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Supplementary Information

For

Metallopolymer Formation Using the (1*R*,2*R*)-*N*,*N*'-Bis(pyridylmethylene)cyclohexane-1,2-diamine (BPID) Ligand Class

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1) Experimental Data

General Procedures: All syntheses and manipulations were carried out under argon inside a Vacuum Atmospheres glove box. Anhydrous solvents were purchased from either Sigma Aldrich or Acros and stored over 4 Å molecular sieves. KH was purchased from Sigma Aldrich and used without further purification. The 2-py-BPID[1] and 4-py-BPID[2] ligands were synthesized according to literature procedure. Elemental Analysis was performed by Midwest Microlab, LLC. NMR spectra were recorded at ambient temperature on a Bruker AV-400 spectrometer. X-ray diffraction data were collected by mounting crystals under Paratone on glass fiber loops on a Bruker Apex II system fitted with an Oxford nitrogen cryostream. Structure solution and refinement against F^2 were performed using SHELX97.

Preparation of $[K(THF)_3\text{-}(2\text{-py-BPID})\text{-}K]_n$ (**2**): A 20 mL scintillation vial was charged with 2-py-BPID ligand (50 mg, 0.171 mmol), KH (28 mg, 0.698 mmol) and THF (5 mL). The mixture was stirred at 50°C for 18 hr resulting in a dark blue solution. The solvent was removed in vacuo and the resulting dark solid dissolved in THF (1.5 mL) and filtered through a PTFE filter. Hexanes were diffused into the clear, dark blue solution and the vial covered with aluminum foil, resulting in a crop of dark, crystalline needles after 3 days. The solution was decanted and the crystals washed with hexanes (3 x 2 mL) and subsequently dried at ambient pressure and temperature. (Yield: 41 mg, 41%). Note: Multiple attempts at obtaining consistent EA data resulted in samples exhibiting varying degrees of loss of THF solvating ligands. Thus, the crystalline samples were dried in vacuo for 2 hours before submitting for EA. ^{1}H NMR (C_6D_6): δ 8.07 (d, 1H, py-*H*), 7.94 (d, 1H, py-*H*), 7.05 (m, 2H, py-*H*), 6.84 (d, 1H, py-*H*), 6.75 (m, 1H, py-*H*), 6.70 (s, 1H, C-*H*), 6.61 (m, 1H, py-*H*), 6.44 (m, 1H, py-*H*), 4.50 (s, 1H, C-*H*), 3.57 (s, 12H, THF), 2.46 (m, 2H, Cy-*H*), 2.01 (m, 2H, Cy-*H*), 1.41 (s, 12H, THF), 1.75-1.58 (m, 4H, Cy-*H*). $^{13}C\{^1H\}$ NMR (THF-d_8): 158.0, 151.4, 132.2, 129.2, 117.9, 104.3, 102.9, 28.1. Anal. calcd for $C_{18}H_{18}N_4K_2$ [**2** - $(THF)_3$]: C, 58.34 H, 5.44. Found: C, 58.82 H, 5.95.

Preparation of $[K(THF)_2\text{-}(4\text{-py-BPID})\text{-}K(THF)]_n$ (**4**): A 20 mL scintillation vial was charged with BPID ligand (50 mg, 0.171 mmol), KH (28 mg, 0.698 mmol) and THF (5 mL). The mixture was stirred at 50°C for 18 hr resulting in a dark green-blue solution. The solvent was

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removed in vacuo and the resulting dark solid dissolved in THF (1.5 mL) and filtered through a PTFE filter. Hexanes were diffused into the resulting clear, dark solution and the vial covered with aluminum foil, resulting in a crop of dark crystals after 3 days. The solution was decanted and the crystals washed with hexanes (3 x 2 mL) and subsequently dried at ambient pressure and temperature. (Yield: 23 mg, 23%). ^{1}H NMR (THF-d_8): δ 8.74-8.33 (m(b), 2H, py-*H*), 8.25 (d, 1H, py-*H*), 8.10-7.74 (m(b), 1H, py-*H*), 7.59-7.04 (m(b), 3H, py-*H*), 6.95 (d, 1H, py-*H*), 6.30 (s(b), 1H, C-*H*), 5.84 (s(b), 1H, C-*H*), 3.08-2.88 (m(b), 1H, Cy-*H*), 2.51 (m, 1H, Cy-*H*), 2.45-2.14 (m(b), 2H, Cy-*H*), 1.97 (m, 1H, Cy-*H*), 1.61 (m, 1H, Cy-*H*), 1.49-1.31 (m, 2H, Cy-*H*).

