Supporting Information

Revealing the reduction process of Cu(II) to Cu(I) by sodiobis(trimethylsilyl)amine

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XANES and EXAFS Data Collection and Analysis

General Information

All experimental manipulations were carried out using Schlenk techniques. Unless ortherwise noted, commercially available chemicals were used as received. Organic solvents were strictly distilled dried under sodium wire or calcium hydride, purged with dry ultrapure nitrogen then stored in glovebox before use. X-ray absorption measurements were acquired on the beam-line 44A of Taiwan Photon Source (TPS), National Synchrotron Radiation Research Center (NSSRC) in Taiwan. The data were collected in transmission quick scan mode. Experiments utilized a cryogenically cooled double-crystal Si (111) monochromator. The monochromator was scanned continuously under quick scan mode during the measurements with 0.5s per spectrum. The ionization chambers were optimized for the maximum current with linear response (~10^{10} photons detected/sec) with 10% absorption (N_2) in the incident ion chamber and 70% absorption (60% N_2 and 40% Ar) in the transmission detector. A Cu foil spectrum (edge energy 8979 eV) was acquired simultaneously with each measurement for energy calibration[1]. Multiple scans were taken to reduce the noise.

All solution samples were placed in a sample holder (the XAS solution cell) made of PEEK (polyether ether ketone) equipped with a screw top and O-ring fitting to prevent exposure to air and water.[2] For solution samples, the Cu concentration was adjusted to be 0.05 - 0.1 M with a path length of 3.5 mm.

The edge energy of the X-Ray absorption near edge structure (XANES) spectrum was determined from the inflection point in the edge, i.e., the maximum in the first derivative of the XANES spectrum. The pre-edge energy was determined from the maximum of the pre-edge peak.

Background removal and normalization procedures were carried out using the Athena software package using standard methods.[3] Standard procedures based on Artemis software (Demeter 0.9.20) were used to extract the extended X-ray absorption fine structure (EXAFS) data. The coordination parameters were obtained by a least square fit in R-space of the nearest neighbor, k^2-weighted Fourier transform data.

Experimental Details

$CuCl_2$ + 4 NaHMDS / DMF solution: $CuCl_2$ (0.5 mmol, 67.5 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (2.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

CuI + 2 NaHMDS /DMF solution: CuI (0.5 mmol, 95.0 mg) were added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (1.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

$CuCl_2$/DMF solution: $CuCl_2$ (0.5 mmol, 67.5 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell and the solution was stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

$CuCl_2$ + 4 NaHMDS / DMF solution: $CuCl_2$ (0.5 mmol, 67.5 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (2.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

$CuCl_2$ + 4 NaHMDS / Toluene solution: $CuCl_2$ (0.5 mmol, 67.5 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of Toluene was injected into the cell. Then NaHMDS (2.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

$CuCl_2$ + 4 NaHMDS / THF solution: $CuCl_2$ (0.5 mmol, 67.5 mg) was added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of THF was injected into the cell. Then NaHMDS (2.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

CuI + 1 NaHMDS /DMF solution: CuI (0.5 mmol, 95.0 mg) were added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (0.5 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

CuI + 2 NaHMDS /DMF solution: CuI (0.5 mmol, 95.0 mg) were added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (1.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

CuI + 3 NaHMDS /DMF solution: CuI (0.5 mmol, 95.0 mg) were added to the XAS solution cell in a glovebox beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (1.5 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

CuI + 4 NaHMDS /DMF solution: CuI (0.5 mmol, 95.0 mg) were added to the XAS solution cell in a glovebox

beforehand. Then, 5.0 mL of DMF was injected into the cell. Then NaHMDS (2.0 mmol) was added into the solution and stirred under N_2 at roon temperature for 20 minutes. XANES spectrum was measured at room temperature.

