Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2013

Supporting Information for:

Neutral Tricoordinated Beryllium (0) Compounds – Isostructural to BH_3 but Isoelectronic to NH_3

Susmita De and Pattiyil Parameswaran*[a]

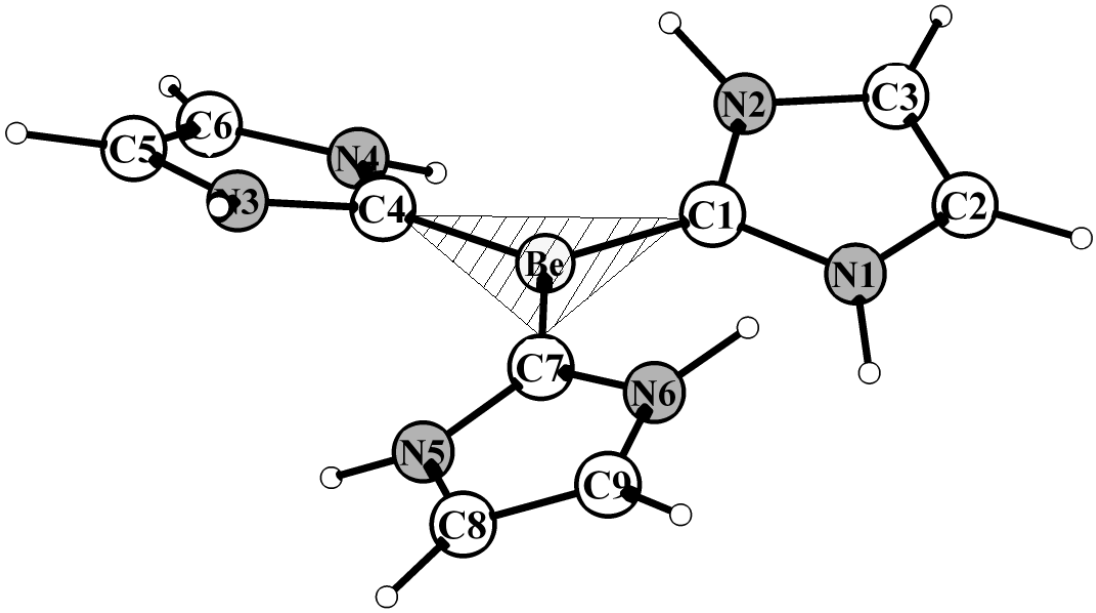
[a]Department of Chemistry, National Institute of Technology Calicut,
Kozhikode, Kerala, India -673 601.
e-mail: param@nitc.ac.in

Figure S1: Optimized equilibrium geometry of $Be(NHC)_3$, indicating the orientation of the NHC rings at the BP86/TZVPP level of theory.

Table S1: Total energies at BP86/TZVPP level (E_{BP86}, in au), zero point energy at BP86/TZVPP level ($E_{ZPE(BP86)}$, in au), total energies at M06/TZVPP//BP86/TZVPP level (E_{M06}, in au) and optimized Cartesian coordinates of all calculated molecules using G09 program package.

Figure S2: Optimized geometries of some BeL_3 molecules (L = CO (**1**), NHC (**2**) and PMe_3 (**3**)) and its protonated, BH_3 and $W(CO)_5$ adducts at the M06/TZVPP level of theory. Distances are given in Å and angles are given in deg. The point group symmetry and the pyramidalization angle θ around Be are given.

This journal is © The Royal Society of Chemistry 2013



Be-C1-C4-C7 = 0.0°
N1-C1-Be-C7 = N4-C4-Be-C7 = 18.0°, N2-C1-Be-C7 = N3-C4-Be-C7 = 18.2° and N5-C7-Be-C4 = N6-C7-Be-C4 = 17.2°

Figure S1: Optimized equilibrium geometry of $Be(NHC)_3$, indicating the orientation of the NHC rings at the BP86/TZVPP level of theory.

This journal is © The Royal Society of Chemistry 2013

Table S1: Total energies at BP86/TZVPP level (E_{BP86}, in au), zero point energy at the BP86/TZVPP level ($E_{ZPE(BP86)}$, in au), total energies at the M06/TZVPP//BP86/TZVPP level (E_{M06}, in au) and optimized Cartesian coordinates of all calculated molecules using G09 program package.

