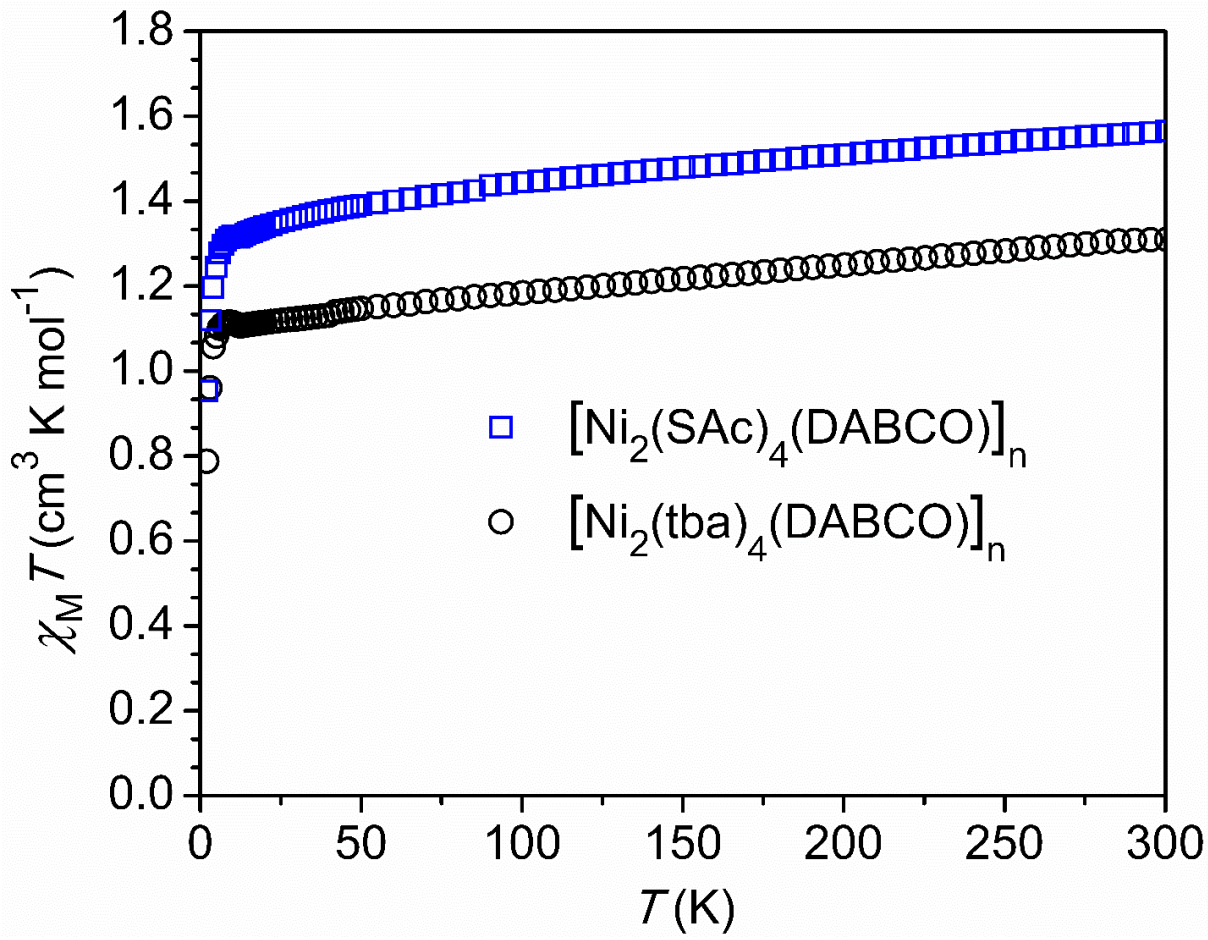

Figure S8. Temperature dependence of magnetic susceptibilities for $[Ni_2(L)_4(DABCO)]_n$, where L = SAc (compound **3**, blue) and tba (compound **1**, black), collected at applied fields of 1000 Oe.

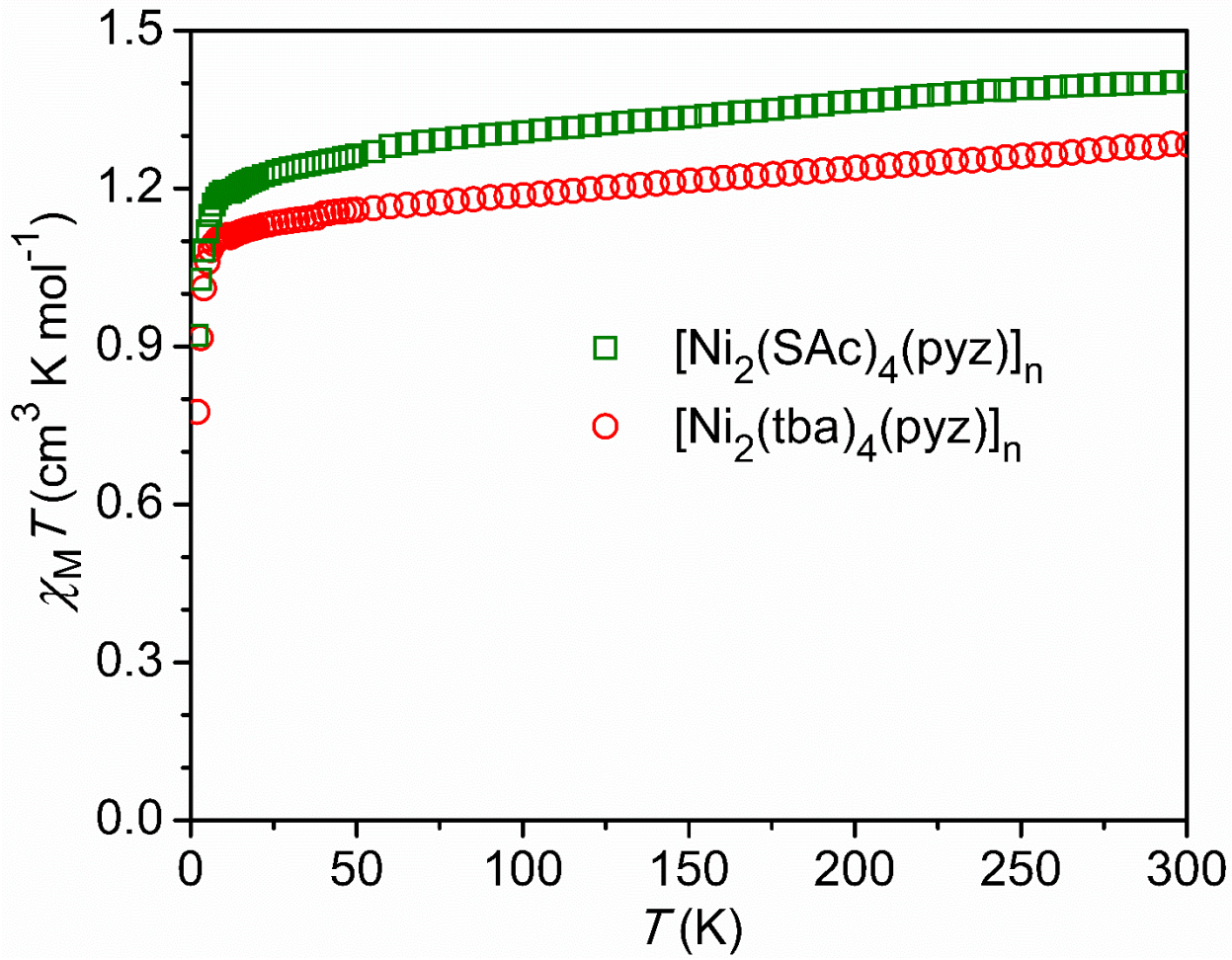

Figure S9. Temperature dependence of magnetic susceptibilities for $[Ni_2(L)_4(pyz)]_n$, where L = SAc (compound **4**, green) and tba (compound **2**, red), collected at applied fields of 1000 Oe.

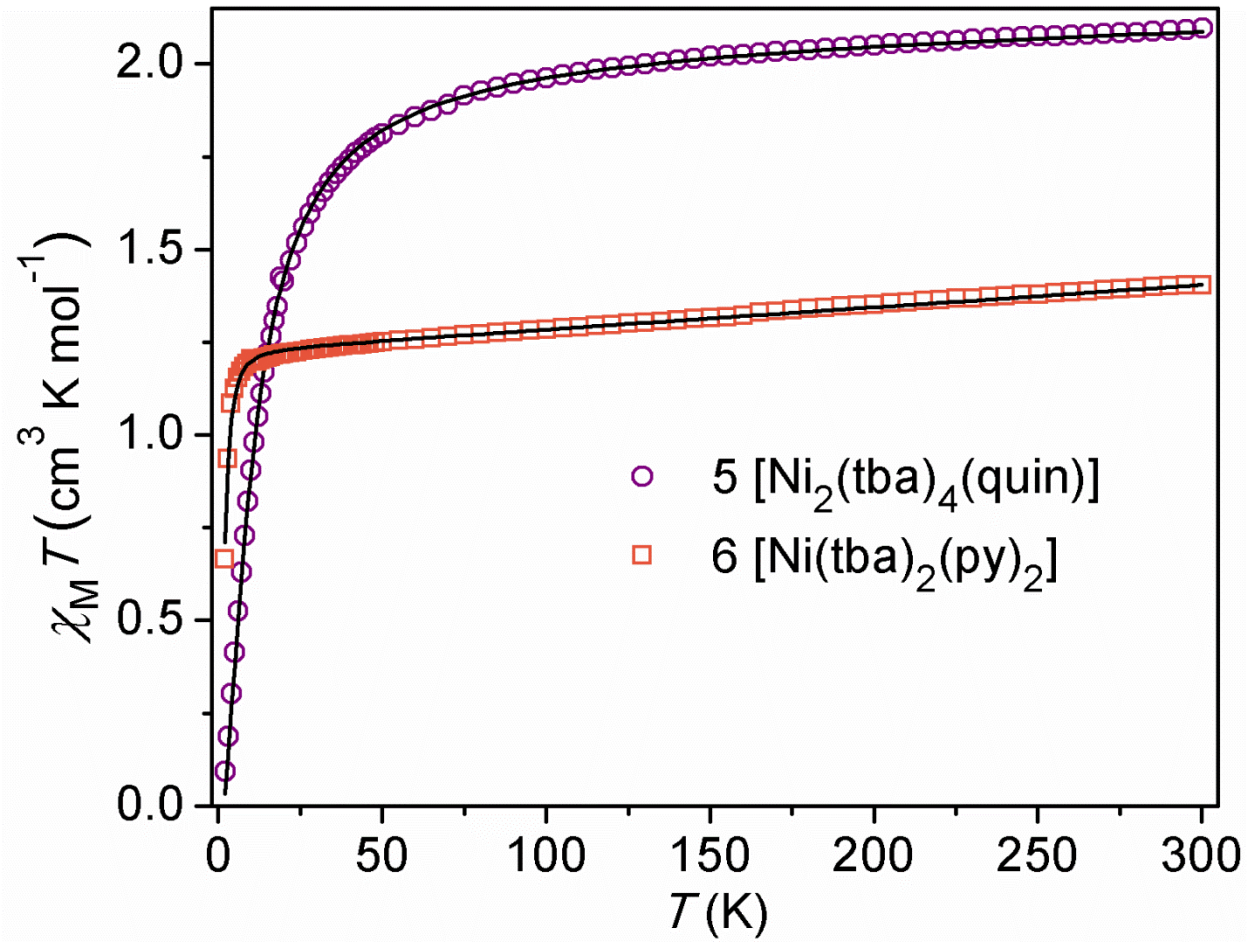

Figure S10. Temperature dependence of magnetic susceptibilities for $[Ni_2(tba)_4(quin)]$ (**5**) and $[Ni(tba)_2(py)_2]$ (**6**) collected at applied fields of 1000 Oe. Fit lines are described in the manuscript.

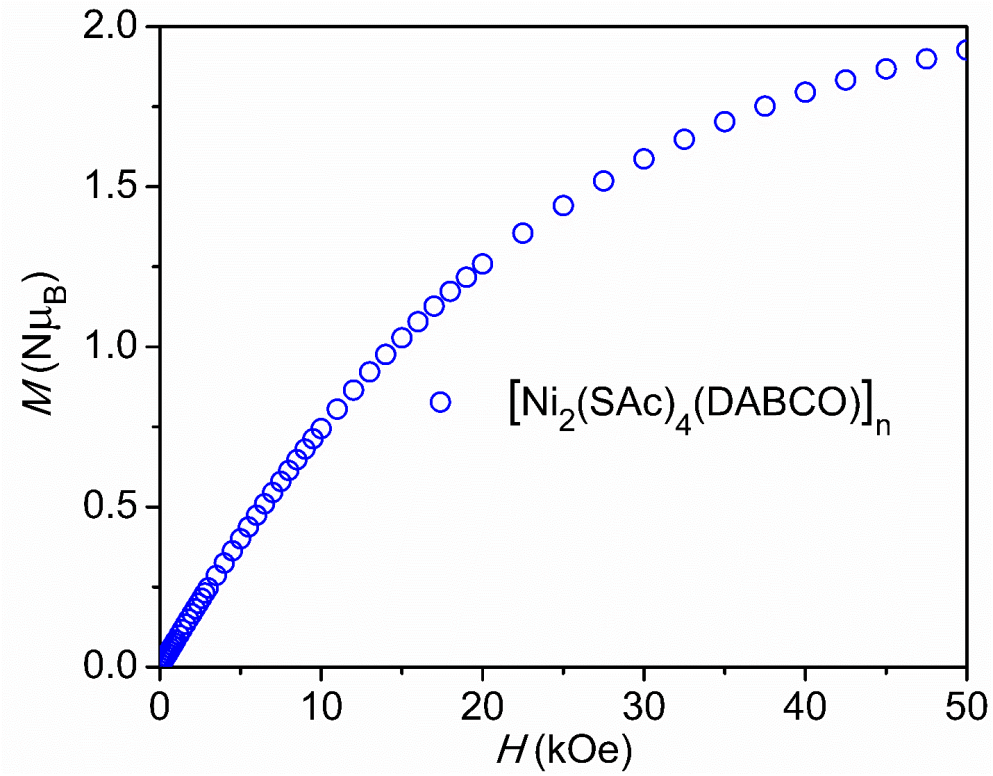

Figure S11. Field dependence of magnetization for $[Ni_2(SAc)_4]_2(DABCO)]_n$, collected at 2 K.

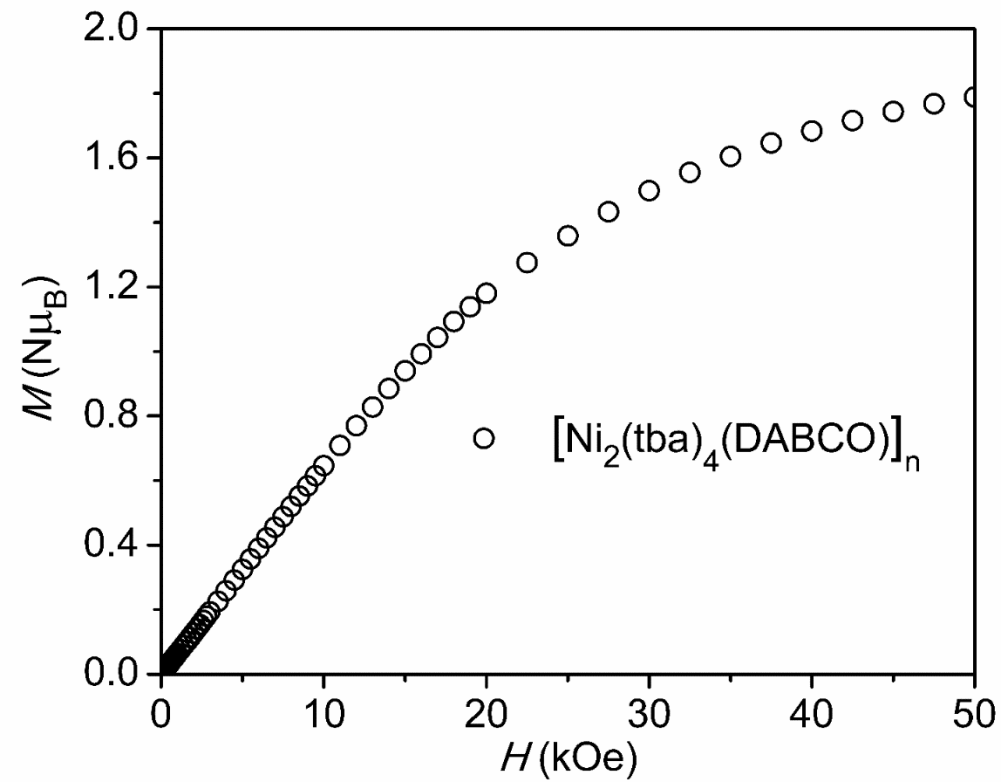

Figure S12. Field dependence of magnetization for $[Ni_2(tba)_4]_2(DABCO)]_n$, collected at 2 K.

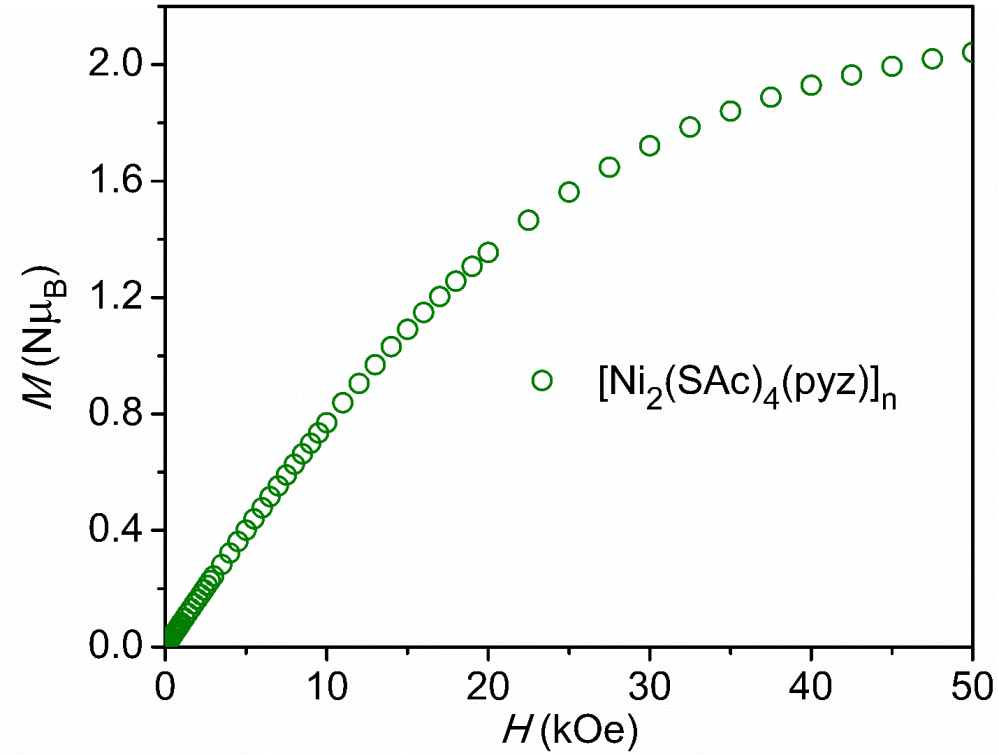

Figure S13. Field dependence of magnetization for $[Ni_2(SAc)_4]_2(pyz)]_n$, collected at 2 K.

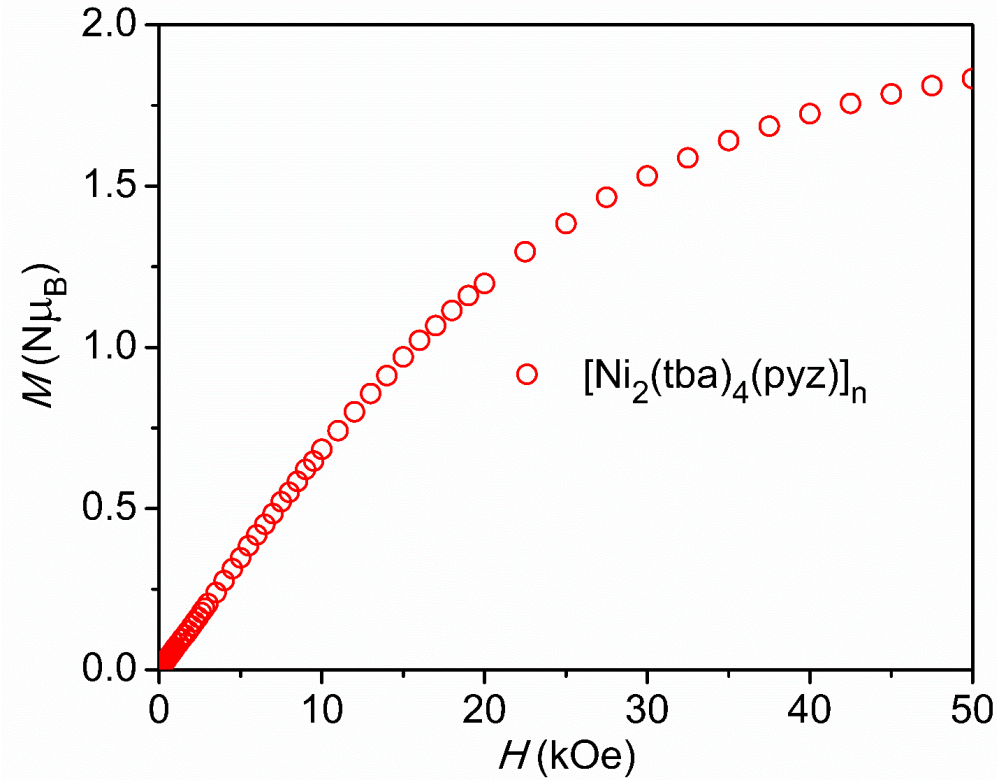

Figure S14. Field dependence of magnetization for $[Ni_2(tba)_4]_2(pyz)]_n$, collected at 2 K.

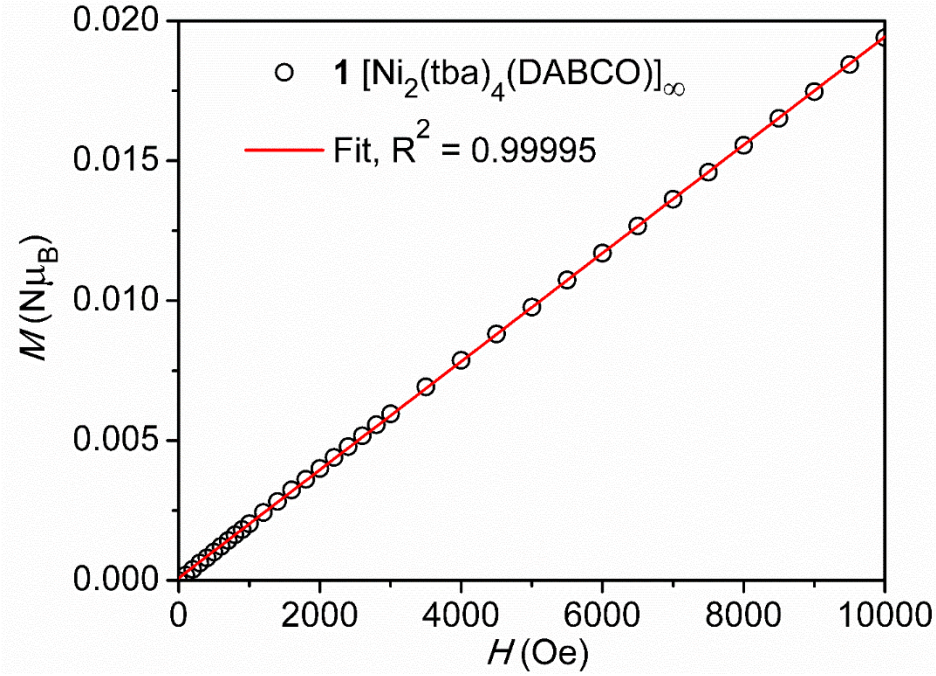

Figure S15. Field dependence of magnetization for $[Ni_2(tba)_4]_2(DABCO)]_\infty$ (**1**), collected at 100 K. Fit: $y = 1.94x10^{-6}(x) + 8.81x10^{-5}$ ($R^2 = 0.99995$)

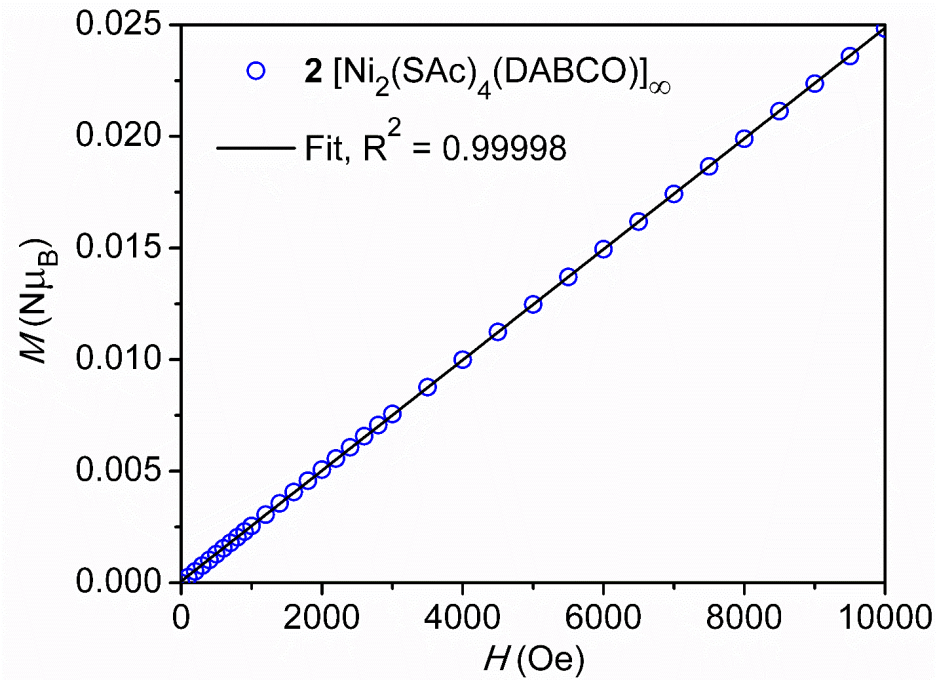

Figure S16. Field dependence of magnetization for $[Ni_2(SAc)_4]_2(DABCO)]_\infty$ (**2**), collected at 100 K. Fit: $y = 2.48x10^{-6}(x) + 6.67x10^{-5}$ ($R^2 = 0.99998$).

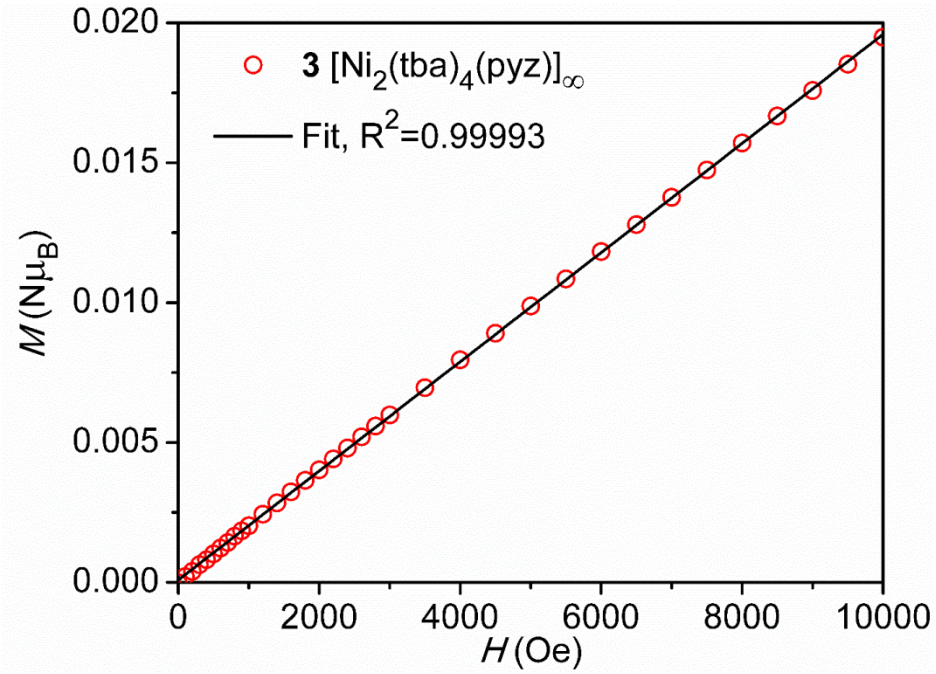

Figure S17. Field dependence of magnetization for $[Ni_2(tba)_4]_2(pyz)]_\infty$ (**3**), collected at 100 K. Fit: $y = 1.95x10^{-6}(x) + 8.37x10^{-5}$ ($R^2 = 0.99993$).

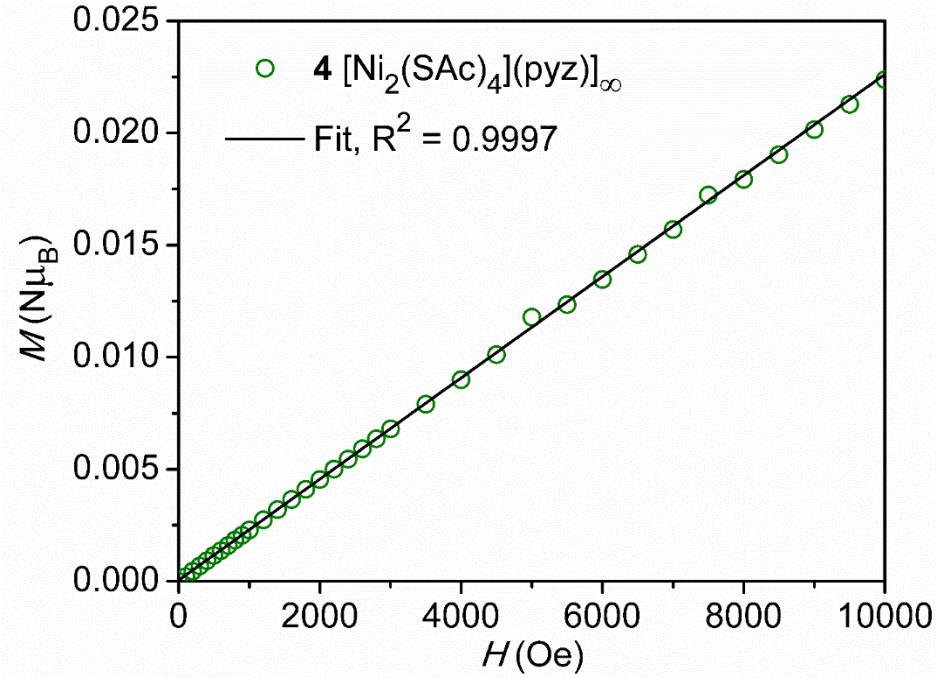

Figure S18. Field dependence of magnetization for $[Ni_2(SAc)_4]_2(pyz)]_\infty$ (**4**), collected at 100 K. Fit: $y = 2.26x10^{-6}(x) + 5.19x10^{-5}$ ($R^2 = 0.9997$).

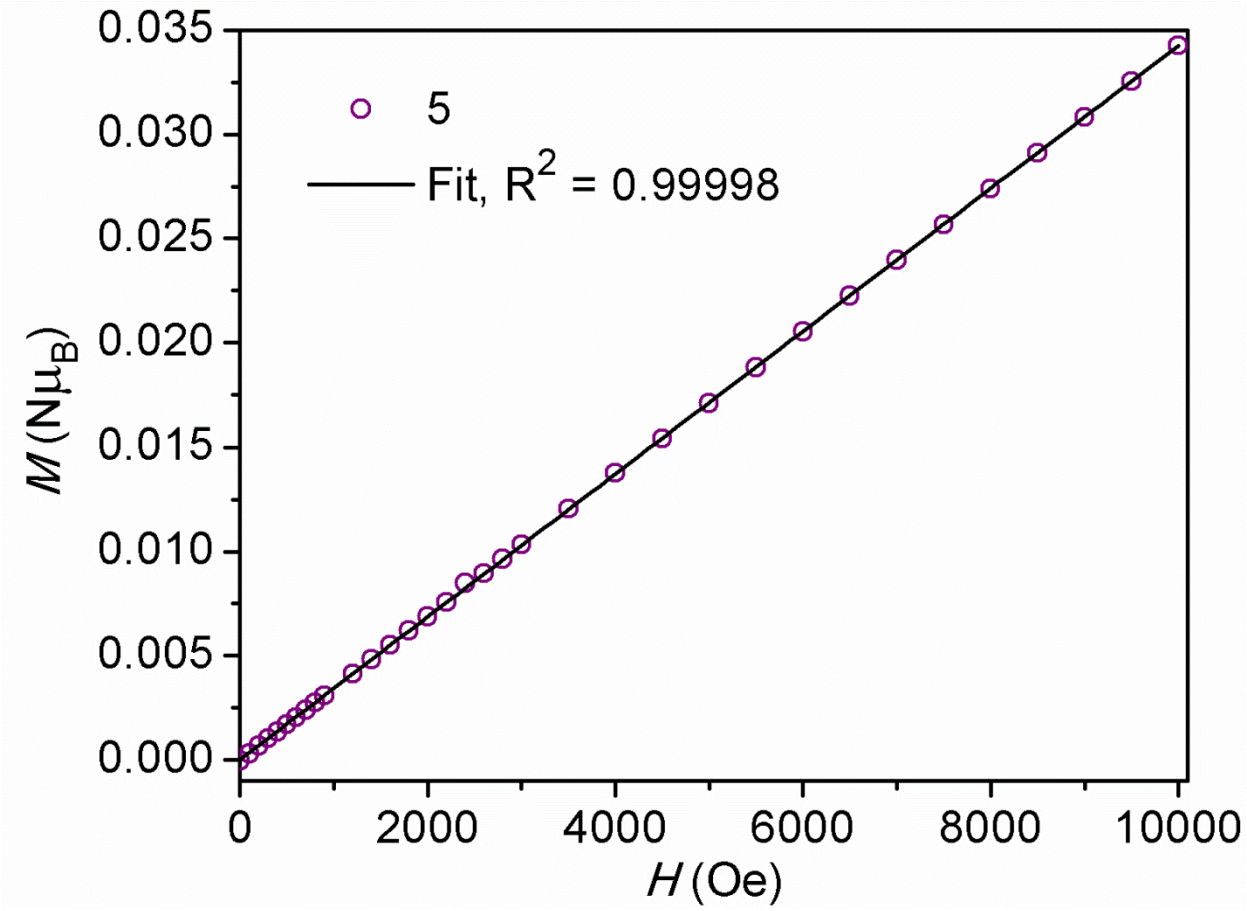

Figure S19. Field dependence of magnetization for $[Ni_2(tba)_4(quin)]$ (**5**), collected at 100 K. Fit: $y = 3.42x10^{-6}(x) + 2.79x10^{-5}$ ($R^2 = 0.99998$)

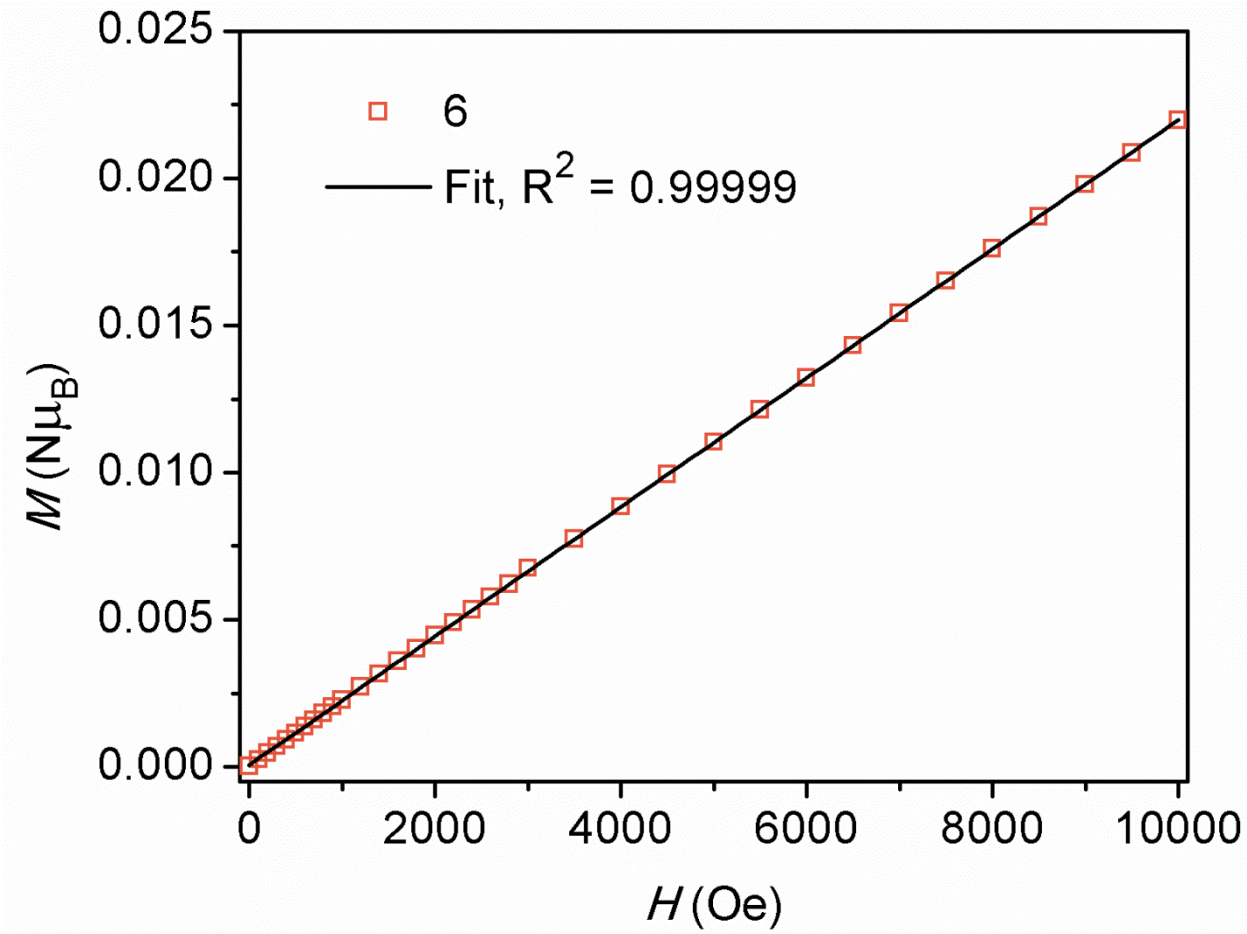

Figure S20. Field dependence of magnetization for $[Ni(tba)_2(py)_2]$ (**6**), collected at 100 K. Fit: $y = 2.19x10^{-6}(x) + 6.00x10^{-5}$ ($R^2 = 0.99999$)

Table S1. Single Crystal X-ray Diffraction Collection Parameters for **2-5**

	2	**3**	**4**	**5**
Chemical formula	$C_{16}H_{12}NNiO_2S_2 \cdot C_3H_6O$	$C_{14}H_{24}N_2Ni_2O_4S_4$	$C_{12}H_{16}N_2Ni_2O_4S_4$	$C_{70}H_{66}N_2Ni_4O_8S_8 \cdot 0.582(CH_2Cl_2)$
Formula weight (g/mol)	431.17	530.01	497.93	1603.72
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
space group	*C*2/*c*	*C*2/*c*	*C*2/*c*	*P*$\bar{1}$
a (Å)	27.620 (6)	13.324 (6)	12.670 (19)	10.9952 (5)
b (Å)	9.630 (2)	9.791 (5)	9.658 (14)	11.5241 (6)
c (Å)	18.507 (4)	16.613 (12)	16.44 (2)	14.5257 (6)
α (°)	90	90	90	82.221 (2)
β (°)	127.04 (3)	110.61 (3)	112.87 (6)	71.516 (1)
γ (°)	90	90	90	88.952 (2)
V (Å^3)	3929.6 (19)	2029 (2)	1854 (5)	1728.94 (14)
Z	8	4	4	1
ρ (calcd), g/cm^{-3}	1.458	1.735	1.784	1.540
μ (mm^{-1})	1.22	2.29	2.50	1.42
Temp, K	100	100	100	100
R(F), %[a]	0.069	0.070	0.058	0.034
R (*wF*^{2}), %[b]	0.207	0.190	0.146	0.073

[a] $R = \Sigma||F_0| - |F_c||/\Sigma|F_0|$. [b] $R(\omega F^2) = \{\Sigma[\omega(F_0^2 - F_c^2)^2]\}/\{\Sigma[\omega(F_0^2)^2]\}^{1/2}$; $\omega = 1/[\sigma^2(F_0^2) + (aP)^2 + bP]$ with *a* and *b* given in CIF, $P = [2F_c^2 + \max(F_0,0)]/3$.