References

1) B. Liu, M.-J. Zhang, J. Cui and J. Zhu, *Acta Cryst.*, **2006**, *E62*, o5359-o5360.

2) X.-J. Yuan, Y.-Z. Li, Y.-J. Liu, Y.-Q. Tian, X.-Z. You, *Acta Cryst., Sect. E: Struct. Rep. Online*, **2002**, *58*, o640-o641.

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2) X-ray Data Tables

Table 1. Crystal data for **2** and **4**.

	2	**4**
Empirical formula	$C_{30}H_{44}N_4O_3K_2$	$C_{30}H_{44}N_4O_3K_2$
M	584.88	584.88
T/K	140(1)	140(1)
Color	Purple	Purple
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	7.3294(5)	16.101(3)
b/Å	17.2843(13)	10.5899(17)
c/Å	24.3967(18)	19.115(3)
β/°	98.320(1)	108.545(2)
U/Å^3	3058.1(4)	3090.0(9)
Z	4	4
Dc/Mg m^{-3}	1.270	1.262
μ/mm^{-1}	0.346	0.343
Crystal size/mm	0.16x0.14x0.06	0.10x0.08x0.03
Reflections collected	33850	30080
R(int)	0.0628	0.0953
Data/restraints/parameters	7121 / 0 / 352	5881 / 0 / 352
Absorption correction	Semi-empirical	Semi-empirical
*R*1 [$I > 2\,(I)$]	0.0416	0.0550
*w*R2 (all data)	0.1240	0.1506
Largest peak, hole / e Å^{-3}	0.551, -0.477	0.509, -0.663

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Table 2. Bond distances for **2** and **4**.

Bond	**2 (Å)**	**4 (Å)**
C7-C12	1.454(2)	1.448(4)
C7-N2	1.317(2)	1.328(4)
C6-N2	1.348(2)	1.360(4)
C12-N3	1.321(2)	1.326(4)
C13-N3	1.352(2)	1.362(4)
C5-C6	1.404(2)	1.400(4)
C13-C14	1.399(2)	1.403(4)
K1-O1	2.7696(11)	2.690(3)
K1-O2	2.8111(12)	2.699(3)
K1-O3	2.9094(12)	
K2-O1	2.7620(12)	
K2-O2	2.8027(12)	
K2-O3	2.8738(13)	2.632(3)
K1-N1	2.9497(13)	
K1-N2	2.8231(13)	2.807(3)
K1-N3	2.7938(13)	2.796(3)
K1-N4	2.9450(14)	2.774(3)
K2-N1	2.9626(13)	2.734(3)
K2-N2	2.7722(13)	2.702(3)
K2-N3	2.7632(13)	2.811(3)
K2-N4	2.9812(14)	

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3) DFT Calculation Data Tables

Gas-phase DFT calculations on the K_2[2-py-BPID*] fragment failed to satisfactorily reproduce the experimental structural parameters and attempts to account for solvent explicitly were also unsatisfactory as the extended structure is needed in order to stabilize the solvent positions. Thus, the solvent-K interaction was modeled implicitly using PCM[3] with parameters for THF. The initial coordinates for 2-py-BPID were obtained from the CSD (structure code MEQFEU) while the X-ray crystal structure reported herein was used to construct K_2[2-py-BPID*]. Geometry optimizations were performed with the R-B3LYP-D functional[4,5,6] using Grimme's empirical dispersion correction[7] (see Tables X and Y for a comparison with the optimized structures obtained from B3LYP and wB97X-D[8,9]). The 6-31++G(d,p) basis set was used for all atoms except K, for which 6-31G(d) was used.[10,11,12] Frequency calculations were performed on all optimized structures and no imaginary frequencies were found. At the U-B3LYP level, the S=1 state was 16.5 kcal/mol higher in energy than the R-B3LYP S=0 state. Single point energies at the B3LYP-D geometries were also computed using the R-M06 functional[13] and the KTZVPP basis set of Ahlrichs and coworkers[14,15] and a triple zeta valence set with 3 d polarization functions for K.[16] All calculations were performed using the GAMESS-US software package.[17] MacMolPlt was used to generate the molecular orbital images.[18]

Table 3. HOMO-LUMO gaps from B3LYP-D and M06.

