Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

Homopolar dihydrogen bonding in Ligand Stabilized Diberyllium Hydride Complexes, $Be_2(CH_3)_2H_2L_2$ (L = H^-, CO, N-heterocyclic carbene and CN^-)

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Captions and Legends

Figure S1: Molecular graph of **1-5** at the M06/def2-TZVPP//BP86/TZ2P level of theory. Small green and red circles correspond to bond critical points (bcp) and ring critical points (rcp), respectively.

Figure S2: Optimized geometries and important geometrical parameters of diborane (**1**), $Be_2(CH_3)_2H_4^{2-}$(**2**), $Be_2(CH_3)_2H_2(CO)_2$ (**3**) and $Be_2(CH_3)_2H_2(NHC)_2$ (**4**) using a) the 'integration 5.0' parameter in the Voronoi integration method and b) the 'very fine' Becke grid for integration at the BP86/TZ2P level of theory.

Figure S3: Plots of selected molecular orbitals of a) B_2H_6 (**1**), b) $Be_2(CH_3)_2H_4^{2-}$ (**2**), c) $Be_2(CH_3)_2H_2CO_2$ (**3**), d) $Be_2(CH_3)_2H_2(NHC)_2$ (**4**) and $Be_2(CH_3)_2H_2(CN)_2^{2-}$ (**5**) at the BP86/def2-TZVPP//BP86/TZ2P level of theory. The eigen values are given in parentheses.

Table S1: The atomic and group charges (q) and Wiberg bond index between atoms (P) of **1-10** given by NBO analysis at the M06/def2-TZVPP//BP86/TZ2P level of theory using 'fine' grid for integration using the Gaussian 09 program package.

Table S2: The atomic and group charges (q) and Wiberg bond index between atoms (P) of **1-4** given by NBO analysis at the M06/def2-TZVPP//BP86/TZ2P level of theory using the default 'fine' and 'ultrafine' (in parenthesis) grid for integration using the Gaussian 09 program package.

Table S3: Topological parameters of electron density of **1-4** at the M06/def2-TZVPP//BP86/TZ2P level of theory using the default 'fine' grid and 'ultrafine' (in parenthesis) grid for integration. Electron density, $\rho_{(r)}$ in eÅ^{-3}, Laplacian of electron density $\nabla^2\rho(r)$ in eÅ^{-5}, the bond ellipticity ε and potential energy density $V(r)$, kinetic energy density $G(r)$ and total energy density $H(r)$ in HartreeÅ^{-3}.

Table S4: The atomic charge q(M), spin density S(M) of M (M = B for **1** and **6** and Be for **2-5**, **7-10**), group charge of ligands, q(L) (L = H^-, CO, NHC and CN^-), charge on bridging hydrogen atoms q(μ-H)$_2$, charge of methyl group q(CH_3) and Wiberg bond index between M atoms P(M–M) given by NBO analysis at the M06/def2-TZVPP//BP86/TZ2P and BP86/def2-TZVPP//BP86/TZ2P (in parenthesis) level of theories using the default 'fine' grid for integration.

Table S5: E_{TBE}(BP86) and ZPE(BP86) are total bonding energy and zero-point energy at the BP86/TZ2P level of theory using the ADF 2013.01 program package, E_{el}(M06) and E_{el}(BP86) represents the electronic energy at the M06/def2-TZVPP//BP86/TZ2P and the BP86/def2-TZVPP//BP86/TZ2P level of theory, respectively. The optimized Cartesian coordinates are also given. The energies are given in atomic unit (a. u.) and the Cartesian coordinates are given in Å.