Details of Magnetic Data Fitting Procedures

The Van Vleck equation (simplified) was employed for fitting chains **1**-**4**, assuming isolated Ni_2 units each with $S = 1$:

$$\chi_M T = \frac{N g^2 \beta^2 S(S+1) T}{3k_B T - zJS(S+1)} + TIP$$

Compound **5** was fit as two $S = 1$ centers interacting in a single lantern:

$$\chi_M T = \frac{N g^2 \beta^2}{3k_B} x \frac{2\exp(2x)+10\exp(6x)}{1+3\exp(2x)+5\exp(6x)} + TIP$$

where $x = J/k_B T$.

The Fisher chain model was also employed for fitting chains **1**-**4**:

$$\chi_M T = \frac{N \mu_B g^2}{3k_B} S(S+1) \frac{(1+u)}{(1-u)} + TIP$$

for which $S = 1$ and u is:

$$u = coth\left[\frac{2JS(S+1)}{k_B T}\right] - \left[\frac{k_B T}{2JS(S+1)}\right]$$

For compound **6,** the following spin Hamiltonian was used:

$$\boldsymbol{H} = g\beta \hat{S} \hat{H} + D\left[\widehat{S_z}^2 - S(S+1)/3\right] + E(\widehat{S_x}^2 - \widehat{S_y}^2)$$

Table S2. Results from fitting magnetic susceptibility of 1-6 with PHI.

entry	compound	g_{iso}	zJ (cm^{-1})	TIP * ($cm^3 mol^{-1}$)	R^2	$\|D\|$ (cm^{-1})	$\|E\|$ (cm^{-1})
1	**1** (tba DABCO)	2.13	-0.081	0.00060	0.98469	-	-
2	**2** (tba pyz)	2.15	-0.093	0.00045	0.99662	-	-
3	**3** (SAc DABCO)	2.36	-0.11	0.00060	0.99923	-	-
4	**4** (SAc pyz)	2.26	-0.11	0.00045	0.99923	-	-
5	**1** (tba DABCO)	2.13	-0.076	0.00060	0.99515	2.2	0.14
6	**2** (tba pyz)	2.14	-0.045	0.00045	0.99932	0.033	0.045
7	**3** (SAc DABCO)	2.36	-0.076	0.00060	0.99941	1.4	0.077
8	**4** (SAc pyz)	2.23	-0.11	0.00045	0.99923	0.051	0.11
9	**5**	2.00, 2.07	J_{ex} = -2.2	0.00020	0.99394	-	-
10	**6**	2.21	-	0.0060	0.99801	3.2	0.026

* TIP value was held constant.

When ZFS parameters (D, E) were included in fits (entries 5-8), the values obtained for the pyz-bridged species were found to be negligibly small and should be reordered so that $|E| < 0.33*|D|$. Even in the case where reasonable parameters are obtained, the negligible improvement of the overall fit does not justify the inclusion of additional terms.

Table S3. Results from fitting magnetic susceptibility of 1-4 with FC model.

	g_{iso}	J (cm^{-1})	TIP ($cm^3\ mol^{-1}$)	R^2
1 (tba DABCO)	2.13	-0.13	0.000584	0.97742
2 (tba pyz)	2.15	-0.17	0.000415	0.98777
3 (SAc DABCO)	2.35	-0.17	0.000649	0.99443
4 (SAc pyz)	2.24	-0.16	0.000551	0.99729

Table S4. Summary of $[Ni_2(EE'CR)_4]$ Structural Parameters

CSD code	Ni…Ni (Å)	Ni-Ni-L (°)	E,E	Magnetism	Reference
ABIZUI	2.733	160.846	O,O	No meas	*Bioinorg. Chem. Appl.*, **2010**, *v2010*, 178034.
AZAYEF	2.693	175.717	O,O	No meas	*Russ.J.Inorg.Chem.*, **2008**, *48*, 1476.
BAZBIO	2.654	176.69	O,O	No meas	*Inorg. Chim. Acta.*, **2003**, *353*, 151.
BAZBIO01	2.635	175.554	O,O	No meas	*J. Inorg. Organomet. Polym.*, **2008**, *17*, 259.
DUSHEG	2.649	180	O,O	No meas	*Dalton Trans.*, **2016**, *45*, 4269.
EZOFEF	2.713	180	O,O	No meas	*Inorg. Chem.*, **2011**, *50*, 5085.
EZOFOP	2.846	180	O,O	No meas	*Inorg. Chem.*, **2011**, *50*, 5085.
FUGLUP	2.606	173.66	O,O	No meas	*Acta Crystallogr. Sect. E: Struct. Rep. Online*, **2009**, *65*, m1484.
FUZFAJ	2.752	158.856	O,O	No meas	*Chem.-Eur.J.*, **2015**, 21, 16593.
ICAROV	2.67	180	O,O	No meas	*Chem.-Eur.J.*, **2011,** 17, 13007.
IDOMOD	2.575	176.71	O,O	No meas	*Inorg.Chem.*, **2002**, *41*, 521.
KUGZOB	2.72	160.835	O,O	No meas	*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **1992**, 48, 1888.
KUGZUH	2.765	165.013	O,O	No meas	*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **1992**, 48, 1888.
KUHBEU	2.734	165.7	O,O	No meas	*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **1992**, 48, 1888.
KUHBIY	2.723	166.003	O,O	No meas	*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **1992**, 48, 1888.
KUHBOE	2.717	169.459	O,O	No meas	*Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, **1992**, 48, 1888.
MACNIA	2.754	no report	O,O	No meas	*Inorg. Chim. Acta.*, **1980**, *40*, 115.
MESTEK	2.623	173.09	O,O	No meas	*Angew. Chem., Int. Ed.*, **2006**, *45*, 281.
MESTEK	2.613	177.83	O,O	No meas	*Angew. Chem., Int. Ed.*, **2006**, *45*, 281.
MESTEK	2.616	174.681	O,O	No meas	*Angew. Chem., Int. Ed.*, **2006**, *45*, 281.
MIFYEG	2.61	170.324	O,O	No meas	*Angew. Chem., Int. Ed.*, **2006**, *45*, 281.
MIFYEG	2.597	171.281	O,O	No meas	*Angew. Chem., Int. Ed.*, **2006**, *45*, 281.
MIXZIC	2.622	172.07	O,O	No meas	*Acta Crystallogr. Sect. E: Struct. Rep. Online*, **2002**, *58*, m242.
QEQYIU	2.497	177.562	O,O	No meas	*Russ.Chem.Bull.*, **1915**, 2000.
RAGPUM	2.758	161.491	O,O	No meas	*Russ.Chem.Bull.*, **2000**, *49*, 1887.
SUWYEQ	2.542	175.87	O,O	No meas	*Dalton Trans.*, **2016**, *45*, 1638.
TEDROK	2.849	178.935	O,O	No meas	*Inorg. Chim. Acta.*, **2006**, *359*, 3104.
WUNSEF	2.683	171.12	O,O	No meas	*Russ.J.Coord.Chem.*, **2015**, *41*, 182.
DUCJIW	2.694	165.166	O,O	AF	*Chem. Commun.*, **2015**, 51, 9479.
KOPVIW	2.651	175.154	O,O	strong AF	*Inorg. Chim. Acta.*, **2015**, *424*, 176.
KOPVIW	2.7	171.89	O,O	strong AF	*Inorg. Chim. Acta.*, **2015**, *424*, 176.
NOYHUG	2.627	179.722	O,O	strong paramagnet	*J.Chin.Chem.Soc.(Taipei, Taiwan)*, **2014**, 61, 1326.

CSD code	Ni…Ni (Å)	Ni-Ni-L (°)	E,E	Magnetism	Reference
PACGIL	2.645	172.934	O,O	AF	*Z.Anorg.Allg.Chem.*, **2010**, *636*, 1441.
PEBPAN	2.708	166.646	O,O	AF	*Acta Chem.Scand.*, **1990,** *44*, 984.
POKREM	2.752	172.423	O,O	AF	*Acta Chem.Scand.*, **1990,** *44*, 984.
POKREM	2.765	166.639	O,O	AF	*Acta Chem.Scand.*, **1990,** *44*, 984.
SUVNEE	2.824	180	O,O		*Chem. Commun.*, **2016**, 52, 2079.
TAXGOP	2.588	178.018	O,O	levels with S=1/2 and S=3/2 of the single {Cr7Ni} wheels	*Angew. Chem., Int. Ed.*, **2005**, *44*, 6496.
WEJQOR	2.604	176.738	O,O	AF	*Inorg.Chem*., **1999**, *38*, 3764.
WEJQUX	2.726	168.296	O,O	AF	*Inorg.Chem*., **1999**, *38*, 3764.
WEJVIQ	2.728	177.719	O,O	AF	*Inorg.Chem*., **1999**, *38*, 3764.
GODCAF	2.508	170.134	S,O	No meas	*Inorg. Chim. Acta*., **2014**, *411*, 119.
NMTBZE	2.49	No report	S,O	No meas	*J. Chem. Soc. D*, **1969**, 697.
NUGROY	2.511	179.525	S,O	No meas	*J. Catal.*, **2015**, *329*, 22.
NUGROY	2.506	177.675	S,O	No meas	*J. Catal.*, **2015**, *329*, 22.
NMTBZE01	2.503	178.17	S,O	AF	*Inorg.Chem*., **1970**, *9*, 1116.
NMTBZE02	2.5	168.234	S,O	AF	*Inorg. Chim. Acta*., **2014**, *411*, 119.
DATPOD	2.514	180	S,S	No meas	*Mol.Cryst.Liq.Cryst.*, **1985**, *120*,p381.
DEPPAP	2.564	165.69,168.85	S,S	No meas	*Inorg. Chem.*, **1985**, *24*, 2815.
DTPANI10	2.551	180	S,S	No meas	*J.Chem.Soc.,Dalton Trans.*, **1977**, 2315.
NECZEB	2.527	180	S,S	No meas	*Inorg. Chem.*, **2006**, *45*, 322.
DATPOD10	2.514	180	S,S	χ(a) -7.00 x 10^{-3}	*Inorg. Chem.*, **1985**, *24*, 2815.
FUFJUM	2.548	180	S,S		*Inorg. Chem.*, **2009**, *48*, 6680.
FUFJUM01	2.539	179.972	S,S		*Inorg. Chem.*, **2009**, *48*, 6680.
FUFKAT	2.5419	180	S,S		*Inorg. Chem.*, **2009**, *48*, 6680.
FUFKAT01	2.5385	180	S,S		*Inorg. Chem.*, **2009**, *48*, 6680.
FUFKAT02	2.532	180	S,S		*Inorg. Chem.*, **2009**, *48*, 6680.
FUFKEX	2.5424	180	S,S		*Inorg. Chem.*, **2009**, *48*, 6680.

Further Details on Computational Studies

All geometries were optimized at the PBE0[1]/TZVP[2]/ZORA[3] level using the Orca[4] electronic structure program. The highly efficient resolution-of-identity (RI) algorithm applied using the chain-of-sphere approach (RIJCOSX[5]) was used to help speed up calculations. Geometries of monomeric lanterns were optimized at the quintet, triplet, and singlet multiplicities. In addition, optimizations were performed with broken symmetry wavefunctions at the BS(2,2), BS(3,1), and BS(1,1) levels. All structures (**1A**-**5A**) were verified as local minima based on the lack of imaginary frequencies observed after harmonic analysis of the Hessian. The coordinates for **1A**-**5A** are shown in Tables S34-S63. Relative energies are summarized in Table S5 based on single point PBE0/TZVP/ZORA calculations with the one-center approximation turned off. The triplet geometries for **1A**-**5A** are compared to experimental geometries in Table S6. The spin densities for each species are displayed in Figures S21-S40 for the quintet, triplet, singlet, and BS(2,2) states. All isosurfaces were generated and displayed with Chemcraft (http://www.chemcraftprog.com) using a contour of 0.005 for spin densities and 0.03 for orbitals. The Löwdin and Mulliken spin populations for the triplet state of **1A**-**5A** are summarized in Tables S7-S11 with the labeling scheme shown in Scheme S1. The natural spin populations with specific orbital contributions calculated at the PBE0/cc-pVTZ//PBE0/TZVP/ZORA level are shown in Tables S12-S16.

Delocalizations between the d-orbitals on the metal centers in **1A**-**5A** were analyzed using second-order perturbation theory in the NBO basis based on the first order density matrix calculated at the PBE0/cc-pVTZ level. NBO 5.9[6] was used as implemented in Firefly 8.1[7]. Interactions between the filled $3d_{z^2}$ on the thio-ligated nickel center and the singly-occupied $3d_{z^2}$ on the oxo-ligated nickel center are summarized in Figures S41-S45.

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[1] (a) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1997**, 78, 1396;
(b) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **1996**, 77, 3865.

[2] D. A. Pantazis, X. Y. Chen, C. R. Landis, F. Neese, *J. Chem. Theory Comput.* **2008**, 4, 908

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[6] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, F. Weinhold, *NBO 5.9*, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, 2012; http://www.chem.wisc.edu/~nbo5

[7] A. A. Granovsky, *Firefly version 8.1.0*, http://classic.chem.msu.su/gran/firefly/index.html.

The lantern dimers (**1B-4B**) were each optimized at the PBE0/TZVP/ZORA level with a quintet spin multiplicity. Broken symmetry solutions for the optimized structures were obtained at the BS(2,2) level. All isotropic magnetic exchange couplings reported use the Noodleman scheme[8], based on the Hamiltonian $\widehat{H} = -2JS_AS_B$.

Geometries of **1B-4B** are shown in Tables S64-S67. An energetic summary including calculated exchange couplings are shown in Table S17. The non-orthogonal corresponding orbitals are shown in Figures S46-S49. Spin populations are shown in Tables S18-S25. The labeling scheme for the di-lanterns is defined in Scheme S2.

DFT calculations of ZFS parameters and g-tensors were performed for **1A-5A** with a triplet multiplicity. The calculations were performed at the PBE0/TZVP/ZORA level in Orca with the RIJCOSX approximation employed. The coupled-perturbed (CP)[9] scheme was used for the calculations, and the gauge origin was chosen to be the center of electron charge. The gauge was also tested at the magnetic Ni(II) center, and little discrepancy was observed (Table S26).

NEVPT2 calculations[10] were also used to verify DFT calculations of SOC and the g-tensors. We felt this was particularly necessary in light of the work of Kubica et al.[11] who showed that DFT calculations of ZFS can be unreliable for Ni(II) centers using the TZVP basis set. We have limited our active space to the magnetic center containing the five d-orbitals correlated with 8 electrons, and the wavefunction was state-averaged over 10 triplet states and 15 singlet states.

We have used the strongly contracted form of NEVPT2 which is based on the Dyall zeroth order Hamiltonian[12]. This Hamiltonian differs from the usual projected Fock operators in that it contains some additional two-electron terms. NEVPT2 has the desirable properties of size-consistency and a lack of intruder states. The ZFS parameters were calculated through quasi-

[8] (a) A. P. Ginsberg, *J. Am. Chem. Soc.* **1980**, 102, 111
(b) L. Noodleman, *J. Chem. Phys.* **1981**, 74, 5737
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[9] (a) F. Neese, *J. Chem. Phys.* **2007**, 127, 164112
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[10] (a) C. Angeli, R. Cimiraglia, S. Evangelisti, T. Leininger, J. P. Malrieu, *J. Chem. Phys.* **2001**, 114, 10252.
(b) C. Angeli, R. Cimiraglia, J. P. Malrieu, *Chem. Phys. Lett.* **2001**, 350, 297.
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(d) C. Angeli, R. Cimiraglia, J. P. Malrieu, *J. Chem. Phys.* **2002**, 117, 9138
[11] A. Kubica, J. Kowalewski, D. Kruk, M. Odelius, *J. Chem. Phys.* **2013**, 138, 064304
[12] K. G. Dyall, *J. Chem. Phys.* **1995**, 102, 4909

degenerate perturbation theory (QDPT)[13], and the Breit-Pauli SOC operator was approximated with the spin-orbit mean-field approach (SOMF)[14]. The effective Hamiltonian theory[15] was used when presenting results. Based on the low magnitude of the SSC contribution to the ZFS observed in the DFT results, the SSC contributions were omitted for the NEVPT2 ZFS parameters.

The g-values for **1A**-**5A** are compared with experiment in Table S26. The calculated ZFS parameters are summarized in Table S27. The list of contributions to the ZFS are shown in Tables S28-S32.

An alternative wavefunction for the lanterns corresponds to each of the nickel centers being in a high-spin configuration, with the spin density primarily localized in the $3d_{x^2-y^2}$ orbitals. To estimate the relative energy of this wavefunction NEVPT2(4,4) calculations were done. The active space included the magnetic Ni(II) d-orbitals correlated with 4 electrons. The magnetic orbitals were the $3d_{x^2-y^2}$ and $3d_{z^2}$ on each metal center. A state-averaged CASSCF(4,4) wavefunction was used for the subsequent NEVPT2 calculation. The relative energies are summarized in Table S33.

[13] D. Ganyushin, F. Neese, *J. Chem. Phys.* **2006**, 125, 024103.
[14] F. Neese, *J. Chem. Phys.* **2005**, 122, 034107.
[15] R. Maurice, R. Bastardis, C. de Graaf, N. Suand, T. Mallah, N. Guihery, *J. Chem. Theor. Comput.* **2009**, 5, 2977

Table S5. Relative energies of **1A**-**5A** with the quintet, triplet, singlet, BS(3,1), BS(2,2), and BS(1,1) wavefunctions (kcal/mol).

	S = 2	**S = 1**	**S = 0**	**BS(3,1)**	**BS(2,2)**	**BS(1,1)**
1A	2.0	0.0	15.9	14.7	0.3	15.9
2A	5.2	0.0	16.0	14.4	2.6	15.8
3A	2.8	0.0	33.0	15.9	1.2	15.9
4A	5.7	0.0	33.6	15.0	3.2	16.0
5A	20.6	0.0	16.0	N/A	19.3	16.0

Table S6. Summary of geometries for triplet states of **1A**-**5A**. All distances in Å and angles in degrees.

	1A	**2A**	**2**-Expt.	**3A**	**3**-Expt.	**4A**	**4**-Expt	**5A**	**5**-Expt.
Ni-Ni	2.565	2.509	2.5316	2.589	2.595	2.525	2.540	2.524	2.575
Ni-O (avg.)	2.042	2.037	2.017	2.044	1.953	2.042	2.099	2.043	2.037
Ni-S (avg.)	2.236	2.243	2.2282	2.238	2.264	2.243	2.205	2.224	2.224
Ni{O4}-N	2.152	2.086	2.057	2.160	2.164	2.087	2.126	2.130	2.124
Ni{S4}-N	2.601	2.321	2.262	2.577	2.434	2.307	2.240	N/A	N/A
Ni-Ni-N	176.9	179.7	180.0	176.9	180.0	179.3	180.0	177.1	175.5
O-Ni-Ni-S	23.8	22.1	19.5	22.3	22.9	22.0	18.5	24.3	22.8

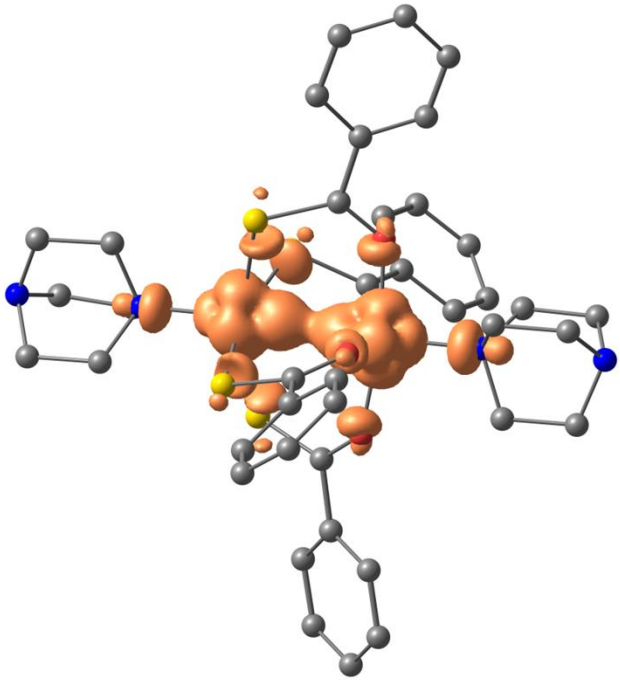

Figure S21. Spin density for the quintet state of **1A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

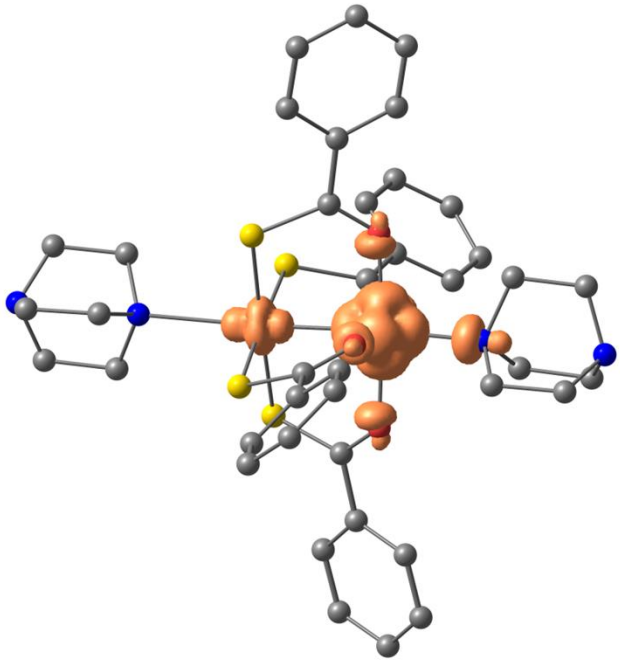

Figure S22. Spin density for the triplet state of **1A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

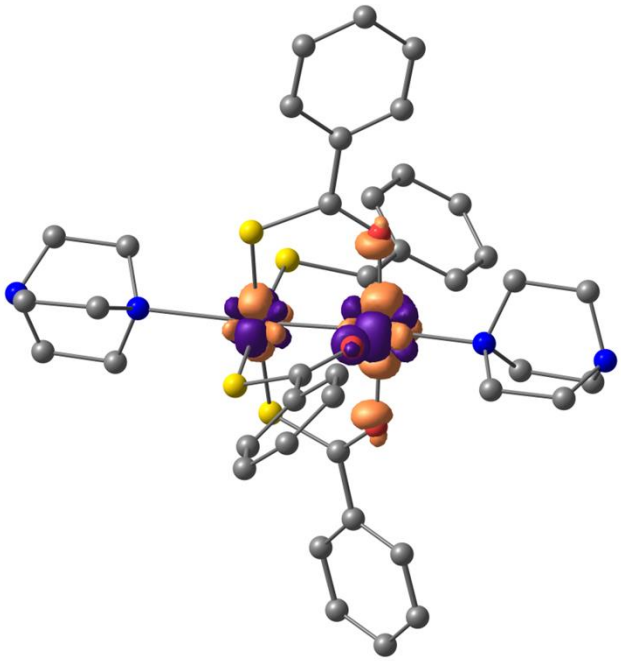

Figure S23. Spin density for the (unrestricted) singlet state of **1A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

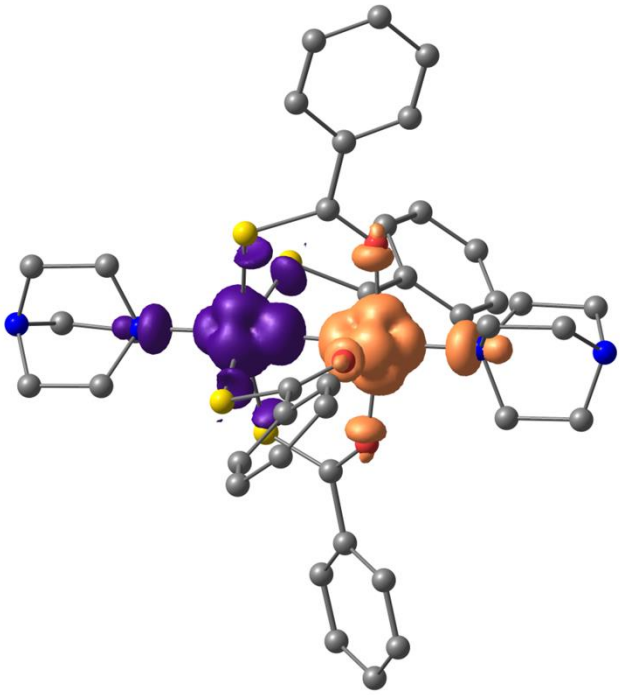

Figure S24. Spin density for the BS(2,2) state of **1A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

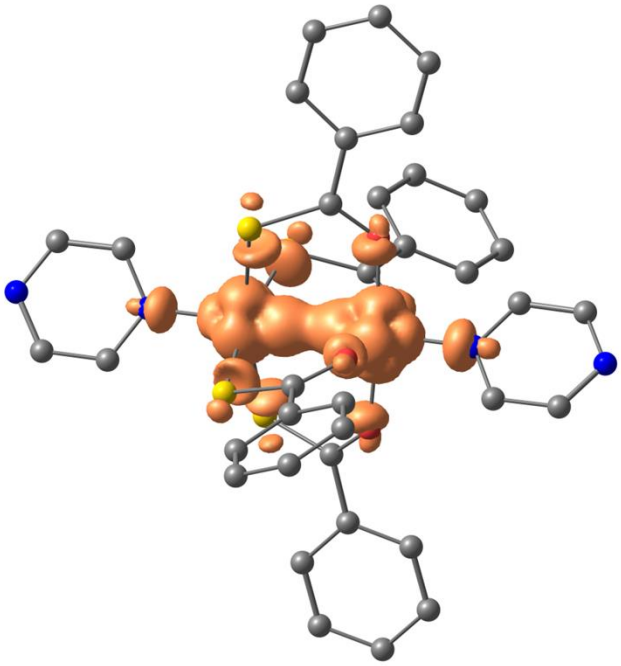

Figure S25. Spin density for the quintet state of **2A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

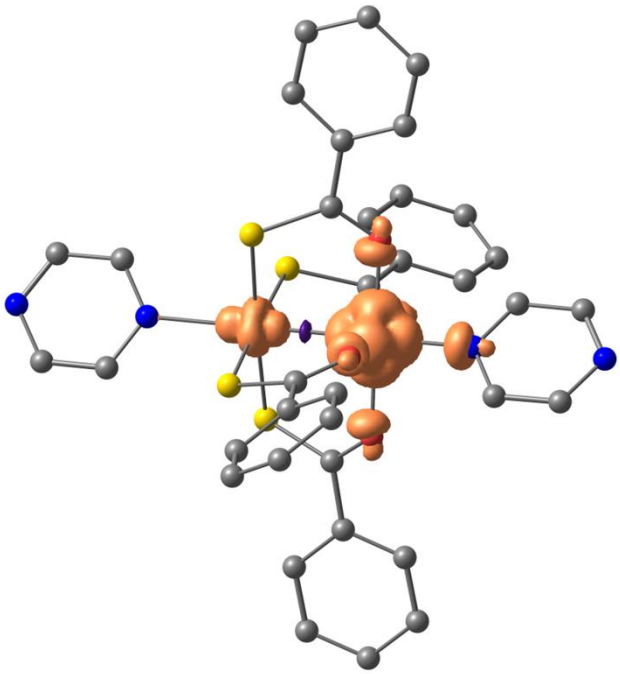

Figure S26. Spin density for the triplet state of **2A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

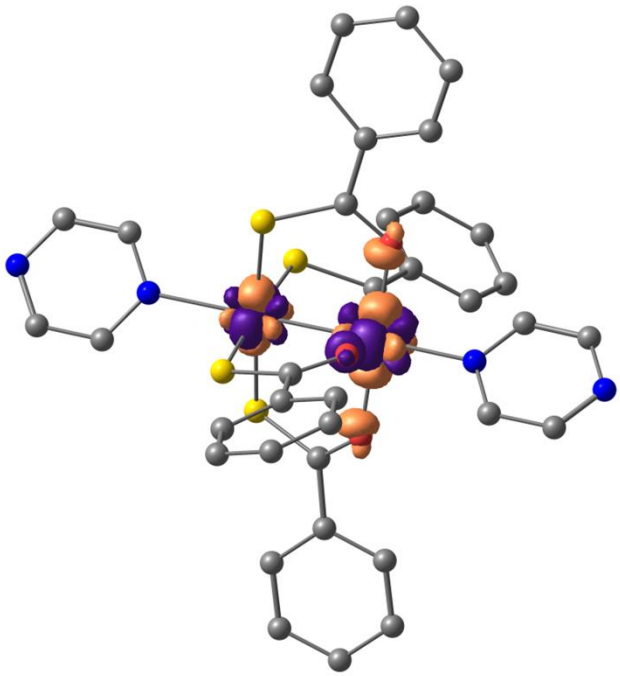

Figure S27. Spin density for the (unrestricted) singlet state of **2A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

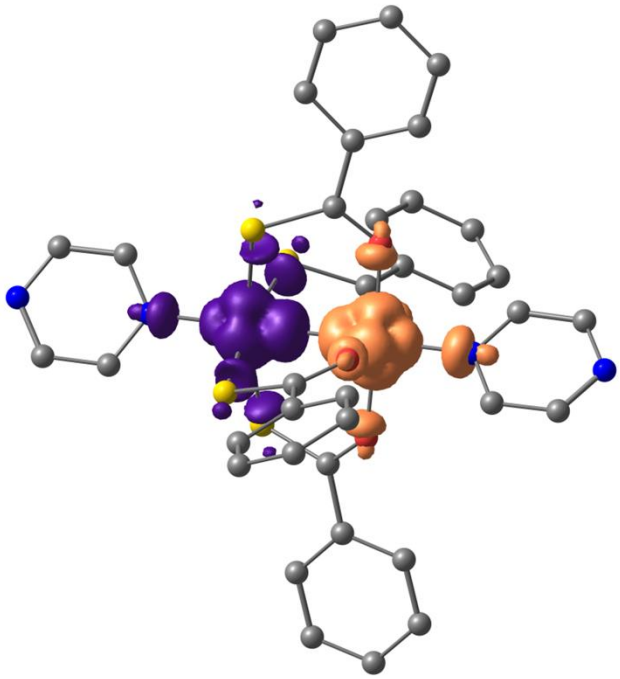

Figure S28. Spin density for the BS(2,2) state of **2A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

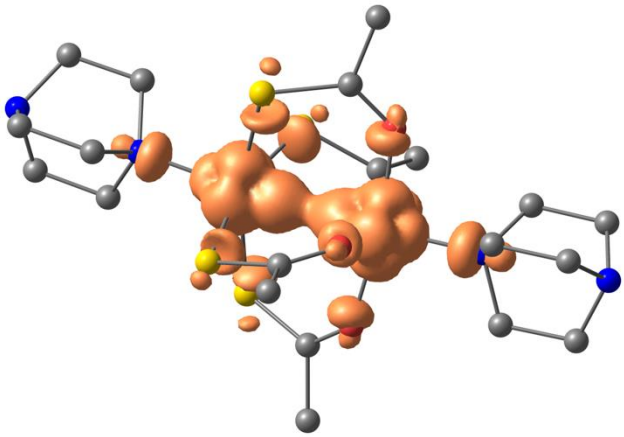

Figure S29. Spin density for the quintet state of **3A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

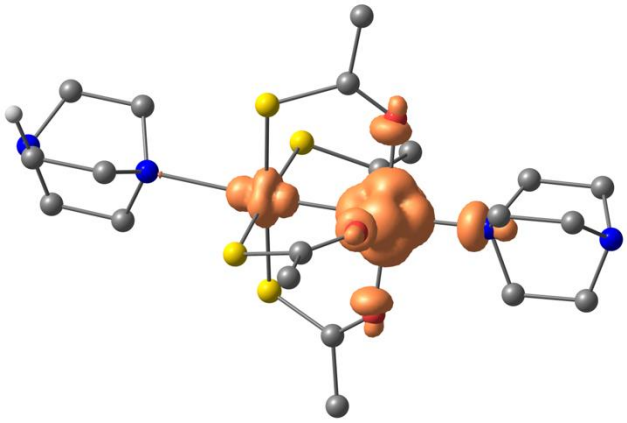

Figure S30. Spin density for the triplet state of **3A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

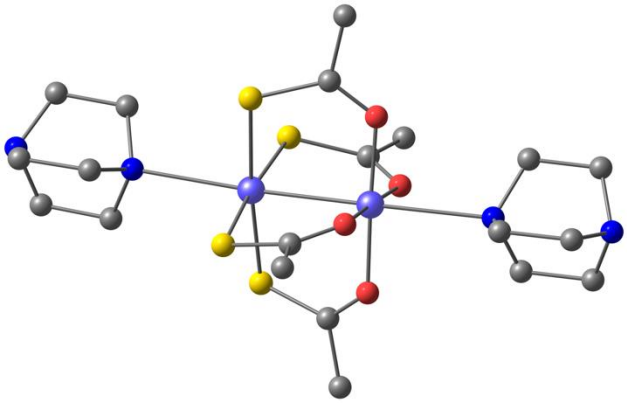

Figure S31. Spin density for the (unrestricted) singlet state of **3A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

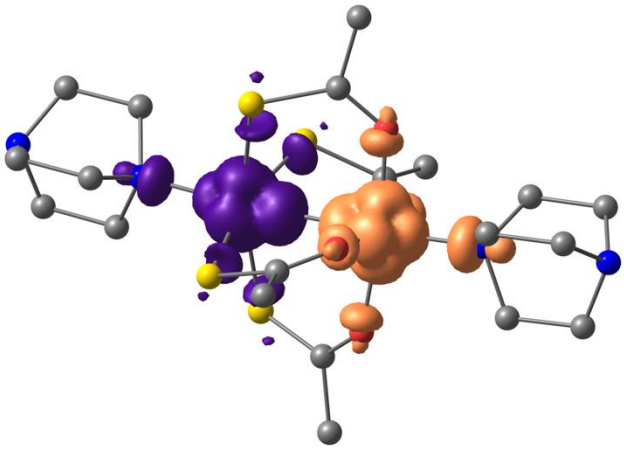

Figure S32. Spin density for the BS(2,2) state of **3A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