	2-py-BPID		**K_2[2-py-BPID*]**	
	B3LYP-D	**M06**	**B3LYP-D**	**M06**
Energy (eV)	5.14	5.62	2.02	1.69

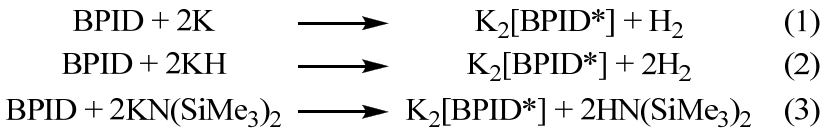

Figure 1. Equations used to calculate the reactions energies in table 1 in the main text.

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Table 4. Experimental and calculated (B3LYP-D) bond lengths for 2-py-BPID.

Bond	**Expt (Å)**	**Calc (Å)**
N1-C1	1.466(2)	1.46
N1-C7	1.267(2)	1.27
N2-C2	1.470(2)	1.46
N2-C13	1.268(2)	1.27
N3-C8	1.349(2)	1.35
N3-C12	1.340(2)	1.34
N4-C14	1.344(2)	1.35
N4-C18	1.341(2)	1.34
C1-C2	1.528(2)	1.55
C1-C6	1.529(2)	1.54
C2-C3	1.529(2)	1.54
C3-C4	1.531(2)	1.54
C4-C5	1.523(2)	1.54
C5-C6	1.532(2)	1.54
C7-C8	1.482(2)	1.48
C8-C9	1.389(2)	1.40
C9-C10	1.389(2)	1.39
C10-C11	1.391(2)	1.40
C11-C12	1.381(2)	1.40
C13-C14	1.482(2)	1.48
C14-C15	1.388(2)	1.40
C15-C16	1.385(3)	1.39
C16-C17	1.390(3)	1.40

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C17-C18	1.380(2)	1.40

Table 5. Experimental and calculated (B3LYP-D) bond angles for 2-py-BPID.

Bond Angle	**Expt (°)**	**Calc (°)**
C1-N1-C7	117.9(1)	118
C2-N2-C13	116.6(1)	118
C8-N3-C12	116.6(1)	118
C14-N4-C18	117.0(2)	118
N1-C1-C2	108.8(1)	109
N1-C1-C6	108.7(1)	110
C2-C1-C6	110.6(1)	110
N2-C2-C1	109.6(1)	109
N2-C2-C3	108.7(1)	110
C1-C2-C3	110.8(1)	110
C2-C3-C4	111.0(1)	112
C3-C4-C5	110.4(1)	111
C4-C5-C6	110.1(1)	111
C1-C6-C5	111.6(1)	111
N1-C7-C8	121.2(2)	123
N3-C8-C7	115.3(1)	115
N3-C8-C9	123.2(2)	123
C7-C8-C9	121.5(2)	122
C8-C9-C10	119.2(2)	119
C9-C10-C11	118.0(2)	119
C10-C11-C12	118.8(2)	118
N3-C12-C11	124.2(2)	123

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N2-C13-C14	122.5(2)	123
N4-C14-C13	114.2(1)	115
N4-C14-C15	123.1(2)	123
C13-C14-C15	122.7(1)	122
C14-C15-C16	119.0(2)	119
C15-C16-C17	118.4(2)	119
C16-C17-C18	118.6(2)	118
N4-C18-C17	123.8(2)	123

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Table 6. Experimental and calculated bond lengths for K_2[2-py-BPID*].