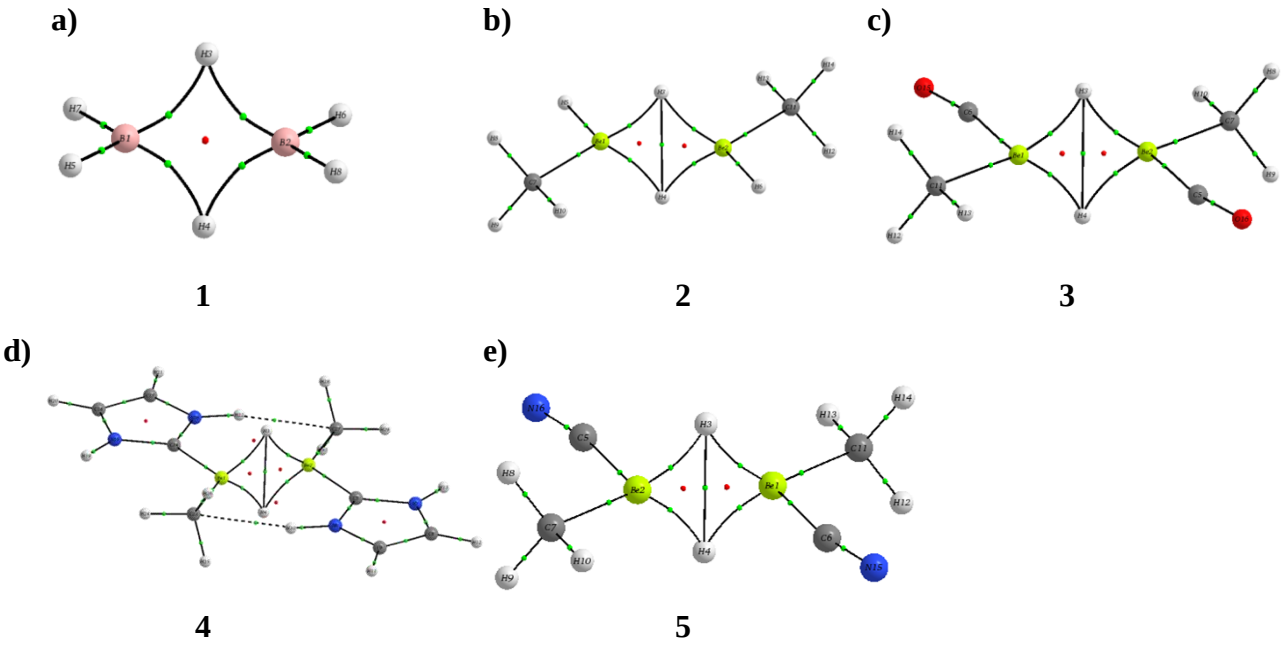
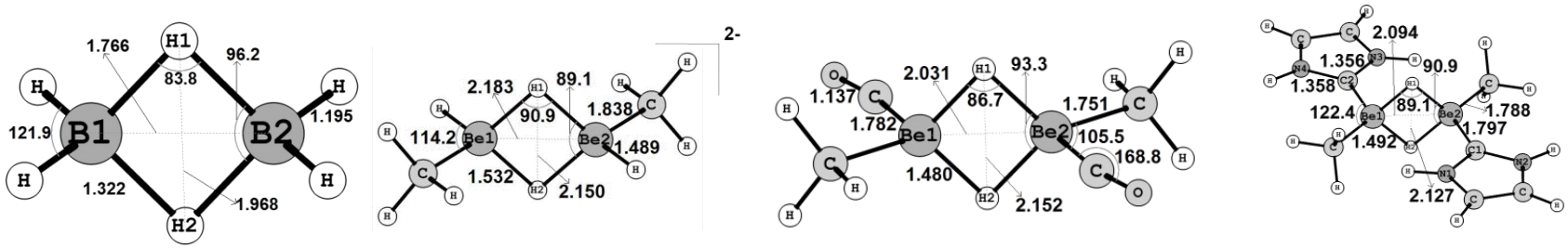


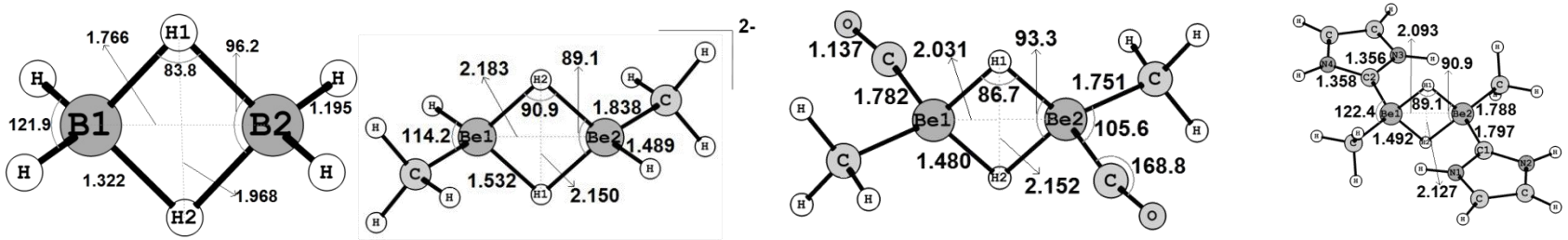
Figure S1: Molecular graph of **1-5** at the M06/def2-TZVPP//BP86/TZ2P level of theory. Small green and red circles correspond to bond critical points (bcp) and ring critical points (rcp), respectively.