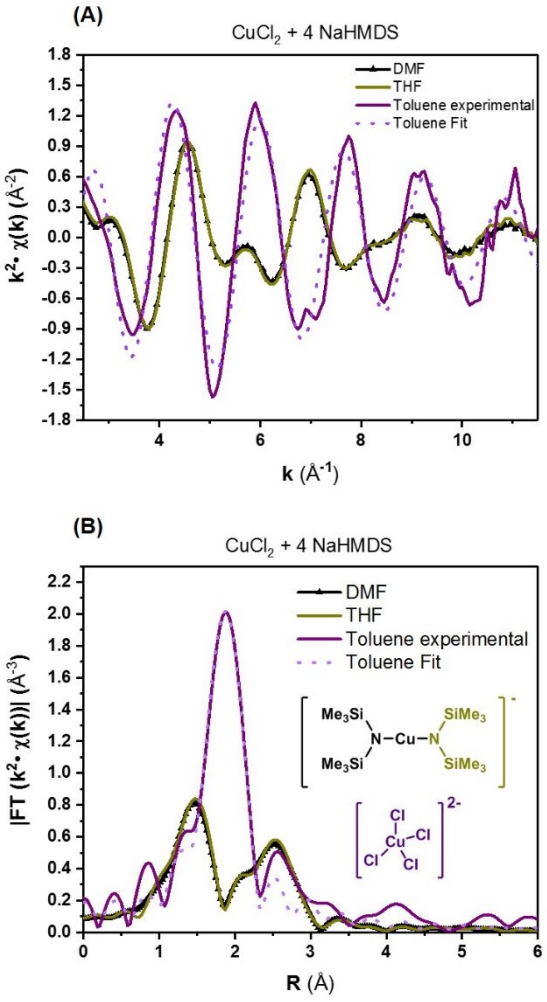

Figure S1. (A) k^2-weighting k-space EXAFS and (B) R-space EXAFS spectrum. Black line: CuCl2 (0.5 mmol) and NaHMDS (2 mmol) in DMF (5 mL) at rt. Purple line: CuCl2 (0.5 mmol) and NaHMDS (2 mmol) in toluene (5 mL) at rt. Olive line: CuCl2 (0.5 mmol) and NaHMDS (2 mmol) in THF (5 mL) at rt. Fitting for reaction in Toluene was shown in dotted line in purple.

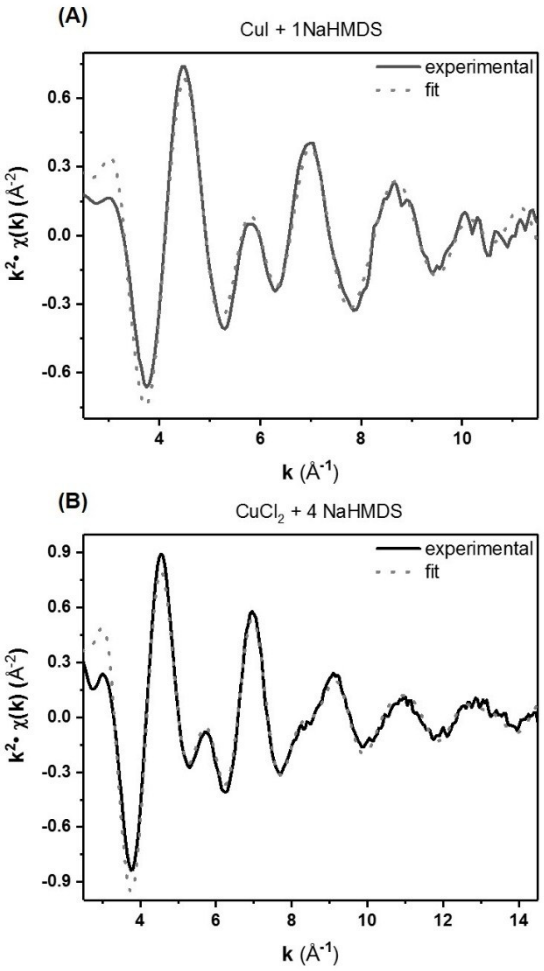

Figure S2. k^2-weighting k-space EXAFS and fitting for (A) CuI + NaHMDS (1 equiv) in DMF solution (3.3 $Å^{-1}$ < k < 11.0 $Å^{-1}$ and 1.05 Å < R < 3.05 Å). (B) $CuCl_2$ + NaHMDS (4 equiv) in DMF solution (3.3 $Å^{-1}$ < k < 14.3 $Å^{-1}$ and 1.05 Å < R < 3.05 Å). Fitting parameters in detail are summarized in ***Table 1***.