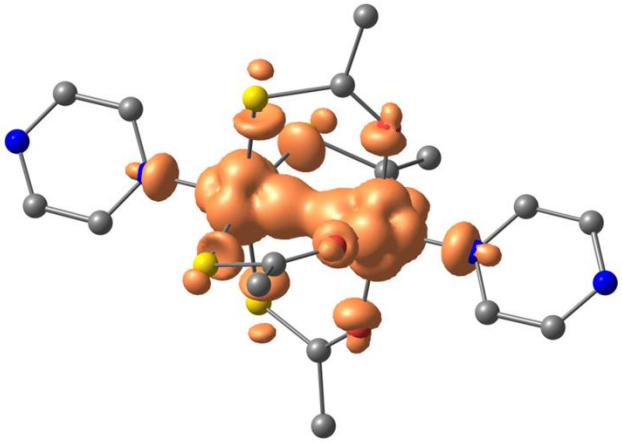

Figure S33. Spin density for the quintet state of **4A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

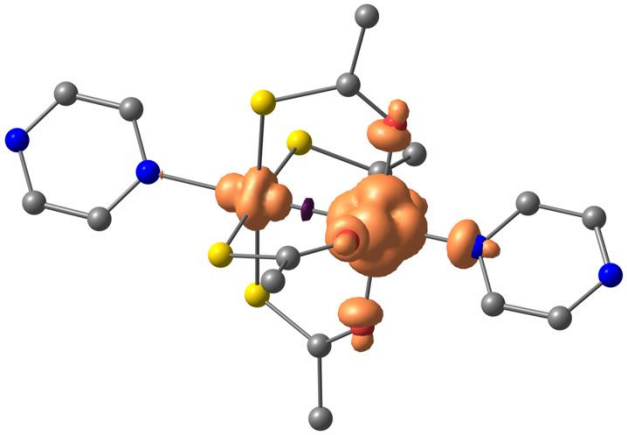

Figure S34. Spin density for the triplet state of **4A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

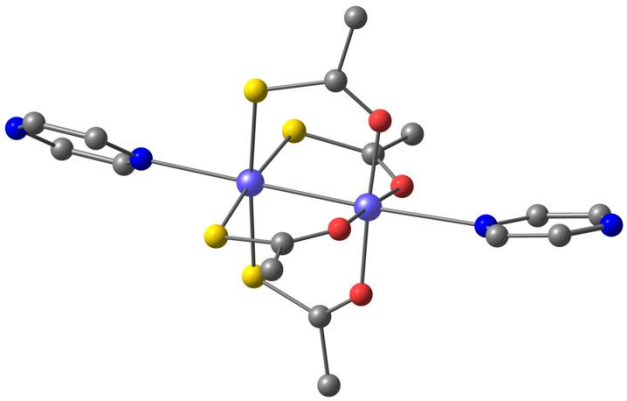

Figure S35. Spin density for the (unrestricted) singlet state of **4A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

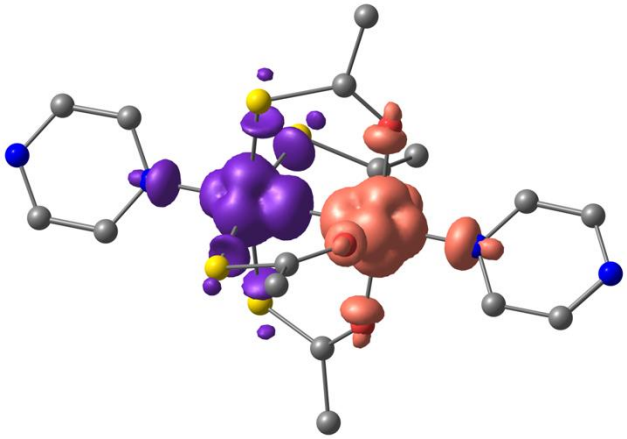

Figure S36. Spin density for the BS(2,2) state of **4A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

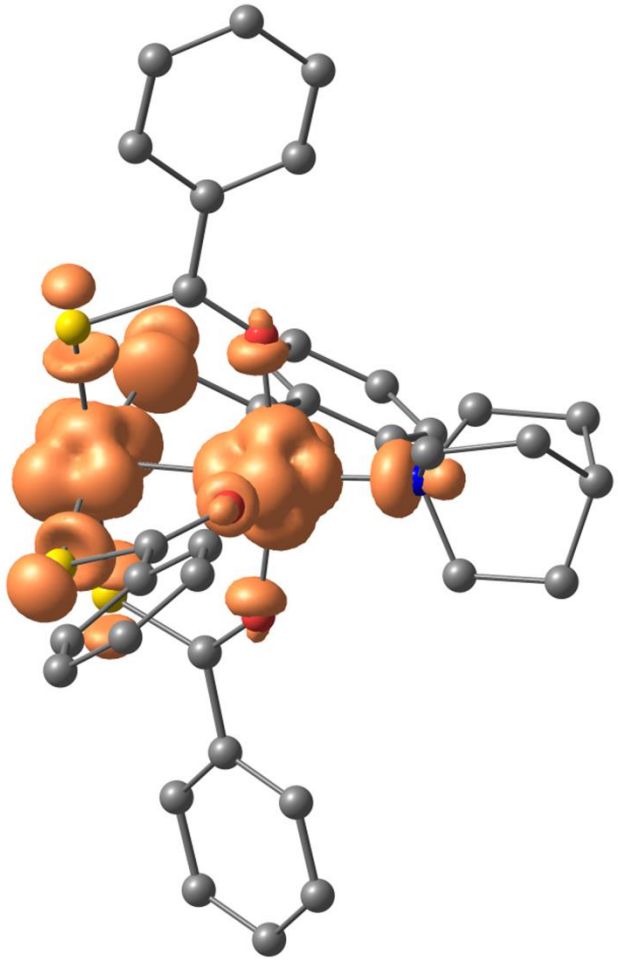

Figure S37. Spin density for the quintet state of **5A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

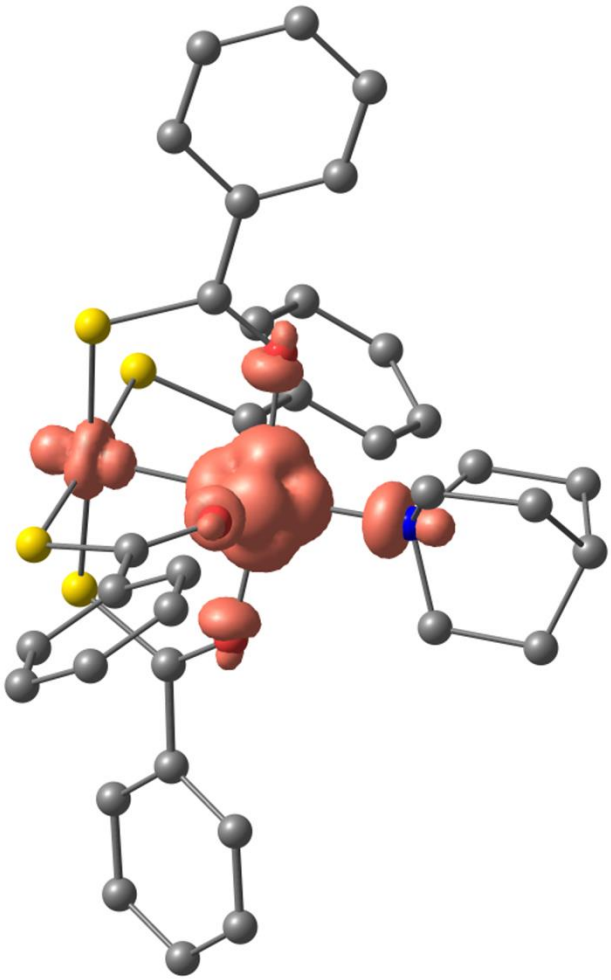

Figure S38. Spin density for the triplet state of **5A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

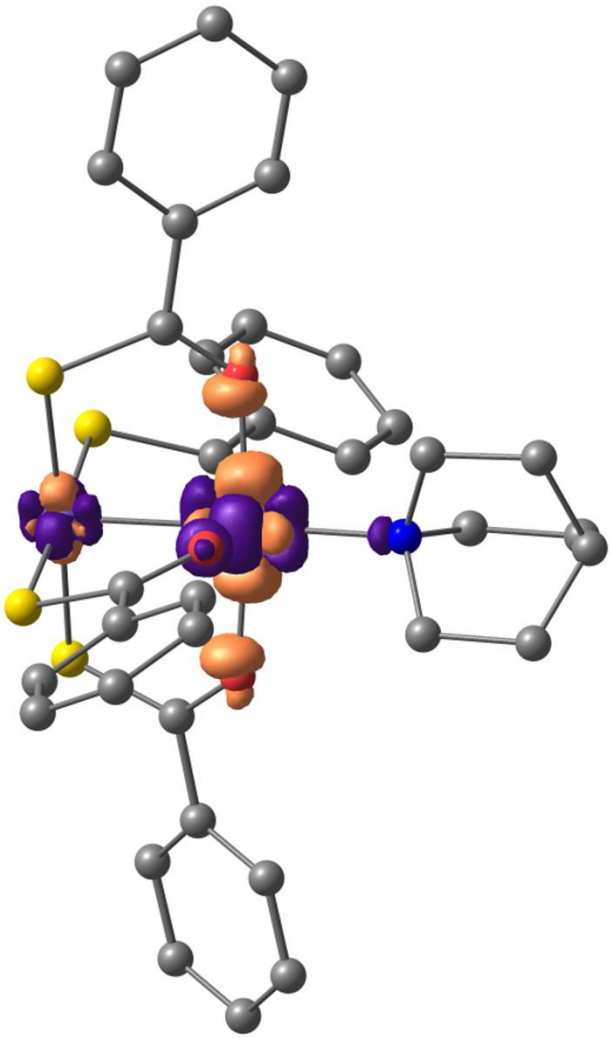

Figure S39. Spin density for the (unrestricted) singlet state of **5A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

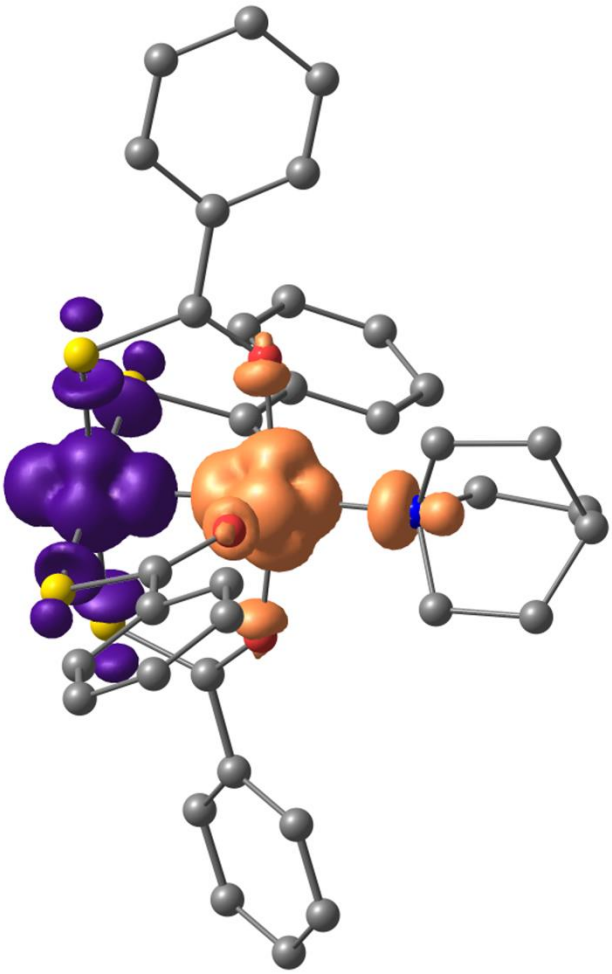

Figure S40. Spin density for the BS(2,2) state of **5A** with an isosurface of 0.005. Hydrogen atoms are omitted for clarity.

Scheme S1. Labeling scheme used throughout.

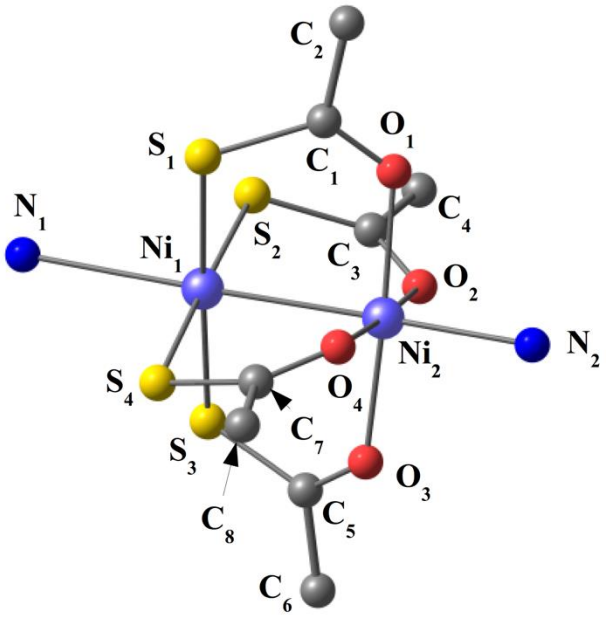

Table S7. Mulliken and Löwdin spin populations for **1A**.

Mulliken				**Löwdin**			
Ni_1	0.092	N_1	0.008	Ni_1	0.103	N_1	0.009
Ni_2	1.668	N_2	0.066	Ni_2	1.667	N_2	0.060
S_1	0.004	C_1	-0.003	S_1	0.002	C_1	-0.001
S_2	0.006	C_2	0.004	S_2	0.002	C_2	0.003
S_3	0.005	C_3	-0.004	S_3	0.002	C_3	-0.001
S_4	0.004	C_4	0.004	S_4	0.001	C_4	0.003
O_1	0.037	C_5	-0.003	O_1	0.036	C_5	-0.002
O_2	0.036	C_6	0.004	O_2	0.035	C_6	0.003
O_3	0.037	C_7	-0.003	O_3	0.036	C_7	-0.002
O_4	0.038	C_8	0.004	O_4	0.037	C_8	0.003

Table S8. Mulliken and Löwdin spin populations for **2A**.

Mulliken				**Löwdin**			
Ni_1	0.116	N_1	0.008	Ni_1	0.129	N_1	0.010
Ni_2	1.666	N_2	0.054	Ni_2	1.657	N_2	0.049
S_1	0.003	C_1	-0.005	S_1	0.000	C_1	-0.002
S_2	0.003	C_2	0.005	S_2	0.000	C_2	0.003
S_3	0.003	C_3	-0.007	S_3	0.000	C_3	-0.003
S_4	0.003	C_4	0.004	S_4	0.000	C_4	0.002
O_1	0.040	C_5	-0.005	O_1	0.039	C_5	-0.002
O_2	0.041	C_6	0.004	O_2	0.039	C_6	0.003
O_3	0.040	C_7	-0.006	O_3	0.039	C_7	-0.003
O_4	0.040	C_8	0.004	O_4	0.039	C_8	0.002

Table S9. Mulliken and Löwdin spin populations for **3A**.

Mulliken				**Löwdin**			
Ni_1	0.093	N_1	0.008	Ni_1	0.105	N_1	0.010
Ni_2	1.668	N_2	0.065	Ni_2	1.665	N_2	0.059
S_1	0.004	C_1	-0.003	S_1	0.001	C_1	-0.002
S_2	0.004	C_2	0.002	S_2	0.001	C_2	0.002
S_3	0.003	C_3	-0.003	S_3	0.001	C_3	-0.002
S_4	0.003	C_4	0.002	S_4	0.001	C_4	0.002
O_1	0.037	C_5	-0.003	O_1	0.037	C_5	-0.002
O_2	0.038	C_6	0.002	O_2	0.037	C_6	0.002
O_3	0.037	C_7	-0.003	O_3	0.037	C_7	-0.002
O_4	0.037	C_8	0.002	O_4	0.037	C_8	0.002

Table S10. Mulliken and Löwdin spin populations for **4A**.

Mulliken				**Löwdin**			
Ni_1	0.118	N_1	0.009	Ni_1	0.131	N_1	0.010
Ni_2	1.662	N_2	0.054	Ni_2	1.656	N_2	0.049
S_1	0.002	C_1	-0.004	S_1	-0.001	C_1	-0.003
S_2	0.003	C_2	0.002	S_2	0.000	C_2	0.002
S_3	0.002	C_3	-0.005	S_3	-0.001	C_3	-0.003
S_4	0.003	C_4	0.002	S_4	0.000	C_4	0.002
O_1	0.040	C_5	-0.004	O_1	0.040	C_5	-0.003
O_2	0.040	C_6	0.002	O_2	0.039	C_6	0.002
O_3	0.040	C_7	-0.004	O_3	0.040	C_7	-0.003
O_4	0.039	C_8	0.002	O_4	0.039	C_8	0.002

Table S11. Mulliken and Löwdin spin populations for **5A**.

Mulliken				**Löwdin**			
Ni_1	0.077	N_1	N/A	Ni_1	0.087	N_1	N/A
Ni_2	1.679	N_2	0.073	Ni_2	1.677	N_2	0.065
S_1	0.005	C_1	-0.002	S_1	0.004	C_1	-0.001
S_2	0.006	C_2	0.004	S_2	0.004	C_2	0.003
S_3	0.006	C_3	-0.003	S_3	0.004	C_3	-0.001
S_4	0.005	C_4	0.004	S_4	0.003	C_4	0.003
O_1	0.036	C_5	-0.002	O_1	0.036	C_5	-0.001
O_2	0.036	C_6	0.004	O_2	0.036	C_6	0.003
O_3	0.036	C_7	-0.002	O_3	0.036	C_7	-0.001
O_4	0.037	C_8	0.004	O_4	0.037	C_8	0.003

Table S12. Natural spin populations for **1A**.

Total				**Natural Atomic Orbital**			
Ni_1	0.078	N_1	0.007	Ni_1-$3d_{z^2}$	0.063	N_1-$2p_z$	0.005
Ni_2	1.619	N_2	0.08	Ni_1-$3d_{x^2-y^2}$	0.017	N_2-$2p_z$	0.056
S_1	0.005	C_1	-0.002	Ni_1-$3d_{xy}$	0.005	S_1-$3p_x$	0.002
S_2	0.006	C_2	0.003	Ni_1-$3d_{xz}$	0.001	S_2-$3p_y$	0.002
S_3	0.005	C_3	-0.002	Ni_1-$3d_{yz}$	0.001	S_3-$3p_x$	0.002
S_4	0.004	C_4	0.003	Ni_2-$3d_{z^2}$	0.776	S_4-$3p_y$	0.002
O_1	0.048	C_5	-0.002	Ni_2-$3d_{x^2-y^2}$	0.702	O_1-$2p_x$	0.028
O_2	0.047	C_6	0.003	Ni_2-$3d_{xy}$	0.134	O_2-$2p_y$	0.029
O_3	0.048	C_7	-0.002	Ni_2-$3d_{xz}$	0.007	O_3-$2p_x$	0.030
O_4	0.049	C_8	0.003	Ni_2-$3d_{yz}$	0.008	O_4-$2p_y$	0.029

Table S13. Natural spin populations for **2A**.

Total				**Natural Atomic Orbital**			
Ni_1	0.099	N_1	0.008	Ni_1-$3d_{z^2}$	0.080	N_1-$2p_z$	0.005
Ni_2	1.606	N_2	0.072	Ni_1-$3d_{x^2-y^2}$	0.025	N_2-$2p_z$	0.040
S_1	0.004	C_1	-0.003	Ni_1-$3d_{xy}$	0.005	S_1-$3p_x$	0.001
S_2	0.004	C_2	0.003	Ni_1-$3d_{xz}$	0.001	S_2-$3p_y$	0.000
S_3	0.004	C_3	-0.003	Ni_1-$3d_{yz}$	0.001	S_3-$3p_x$	0.001
S_4	0.003	C_4	0.003	Ni_2-$3d_{z^2}$	0.775	S_4-$3p_y$	0.001
O_1	0.052	C_5	-0.003	Ni_2-$3d_{x^2-y^2}$	0.712	O_1-$2p_x$	0.031
O_2	0.052	C_6	0.003	Ni_2-$3d_{xy}$	0.119	O_2-$2p_y$	0.032
O_3	0.052	C_7	-0.003	Ni_2-$3d_{xz}$	0.004	O_3-$2p_x$	0.032
O_4	0.051	C_8	0.003	Ni_2-$3d_{yz}$	0.008	O_4-$2p_y$	0.031

Table S14. Natural spin populations for **3A**.

Total				**Natural Atomic Orbital**			
Ni_1	0.079	N_1	0.007	Ni_1-$3d_{z^2}$	0.065	N_1-$2p_z$	0.005
Ni_2	1.618	N_2	0.079	Ni_1-$3d_{x^2-y^2}$	0.020	N_2-$2p_z$	0.055
S_1	0.004	C_1	-0.003	Ni_1-$3d_{xy}$	0.004	S_1-$3p_x$	0.002
S_2	0.004	C_2	0.003	Ni_1-$3d_{xz}$	0.000	S_2-$3p_y$	0.002
S_3	0.004	C_3	-0.003	Ni_1-$3d_{yz}$	0.000	S_3-$3p_x$	0.001
S_4	0.004	C_4	0.003	Ni_2-$3d_{z^2}$	0.775	S_4-$3p_y$	0.001
O_1	0.048	C_5	-0.003	Ni_2-$3d_{x^2-y^2}$	0.688	O_1-$2p_x$	0.030
O_2	0.049	C_6	0.003	Ni_2-$3d_{xy}$	0.147	O_2-$2p_y$	0.031
O_3	0.048	C_7	-0.003	Ni_2-$3d_{xz}$	0.002	O_3-$2p_x$	0.030
O_4	0.048	C_8	0.003	Ni_2-$3d_{yz}$	0.013	O_4-$2p_y$	0.029

Table S15. Natural spin populations for **4A**.

Total				**Natural Atomic Orbital**			
Ni_1	0.100	N_1	0.008	Ni_1-$3d_{z^2}$	0.080	N_1-$2p_z$	0.005
Ni_2	1.606	N_2	0.072	Ni_1-$3d_{x^2-y^2}$	0.022	N_2-$2p_z$	0.040
S_1	0.003	C_1	-0.003	Ni_1-$3d_{xy}$	0.009	S_1-$3p_x$	0.001
S_2	0.004	C_2	0.003	Ni_1-$3d_{xz}$	0.001	S_2-$3p_y$	0.000
S_3	0.003	C_3	-0.003	Ni_1-$3d_{yz}$	0.001	S_3-$3p_x$	0.000
S_4	0.004	C_4	0.003	Ni_2-$3d_{z^2}$	0.767	S_4-$3p_y$	0.001
O_1	0.052	C_5	-0.004	Ni_2-$3d_{x^2-y^2}$	0.782	O_1-$2p_x$	0.032
O_2	0.051	C_6	0.003	Ni_2-$3d_{xy}$	0.046	O_2-$2p_y$	0.033
O_3	0.052	C_7	-0.003	Ni_2-$3d_{xz}$	0.010	O_3-$2p_x$	0.034
O_4	0.051	C_8	0.003	Ni_2-$3d_{yz}$	0.013	O_4-$2p_y$	0.031

Table S16. Natural spin populations for **5A**.

Total				**Natural Atomic Orbital**			
Ni_1	0.064	N_1	N/A	Ni_1-$3d_{z^2}$	0.052	N_1-$2p_z$	N/A
Ni_2	1.628	N_2	0.088	Ni_1-$3d_{x^2-y^2}$	0.011	N_2-$2p_z$	0.064
S_1	0.006	C_1	-0.002	Ni_1-$3d_{xy}$	0.005	S_1-$3p_x$	0.004
S_2	0.006	C_2	0.003	Ni_1-$3d_{xz}$	0.001	S_2-$3p_y$	0.003
S_3	0.006	C_3	-0.002	Ni_1-$3d_{yz}$	0.001	S_3-$3p_x$	0.003
S_4	0.005	C_4	0.004	Ni_2-$3d_{z^2}$	0.782	S_4-$3p_y$	0.003
O_1	0.048	C_5	-0.002	Ni_2-$3d_{x^2-y^2}$	0.726	O_1-$2p_x$	0.028
O_2	0.047	C_6	0.004	Ni_2-$3d_{xy}$	0.108	O_2-$2p_y$	0.029
O_3	0.048	C_7	-0.002	Ni_2-$3d_{xz}$	0.006	O_3-$2p_x$	0.030
O_4	0.049	C_8	0.004	Ni_2-$3d_{yz}$	0.010	O_4-$2p_y$	0.029

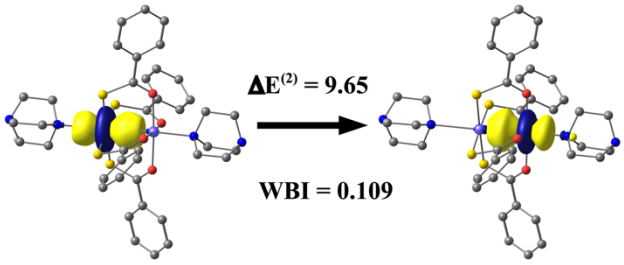

Figure S41. NBOs with σ-symmetry on metal centers in **1A**. Second order delocalization energy in kcal/mol, and Wiberg Bond Index (WBI) refers to all interactions between metal centers.

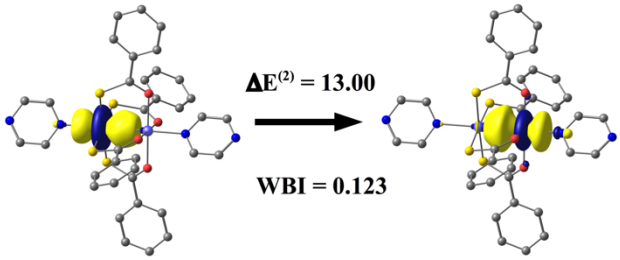

Figure S42. NBOs with σ-symmetry on metal centers in **2A**. Second order delocalization energy in kcal/mol, and Wiberg Bond Index (WBI) refers to all interactions between metal centers.

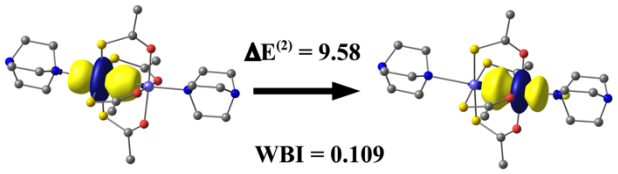

Figure S43. NBOs with σ-symmetry on metal centers in **3A**. Second order delocalization energy in kcal/mol, and Wiberg Bond Index (WBI) refers to all interactions between metal centers.

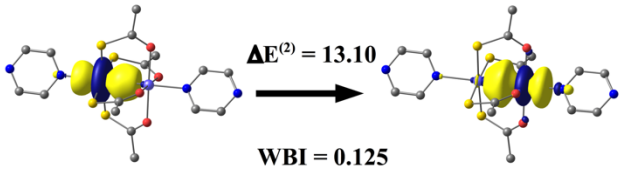

Figure S44. NBOs with σ-symmetry on metal centers in **4A**. Second order delocalization energy in kcal/mol, and Wiberg Bond Index (WBI) refers to all interactions between metal centers.

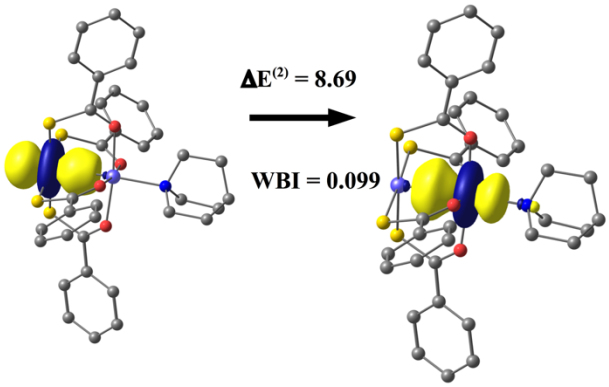

Figure S45. NBOs with σ-symmetry on metal centers in **5A**. Second order delocalization energy in kcal/mol, and Wiberg Bond Index (WBI) refers to all interactions between metal centers.

Table S17. Energetic summary of **1B-4B**. All relative energies in kcal/mol, exchange coupling in Kelvin, and absolute energies in hartree.

	S = 2	**BS(2,2)**	**ΔE (HS-BS)**	**J**	**J_{BF}**	**J_{VV}**
1B	-13104.162375	-13104.162376	$3.40*10^{-4}$	-0.0	-0.185	-0.116
2B	-12861.173873	-12861.173875	$1.65*10^{-3}$	-0.2	-0.242	-0.134
3B	-11570.574176	-11570.574176	$2.00*10^{-5}$	-0.0	-0.243	-0.151
4B	-11327.582853	-11327.582856	$1.62*10^{-3}$	-0.2	-0.227	-0.153

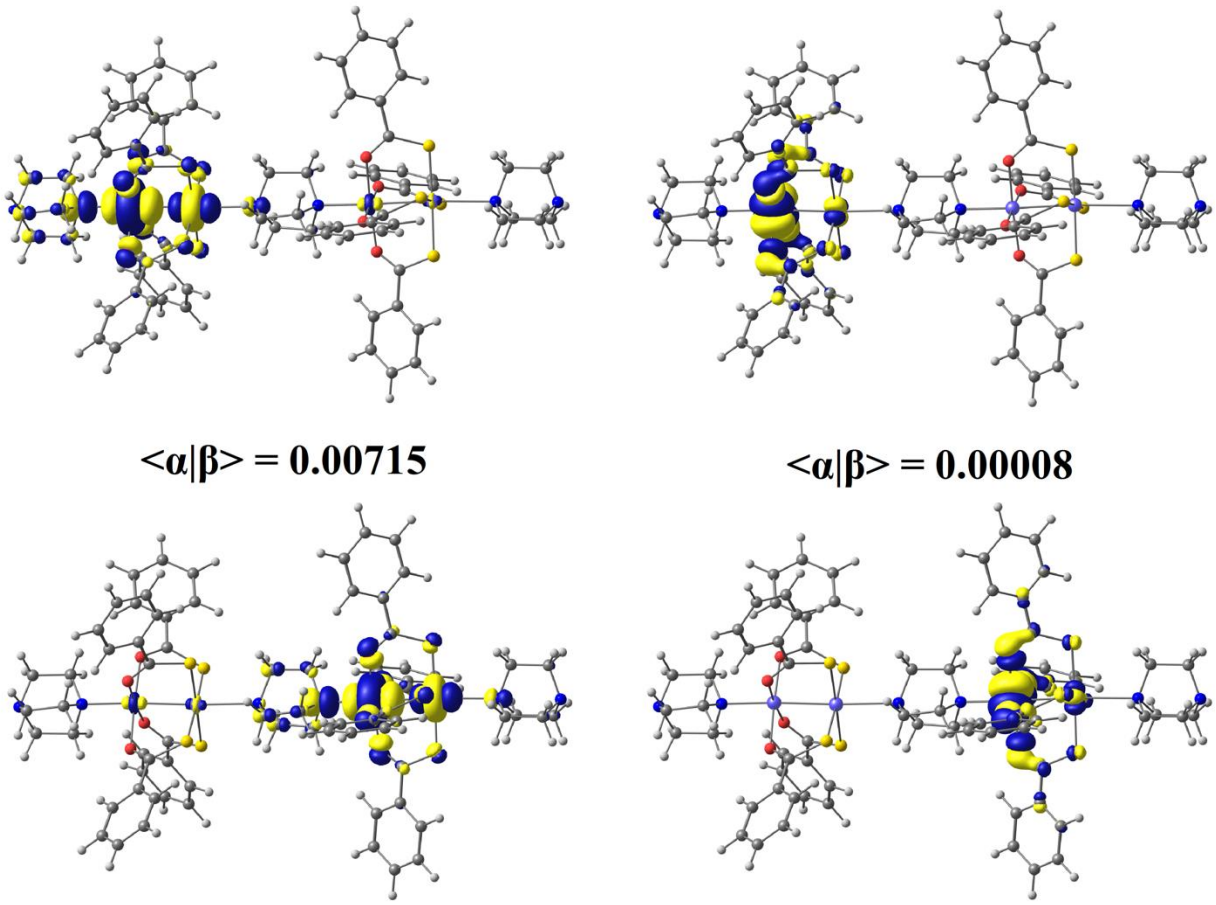

Figure S46. Non-orthogonal magnetic corresponding orbitals for the BS(2,2) wavefunction of **1B** with an isosurface of 0.03. Insets show the α-β overlap integrals.

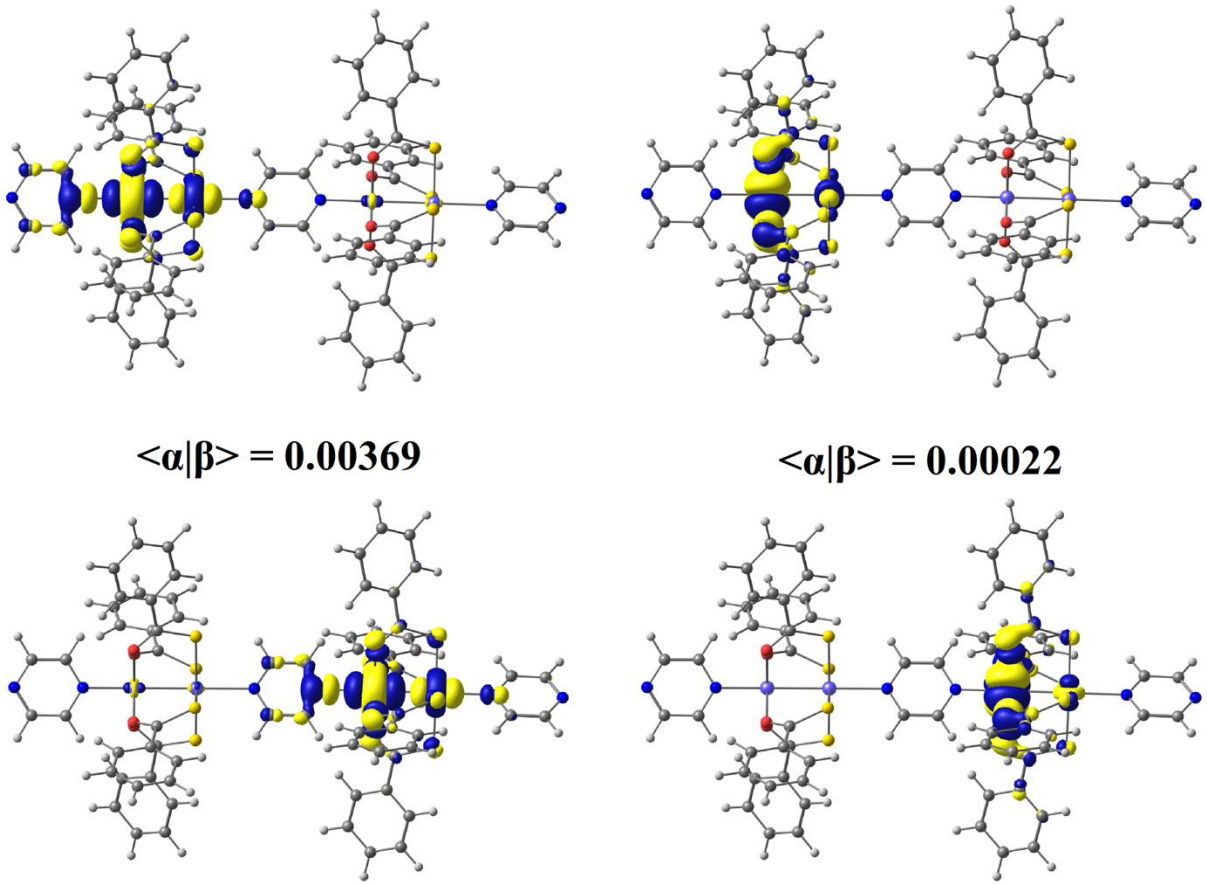

Figure S47. Non-orthogonal magnetic corresponding orbitals for the BS(2,2) wavefunction of **2B** with an isosurface of 0.03. Insets show the α-β overlap integrals.

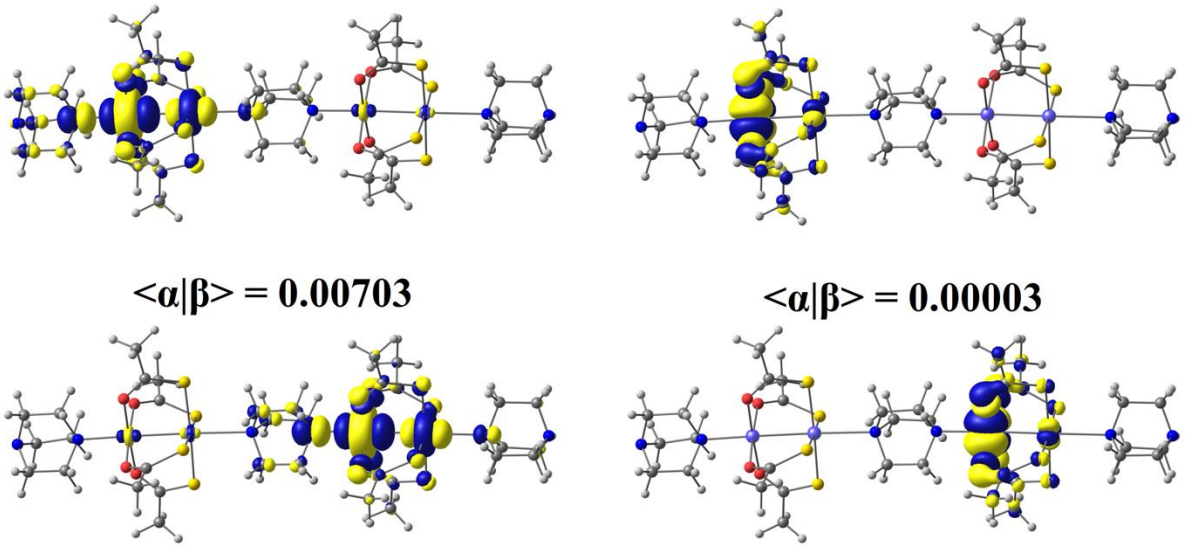

Figure S48. Non-orthogonal magnetic corresponding orbitals for the BS(2,2) wavefunction of **3B** with an isosurface of 0.03. Insets show the α-β overlap integrals.

