Supporting Information

Be≡Be triple bond in $Be_2X_4Y_2$ clusters (X = Li, Na and Y = Li, Na, K) and a perfect classical Be≡Be triple bond presented in $Be_2Na_4K_2$

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METHOD

The initial structures were generated using CALYPSO algorithm,[34] and then the initial geometries were re-optimized and filtrated using B3LYP/6-31G(D) approaches. In this process, only structures without imaginary frequencies were further studied. The D_{4h}-$Be_2Na_4K_2$ and C_{2h}-$Be_2Li_4K_2$ data were calculated at the CCSD/cc-pVTZ/6-311G(d) level, where 6-311G(d) basis set is for K and cc-pVTZ basis set is for Be, Li and Na. For other clusters, their ground state structure and the corresponding electron structure analysis were all confirmed at the CCSD/cc-pVTZ level. The Born-Oppenheimer molecular dynamics were also executed to check their dynamic stability. Gibbs free energy changes of different reactions (Scheme S1) were also performed and the data clearly declare their excellent stability. Various bonding analysis strategies including AdNDP, EFL, LOL and AIM were all carried out using Multiwfn program.[35] The Compliance program was used to calculate the force constants FC.[36,37] The Laplacian, FMO and ESP analysis were performed by Gaussian 09 package.[38] NBO analysis was conducted with NBO program implemented in the Gaussian.

Reference

34. Y. Wang, J. Lv, L. Zhu, and Y. Ma, CALYPSO: a method for crystal structure prediction. *Comput. Phys. Commun.*, http://www.calypso.cn (2012).

35. T. Lu and F. Chen, Multiwfn: a multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**, 580–592.

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37. K. Brandhorst and J. Grunenberg, How strong is it? The interpretation of force and compliance constants as bond strength descriptors, *Chem. Soc. Rev.*, 2008, **37**, 1558-1567.

38. M. J. Frisch et al., Gaussian09 (RevisionD.01), Gaussian, Inc., Wallingford, Connecticut, 2009.

Table of Contents

SI1

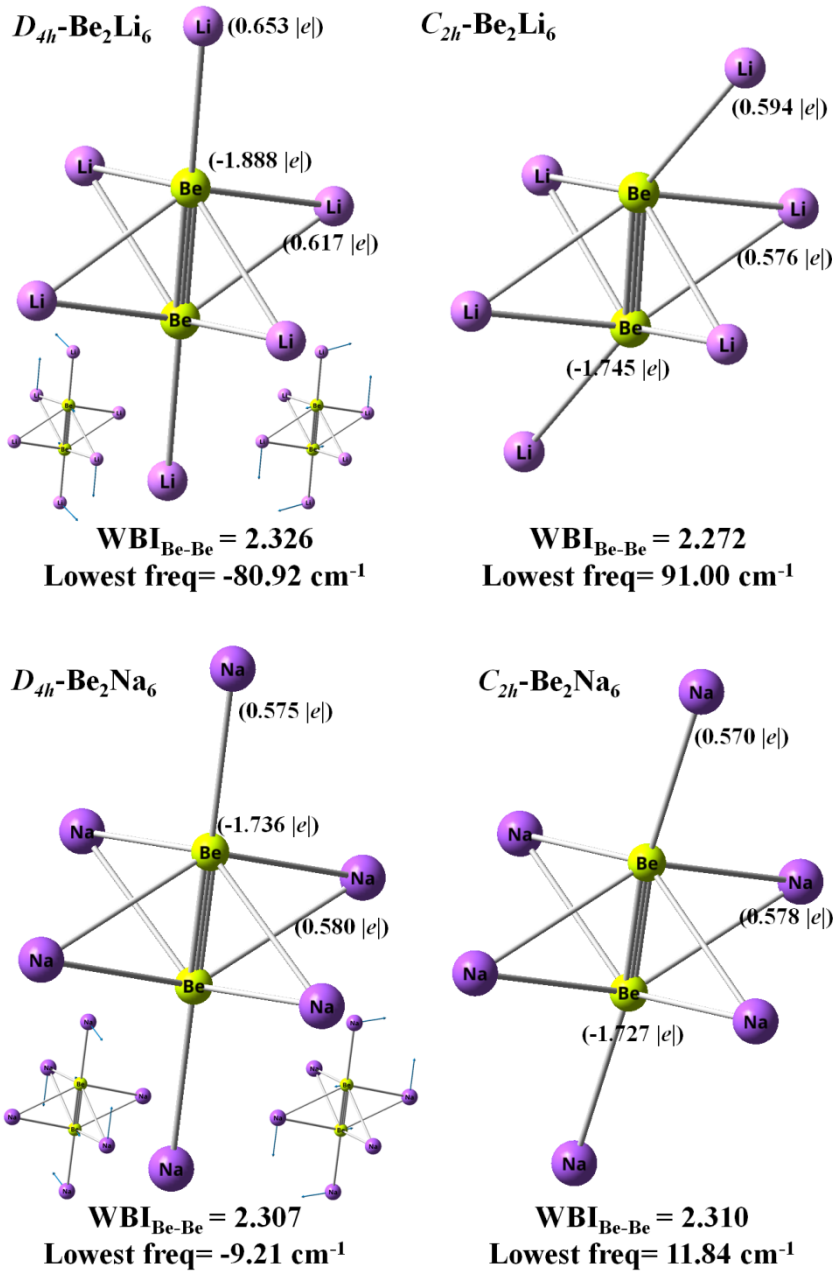
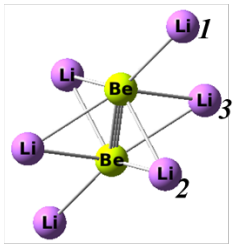