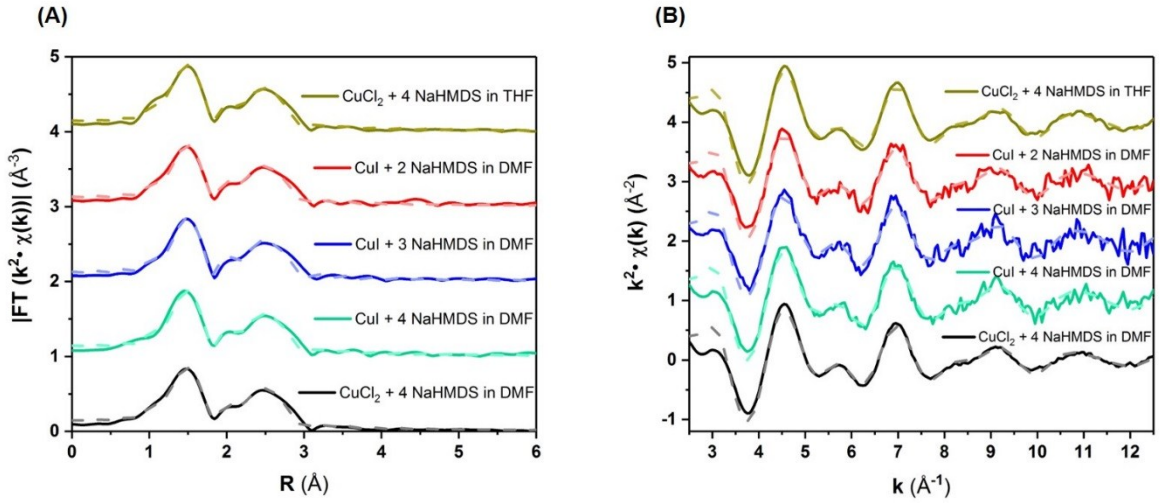

Figure S3. k^2-weighting (A) R-space and (B) k-space EXAFS for experimental data (solid line) and fitting (dash line) for CuI + NaHMDS (1 – 4 equiv.) and CuCl2 + NaHMDS (4 equiv.) in THF and DMF solution. All the experiments gives the linear Cu(I) Cu[N(TMS)2]2Na ate complex. Fitting results summarized in ***Table S1***.

Table S1 Table for fitting results of CuI + NaHMDS (1 – 4 equiv.) and CuCl2 + NaHMDS (4 equiv.) in THF and DMF solution.

Entry	Path	CN	AMP	ΔE_0	DWF	R (Å)
$CuCl_2$ + 4 NaHMDS in THF	Cu-N	1.9 ± 0.1	0.934	8.5 ± 0.9	0.0022	1.88 ± 0.00
	Cu-Si	4.0 ± 0.4			0.0104	3.01 ± 0.00
CuI + 2 NaHMDS in DMF	Cu-N	1.6 ± 0.9			0.0014	1.88 ± 0.02
	Cu-Si	4.0 ± 4.2			0.0112	3.02 ± 0.04
CuI + 3 NaHMDS in DMF	Cu-N	1.5 ± 0.9			0.0033	1.88 ± 0.02
	Cu-Si	3.7 ± 4.2			0.0128	3.02 ± 0.04
CuI + 4 NaHMDS in DMF	Cu-N	1.8 ± 0.8			0.0016	1.88 ± 0.02
	Cu-Si	4.0 ± 3.4			0.0106	3.02 ± 0.03
$CuCl_2$ + 4 NaHMDS in DMF	Cu-N	2	0.934 ± 0.078		0.0031	1.89 ± 0.01
	Cu-Si	4			0.0108	3.01 ± 0.01

Note: FT range: 3.3 $Å^{-1}$ – 12 $Å^{-1}$, Fitting range: 1 Å - 3 Å. Fitting results gives averaged Cu-Si bond distances rather than two different types of Cu-Si bond (in the manuscript) due to shorter fitting data range.