1

E_{BP86} = -354.869029269
$E_{ZPE(BP86)}$ = 0.025027269
E_{M06} = -354.670345075

Be	0.00000	0.00000	0.00000
C	0.00000	1.65770	0.00000
O	0.00000	2.81225	0.00000
C	1.43561	-0.82885	0.00000
O	2.43548	-1.40613	0.00000
C	-1.43561	-0.82885	0.00000
O	-2.43548	-1.40613	0.00000

1-H^+

E_{BP86} = -355.200710463
$E_{ZPE(BP86)}$ = 0.031528463
E_{M06} = -355.021153264

Be	0.00000	0.00000	0.39465
C	0.00000	1.72519	-0.01807
O	0.00000	2.84707	-0.12582
C	-1.49406	-0.86260	-0.01807
O	-2.46564	-1.42354	-0.12582
C	1.49406	-0.86260	-0.01807
O	2.46564	-1.42354	-0.12582
H	0.00000	0.00000	1.76627

1-BH_3

E_{BP86} = -381.499673807
$E_{ZPE(BP86)}$ = 0.053536807
E_{M06} = -381.290673702

Be	0.00250	-0.00050	-0.34899
C	1.64629	-0.29787	-0.37593
O	2.77042	-0.50165	-0.27989
C	-0.56191	1.57144	-0.38391
O	-0.94887	2.64687	-0.29351
C	-1.07794	-1.27411	-0.39439
O	-1.81804	-2.14573	-0.31122
H	-1.18344	0.21311	2.04733
H	0.39277	-1.12071	2.05687
H	0.75969	0.91144	2.05750
B	-0.00914	0.00108	1.84733

1-$W(CO)_5$

E_{BP86} = -989.157820125
$E_{ZPE(BP86)}$ = 0.065650125
E_{M06} = -988.4996017

Be	-2.16872	-0.02437	-0.03852
C	-2.38370	1.60921	-0.38774
O	-2.48963	2.72594	-0.62720
C	-2.34141	-0.54332	1.55492
O	-2.41662	-0.89735	2.64322
C	-2.36613	-1.13898	-1.28446
O	-2.45949	-1.90051	-2.13741
W	0.49662	0.00364	0.00195
C	0.62887	-1.12182	-1.71731
C	0.56108	1.70897	-1.15168
C	2.48757	0.04103	0.13994
C	0.36253	1.15229	1.70826
C	0.47742	-1.73118	1.11488
O	0.71741	-1.75368	-2.68464
O	3.64590	0.06364	0.22579
O	0.30485	1.80285	2.66629
O	0.49538	-2.71026	1.73512
O	0.62318	2.66574	-1.80259

2

E_{BP86} = -693.636277601

$E_{ZPE(BP86)}$ = 0.211841601

E_{M06} = -693.129313413

Be	0.00000	0.00000	-0.00397
N	0.43983	-0.98682	2.59463
C	0.00000	0.00000	1.70086
C	0.28792	-0.61561	3.92843
C	-0.28792	0.61561	3.92843
N	-0.43983	0.98682	2.59463
H	-1.01696	1.75627	2.28229
H	-0.59227	1.24657	4.75489
H	0.59227	-1.24657	4.75489
H	1.01696	-1.75627	2.28229
N	-0.54238	1.68894	-2.18913
C	-0.17671	1.46702	-0.85415
C	-0.59532	3.04129	-2.51817
C	-0.23008	3.72933	-1.40428
N	0.00000	2.78431	-0.40716
H	0.47914	2.98132	0.46135
H	-0.12306	4.79536	-1.24325
H	-0.88048	3.39885	-3.50032
H	-0.95073	0.95247	-2.74890
N	0.54238	-1.68894	-2.18913
C	0.17671	-1.46702	-0.85415
C	0.59532	-3.04129	-2.51817
C	0.23008	-3.72933	-1.40428
N	0.00000	-2.78431	-0.40716
H	-0.47914	-2.98132	0.46135
H	0.12306	-4.79536	-1.24325
H	0.88048	-3.39885	-3.50032