	Expt (Å)	**B3LYP**	**B3LYP w/ THF**	**B3LYP-D w/ THF**	**wB97X-D w/ THF**
K1-N1	2.9439(4)	2.83	2.86	2.90	2.87
K1-N2	2.8196(4)	2.77	2.80	2.84	2.78
K1-N3	2.7903(4)	2.81	2.83	2.85	2.77
K1-N4	2.9400(5)	2.82	2.87	2.89	2.83
K2-N1	2.9563(4)	2.89	2.93	2.96	2.91
K2-N2	2.7654(4)	2.75	2.77	2.79	2.76
K2-N3	2.7571(4)	2.69	2.72	2.76	2.72
K2-N4	2.9692(4)	2.88	2.90	2.92	2.87
N1-C1	1.3481(3)	1.35	1.35	1.35	1.34
N1-C5	1.3907(2)	1.39	1.39	1.39	1.38
N2-C6	1.3551(3)	1.35	1.35	1.35	1.36
N2-C7	1.3205(3)	1.32	1.32	1.32	1.31
N3-C12	1.3261(2)	1.32	1.32	1.32	1.31
N3-C13	1.3556(3)	1.35	1.35	1.35	1.36
N4-C14	1.3847(2)	1.39	1.39	1.39	1.38
N4-C18	1.3432(2)	1.35	1.35	1.35	1.34
C1-C2	1.3804(3)	1.39	1.39	1.39	1.38
C2-C3	1.3995(2)	1.42	1.42	1.42	1.41
C3-C4	1.3582(3)	1.37	1.38	1.38	1.37
C4-C5	1.4212(3)	1.44	1.44	1.44	1.44

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C5-C6	1.3918(3)	1.42	1.42	1.42	1.41
C7-C8	1.4977(3)	1.51	1.52	1.51	1.51
C7-C12	1.4487(3)	1.46	1.46	1.46	1.47
C8-C9	1.5187(3)	1.54	1.54	1.54	1.53
C9-C10	1.5091(2)	1.53	1.53	1.53	1.53
C10-C11	1.5143(2)	1.54	1.54	1.54	1.53
C11-C12	1.4987(3)	1.52	1.52	1.52	1.51
C13-C14	1.3938(3)	1.42	1.42	1.42	1.41
C14-C15	1.4294(3)	1.44	1.44	1.44	1.44
C15-C16	1.3575(3)	1.37	1.38	1.38	1.37
C16-C17	1.4057(2)	1.42	1.42	1.42	1.42
C17-C18	1.3716(3)	1.39	1.39	1.39	1.38

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Table 7. Experimental and calculated bond angles for K_2[2-py-BPID*].

	Expt (°)	**B3LYP**	**B3LYP w/ THF**	**B3LYP-D w/ THF**	**wB97X-D w/ THF**
N1-K1-N2	57.3	60	59	58	59
N1-K1-N3	100.9	102	102	101	102
N1-K1-N4	101.7	100	100	99	99
N2-K1-N3	56.2	56	56	56	57
N2-K1-N4	101.2	103	102	101	102
N3-K1-N4	57.5	59	59	58	59
N1-K2-N2	57.7	59	59	58	58
N1-K2-N3	101.4	103	102	101	102
N1-K2-N4	100.7	97	97	97	97
N2-K2-N3	57.2	58	58	57	58
N2-K2-N4	101.8	102	102	101	102
N3-K2-N4	57.4	60	60	59	59
K1-N1-K2	69.8	70	70	71	71
K1-N1-C1	124.6	122	121	120	121
K1-N1-C5	108.5	102	103	103	104
K2-N1-C1	123.2	125	126	126	125
K2-N1-C5	103.4	109	108	108	108
C1-N1-C5	117.4	118	118	118	118
K1-N2-K2	74.3	73	74	75	74
K1-N2-C6	113.4	105	106	107	108