a)



1 **2** **3** **4**

b)



1 **2** **3** **4**

Figure S2: Optimized geometries and important geometrical parameters of diborane (**1**), $Be_2(CH_3)_2H_4^{2-}$(**2**), $Be_2(CH_3)_2H_2(CO)_2$ (**3**) and $Be_2(CH_3)_2H_2(NHC)_2$ (**4**) using a) the 'integration 5.0' parameter in the Voronoi integration method and b) the ‘very fine’ Becke grid for integration at the BP86/TZ2P level of theory.

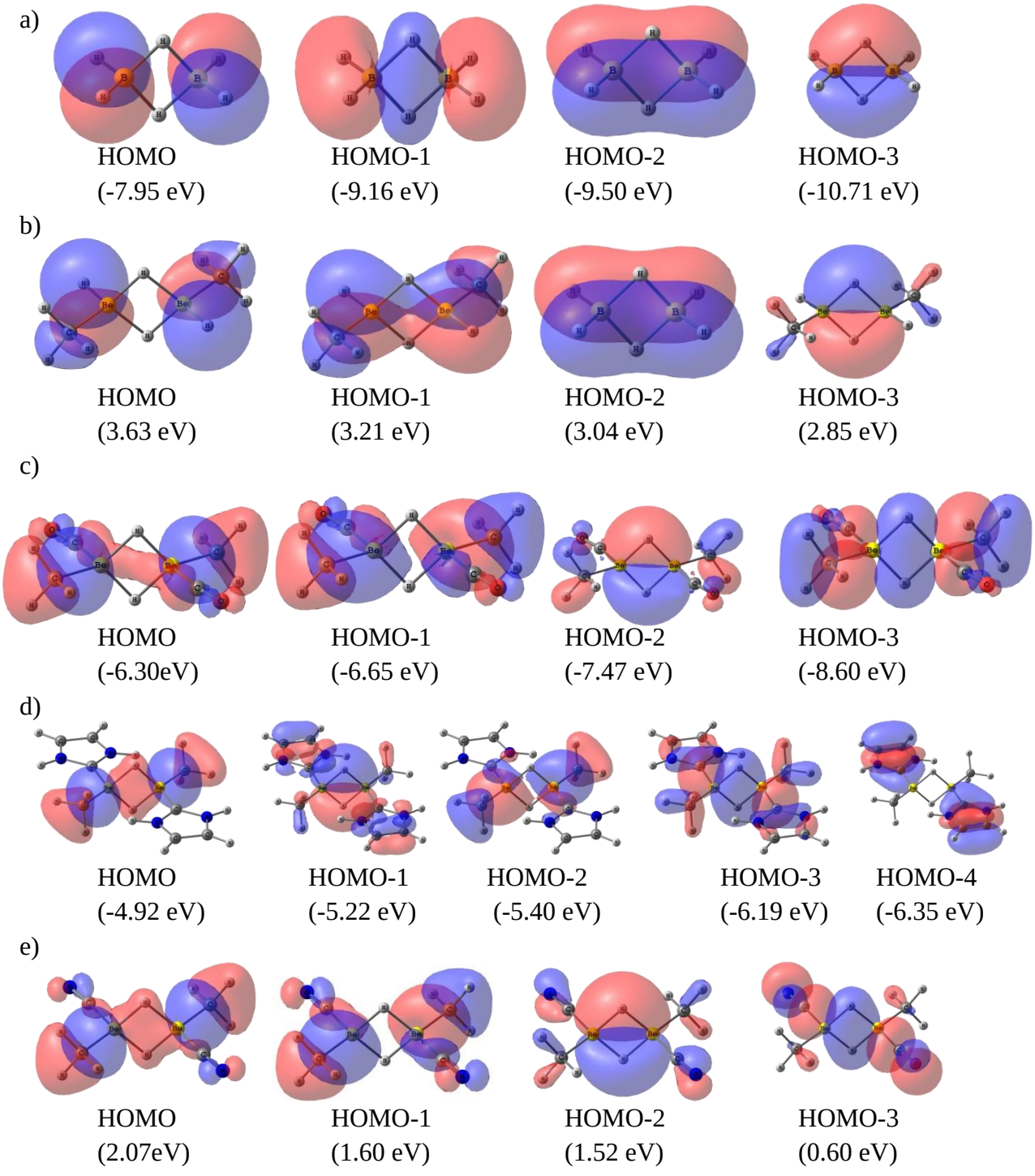


Figure S3: Plots of selected molecular orbitals of a) B_2H_6 (**1**), b) $Be_2(CH_3)_2H_4^{2-}$ (**2**), c) $Be_2(CH_3)_2H_2CO_2$ (**3**), d) $Be_2(CH_3)_2H_2(NHC)_2$ (**4**) and $Be_2(CH_3)_2H_2(CN)_2^{2-}$ (**5**) at the BP86/def2-TZVPP//BP86/TZ2P level of theory. The eigen values are given in parentheses.

Table S1: The atomic and group charges (q) and Wiberg bond index between atoms (P) of **1-10** given by NBO analysis at the M06/def2-TZVPP//BP86/TZ2P level of theory using 'fine' grid for integration using the Gaussian 09 program package.

	NBO charge					Wiberg bond index			
	q(M)[a]	q(CH_3)	q(L)	q(μ-H)	q(X)[b]	P(M–M)[a]	Pμ(M–H)	P(M–C)	P(M─X)[b]
1	-0.12			0.12		0.66	0.48		
2	0.37	-0.67	-0.42	-0.29	-0.42	0.27	0.45	0.56	0.80
3	0.35	-0.46	0.29	-0.19	0.70	0.32	0.45	0.69	0.65
4	0.47	-0.58	0.33	-0.23	0.20	0.29	0.44	0.64	0.58
5	0.44	-0.61	-0.57	-0.25	0.05	0.27	0.45	0.60	0.68
6	0.33								
7	0.21	-0.73	-0.49		-0.49			0.50	0.73
8	0.90	-0.59	-0.31		0.13			0.66	0.80
9	0.96	-0.62	-0.34		-0.29			0.63	0.76
10	0.37	-0.68	-0.69		-0.17			0.54	0.64