H	0.95073	-0.95247	-2.74890

2-H^+

E_{BP86} = -694.130355637
$E_{ZPE(BP86)}$ = 0.225709637
E_{M06} = -693.637146563

Be	0.00005	0.01581	-0.52382
N	2.25693	-1.45800	-1.01561
C	1.52825	-0.84701	-0.04693
C	3.37466	-2.11037	-0.52488
C	3.36434	-1.90389	0.82423
N	2.23706	-1.13436	1.08176
H	1.95955	-0.82264	2.00550
H	4.04713	-2.23170	1.59855
H	4.07036	-2.65313	-1.15270
H	1.94901	-1.39996	-1.98482
N	-2.25532	-1.46051	-1.01564
C	-1.52701	-0.84915	-0.04693
C	-3.37209	-2.11448	-0.52481
C	-3.36154	-1.90860	0.82439
N	-2.23503	-1.13791	1.08190
H	-1.95762	-0.82622	2.00567
H	-4.04366	-2.23756	1.59881
H	-4.06740	-2.65770	-1.15266
H	-1.94773	-1.40189	-1.98492
N	-1.06259	2.62464	-0.05389
C	-0.00122	1.77684	-0.13844
C	-0.68385	3.95573	0.05967
C	0.67836	3.95671	0.05950
N	1.05901	2.62617	-0.05413
H	2.01884	2.30563	-0.11715
H	1.38803	4.77153	0.12966
H	-1.39469	4.76950	0.13002
H	-2.02196	2.30259	-0.11638
H	0.00012	-0.13661	-1.94975

2-BH_3

E_{BP86} = -720.303605239
$E_{ZPE(BP86)}$ = 0.242932239
E_{M06} = -719.785534217

Be	-0.00010	0.01154	0.11909
N	-1.98559	-1.83088	0.63644
C	-1.50858	-0.86410	-0.19751
C	-3.23363	-2.29618	0.26583
C	-3.58178	-1.61110	-0.86237
N	-2.51958	-0.74747	-1.12123
H	-2.44473	-0.13960	-1.92771
H	-4.47065	-1.66254	-1.47924
H	-3.77178	-3.05455	0.82155
H	-1.48418	-1.97364	1.52331

N	1.98818	-1.82697	0.63856
C	1.50978	-0.86231	-0.19698
C	3.23649	-2.29174	0.26833
C	3.58360	-1.60829	-0.86119
N	2.52042	-0.74618	-1.12115
H	2.44440	-0.14035	-1.92905
H	4.47240	-1.65975	-1.47817
H	3.77568	-3.04846	0.82530
H	1.48672	-1.96940	1.52547
N	1.06871	2.60481	-0.09125
C	-0.00109	1.72931	-0.13812
C	0.67768	3.93011	0.08181
C	-0.68154	3.92909	0.08631
N	-1.07187	2.60331	-0.08436
H	-2.01749	2.26677	0.04374
H	-1.38757	4.74469	0.18139
H	1.38315	4.74672	0.17211
H	2.01593	2.26982	0.02869
H	0.00000	-1.36094	2.29867
H	1.02809	0.35682	2.66175
H	-1.03191	0.35492	2.65986
B	-0.00103	-0.10035	2.18403

2-W(CO)$_5$

E_{BP86} = -1327.98970611

$E_{ZPE(BP86)}$ = 0.25762911

E_{M06} = -1327.0267119

Be	-1.24032	0.13259	-0.15573
N	-2.11270	-0.61294	2.46691
C	-2.03703	0.29133	1.44500
C	-2.71908	-0.08792	3.59689
C	-3.07716	1.18976	3.28377
N	-2.66096	1.38729	1.97404
H	-2.77207	2.24744	1.44939
H	-3.57231	1.95392	3.86944
H	-2.83748	-0.65073	4.51443
H	-1.58039	-1.48923	2.43875
N	-1.66033	-1.89987	-2.16940
C	-2.04747	-1.18446	-1.07476
C	-2.59170	-2.85897	-2.53279
C	-3.63012	-2.74301	-1.65633
N	-3.27490	-1.71957	-0.78925
H	-3.83652	-1.38420	-0.01498
H	-4.56041	-3.29138	-1.57734
H	-2.43757	-3.53908	-3.36140
H	-0.69101	-1.87618	-2.51735
N	-1.51990	1.94653	-2.33399
C	-1.24949	1.68569	-1.01829
C	-1.30566	3.27806	-2.67377
C	-0.91035	3.89635	-1.52749