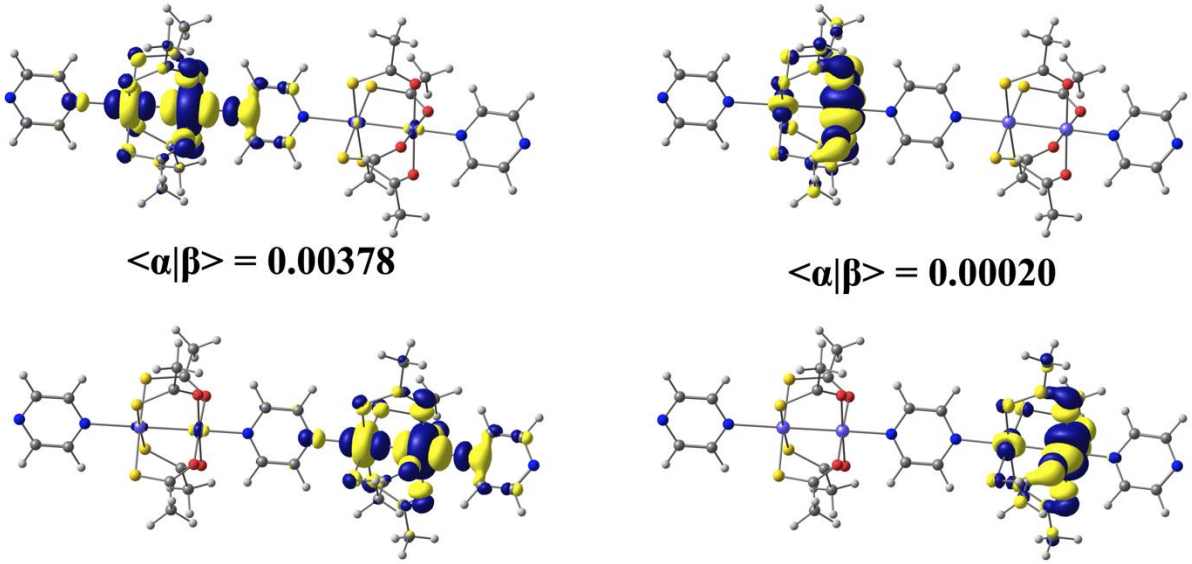

Figure S49. Non-orthogonal magnetic corresponding orbitals for the BS(2,2) wavefunction of **4B** with an isosurface of 0.03. Insets show the α-β overlap integrals.

Scheme S2. Labeling scheme used for dilanterns **1B-4B** (a)

(a)

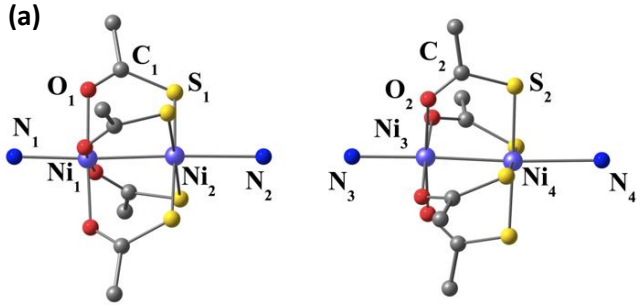

Table S18. Mulliken and Löwdin spin populations for quintet **1B**.

Mulliken				**Löwdin**			
Ni_1	1.669	N_1	0.066	Ni_1	1.667	N_1	0.060
Ni_2	-0.081	N_2	0.007	Ni_2	0.104	N_2	0.009
Ni_3	1.670	N_3	0.065	Ni_3	1.667	N_3	0.059
Ni_4	0.092	N_4	0.007	Ni_4	0.104	N_4	0.009
S_1	0.005	C_1	-0.005	S_1	0.002	C_1	-0.002
S_2	0.004	C_2	-0.003	S_2	0.001	C_2	-0.002
O_1	0.038	O_2	0.037	O_1	0.037	O_2	0.036

Table S19. Mulliken and Löwdin spin populations for BS(2,2) **1B**.

Mulliken				**Löwdin**			
Ni_1	1.669	N_1	0.066	Ni_1	1.667	N_1	0.060
Ni_2	0.092	N_2	0.006	Ni_2	0.104	N_2	0.008
Ni_3	-1.670	N_3	-0.065	Ni_3	-1.667	N_3	-0.059
Ni_4	-0.092	N_4	-0.007	Ni_4	-0.104	N_4	-0.009
S_1	0.005	C_1	-0.005	S_1	0.002	C_1	-0.002
S_2	-0.004	C_2	0.003	S_2	-0.001	C_2	0.002
O_1	0.038	O_2	-0.037	O_1	0.037	O_2	-0.036

Table S20. Mulliken and Löwdin spin populations for quintet **2B**.

Mulliken				**Löwdin**			
Ni_1	1.669	N_1	0.055	Ni_1	1.660	N_1	0.050
Ni_2	0.112	N_2	0.002	Ni_2	0.125	N_2	0.004
Ni_3	1.665	N_3	0.053	Ni_3	1.657	N_3	0.048
Ni_4	0.117	N_4	0.008	Ni_4	0.130	N_4	0.010
S_1	0.003	C_1	-0.006	S_1	-0.000	C_1	-0.002
S_2	0.003	C_2	-0.005	S_2	-0.000	C_2	-0.002
O_1	0.041	O_2	0.041	O_1	0.040	O_2	0.039

Table S21. Mulliken and Löwdin spin populations for BS(2,2) **2B**.

Mulliken				**Löwdin**			
Ni_1	-1.669	N_1	-0.055	Ni_1	-1.660	N_1	-0.050
Ni_2	-0.112	N_2	-0.013	Ni_2	-0.125	N_2	-0.014
Ni_3	1.665	N_3	0.054	Ni_3	1.657	N_3	0.050
Ni_4	0.117	N_4	0.008	Ni_4	0.130	N_4	0.010
S_1	-0.003	C_1	0.006	S_1	0.000	C_1	0.002
S_2	0.003	C_2	-0.005	S_2	-0.000	C_2	-0.002
O_1	-0.041	O_2	0.041	O_1	-0.040	O_2	0.039

Table S22. Mulliken and Löwdin spin populations for quintet **3B**.

Mulliken				**Löwdin**			
Ni_1	1.669	N_1	0.066	Ni_1	1.666	N_1	0.060
Ni_2	0.092	N_2	0.007	Ni_2	0.103	N_2	0.009
Ni_3	1.669	N_3	0.064	Ni_3	1.665	N_3	0.059
Ni_4	0.094	N_4	0.008	Ni_4	0.106	N_4	0.010
S_1	0.004	C_1	-0.003	S_1	0.002	C_1	-0.002
S_2	0.004	C_2	-0.004	S_2	0.001	C_2	-0.002
O_1	0.037	O_2	0.038	O_1	0.037	O_2	0.037

Table S23. Mulliken and Löwdin spin populations for BS(2,2) **3B**.

Mulliken				**Löwdin**			
Ni_1	1.669	N_1	0.066	Ni_1	1.666	N_1	0.060
Ni_2	0.092	N_2	0.007	Ni_2	0.104	N_2	0.009
Ni_3	-1.669	N_3	-0.064	Ni_3	-1.665	N_3	-0.059
Ni_4	-0.094	N_4	-0.008	Ni_4	-0.106	N_4	-0.010
S_1	0.004	C_1	-0.003	S_1	0.001	C_1	-0.002
S_2	-0.004	C_2	0.004	S_2	-0.001	C_2	0.002
O_1	0.037	O_2	-0.038	O_1	0.037	O_2	-0.037

Table S24. Mulliken and Löwdin spin populations for quintet **4B**.

Mulliken				**Löwdin**			
Ni_1	1.664	N_1	0.055	Ni_1	1.657	N_1	0.050
Ni_2	0.115	N_2	0.003	Ni_2	0.128	N_2	0.005
Ni_3	1.662	N_3	0.053	Ni_3	1.655	N_3	0.049
Ni_4	0.118	N_4	0.009	Ni_4	0.131	N_4	0.010
S_1	0.002	C_1	-0.004	S_1	-0.001	C_1	-0.003
S_2	0.002	C_2	-0.004	S_2	-0.001	C_2	-0.003
O_1	0.040	O_2	0.040	O_1	0.040	O_2	0.040

Table S25. Mulliken and Löwdin spin populations for BS(2,2) **4B**.

Mulliken				**Löwdin**			
Ni_1	1.663	N_1	0.055	Ni_1	1.657	N_1	0.050
Ni_2	0.116	N_2	0.014	Ni_2	0.129	N_2	0.015
Ni_3	-1.662	N_3	-0.055	Ni_3	-1.655	N_3	-0.050
Ni_4	-0.118	N_4	-0.009	Ni_4	-0.131	N_4	-0.010
S_1	0.002	C_1	-0.004	S_1	-0.001	C_1	-0.003
S_2	-0.002	C_2	0.004	S_2	0.001	C_2	0.003
O_1	0.040	O_2	-0.040	O_1	0.040	O_2	-0.040

Table S26. Experimental and calculated g-values for **1A-5A**. g_{DFT}-1 refers to the calculations performed with the gauge origin at the center of electronic charge, and g_{DFT}-2 refers to calculations done with the gauge origin at the $\{NiO_4\}$ center.

		1A	**2A**	**3A**	**4A**	**5A**
g_{DFT}-1	g_x	2.1353	2.1309	2.1351	2.1320	2.1341
	g_y	2.1401	2.1332	2.1398	2.1335	2.1415
	g_z	2.1402	2.1337	2.1412	2.1349	2.1420
	g_{iso}	**2.1385**	**2.1326**	**2.1387**	**2.1335**	**2.1392**
g_{DFT}-2	g_x	2.1352	2.1306	2.1351	2.1316	2.1341
	g_y	2.1397	2.1330	2.1393	2.1333	2.1413
	g_z	2.1398	2.1337	2.1407	2.1349	2.1418
	g_{iso}	**2.1382**	**2.1324**	**2.1383**	**2.1332**	**2.1391**
g_{NEVPT2}	g_x	2.2227	2.2159	2.2202	2.2171	2.2246
	g_y	2.3133	2.2831	2.3117	2.2851	2.3156
	g_z	2.3157	2.2866	2.3173	2.2855	2.3187
	g_{iso}	**2.2839**	**2.2619**	**2.2830**	**2.2626**	**2.2863**
$g_{BF\ Model}$	g_{iso}	2.13	2.35	2.15	2.24	N/A
$g_{VV\ Eq.}$	g_{iso}	2.13	2.36	2.15	2.25	N/A

Table S27. ZFS parameters for **1A**-**5A** (cm^{-1}).

		1A	**2A**	**3A**	**4A**	**5A**
NEVPT2	D	10.725	7.816	10.897	7.566	11.232
	E	0.173	0.251	0.435	0.059	0.253
DFT	D	13.379	13.863	7.618	9.526	-11.402
	E	0.488	0.239	0.091	0.214	-0.060

Table S28. Individual contributions to the NEVPT2 ZFS for **1A** (cm^{-1}) with relative energies of states.

State	Multiplicity	Energy	D	E
1	3	0.0	0.000	0.000
2	3	7022.8	28.179	12.159
3	3	7051.2	27.265	-11.832
4	3	10195.2	-41.485	-0.133
5	3	12829.8	0.013	0.003
6	1	14101.3	-0.008	0.002
7	3	15033.5	0.597	0.593
8	3	15073.7	0.575	-0.580
9	1	16092.9	-0.000	-0.000
10	1	22478.7	-7.478	-6.335
11	1	22511.3	-7.329	6.283
12	1	25389.1	13.912	0.021
13	3	25544.9	0.001	0.000
14	1	27701.6	-0.002	-0.000
15	3	28060.6	0.061	-0.063
16	3	28154.6	0.062	0.062
17	1	29355.3	-0.002	0.001
18	1	34005.8	0.014	-0.000
19	1	34062.7	0.001	-0.000
20	1	36322.7	-0.001	0.001
21	1	37448.8	-0.989	0.436
22	1	37531.0	-0.994	-0.374
23	1	38346.6	-0.129	-0.068
24	1	39310.0	1.851	0.016
25	1	61880.5	-0.000	0.000

Table S29. Individual contributions to the NEVPT2 ZFS for **2A** (cm^{-1}) with relative energies of states.

State	Multiplicity	Energy	D	E
1	3	0.0	0.000	0.000
2	3	7710.1	25.557	25.474
3	3	7911.1	25.298	-25.212
4	3	10604.8	-40.778	-0.001
5	3	13646.9	-0.003	-0.000
6	1	14122.8	0.001	0.000
7	3	15851.8	0.528	-0.524
8	1	16177.2	0.000	-0.000
9	3	16244.0	0.531	0.523
10	1	23194.2	-7.303	-7.302
11	1	23317.7	-7.262	7.261
12	1	25942.0	14.060	0.000
13	3	26595.4	-0.000	0.000
14	1	28065.3	0.004	0.000
15	3	28880.4	0.057	-0.042
16	3	28973.8	0.062	0.052
17	1	29579.0	0.000	0.000
18	1	34590.0	-0.003	-0.000
19	1	34873.6	-0.008	-0.008
20	1	37238.9	0.007	0.000
21	1	38505.1	-1.055	0.942
22	1	38622.9	-1.042	-0.927
23	1	39591.9	-0.000	-0.000
24	1	40550.9	1.698	0.000
25	1	62811.1	0.000	-0.000

Table S30. Individual contributions to the NEVPT2 ZFS for **3A** (cm^{-1}) with relative energies of states.

State	Multiplicity	Energy	D	E
1	3	0.0	0.000	0.000
2	3	7057.0	25.576	24.691
3	3	7094.0	27.739	-24.434
4	3	10321.3	-41.125	0.238
5	3	12897.0	0.011	-0.008
6	1	14041.3	-0.008	-0.005
7	3	15142.3	0.593	0.538
8	3	15226.5	0.578	-0.525
9	1	16108.6	-0.000	0.001
10	1	22512.6	-7.396	-7.457
11	1	22572.0	-7.433	7.431
12	1	25525.8	13.860	-0.032
13	3	25633.2	0.001	-0.001
14	1	27718.2	-0.002	0.002
15	3	28188.1	0.064	-0.064
16	3	28295.6	0.060	0.062
17	1	29459.2	-0.002	-0.001
18	1	34094.0	0.014	0.000
19	1	34160.0	0.002	0.000
20	1	36477.7	-0.000	-0.000
21	1	37550.1	-1.010	0.993
22	1	37734.1	-0.997	-1.044
23	1	38487.6	-0.110	0.104
24	1	39464.9	1.859	-0.031
25	1	62038.7	-0.000	-0.000

Table S31. Individual contributions to the NEVPT2 ZFS for **4A** (cm^{-1}) with relative energies of states.

State	**Multiplicity**	**Energy**	**D**	**E**
1	3	0.0	0.000	0.000
2	3	7768.4	25.345	6.100
3	3	7938.0	25.363	-6.115
4	3	10555.6	-40.943	0.000
5	3	13715.1	-0.012	0.000
6	1	14223.0	0.001	0.000
7	3	15816.7	0.515	-0.096
8	1	16181.0	0.000	0.000
9	3	16237.4	0.512	0.134
10	1	23268.4	-7.276	-1.081
11	1	23345.0	-7.276	1.084
12	1	25902.8	14.062	-0.000
13	3	26618.5	-0.000	-0.000
14	1	28201.3	0.013	0.000
15	3	28830.0	0.059	0.058
16	3	28969.8	0.054	-0.054
17	1	29552.4	0.000	-0.000
18	1	34506.7	-0.008	-0.007
19	1	34876.4	-0.008	-0.003
20	1	37266.9	0.003	-0.000
21	1	38524.2	-1.046	1.033
22	1	38653.4	-1.041	-1.027
23	1	39572.8	-0.000	-0.000
24	1	40524.9	1.706	-0.000
25	1	62850.5	0.000	0.000

Table S32. Individual contributions to the ZFS for **5A** (cm^{-1}) with relative energies of states.

State	**Multiplicity**	**Energy**	**D**	**E**
1	3	0.0	0.000	0.000
2	3	6844.7	28.325	28.567
3	3	6881.7	28.269	-28.395
4	3	10097.2	-41.938	0.099
5	3	12597.5	0.012	0.012
6	1	14054.8	-0.008	0.007
7	3	14880.5	0.627	-0.493
8	3	14895.8	0.594	0.484
9	1	16029.2	-0.000	0.000
10	1	22263.9	-7.445	-7.367
11	1	22299.0	-7.432	7.354
12	1	25223.2	13.978	-0.012
13	3	25282.9	0.001	0.001
14	1	27556.4	-0.002	-0.002
15	3	27830.4	0.064	-0.057
16	3	27916.0	0.064	0.055
17	1	29249.9	-0.002	0.002
18	1	33807.3	0.018	-0.000
19	1	33830.3	-0.000	-0.000
20	1	36059.0	-0.001	0.001
21	1	37166.7	-0.992	0.909
22	1	37242.3	-1.006	-0.930
23	1	38011.1	-0.146	0.042
24	1	38974.7	1.893	-0.012
25	1	61568.3	-0.000	0.000

Table S33. Absolute (Hartree) and relative energies (kcal/mol) of two lowest triplet states for **1A-5A** at the NEVPT2(4,4)/TZVP/ZORA level.

	T_0	T_1	ΔE
1A	-6718.9535	-6718.9391	9.1
2A	-6557.2509	-6557.2411	6.2
3A	-5953.1873	-5953.1724	9.3
4A	-5791.4853	-5791.4748	6.6
5A	-6358.1048	-6358.0678	23.2

Table S34. Cartesian coordinates for quintet state of **1A** at the PBE0/TZVP/ZORA level.

O	-1.897574000000	-0.378520000000	-0.786176000000
O	0.418211000000	-1.986550000000	-0.563153000000
O	2.069633000000	0.298453000000	-0.634133000000
O	-0.235331000000	1.977165000000	-0.867640000000
C	-2.745128000000	0.072462000000	0.014256000000
C	-0.016295000000	-2.727306000000	0.343310000000
C	2.809109000000	-0.045486000000	0.313045000000
C	0.120519000000	2.823103000000	-0.016915000000
S	-2.369692000000	0.820926000000	1.509498000000
S	-0.711496000000	-2.173243000000	1.810178000000
S	2.264726000000	-0.494393000000	1.872599000000
S	0.599008000000	2.457609000000	1.586294000000
Ni	0.089292000000	-0.014701000000	-0.878172000000
Ni	-0.078443000000	0.154210000000	2.015515000000
C	-4.177221000000	-0.068568000000	-0.375556000000
C	-4.508390000000	-0.968052000000	-1.389519000000
C	-5.191485000000	0.668151000000	0.234424000000
C	-5.826935000000	-1.131329000000	-1.781614000000
C	-6.507083000000	0.516410000000	-0.171051000000
C	-6.829652000000	-0.385295000000	-1.177045000000
H	-3.718151000000	-1.547747000000	-1.849983000000
H	-4.935245000000	1.363475000000	1.024621000000
H	-6.074348000000	-1.843892000000	-2.560621000000
H	-7.286130000000	1.102335000000	0.303429000000
H	-7.861437000000	-0.507865000000	-1.487448000000
C	0.128723000000	4.250119000000	-0.454614000000
C	-0.450695000000	4.578194000000	-1.680889000000
C	0.706080000000	5.262940000000	0.310346000000
C	-0.454808000000	5.887896000000	-2.131394000000
C	0.711773000000	6.570254000000	-0.146394000000
C	0.130986000000	6.887905000000	-1.367144000000
H	-0.908104000000	3.791582000000	-2.267262000000
H	1.154468000000	5.011319000000	1.263702000000
H	-0.917352000000	6.130253000000	-3.081706000000
H	1.171725000000	7.346585000000	0.454530000000
H	0.132997000000	7.913170000000	-1.720067000000
C	4.277015000000	-0.047747000000	0.053073000000
C	5.164941000000	-0.800225000000	0.820118000000
C	4.771820000000	0.717680000000	-1.002796000000
C	6.519135000000	-0.793455000000	0.529321000000
C	6.129109000000	0.738459000000	-1.279592000000
C	7.005880000000	-0.022390000000	-0.518061000000
H	4.780386000000	-1.394595000000	1.640115000000
H	4.078110000000	1.308034000000	-1.588543000000
H	7.199138000000	-1.392449000000	1.124533000000
H	6.505098000000	1.349846000000	-2.092317000000
H	8.067564000000	-0.012972000000	-0.738474000000
C	0.097769000000	-4.197575000000	0.123602000000
C	-0.647696000000	-5.120151000000	0.855800000000
C	0.977953000000	-4.660211000000	-0.855026000000
C	-0.520251000000	-6.476682000000	0.607446000000
C	1.118437000000	-6.018373000000	-1.088621000000
C	0.365615000000	-6.930354000000	-0.361298000000

H	-1.330618000000	-4.761511000000	1.616364000000
H	1.559154000000	-3.938607000000	-1.415262000000
H	-1.112994000000	-7.184701000000	1.175634000000
H	1.817084000000	-6.367596000000	-1.840662000000
H	0.469859000000	-7.993575000000	-0.547359000000
N	0.280848000000	-0.041509000000	-5.538315000000
N	0.183344000000	-0.038268000000	-2.970121000000
C	-1.032952000000	0.397533000000	-5.084616000000
C	-1.104771000000	0.421213000000	-3.540551000000
C	1.284095000000	0.866854000000	-4.996997000000
C	1.254430000000	0.865213000000	-3.450854000000
C	0.533630000000	-1.380539000000	-5.019893000000
C	0.463808000000	-1.400509000000	-3.474193000000
H	-1.226536000000	1.389285000000	-5.501108000000
H	-1.783462000000	-0.279831000000	-5.499978000000
H	-1.292330000000	1.420468000000	-3.146674000000
H	-1.887469000000	-0.228705000000	-3.153460000000
H	2.265053000000	0.559960000000	-5.368921000000
H	1.087169000000	1.867276000000	-5.390606000000
H	2.190874000000	0.515544000000	-3.018584000000
H	1.054102000000	1.854913000000	-3.039471000000
H	1.517773000000	-1.702789000000	-5.369404000000
H	-0.203384000000	-2.062049000000	-5.451947000000
H	-0.321400000000	-2.060007000000	-3.103494000000
H	1.400141000000	-1.730823000000	-3.023289000000
N	-0.212956000000	0.149731000000	4.131882000000
N	-0.374725000000	0.145682000000	6.704473000000
C	-1.534568000000	-0.356109000000	4.579505000000
C	-1.646037000000	-0.258110000000	6.117795000000
C	-0.031124000000	1.517259000000	4.671662000000
C	-0.041561000000	1.478819000000	6.218247000000
C	0.833458000000	-0.716829000000	4.727374000000
C	0.653717000000	-0.786787000000	6.260461000000
H	-2.309071000000	0.222412000000	4.076579000000
H	-1.623290000000	-1.386360000000	4.232063000000
H	-2.402869000000	0.474675000000	6.408626000000
H	-1.941156000000	-1.218295000000	6.548137000000
H	0.911974000000	1.907544000000	4.286877000000
H	-0.830200000000	2.141207000000	4.267802000000
H	0.936626000000	1.753313000000	6.621122000000
H	-0.769159000000	2.188456000000	6.619614000000
H	1.800424000000	-0.289756000000	4.459699000000
H	0.764155000000	-1.698372000000	4.255596000000
H	0.361979000000	-1.791247000000	6.577250000000
H	1.590119000000	-0.544993000000	6.769398000000

Table S35. Cartesian coordinates for triplet state of **1A** at the PBE0/TZVP/ZORA level.

O	-1.863747000000	-0.483741000000	-0.946429000000
O	0.506952000000	-2.032683000000	-0.724612000000
O	2.128841000000	0.335199000000	-0.792458000000
O	-0.274255000000	1.966193000000	-1.020931000000
C	-2.669721000000	-0.055648000000	-0.099924000000
C	0.076393000000	-2.713785000000	0.223650000000
C	2.812557000000	0.028460000000	0.201799000000
C	0.034984000000	2.774346000000	-0.124490000000
S	-2.199633000000	0.614588000000	1.411224000000
S	-0.506047000000	-2.046610000000	1.698605000000
S	2.157984000000	-0.345330000000	1.744967000000
S	0.464256000000	2.310902000000	1.473467000000
Ni	0.127429000000	-0.033266000000	-0.937008000000
Ni	-0.022420000000	0.133599000000	1.617988000000
C	-4.121613000000	-0.148225000000	-0.409927000000
C	-4.530270000000	-1.021410000000	-1.418174000000
C	-5.080065000000	0.604321000000	0.267407000000
C	-5.872404000000	-1.146384000000	-1.736735000000
C	-6.419730000000	0.490047000000	-0.064581000000
C	-6.820386000000	-0.387745000000	-1.063577000000
H	-3.781085000000	-1.609028000000	-1.934098000000
H	-4.767139000000	1.286088000000	1.049126000000
H	-6.180740000000	-1.838165000000	-2.512563000000
H	-7.156103000000	1.087119000000	0.461205000000
H	-7.870787000000	-0.480666000000	-1.316185000000
C	0.034980000000	4.224192000000	-0.463335000000
C	-0.501631000000	4.620216000000	-1.688810000000
C	0.553699000000	5.194230000000	0.394132000000
C	-0.522998000000	5.957456000000	-2.048223000000
C	0.541205000000	6.529642000000	0.028510000000
C	0.002078000000	6.915661000000	-1.191770000000
H	-0.910594000000	3.863391000000	-2.346178000000
H	0.971382000000	4.893518000000	1.347436000000
H	-0.950581000000	6.254044000000	-2.999427000000
H	0.953383000000	7.274284000000	0.699845000000
H	-0.010046000000	7.962745000000	-1.473087000000
C	4.292103000000	-0.003839000000	0.048453000000
C	5.118689000000	-0.698333000000	0.930581000000
C	4.864220000000	0.680014000000	-1.024038000000
C	6.490210000000	-0.710729000000	0.739104000000
C	6.237415000000	0.678859000000	-1.204466000000
C	7.053867000000	-0.020606000000	-0.326002000000
H	4.677810000000	-1.236529000000	1.761140000000
H	4.215981000000	1.221557000000	-1.701750000000
H	7.123231000000	-1.262476000000	1.424724000000
H	6.673283000000	1.224156000000	-2.034029000000
H	8.128517000000	-0.027487000000	-0.470024000000
C	0.068101000000	-4.194791000000	0.072582000000
C	-0.640801000000	-5.031405000000	0.933862000000
C	0.785214000000	-4.757844000000	-0.983202000000
C	-0.633646000000	-6.402474000000	0.739562000000
C	0.801557000000	-6.130375000000	-1.167823000000
C	0.088310000000	-6.956273000000	-0.309591000000

H	-1.204712000000	-4.599392000000	1.751860000000
H	1.333913000000	-4.101354000000	-1.646705000000
H	-1.195600000000	-7.042871000000	1.409879000000
H	1.370447000000	-6.558184000000	-1.985671000000
H	0.095230000000	-8.030517000000	-0.456871000000
N	0.341962000000	-0.036458000000	-5.658538000000
N	0.232219000000	-0.049828000000	-3.086811000000
C	-0.996163000000	0.326529000000	-5.207525000000
C	-1.069670000000	0.354440000000	-3.663670000000
C	1.290548000000	0.923705000000	-5.107145000000
C	1.262245000000	0.901942000000	-3.561461000000
C	0.667526000000	-1.361019000000	-5.142126000000
C	0.576622000000	-1.392860000000	-3.597887000000
H	-1.248928000000	1.302000000000	-5.631351000000
H	-1.703137000000	-0.397977000000	-5.620192000000
H	-1.297543000000	1.348028000000	-3.276121000000
H	-1.828293000000	-0.323045000000	-3.276179000000
H	2.287412000000	0.678846000000	-5.483480000000
H	1.035614000000	1.914703000000	-5.492122000000
H	2.214213000000	0.586845000000	-3.136857000000
H	1.025077000000	1.878475000000	-3.138215000000
H	1.674476000000	-1.619817000000	-5.479968000000
H	-0.019740000000	-2.083619000000	-5.589869000000
H	-0.185662000000	-2.087530000000	-3.243713000000
H	1.519279000000	-1.688477000000	-3.135842000000
N	-0.177296000000	0.168861000000	4.214297000000
N	-0.319771000000	0.190650000000	6.778369000000
C	-1.496945000000	-0.302271000000	4.660831000000
C	-1.590364000000	-0.242312000000	6.205551000000
C	0.032465000000	1.529440000000	4.727784000000
C	-0.010992000000	1.526208000000	6.276773000000
C	0.850352000000	-0.707831000000	4.795281000000
C	0.724446000000	-0.728718000000	6.338666000000
H	-2.260538000000	0.316547000000	4.185872000000
H	-1.633049000000	-1.319757000000	4.286992000000
H	-2.364385000000	0.459583000000	6.528169000000
H	-1.842827000000	-1.219419000000	6.626663000000
H	0.994738000000	1.888329000000	4.354785000000
H	-0.739330000000	2.173443000000	4.299849000000
H	0.949223000000	1.834043000000	6.700170000000
H	-0.768587000000	2.218924000000	6.653749000000
H	1.825847000000	-0.330302000000	4.482020000000
H	0.732423000000	-1.703488000000	4.361712000000
H	0.472208000000	-1.728137000000	6.704126000000
H	1.664317000000	-0.437451000000	6.815932000000

Table S36. Cartesian coordinates for singlet state of **1A** at the PBE0/TZVP/ZORA level.

O	-1.840602772181	-0.461268876001	-0.905769700447
O	0.489773005942	-2.009043669909	-0.684924853189
O	2.094271966807	0.320082878441	-0.751361588851
O	-0.258198931013	1.932029255900	-0.976226519945
C	-2.658238338885	-0.035691794582	-0.065240296600
C	0.063032382132	-2.705623606725	0.257415148533
C	2.794112451243	0.018830526490	0.236524465178
C	0.047877836313	2.753379017106	-0.087538665738
S	-2.218067153456	0.619759521618	1.457430318757
S	-0.518284965818	-2.067936230455	1.742363823914
S	2.172057203717	-0.355306052731	1.789899590220
S	0.466901841017	2.321669098313	1.518984824142
Ni	0.122937743379	-0.040886033772	-0.885463031968
Ni	-0.027748808597	0.130270475658	1.703033649214
C	-4.103816432935	-0.126508236577	-0.404943048143
C	-4.494120853867	-0.997294746957	-1.422634090026
C	-5.074283243851	0.626919873271	0.254231277129
C	-5.829987910303	-1.118863231400	-1.768048496932
C	-6.407223449095	0.516030804241	-0.104685805778
C	-6.789723463953	-0.359303605781	-1.112940221743
H	-3.736576772150	-1.585878421733	-1.924939345567
H	-4.775267889387	1.306484489497	1.043187859035
H	-6.124055314522	-1.808881816496	-2.550959423264
H	-7.152571633125	1.114015632944	0.407220110704
H	-7.834995942108	-0.449534024443	-1.386882808222
C	0.045528068355	4.196648251751	-0.454787394884
C	-0.490818000319	4.569060332462	-1.687926654088
C	0.562836973351	5.183601559809	0.384063907311
C	-0.513526225713	5.899275549633	-2.072535938670
C	0.549088188965	6.511796629067	-0.006860674175
C	0.010106953863	6.874235470125	-1.234394399165
H	-0.898557459718	3.800139397740	-2.331731319568
H	0.980232611957	4.901113531268	1.342955581337
H	-0.941178062696	6.177100037841	-3.029360438847
H	0.960524529446	7.269267161593	0.650448800178
H	-0.003024825948	7.915777119029	-1.535501230137
C	4.270696181536	0.000002397523	0.054555572579
C	5.118149327941	-0.696729150992	0.914830504390
C	4.818043275974	0.698096114718	-1.021801890090
C	6.485912981955	-0.697805136879	0.697811263783
C	6.187808444533	0.708490215101	-1.227163772537
C	7.025054657812	0.006347111825	-0.370780974571
H	4.695938586842	-1.245008662349	1.748412101875
H	4.154227877271	1.241880045125	-1.682323570383
H	7.135168195281	-1.251827504470	1.366206106341
H	6.604438251150	1.265188089504	-2.059024450688
H	8.096888010538	0.008444106230	-0.534600306482
C	0.064580078459	-4.183426814151	0.077893552711
C	-0.627843400955	-5.041159374396	0.931938500942
C	0.773086011881	-4.721999300336	-0.996512840832
C	-0.613673520979	-6.408241373901	0.712045965771
C	0.796522405491	-6.090759482491	-1.206740985679
C	0.099397091153	-6.937463272900	-0.355666290926

H	-1.183947389556	-4.628102890878	1.764844867719
H	1.309726781191	-4.050298643455	-1.654443482317
H	-1.163105705556	-7.064793480462	1.377076400818
H	1.358535604953	-6.499193754634	-2.039096148062
H	0.111894139971	-8.008715709398	-0.523012500446
N	0.340093322442	-0.046238081702	-5.655377424237
N	0.231116965689	-0.058565311511	-3.085461560216
C	-0.995084556803	0.328596285847	-5.203917844503
C	-1.066325952630	0.355420170712	-3.659444062314
C	1.297828862421	0.905515350265	-5.104040222073
C	1.267171129217	0.883647295389	-3.557751072526
C	0.653673789518	-1.374202447286	-5.139370795529
C	0.563881575924	-1.402935695106	-3.594466246314
H	-1.238514634221	1.306787759996	-5.627204784478
H	-1.708504277401	-0.388985017489	-5.617863876863
H	-1.287089952143	1.350946954438	-3.272105264591
H	-1.830688933034	-0.315889818514	-3.271470235006
H	2.292353806730	0.651308488022	-5.480639995959
H	1.051569764540	1.898580153772	-5.489600327652
H	2.217065769652	0.562135537791	-3.132234227508
H	1.037390116655	1.862902968353	-3.135899642603
H	1.657705233596	-1.642574645242	-5.478755284797
H	-0.041311226831	-2.089806041334	-5.586680398918
H	-0.203421409551	-2.091988706960	-3.239191649257
H	1.505449375689	-1.706057098280	-3.134206347326
N	-0.180552041826	0.166818808396	4.230868422571
N	-0.323952662845	0.188953260014	6.796901069185
C	-1.498942293663	-0.310292434491	4.679522942018
C	-1.593117875761	-0.246916961043	6.223624699513
C	0.022867656513	1.529226066615	4.745929186023
C	-0.018114385139	1.524818943246	6.294583855395
C	0.851569990311	-0.705071059662	4.814764312740
C	0.722113279964	-0.728204336829	6.357391222337
H	-2.265537403341	0.303418181518	4.203181918058
H	-1.629581207537	-1.329313568047	4.308284439578
H	-2.368476586330	0.454594996164	6.543623560084
H	-1.844967613876	-1.223463577485	6.646209739315
H	0.982629455992	1.893228112825	4.371830171952
H	-0.752956882736	2.169011201047	4.319224519016
H	0.942393019827	1.834105477104	6.716080297224
H	-0.775949344845	2.216593780489	6.672595899349
H	1.825267828980	-0.320604524580	4.504865905803
H	0.740944967473	-1.700761990889	4.379620415655
H	0.470602433636	-1.728551300725	6.720584511324
H	1.660951900009	-0.436691006391	6.836374776908

Table S37. Cartesian coordinates for the BS(3,1) state of **1A** at the PBE0/TZVP/ZORA level.