Table S2 XAS Pre-Edge Energies and Edge Energy and Oxidation States for Copper Complexes

Sample	Pre-edge Energy (eV)	Edge Energy (eV)	Oxidation State
Cu foil	N.A.	8979	0
$CuCl_2$ (DMF solution)	8977.0	8984.5	+2
$CuCl_2$ + 4 NaHMDS in DMF	N.A.	8981.1	+1
$CuCl_2$ + 4 NaHMDS in THF	N.A.	8981.1	+1
$CuCl_2$ + 4 NaHMDS in toluene	8977.0	8984.5	+2
CuI + 1 NaHMDS in DMF	N.A.	8980.8	+1
CuI + 2 NaHMDS in DMF	N.A.	8980.8	+1
CuI + 3 NaHMDS in DMF	N.A.	8980.8	+1
CuI + 4 NaHMDS in DMF	N.A.	8980.8	+1

EPR Experimental Details

General Information

EPR spectra were recorded on a Bruker X-band A200 spectrometer. The samples were taken out into a thin small tube and frozen by liquid nitrogen, then recorded by EPR spectrometer at indicated temperature and parameters.

EPR Experiments Data Collection and Analysis

Experimental Details

<u>$CuCl_2$ in DMF solution</u>

A dried Schlenk tube equipped with a stir bar was loaded with $CuCl_2$ (0.5 mmol, 67.5 mg) under the atmosphere of nitrogen at room temperature. After 20 mins, the solution sample was taken out into a small tube, and then analyzed by EPR. EPR spectra was recorded at rt on EPR spectrometer operated at 9.838 GHz. Typical spectrometer

parameters are shown as follows, scan range: 2000 G; center field set: 3200 G; time constant: 40.96 ms; scan time: 15.36 s; modulation amplitude:5.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^5; microwave power: 2.09 mW.

CuCl2 + 4 NaHMDS in DMF solution

A dried Schlenk tube equipped with a stir bar was loaded with $CuCl_2$ (0.5 mmol, 67.5 mg), NaHMDS (2.0 mmol) under the atmosphere of nitrogen at room temperature. After 20 mins, the solution sample was taken out into a small tube and then analyzed by EPR. . EPR spectra was recorded at rt on EPR spectrometer operated at 9.838 GHz. Typical spectrometer parameters are shown as follows, scan range: 2000 G; center field set: 3200 G; time constant: 40.96 ms; scan time: 15.36 s; modulation amplitude:5.0 G; modulation frequency: 100 kHz; receiver gain: 1.00×10^5; microwave power: 2.09 mW.

3. DFT caclulations

3.1. Complete reference for Gaussian 09

Gaussian 09, Revision A.2, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

3.2. B3LYP absolute calculation energies, enthalpies, and free energies.

All the Density functional theory (DFT) calculations were carried out with the GAUSSIAN 09 series of programs. The DFT method B3LYP[4] with a standard 6-31G(d) basis set (LanL2dz basis set for Cu) was used for geometry optimizations. Harmonic frequency calculations were performed for all stationary points to confirm them as a local minima or transition structures and to derive the thermochemical corrections for the enthalpies and free energies. The solvent effects were considered with an integral equation formalism polarizable continuum solvation model (IEFPCM).[5] The larger basis set 6-311+G (d, p) (def2-TZVP basis set for Cu) is used in the solvation single point calculations. The energies given in this paper are the B3LYP calculated Gibbs free energies in N, N-dimethylformamide solvent.

Geometry	$E_{(elec)}$	$E_{(DMF)}$	$H_{(gas\ phase)}$	$G_{(gas\ phase)}$	IF*
$Cu[N(TMS)_2]_2$	-1942.830457	-3387.565810	-1942.334384	-1942.435958	-
$Cu[N(TMS)_2]_3^-$	-2816.209031	-4261.152054	-2815.464691	-2815.602018	-
$Cu[N(TMS)_2]_2^-$	-1942.929795	-3387.725770	-1942.434822	-1942.540543	-

$N(TMS)_2^-$	-873.343115	-873.582953	-873.099447	-873.161518	-
$N(TMS)_2$ radical	-873.267339	-873.426395	-873.022783	-873.082888	-
$(TMS)_2N–N(TMS)_2$	1746.604504	-1746.915164	-1746.108891	-1746.203055	-

* IF: The imaginary frequencies for the transition states.