[a]M = B for **1** and **6** and M = Be for others; [b]X = atom of the ligand, which is directly attached to M.

Table S2: The atomic and group charges (q) and Wiberg bond index between atoms (P) of **1-4** given by NBO analysis at the M06/def2-TZVPP//BP86/TZ2P level of theory using the default 'fine' and 'ultrafine' (in parenthesis) grid for integration using the Gaussian 09 program package.

	NBO Charge					Wiberg bond index			
	q(M)[a]	q(CH_3)	q(L)	q(μ-H)	q(X)[b]	P(M–M)[a]	Pμ(M–H)	P(M–C)	P(M─X)[b]
1	-0.12			0.12		0.66	0.48		
	(-0.12)			(0.12)		(0.66)	(0.48)		
2	0.37	-0.67	-0.42	-0.29	-0.42	0.27	0.45	0.56	0.80
	(0.37)	(-0.67)	(-0.42)	(-0.29)	(-0.42)	(0.27)	(0.45)	(0.56)	(0.80)
3	0.35	-0.46	0.29	-0.19	0.70	0.32	0.45	0.69	0.65
	(0.35)	(-0.46)	(0.29)	(-0.19)	(0.70)	(0.32)	(0.45)	(0.69)	(0.65)
4	0.47	-0.58	0.33	-0.23	0.20	0.29	0.44	0.64	0.58
	(0.47)	(-0.58)	(0.33)	(-0.23)	(0.20)	(0.29)	(0.44)	(0.64)	(0.58)

[a]M = B for **1** and **6** and M = Be for others; [b]X = atom of the ligand, which is directly attached to M.

Table S3: Topological parameters of electron density of **1-4** at the M06/def2-TZVPP//BP86/TZ2P level of theory using the default 'fine' grid and 'ultrafine' (in parenthesis) grid for integration. Electron density, $\rho_{(r)}$ in eÅ^{-3}, Laplacian of electron density $\nabla^2\rho(r)$ in eÅ^{-5}, the bond ellipticity ε and potential energy density $V(r)$, kinetic energy density $G(r)$ and total energy density $H(r)$ in HartreeÅ^{-3}.