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K1-N2-C7	112.3	114	113	113	111
K2-N2-C6	109.6	114	114	113	114
K2-N2-C7	108.8	109	109	109	109
C6-N2-C7	126.2	128	128	128	128
K1-N3-K2	74.9	73	74	75	75
K1-N3-C12	111.1	113	113	113	112
K1-N3-C13	111.2	113	112	112	112
K2-N3-C12	110.6	110	110	109	110
K2-N3-C13	112.7	106	107	107	108
C12-N3-C13	125.3	128	128	127	128
K1-N4-K2	69.7	71	71	72	72
K1-N4-C14	106.0	111	110	110	109
K1-N4-C18	123.2	122	122	122	123
K2-N4-C14	105.4	100	101	102	102
K2-N4-C18	126.2	125	125	124	123
C14-N4-C18	116.8	118	118	118	118
N1-C1-C2	124.8	125	125	125	125
C1-C2-C3	117.7	117	117	117	117
C2-C3-C4	119.6	120	120	120	120
C3-C4-C5	120.9	121	121	121	121
N1-C5-C4	119.6	119	119	119	119
N1-C5-C6	120.1	120	120	120	120
C4-C5-C6	120.4	121	121	121	121
N2-C6-C5	119.9	120	120	120	119
N2-C7-C8	122.5	123	123	123	123

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N2-C7-C12	116.6	116	117	117	117
C8-C7-C12	120.9	121	121	121	121
C7-C8-C9	113.5	113	113	113	113
C8-C9-C10	110.6	111	111	111	111
C9-C10-C11	110.8	111	111	111	111
C10-C11-C12	113.1	114	114	114	113
N3-C12-C7	116.9	116	117	117	117
N3-C12-C11	122.0	123	123	122	123
C7-C12-C11	121.1	121	121	121	121
N3-C13-C14	119.6	120	120	120	119
N4-C14-C13	120.1	120	120	120	120
N4-C14-C15	119.6	119	119	119	119
C13-C14-C15	120.2	121	121	121	121
C14-C15-C16	121.0	121	121	121	121
C15-C16-C17	119.0	120	120	120	120
C16-C17-C18	117.6	117	117	117	117
N4-C18-C17	125.8	126	125	125	125

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Table 8. Final coordinates for 2-py-BPID.

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	3.6812018936	6.1543652820	0.8670991906
N	7.0	1.9103903977	3.9528224125	1.4046471703
N	7.0	4.8812793933	7.6080705724	3.9039772049
N	7.0	-0.9029810504	5.1014615404	3.2880678256
C	6.0	3.8347672344	4.8664593044	0.2051082145
H	1.0	4.4716682085	4.1856416560	0.7966211209
C	6.0	2.4410138351	4.1990582301	0.0709630792
H	1.0	1.7956276912	4.8924882018	-0.4960901383
C	6.0	2.5541702183	2.8708236326	-0.6986102670
H	1.0	1.5540018777	2.4326641982	-0.7976888323
H	1.0	3.1530573118	2.1711902900	-0.0999579115
C	6.0	3.2024950760	3.0662023452	-2.0769342070
H	1.0	3.2961104521	2.0977440554	-2.5825923328
H	1.0	2.5493005997	3.6894780131	-2.7042320460
C	6.0	4.5766913119	3.7400949126	-1.9486125557
H	1.0	5.0114980998	3.9171811637	-2.9395873123
H	1.0	5.2627831420	3.0657379715	-1.4164811750
C	6.0	4.4695156695	5.0664356516	-1.1831249261
H	1.0	5.4570732742	5.5256642953	-1.0565417861
H	1.0	3.8547994270	5.7784694664	-1.7505852029
C	6.0	4.2693492622	6.3273169051	1.9846618452
H	1.0	4.8933632794	5.5535171176	2.4544447656
C	6.0	4.1625935779	7.5817040135	2.7629228569
C	6.0	3.3611134282	8.6566349562	2.3461569911
H	1.0	2.8001510044	8.5741077871	1.4218577870
C	6.0	3.3072898972	9.7993919044	3.1409542667
H	1.0	2.6936131698	10.6457209727	2.8461496368
C	6.0	4.0526594477	9.8338783671	4.3235224853
H	1.0	4.0398972235	10.7018175963	4.9753715204
C	6.0	4.8204783067	8.7148215664	4.6580017026
H	1.0	5.4111128791	8.7060425118	5.5716597479