3.3. B3LYP geometries for all the optimized compounds.

$Cu[N(TMS)_2]_2$

Cu	0.00003300	-0.00009100	-0.00061600
N	-1.84450500	-0.00019000	-0.00035700
N	1.84457200	0.00014300	-0.00042700
Si	-2.64064500	-1.50381500	0.45861200
Si	-2.64035600	1.50384000	-0.45855400
Si	2.64047700	1.50385900	0.45862000
Si	2.64055600	-1.50386000	-0.45851600
C	-4.19345700	-1.18711900	1.50535200
H	-4.96937300	-0.63270500	0.96630200
H	-4.63295300	-2.14294200	1.81899200
H	-3.95031300	-0.62406800	2.41444500
C	-1.47508000	-2.55061800	1.52752000
H	-0.56163300	-2.84550800	0.99804600
H	-1.17430300	-2.00345100	2.42956700
H	-1.97675000	-3.47208500	1.85108500
C	-3.12073800	-2.49881000	-1.08306500
H	-2.23783300	-2.73579800	-1.68879500
H	-3.59967600	-3.44564100	-0.80242500
H	-3.82107800	-1.94493100	-1.71856700
C	-1.47690400	2.54764900	-1.53271200
H	-1.17980300	1.99865700	-2.43486400
H	-1.97841800	3.46927200	-1.85607000
H	-0.56132100	2.84212200	-1.00669300
C	-4.19709000	1.18815000	-1.49975000
H	-4.97201200	0.63548900	-0.95748200
H	-4.63623300	2.14425700	-1.81301300
H	-3.95784500	0.62374500	-2.40903800
C	-3.11409600	2.50112100	1.08360000
H	-3.81315600	1.94874300	1.72182200
H	-2.22897700	2.73749200	1.68632300
H	-3.59267400	3.44832100	0.80360000
C	3.11976100	2.49927700	-1.08303600
H	3.82001000	1.94566700	-1.71887600
H	2.23657600	2.73612600	-1.68841100
H	3.59856700	3.44618300	-0.80243000
C	1.47490000	2.55008900	1.52809400
H	1.97637800	3.47161600	1.85178700
H	0.56124500	2.84485000	0.99890100
H	1.17447600	2.00260200	2.43006300
C	4.19368200	1.18750600	1.50488000
H	4.96966700	0.63342300	0.96559900
H	4.63291700	2.14343900	1.81854700
H	3.95093600	0.62426700	2.41396600
C	3.11429000	-2.50106800	1.08368400
H	3.59316000	-3.44812800	0.80370300
H	3.81309300	-1.94855700	1.72206700
H	2.22912300	-2.73771600	1.68623200
C	1.47724000	-2.54781100	-1.53267100
H	0.56148000	-2.84199600	-1.00680400
H	1.18045500	-1.99903900	-2.43506000
H	1.97870700	-3.46960300	-1.85562000
C	4.19730800	-1.18807500	-1.49966000
H	3.95816600	-0.62325800	-2.40871800
H	4.97236300	-0.63580600	-0.95718700
H	4.63624300	-2.14415000	-1.81332000

$Cu[N(TMS)_2]_3^-$

Cu	-0.02637000	-0.10325000	-0.01728400
N	-1.87088500	-0.91274500	-0.04950500
N	-0.00725500	1.92710100	-0.03014600
N	1.76967700	-0.96286500	0.04234100
Si	2.11092700	-1.92152900	1.45031700
Si	2.94809100	-0.75784900	-1.21856500
Si	-2.07373100	-2.28960500	-1.08330200
Si	-3.13972100	-0.35749800	0.99566600
Si	0.61940300	2.71934800	1.37003000
Si	-0.46355800	2.68471000	-1.51355400
C	-3.50730200	-2.15305700	-2.34362800
H	-3.44619400	-1.20200300	-2.88774300
H	-3.43769100	-2.96242000	-3.08412900
H	-4.49929400	-2.21081300	-1.88430500
C	-0.55821500	-2.64703800	-2.16917000
H	0.36692200	-2.70036600	-1.58813400
H	-0.70163300	-3.60640600	-2.68603500
H	-0.42914700	-1.87559200	-2.93673300
C	-2.36443000	-3.89837200	-0.08811900
H	-3.24778400	-3.83811700	0.55866700