Compound	Bond/Ring	$\rho_{(r)}$	$\nabla^2_{(r)}$	ε	$V_{(r)}$	$G_{(r)}$	$H_{(r)}$
	B─H	1.226	-8.750	0.09	-2.104	0.746	-1.358
		(1.227)	(8.719)	(0.09)	(-2.105)	(0.746)	(-1.359)
1	μ(B─H)	0.854	0.460	0.73	-1.590	0.811	-0.779
		(0.854)	(0.460)	(0.73)	(-1.590)	(0.811)	(-0.779)
	(B1─H3─H4─B2)[a]	0.788	-0.952	-	-0.769	0.351	-0.472
		(0.788)	(-0.957)		(-0.769)	0.351	(-0.472)
	Be─$C_{(CH3)}$	0.434	6.148	0.05	-0.580	0.505	-0.075
		(0.434)	(6.148)	(0.05)	(-0.580)	(0.505)	(-0.075)
	Be─$L_{(H-)}$	0.385	5.068	0.07	-0.502	0.429	-0.074
		(0.385)	(5.066)	(0.07)	(-0.501)	(0.429)	(-0.073)
2	μ(Be─H)	0.334	5.090	0.49	-0.444	0.400	-0.044
		(0.334)	(5.090)	(0.49)	(0.444)	(0.400)	(-0.044)
	H1─H2	0.327	0.236	2.52	-0.203	0.110	-0.093
		(0.237)	(0.238)	(2.52)	(0.203)	(0.110)	(-0.093)
	(Be─H1─H2)[a]	0.306	1.930	-	-0.356	0.246	-0.110
		(0.306)	(1.930)		(-0.356)	(0.246)	(-0.110)
	Be─$C_{(CH3)}$	0.568	6.420	0.03	-0.789	0.619	-0.169
		(0.568)	(6.422)	(0.03)	(-0.789)	(0.619)	(-0.169)
	Be─$L_{(CO)}$	0.366	9.179	0.36	-0.588	0.615	0.027
		(0.366)	(9.179)	(0.36)	(-0.588)	(0.615)	(0.027)
3	μ(Be─H)	0.406	5.931	0.51	-0.567	0.491	-0.075
		(0.406)	(5.931)	(0.51)	(-0.567)	(0.491)	(-0.075)
	H1─H2	0.376	0.210	2.96	-0.265	0.140	-0.125
		(0.376)	(0.210)	(2.95)	(-0.265)	(0.140)	(-0.125)
	(Be─H1─H2)[a]	0.364	1.764	-	-0.425	0.275	-0.150
		(0.364)	(6.422)		(-0.425)	(0.275)	(-0.150)
	Be─$C_{(CH3)}$	0.514	6.434	0.04	-0.705	0.578	-0.128
		(0.512)	(6.422)	(0.04)	(-0.704)	(0.578)	(-0.126)
	Be─$L_{(NHC)}$	0.437	8.090	0.06	-0.641	0.603	-0.038
		(0.435)	(8.076)	(0.06)	(-0.639)	(0.603)	(-0.036)
4	μ(Be─H)	0.385	5.798	0.43	-0.538	0.472	-0.066
		(0.385)	(5.801)	(0.43)	(-0.538)	(0.472)	(-0.066)
	H1─H2	0.368	0.231	2.74	-0.250	0.134	-0.118
		(0.368)	(0.231)	(2.73)	(-0.250)	(0.134)	(-0.116)
	(Be─H1─H2)[a]	0.349	2.034	-	-0.421	0.282	-0.139
		(0.349)	(2.034)		(-0.422)	(0.282)	(-0.140)

Table S4: The atomic charge q(M), spin density S(M) of M (M = B for **1** and **6** and Be for **2-5**, **7-10**), group charge of ligands, q(L) (L = H^-, CO, NHC and CN^-), charge on bridging hydrogen atoms q(μ-$H)_2$, charge of methyl group q(CH_3) and Wiberg bond index between M atoms P(M–M) given by NBO analysis at the M06/def2-TZVPP//BP86/TZ2P and BP86/def2-TZVPP//BP86/TZ2P (in parenthesis) level of theories using the default 'fine' grid for integration.