O	-1.894006000000	-0.384736000000	-0.791226000000
O	0.428354000000	-1.984519000000	-0.566787000000
O	2.072178000000	0.308067000000	-0.642116000000
O	-0.236536000000	1.979302000000	-0.874134000000
C	-2.738221000000	0.067896000000	0.011542000000
C	-0.007842000000	-2.722071000000	0.341220000000
C	2.807146000000	-0.034840000000	0.308714000000
C	0.118914000000	2.821429000000	-0.019834000000
S	-2.356046000000	0.817330000000	1.504677000000
S	-0.702342000000	-2.161310000000	1.806017000000
S	2.256361000000	-0.481937000000	1.866581000000
S	0.592268000000	2.449061000000	1.583392000000
Ni	0.092034000000	-0.013022000000	-0.881859000000
Ni	-0.078030000000	0.157105000000	2.011148000000
C	-4.172263000000	-0.072337000000	-0.371633000000
C	-4.507899000000	-0.970693000000	-1.385157000000
C	-5.184238000000	0.662733000000	0.244237000000
C	-5.828326000000	-1.134570000000	-1.770770000000
C	-6.501766000000	0.510254000000	-0.154586000000
C	-6.828691000000	-0.390483000000	-1.160062000000
H	-3.719634000000	-1.549093000000	-1.850589000000
H	-4.924894000000	1.357596000000	1.033823000000
H	-6.078934000000	-1.846258000000	-2.549556000000
H	-7.278851000000	1.094885000000	0.324681000000
H	-7.861935000000	-0.513702000000	-1.465301000000
C	0.131337000000	4.250185000000	-0.451711000000
C	-0.442524000000	4.583405000000	-1.679229000000
C	0.706597000000	5.259638000000	0.319346000000
C	-0.443453000000	5.894775000000	-2.124843000000
C	0.715371000000	6.568655000000	-0.132437000000
C	0.139975000000	6.891394000000	-1.354425000000
H	-0.897840000000	3.799295000000	-2.270502000000
H	1.150990000000	5.004176000000	1.273561000000
H	-0.901614000000	6.141091000000	-3.076267000000
H	1.173565000000	7.342284000000	0.473289000000
H	0.144419000000	7.917952000000	-1.703542000000
C	4.276426000000	-0.037325000000	0.055801000000
C	5.161467000000	-0.788809000000	0.827118000000
C	4.775210000000	0.727363000000	-0.998812000000
C	6.516916000000	-0.781336000000	0.542108000000
C	6.133656000000	0.748622000000	-1.269897000000
C	7.007608000000	-0.010955000000	-0.503926000000
H	4.773851000000	-1.383015000000	1.645791000000
H	4.083404000000	1.316259000000	-1.588251000000
H	7.194777000000	-1.379500000000	1.140591000000
H	6.512665000000	1.359318000000	-2.081743000000
H	8.070201000000	-0.001161000000	-0.719888000000
C	0.102503000000	-4.193179000000	0.126341000000
C	-0.645273000000	-5.111840000000	0.861186000000
C	0.981634000000	-4.660731000000	-0.850889000000
C	-0.520853000000	-6.469408000000	0.616957000000
C	1.118834000000	-6.019925000000	-1.080525000000
C	0.363942000000	-6.927959000000	-0.350474000000

H	-1.327719000000	-4.749429000000	1.620382000000
H	1.564424000000	-3.942046000000	-1.413195000000
H	-1.115302000000	-7.174328000000	1.187211000000
H	1.816555000000	-6.372906000000	-1.831668000000
H	0.465674000000	-7.991956000000	-0.533475000000
N	0.273813000000	-0.048243000000	-5.543569000000
N	0.180893000000	-0.040747000000	-2.975383000000
C	-1.034423000000	0.405490000000	-5.088190000000
C	-1.102222000000	0.434294000000	-3.544061000000
C	1.287982000000	0.849622000000	-5.005121000000
C	1.262231000000	0.848807000000	-3.458930000000
C	0.512290000000	-1.389439000000	-5.023928000000
C	0.442878000000	-1.406909000000	-3.478216000000
H	-1.219104000000	1.397929000000	-5.507143000000
H	-1.792501000000	-0.265460000000	-5.500299000000
H	-1.275328000000	1.437144000000	-3.152793000000
H	-1.892733000000	-0.203761000000	-3.152909000000
H	2.264636000000	0.532150000000	-5.379516000000
H	1.100550000000	1.851785000000	-5.399002000000
H	2.195427000000	0.487928000000	-3.028902000000
H	1.075473000000	1.841123000000	-3.047320000000
H	1.492784000000	-1.722635000000	-5.373484000000
H	-0.232179000000	-2.063217000000	-5.455382000000
H	-0.350957000000	-2.055302000000	-3.106120000000
H	1.374815000000	-1.749928000000	-3.027849000000
N	-0.213777000000	0.147554000000	4.119834000000
N	-0.379214000000	0.141106000000	6.692793000000
C	-1.533830000000	-0.363898000000	4.565950000000
C	-1.649165000000	-0.263131000000	6.103858000000
C	-0.038453000000	1.515046000000	4.661067000000
C	-0.046686000000	1.474665000000	6.207883000000
C	0.835164000000	-0.714789000000	4.716566000000
C	0.650081000000	-0.790281000000	6.248942000000
H	-2.310349000000	0.209314000000	4.060326000000
H	-1.616680000000	-1.395346000000	4.220925000000
H	-2.406424000000	0.470411000000	6.391689000000
H	-1.945814000000	-1.222532000000	6.534933000000
H	0.902135000000	1.910957000000	4.276143000000
H	-0.841215000000	2.135330000000	4.258970000000
H	0.932245000000	1.748320000000	6.609531000000
H	-0.773582000000	2.184070000000	6.610924000000
H	1.800531000000	-0.281367000000	4.453571000000
H	0.773065000000	-1.695510000000	4.242234000000
H	0.355850000000	-1.795659000000	6.560460000000
H	1.585031000000	-0.551696000000	6.762042000000

Table S38. Cartesian coordinates for the BS(2,2) state of **1A** at the PBE0/TZVP/ZORA level.

O	-1.894084000000	-0.380615000000	-0.779312000000
O	0.427561000000	-1.978762000000	-0.557786000000
O	2.068970000000	0.314018000000	-0.632111000000
O	-0.230776000000	1.983066000000	-0.861792000000
C	-2.745251000000	0.071828000000	0.016521000000
C	-0.011481000000	-2.725511000000	0.341061000000
C	2.810047000000	-0.034697000000	0.311966000000
C	0.132105000000	2.827382000000	-0.012213000000
S	-2.368036000000	0.828851000000	1.505722000000
S	-0.719850000000	-2.173307000000	1.801780000000
S	2.261413000000	-0.500772000000	1.864109000000
S	0.603656000000	2.454405000000	1.589883000000
Ni	0.088691000000	-0.005312000000	-0.842364000000
Ni	-0.080982000000	0.149677000000	1.980984000000
C	-4.176123000000	-0.076890000000	-0.373050000000
C	-4.502488000000	-0.975306000000	-1.389558000000
C	-5.194595000000	0.650857000000	0.240805000000
C	-5.820439000000	-1.145860000000	-1.780608000000
C	-6.509696000000	0.491396000000	-0.163152000000
C	-6.827375000000	-0.408954000000	-1.171982000000
H	-3.709125000000	-1.548321000000	-1.852998000000
H	-4.942070000000	1.345165000000	1.033116000000
H	-6.064042000000	-1.857255000000	-2.561868000000
H	-7.292130000000	1.070037000000	0.314643000000
H	-7.858720000000	-0.537605000000	-1.481371000000
C	0.152554000000	4.253667000000	-0.450052000000
C	-0.413373000000	4.585212000000	-1.681650000000
C	0.729295000000	5.262949000000	0.320160000000
C	-0.405120000000	5.894842000000	-2.132156000000
C	0.747083000000	6.570207000000	-0.136318000000
C	0.179502000000	6.891288000000	-1.362408000000
H	-0.869404000000	3.801406000000	-2.272670000000
H	1.167554000000	5.008548000000	1.277510000000
H	-0.856851000000	6.139926000000	-3.086959000000
H	1.206096000000	7.343757000000	0.468871000000
H	0.191058000000	7.916473000000	-1.715359000000
C	4.278013000000	-0.025875000000	0.054516000000
C	5.170101000000	-0.771519000000	0.823453000000
C	4.768843000000	0.743106000000	-1.000726000000
C	6.524746000000	-0.754462000000	0.535337000000
C	6.126449000000	0.773700000000	-1.275074000000
C	7.007459000000	0.019869000000	-0.511525000000
H	4.788500000000	-1.368639000000	1.642856000000
H	4.071702000000	1.327635000000	-1.588210000000
H	7.208239000000	-1.347896000000	1.132102000000
H	6.499303000000	1.387306000000	-2.087557000000
H	8.069436000000	0.037182000000	-0.730036000000
C	0.109283000000	-4.194174000000	0.118824000000
C	-0.635339000000	-5.120595000000	0.847124000000
C	0.995156000000	-4.651932000000	-0.856895000000
C	-0.501535000000	-6.476279000000	0.597660000000
C	1.141653000000	-6.009219000000	-1.091809000000
C	0.389746000000	-6.925049000000	-0.368422000000

H	-1.322637000000	-4.765739000000	1.605547000000
H	1.575901000000	-3.927330000000	-1.413649000000
H	-1.093342000000	-7.187366000000	1.162956000000
H	1.844370000000	-6.354669000000	-1.841774000000
H	0.498970000000	-7.987591000000	-0.555499000000
N	0.249356000000	-0.061499000000	-5.518160000000
N	0.167999000000	-0.042687000000	-2.948150000000
C	-1.043166000000	0.430790000000	-5.058263000000
C	-1.101058000000	0.471251000000	-3.513876000000
C	1.291130000000	0.808152000000	-4.986498000000
C	1.275074000000	0.809035000000	-3.439946000000
C	0.450851000000	-1.407072000000	-4.994413000000
C	0.382237000000	-1.417703000000	-3.448558000000
H	-1.203242000000	1.425340000000	-5.482426000000
H	-1.821639000000	-0.221717000000	-5.462096000000
H	-1.238769000000	1.481824000000	-3.128963000000
H	-1.910540000000	-0.137616000000	-3.115024000000
H	2.256338000000	0.463193000000	-5.366266000000
H	1.128980000000	1.814850000000	-5.380107000000
H	2.198695000000	0.417343000000	-3.016464000000
H	1.125547000000	1.807917000000	-3.028828000000
H	1.421781000000	-1.767933000000	-5.343357000000
H	-0.311939000000	-2.061667000000	-5.423501000000
H	-0.433491000000	-2.036954000000	-3.074061000000
H	1.301941000000	-1.792791000000	-2.999262000000
N	-0.220219000000	0.149411000000	4.106775000000
N	-0.388291000000	0.140341000000	6.679609000000
C	-1.537793000000	-0.369675000000	4.551854000000
C	-1.657498000000	-0.263636000000	6.088679000000
C	-0.052399000000	1.517191000000	4.649358000000
C	-0.056133000000	1.474550000000	6.195826000000
C	0.832492000000	-0.707814000000	4.704261000000
C	0.641702000000	-0.790343000000	6.235282000000
H	-2.317971000000	0.194833000000	4.042017000000
H	-1.611672000000	-1.403360000000	4.211399000000
H	-2.413934000000	0.472416000000	6.372341000000
H	-1.957410000000	-1.221039000000	6.522012000000
H	0.884410000000	1.920281000000	4.262877000000
H	-0.860231000000	2.132727000000	4.249917000000
H	0.924329000000	1.746247000000	6.595136000000
H	-0.780889000000	2.184143000000	6.602410000000
H	1.795712000000	-0.266538000000	4.446266000000
H	0.779255000000	-1.687487000000	4.226399000000
H	0.344263000000	-1.796616000000	6.540879000000
H	1.575067000000	-0.556059000000	6.753258000000

Table S39. Cartesian coordinates for the BS(1,1) state of **1A** at the PBE0/TZVP/ZORA level.

O	-1.840536000000	-0.461272000000	-0.905831000000
O	0.489801000000	-2.009111000000	-0.684933000000
O	2.094249000000	0.320051000000	-0.751407000000
O	-0.258204000000	1.932080000000	-0.976260000000
C	-2.658184000000	-0.035694000000	-0.065308000000
C	0.063045000000	-2.705654000000	0.257418000000
C	2.794096000000	0.018815000000	0.236484000000
C	0.047876000000	2.753397000000	-0.087553000000
S	-2.218049000000	0.619721000000	1.457386000000
S	-0.518261000000	-2.067909000000	1.742353000000
S	2.172058000000	-0.355295000000	1.789870000000
S	0.466899000000	2.321629000000	1.518963000000
Ni	0.122957000000	-0.040892000000	-0.885517000000
Ni	-0.027736000000	0.130259000000	1.702951000000
C	-4.103757000000	-0.126574000000	-0.405013000000
C	-4.494026000000	-0.997407000000	-1.422678000000
C	-5.074253000000	0.626838000000	0.254135000000
C	-5.829888000000	-1.119035000000	-1.768093000000
C	-6.407188000000	0.515891000000	-0.104784000000
C	-6.789653000000	-0.359489000000	-1.113013000000
H	-3.736460000000	-1.585980000000	-1.924963000000
H	-4.775265000000	1.306438000000	1.043072000000
H	-6.123928000000	-1.809089000000	-2.550983000000
H	-7.152559000000	1.113866000000	0.407100000000
H	-7.834921000000	-0.449765000000	-1.386956000000
C	0.045537000000	4.196685000000	-0.454744000000
C	-0.490807000000	4.569147000000	-1.687869000000
C	0.562849000000	5.183603000000	0.384147000000
C	-0.513507000000	5.899377000000	-2.072427000000
C	0.549109000000	6.511813000000	-0.006727000000
C	0.010131000000	6.874302000000	-1.234248000000
H	-0.898549000000	3.800252000000	-2.331702000000
H	0.980242000000	4.901077000000	1.343028000000
H	-0.941156000000	6.177241000000	-3.029241000000
H	0.960548000000	7.269257000000	0.650612000000
H	-0.002994000000	7.915855000000	-1.535315000000
C	4.270681000000	0.000068000000	0.054519000000
C	5.118166000000	-0.696639000000	0.914782000000
C	4.817996000000	0.698214000000	-1.021821000000
C	6.485930000000	-0.697641000000	0.697767000000
C	6.187762000000	0.708683000000	-1.227177000000
C	7.025040000000	0.006563000000	-0.370807000000
H	4.695980000000	-1.244958000000	1.748350000000
H	4.154156000000	1.241979000000	-1.682334000000
H	7.135211000000	-1.251647000000	1.366151000000
H	6.604367000000	1.265422000000	-2.059023000000
H	8.096874000000	0.008718000000	-0.534623000000
C	0.064499000000	-4.183463000000	0.077927000000
C	-0.627985000000	-5.041137000000	0.931981000000
C	0.772970000000	-4.722098000000	-0.996471000000
C	-0.613906000000	-6.408223000000	0.712108000000
C	0.796314000000	-6.090863000000	-1.206681000000
C	0.099129000000	-6.937508000000	-0.355596000000

H	-1.184064000000	-4.628033000000	1.764881000000
H	1.309655000000	-4.050441000000	-1.654410000000
H	-1.163385000000	-7.064730000000	1.377145000000
H	1.358301000000	-6.499347000000	-2.039029000000
H	0.111552000000	-8.008763000000	-0.522929000000
N	0.340114000000	-0.046272000000	-5.655404000000
N	0.231135000000	-0.058570000000	-3.085488000000
C	-0.995057000000	0.328594000000	-5.203950000000
C	-1.066295000000	0.355451000000	-3.659477000000
C	1.297868000000	0.905468000000	-5.104075000000
C	1.267216000000	0.883608000000	-3.557785000000
C	0.653667000000	-1.374238000000	-5.139383000000
C	0.563861000000	-1.402956000000	-3.594479000000
H	-1.238471000000	1.306781000000	-5.627255000000
H	-1.708489000000	-0.388983000000	-5.617881000000
H	-1.287019000000	1.350994000000	-3.272159000000
H	-1.830682000000	-0.315822000000	-3.271487000000
H	2.292387000000	0.651244000000	-5.480677000000
H	1.051621000000	1.898535000000	-5.489638000000
H	2.217103000000	0.562071000000	-3.132271000000
H	1.037465000000	1.862873000000	-3.135939000000
H	1.657697000000	-1.642629000000	-5.478756000000
H	-0.041326000000	-2.089833000000	-5.586693000000
H	-0.203466000000	-2.091982000000	-3.239203000000
H	1.505415000000	-1.706105000000	-3.134210000000
N	-0.180532000000	0.166829000000	4.230889000000
N	-0.323896000000	0.188961000000	6.796923000000
C	-1.498949000000	-0.310192000000	4.679556000000
C	-1.593088000000	-0.246854000000	6.223663000000
C	0.022988000000	1.529219000000	4.745951000000
C	-0.018006000000	1.524815000000	6.294605000000
C	0.851538000000	-0.705134000000	4.814765000000
C	0.722125000000	-0.728240000000	6.357396000000
H	-2.265507000000	0.303595000000	4.203252000000
H	-1.629680000000	-1.329191000000	4.308290000000
H	-2.368419000000	0.454671000000	6.543699000000
H	-1.844956000000	-1.223405000000	6.646229000000
H	0.982781000000	1.893146000000	4.371858000000
H	-0.752783000000	2.169065000000	4.319240000000
H	0.942508000000	1.834069000000	6.716110000000
H	-0.775821000000	2.216616000000	6.672612000000
H	1.825257000000	-0.320749000000	4.504834000000
H	0.740821000000	-1.700821000000	4.379636000000
H	0.470591000000	-1.728573000000	6.720612000000
H	1.660986000000	-0.436751000000	6.836350000000

Table S40. Cartesian coordinates for the quintet state of **2A** at the PBE0/TZVP/ZORA level.

O	-1.926660000000	-0.351514000000	-0.725603000000
O	0.392335000000	-2.040836000000	-0.586849000000
O	2.043449000000	0.231887000000	-0.613069000000
O	-0.263881000000	1.921790000000	-0.762670000000
C	-2.768085000000	0.035203000000	0.115746000000
C	0.010747000000	-2.796482000000	0.333660000000
C	2.808122000000	-0.078757000000	0.327978000000
C	0.038566000000	2.771744000000	0.103138000000
S	-2.381239000000	0.634715000000	1.674626000000
S	-0.641806000000	-2.252158000000	1.824269000000
S	2.288370000000	-0.497938000000	1.905768000000
S	0.537674000000	2.400279000000	1.701284000000
Ni	0.063937000000	-0.064884000000	-0.766358000000
Ni	-0.056911000000	0.086869000000	2.026665000000
N	0.204040000000	-0.208219000000	-5.561832000000
C	1.106921000000	-0.834973000000	-4.817023000000
C	1.077723000000	-0.799215000000	-3.431103000000
N	0.124234000000	-0.123706000000	-2.794950000000
C	-0.789009000000	0.511659000000	-3.524841000000
C	-0.738339000000	0.462414000000	-4.909707000000
H	1.883678000000	-1.385143000000	-5.337406000000
H	1.812126000000	-1.304496000000	-2.816096000000
H	-1.554051000000	1.055930000000	-2.985198000000
H	-1.482030000000	0.979828000000	-5.506383000000
C	-4.201160000000	-0.037166000000	-0.288832000000
C	-4.520712000000	-0.635682000000	-1.508501000000
C	-5.228102000000	0.474527000000	0.503348000000
C	-5.838446000000	-0.720777000000	-1.925945000000
C	-6.544229000000	0.395860000000	0.080515000000
C	-6.853957000000	-0.201553000000	-1.134206000000
H	-3.720123000000	-1.042321000000	-2.113402000000
H	-4.982400000000	0.934628000000	1.452670000000
H	-6.075207000000	-1.195868000000	-2.871400000000
H	-7.333431000000	0.801727000000	0.703144000000
H	-7.886002000000	-0.265332000000	-1.460721000000
C	0.000363000000	4.199986000000	-0.316419000000
C	-0.005373000000	4.495464000000	-1.680047000000
C	-0.038373000000	5.245280000000	0.604550000000
C	-0.041270000000	5.809563000000	-2.114194000000
C	-0.084025000000	6.559058000000	0.168662000000
C	-0.083507000000	6.845183000000	-1.190084000000
H	0.027664000000	3.677721000000	-2.388965000000
H	-0.036725000000	5.014357000000	1.662827000000
H	-0.035906000000	6.028045000000	-3.176203000000
H	-0.120968000000	7.365089000000	0.892738000000
H	-0.115642000000	7.874872000000	-1.528550000000
C	4.268998000000	-0.074854000000	0.032191000000
C	5.210112000000	-0.607029000000	0.912589000000
C	4.703292000000	0.470951000000	-1.176644000000
C	6.555929000000	-0.598997000000	0.586673000000
C	6.050892000000	0.488219000000	-1.495567000000
C	6.980697000000	-0.050613000000	-0.616376000000
H	4.874017000000	-1.028935000000	1.851983000000

H	3.967804000000	0.890412000000	-1.851472000000
H	7.278255000000	-1.021818000000	1.275633000000
H	6.378222000000	0.924465000000	-2.432715000000
H	8.035782000000	-0.041394000000	-0.866537000000
C	0.101404000000	-4.262796000000	0.085432000000
C	-0.089961000000	-5.201613000000	1.098212000000
C	0.395858000000	-4.708028000000	-1.203870000000
C	0.008812000000	-6.555731000000	0.826148000000
C	0.492562000000	-6.062468000000	-1.475075000000
C	0.299821000000	-6.990366000000	-0.460102000000
H	-0.315292000000	-4.855485000000	2.099575000000
H	0.541885000000	-3.974353000000	-1.986455000000
H	-0.140747000000	-7.276234000000	1.622246000000
H	0.717441000000	-6.397140000000	-2.481589000000
H	0.375661000000	-8.051325000000	-0.671061000000
N	-0.130560000000	0.142736000000	4.062239000000
N	-0.257884000000	0.220679000000	6.835316000000
C	0.403076000000	-0.826647000000	4.805101000000
C	0.335045000000	-0.775432000000	6.188587000000
C	-0.725884000000	1.151599000000	4.698110000000
C	-0.784937000000	1.178560000000	6.082460000000
H	0.877661000000	-1.646676000000	4.279415000000
H	0.772066000000	-1.566383000000	6.788540000000
H	-1.149270000000	1.938935000000	4.085772000000
H	-1.272710000000	2.001009000000	6.594478000000

Table S41. Cartesian coordinates for the triplet state of **2A** at the PBE0/TZVP/ZORA level.

O	-1.932476000000	-0.446009000000	-0.878054000000
O	0.460375000000	-2.077692000000	-0.715947000000
O	2.067660000000	0.280231000000	-0.766918000000
O	-0.328297000000	1.919594000000	-0.922750000000
C	-2.724426000000	-0.060843000000	0.001779000000
C	0.109615000000	-2.787093000000	0.244078000000
C	2.785938000000	-0.015783000000	0.205779000000
C	-0.043898000000	2.719678000000	-0.013125000000
S	-2.226726000000	0.471557000000	1.559400000000
S	-0.477475000000	-2.153984000000	1.733994000000
S	2.172155000000	-0.388526000000	1.768466000000
S	0.421815000000	2.234565000000	1.571227000000
Ni	0.065447000000	-0.077766000000	-0.800780000000
Ni	-0.028572000000	0.040844000000	1.703800000000
N	0.228976000000	-0.286993000000	-5.654228000000
C	1.130868000000	-0.899189000000	-4.895876000000
C	1.094865000000	-0.843703000000	-3.510473000000
N	0.138019000000	-0.165185000000	-2.883633000000
C	-0.772464000000	0.454869000000	-3.629050000000
C	-0.717851000000	0.388487000000	-5.013178000000
H	1.912180000000	-1.453521000000	-5.405330000000
H	1.829542000000	-1.339651000000	-2.888333000000
H	-1.542415000000	1.004645000000	-3.102065000000
H	-1.461377000000	0.895358000000	-5.619463000000
C	-4.176934000000	-0.056915000000	-0.321296000000
C	-4.582270000000	-0.591725000000	-1.544779000000
C	-5.137667000000	0.468725000000	0.541980000000
C	-5.921340000000	-0.601299000000	-1.897160000000
C	-6.475194000000	0.464737000000	0.184187000000
C	-6.870967000000	-0.069881000000	-1.034930000000
H	-3.829973000000	-1.004470000000	-2.205105000000
H	-4.828960000000	0.883186000000	1.494129000000
H	-6.226258000000	-1.024826000000	-2.847504000000
H	-7.213693000000	0.880452000000	0.860038000000
H	-7.919547000000	-0.073558000000	-1.310865000000
C	-0.057398000000	4.172484000000	-0.328681000000
C	-0.022517000000	4.559357000000	-1.668611000000
C	-0.114872000000	5.152340000000	0.661307000000
C	-0.038301000000	5.900644000000	-2.011415000000
C	-0.137452000000	6.493434000000	0.315570000000
C	-0.097776000000	6.871158000000	-1.019953000000
H	0.023579000000	3.791177000000	-2.430423000000
H	-0.150550000000	4.854023000000	1.702221000000
H	-0.003677000000	6.191677000000	-3.055347000000
H	-0.189185000000	7.248012000000	1.092161000000
H	-0.114041000000	7.921832000000	-1.287758000000
C	4.259322000000	-0.035864000000	0.003322000000
C	5.133069000000	-0.630411000000	0.912742000000
C	4.775236000000	0.554365000000	-1.150733000000
C	6.496223000000	-0.636748000000	0.668923000000
C	6.140048000000	0.557156000000	-1.385897000000
C	7.003751000000	-0.041190000000	-0.478297000000
H	4.736288000000	-1.093922000000	1.808012000000

H	4.089115000000	1.016410000000	-1.849622000000
H	7.166838000000	-1.108475000000	1.378007000000
H	6.532332000000	1.027529000000	-2.280527000000
H	8.072036000000	-0.043348000000	-0.664138000000
C	0.153993000000	-4.264131000000	0.080235000000
C	0.119079000000	-5.136265000000	1.167371000000
C	0.247027000000	-4.787948000000	-1.209435000000
C	0.175210000000	-6.505453000000	0.967210000000
C	0.297661000000	-6.157403000000	-1.407492000000
C	0.263382000000	-7.019734000000	-0.319476000000
H	0.055961000000	-4.731171000000	2.169961000000
H	0.272029000000	-4.103581000000	-2.048230000000
H	0.153088000000	-7.174662000000	1.819733000000
H	0.363301000000	-6.555325000000	-2.413852000000
H	0.306203000000	-8.092193000000	-0.473664000000
N	-0.122835000000	0.143618000000	4.020632000000
N	-0.291027000000	0.241039000000	6.800819000000
C	0.445170000000	-0.784238000000	4.785699000000
C	0.360240000000	-0.728609000000	6.169342000000
C	-0.772759000000	1.121454000000	4.645442000000
C	-0.855272000000	1.162954000000	6.029668000000
H	0.971341000000	-1.586636000000	4.279740000000
H	0.829962000000	-1.490457000000	6.783140000000
H	-1.230501000000	1.884389000000	4.024844000000
H	-1.391571000000	1.964302000000	6.527699000000

Table S42. Cartesian coordinates for the singlet state of **2A** at the PBE0/TZVP/ZORA level.

O	-1.899983000000	-0.437555000000	-0.829717000000
O	0.444949000000	-2.056399000000	-0.671771000000
O	2.036164000000	0.263341000000	-0.721052000000
O	-0.310655000000	1.884786000000	-0.874520000000
C	-2.706546000000	-0.053306000000	0.041659000000
C	0.092760000000	-2.779982000000	0.280732000000
C	2.771907000000	-0.024113000000	0.245103000000
C	-0.028734000000	2.699411000000	0.026698000000
S	-2.242290000000	0.473290000000	1.606918000000
S	-0.485613000000	-2.175668000000	1.781702000000
S	2.190362000000	-0.400272000000	1.815219000000
S	0.429016000000	2.246804000000	1.618951000000
Ni	0.066805000000	-0.084840000000	-0.758013000000
Ni	-0.028752000000	0.037421000000	1.785948000000
N	0.229825000000	-0.273950000000	-5.654865000000
C	1.118455000000	-0.909318000000	-4.899706000000
C	1.081092000000	-0.862218000000	-3.513734000000
N	0.138280000000	-0.169716000000	-2.882008000000
C	-0.758108000000	0.472519000000	-3.624892000000
C	-0.704358000000	0.415275000000	-5.009747000000
H	1.889127000000	-1.475333000000	-5.412731000000
H	1.805442000000	-1.378017000000	-2.894853000000
H	-1.517533000000	1.035119000000	-3.095356000000
H	-1.437059000000	0.940891000000	-5.613441000000
C	-4.151600000000	-0.052793000000	-0.313584000000
C	-4.530035000000	-0.578946000000	-1.549518000000
C	-5.132005000000	0.463014000000	0.533542000000
C	-5.861500000000	-0.589219000000	-1.929645000000
C	-6.461691000000	0.458306000000	0.147989000000
C	-6.830501000000	-0.067360000000	-1.083371000000
H	-3.763513000000	-0.984249000000	-2.197880000000
H	-4.843657000000	0.870254000000	1.495018000000
H	-6.145202000000	-1.005848000000	-2.889533000000
H	-7.215198000000	0.866548000000	0.811741000000
H	-7.873083000000	-0.071402000000	-1.381193000000
C	-0.046492000000	4.144975000000	-0.319873000000
C	0.009043000000	4.505096000000	-1.666745000000
C	-0.128272000000	5.143901000000	0.649253000000
C	-0.009487000000	5.839048000000	-2.036550000000
C	-0.154926000000	6.477408000000	0.276142000000
C	-0.093792000000	6.828562000000	-1.065841000000
H	0.074365000000	3.722207000000	-2.412031000000
H	-0.179604000000	4.865241000000	1.694852000000
H	0.042185000000	6.109308000000	-3.085325000000
H	-0.226171000000	7.247225000000	1.036141000000
H	-0.112501000000	7.873497000000	-1.354885000000
C	4.241033000000	-0.027960000000	0.010777000000
C	5.144764000000	-0.556999000000	0.931669000000
C	4.722707000000	0.511261000000	-1.182723000000
C	6.502611000000	-0.549576000000	0.660748000000
C	6.082189000000	0.527161000000	-1.446143000000
C	6.975359000000	-0.006072000000	-0.526612000000
H	4.774459000000	-0.977970000000	1.858640000000

H	4.014156000000	0.923917000000	-1.889854000000
H	7.196544000000	-0.969079000000	1.380116000000
H	6.447253000000	0.957228000000	-2.372067000000
H	8.039668000000	0.002542000000	-0.733856000000
C	0.135370000000	-4.253131000000	0.084532000000
C	0.098347000000	-5.148694000000	1.152516000000
C	0.226705000000	-4.749539000000	-1.216187000000
C	0.150851000000	-6.513245000000	0.922621000000
C	0.273194000000	-6.114496000000	-1.443805000000
C	0.237092000000	-7.000045000000	-0.374813000000
H	0.035340000000	-4.764993000000	2.163423000000
H	0.252621000000	-4.047766000000	-2.040379000000
H	0.126769000000	-7.200569000000	1.760558000000
H	0.336879000000	-6.490644000000	-2.458610000000
H	0.276516000000	-8.069026000000	-0.552106000000
N	-0.120334000000	0.137353000000	4.068228000000
N	-0.282203000000	0.236700000000	6.848597000000
C	0.447392000000	-0.791676000000	4.832694000000
C	0.365283000000	-0.734932000000	6.216318000000
C	-0.766900000000	1.117265000000	4.694041000000
C	-0.845925000000	1.159589000000	6.078281000000
H	0.970688000000	-1.595307000000	4.325885000000
H	0.834333000000	-1.497560000000	6.829530000000
H	-1.224243000000	1.880714000000	4.073933000000
H	-1.379010000000	1.962515000000	6.577085000000

Table S43. Cartesian coordinates for the BS(3,1) state of **2A** at the PBE0/TZVP/ZORA level.

O	-1.929038146774	-0.373614753050	-0.725329243575
O	0.397691866434	-2.051505060943	-0.572669687802
O	2.041728117492	0.231979064410	-0.599948312387
O	-0.278800033663	1.908254274235	-0.762647943813
C	-2.767658251177	0.021644669734	0.113862261831
C	0.009526419608	-2.814143482335	0.338158163005
C	2.811854990293	-0.080197327320	0.334678419996
C	0.041203364613	2.755861670525	0.098241749377
S	-2.360579882075	0.618720529326	1.666779136390
S	-0.643786794253	-2.267050272457	1.826587044820
S	2.285405443350	-0.526720369148	1.902281145373
S	0.561451055868	2.360706274934	1.683042884269
Ni	0.057950970888	-0.073054397856	-0.698426981654
Ni	-0.044218782920	0.054501523457	1.959696570704
N	0.219168435051	-0.253295779881	-5.511715941086
C	1.122272638648	-0.869505670664	-4.758384312794
C	1.087363667914	-0.823054706607	-3.372767548854
N	0.128685472901	-0.148413137693	-2.744408731783
C	-0.784226775215	0.476175807237	-3.483214541334
C	-0.728712546716	0.417393350355	-4.867597429094
H	1.903869926320	-1.419655761395	-5.271611346062
H	1.822135027529	-1.320064136029	-2.751642136321
H	-1.554549213591	1.020073098137	-2.950830175706
H	-1.472889631638	0.926636745633	-5.470790888186
C	-4.201585233039	-0.036042756645	-0.286276994622
C	-4.529760238510	-0.619845227236	-1.510685830647
C	-5.220866094528	0.479056498996	0.513509532349
C	-5.849252619591	-0.686378424522	-1.925840881401
C	-6.538717252735	0.418301729751	0.093297889678
C	-6.857236409462	-0.163846509628	-1.126646684946
H	-3.734706758851	-1.028526239277	-2.121552556352
H	-4.968044262985	0.928054824418	1.466427861883
H	-6.093349069587	-1.149061257824	-2.875569666310
H	-7.322286078039	0.826487352476	0.721460278392
H	-7.890549901497	-0.212895084705	-1.451662764125
C	0.003282935496	4.185909479150	-0.312420934539
C	-0.074927252919	4.488490864912	-1.672280077845
C	0.037097767522	5.227001469417	0.613820890158
C	-0.112066741148	5.805337891137	-2.097869023745
C	-0.006480631638	6.543648036341	0.186769284365
C	-0.079964378305	6.836604139132	-1.168576653895
H	-0.098193033011	3.673981887544	-2.385222451570
H	0.094531952886	4.991099393314	1.669539584040
H	-0.165282325168	6.029405712016	-3.157380612902
H	0.015564754384	7.346530696015	0.914905221161
H	-0.111718447201	7.868474341819	-1.500398603932
C	4.272501313903	-0.051976535758	0.043286515268
C	5.219473890223	-0.562919617249	0.929920664208
C	4.701000893717	0.496869763590	-1.166171119726
C	6.566225174685	-0.530846980554	0.609693268667
C	6.049319190766	0.537376654196	-1.479840945683
C	6.985298157415	0.019923977783	-0.594352252218
H	4.887566526616	-0.986742790088	1.870085321742

H	3.960449118682	0.899854017265	-1.845529603253
H	7.293674649023	-0.936430966001	1.303570179480
H	6.372381442422	0.975055639775	-2.417785830960
H	8.041015810949	0.047744270151	-0.840426336065
C	0.093548171242	-4.278318543140	0.082302265600
C	-0.097945820242	-5.220780051774	1.091711011778
C	0.380491045268	-4.717927473824	-1.210545035814
C	-0.006640684739	-6.573974768582	0.812611460833
C	0.469552146767	-6.071485268988	-1.488565686960
C	0.276845437311	-7.003271451350	-0.477161287250
H	-0.317000390264	-4.878600577962	2.095929113070
H	0.526168055073	-3.980866661901	-1.990081326694
H	-0.155977019733	-7.297841180181	1.605661908995
H	0.688372939651	-6.402416755938	-2.497637366300
H	0.346819348677	-8.063497029166	-0.693726651619
N	-0.127186641620	0.133738608672	3.982979067557
N	-0.263941088761	0.239412014267	6.755904881610
C	0.394842086051	-0.832830441058	4.737731548757
C	0.322445976102	-0.767677637411	6.120418590637
C	-0.715226839650	1.153836788996	4.607600278511
C	-0.779305577439	1.194319719209	5.991462350329
H	0.863161650937	-1.662802063236	4.222243212697
H	0.750744601153	-1.557050182291	6.728707439757
H	-1.127669394043	1.940220508908	3.986748924611
H	-1.261915881105	2.026351779435	6.492834899927

Table S44. Cartesian coordinates for the BS(2,2) state of **2A** at the PBE0/TZVP/ZORA level.