H	-2.49912700	-4.76026900	-0.75658700
H	-1.50098900	-4.10728500	0.55627100
C	-3.45740600	1.50858700	0.86026200
H	-3.87850900	1.75191600	-0.12375300
H	-4.17309200	1.84291300	1.62421500
H	-2.53035500	2.07521500	0.96943000
C	-2.83984300	-0.76158700	2.83696000
H	-3.68669600	-0.41952800	3.44841500
H	-2.73842000	-1.84437700	2.98697000
H	-1.93566500	-0.28811200	3.23104200
C	-4.86779800	-1.12251000	0.65996000
H	-5.55614300	-0.76631500	1.43941200
H	-5.27910300	-0.80527500	-0.30536100
H	-4.88717100	-2.21822600	0.68744400
C	1.97236600	-3.79501100	1.10677700
H	2.11448800	-4.37037000	2.03224100
H	0.97916500	-4.03958800	0.71071800
H	2.71361200	-4.14427100	0.37921900
C	0.89285600	-1.57168000	2.86048900
H	1.09588200	-2.24084200	3.70818300
H	0.97920200	-0.54183700	3.22501400
H	-0.14384000	-1.73307700	2.54806900
C	3.84598600	-1.63607900	2.20474900
H	3.97665300	-2.26045500	3.09965300
H	4.66259100	-1.87872100	1.51437700
H	3.97354600	-0.59020200	2.51027800
C	2.21493300	-0.32477600	-2.91654800
H	1.55541500	0.54598500	-2.88315300
H	3.03223600	-0.09169600	-3.61334700
H	1.64775400	-1.16146300	-3.33723400
C	4.24044000	0.59923600	-0.86741900
H	4.74716200	0.45309700	0.09335000
H	5.00652200	0.61107500	-1.65540300
H	3.76777700	1.58704700	-0.84383800
C	3.95294400	-2.35435000	-1.55517700
H	4.65454800	-2.17727100	-2.38211500
H	4.54159900	-2.69129900	-0.69391500
H	3.29607600	-3.18108600	-1.85231400
C	-1.30975700	1.46730200	-2.70550400
H	-0.66433200	0.63500400	-3.00526500
H	-2.19826800	1.03427300	-2.23408600
H	-1.61960200	1.99335600	-3.61938500
C	-1.72113200	4.11898900	-1.34914000
H	-1.30168400	4.99847700	-0.84896700
H	-2.04738400	4.43566200	-2.35008100
H	-2.61179400	3.80821500	-0.79205600
C	1.01333500	3.46385000	-2.45144700
H	0.69615200	3.88051000	-3.41796000
H	1.45869000	4.28264200	-1.87144000
H	1.80828500	2.73516600	-2.64598100
C	-0.34022900	2.31179900	2.96772700
H	0.11583500	2.82585400	3.82545500
H	-1.38657600	2.63235900	2.90291900
H	-0.34181400	1.23975400	3.19047200
C	2.44238300	2.33404700	1.76234700
H	3.11477700	2.82191900	1.04623700
H	2.70841600	2.69210400	2.76688700
H	2.64222300	1.25988400	1.71240600
C	0.55009300	4.63098700	1.26823500
H	1.05714800	5.04925400	2.14887500
H	1.05592500	5.02954600	0.38071100
H	-0.47745900	5.01179800	1.26839400