Figure S1. The comparison of D_{4h}-Be_2X_6 and C_{2h}-Be_2X_6 (X=Li, Na) structures. The values in parentheses correspond to the NPA charges. The vibration modes of degenerate lowest imaginary frequency of the D_{4h}-Be_2X_6 structures are also given.

SI2

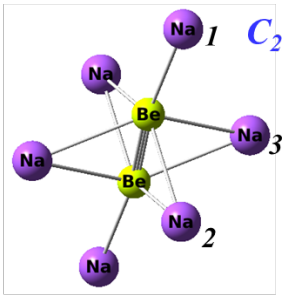


C_{2h}-Be_2Li_6

NPA_{Be}= -1.75 |*e*|
NPA_{Li1}= 0.59 |*e*|
NPA_{Li3}= 0.58 |*e*|

$WBI_{Be\text{-}Be}$= 2.272
$WBI_{Li1\text{-}Be}$= 0.427
$WBI_{Li3\text{-}Be}$= 0.355
$WBI_{Li1\text{-}Li3}$= 0.069

$R_{Be\text{-}Be}$ = 1.982 Å
$R_{Be\text{-}Li1}$ = 2.462 Å
$R_{Be\text{-}Li3}$ = 2.378 Å
$R_{Li1\text{-}Li3}$ = 3.373 Å
$R_{Li2\text{-}Li3}$ = 3.076 Å
$A_{Be\text{-}Be\text{-}Li1}$ = 150.14 °

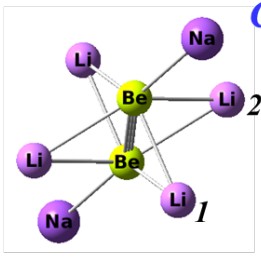


C_{2h}-Be_2Na_6

NPA_{Be}= -1.73 |*e*|
NPA_{Na1}= 0.57 |*e*|
NPA_{Na3}= 0.58 |*e*|

$WBI_{Be\text{-}Be}$ = 2.310
$WBI_{Na1\text{-}Be}$ = 0.449
$WBI_{Na2\text{-}Be}$ = 0.285
$WBI_{Na2\text{-}Na3}$ = 0.052
$WBI_{Na1\text{-}Na3}$ = 0.060