This journal is © The Royal Society of Chemistry 2013

N	-0.91136	2.92510	-0.53509
H	-0.46624	3.02239	0.38313
H	-0.62469	4.92409	-1.34184
H	-1.44073	3.66034	-3.67750
H	-1.79961	1.22010	-2.98195
W	1.52567	-0.29367	0.19226
C	1.35476	-1.48114	-1.42363
O	1.14627	-2.08597	-2.42470
C	2.10591	1.13807	-1.16008
O	2.39445	1.95131	-1.94681
C	3.39878	-0.68897	0.78781
O	4.47934	-0.93200	1.15905
C	1.01307	1.27042	1.36913
O	0.63279	2.26953	1.88516
C	0.65978	-1.67589	1.39718
O	0.08172	-2.44756	2.08290

3

E_{BP86} = -1398.30268168

$E_{ZPE(BP86)}$ = 0.33362268

E_{M06} = -1397.84355136

Be	0.00500	-0.00338	-0.14617
P	0.35187	2.00942	-0.03202
P	1.56919	-1.31694	-0.03019
P	-1.91581	-0.69233	-0.00140
C	2.57248	-1.50911	1.53812
H	3.36748	-2.26889	1.45568
H	3.03084	-0.54239	1.79053
H	1.88965	-1.77421	2.35641
C	1.07268	-3.07728	-0.29826
H	0.32032	-3.37140	0.44532
H	0.64531	-3.19087	-1.30170
H	1.94257	-3.74165	-0.19646
C	-2.45646	-2.07904	-1.11192
H	-2.30380	-1.77529	-2.15501
H	-1.83523	-2.96446	-0.92094
H	-3.51153	-2.34847	-0.94842
C	-2.59773	-1.34625	1.61389
H	-2.50056	-0.55713	2.37172
H	-3.64954	-1.67076	1.54699
H	-1.98033	-2.19425	1.94166
C	-3.19037	0.59403	-0.37515
H	-3.06865	1.45098	0.30056
H	-3.07023	0.93777	-1.40948
H	-4.20282	0.18651	-0.24138
C	-0.48097	3.15075	-1.24116
H	-0.20735	2.84798	-2.25957
H	-1.57055	3.05380	-1.14125
H	-0.20415	4.20373	-1.07350
C	-0.02169	2.95884	1.53497

H	0.54657	2.50620	2.35826
H	0.21539	4.03333	1.46320
H	-1.08937	2.84420	1.76989
C	2.12668	2.46089	-0.27551
H	2.74964	1.93578	0.46006
H	2.44308	2.16863	-1.28404
H	2.27170	3.54326	-0.15020
C	2.97802	-1.14808	-1.23124
H	2.58267	-1.22793	-2.25153
H	3.43458	-0.15489	-1.12149
H	3.75476	-1.91159	-1.06693

3-H$^+$

E_{BP86} = -1398.79623900

$E_{ZPE(BP86)}$ = 0.34302300

E_{M06} = -1398.34653095

Be	0.00000	0.00000	0.54241
P	0.00000	2.10547	0.03310
P	1.82339	-1.05274	0.03310
P	-1.82339	-1.05274	0.03310
H	0.00000	0.00000	1.92835
C	1.60069	2.92547	0.40347
H	1.89345	2.70579	1.43822
H	2.38428	2.55808	-0.27213
H	1.51374	4.01370	0.27954
C	-1.18326	3.03220	1.08179
H	-2.21148	2.71353	0.86948
H	-0.96708	2.81770	2.13598
H	-1.10159	4.11288	0.90156
C	-0.38219	2.67415	-1.67284
H	0.33408	2.24139	-2.38368
H	-1.39003	2.34645	-1.96061
H	-0.33605	3.76963	-1.74537
C	-3.33388	-0.07650	0.40347
H	-3.29001	0.28688	1.43822
H	-3.40750	0.78580	-0.27213
H	-4.23283	-0.69592	0.27954
C	-2.03433	-2.54083	1.08179
H	-1.24425	-3.27196	0.86948
H	-1.95666	-2.24637	2.13598
H	-3.01106	-3.01044	0.90156
C	-2.12478	-1.66806	-1.67284
H	-2.10814	-0.83138	-2.38368
H	-1.33708	-2.37702	-1.96061
H	-3.09657	-2.17584	-1.74537
C	1.73319	-2.84897	0.40347
H	1.39656	-2.99267	1.43822
H	1.02323	-3.34389	-0.27213
H	2.71910	-3.31778	0.27954
C	3.21759	-0.49137	1.08179