$Cu[N(TMS)_2]_2^-$

Cu	-0.00313300	-0.07791800	-0.00305400
N	-1.92144500	-0.06189600	-0.05682000
N	1.91417300	-0.07887100	0.06069300
Si	-2.72016200	-1.15766100	0.98709100
Si	-2.55332400	1.16394500	-1.07168300
Si	2.54807300	1.06158700	1.17013500
Si	2.72405700	-1.06231300	-1.08218500
C	-3.82957000	-0.30289000	2.29459300
H	-4.62408700	0.29396800	1.82786600
H	-4.31192300	-1.03091500	2.96219900
H	-3.23274700	0.37726500	2.91614500
C	-1.48913400	-2.22477700	1.97488000
H	-0.84822300	-2.81259800	1.30601200
H	-0.82914900	-1.60252600	2.59124000
H	-2.01512300	-2.92492800	2.63997400
C	-3.85360800	-2.40081900	0.07226700
H	-3.27561700	-2.96752300	-0.66933400
H	-4.30851600	-3.12224000	0.76589900
H	-4.66760600	-1.89587400	-0.46235000
C	-1.69685500	1.19407800	-2.77622700
H	-1.82756000	0.23247400	-3.28938900
H	-2.10112700	1.98328800	-3.42614500
H	-0.61800700	1.36268600	-2.66965800
C	-4.42312500	0.97830900	-1.44809400
H	-5.03429100	0.98405600	-0.53656300
H	-4.77302500	1.80454500	-2.08256100
H	-4.63279600	0.04168600	-1.97968700
C	-2.34794000	2.91696200	-0.33967800
H	-2.88133400	3.00664800	0.61584700
H	-1.28885100	3.12548600	-0.14154800
H	-2.72641500	3.69956600	-1.01266000
C	2.41277200	2.86270400	0.54600400

H	2.96302500	2.99100900	-0.39541400
H	1.36426800	3.11865400	0.34683700
H	2.80657200	3.59013800	1.27003500
C	1.64288800	1.00685900	2.84828900
H	2.05486200	1.73594900	3.56059400
H	0.57375800	1.22015200	2.72568200
H	1.72683600	0.00894500	3.29792700
C	4.40011300	0.79672500	1.58597400
H	5.03869200	0.83920400	0.69441900
H	4.75506300	1.57082000	2.28056900
H	4.56575800	-0.17715600	2.06354000
C	3.85217700	-2.39142400	-0.28937100
H	4.30385600	-3.04421100	-1.04988800
H	4.66841800	-1.94508100	0.29197300
H	3.27185000	-3.02572800	0.39339900
C	1.50645700	-2.02853900	-2.18380300
H	0.86453400	-2.68342000	-1.58155500
H	0.84735700	-1.35238100	-2.74154200
H	2.04206800	-2.65619700	-2.91069800
C	3.84226900	-0.07320700	-2.28264100
H	3.24105600	0.63638800	-2.86594300
H	4.60069300	0.50894300	-1.74310100
H	4.36979100	-0.72779200	-2.99086200

$N(TMS)_2^-$

N	0.00000200	0.00020400	0.00046200
Si	1.64484800	-0.00001000	-0.00001200
Si	-1.64484400	0.00008000	0.00020200
C	-2.44672200	-1.69688300	-0.43498300
H	-2.13128900	-2.46995400	0.27904700
H	-3.54690400	-1.66314900	-0.42673800
H	-2.13067800	-2.03143700	-1.43255300
C	-2.44849800	0.47132700	1.68617500
H	-2.13543900	1.47710400	1.99815500
H	-3.54853200	0.45928700	1.65094200
H	-2.13190900	-0.22433100	2.47527700
C	-2.44808700	1.22459000	-1.25164600
H	-2.13289000	0.99299700	-2.27826500
H	-3.54818700	1.19912400	-1.22567100
H	-2.13328500	2.25617400	-1.04267400
C	2.44770500	-0.47961200	-1.68401900
H	2.13087800	0.21223500	-2.47637400
H	3.54775600	-0.46756100	-1.64932000
H	2.13436100	-1.48684900	-1.99096700
C	2.44725500	1.69890700	0.42644900
H	2.13172700	2.03852500	1.42247100
H	3.54742800	1.66489700	0.41787300
H	2.13166800	2.46845100	-0.29131100
C	2.44834200	-1.21857100	1.25745800
H	2.13328900	-2.25110000	1.05359100
H	3.54843600	-1.19341800	1.23098900
H	2.13353100	-0.98194700	2.28304600