O	-1.930686000000	-0.367612000000	-0.719392000000
O	0.395083000000	-2.044781000000	-0.568723000000
O	2.035346000000	0.235466000000	-0.592106000000
O	-0.279725000000	1.911544000000	-0.754783000000
C	-2.772343000000	0.025527000000	0.119055000000
C	0.006996000000	-2.809896000000	0.340977000000
C	2.808526000000	-0.079102000000	0.340375000000
C	0.041588000000	2.760946000000	0.104798000000
S	-2.375897000000	0.623603000000	1.673659000000
S	-0.646594000000	-2.270346000000	1.831710000000
S	2.292485000000	-0.523128000000	1.911348000000
S	0.556267000000	2.374065000000	1.693129000000
Ni	0.054654000000	-0.069159000000	-0.710971000000
Ni	-0.048918000000	0.060308000000	1.982914000000
N	0.215842000000	-0.245673000000	-5.517117000000
C	1.124250000000	-0.854737000000	-4.764391000000
C	1.089597000000	-0.808816000000	-3.378800000000
N	0.125482000000	-0.141738000000	-2.750506000000
C	-0.792958000000	0.475830000000	-3.488498000000
C	-0.737227000000	0.417452000000	-4.872873000000
H	1.909996000000	-1.398544000000	-5.277990000000
H	1.828636000000	-1.299516000000	-2.757694000000
H	-1.567689000000	1.012920000000	-2.955557000000
H	-1.485647000000	0.920646000000	-5.475838000000
C	-4.204670000000	-0.038696000000	-0.286702000000
C	-4.526891000000	-0.635057000000	-1.506721000000
C	-5.228494000000	0.481596000000	0.503912000000
C	-5.844614000000	-0.709169000000	-1.926249000000
C	-6.544527000000	0.413538000000	0.079093000000
C	-6.857031000000	-0.181390000000	-1.136204000000
H	-3.728684000000	-1.048079000000	-2.110470000000
H	-4.980325000000	0.940313000000	1.453336000000
H	-6.083817000000	-1.182149000000	-2.872143000000
H	-7.331434000000	0.826055000000	0.700228000000
H	-7.888974000000	-0.236436000000	-1.464605000000
C	0.008818000000	4.189233000000	-0.313546000000
C	-0.081619000000	4.484809000000	-1.674257000000
C	0.060032000000	5.235686000000	0.605902000000
C	-0.113848000000	5.799324000000	-2.107366000000
C	0.021965000000	6.550074000000	0.171442000000
C	-0.063975000000	6.835797000000	-1.184709000000
H	-0.118474000000	3.666461000000	-2.382140000000
H	0.127168000000	5.005668000000	1.662295000000
H	-0.176979000000	6.017409000000	-3.167582000000
H	0.058239000000	7.356946000000	0.894587000000
H	-0.091491000000	7.865931000000	-1.522245000000
C	4.267690000000	-0.054653000000	0.039909000000
C	5.218706000000	-0.570300000000	0.919556000000
C	4.690758000000	0.494841000000	-1.171266000000
C	6.563480000000	-0.542508000000	0.590703000000
C	6.037186000000	0.531206000000	-1.493507000000
C	6.976961000000	0.008796000000	-0.615005000000
H	4.891103000000	-0.994443000000	1.861007000000

H	3.947561000000	0.902033000000	-1.845177000000
H	7.293819000000	-0.951973000000	1.279262000000
H	6.355803000000	0.969624000000	-2.432633000000
H	8.031193000000	0.033271000000	-0.867721000000
C	0.095153000000	-4.273316000000	0.080097000000
C	-0.124063000000	-5.220685000000	1.079348000000
C	0.415233000000	-4.707487000000	-1.206863000000
C	-0.027993000000	-6.572640000000	0.795932000000
C	0.510499000000	-6.059774000000	-1.488985000000
C	0.289444000000	-6.996226000000	-0.487764000000
H	-0.368808000000	-4.883041000000	2.079111000000
H	0.582819000000	-3.967013000000	-1.978643000000
H	-0.200093000000	-7.300069000000	1.581075000000
H	0.756366000000	-6.386011000000	-2.493353000000
H	0.363660000000	-8.055505000000	-0.707543000000
N	-0.132353000000	0.135845000000	4.019815000000
N	-0.268489000000	0.236419000000	6.792164000000
C	0.386837000000	-0.833943000000	4.772182000000
C	0.314844000000	-0.771464000000	6.155058000000
C	-0.717360000000	1.156497000000	4.646087000000
C	-0.781261000000	1.194635000000	6.030064000000
H	0.852777000000	-1.664079000000	4.254548000000
H	0.740633000000	-1.563050000000	6.762211000000
H	-1.127870000000	1.944960000000	4.026372000000
H	-1.261247000000	2.026835000000	6.533643000000

Table S45. Cartesian coordinates for the BS(1,1) state of **2A** at the PBE0/TZVP/ZORA level.

O	-1.929264282056	-0.446598937392	-0.870630920842
O	0.462782711060	-2.076124287486	-0.706961775802
O	2.060469617640	0.284108690975	-0.756882503528
O	-0.335156960433	1.922052625196	-0.913175060545
C	-2.724920795063	-0.059615755549	0.004282043113
C	0.109590606896	-2.786792220489	0.249760324841
C	2.781865464735	-0.016053560008	0.211532123373
C	-0.045947229893	2.722808097647	-0.007166241426
S	-2.231706631732	0.476892130530	1.561840335699
S	-0.485301991145	-2.153940876339	1.737614452441
S	2.171221365765	-0.391136651440	1.774757471163
S	0.424396519369	2.236537186564	1.576372563256
Ni	0.063229524453	-0.075424353063	-0.785884020407
Ni	-0.031283345873	0.041233842560	1.696424488192
N	0.228883031099	-0.280180313932	-5.645412921774
C	1.129136840264	-0.895120381482	-4.887410987561
C	1.092461060575	-0.841170210700	-3.501801280124
N	0.136933429925	-0.161809837115	-2.874679545946
C	-0.771818056767	0.460791032085	-3.619437881216
C	-0.716854271572	0.396284835810	-5.003785394040
H	1.909547126614	-1.450395480208	-5.397310717590
H	1.825838119808	-1.339476446979	-2.879903369788
H	-1.540832285569	1.011506635272	-3.091947275608
H	-1.459023363106	0.905527319202	-5.609796159356
C	-4.176333316022	-0.057537055031	-0.324165089995
C	-4.575898237242	-0.586221072283	-1.552033118425
C	-5.141506369863	0.460196629150	0.538959408703
C	-5.913688747654	-0.597279223190	-1.908995631146
C	-6.477873356227	0.454464765233	0.176790728328
C	-6.867866242463	-0.073810511004	-1.046833095470
H	-3.820204878506	-0.992971651727	-2.212229512300
H	-4.837175597459	0.869627104500	1.494670519972
H	-6.214137848101	-1.015701000076	-2.862966789453
H	-7.219887633848	0.863761835907	0.852700731985
H	-7.915465121845	-0.078877458292	-1.326418210076
C	-0.057348144140	4.175663766075	-0.323131378522
C	-0.029182072835	4.561794408488	-1.663235188534
C	-0.106568496173	5.155926162465	0.666833876714
C	-0.043491478645	5.902908494740	-2.006305823212
C	-0.127577733359	6.496911258422	0.320815108617
C	-0.094628461351	6.873913883332	-1.014883073830
H	0.010373647658	3.793049167722	-2.424819978174
H	-0.136856622686	4.857828716207	1.707857366028
H	-0.014167432327	6.193710913225	-3.050316988892
H	-0.172741471545	7.251973412020	1.097275808122
H	-0.109678437327	7.924456853031	-1.283062731802
C	4.254526320857	-0.038960234901	0.003513043971
C	5.129994015085	-0.635895369680	0.909637269131
C	4.767565662278	0.549891560843	-1.152469582457
C	6.492229884125	-0.645947214915	0.660793774481
C	6.131413841435	0.548642597180	-1.392865920753
C	6.996915435625	-0.052019882300	-0.488581363540
H	4.735304384257	-1.098393763483	1.806396957954

H	4.080056095317	1.013782769764	-1.848744701313
H	7.164256165476	-1.119409469886	1.367320526014
H	6.521511990970	1.017669056926	-2.289143379079
H	8.064437036710	-0.057346717648	-0.678582419245
C	0.157064228396	-4.263738754661	0.086594178350
C	0.140003521467	-5.134607137134	1.174953833625
C	0.236802564880	-4.788100390048	-1.203612522194
C	0.201841762616	-6.503712172663	0.975343838954
C	0.291772624222	-6.157430391126	-1.400986395208
C	0.276387812325	-7.018726521358	-0.311783561128
H	0.087203730367	-4.728171030219	2.177628163111
H	0.248190671151	-4.104280232183	-2.043124077587
H	0.194881442408	-7.172268318321	1.828594250172
H	0.346415174395	-6.556340198238	-2.407535813463
H	0.323471914006	-8.091042021125	-0.465675764994
N	-0.126582418248	0.143371483790	4.005584833252
N	-0.294559444358	0.241577068566	6.785433723977
C	0.433458895037	-0.789672563809	4.770295439186
C	0.348536498056	-0.733471322294	6.153950949802
C	-0.768440742522	1.126712186702	4.630218156027
C	-0.850766719395	1.168449068654	6.014474011848
H	0.952250216526	-1.596771754263	4.264243181828
H	0.811486482115	-1.499636833096	6.767481665326
H	-1.219183103613	1.893753530151	4.009623351199
H	-1.380361785003	1.974308223205	6.512388089592

Table S46. Cartesian coordinates for the quintet state of **3A** at the PBE0/TZVP/ZORA level.

O	-1.975832000000	-0.298715000000	-0.865619000000
O	0.361366000000	-1.929027000000	-0.740223000000
O	1.981103000000	0.467543000000	-0.838179000000
O	-0.377031000000	2.025159000000	-0.952564000000
C	-2.783975000000	0.094737000000	-0.000775000000
C	0.025171000000	-2.674575000000	0.201352000000
C	2.766187000000	0.226636000000	0.099847000000
C	-0.082840000000	2.871736000000	-0.085832000000
C	-4.245877000000	-0.031325000000	-0.330358000000
C	0.185555000000	-4.154046000000	-0.011277000000
C	4.229142000000	0.448453000000	-0.163269000000
C	-0.265845000000	4.316571000000	-0.459826000000
H	-4.417285000000	0.262973000000	-1.367665000000
H	-0.083998000000	-4.413581000000	-1.036705000000
H	4.475686000000	0.137173000000	-1.180057000000
H	0.012726000000	4.467677000000	-1.504230000000
H	-4.523920000000	-1.084868000000	-0.231418000000
H	1.241951000000	-4.401548000000	0.130538000000
H	4.425060000000	1.522090000000	-0.083939000000
H	-1.328244000000	4.557728000000	-0.356859000000
H	-4.866932000000	0.557202000000	0.341035000000
H	-0.402659000000	-4.732416000000	0.697770000000
H	4.854996000000	-0.070756000000	0.559178000000
H	0.301688000000	4.979342000000	0.189799000000
S	-2.384342000000	0.737994000000	1.531210000000
S	-0.577862000000	-2.164304000000	1.718086000000
S	2.324406000000	-0.312274000000	1.662296000000
S	0.480030000000	2.542884000000	1.496451000000
Ni	0.011545000000	0.044201000000	-0.998785000000
Ni	-0.042155000000	0.194253000000	1.929613000000
N	0.233707000000	-0.440571000000	-5.632795000000
N	0.110153000000	-0.162221000000	-3.081833000000
C	-0.937802000000	-1.130042000000	-5.106191000000
C	-1.030436000000	-0.968875000000	-3.571538000000
C	0.142255000000	0.971372000000	-5.281307000000
C	0.075179000000	1.158410000000	-3.746926000000
C	1.423402000000	-1.003365000000	-5.006169000000
C	1.365926000000	-0.847588000000	-3.469046000000
H	-1.825751000000	-0.721909000000	-5.595987000000
H	-0.869462000000	-2.184242000000	-5.386997000000
H	-1.945769000000	-0.467536000000	-3.261054000000
H	-0.996859000000	-1.925988000000	-3.049584000000
H	1.010876000000	1.485915000000	-5.700203000000
H	-0.745702000000	1.387142000000	-5.764550000000
H	0.916512000000	1.737788000000	-3.364485000000
H	-0.834724000000	1.666790000000	-3.428699000000
H	2.300141000000	-0.496538000000	-5.417735000000
H	1.493332000000	-2.056599000000	-5.290313000000
H	1.381017000000	-1.806874000000	-2.951991000000
H	2.191560000000	-0.251860000000	-3.081939000000
N	-0.053139000000	0.171865000000	4.051733000000
N	-0.068883000000	0.152909000000	6.628403000000
C	-1.399322000000	-0.175147000000	4.567473000000

C	-1.391133000000	-0.179127000000	6.113855000000
C	0.321276000000	1.501193000000	4.586617000000
C	0.313060000000	1.470007000000	6.133726000000
C	0.913667000000	-0.822945000000	4.578798000000
C	0.881450000000	-0.829683000000	6.124441000000
H	-2.107177000000	0.553025000000	4.172543000000
H	-1.672533000000	-1.147192000000	4.153853000000
H	-2.106279000000	0.547390000000	6.507644000000
H	-1.675635000000	-1.159426000000	6.504096000000
H	1.306636000000	1.749838000000	4.188402000000
H	-0.384985000000	2.231063000000	4.188603000000
H	1.300410000000	1.713406000000	6.533867000000
H	-0.389746000000	2.204775000000	6.534238000000
H	1.901227000000	-0.554969000000	4.202965000000
H	0.655171000000	-1.793662000000	4.153636000000
H	0.594671000000	-1.812611000000	6.506762000000
H	1.867616000000	-0.597899000000	6.534636000000

Table S47. Cartesian coordinates for the triplet state of **3A** at the PBE0/TZVP/ZORA level.

O	-2.007982000000	-0.360894000000	-0.966930000000
O	0.389454000000	-1.961085000000	-0.850940000000
O	1.985928000000	0.511077000000	-0.933769000000
O	-0.444236000000	2.033486000000	-1.056216000000
C	-2.760386000000	0.010768000000	-0.051523000000
C	0.064451000000	-2.648021000000	0.132422000000
C	2.717010000000	0.257838000000	0.037785000000
C	-0.150534000000	2.825314000000	-0.146382000000
C	-4.243272000000	-0.054143000000	-0.282114000000
C	0.137448000000	-4.142786000000	0.007451000000
C	4.202650000000	0.382781000000	-0.140103000000
C	-0.250420000000	4.297227000000	-0.428061000000
H	-4.476921000000	0.357285000000	-1.265977000000
H	-0.282604000000	-4.449913000000	-0.952096000000
H	4.493957000000	-0.041209000000	-1.102735000000
H	0.161871000000	4.509166000000	-1.416170000000
H	-4.541805000000	-1.106248000000	-0.280483000000
H	1.191894000000	-4.433119000000	0.019677000000
H	4.453912000000	1.447332000000	-0.152368000000
H	-1.310029000000	4.568375000000	-0.441869000000
H	-4.802804000000	0.471207000000	0.489144000000
H	-0.374165000000	-4.648633000000	0.823752000000
H	4.753764000000	-0.095402000000	0.667231000000
H	0.252333000000	4.895268000000	0.329444000000
S	-2.242540000000	0.584372000000	1.477189000000
S	-0.451985000000	-2.022516000000	1.641619000000
S	2.158951000000	-0.212416000000	1.588920000000
S	0.348817000000	2.374283000000	1.430655000000
Ni	-0.003431000000	0.039396000000	-1.001009000000
Ni	-0.045616000000	0.175910000000	1.584042000000
N	0.259100000000	-0.420986000000	-5.704429000000
N	0.112742000000	-0.154550000000	-3.148667000000
C	-0.911828000000	-1.120067000000	-5.188456000000
C	-1.018707000000	-0.961237000000	-3.654277000000
C	0.156529000000	0.988595000000	-5.345364000000
C	0.080052000000	1.166174000000	-3.810205000000
C	1.447007000000	-0.978578000000	-5.069559000000
C	1.372348000000	-0.832889000000	-3.532211000000
H	-1.798350000000	-0.718351000000	-5.686495000000
H	-0.832426000000	-2.173242000000	-5.471071000000
H	-1.939531000000	-0.463405000000	-3.354126000000
H	-0.990300000000	-1.920311000000	-3.135294000000
H	1.023684000000	1.510919000000	-5.758248000000
H	-0.731710000000	1.400496000000	-5.831900000000
H	0.918243000000	1.745858000000	-3.420794000000
H	-0.831889000000	1.673993000000	-3.497457000000
H	2.323304000000	-0.461928000000	-5.470389000000
H	1.528472000000	-2.029319000000	-5.360638000000
H	1.387082000000	-1.796733000000	-3.024007000000
H	2.194080000000	-0.238407000000	-3.135116000000
N	-0.052110000000	0.175992000000	4.160928000000
N	-0.059062000000	0.183356000000	6.729025000000
C	-1.380264000000	-0.192942000000	4.672680000000

C	-1.380684000000	-0.170953000000	6.221339000000
C	0.293142000000	1.510269000000	4.670242000000
C	0.302812000000	1.502706000000	6.219583000000
C	0.930026000000	-0.787210000000	4.681769000000
C	0.905872000000	-0.790872000000	6.230209000000
H	-2.110080000000	0.506932000000	4.261721000000
H	-1.628973000000	-1.181713000000	4.279894000000
H	-2.100218000000	0.557154000000	6.606042000000
H	-1.655345000000	-1.146360000000	6.632336000000
H	1.268561000000	1.784419000000	4.260988000000
H	-0.434276000000	2.222087000000	4.273887000000
H	1.291172000000	1.759358000000	6.610829000000
H	-0.404962000000	2.231786000000	6.623663000000
H	1.912951000000	-0.505293000000	4.298918000000
H	0.692561000000	-1.769336000000	4.267149000000
H	0.630820000000	-1.774418000000	6.621457000000
H	1.888165000000	-0.542760000000	6.641996000000

Table S48. Cartesian coordinates for the singlet state of **3A** at the PBE0/TZVP/ZORA level.

O	-1.860651000000	-0.396953000000	-0.862083000000
O	0.360547000000	-1.858533000000	-0.725443000000
O	1.830241000000	0.378139000000	-0.858183000000
O	-0.410391000000	1.827168000000	-0.980706000000
C	-2.673868000000	-0.124151000000	0.051525000000
C	0.138603000000	-2.588692000000	0.268530000000
C	2.612349000000	0.250533000000	0.112635000000
C	-0.230102000000	2.687180000000	-0.087400000000
C	-4.127336000000	-0.303752000000	-0.273473000000
C	0.299513000000	-4.065586000000	0.061142000000
C	4.073856000000	0.415952000000	-0.182284000000
C	-0.416925000000	4.119568000000	-0.492534000000
H	-4.336073000000	0.111145000000	-1.261176000000
H	-0.171957000000	-4.356287000000	-0.879211000000
H	4.330546000000	-0.138507000000	-1.086736000000
H	0.059513000000	4.293954000000	-1.458839000000
H	-4.340719000000	-1.375919000000	-0.309481000000
H	1.367710000000	-4.286642000000	-0.017312000000
H	4.265932000000	1.475606000000	-0.373546000000
H	-1.488778000000	4.304295000000	-0.608875000000
H	-4.768789000000	0.155747000000	0.475433000000
H	-0.116455000000	-4.637785000000	0.887535000000
H	4.694225000000	0.091371000000	0.650252000000
H	-0.023734000000	4.805440000000	0.254800000000
S	-2.283590000000	0.402166000000	1.623412000000
S	-0.301080000000	-2.060125000000	1.827591000000
S	2.170129000000	-0.067539000000	1.726829000000
S	0.176931000000	2.382560000000	1.538579000000
Ni	-0.017202000000	-0.010083000000	-0.815142000000
Ni	-0.058615000000	0.166583000000	1.784652000000
N	0.269126000000	-0.312922000000	-6.005336000000
N	0.123367000000	-0.177672000000	-3.456297000000
C	-1.079284000000	-0.652770000000	-5.558219000000
C	-1.172369000000	-0.567977000000	-4.013092000000
C	0.587823000000	1.039125000000	-5.553101000000
C	0.507595000000	1.123025000000	-4.007348000000
C	1.214085000000	-1.245392000000	-5.395762000000
C	1.125660000000	-1.169335000000	-3.849323000000
H	-1.781225000000	0.034096000000	-6.040213000000
H	-1.313080000000	-1.659138000000	-5.917812000000
H	-1.912657000000	0.167736000000	-3.689558000000
H	-1.456982000000	-1.524551000000	-3.567867000000
H	1.588220000000	1.292502000000	-5.915981000000
H	-0.113813000000	1.730604000000	-6.028851000000
H	1.466955000000	1.401895000000	-3.564078000000
H	-0.227848000000	1.859432000000	-3.676002000000
H	2.217490000000	-0.995330000000	-5.752909000000
H	0.984212000000	-2.250870000000	-5.760516000000
H	0.842415000000	-2.127736000000	-3.408340000000
H	2.078076000000	-0.877242000000	-3.399782000000
N	-0.056098000000	0.216992000000	4.400754000000
N	-0.057205000000	0.251305000000	6.964213000000
C	-1.350959000000	-0.244213000000	4.917292000000

C	-1.354730000000	-0.194963000000	6.465931000000
C	0.188586000000	1.578348000000	4.891544000000
C	0.213798000000	1.587527000000	6.441296000000
C	0.996198000000	-0.663495000000	4.924403000000
C	0.969907000000	-0.662236000000	6.473556000000
H	-2.133584000000	0.389032000000	4.493326000000
H	-1.520520000000	-1.257325000000	4.543837000000
H	-2.117902000000	0.493485000000	6.839556000000
H	-1.567404000000	-1.178286000000	6.894587000000
H	1.136132000000	1.925145000000	4.470951000000
H	-0.597121000000	2.226645000000	4.495698000000
H	1.187611000000	1.910005000000	6.820328000000
H	-0.535492000000	2.273005000000	6.846951000000
H	1.954809000000	-0.307417000000	4.539948000000
H	0.836368000000	-1.664235000000	4.516232000000
H	0.754496000000	-1.659173000000	6.868249000000
H	1.933234000000	-0.351545000000	6.887783000000

Table S49. Cartesian coordinates for the BS(3,1) state of **3A** at the PBE0/TZVP/ZORA level.

O	-1.976739000000	-0.303851000000	-0.857920000000
O	0.367122000000	-1.931513000000	-0.735466000000
O	1.981071000000	0.472155000000	-0.833569000000
O	-0.378399000000	2.024499000000	-0.946402000000
C	-2.782430000000	0.100370000000	0.003394000000
C	0.025095000000	-2.675327000000	0.204654000000
C	2.767066000000	0.226461000000	0.101539000000
C	-0.075504000000	2.870393000000	-0.082934000000
C	-4.245647000000	-0.022834000000	-0.318491000000
C	0.189277000000	-4.155079000000	0.001991000000
C	4.229788000000	0.452282000000	-0.155810000000
C	-0.254068000000	4.316375000000	-0.452467000000
H	-4.420880000000	0.266439000000	-1.356528000000
H	-0.070379000000	-4.420959000000	-1.024305000000
H	4.479830000000	0.147609000000	-1.173701000000
H	0.024275000000	4.469325000000	-1.496642000000
H	-4.526801000000	-1.074809000000	-0.212214000000
H	1.244549000000	-4.400472000000	0.155373000000
H	4.423866000000	1.525666000000	-0.069040000000
H	-1.315477000000	4.561013000000	-0.347861000000
H	-4.861593000000	0.571905000000	0.352297000000
H	-0.405033000000	-4.730133000000	0.708831000000
H	4.854431000000	-0.070729000000	0.565112000000
H	0.316805000000	4.975443000000	0.198157000000
S	-2.366963000000	0.754728000000	1.525418000000
S	-0.589825000000	-2.150498000000	1.711061000000
S	2.314840000000	-0.323116000000	1.656404000000
S	0.494023000000	2.529396000000	1.493378000000
Ni	0.010195000000	0.044879000000	-0.945429000000
Ni	-0.038755000000	0.191194000000	1.881737000000
N	0.230585000000	-0.440215000000	-5.604196000000
N	0.106605000000	-0.160944000000	-3.050690000000
C	-0.936437000000	-1.135729000000	-5.075535000000
C	-1.026580000000	-0.977049000000	-3.540455000000
C	0.131545000000	0.971158000000	-5.252067000000
C	0.060186000000	1.157695000000	-3.717729000000
C	1.423288000000	-0.996009000000	-4.977079000000
C	1.367082000000	-0.835818000000	-3.440422000000
H	-1.827210000000	-0.730773000000	-5.562979000000
H	-0.864218000000	-2.189273000000	-5.358110000000
H	-1.946304000000	-0.485087000000	-3.228470000000
H	-0.983415000000	-1.934692000000	-3.020195000000
H	0.998764000000	1.489704000000	-5.669133000000
H	-0.757209000000	1.383026000000	-5.737326000000
H	0.895019000000	1.746024000000	-3.334819000000
H	-0.855053000000	1.657763000000	-3.401888000000
H	2.297556000000	-0.486876000000	-5.391253000000
H	1.497176000000	-2.049796000000	-5.258454000000
H	1.392741000000	-1.793641000000	-2.921318000000
H	2.188565000000	-0.231690000000	-3.057987000000
N	-0.053249000000	0.168251000000	4.010413000000
N	-0.071935000000	0.149775000000	6.589879000000
C	-1.398906000000	-0.179608000000	4.526282000000

C	-1.393033000000	-0.181873000000	6.073010000000
C	0.319251000000	1.497125000000	4.546583000000
C	0.311089000000	1.465930000000	6.094131000000
C	0.913347000000	-0.824875000000	4.540458000000
C	0.877632000000	-0.833319000000	6.086323000000
H	-2.107813000000	0.547068000000	4.131383000000
H	-1.671136000000	-1.152437000000	4.114181000000
H	-2.108636000000	0.545594000000	6.464227000000
H	-1.679161000000	-1.161603000000	6.463501000000
H	1.304713000000	1.747271000000	4.149856000000
H	-0.387531000000	2.226703000000	4.149369000000
H	1.298871000000	1.708639000000	6.493650000000
H	-0.390784000000	2.201865000000	6.494147000000
H	1.901841000000	-0.554247000000	4.169776000000
H	0.658353000000	-1.795861000000	4.114090000000
H	0.588743000000	-1.816391000000	6.466696000000
H	1.863640000000	-0.603661000000	6.498121000000

Table S50. Cartesian coordinates for the BS(2,2) state of **3A** at the PBE0/TZVP/ZORA level.

O	-1.974986000000	-0.303528000000	-0.859104000000
O	0.365749000000	-1.929510000000	-0.735144000000
O	1.978720000000	0.470542000000	-0.833770000000
O	-0.379654000000	2.022030000000	-0.945561000000
C	-2.784209000000	0.097302000000	0.001314000000
C	0.024728000000	-2.677877000000	0.202355000000
C	2.767470000000	0.222339000000	0.099076000000
C	-0.077692000000	2.870145000000	-0.083064000000
C	-4.245709000000	-0.028570000000	-0.328182000000
C	0.190375000000	-4.156337000000	-0.009831000000
C	4.229341000000	0.446562000000	-0.165597000000
C	-0.260132000000	4.314551000000	-0.457581000000
H	-4.415888000000	0.257097000000	-1.368039000000
H	-0.064054000000	-4.415448000000	-1.039135000000
H	4.473373000000	0.145520000000	-1.186013000000
H	0.008269000000	4.463213000000	-1.504936000000
H	-4.526001000000	-1.080614000000	-0.220175000000
H	1.245033000000	-4.402200000000	0.147018000000
H	4.425534000000	1.519328000000	-0.075965000000
H	-1.320657000000	4.559107000000	-0.344046000000
H	-4.866059000000	0.567030000000	0.337644000000
H	-0.406684000000	-4.736488000000	0.690396000000
H	4.857099000000	-0.079867000000	0.549997000000
H	0.315947000000	4.976733000000	0.185147000000
S	-2.378950000000	0.747713000000	1.527561000000
S	-0.588438000000	-2.164379000000	1.713142000000
S	2.323628000000	-0.327596000000	1.656037000000
S	0.492503000000	2.536955000000	1.494447000000
Ni	0.010234000000	0.043891000000	-0.962557000000
Ni	-0.039831000000	0.189192000000	1.894924000000
N	0.232330000000	-0.437966000000	-5.611621000000
N	0.107618000000	-0.160855000000	-3.058876000000
C	-0.937581000000	-1.129975000000	-5.084830000000
C	-1.028745000000	-0.972211000000	-3.549713000000
C	0.138029000000	0.973457000000	-5.258654000000
C	0.066809000000	1.159074000000	-3.724229000000
C	1.422746000000	-0.998613000000	-4.984567000000
C	1.366019000000	-0.840301000000	-3.447718000000
H	-1.826563000000	-0.721768000000	-5.572764000000
H	-0.868534000000	-2.183541000000	-5.367986000000
H	-1.946587000000	-0.476632000000	-3.237776000000
H	-0.989730000000	-1.930309000000	-3.029950000000
H	1.007119000000	1.489425000000	-5.674929000000
H	-0.749162000000	1.388749000000	-5.743780000000
H	0.903981000000	1.743356000000	-3.340199000000
H	-0.846505000000	1.662442000000	-3.408001000000
H	2.299018000000	-0.491890000000	-5.397367000000
H	1.493314000000	-2.052270000000	-5.267150000000
H	1.387278000000	-1.798754000000	-2.929518000000
H	2.189293000000	-0.239697000000	-3.063444000000
N	-0.053530000000	0.171570000000	4.027074000000
N	-0.070961000000	0.153395000000	6.605555000000
C	-1.399332000000	-0.176266000000	4.543303000000

C	-1.392449000000	-0.179134000000	6.089717000000
C	0.319472000000	1.500889000000	4.562789000000
C	0.310927000000	1.470106000000	6.109972000000
C	0.913551000000	-0.821847000000	4.556364000000
C	0.879432000000	-0.829180000000	6.101995000000
H	-2.108175000000	0.550697000000	4.148316000000
H	-1.671818000000	-1.148929000000	4.130739000000
H	-2.108204000000	0.547573000000	6.482069000000
H	-1.677369000000	-1.159194000000	6.480270000000
H	1.305035000000	1.750480000000	4.165755000000
H	-0.386813000000	2.230586000000	4.164654000000
H	1.298263000000	1.713840000000	6.509981000000
H	-0.391856000000	2.205203000000	6.509940000000
H	1.901599000000	-0.552130000000	4.183328000000
H	0.657389000000	-1.793021000000	4.130825000000
H	0.591951000000	-1.812208000000	6.483547000000
H	1.865402000000	-0.598051000000	6.513061000000

Table S51. Cartesian coordinates for the BS(1,1) state of **3A** at the PBE0/TZVP/ZORA level.

O	-1.976963000000	-0.352340000000	-0.942234000000
O	0.382152000000	-1.925540000000	-0.830934000000
O	1.964117000000	0.489820000000	-0.910685000000
O	-0.423686000000	1.999631000000	-1.032639000000
C	-2.743237000000	0.012939000000	-0.032585000000
C	0.064454000000	-2.629724000000	0.145873000000
C	2.706674000000	0.244569000000	0.056955000000
C	-0.138165000000	2.806919000000	-0.129808000000
C	-4.221192000000	-0.063674000000	-0.290354000000
C	0.148883000000	-4.120799000000	-0.012300000000
C	4.188850000000	0.370967000000	-0.148453000000
C	-0.244425000000	4.271547000000	-0.445387000000
H	-4.440162000000	0.347949000000	-1.277516000000
H	-0.274202000000	-4.410285000000	-0.976005000000
H	4.463422000000	-0.061408000000	-1.112274000000
H	0.179628000000	4.464520000000	-1.432438000000
H	-4.511226000000	-1.118145000000	-0.296429000000
H	1.205620000000	-4.402934000000	-0.012471000000
H	4.437617000000	1.435830000000	-0.175281000000
H	-1.305512000000	4.534976000000	-0.479748000000
H	-4.798574000000	0.455322000000	0.471715000000
H	-0.353976000000	-4.648015000000	0.795611000000
H	4.755077000000	-0.098582000000	0.653207000000
H	0.244145000000	4.889212000000	0.305304000000
S	-2.254726000000	0.581356000000	1.504474000000
S	-0.446094000000	-2.038174000000	1.667200000000
S	2.174807000000	-0.208993000000	1.619265000000
S	0.348270000000	2.389775000000	1.456655000000
Ni	-0.001670000000	0.041049000000	-0.969767000000
Ni	-0.044288000000	0.177616000000	1.645554000000
N	0.251794000000	-0.417295000000	-5.722564000000
N	0.112790000000	-0.153008000000	-3.168064000000
C	-0.922076000000	-1.110956000000	-5.204818000000
C	-1.020686000000	-0.955494000000	-3.669152000000
C	0.157049000000	0.992861000000	-5.362236000000
C	0.080738000000	1.167089000000	-3.826162000000
C	1.438692000000	-0.981692000000	-5.090819000000
C	1.368174000000	-0.832583000000	-3.553011000000
H	-1.807503000000	-0.701758000000	-5.698970000000
H	-0.850142000000	-2.163687000000	-5.491461000000
H	-1.940129000000	-0.457485000000	-3.363550000000
H	-0.991910000000	-1.916687000000	-3.153498000000
H	1.027788000000	1.510081000000	-5.774297000000
H	-0.728365000000	1.410372000000	-5.849376000000
H	0.919162000000	1.747020000000	-3.436864000000
H	-0.831468000000	1.675123000000	-3.513061000000
H	2.316894000000	-0.471186000000	-5.495592000000
H	1.511995000000	-2.033310000000	-5.381287000000
H	1.384417000000	-1.796119000000	-3.043440000000
H	2.192921000000	-0.239102000000	-3.159422000000
N	-0.055528000000	0.179548000000	4.175261000000
N	-0.063967000000	0.187037000000	6.744053000000
C	-1.384400000000	-0.189562000000	4.687279000000

C	-1.384591000000	-0.169596000000	6.235800000000
C	0.289154000000	1.514418000000	4.685651000000
C	0.295996000000	1.506897000000	6.234868000000
C	0.926932000000	-0.783663000000	4.697806000000
C	0.902701000000	-0.785685000000	6.246065000000
H	-2.113516000000	0.511827000000	4.277844000000
H	-1.634062000000	-1.177395000000	4.292925000000
H	-2.106044000000	0.556185000000	6.621166000000
H	-1.656974000000	-1.146223000000	6.645274000000
H	1.265390000000	1.788085000000	4.278139000000
H	-0.437625000000	2.226146000000	4.288062000000
H	1.283032000000	1.766041000000	6.627658000000
H	-0.414199000000	2.234504000000	6.637212000000
H	1.909975000000	-0.502288000000	4.315039000000
H	0.689371000000	-1.766140000000	4.284246000000
H	0.629729000000	-1.769464000000	6.638034000000
H	1.884594000000	-0.535305000000	6.657295000000

Table S52. Cartesian coordinates for the quintet state of **4A** at the PBE0/TZVP/ZORA level.

O	-1.982696000000	-0.212184000000	-0.949129000000
O	0.201531000000	-2.048830000000	-0.695958000000
O	2.016941000000	0.107190000000	-0.719451000000
O	-0.172054000000	1.952587000000	-0.970325000000
C	-2.797272000000	0.211938000000	-0.105174000000
C	-0.225939000000	-2.756839000000	0.238279000000
C	2.731493000000	-0.189998000000	0.258988000000
C	0.161583000000	2.778427000000	-0.096656000000
C	-4.252986000000	0.147485000000	-0.470651000000
C	-0.170404000000	-4.245730000000	0.044189000000
C	4.219128000000	-0.159139000000	0.049354000000
C	0.146791000000	4.227778000000	-0.491682000000
H	-4.376468000000	0.331562000000	-1.538956000000
H	-0.453344000000	-4.494833000000	-0.980129000000
H	4.460879000000	-0.525106000000	-0.949889000000
H	0.558788000000	4.338967000000	-1.496390000000
H	-4.605469000000	-0.866764000000	-0.260284000000
H	0.865018000000	-4.566129000000	0.194401000000
H	4.543744000000	0.883793000000	0.111913000000
H	-0.895453000000	4.559736000000	-0.518284000000
H	-4.849225000000	0.844563000000	0.114263000000
H	-0.803100000000	-4.772368000000	0.754957000000
H	4.748529000000	-0.730958000000	0.808365000000
H	0.692044000000	4.848253000000	0.215689000000
S	-2.408871000000	0.827144000000	1.444897000000
S	-0.856914000000	-2.178407000000	1.720674000000
S	2.172512000000	-0.596447000000	1.825418000000
S	0.622714000000	2.401320000000	1.507460000000
Ni	0.020870000000	-0.054446000000	-0.930419000000
Ni	-0.133983000000	0.128646000000	1.883995000000
N	0.392856000000	-0.327460000000	-5.711507000000
C	1.027813000000	-1.172908000000	-4.908684000000
C	0.922587000000	-1.105097000000	-3.527956000000
N	0.167116000000	-0.172060000000	-2.954148000000
C	-0.477478000000	0.683532000000	-3.743111000000
C	-0.356807000000	0.595839000000	-5.121519000000
H	1.643723000000	-1.933291000000	-5.376996000000
H	1.429155000000	-1.796589000000	-2.866629000000
H	-1.076493000000	1.441102000000	-3.253909000000
H	-0.882105000000	1.293224000000	-5.765336000000
H	0.511691000000	-1.620351000000	4.219595000000
H	0.350748000000	-1.433816000000	6.720648000000
C	0.031000000000	-0.618283000000	6.081011000000
C	0.127276000000	-0.729697000000	4.702681000000
N	-0.264288000000	0.268090000000	3.910409000000
C	-0.746194000000	1.365684000000	4.493466000000
H	-1.052798000000	2.175448000000	3.841792000000
H	-1.226405000000	2.349525000000	6.341883000000
C	-0.833038000000	1.453633000000	5.873727000000
N	-0.447450000000	0.468150000000	6.675356000000

Table S53. Cartesian coordinates for the triplet state of **4A** at the PBE0/TZVP/ZORA level.