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C	6.0	0.8492483876	4.5667074210	1.7537108790
H	1.0	0.3092789350	5.2501181817	1.0828455699
C	6.0	0.2489853750	4.4258594487	3.0996294320
C	6.0	0.8499858329	3.6548804094	4.1074308951
H	1.0	1.7828332866	3.1426640413	3.8990727700
C	6.0	0.2291574141	3.5768812489	5.3514250220
H	1.0	0.6707127522	2.9905836907	6.1521071191
C	6.0	-0.9691231691	4.2700624853	5.5515188488
H	1.0	-1.4877055102	4.2402433325	6.5045580785
C	6.0	-1.4899737181	5.0164185602	4.4905837290
H	1.0	-2.4169287230	5.5728773228	4.6107626124

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Table 9. Final B3LYP-D coordinates for K_2[2-py-BPID*].

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
K	19.0	-0.8457100000	4.9898500000	9.1004900000
K	19.0	-4.1770600000	4.8832100000	9.3414500000
N	7.0	-2.6604600000	5.9718400000	7.1038100000
N	7.0	-2.5784800000	3.2861100000	7.7600000000
N	7.0	-2.4131400000	3.1020200000	10.3913700000
N	7.0	-2.3446200000	5.6727100000	11.4077600000
C	6.0	-2.6487900000	7.2655700000	6.7397400000
H	1.0	-2.6916300000	7.9793900000	7.5631300000
C	6.0	-2.5879000000	7.7307600000	5.4388300000
H	1.0	-2.5776300000	8.7931400000	5.2242600000
C	6.0	-2.5375800000	6.7575400000	4.4135000000
H	1.0	-2.4892400000	7.0615600000	3.3709600000
C	6.0	-2.5546400000	5.4263900000	4.7393300000
H	1.0	-2.5159500000	4.6646900000	3.9651600000
C	6.0	-2.6043800000	5.0112600000	6.1127100000
C	6.0	-2.5828000000	3.6394000000	6.4498200000
H	1.0	-2.5223300000	2.9073100000	5.6420300000
C	6.0	-2.5358600000	2.0805500000	8.2619300000
C	6.0	-2.5457800000	0.8375200000	7.4034100000
H	1.0	-1.5527200000	0.7077200000	6.9425900000
H	1.0	-3.2438600000	0.9840300000	6.5680400000
C	6.0	-2.9152300000	-0.4302800000	8.1773800000
H	1.0	-3.9854700000	-0.4108500000	8.4251300000
H	1.0	-2.7509400000	-1.3111000000	7.5470500000
C	6.0	-2.1073000000	-0.5292500000	9.4689100000
H	1.0	-1.0366000000	-0.5022100000	9.2245700000
H	1.0	-2.2948500000	-1.4839000000	9.9721000000
C	6.0	-2.4478100000	0.6292100000	10.4100000000
H	1.0	-3.4381100000	0.4543200000	10.8617200000
H	1.0	-1.7404100000	0.6529200000	11.2497800000
C	6.0	-2.4511100000	1.9772700000	9.7286300000

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C	6.0	-2.4079400000	3.2734500000	11.7391200000
H	1.0	-2.4521200000	2.4373400000	12.4397400000
C	6.0	-2.3812000000	4.5854100000	12.2606400000
C	6.0	-2.3956000000	4.8122400000	13.6789900000
H	1.0	-2.4267000000	3.9532500000	14.3438100000
C	6.0	-2.3804600000	6.0868900000	14.1816800000
H	1.0	-2.3968500000	6.2479300000	15.2566200000
C	6.0	-2.3355600000	7.1902000000	13.2965400000
H	1.0	-2.3210800000	8.2140200000	13.6520700000
C	6.0	-2.3257800000	6.9052900000	11.9434900000
H	1.0	-2.2984200000	7.7225000000	11.2219200000

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Table 10. Final coordinates for $KN(SiMe_3)_2$.