Compound	q(M)	S(M)	q(L)	q(μ-$H)_2$	q(CH_3)	P(M–M)
1	-0.12	-	-	0.24	-	0.66
	(-0.19)			(0.28)		0.70
2	0.37	-	-0.42	-0.57	-0.67	0.27
	(0.29)		(-0.39)	(-0.50)	(-0.65)	(0.29)
3	0.35	-	0.29	-0.37	-0.46	0.32
	(0.29)		(0.27)	(-0.30)	(-0.41)	(0.34)
4	0.47	-	0.33	-0.48	-0.58	0.29
	(0.40)		(0.35)	(-0.38)	(-0.55)	(0.31)
5	0.44	-	-0.57	-0.51	-0.61	0.27
	(0.36)		(-0.43)	(-0.56)	(-0.59)	(0.30)
6	0.33	0.99	-	-	-	-
	(0.30)	(1.04)				
7	0.21	0.92	-0.49	-	-0.73	-
	(0.20)	(0.93)	(-0.48)		(-0.72)	
8	0.90	0.28	-0.31	-	-0.59	-
	(0.85)	(0.32)	(-0.28)		(-0.57)	
9	0.96	0.27	-0.34	-	-0.62	-
	(0.89)	(0.33)	(0.28)		(-0.60)	
10	0.37	0.86	-0.69	-	-0.68	
	(0.36)	(0.87)	(0.68)		(0.68)	

Table S5: E_{TBE}(BP86) and ZPE(BP86) are total bonding energy and zero-point energy at the BP86/TZ2P level of theory using the ADF 2013.01 program package, E_{el}(M06) and E_{el}(BP86) represents the electronic energy at the M06/def2-TZVPP//BP86/TZ2P and the BP86/def2-TZVPP//BP86/TZ2P level of theory, respectively. The optimized Cartesian coordinates are also given. The energies are given in atomic unit (a. u.) and the Cartesian coordinates are given in Å.

H^-

E_{TBE}(BP86) = 0.0 a. u.
ZPE(BP86) = 0.0 a. u.
E_{el}(M06) = -0.5022894 a. u.
E_{el}(BP86) = -0.5102459 a. u.

CO

E_{TBE}(BP86) = -0.544954 a. u.
ZPE(BP86) = 0.004830 a. u.
E_{el}(M06) = -113.3010388 a. u.
E_{el}(BP86) = -113.3591813 a. u.

6	0.000000000	0.000000000	2.305073000
8	0.000000000	0.000000000	3.441253000

NHC

E_{TBE}(BP86) = -2.056013 a. u.
ZPE(BP86) = 0.069329 a. u.
E_{el}(M06) = -226.1053246 a. u.
E_{el}(BP86) = -226.2704192 a. u.

6	2.552444000	0.388593000	0.000000000
7	3.831883000	0.876672000	0.000000000
7	2.807755000	-0.956885000	0.000000000
6	4.160503000	-1.288331000	0.000000000
6	4.823623000	-0.101654000	0.000000000
1	4.018410000	1.870223000	0.000000000
1	5.883888000	0.114248000	0.000000000
1	4.532820000	-2.304340000	0.000000000
1	2.059118000	-1.636295000	0.000000000

CN^-

E_{TBE}(BP86) = -0.607905a. u.
ZPE(BP86) = 0.004625 a. u.
E_{el}(M06) = -92.8234401 a. u.
E_{el}(BP86) = -92.889702 a. u.

6	0.000000000	0.000000000	2.166767000
7	0.000000000	0.000000000	3.349446000

$Be_2(CH_3)_2(\mu\text{-}H)_2$

E_{TBE}(BP86) = -1.926690 a. u.
ZPE(BP86) = 0.087999 a. u.
E_{el}(M06) = -110.4853677 a. u.
E_{el}(BP86) = -110.5508228 a. u.

4	1.003942000	-0.031447000	0.000000000
4	-1.003942000	0.031447000	0.000000000
1	0.000000000	0.000000000	-1.086026000
1	0.000000000	0.000000000	1.086026000
6	2.690384000	-0.057629000	0.000000000
1	3.119997000	-0.548479000	0.887690000
1	3.119997000	-0.548479000	-0.887690000
1	3.093823000	0.971667000	0.000000000
6	-2.690384000	0.057629000	0.000000000
1	-3.119997000	0.548479000	-0.887690000
1	-3.093823000	-0.971667000	0.000000000
1	-3.119997000	0.548479000	0.887690000

B_2H_6 (1)

E_{TBE}(BP86) = -1.231248 a. u.
ZPE(BP86) = 0.060918 a. u.
E_{el}(M06) = -53.25667 a. u.
E_{el}(BP86) = -53.2897788 a. u.