O	-1.978156000000	-0.271314000000	-1.019099000000
O	0.283464000000	-2.084088000000	-0.767502000000
O	2.072659000000	0.151988000000	-0.813442000000
O	-0.198505000000	1.968061000000	-1.034516000000
C	-2.746254000000	0.156222000000	-0.143173000000
C	-0.153918000000	-2.733993000000	0.195382000000
C	2.730133000000	-0.147190000000	0.195872000000
C	0.137883000000	2.742971000000	-0.125108000000
C	-4.218306000000	0.186590000000	-0.436975000000
C	-0.200524000000	-4.230316000000	0.084885000000
C	4.226235000000	-0.198837000000	0.081811000000
C	0.217389000000	4.210504000000	-0.431626000000
H	-4.378820000000	0.497425000000	-1.470571000000
H	-0.577277000000	-4.510094000000	-0.900428000000
H	4.504932000000	-0.686623000000	-0.853782000000
H	0.755824000000	4.354939000000	-1.370245000000
H	-4.605811000000	-0.830585000000	-0.328457000000
H	0.821556000000	-4.609509000000	0.174777000000
H	4.597618000000	0.829403000000	0.046162000000
H	-0.800573000000	4.586503000000	-0.568489000000
H	-4.759915000000	0.837726000000	0.246637000000
H	-0.809839000000	-4.680840000000	0.865873000000
H	4.686147000000	-0.706141000000	0.927651000000
H	0.696054000000	4.772443000000	0.367847000000
S	-2.256378000000	0.696331000000	1.409825000000
S	-0.711880000000	-2.047904000000	1.666622000000
S	2.060405000000	-0.485848000000	1.739006000000
S	0.521710000000	2.256772000000	1.474492000000
Ni	0.045154000000	-0.056676000000	-0.884402000000
Ni	-0.100736000000	0.107761000000	1.631102000000
N	0.323958000000	-0.322967000000	-5.731727000000
C	1.040154000000	-1.116358000000	-4.944091000000
C	0.967312000000	-1.049277000000	-3.560931000000
N	0.164076000000	-0.173035000000	-2.964912000000
C	-0.560195000000	0.628706000000	-3.740162000000
C	-0.473070000000	0.546047000000	-5.121543000000
H	1.696434000000	-1.832334000000	-5.427744000000
H	1.541987000000	-1.701019000000	-2.915263000000
H	-1.200592000000	1.342674000000	-3.238363000000
H	-1.065063000000	1.201508000000	-5.751704000000
H	0.645998000000	-1.543922000000	4.275194000000
H	0.422705000000	-1.357664000000	6.766948000000
C	0.054878000000	-0.571590000000	6.115277000000
C	0.184677000000	-0.677765000000	4.737814000000
N	-0.259276000000	0.278182000000	3.926446000000
C	-0.831044000000	1.334127000000	4.499197000000
H	-1.187126000000	2.120134000000	3.841604000000
H	-1.429968000000	2.291977000000	6.331523000000
C	-0.958764000000	1.425976000000	5.877489000000
N	-0.518059000000	0.476802000000	6.695057000000

Table S54. Cartesian coordinates for the singlet state of **4A** at the PBE0/TZVP/ZORA level.

O	-1.704876000000	-0.221607000000	-0.971012000000
O	0.326686000000	-1.918577000000	-0.676425000000
O	2.028896000000	0.128924000000	-0.660338000000
O	-0.001861000000	1.826818000000	-0.966777000000
C	-2.566327000000	0.095986000000	-0.119219000000
C	-0.016961000000	-2.626189000000	0.300045000000
C	2.715336000000	-0.055754000000	0.370678000000
C	0.165294000000	2.669456000000	-0.053151000000
C	-3.996101000000	0.058205000000	-0.571487000000
C	-0.000747000000	-4.110784000000	0.085185000000
C	4.203773000000	-0.069564000000	0.185184000000
C	0.202230000000	4.109424000000	-0.472890000000
H	-4.081367000000	0.541831000000	-1.546062000000
H	-0.552626000000	-4.350495000000	-0.826065000000
H	4.456356000000	-0.705556000000	-0.665089000000
H	0.913832000000	4.230074000000	-1.292448000000
H	-4.290155000000	-0.988169000000	-0.692622000000
H	1.035407000000	-4.428409000000	-0.059623000000
H	4.529725000000	0.947093000000	-0.051792000000
H	-0.787082000000	4.386553000000	-0.847436000000
H	-4.661660000000	0.530299000000	0.147835000000
H	-0.423876000000	-4.647739000000	0.931080000000
H	4.721501000000	-0.407667000000	1.080107000000
H	0.467956000000	4.765682000000	0.352703000000
S	-2.266980000000	0.531962000000	1.499977000000
S	-0.491972000000	-2.062221000000	1.834923000000
S	2.121038000000	-0.262204000000	1.954682000000
S	0.347480000000	2.331553000000	1.605409000000
Ni	0.157947000000	-0.041941000000	-0.759658000000
Ni	-0.081334000000	0.141737000000	1.825887000000
N	-0.087830000000	-0.365730000000	-6.131423000000
C	0.151997000000	-1.437498000000	-5.384007000000
C	0.323305000000	-1.355353000000	-4.008514000000
N	0.258646000000	-0.194437000000	-3.368009000000
C	0.017467000000	0.880397000000	-4.109122000000
C	-0.153419000000	0.792479000000	-5.484069000000
H	0.207997000000	-2.393163000000	-5.896290000000
H	0.513837000000	-2.235888000000	-3.403260000000
H	-0.042481000000	1.828110000000	-3.584074000000
H	-0.350059000000	1.679488000000	-6.078693000000
H	0.766748000000	-1.412582000000	4.595137000000
H	0.468078000000	-1.274640000000	7.081327000000
C	0.033772000000	-0.526339000000	6.425953000000
C	0.203128000000	-0.604708000000	5.050722000000
N	-0.321183000000	0.303965000000	4.233983000000
C	-1.013204000000	1.287129000000	4.801625000000
H	-1.442209000000	2.035069000000	4.142486000000
H	-1.747689000000	2.163432000000	6.627810000000

C	-1.179074000000	1.355776000000	6.177775000000
N	-0.658067000000	0.451657000000	6.999281000000

Table S55. Cartesian coordinates for the BS(3,1) state of **4A** at the PBE0/TZVP/ZORA level.

O	-1.969553000000	-0.208816000000	-0.940571000000
O	0.214849000000	-2.054764000000	-0.690014000000
O	2.032765000000	0.100221000000	-0.712342000000
O	-0.156026000000	1.949707000000	-0.957529000000
C	-2.785368000000	0.225516000000	-0.103944000000
C	-0.223616000000	-2.758780000000	0.240925000000
C	2.746060000000	-0.198136000000	0.265848000000
C	0.182356000000	2.777559000000	-0.089021000000
C	-4.241129000000	0.170307000000	-0.468417000000
C	-0.175405000000	-4.248563000000	0.058596000000
C	4.234292000000	-0.165272000000	0.066291000000
C	0.164142000000	4.227355000000	-0.479199000000
H	-4.361653000000	0.320056000000	-1.542303000000
H	-0.427517000000	-4.502412000000	-0.972423000000
H	4.482018000000	-0.507967000000	-0.939589000000
H	0.547318000000	4.339987000000	-1.494937000000
H	-4.611088000000	-0.829395000000	-0.221662000000
H	0.851102000000	-4.577997000000	0.246060000000
H	4.561110000000	0.874874000000	0.157688000000
H	-0.876518000000	4.565354000000	-0.472927000000
H	-4.826156000000	0.896897000000	0.091981000000
H	-0.835728000000	-4.764102000000	0.752600000000
H	4.757380000000	-0.756323000000	0.815245000000
H	0.732748000000	4.842550000000	0.214674000000
S	-2.383678000000	0.843879000000	1.439415000000
S	-0.859851000000	-2.158368000000	1.711258000000
S	2.169201000000	-0.604582000000	1.824125000000
S	0.649060000000	2.386843000000	1.509030000000
Ni	0.032672000000	-0.054897000000	-0.861619000000
Ni	-0.118728000000	0.127517000000	1.817425000000
N	0.349014000000	-0.326485000000	-5.663374000000
C	1.042815000000	-1.132983000000	-4.869185000000
C	0.957849000000	-1.064870000000	-3.486913000000
N	0.163769000000	-0.172199000000	-2.902588000000
C	-0.539239000000	0.643710000000	-3.682850000000
C	-0.438667000000	0.557627000000	-5.062999000000
H	1.690557000000	-1.860899000000	-5.346210000000
H	1.512644000000	-1.725432000000	-2.832891000000
H	-1.171105000000	1.368399000000	-3.185567000000
H	-1.012036000000	1.222989000000	-5.699773000000
H	0.527051000000	-1.619114000000	4.149143000000
H	0.342460000000	-1.438045000000	6.646671000000
C	0.022056000000	-0.623182000000	6.006434000000
C	0.132530000000	-0.731287000000	4.628927000000
N	-0.259013000000	0.264583000000	3.834201000000
C	-0.754764000000	1.356964000000	4.415398000000

H	-1.061023000000	2.166402000000	3.763356000000
H	-1.262503000000	2.333109000000	6.259847000000
C	-0.856618000000	1.441025000000	5.795003000000
N	-0.471545000000	0.457330000000	6.598942000000

Table S56. Cartesian coordinates for the BS(2,2) state of **4A** at the PBE0/TZVP/ZORA level.

O	-1.971581000000	-0.209938000000	-0.942178000000
O	0.213017000000	-2.051233000000	-0.692579000000
O	2.025937000000	0.103303000000	-0.709776000000
O	-0.163079000000	1.947998000000	-0.960318000000
C	-2.789044000000	0.224231000000	-0.105967000000
C	-0.224210000000	-2.759934000000	0.236358000000
C	2.741830000000	-0.196443000000	0.267040000000
C	0.174945000000	2.778875000000	-0.093503000000
C	-4.243549000000	0.167203000000	-0.475905000000
C	-0.169832000000	-4.248638000000	0.045619000000
C	4.229311000000	-0.162296000000	0.060609000000
C	0.152669000000	4.226900000000	-0.490596000000
H	-4.360415000000	0.311661000000	-1.550891000000
H	-0.413496000000	-4.497892000000	-0.988526000000
H	4.472794000000	-0.496972000000	-0.948972000000
H	0.528073000000	4.335478000000	-1.509650000000
H	-4.614118000000	-0.831409000000	-0.225619000000
H	0.856530000000	-4.575422000000	0.238603000000
H	4.556528000000	0.877118000000	0.158780000000
H	-0.888366000000	4.563623000000	-0.478177000000
H	-4.830664000000	0.896027000000	0.079230000000
H	-0.832815000000	-4.770271000000	0.732348000000
H	4.755594000000	-0.758801000000	0.802875000000
H	0.725241000000	4.845815000000	0.196520000000
S	-2.395792000000	0.843151000000	1.439190000000
S	-0.863235000000	-2.171222000000	1.709793000000
S	2.173951000000	-0.605011000000	1.827760000000
S	0.644042000000	2.398269000000	1.506005000000
Ni	0.029595000000	-0.055085000000	-0.882049000000
Ni	-0.123499000000	0.127836000000	1.834404000000
N	0.360275000000	-0.329250000000	-5.675211000000
C	1.048978000000	-1.137426000000	-4.878323000000
C	0.959433000000	-1.068486000000	-3.496427000000
N	0.165681000000	-0.172897000000	-2.915852000000
C	-0.532372000000	0.644968000000	-3.698651000000
C	-0.427009000000	0.557574000000	-5.078351000000
H	1.696301000000	-1.867410000000	-5.352702000000
H	1.509866000000	-1.730144000000	-2.839803000000
H	-1.163660000000	1.371836000000	-3.203757000000
H	-0.996109000000	1.224188000000	-5.717593000000
H	0.484704000000	-1.635538000000	4.175540000000
H	0.312018000000	-1.451947000000	6.674888000000
C	0.007503000000	-0.630248000000	6.035639000000
C	0.110709000000	-0.739951000000	4.657677000000

N	-0.261787000000	0.264754000000	3.865099000000
C	-0.731903000000	1.367394000000	4.447968000000
H	-1.023475000000	2.182950000000	3.796564000000
H	-1.210453000000	2.353937000000	6.295207000000
C	-0.826288000000	1.453514000000	5.828023000000
N	-0.459481000000	0.461146000000	6.629876000000

Table S57. Cartesian coordinates for the BS(1,1) state of **4A** at the PBE0/TZVP/ZORA level.

O	-1.944340000000	-0.263729000000	-0.994191000000
O	0.267841000000	-2.054289000000	-0.750221000000
O	2.035414000000	0.144832000000	-0.795335000000
O	-0.187997000000	1.941908000000	-1.012053000000
C	-2.728828000000	0.156679000000	-0.124902000000
C	-0.159620000000	-2.719239000000	0.210360000000
C	2.712001000000	-0.149811000000	0.206560000000
C	0.141172000000	2.730163000000	-0.107748000000
C	-4.194398000000	0.170017000000	-0.450160000000
C	-0.194563000000	-4.213515000000	0.071143000000
C	4.204968000000	-0.192268000000	0.054571000000
C	0.208488000000	4.192577000000	-0.440638000000
H	-4.336388000000	0.482052000000	-1.486077000000
H	-0.581811000000	-4.477228000000	-0.914609000000
H	4.462664000000	-0.680506000000	-0.886810000000
H	0.746996000000	4.324558000000	-1.381012000000
H	-4.572754000000	-0.851683000000	-0.353239000000
H	0.831445000000	-4.586312000000	0.139867000000
H	4.569982000000	0.837736000000	0.007046000000
H	-0.812003000000	4.558411000000	-0.585433000000
H	-4.757350000000	0.812623000000	0.223814000000
H	-0.790033000000	-4.683745000000	0.850881000000
H	4.688268000000	-0.694929000000	0.889790000000
H	0.681363000000	4.771848000000	0.349525000000
S	-2.273142000000	0.694672000000	1.434954000000
S	-0.708848000000	-2.062661000000	1.694412000000
S	2.079140000000	-0.484536000000	1.761894000000
S	0.521158000000	2.272681000000	1.497781000000
Ni	0.043813000000	-0.055429000000	-0.872706000000
Ni	-0.101053000000	0.110254000000	1.684941000000
N	0.332045000000	-0.323131000000	-5.762389000000
C	1.010576000000	-1.147620000000	-4.973154000000
C	0.933227000000	-1.080040000000	-3.590013000000
N	0.165392000000	-0.173017000000	-2.994119000000
C	-0.520362000000	0.659080000000	-3.771768000000
C	-0.431015000000	0.576880000000	-5.153340000000
H	1.638568000000	-1.889326000000	-5.455883000000
H	1.477037000000	-1.757710000000	-2.943551000000
H	-1.133006000000	1.398835000000	-3.271618000000
H	-0.992387000000	1.257719000000	-5.784849000000
H	0.650781000000	-1.536622000000	4.313293000000
H	0.420868000000	-1.349186000000	6.804368000000

C	0.052313000000	-0.564872000000	6.151160000000
C	0.185464000000	-0.671864000000	4.774309000000
N	-0.259984000000	0.281887000000	3.960742000000
C	-0.836169000000	1.336676000000	4.531724000000
H	-1.193696000000	2.120544000000	3.872495000000
H	-1.440745000000	2.294542000000	6.362014000000
C	-0.966456000000	1.429567000000	5.909518000000
N	-0.524743000000	0.482412000000	6.728895000000

Table S58. Cartesian coordinates for the quintet state of **5A** at the PBE0/TZVP/ZORA level.

O	-1.935944000000	-0.351738000000	-1.013712000000
O	0.279786000000	-1.939790000000	-0.605633000000
O	2.069651000000	0.316061000000	-0.769499000000
O	-0.116545000000	2.072114000000	-0.933808000000
C	-2.780298000000	0.029439000000	-0.180059000000
C	-0.169116000000	-2.631038000000	0.330841000000
C	2.774667000000	-0.001768000000	0.209673000000
C	0.216627000000	2.888251000000	-0.047961000000
S	-2.354867000000	0.984313000000	1.191576000000
S	-0.835823000000	-1.996896000000	1.790364000000
S	2.134792000000	-0.504842000000	1.719676000000
S	0.562957000000	2.487783000000	1.591114000000
Ni	0.068464000000	0.053445000000	-0.988843000000
Ni	-0.149135000000	0.245651000000	1.673943000000
C	-4.202845000000	-0.323646000000	-0.418100000000
C	-4.531609000000	-1.069874000000	-1.551217000000
C	-5.212783000000	0.042841000000	0.470597000000
C	-5.844018000000	-1.438448000000	-1.791776000000
C	-6.525811000000	-0.321899000000	0.225182000000
C	-6.844343000000	-1.064864000000	-0.903861000000
H	-3.740490000000	-1.366634000000	-2.228131000000
H	-4.954963000000	0.608739000000	1.357710000000
H	-6.088713000000	-2.024174000000	-2.670570000000
H	-7.303187000000	-0.031744000000	0.922487000000
H	-7.872009000000	-1.356815000000	-1.089599000000
C	0.324372000000	4.318420000000	-0.454980000000
C	-0.183892000000	4.699894000000	-1.697328000000
C	0.926261000000	5.281568000000	0.354064000000
C	-0.098343000000	6.016159000000	-2.119015000000
C	1.022990000000	6.594760000000	-0.074895000000
C	0.509549000000	6.966994000000	-1.310237000000
H	-0.656797000000	3.949910000000	-2.318320000000
H	1.322407000000	4.990010000000	1.319179000000
H	-0.507272000000	6.302421000000	-3.081595000000
H	1.500446000000	7.332644000000	0.559678000000
H	0.581594000000	7.997205000000	-1.640742000000
C	4.252106000000	0.043033000000	0.036043000000
C	5.125123000000	-0.555570000000	0.943469000000
C	4.775816000000	0.702967000000	-1.076131000000
C	6.493140000000	-0.504374000000	0.735132000000

C	6.144993000000	0.766361000000	-1.274077000000
C	7.007250000000	0.157998000000	-0.371783000000
H	4.721345000000	-1.064534000000	1.810550000000
H	4.093775000000	1.176989000000	-1.770625000000
H	7.162271000000	-0.981287000000	1.442123000000
H	6.542202000000	1.292447000000	-2.134881000000
H	8.079224000000	0.202529000000	-0.528937000000
C	-0.129269000000	-4.111308000000	0.163184000000
C	-0.721426000000	-4.983039000000	1.076498000000
C	0.519992000000	-4.639317000000	-0.953440000000
C	-0.671121000000	-6.351549000000	0.871845000000
C	0.579300000000	-6.008608000000	-1.150489000000
C	-0.019671000000	-6.868859000000	-0.239956000000
H	-1.222294000000	-4.577738000000	1.947293000000
H	0.983953000000	-3.958333000000	-1.655320000000
H	-1.140146000000	-7.018626000000	1.586151000000
H	1.093800000000	-6.407468000000	-2.017532000000
H	0.022917000000	-7.941214000000	-0.395093000000
C	0.353965000000	0.021471000000	-5.662201000000
N	0.203523000000	0.040200000000	-3.085696000000
C	-1.033259000000	0.468594000000	-5.212001000000
C	-1.023066000000	0.624823000000	-3.680221000000
C	1.376661000000	0.988813000000	-5.073166000000
C	1.369710000000	0.835846000000	-3.541298000000
C	0.621198000000	-1.371787000000	-5.096844000000
C	0.363756000000	-1.346860000000	-3.577840000000
H	-1.303826000000	1.414684000000	-5.688021000000
H	-1.780503000000	-0.268838000000	-5.519548000000
H	-1.047533000000	1.671939000000	-3.376195000000
H	-1.879452000000	0.138118000000	-3.218267000000
H	2.375028000000	0.779909000000	-5.466290000000
H	1.127992000000	2.013872000000	-5.363551000000
H	2.260438000000	0.320557000000	-3.185264000000
H	1.331176000000	1.798698000000	-3.031625000000
H	1.653803000000	-1.665339000000	-5.307385000000
H	-0.024472000000	-2.110525000000	-5.578642000000
H	-0.542898000000	-1.890897000000	-3.307853000000
H	1.183660000000	-1.799735000000	-3.020647000000
H	0.418872000000	0.009449000000	-6.752409000000

Table S59. Cartesian coordinates for the triplet state of **5A** at the PBE0/TZVP/ZORA level.

O	-1.864528000000	-0.422493000000	-0.943335000000
O	0.487622000000	-2.007659000000	-0.722062000000
O	2.140445000000	0.324948000000	-0.805869000000
O	-0.231173000000	1.995922000000	-1.045954000000
C	-2.656141000000	-0.004533000000	-0.076619000000
C	0.076535000000	-2.677164000000	0.244342000000
C	2.820518000000	0.015143000000	0.191618000000
C	0.069257000000	2.800876000000	-0.142762000000
S	-2.151629000000	0.695061000000	1.414592000000
S	-0.529102000000	-1.986232000000	1.701335000000
S	2.156528000000	-0.362776000000	1.732389000000
S	0.541148000000	2.322260000000	1.443224000000
Ni	0.137671000000	-0.011491000000	-0.997558000000
Ni	0.006956000000	0.164049000000	1.516452000000
C	-4.113296000000	-0.108204000000	-0.354493000000
C	-4.526450000000	-0.816201000000	-1.483583000000
C	-5.075118000000	0.474182000000	0.470723000000
C	-5.873147000000	-0.939967000000	-1.781176000000
C	-6.420725000000	0.359081000000	0.164904000000
C	-6.823791000000	-0.348710000000	-0.959982000000
H	-3.775178000000	-1.277612000000	-2.111779000000
H	-4.761622000000	1.020037000000	1.352447000000
H	-6.183403000000	-1.500355000000	-2.655896000000
H	-7.159663000000	0.821602000000	0.809163000000
H	-7.878644000000	-0.442012000000	-1.193533000000
C	0.041986000000	4.252932000000	-0.464451000000
C	-0.403402000000	4.648784000000	-1.725925000000
C	0.443391000000	5.227414000000	0.448999000000
C	-0.447723000000	5.989905000000	-2.067071000000
C	0.408071000000	6.567322000000	0.102472000000
C	-0.038105000000	6.952685000000	-1.154536000000
H	-0.722159000000	3.887986000000	-2.427064000000
H	0.783091000000	4.928265000000	1.433205000000
H	-0.802543000000	6.286094000000	-3.047717000000
H	0.726776000000	7.315699000000	0.818796000000
H	-0.068710000000	8.003259000000	-1.420935000000
C	4.298853000000	-0.031665000000	0.039870000000
C	5.120710000000	-0.700054000000	0.946582000000
C	4.875495000000	0.610721000000	-1.055798000000
C	6.491933000000	-0.729054000000	0.755518000000
C	6.248596000000	0.593710000000	-1.235647000000
C	7.060179000000	-0.080502000000	-0.333082000000
H	4.678019000000	-1.204559000000	1.797167000000
H	4.231422000000	1.133297000000	-1.752142000000
H	7.121057000000	-1.259855000000	1.461052000000
H	6.688221000000	1.106925000000	-2.083529000000
H	8.134823000000	-0.099551000000	-0.476511000000
C	0.097951000000	-4.160077000000	0.125725000000
C	-0.502943000000	-4.994284000000	1.068075000000
C	0.738454000000	-4.729991000000	-0.974767000000
C	-0.468729000000	-6.369083000000	0.907297000000
C	0.782226000000	-6.105713000000	-1.126924000000
C	0.175254000000	-6.929069000000	-0.188382000000

H	-1.001233000000	-4.559446000000	1.926350000000
H	1.206503000000	-4.076711000000	-1.700074000000
H	-0.945046000000	-7.007392000000	1.642631000000
H	1.289853000000	-6.538230000000	-1.981752000000
H	0.204840000000	-8.006266000000	-0.309195000000
C	0.343769000000	-0.066805000000	-5.703290000000
N	0.239641000000	-0.050780000000	-3.124388000000
C	-1.042671000000	0.361074000000	-5.232722000000
C	-1.052794000000	0.398969000000	-3.691650000000
C	1.366732000000	0.913461000000	-5.138318000000
C	1.307889000000	0.859150000000	-3.598760000000
C	0.641915000000	-1.457548000000	-5.149170000000
C	0.530976000000	-1.416482000000	-3.611398000000
H	-1.291173000000	1.343493000000	-5.643627000000
H	-1.795715000000	-0.339340000000	-5.605005000000
H	-1.233553000000	1.403064000000	-3.307271000000
H	-1.828805000000	-0.240554000000	-3.275935000000
H	2.369601000000	0.657917000000	-5.491702000000
H	1.151409000000	1.923835000000	-5.497765000000
H	2.242311000000	0.502469000000	-3.169007000000
H	1.111004000000	1.839243000000	-3.164182000000
H	1.643959000000	-1.773035000000	-5.453699000000
H	-0.060492000000	-2.185501000000	-5.564359000000
H	-0.262140000000	-2.067709000000	-3.242973000000
H	1.453372000000	-1.741194000000	-3.129471000000
H	0.388397000000	-0.077034000000	-6.794870000000

Table S60. Cartesian coordinates for the singlet state of **5A** at the PBE0/TZVP/ZORA level.

O	-1.852402000000	-0.419961000000	-0.908185000000
O	0.478301000000	-1.981582000000	-0.701096000000
O	2.116418000000	0.323556000000	-0.766620000000
O	-0.238178000000	1.956425000000	-1.004469000000
C	-2.652269000000	-0.006429000000	-0.045196000000
C	0.068833000000	-2.663162000000	0.261160000000
C	2.801964000000	0.019746000000	0.230564000000
C	0.067296000000	2.773144000000	-0.110002000000
S	-2.170616000000	0.671091000000	1.460997000000
S	-0.523200000000	-1.997300000000	1.731565000000
S	2.150899000000	-0.347629000000	1.777424000000
S	0.509396000000	2.324101000000	1.488503000000
Ni	0.131006000000	-0.018110000000	-0.950875000000
Ni	-0.004584000000	0.160324000000	1.567369000000
C	-4.105325000000	-0.110623000000	-0.341894000000
C	-4.508825000000	-0.891466000000	-1.425407000000
C	-5.071853000000	0.541710000000	0.422906000000
C	-5.852339000000	-1.021903000000	-1.734577000000
C	-6.413585000000	0.421124000000	0.103038000000
C	-6.808038000000	-0.362505000000	-0.973628000000
H	-3.753822000000	-1.403851000000	-2.008129000000
H	-4.764911000000	1.148338000000	1.266378000000
H	-6.155819000000	-1.640789000000	-2.571413000000
H	-7.156194000000	0.939007000000	0.699075000000
H	-7.860060000000	-0.460954000000	-1.217147000000
C	0.056466000000	4.217748000000	-0.462686000000
C	-0.457559000000	4.598175000000	-1.702972000000
C	0.543743000000	5.199675000000	0.399777000000
C	-0.487370000000	5.932441000000	-2.071910000000
C	0.523354000000	6.531951000000	0.024114000000
C	0.007130000000	6.902613000000	-1.210690000000
H	-0.842319000000	3.832374000000	-2.364402000000
H	0.941520000000	4.912232000000	1.365603000000
H	-0.897454000000	6.217263000000	-3.034305000000
H	0.910663000000	7.286123000000	0.699470000000
H	-0.011549000000	7.947534000000	-1.499501000000
C	4.279155000000	-0.024332000000	0.068096000000
C	5.107671000000	-0.691937000000	0.969149000000
C	4.847755000000	0.618539000000	-1.031522000000
C	6.477552000000	-0.719381000000	0.768832000000
C	6.219631000000	0.603165000000	-1.220374000000
C	7.037864000000	-0.070137000000	-0.323373000000
H	4.671189000000	-1.197350000000	1.822336000000
H	4.198667000000	1.139712000000	-1.724001000000
H	7.111790000000	-1.249884000000	1.469786000000
H	6.652844000000	1.116696000000	-2.071291000000
H	8.111472000000	-0.088211000000	-0.474037000000
C	0.088483000000	-4.143170000000	0.116052000000
C	-0.525637000000	-4.991911000000	1.036724000000
C	0.740111000000	-4.695642000000	-0.987091000000
C	-0.492934000000	-6.363692000000	0.852509000000
C	0.782502000000	-6.068707000000	-1.162025000000
C	0.162644000000	-6.906454000000	-0.244873000000

H	-1.033262000000	-4.570384000000	1.896019000000
H	1.218390000000	-4.031562000000	-1.695686000000
H	-0.979958000000	-7.013345000000	1.570653000000
H	1.299518000000	-6.487707000000	-2.017933000000
H	0.191093000000	-7.981464000000	-0.383723000000
C	0.343735000000	-0.044290000000	-5.699005000000
N	0.236766000000	-0.046214000000	-3.121781000000
C	-1.049493000000	0.360372000000	-5.227152000000
C	-1.066689000000	0.366831000000	-3.684996000000
C	1.351812000000	0.947616000000	-5.127376000000
C	1.276820000000	0.896618000000	-3.587653000000
C	0.663274000000	-1.433953000000	-5.153841000000
C	0.568686000000	-1.398186000000	-3.614163000000
H	-1.304408000000	1.348259000000	-5.620835000000
H	-1.794319000000	-0.339087000000	-5.617184000000
H	-1.287826000000	1.355635000000	-3.281913000000
H	-1.820895000000	-0.309462000000	-3.286813000000
H	2.360074000000	0.700246000000	-5.471280000000
H	1.130741000000	1.954852000000	-5.491941000000
H	2.219035000000	0.574909000000	-3.146450000000
H	1.041890000000	1.871596000000	-3.159987000000
H	1.665076000000	-1.737312000000	-5.471053000000
H	-0.036013000000	-2.167392000000	-5.564743000000
H	-0.196803000000	-2.078214000000	-3.239269000000
H	1.507995000000	-1.691286000000	-3.143722000000
H	0.389097000000	-0.046866000000	-6.790653000000

Table S61. Cartesian coordinates for the BS(3,1) state of **5A** at the PBE0/TZVP/ZORA level.

O	-1.869813000000	-0.428198000000	-0.942695000000
O	0.486975000000	-2.003718000000	-0.723786000000
O	2.130679000000	0.330792000000	-0.798958000000
O	-0.248013000000	1.995141000000	-1.035780000000
C	-2.664759000000	-0.013136000000	-0.078022000000
C	0.070861000000	-2.674446000000	0.239800000000
C	2.809889000000	0.021822000000	0.199236000000
C	0.065082000000	2.799693000000	-0.136087000000
S	-2.169179000000	0.686772000000	1.415532000000
S	-0.537512000000	-1.987271000000	1.697225000000
S	2.144596000000	-0.354613000000	1.739714000000
S	0.519380000000	2.325097000000	1.454250000000
Ni	0.127556000000	-0.009492000000	-0.995851000000
Ni	-0.006595000000	0.165082000000	1.519625000000
C	-4.120353000000	-0.132205000000	-0.354726000000
C	-4.531451000000	-0.948373000000	-1.408894000000
C	-5.081589000000	0.538049000000	0.401093000000
C	-5.877750000000	-1.096066000000	-1.697957000000
C	-6.426189000000	0.400995000000	0.100123000000
C	-6.828425000000	-0.418240000000	-0.946815000000
H	-3.780252000000	-1.474942000000	-1.984119000000
H	-4.768633000000	1.171681000000	1.222296000000
H	-6.187205000000	-1.742891000000	-2.511178000000
H	-7.164889000000	0.933309000000	0.688356000000
H	-7.882602000000	-0.530008000000	-1.174842000000
C	0.061253000000	4.249955000000	-0.466813000000
C	-0.451294000000	4.649928000000	-1.701379000000
C	0.553534000000	5.217430000000	0.408949000000
C	-0.474543000000	5.989236000000	-2.052019000000
C	0.539586000000	6.554947000000	0.051782000000
C	0.024884000000	6.945033000000	-1.177604000000
H	-0.839767000000	3.894621000000	-2.372719000000
H	0.950131000000	4.914458000000	1.370501000000
H	-0.883292000000	6.289467000000	-3.010262000000
H	0.930468000000	7.298004000000	0.737315000000
H	0.011290000000	7.993909000000	-1.452032000000
C	4.288399000000	-0.025512000000	0.049124000000
C	5.108772000000	-0.694523000000	0.956517000000
C	4.866595000000	0.616481000000	-1.045922000000
C	6.480155000000	-0.724417000000	0.766695000000
C	6.239868000000	0.598611000000	-1.224443000000
C	7.049961000000	-0.076205000000	-0.321224000000
H	4.664810000000	-1.198992000000	1.806419000000
H	4.223681000000	1.139200000000	-1.742959000000
H	7.108162000000	-1.255786000000	1.472607000000
H	6.680635000000	1.111483000000	-2.071895000000
H	8.124713000000	-0.096068000000	-0.463650000000
C	0.089933000000	-4.157056000000	0.116772000000
C	-0.532318000000	-4.992889000000	1.043622000000
C	0.750278000000	-4.724658000000	-0.973441000000
C	-0.499245000000	-6.367133000000	0.877947000000
C	0.793181000000	-6.099920000000	-1.129848000000
C	0.164926000000	-6.924906000000	-0.206757000000

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H    -1.046455000000     -4.559394000000      1.893143000000
H     1.234736000000     -4.069707000000     -1.686478000000
H    -0.992513000000     -7.006953000000      1.600682000000
H     1.316999000000     -6.530796000000     -1.975768000000
H     0.193706000000     -8.001693000000     -0.331070000000
C     0.341827000000     -0.035910000000     -5.699352000000
N     0.232832000000     -0.035671000000     -3.120960000000
C    -1.052452000000      0.365707000000     -5.228984000000
C    -1.070684000000      0.380931000000     -3.687583000000
C     1.346525000000      0.959047000000     -5.127720000000
C     1.276445000000      0.906068000000     -3.588591000000
C     0.664396000000     -1.423891000000     -5.152195000000
C     0.563390000000     -1.390176000000     -3.613559000000
H    -1.311619000000      1.350550000000     -5.627147000000
H    -1.794609000000     -0.338889000000     -5.614578000000
H    -1.285221000000      1.373014000000     -3.289514000000
H    -1.827858000000     -0.289123000000     -3.285294000000
H     2.355188000000      0.716283000000     -5.473347000000
H     1.120698000000      1.965969000000     -5.489967000000
H     2.217889000000      0.579351000000     -3.150374000000
H     1.045511000000      1.880247000000     -3.157588000000
H     1.668806000000     -1.723219000000     -5.464642000000
H    -0.030084000000     -2.160341000000     -5.565561000000
H    -0.205556000000     -2.067615000000     -3.241673000000
H     1.499213000000     -1.685755000000     -3.138529000000
H     0.388139000000     -0.039629000000     -6.790915000000
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Table S62. Cartesian coordinates for the BS(2,2) state of **5A** at the PBE0/TZVP/ZORA level.

O	-1.895817000000	-0.318618000000	-0.874434000000
O	0.372637000000	-1.948859000000	-0.600074000000
O	2.067629000000	0.298618000000	-0.637672000000
O	-0.183062000000	2.024203000000	-0.934454000000
C	-2.736285000000	0.083068000000	-0.038149000000
C	-0.057681000000	-2.666624000000	0.330382000000
C	2.797695000000	-0.039329000000	0.321401000000
C	0.146560000000	2.870083000000	-0.071533000000
S	-2.327392000000	0.864802000000	1.434144000000
S	-0.723824000000	-2.057614000000	1.789821000000
S	2.226131000000	-0.451066000000	1.883130000000
S	0.617771000000	2.487170000000	1.532472000000
Ni	0.090828000000	0.025110000000	-0.959100000000
Ni	-0.046468000000	0.214725000000	1.675251000000
C	-4.171809000000	-0.138236000000	-0.363672000000
C	-4.495669000000	-0.884437000000	-1.497932000000
C	-5.200721000000	0.361360000000	0.434108000000
C	-5.818702000000	-1.126375000000	-1.826809000000
C	-6.523292000000	0.126639000000	0.098534000000
C	-6.836546000000	-0.618969000000	-1.030538000000
H	-3.693350000000	-1.285088000000	-2.104304000000
H	-4.952313000000	0.931891000000	1.320772000000
H	-6.057852000000	-1.716538000000	-2.704306000000
H	-7.314470000000	0.523008000000	0.724575000000
H	-7.873133000000	-0.808442000000	-1.286351000000
C	0.136566000000	4.299697000000	-0.490677000000
C	-0.387429000000	4.629971000000	-1.741189000000
C	0.638787000000	5.316359000000	0.321313000000
C	-0.411830000000	5.946556000000	-2.169448000000
C	0.623720000000	6.630987000000	-0.112743000000
C	0.098015000000	6.950789000000	-1.357615000000
H	-0.785884000000	3.839650000000	-2.364148000000
H	1.042476000000	5.065014000000	1.294619000000
H	-0.830810000000	6.191252000000	-3.139116000000
H	1.022596000000	7.411274000000	0.525275000000
H	0.083048000000	7.981946000000	-1.692484000000
C	4.265247000000	-0.071805000000	0.072594000000
C	5.139934000000	-0.782849000000	0.892851000000
C	4.775556000000	0.621719000000	-1.025112000000
C	6.496096000000	-0.806618000000	0.613348000000
C	6.134622000000	0.611288000000	-1.292034000000
C	6.997907000000	-0.108450000000	-0.477056000000
H	4.745454000000	-1.322166000000	1.745638000000
H	4.092849000000	1.181438000000	-1.652006000000
H	7.165818000000	-1.372100000000	1.251168000000
H	6.522795000000	1.166167000000	-2.138835000000
H	8.061174000000	-0.123005000000	-0.689223000000
C	0.011932000000	-4.141976000000	0.137081000000
C	-0.506063000000	-5.039879000000	1.070229000000
C	0.615067000000	-4.640070000000	-1.018637000000
C	-0.428431000000	-6.404143000000	0.847244000000
C	0.700489000000	-6.005004000000	-1.235548000000
C	0.175805000000	-6.891101000000	-0.304384000000

H	-0.969364000000	-4.656995000000	1.971522000000
H	1.022567000000	-3.939544000000	-1.735788000000
H	-0.838349000000	-7.091828000000	1.578030000000
H	1.177915000000	-6.380265000000	-2.133847000000
H	0.239685000000	-7.960177000000	-0.474263000000
C	0.400625000000	-0.007607000000	-5.605651000000
N	0.236838000000	0.000902000000	-3.032079000000
C	-1.002645000000	0.394723000000	-5.162375000000
C	-1.009900000000	0.539362000000	-3.629500000000
C	1.391717000000	0.988217000000	-5.009587000000
C	1.377145000000	0.838191000000	-3.477207000000
C	0.707825000000	-1.393539000000	-5.043170000000
C	0.448859000000	-1.379540000000	-3.524470000000
H	-1.296419000000	1.336460000000	-5.633048000000
H	-1.725595000000	-0.361131000000	-5.482473000000
H	-1.081245000000	1.581284000000	-3.317040000000
H	-1.847235000000	0.014091000000	-3.174241000000
H	2.398262000000	0.805736000000	-5.394514000000
H	1.117540000000	2.005719000000	-5.302879000000
H	2.282156000000	0.356042000000	-3.109847000000
H	1.296951000000	1.800371000000	-2.971615000000
H	1.748422000000	-1.657120000000	-5.253351000000
H	0.083499000000	-2.149422000000	-5.526392000000
H	-0.437679000000	-1.955701000000	-3.255192000000
H	1.284346000000	-1.801344000000	-2.966653000000
H	0.471519000000	-0.014366000000	-6.695475000000

Table S63. Cartesian coordinates for the BS(1,1) state of **5A** at the PBE0/TZVP/ZORA level.