H	3.45573	0.55843	0.86948
H	2.92374	-0.57133	2.13598
H	4.11265	-1.10244	0.90156
C	2.50697	-1.00608	-1.67284
H	1.77407	-1.41002	-2.38368
H	2.72710	0.03057	-1.96061
H	3.43262	-1.59379	-1.74537

3-BH_3

E_{BP86} = -1424.98713678

$E_{ZPE(BP86)}$ = 0.36317878

E_{M06} = -1424.52179316

Be	0.00178	-0.00032	-0.25178
P	2.06988	-0.07980	0.13245
P	-0.96455	1.82904	0.13875
P	-1.10447	-1.75029	0.13093
C	2.90153	1.48985	-0.34490
H	2.58293	1.74631	-1.36306
H	2.61090	2.29674	0.34099
H	3.99417	1.37523	-0.31226
C	2.92149	-1.30991	-0.93460
H	2.67606	-2.32843	-0.60701
H	2.54999	-1.17425	-1.95907
H	4.01228	-1.17771	-0.89727
C	2.85013	-0.41150	1.78707
H	2.50887	0.34523	2.50701
H	2.52523	-1.39504	2.15423
H	3.95007	-0.39539	1.74237
C	-0.16062	-3.25796	-0.34100
H	0.21601	-3.12095	-1.36269
H	0.68689	-3.40328	0.34224
H	-0.80463	-4.14778	-0.29623
C	-2.59135	-1.87498	-0.94062
H	-3.34663	-1.14324	-0.62606
H	-2.28063	-1.63522	-1.96611
H	-3.02921	-2.88230	-0.89261
C	-1.78538	-2.25621	1.78452
H	-0.95998	-2.35622	2.50282
H	-2.46012	-1.47253	2.15612
H	-2.33775	-3.20720	1.73649
C	-2.74266	1.76256	-0.32960
H	-2.81022	1.36652	-1.35089
H	-3.29171	1.10097	0.35373
H	-3.19256	2.76474	-0.28722
C	-0.33814	3.18463	-0.93263
H	0.67704	3.46882	-0.62720
H	-0.29868	2.80451	-1.96210
H	-0.98931	4.06842	-0.87116
C	-1.05725	2.67291	1.79228
H	-1.53628	2.00227	2.51879

H	-0.04024	2.88515	2.15013
H	-1.62178	3.61665	1.74717
H	-1.07454	0.45373	-2.64223
H	0.92818	0.70755	-2.64714
H	0.14451	-1.15434	-2.64373
B	0.00094	0.00234	-2.24117