5	0.882837000	0.000000000	0.000000000
5	-0.882837000	0.000000000	0.000000000
1	0.000000000	0.984174000	0.000000000
1	0.000000000	-0.984174000	0.000000000
1	1.463214000	0.000000000	-1.044508000
1	-1.463214000	0.000000000	1.044508000
1	1.463214000	0.000000000	1.044508000
1	-1.463214000	0.000000000	-1.044508000

$Be_2(CH_3)_2H_4^{2-}$ (2)

E_{TBE}(BP86) = -2.110405 a. u.
ZPE(BP86) = 0.095351 a. u.
E_{el}(M06) = -111.5710234 a. u.
E_{el}(BP86) = -111.6587802 a. u.

4	-0.852326000	0.681572000	0.000000000
4	0.852326000	-0.681572000	0.000000000
1	0.000000000	0.000000000	-1.074986000
1	0.000000000	0.000000000	1.074986000
1	-0.672750000	2.159698000	0.000000000

1	0.672750000	-2.159698000	0.000000000
6	-2.607588000	0.136453000	0.000000000
1	-3.159233000	0.520054000	0.886969000
1	-3.159233000	0.520054000	-0.886969000
1	-2.725231000	-0.967146000	0.000000000
6	2.607588000	-0.136453000	0.000000000
1	3.159233000	-0.520054000	-0.886969000
1	2.725231000	0.967146000	0.000000000
1	3.159233000	-0.520054000	0.886969000

$Be_2(CH_3)_2H_2(CO)_2$ (3)

E_{TBE}(BP86) = -3.057743 a. u.

ZPE(BP86) = 0.104662 a. u.

E_{el}(M06) = -337.1162766 a. u.

E_{el}(BP86) = -337.3109512 a. u.

4	-0.779296000	0.651264000	0.000000000
4	0.779296000	-0.651264000	0.000000000
1	0.000000000	0.000000000	-1.076178000
1	0.000000000	0.000000000	1.076178000
6	2.350597000	0.190040000	0.000000000
6	-2.350597000	-0.190040000	0.000000000
6	1.161883000	-2.359895000	0.000000000
1	1.728305000	-2.684733000	-0.886272000
1	1.728305000	-2.684733000	0.886272000
1	0.210006000	-2.916773000	0.000000000
6	-1.161883000	2.359895000	0.000000000
1	-1.728305000	2.684733000	0.886272000
1	-0.210006000	2.916773000	0.000000000
1	-1.728305000	2.684733000	-0.886272000
8	-3.438523000	-0.521085000	0.000000000
8	3.438523000	0.521085000	0.000000000

$Be_2(CH_3)_2H_2(NHC)_2$ (4)

E_{TBE}(BP86) = -6.154228 a. u.

ZPE(BP86) = 0.233196 a. u.

E_{el}(M06) = -562.8108887 a. u.

E_{el}(BP86) = -563.2069525 a. u.

6	-2.333669000	-0.075463000	0.000000000
7	-2.553362000	1.262318000	0.000000000
7	-3.591161000	-0.588677000	0.000000000
6	-4.569448000	0.395943000	0.000000000
6	-3.897674000	1.582177000	0.000000000
1	-1.762889000	1.912367000	0.000000000
1	-4.264716000	2.599402000	0.000000000
1	-5.628984000	0.180460000	0.000000000
1	-3.763272000	-1.586106000	0.000000000
6	2.333669000	0.075463000	0.000000000
7	3.591161000	0.588677000	0.000000000
7	2.553362000	-1.262318000	0.000000000
6	3.897674000	-1.582177000	0.000000000
6	4.569448000	-0.395943000	0.000000000
1	3.763272000	1.586106000	0.000000000
1	5.628984000	-0.180460000	0.000000000
1	4.264716000	-2.599402000	0.000000000
1	1.762889000	-1.912367000	0.000000000
4	0.685813000	0.791075000	0.000000000
4	-0.685813000	-0.791075000	0.000000000
6	0.407545000	2.556886000	0.000000000
1	-0.137835000	2.930715000	-0.888574000
1	-0.137835000	2.930715000	0.888574000
1	1.344811000	3.145040000	0.000000000
6	-0.407545000	-2.556886000	0.000000000
1	0.137835000	-2.930715000	0.888574000
1	-1.344811000	-3.145040000	0.000000000
1	0.137835000	-2.930715000	-0.888574000
1	0.000000000	0.000000000	-1.063583000
1	0.000000000	0.000000000	1.063583000

$Be_2(CH_3)_2H_2(CN)_2^{2-}$ (5)

E_{TBE}(BP86) = -3.206161 a. u.