$N(TMS)_2$ radical

N	-0.00030500	0.01512400	-0.49343100
Si	-1.67560200	0.00426100	-0.04155400
Si	1.67521200	-0.00416000	-0.04279200
C	-2.58684800	-1.19403000	-1.18926200
H	-3.66096400	-1.20916900	-0.96474100
H	-2.45948500	-0.90140200	-2.23718400
H	-2.21138200	-2.21825700	-1.08024600
C	-2.28734400	1.77805500	-0.33301900
H	-1.76709000	2.49637200	0.31048100
H	-2.13468700	2.08132400	-1.37404900
H	-3.35991000	1.84437600	-0.11019600
C	-2.00776600	-0.48678000	1.75987500
H	-3.08214200	-0.47246000	1.98500900
H	-1.64248700	-1.49883200	1.97393400
H	-1.51251400	0.19825000	2.45843000
C	2.31388300	-1.72270800	-0.53531000
H	1.81020100	-2.51705300	0.02696200
H	2.15707400	-1.91009000	-1.60268900
H	3.38908400	-1.79621700	-0.32788300
C	2.00479400	0.28108200	1.80289700
H	3.07942400	0.25084100	2.02495700
H	1.62967600	1.25862200	2.13019900
H	1.51631400	-0.48390800	2.41833100
C	2.56421500	1.33373200	-1.04505600
H	3.63927700	1.33506900	-0.82466100
H	2.43419800	1.16626500	-2.11974600
H	2.17739300	2.33287300	-0.81279000

$(TMS)_2N\text{-}N(TMS)_2$

N	-0.73756800	0.00010100	0.00013200
Si	-1.55971500	-1.16542200	1.06632300
Si	-1.55993300	1.16541300	-1.06613800
C	-0.45339300	-1.74662100	2.48762200
H	-0.89654200	-2.64880000	2.92885000
H	0.56097300	-1.99861500	2.16774700
H	-0.38195500	-0.99763900	3.28195900
C	-2.13108600	-2.71942400	0.13398600
H	-2.77596900	-2.47728800	-0.71832400
H	-1.28579800	-3.30514300	-0.24574700
H	-2.70398300	-3.37176200	0.80625000
C	-3.09738400	-0.36661100	1.84373600
H	-3.58277500	-1.09411900	2.50759800

H	-2.82841200	0.50466900	2.45226100
H	-3.84903900	-0.04595300	1.11505100
C	-2.13158300	2.71927700	-0.13375300
H	-2.77617100	2.47700300	0.71873800
H	-1.28633500	3.30521900	0.24573100
H	-2.70482100	3.37145400	-0.80588200
C	-3.09738300	0.36630600	-1.84369500
H	-3.58294500	1.09376100	-2.50748800
H	-2.82816000	-0.50483500	-2.45231100
H	-3.84897600	0.04535900	-1.11507200
C	-0.45376100	1.74689100	-2.48742200
H	-0.89789300	2.64822900	-2.92939300
H	0.56020400	2.00034800	-2.16742800
H	-0.38116600	0.99747900	-3.28124400
N	0.73757700	0.00009700	-0.00011100
Si	1.55992200	1.16541400	1.06617300
Si	1.55973400	-1.16537300	-1.06635600
C	0.45374000	1.74674300	2.48751600
H	0.38160100	0.99746500	3.28150600
H	0.89752000	2.64838000	2.92922600
H	-0.56037800	1.99966600	2.16759800
C	3.09744100	0.36631600	1.84359700
H	3.84898500	0.04540800	1.11490600
H	3.58304600	1.09372600	2.50740200
H	2.82825400	-0.50486500	2.45217000
C	2.13143500	2.71937600	0.13386500
H	1.28611500	3.30535500	-0.24539800
H	2.70479100	3.37148400	0.80595800
H	2.77586900	2.47719800	-0.71876800
C	2.13128500	-2.71931300	-0.13402600
H	2.70440900	-3.37151600	-0.80622800
H	2.77600000	-2.47708600	0.71838200
H	1.28606100	-3.30521300	0.24556500
C	0.45336900	-1.74666500	-2.48757900
H	0.38176700	-0.99766500	-3.28188200
H	0.89662200	-2.64875400	-2.92888800
H	-0.56093800	-1.99883000	-2.16765900
C	3.09730500	-0.36645900	-1.84385800
H	3.84898300	-0.04583000	-1.11518300
H	3.58269400	-1.09388900	-2.50780100
H	2.82827600	0.50486500	-2.45229200

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