O	-1.852662000000	-0.419784000000	-0.907031000000
O	0.476744000000	-1.976880000000	-0.700527000000
O	2.116044000000	0.325549000000	-0.767342000000
O	-0.238187000000	1.957746000000	-1.003901000000
C	-2.653069000000	-0.008448000000	-0.043644000000
C	0.068859000000	-2.659614000000	0.261679000000
C	2.801615000000	0.022118000000	0.230038000000
C	0.066006000000	2.775107000000	-0.109402000000
S	-2.172204000000	0.669703000000	1.462788000000
S	-0.518953000000	-1.995842000000	1.734695000000
S	2.151273000000	-0.341992000000	1.778244000000
S	0.506072000000	2.327189000000	1.490061000000
Ni	0.130267000000	-0.014884000000	-0.948818000000
Ni	-0.005475000000	0.163190000000	1.571353000000
C	-4.106110000000	-0.115996000000	-0.339374000000
C	-4.508347000000	-0.897945000000	-1.422558000000
C	-5.073734000000	0.534384000000	0.425702000000
C	-5.851706000000	-1.031354000000	-1.731157000000
C	-6.415347000000	0.410772000000	0.106410000000
C	-6.808528000000	-0.373898000000	-0.969955000000
H	-3.752535000000	-1.408828000000	-2.005560000000
H	-4.767757000000	1.141948000000	1.268843000000
H	-6.154125000000	-1.651029000000	-2.567793000000
H	-7.158816000000	0.927208000000	0.702628000000
H	-7.860431000000	-0.474652000000	-1.213055000000
C	0.057743000000	4.219292000000	-0.463670000000
C	-0.451579000000	4.598838000000	-1.706153000000
C	0.542783000000	5.201739000000	0.399478000000
C	-0.479006000000	5.932742000000	-2.076562000000
C	0.524757000000	6.533652000000	0.022392000000
C	0.013177000000	6.903424000000	-1.214591000000
H	-0.834597000000	3.832743000000	-2.368249000000
H	0.937032000000	4.914923000000	1.366933000000
H	-0.885375000000	6.216858000000	-3.040741000000
H	0.910193000000	7.288207000000	0.698389000000
H	-0.003618000000	7.948043000000	-1.504605000000
C	4.278846000000	-0.024231000000	0.067360000000
C	5.106847000000	-0.689618000000	0.970581000000
C	4.847954000000	0.614490000000	-1.034401000000
C	6.476710000000	-0.718851000000	0.770365000000
C	6.219807000000	0.597279000000	-1.223216000000
C	7.037499000000	-0.073594000000	-0.323914000000
H	4.669795000000	-1.191938000000	1.825275000000
H	4.199312000000	1.134044000000	-1.728478000000
H	7.110559000000	-1.247484000000	1.473073000000
H	6.653495000000	1.107573000000	-2.075839000000
H	8.111096000000	-0.092978000000	-0.474508000000
C	0.087262000000	-4.139460000000	0.114650000000
C	-0.532201000000	-4.988559000000	1.031412000000
C	0.742807000000	-4.691297000000	-0.986495000000
C	-0.500743000000	-6.360133000000	0.845354000000
C	0.783895000000	-6.064180000000	-1.163176000000
C	0.158809000000	-6.902289000000	-0.249912000000

H	-1.043361000000	-4.567415000000	1.888790000000
H	1.225272000000	-4.026899000000	-1.691955000000
H	-0.992029000000	-7.010089000000	1.560315000000
H	1.303992000000	-6.482748000000	-2.017428000000
H	0.186212000000	-7.977143000000	-0.390179000000
C	0.344199000000	-0.043360000000	-5.697908000000
N	0.236395000000	-0.043750000000	-3.120515000000
C	-1.050078000000	0.358554000000	-5.226693000000
C	-1.067411000000	0.366896000000	-3.684526000000
C	1.349944000000	0.951108000000	-5.126620000000
C	1.275099000000	0.900386000000	-3.586871000000
C	0.666624000000	-1.431942000000	-5.151575000000
C	0.570721000000	-1.395432000000	-3.611974000000
H	-1.307549000000	1.345306000000	-5.621543000000
H	-1.793074000000	-0.343309000000	-5.615897000000
H	-1.289698000000	1.356083000000	-3.282948000000
H	-1.820984000000	-0.309607000000	-3.285521000000
H	2.358777000000	0.705942000000	-5.470420000000
H	1.126591000000	1.957751000000	-5.491460000000
H	2.217693000000	0.579706000000	-3.145828000000
H	1.039363000000	1.875230000000	-3.159373000000
H	1.669446000000	-1.733120000000	-5.467636000000
H	-0.030514000000	-2.167355000000	-5.562609000000
H	-0.193983000000	-2.076408000000	-3.237258000000
H	1.510096000000	-1.686834000000	-3.140638000000
H	0.389912000000	-0.046610000000	-6.789541000000

Table S64. Cartesian coordinates for quintet state of **1B** at the PBE0/TZVP/ZORA level.

O	-1.886126000000	0.391551000000	-0.990746000000
O	-0.309371000000	-1.987003000000	-0.790087000000
O	2.123321000000	-0.389433000000	-0.862358000000
O	0.473219000000	2.017075000000	-1.031952000000
C	-2.465476000000	1.049365000000	-0.107776000000
C	-0.950427000000	-2.466149000000	0.162536000000
C	2.657122000000	-0.945240000000	0.116299000000
C	1.072418000000	2.639829000000	-0.136142000000
S	-1.744822000000	1.463672000000	1.400128000000
S	-1.209020000000	-1.650774000000	1.654101000000
S	1.909037000000	-1.098231000000	1.656137000000
S	1.356842000000	2.005124000000	1.437493000000
Ni	0.122305000000	0.005393000000	-0.979292000000
Ni	0.072289000000	0.177699000000	1.571459000000
C	-3.844347000000	1.534975000000	-0.384906000000
C	-4.349411000000	1.402429000000	-1.678810000000
C	-4.649477000000	2.104142000000	0.601494000000
C	-5.628489000000	1.837111000000	-1.982113000000
C	-5.927554000000	2.540825000000	0.295952000000
C	-6.420454000000	2.409372000000	-0.995486000000
H	-3.721960000000	0.952682000000	-2.437488000000
H	-4.268157000000	2.196057000000	1.611089000000
H	-6.010176000000	1.729551000000	-2.991157000000
H	-6.544554000000	2.981204000000	1.070824000000
H	-7.422773000000	2.749196000000	-1.231495000000
C	1.569262000000	4.006659000000	-0.450301000000
C	1.159701000000	4.602705000000	-1.643496000000
C	2.423858000000	4.708422000000	0.399263000000
C	1.595569000000	5.873177000000	-1.980446000000
C	2.867188000000	5.974403000000	0.055410000000
C	2.453085000000	6.561381000000	-1.133203000000
H	0.485365000000	4.058319000000	-2.292413000000
H	2.742646000000	4.252892000000	1.328998000000
H	1.264463000000	6.330038000000	-2.906248000000
H	3.536494000000	6.507806000000	0.720616000000
H	2.796145000000	7.555561000000	-1.397017000000
C	4.025221000000	-1.506111000000	-0.055413000000
C	4.595750000000	-2.377381000000	0.871994000000
C	4.758582000000	-1.142288000000	-1.184968000000
C	5.872106000000	-2.874932000000	0.671182000000
C	6.040162000000	-1.631348000000	-1.377633000000
C	6.599303000000	-2.501153000000	-0.451419000000
H	4.029471000000	-2.666370000000	1.749085000000
H	4.312727000000	-0.461321000000	-1.898958000000
H	6.303050000000	-3.555975000000	1.396090000000
H	6.605988000000	-1.332376000000	-2.252809000000
H	7.601396000000	-2.886556000000	-0.602870000000
C	-1.518320000000	-3.832211000000	0.009750000000
C	-2.565451000000	-4.295415000000	0.805153000000
C	-0.984828000000	-4.669757000000	-0.969573000000
C	-3.069575000000	-5.572157000000	0.622009000000
C	-1.480567000000	-5.951956000000	-1.140239000000
C	-2.526007000000	-6.405305000000	-0.347029000000

H	-2.988914000000	-3.643366000000	1.559614000000
H	-0.169796000000	-4.303967000000	-1.581567000000
H	-3.890384000000	-5.919334000000	1.239130000000
H	-1.050033000000	-6.601044000000	-1.894459000000
H	-2.917147000000	-7.407288000000	-0.483795000000
N	0.520174000000	-0.354078000000	-5.675857000000
N	0.281385000000	-0.157003000000	-3.119288000000
C	-0.868720000000	-0.099353000000	-5.310188000000
C	-1.003135000000	0.136839000000	-3.787976000000
C	1.339775000000	0.741770000000	-5.172125000000
C	1.296526000000	0.793569000000	-3.629003000000
C	0.953384000000	-1.586712000000	-5.026709000000
C	0.700015000000	-1.524151000000	-3.503994000000
H	-1.225068000000	0.767420000000	-5.873352000000
H	-1.464086000000	-0.959466000000	-5.627938000000
H	-1.259752000000	1.171955000000	-3.555177000000
H	-1.769155000000	-0.494743000000	-3.337925000000
H	2.363585000000	0.606374000000	-5.530662000000
H	0.965930000000	1.671927000000	-5.608635000000
H	2.249117000000	0.514100000000	-3.178307000000
H	1.042909000000	1.784883000000	-3.257358000000
H	2.015477000000	-1.726689000000	-5.244540000000
H	0.416735000000	-2.426641000000	-5.475783000000
H	-0.091602000000	-2.204091000000	-3.191174000000
H	1.590299000000	-1.773839000000	-2.925802000000
N	-0.072738000000	0.225477000000	4.163843000000
O	-1.992324000000	-0.908700000000	8.879364000000
O	0.801951000000	-1.421025000000	9.143330000000
O	1.375334000000	1.404870000000	9.058259000000
O	-1.451247000000	1.963052000000	8.735234000000
C	-2.907669000000	-0.818055000000	9.718469000000
C	0.687347000000	-2.177751000000	10.124579000000
C	2.100040000000	1.436407000000	10.069203000000
C	-1.524809000000	2.838636000000	9.618052000000
S	-2.753504000000	0.009618000000	11.218116000000
S	-0.181379000000	-1.775399000000	11.553786000000
S	1.624247000000	0.824571000000	11.605249000000
S	-0.963239000000	2.616527000000	11.228732000000
Ni	-0.321624000000	0.269935000000	8.896083000000
Ni	-0.566706000000	0.421772000000	11.438431000000
C	-4.206307000000	-1.474985000000	9.408056000000
C	-4.245096000000	-2.412599000000	8.376067000000
C	-5.376594000000	-1.188673000000	10.110120000000
C	-5.427999000000	-3.059888000000	8.059396000000
C	-6.561509000000	-1.825330000000	9.781158000000
C	-6.590084000000	-2.765410000000	8.759278000000
H	-3.331032000000	-2.634661000000	7.839788000000
H	-5.352652000000	-0.458951000000	10.910640000000
H	-5.443592000000	-3.796538000000	7.263986000000
H	-7.467584000000	-1.589915000000	10.327707000000
H	-7.517812000000	-3.268278000000	8.509860000000
C	-2.101319000000	4.160264000000	9.243119000000
C	-2.448871000000	4.380338000000	7.909667000000
C	-2.312667000000	5.178415000000	10.172794000000
C	-2.986903000000	5.592538000000	7.511786000000
C	-2.846577000000	6.392148000000	9.772892000000
C	-3.184708000000	6.603313000000	8.442572000000

H	-2.293297000000	3.584457000000	7.192822000000
H	-2.056731000000	5.010838000000	11.211952000000
H	-3.251819000000	5.750116000000	6.472346000000
H	-3.004845000000	7.176641000000	10.504156000000
H	-3.604659000000	7.553728000000	8.132431000000
C	3.450892000000	2.049451000000	9.946127000000
C	4.422206000000	1.923748000000	10.938750000000
C	3.745957000000	2.784445000000	8.797926000000
C	5.661784000000	2.520810000000	10.784571000000
C	4.982694000000	3.390798000000	8.650621000000
C	5.944634000000	3.259266000000	9.642921000000
H	4.199762000000	1.352225000000	11.831678000000
H	2.985408000000	2.882757000000	8.033541000000
H	6.410826000000	2.411314000000	11.560615000000
H	5.197523000000	3.968733000000	7.758814000000
H	6.913590000000	3.732193000000	9.527907000000
C	1.301683000000	-3.530416000000	10.044858000000
C	1.537658000000	-4.309438000000	11.176780000000
C	1.663070000000	-4.025988000000	8.791969000000
C	2.117263000000	-5.561441000000	11.055392000000
C	2.238222000000	-5.279784000000	8.671946000000
C	2.467483000000	-6.050585000000	9.803996000000
H	1.272885000000	-3.920070000000	12.152295000000
H	1.481067000000	-3.412970000000	7.918553000000
H	2.301114000000	-6.157043000000	11.942335000000
H	2.509400000000	-5.657788000000	7.692612000000
H	2.921577000000	-7.030927000000	9.711559000000
N	-0.199244000000	0.235574000000	6.747369000000
C	-1.463730000000	0.112752000000	4.620351000000
C	-1.552073000000	0.278787000000	6.149935000000
C	0.481552000000	1.469242000000	4.707737000000
C	0.555322000000	1.404698000000	6.247120000000
C	0.681827000000	-0.898099000000	4.730734000000
C	0.475755000000	-0.982741000000	6.256834000000
H	-2.061859000000	0.867312000000	4.106545000000
H	-1.838258000000	-0.863343000000	4.305156000000
H	-1.997208000000	1.231588000000	6.435124000000
H	-2.148587000000	-0.507168000000	6.610456000000
H	1.473423000000	1.628459000000	4.279919000000
H	-0.150161000000	2.292841000000	4.366805000000
H	1.581473000000	1.299128000000	6.597116000000
H	0.143714000000	2.299041000000	6.715810000000
H	1.734861000000	-0.750997000000	4.482712000000
H	0.357856000000	-1.816954000000	4.236894000000
H	-0.149955000000	-1.832364000000	6.537119000000
H	1.420952000000	-1.085252000000	6.789142000000
N	-0.664670000000	0.571272000000	14.036857000000
N	-0.746044000000	0.714123000000	16.599155000000
C	-2.011577000000	0.245870000000	14.524650000000
C	-2.053663000000	0.336744000000	16.071197000000
C	-0.320528000000	1.927981000000	14.486263000000
C	-0.361791000000	2.003614000000	16.032929000000
C	0.289386000000	-0.373314000000	14.636939000000
C	0.231431000000	-0.284908000000	16.181660000000
H	-2.715178000000	0.941482000000	14.061153000000
H	-2.267623000000	-0.754605000000	14.168713000000
H	-2.783941000000	1.079296000000	16.404712000000

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H    -2.338162000000     -0.620538000000     16.516869000000
H     0.668163000000      2.172082000000     14.090601000000
H    -1.031062000000      2.622253000000     14.032845000000
H     0.613918000000      2.278307000000     16.443356000000
H    -1.079958000000      2.754646000000     16.373647000000
H     1.284735000000     -0.135348000000     14.254999000000
H     0.043665000000     -1.375565000000     14.281503000000
H    -0.050972000000     -1.244989000000     16.622893000000
H     1.203242000000     -0.009326000000     16.600924000000
H     1.590119000000     -0.544993000000      6.769398000000
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Table S65. Cartesian coordinates for quintet state of **2B** at the PBE0/TZVP/ZORA level.

O	-2.034363000000	-0.142175000000	-0.863513000000
O	0.087807000000	-2.132547000000	-0.761634000000
O	2.022067000000	-0.032473000000	-0.790170000000
O	-0.098567000000	1.946451000000	-0.888057000000
C	-2.747460000000	0.340386000000	0.035612000000
C	-0.353932000000	-2.795608000000	0.193939000000
C	2.708350000000	-0.425252000000	0.171244000000
C	0.315525000000	2.679642000000	0.027648000000
S	-2.162029000000	0.760388000000	1.598312000000
S	-0.835066000000	-2.098860000000	1.693876000000
S	2.057222000000	-0.762495000000	1.727931000000
S	0.729634000000	2.097920000000	1.594762000000
Ni	-0.006291000000	-0.092592000000	-0.804132000000
Ni	-0.053646000000	-0.000289000000	1.698050000000
N	0.192023000000	-0.191966000000	-5.648914000000
C	0.898820000000	-1.038258000000	-4.906008000000
C	0.836686000000	-1.016005000000	-3.522389000000
N	0.052738000000	-0.149143000000	-2.888304000000
C	-0.664736000000	0.694287000000	-3.624235000000
C	-0.586862000000	0.673823000000	-5.007639000000
H	1.527290000000	-1.750365000000	-5.428968000000
H	1.411655000000	-1.696151000000	-2.906788000000
H	-1.297210000000	1.392432000000	-3.090557000000
H	-1.158270000000	1.368574000000	-5.613078000000
C	-4.189618000000	0.552122000000	-0.260779000000
C	-4.720890000000	-0.039788000000	-1.407060000000
C	-5.018103000000	1.322438000000	0.554082000000
C	-6.058059000000	0.127570000000	-1.726083000000
C	-6.351780000000	1.498610000000	0.225586000000
C	-6.876264000000	0.899356000000	-0.912222000000
H	-4.069849000000	-0.636637000000	-2.033515000000
H	-4.608791000000	1.787250000000	1.443084000000
H	-6.463641000000	-0.344983000000	-2.613590000000
H	-6.986295000000	2.105199000000	0.861606000000
H	-7.922515000000	1.033655000000	-1.163545000000
C	0.507463000000	4.125267000000	-0.262315000000
C	0.512957000000	4.539716000000	-1.594443000000
C	0.669549000000	5.075072000000	0.745555000000
C	0.682934000000	5.876448000000	-1.912262000000
C	0.836895000000	6.412070000000	0.425474000000
C	0.843986000000	6.816314000000	-0.902750000000
H	0.389130000000	3.795823000000	-2.371404000000
H	0.656524000000	4.757485000000	1.781114000000
H	0.692070000000	6.187108000000	-2.950898000000
H	0.959054000000	7.143063000000	1.216595000000
H	0.974915000000	7.863776000000	-1.150793000000
C	4.168465000000	-0.610223000000	-0.046520000000
C	5.013006000000	-1.141547000000	0.927750000000
C	4.704618000000	-0.230879000000	-1.277747000000
C	6.365143000000	-1.294738000000	0.671935000000
C	6.058777000000	-0.376811000000	-1.527831000000
C	6.892088000000	-0.911312000000	-0.554518000000
H	4.603041000000	-1.433433000000	1.887134000000

H	4.043044000000	0.187564000000	-2.025755000000
H	7.012652000000	-1.711139000000	1.435038000000
H	6.466124000000	-0.071175000000	-2.484956000000
H	7.952567000000	-1.026454000000	-0.749483000000
C	-0.522497000000	-4.262228000000	0.017606000000
C	-0.708321000000	-5.125074000000	1.097145000000
C	-0.478530000000	-4.788235000000	-1.273969000000
C	-0.852808000000	-6.486124000000	0.887394000000
C	-0.625361000000	-6.149291000000	-1.481616000000
C	-0.811920000000	-7.001664000000	-0.401158000000
H	-0.731973000000	-4.720395000000	2.101502000000
H	-0.335111000000	-4.111560000000	-2.107096000000
H	-0.993942000000	-7.148735000000	1.733672000000
H	-0.596002000000	-6.547657000000	-2.489438000000
H	-0.924498000000	-8.067979000000	-0.562802000000
N	-0.092519000000	0.072110000000	4.032221000000
N	-0.117719000000	0.166298000000	6.819293000000
C	0.234385000000	-0.986050000000	4.768783000000
C	0.220383000000	-0.932857000000	6.155265000000
C	-0.432411000000	1.177323000000	4.689641000000
C	-0.443515000000	1.217697000000	6.076542000000
H	0.507461000000	-1.891177000000	4.236573000000
H	0.490059000000	-1.803653000000	6.744219000000
H	-0.694377000000	2.044652000000	4.092888000000
H	-0.723144000000	2.126194000000	6.600318000000
O	2.421159000000	0.188335000000	-10.429728000000
O	-0.079494000000	1.653542000000	-10.597311000000
O	-1.516772000000	-0.824004000000	-10.603768000000
O	0.993492000000	-2.276317000000	-10.427022000000
C	3.149053000000	-0.041796000000	-9.446917000000
C	0.102488000000	2.453862000000	-9.661929000000
C	-2.342880000000	-0.557330000000	-9.711953000000
C	0.722373000000	-3.025455000000	-9.471640000000
S	2.548583000000	-0.477914000000	-7.894768000000
S	0.574100000000	1.980939000000	-8.074969000000
S	-1.902202000000	-0.007663000000	-8.142644000000
S	0.072808000000	-2.469924000000	-7.976921000000
Ni	0.449187000000	-0.311513000000	-10.497100000000
Ni	0.321195000000	-0.243474000000	-7.987603000000
N	0.665739000000	-0.515902000000	-15.343624000000
C	-0.319241000000	0.112951000000	-14.712864000000
C	-0.386097000000	0.185358000000	-13.329520000000
N	0.551260000000	-0.381120000000	-12.574752000000
C	1.546960000000	-1.011666000000	-13.191329000000
C	1.594430000000	-1.073955000000	-14.576034000000
H	-1.085133000000	0.575059000000	-15.326933000000
H	-1.188024000000	0.695876000000	-12.810819000000
H	2.301056000000	-1.466804000000	-12.561403000000
H	2.406939000000	-1.589785000000	-15.076998000000
C	4.621054000000	0.075341000000	-9.625221000000
C	5.099263000000	0.687230000000	-10.784302000000
C	5.530960000000	-0.409214000000	-8.686229000000
C	6.461548000000	0.818421000000	-10.995894000000
C	6.892581000000	-0.286626000000	-8.905771000000
C	7.361648000000	0.329095000000	-10.058856000000
H	4.384811000000	1.063968000000	-11.505561000000
H	5.164109000000	-0.888055000000	-7.786254000000

H	6.823506000000	1.304184000000	-11.895043000000
H	7.592140000000	-0.673370000000	-8.173616000000
H	8.428462000000	0.427648000000	-10.226010000000
C	0.924943000000	-4.487520000000	-9.644784000000
C	1.003172000000	-5.000695000000	-10.939775000000
C	1.061031000000	-5.352483000000	-8.559983000000
C	1.205730000000	-6.354866000000	-11.144858000000
C	1.273382000000	-6.705245000000	-8.767801000000
C	1.343787000000	-7.210051000000	-10.059169000000
H	0.895966000000	-4.321388000000	-11.776336000000
H	1.011646000000	-4.952926000000	-7.554474000000
H	1.256612000000	-6.746533000000	-12.154486000000
H	1.388296000000	-7.368574000000	-7.918133000000
H	1.507779000000	-8.269865000000	-10.219409000000
C	-3.788458000000	-0.719006000000	-10.024738000000
C	-4.794551000000	-0.347475000000	-9.133372000000
C	-4.141860000000	-1.265657000000	-11.258902000000
C	-6.126232000000	-0.514918000000	-9.473123000000
C	-5.474517000000	-1.440166000000	-11.593070000000
C	-6.470082000000	-1.062276000000	-10.702273000000
H	-4.526086000000	0.073497000000	-8.171923000000
H	-3.354480000000	-1.560047000000	-11.941464000000
H	-6.900313000000	-0.218785000000	-8.774488000000
H	-5.738182000000	-1.873615000000	-12.551237000000
H	-7.513849000000	-1.196400000000	-10.963601000000
C	-0.043541000000	3.905956000000	-9.943192000000
C	-0.256825000000	4.843571000000	-8.933712000000
C	0.021450000000	4.334512000000	-11.269236000000
C	-0.404793000000	6.184675000000	-9.246856000000
C	-0.117535000000	5.676828000000	-11.578636000000
C	-0.333262000000	6.604890000000	-10.568120000000
H	-0.317655000000	4.510327000000	-7.904736000000
H	0.189632000000	3.599020000000	-12.046096000000
H	-0.580616000000	6.905340000000	-8.456392000000
H	-0.057529000000	6.002199000000	-12.611102000000
H	-0.447569000000	7.655615000000	-10.810342000000

Table S66. Cartesian coordinates for quintet state of **3B** at the PBE0/TZVP/ZORA level.

O	-2.196462000000	-0.405962000000	-3.907323000000
O	0.213275000000	-1.877924000000	-3.484727000000
O	1.759305000000	0.572120000000	-3.632783000000
O	-0.734868000000	2.063428000000	-4.030893000000
C	-3.037511000000	-0.013294000000	-3.083108000000
C	-0.163143000000	-2.510390000000	-2.484754000000
C	2.408337000000	0.419203000000	-2.584484000000
C	-0.555030000000	2.923536000000	-3.153483000000
C	-4.491470000000	-0.191529000000	-3.413834000000
C	-0.041614000000	-4.007210000000	-2.506089000000
C	3.903636000000	0.540482000000	-2.652028000000
C	-0.720795000000	4.367914000000	-3.529184000000
H	-4.667467000000	0.094922000000	-4.452278000000
H	-0.448599000000	-4.390102000000	-3.444093000000
H	4.274093000000	0.016284000000	-3.534838000000
H	-0.261499000000	4.550332000000	-4.502365000000
H	-4.733472000000	-1.253651000000	-3.315027000000
H	1.021129000000	-4.263309000000	-2.475225000000
H	4.153494000000	1.599859000000	-2.761181000000
H	-1.791693000000	4.572134000000	-3.619743000000
H	-5.137537000000	0.377646000000	-2.748522000000
H	-0.542677000000	-4.473646000000	-1.660511000000
H	4.387272000000	0.159404000000	-1.754870000000
H	-0.301823000000	5.037081000000	-2.780265000000
S	-2.670468000000	0.710972000000	-1.572496000000
S	-0.811264000000	-1.805278000000	-1.063680000000
S	1.730766000000	0.090114000000	-1.045819000000
S	-0.146162000000	2.592874000000	-1.521140000000
Ni	-0.217973000000	0.095435000000	-3.815161000000
Ni	-0.477493000000	0.397605000000	-1.257115000000
N	0.478761000000	-0.269997000000	-8.478965000000
N	0.083033000000	-0.075184000000	-5.941919000000
C	-0.947369000000	-0.326447000000	-8.178713000000
C	-1.190553000000	-0.316571000000	-6.651583000000
C	1.009739000000	0.992211000000	-7.977020000000
C	0.680038000000	1.170290000000	-6.477806000000
C	1.144055000000	-1.360232000000	-7.774885000000
C	1.004118000000	-1.193409000000	-6.244939000000
H	-1.427789000000	0.530314000000	-8.658770000000
H	-1.364261000000	-1.228395000000	-8.634577000000
H	-1.893145000000	0.461320000000	-6.351467000000
H	-1.590789000000	-1.264681000000	-6.291547000000
H	2.089990000000	0.993518000000	-8.145892000000
H	0.588130000000	1.808927000000	-8.569192000000
H	1.566131000000	1.394429000000	-5.883802000000
H	-0.040267000000	1.969922000000	-6.307565000000
H	2.195976000000	-1.375124000000	-8.072202000000
H	0.698629000000	-2.300996000000	-8.109503000000
H	0.614722000000	-2.089498000000	-5.764751000000
H	1.956678000000	-0.958213000000	-5.767672000000
N	-0.733839000000	0.544438000000	1.307863000000
N	-0.984889000000	0.644523000000	3.879613000000
C	-2.010428000000	-0.043576000000	1.732006000000

C	-2.205648000000	0.097245000000	3.256089000000
C	-0.686514000000	1.932268000000	1.777253000000
C	-0.748443000000	1.992672000000	3.319223000000
C	0.351199000000	-0.192972000000	1.965691000000
C	0.152287000000	-0.217796000000	3.494911000000
H	-2.817318000000	0.447773000000	1.185941000000
H	-2.011244000000	-1.092531000000	1.428252000000
H	-3.026374000000	0.773002000000	3.500144000000
H	-2.427421000000	-0.859060000000	3.728867000000
H	0.232494000000	2.388940000000	1.403609000000
H	-1.521040000000	2.469873000000	1.321702000000
H	0.182609000000	2.361493000000	3.751015000000
H	-1.551560000000	2.640613000000	3.666887000000
H	1.292892000000	0.289637000000	1.697260000000
H	0.376444000000	-1.204059000000	1.553542000000
H	-0.058140000000	-1.219959000000	3.864965000000
H	1.033282000000	0.143738000000	4.025557000000
O	-0.359640000000	-1.137690000000	6.234572000000
O	0.707792000000	1.564746000000	6.081151000000
O	-2.036922000000	2.582642000000	5.933081000000
O	-3.026007000000	-0.096987000000	6.057442000000
C	-0.544208000000	-1.856258000000	7.230265000000
C	1.460237000000	1.480005000000	7.066457000000
C	-1.937428000000	3.435134000000	6.829897000000
C	-3.848460000000	0.101555000000	6.965387000000
C	-0.152164000000	-3.303666000000	7.143935000000
C	2.898299000000	1.877669000000	6.898234000000
C	-2.397382000000	4.834022000000	6.537339000000
C	-5.269218000000	-0.331088000000	6.741811000000
H	-0.466697000000	-3.710363000000	6.181136000000
H	3.276036000000	1.497094000000	5.947637000000
H	-2.089205000000	5.120696000000	5.530415000000
H	-5.580893000000	-0.054287000000	5.733079000000
H	0.939019000000	-3.362090000000	7.193259000000
H	2.945001000000	2.970095000000	6.865543000000
H	-3.490857000000	4.842672000000	6.569449000000
H	-5.306097000000	-1.421853000000	6.815706000000
H	-0.570036000000	-3.891368000000	7.958894000000
H	3.519140000000	1.527951000000	7.720687000000
H	-2.023578000000	5.549098000000	7.267577000000
H	-5.948592000000	0.092177000000	7.478998000000
S	-1.198087000000	-1.326773000000	8.723178000000
S	0.980102000000	0.956311000000	8.625185000000
S	-1.329863000000	3.131993000000	8.404952000000
S	-3.492125000000	0.821682000000	8.480941000000
Ni	-1.159595000000	0.735207000000	6.029337000000
Ni	-1.257547000000	0.904673000000	8.606766000000
N	-1.312121000000	1.214334000000	11.156467000000
N	-1.375935000000	1.534752000000	13.703960000000
C	-1.054961000000	-0.059994000000	11.841082000000
C	-1.151244000000	0.130585000000	13.375423000000
C	-2.629448000000	1.711772000000	11.578761000000
C	-2.638204000000	1.961504000000	13.107174000000
C	-0.293167000000	2.187056000000	11.580667000000
C	-0.295972000000	2.324834000000	13.122436000000
H	-1.780854000000	-0.793004000000	11.482941000000
H	-0.066756000000	-0.411092000000	11.534651000000

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H    -1.975478000000     -0.452346000000     13.796026000000
H    -0.234897000000     -0.197662000000     13.874005000000
H    -2.845048000000      2.622815000000     11.015078000000
H    -3.374897000000      0.967961000000     11.289796000000
H    -2.777509000000      3.022001000000     13.334775000000
H    -3.452141000000      1.415329000000     13.592096000000
H    -0.518354000000      3.138076000000     11.092712000000
H     0.676426000000      1.855063000000     11.205121000000
H     0.647292000000      1.977817000000     13.553776000000
H    -0.426496000000      3.366995000000     13.427305000000
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Table S67. Cartesian coordinates for quintet state of **4B** at the PBE0/TZVP/ZORA level.

O	-1.961428000000	-0.498221000000	-0.930209000000
O	0.475575000000	-2.085556000000	-0.829196000000
O	2.040438000000	0.307321000000	-0.915585000000
O	-0.410063000000	1.903415000000	-1.000524000000
C	-2.720041000000	-0.173378000000	-0.003592000000
C	0.163118000000	-2.793872000000	0.141039000000
C	2.775482000000	0.061339000000	0.053770000000
C	-0.116918000000	2.692657000000	-0.088662000000
C	-4.201195000000	-0.285633000000	-0.219888000000
C	0.254022000000	-4.284852000000	-0.004528000000
C	4.261779000000	0.149852000000	-0.137312000000
C	-0.218936000000	4.165556000000	-0.357172000000
H	-4.452768000000	0.076734000000	-1.218080000000
H	-0.174445000000	-4.581953000000	-0.963414000000
H	4.532365000000	-0.283546000000	-1.101549000000
H	0.199773000000	4.385612000000	-1.340728000000
H	-4.470645000000	-1.344589000000	-0.171041000000
H	1.311985000000	-4.562494000000	-0.009055000000
H	4.537898000000	1.208049000000	-0.156383000000
H	-1.278905000000	4.435304000000	-0.374982000000
H	-4.769321000000	0.253522000000	0.535609000000
H	-0.242021000000	-4.808439000000	0.810210000000
H	4.809228000000	-0.337609000000	0.667085000000
H	0.279028000000	4.757689000000	0.408011000000
S	-2.201839000000	0.377337000000	1.536403000000
S	-0.369818000000	-2.191533000000	1.657326000000
S	2.222267000000	-0.352484000000	1.624960000000
S	0.399615000000	2.219237000000	1.477259000000
Ni	0.037762000000	-0.090125000000	-0.900985000000
Ni	0.011867000000	0.015658000000	1.621562000000
N	0.071449000000	-0.267283000000	-5.757298000000
C	0.893426000000	-1.008321000000	-5.023655000000
C	0.892799000000	-0.965834000000	-3.637539000000
N	0.054167000000	-0.168047000000	-2.982668000000
C	-0.776499000000	0.579869000000	-3.703501000000
C	-0.759856000000	0.523259000000	-5.088830000000
H	1.578928000000	-1.660303000000	-5.554944000000
H	1.554901000000	-1.575644000000	-3.036028000000
H	-1.445509000000	1.230904000000	-3.155433000000
H	-1.438666000000	1.135141000000	-5.673723000000
H	0.970102000000	-1.630046000000	4.232278000000
H	0.708255000000	-1.548079000000	6.743605000000
C	0.314926000000	-0.771637000000	6.100502000000
C	0.454484000000	-0.811758000000	4.722526000000
N	-0.050709000000	0.140410000000	3.944208000000
C	-0.686116000000	1.142031000000	4.545186000000
H	-1.088381000000	1.923544000000	3.910188000000
H	-1.346095000000	1.997648000000	6.421143000000
C	-0.829973000000	1.188503000000	5.921476000000
N	-0.332878000000	0.226611000000	6.692938000000
O	-2.624805000000	0.627393000000	8.380124000000
O	-0.978998000000	-1.770496000000	8.690051000000
O	1.323040000000	-0.136274000000	9.068562000000

O	-0.308371000000	2.260272000000	8.772316000000
C	-3.369269000000	1.172490000000	9.210840000000
C	-1.691826000000	-2.347852000000	9.525311000000
C	1.735158000000	-0.669028000000	10.111248000000
C	0.085852000000	2.847428000000	9.792618000000
C	-4.721776000000	1.638065000000	8.754062000000
C	-2.103184000000	-3.765867000000	9.255930000000
C	3.160929000000	-1.137052000000	10.158890000000
C	0.618363000000	4.243795000000	9.648482000000
H	-4.616438000000	2.207274000000	7.828338000000
H	-2.377220000000	-3.871006000000	8.204864000000
H	3.428474000000	-1.592018000000	9.203823000000
H	1.371360000000	4.260055000000	8.857698000000
H	-5.327451000000	0.754967000000	8.532596000000
H	-1.241410000000	-4.412444000000	9.445776000000
H	3.800996000000	-0.262092000000	10.304564000000
H	-0.204021000000	4.893661000000	9.337022000000
H	-5.229446000000	2.236062000000	9.508097000000
H	-2.923536000000	-4.083561000000	9.896637000000
H	3.336554000000	-1.834637000000	10.975686000000
H	1.041066000000	4.622365000000	10.576723000000
S	-2.975536000000	1.424316000000	10.860752000000
S	-2.245475000000	-1.640014000000	10.987874000000
S	0.801981000000	-0.892979000000	11.533536000000
S	0.077006000000	2.175240000000	11.371661000000
Ni	-0.655090000000	0.247550000000	8.753224000000
Ni	-1.093078000000	0.267968000000	11.238403000000
H	-1.224724000000	-1.766180000000	13.710937000000
H	-1.646041000000	-1.763457000000	16.183253000000
C	-1.689081000000	-0.842321000000	15.610929000000
C	-1.450656000000	-0.848702000000	14.244099000000
N	-1.496896000000	0.271661000000	13.528480000000
C	-1.784383000000	1.391191000000	14.186606000000
H	-1.817669000000	2.308842000000	13.608832000000
H	-2.258668000000	2.304800000000	16.077599000000
C	-2.023964000000	1.383979000000	15.553304000000
N	-1.977809000000	0.270466000000	16.275502000000