ZPE(BP86) = 0.102340 a. u.

E_{el}(M06) = -296.178735 a. u.

E_{el}(BP86) = -296.3793072 a. u.

4	0.006923000	1.066319000	0.000000000
4	-0.006923000	-1.066319000	0.000000000
1	0.000000000	0.000000000	1.072465000
1	0.000000000	0.000000000	-1.072465000
6	-1.590450000	-1.952034000	0.000000000
6	1.590450000	1.952034000	0.000000000
6	1.426692000	-2.156655000	0.000000000
1	1.448919000	-2.825676000	0.885266000
1	1.448919000	-2.825676000	-0.885266000
1	2.378392000	-1.592170000	0.000000000
6	-1.426692000	2.156655000	0.000000000
1	-1.448919000	2.825676000	-0.885266000
1	-2.378392000	1.592170000	0.000000000
1	-1.448919000	2.825676000	0.885266000
7	2.565483000	2.607309000	0.000000000
7	-2.565483000	-2.607309000	0.000000000

BH_2 (6)

E_{TBE}(BP86) = -0.369198 a. u.

ZPE(BP86) = 0.013989 a. u.

E_{el}(M06) = -25.9172266 a. u.

E_{el}(BP86) = -25.9319118 a. u.

5	0.000000000	0.000000000	0.932550000
1	1.082555000	0.000000000	1.438264000
1	-1.082555000	0.000000000	1.438264000

$Be(CH_3)H^-$ (7)

E_{TBE}(BP86) = -0.920884 a. u.

ZPE(BP86) = 0.038125 a. u.

E_{el}(M06) = -55.1830476 a. u.

E_{el}(BP86) = -55.2293501 a. u.

4	-0.956661000	0.753817000	0.000000000
1	-0.594338000	2.120545000	0.000000000
6	-2.599132000	0.124876000	0.000000000
1	-3.153016000	0.511425000	0.883846000
1	-3.153016000	0.511425000	-0.883846000
1	-2.720198000	-0.971404000	0.000000000

$Be(CH_3)CO$ (8)

E_{TBE}(BP86) = -1.343916 a. u.

ZPE(BP86) = 0.043479 a. u.

E_{el}(M06) = -167.9088916 a. u.

E_{el}(BP86) = -168.0057665 a. u.

4	-1.845445000	1.060760000	0.000000000
6	-2.685622000	-0.355550000	0.000000000
6	-1.036122000	2.532038000	0.000000000
1	-1.306202000	3.139873000	0.879780000
1	0.060042000	2.437588000	0.000000000
1	-1.306202000	3.139873000	-0.879780000
8	-3.277364000	-1.368309000	0.000000000

$Be(CH_3)NHC$ (9)

E_{TBE}(BP86) = -2.878044 a. u.

ZPE(BP86) = 0.104132 a. u.

E_{el}(M06) = -280.7389139 a. u.

E_{el}(BP86) = -280.9389677 a. u.

6	-2.606040000	-0.335371000	0.007803000
7	-2.521496000	1.067680000	0.117236000
7	-4.000597000	-0.519814000	-0.076074000
6	-4.689357000	0.685221000	-0.077652000
6	-3.768161000	1.674251000	0.037919000
1	-1.647250000	1.570028000	0.103670000
1	-3.899310000	2.746309000	0.091877000
1	-5.767521000	0.740451000	-0.141369000
1	-4.433468000	-1.421014000	-0.206389000
4	-1.398324000	-1.459088000	-0.046509000
6	-0.169046000	-2.627092000	0.060540000
1	0.729437000	-2.206869000	0.547137000
1	-0.468270000	-3.485903000	0.686762000
1	0.164795000	-3.037496000	-0.905986000

$Be(CH_3)CN^-$ (10)

E_{TBE}(BP86) = -1.452376 a. u.

ZPE(BP86) = 0.041441 a. u.

E_{el}(M06) = -147.4688203 a. u.

E_{el}(BP86) = -147.5749344 a. u.

4	0.000000000	0.966713000	0.000000000
6	-0.939405000	-0.488222000	0.000000000
6	1.743864000	1.030407000	0.000000000
1	2.150168000	0.493561000	0.882309000
1	2.150168000	0.493561000	-0.882309000
1	2.195717000	2.034968000	0.000000000
7	-1.617544000	-1.448865000	0.000000000