3-W(CO)$_5$

E_{BP86} = -2032.64504086

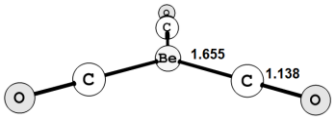
$E_{ZPE(BP86)}$ = 0.37637886

E_{M06} = -2031.7366415

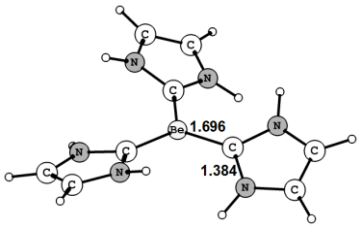
Be	-0.04387	1.10023	0.00000
P	-1.10976	1.77282	1.77083
P	1.88017	2.18329	0.00000
P	-1.10976	1.77282	-1.77083
C	-0.46273	1.07305	3.34267
H	-0.56687	-0.01739	3.32798
H	0.60246	1.31068	3.45564
H	-1.01711	1.48482	4.19817
C	-2.89346	1.32959	1.83517
H	-3.45139	1.92043	1.09784
H	-3.03060	0.26457	1.62192
H	-3.29402	1.55109	2.83469
C	-1.21303	3.57316	2.21953
H	-0.21278	3.96761	2.44074
H	-1.63287	4.14731	1.38285
H	-1.84707	3.72305	3.10591
C	-2.89346	1.32959	-1.83517
H	-3.03060	0.26457	-1.62192
H	-3.45139	1.92043	-1.09784
H	-3.29402	1.55109	-2.83469
C	-0.46273	1.07305	-3.34267
H	0.60246	1.31068	-3.45564
H	-0.56687	-0.01739	-3.32798
H	-1.01711	1.48482	-4.19817
C	-1.21303	3.57316	-2.21953
H	-1.63287	4.14731	-1.38285
H	-0.21278	3.96761	-2.44074
H	-1.84707	3.72305	-3.10591
C	2.98308	1.85189	-1.43229
H	3.18660	0.77914	-1.51885
H	2.50125	2.18216	-2.36205
H	3.92776	2.40135	-1.31255
C	2.98308	1.85189	1.43229
H	2.50125	2.18216	2.36205
H	3.18660	0.77914	1.51885
H	3.92776	2.40135	1.31255
C	1.89028	4.03843	0.00000
H	1.37380	4.42396	-0.88816
H	1.37380	4.42396	0.88816

This journal is © The Royal Society of Chemistry 2013

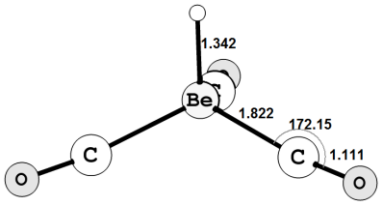
H	2.92313	4.41745	0.00000
W	0.09711	-1.61533	0.00000
C	1.48165	-1.36685	1.48280
C	0.42273	-3.58573	0.00000
C	-1.36446	-1.82150	1.41306
C	-1.36446	-1.82150	-1.41306
C	1.48165	-1.36685	-1.48280
O	2.25874	-1.26658	2.35310
O	2.25874	-1.26658	-2.35310
O	-2.20854	-1.98370	-2.20894
O	-2.20854	-1.98370	2.20894
O	0.62801	-4.73495	0.00000



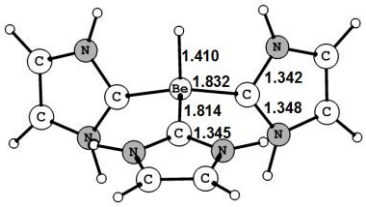
1(D_{3h})
θ = 0.0°



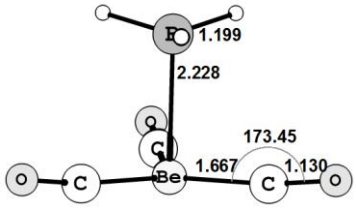
2(C_2)
θ = 0.0°



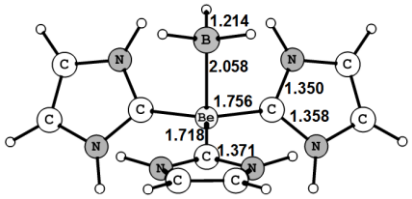
1-H$^+$ (C_{3v})
θ = 24.3°



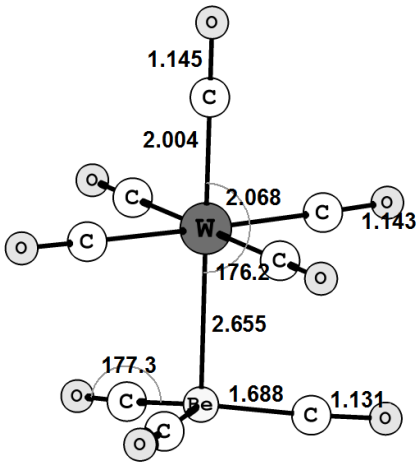
2-H$^+$ (C_1)
θ = 20.8°



1-BH_3 (C_1)
θ = 0.6°



2-BH_3 (C_1)
θ = 3.8°



1-WCO_5 (C_1)
θ = 3.1°

Figure S2: Optimized geometries of some BeL_3 molecules (L = CO (**1**), NHC (**2**) and PMe_3 (**3**)) and its protonated, BH_3 and $W(CO)_5$ adducts at the M06/TZVPP level of theory. Distances are given in Å and angles are given in deg. The point group symmetry and the pyramidalization angle θ around Be are given.