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	0.3120032936	-0.1612533094	0.5080868484
SI	14.0	1.3435342378	-0.4319917185	-0.8212582016
SI	14.0	0.4232087390	1.1532715014	1.5879931667
C	6.0	2.1834780063	1.4781710119	2.2690268040
C	6.0	-0.1657188018	2.8224462411	0.8703099744
C	6.0	-0.6617465230	0.8511875635	3.1413061949
C	6.0	2.9962624338	-1.2913695254	-0.3480523887
C	6.0	0.5285405221	-1.5986439060	-2.0944435130
C	6.0	1.8586280362	1.1328328353	-1.7906600796
H	1.0	2.1859141574	2.2918254233	3.0069022702
H	1.0	2.8782452788	1.7513702603	1.4648310667
H	1.0	2.5829324375	0.5782575036	2.7556151074
H	1.0	-1.2164297454	2.7637819302	0.5577989402
H	1.0	0.4294070498	3.0801657928	-0.0136602640
H	1.0	-0.0692992575	3.6361442087	1.6011420826
H	1.0	-0.6955899053	1.7605737160	3.7552210459
H	1.0	-0.2803740408	0.0531313927	3.7965410585
H	1.0	-1.6952736035	0.6009151524	2.8671706472
H	1.0	3.5049194621	-0.7317442234	0.4468382489
H	1.0	3.6702769161	-1.3441996286	-1.2136984608
H	1.0	2.8546588917	-2.3221559679	0.0094799694
H	1.0	0.2216074564	-2.5504873068	-1.6389840093
H	1.0	1.2207383707	-1.8329698457	-2.9136562579
H	1.0	-0.3670923202	-1.1382663946	-2.5304920355
H	1.0	2.4169958805	1.8279170700	-1.1511262022
H	1.0	0.9736783703	1.6637552118	-2.1633445974
H	1.0	2.4925288491	0.8804241490	-2.6508702746
K	19.0	0.0365320914	-2.3486534406	1.8865811940

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Table 11. Final coordinates for $HN(SiMe_3)_2$.

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
N	7.0	0.2871189535	-0.0295660852	0.4114076192
SI	14.0	1.3496934732	-0.4349029511	-0.9271483532
SI	14.0	0.3666056161	1.2655361893	1.5972012515
C	6.0	2.1100243056	1.3976709214	2.3250277740
C	6.0	-0.0731155810	2.9349087610	0.8218718990
C	6.0	-0.8792871545	0.8633908055	2.9594827235
C	6.0	2.8182925930	-1.4814002679	-0.3511576154
C	6.0	0.3401920885	-1.4055667953	-2.1962034233
C	6.0	2.0071733307	1.1623531368	-1.6952467273
H	1.0	-0.4113584766	-0.7356465657	0.6253116565
H	1.0	2.1599052083	2.2071561180	3.0638791926
H	1.0	2.8511618435	1.6133540540	1.5462573787
H	1.0	2.4011913801	0.4635129453	2.8192721718
H	1.0	-1.0841578215	2.9116848010	0.3981721571
H	1.0	0.6232397946	3.1976680216	0.0180426875
H	1.0	-0.0361668509	3.7318639252	1.5753390959
H	1.0	-0.9039304380	1.6672745057	3.7050076741
H	1.0	-0.6177984751	-0.0678479712	3.4759328701
H	1.0	-1.8911609568	0.7565002062	2.5498463878
H	1.0	3.3936170352	-0.9432867037	0.4116476795
H	1.0	3.4921413525	-1.7215198669	-1.1831007748
H	1.0	2.4733211644	-2.4239712201	0.0909473330
H	1.0	-0.0503212161	-2.3335116521	-1.7603535080
H	1.0	0.9549053042	-1.6754686056	-3.0632515355
H	1.0	-0.5104856052	-0.8108650275	-2.5481753411
H	1.0	2.5696088623	1.7636058369	-0.9717344443
H	1.0	1.1851051931	1.7767523405	-2.0793770051
H	1.0	2.6807327350	0.9304799684	-2.5289550634

Table 12. Final coordinates for KH.

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
K	19.0	-0.3696400000	0.1846748160	0.0000000000
H	1.0	-0.3696400000	2.5503851840	0.0000000000

Table 13. Final coordinates for H_2.

COORDINATES OF ALL ATOMS ARE (ANGS)

ATOM	CHARGE	X	Y	Z
H	1.0	0.0000000000	0.0000000000	0.0777755782
H	1.0	0.0000000000	0.0000000000	0.8222244218

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