$R_{Be\text{-}Be}$ = 1.982 Å
$R_{Be\text{-}Na1}$ = 2.719 Å
$R_{Be\text{-}Na2}$ = 2.798 Å
$R_{Na1\text{-}Na3}$ = 4.349 Å
$R_{Na2\text{-}Na3}$ = 3.714 Å
$A_{Be\text{-}Be\text{-}Na1}$ = 171.63 °

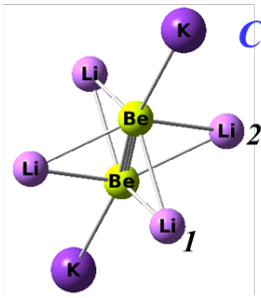


C_{2h}-$Be_2Li_4Na_2$

NPA_{Be}= -1.75 |*e*|
NPA_{Li}= 0.57 |*e*|
NPA_{Na}= 0.54 |*e*|

$WBI_{Be\text{-}Be}$= 2.382
$WBI_{Na\text{-}Be}$= 0.428
$WBI_{Li1\text{-}Be}$= 0.334
$WBI_{Li1\text{-}Na}$= 0.085
$WBI_{Li\text{-}Li}$ = 0.056

$R_{Be\text{-}Be}$ = 1.973 Å
$R_{Be\text{-}Na}$ = 2.754 Å
$R_{Be\text{-}Li2}$ = 2.406 Å
$R_{Na\text{-}Li2}$ = 3.676 Å
$R_{Li\text{-}Li}$ = 3.110 Å
$A_{Be\text{-}Be\text{-}Na}$ = 151.63 °



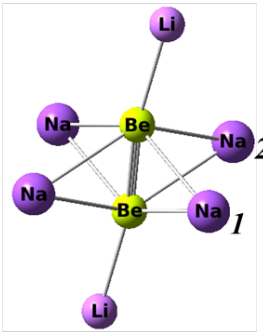
C_{2h}-$Be_2Li_4K_2$

NPA_{Be}= -1.68 |*e*|
NPA_{Li}= 0.51 |*e*|
NPA_{K}= 0.66 |*e*|

$WBI_{Be\text{-}Be}$ = 2.469
$WBI_{K\text{-}Be}$= 0.293
$WBI_{Li1\text{-}Be}$= 0.314
$WBI_{Li1\text{-}K}$= 0.072
$WBI_{Li\text{-}Li}$ = 0.070

$R_{Be\text{-}Be}$ = 1.964 Å
$R_{Be\text{-}K}$ = 3.154 Å
$R_{Be\text{-}Li2}$ = 2.427 Å
$R_{K\text{-}Li2}$ = 4.464 Å
$R_{Li\text{-}Li}$ = 3.145 Å
$A_{Be\text{-}Be\text{-}K}$ = 169.33 °

SI3

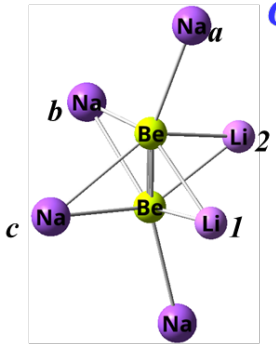


C_{2h}-$Be_2Na_4Li_2$

NPA_{Be}= -1.75 |*e*|
NPA_{Li}= 0.61 |*e*|
NPA_{Na}= 0.60 |*e*|

$WBI_{Be\text{-}Be}$= 2.189
$WBI_{Li\text{-}Be}$= 0.437
$WBI_{Na1\text{-}Be}$= 0.292
$WBI_{Li1\text{-}Na}$= 0.048
$WBI_{Na\text{-}Na}$ = 0.048

$R_{Be\text{-}Be}$ = 1.989 Å
$R_{Be\text{-}Li}$ = 2.430 Å
$R_{Be\text{-}Na2}$ = 2.775 Å
$R_{Li\text{-}Na2}$ = 4.055 Å
$R_{Na\text{-}Na}$ = 3.695 Å
$A_{Be\text{-}Be\text{-}Li}$ = 169.97 °

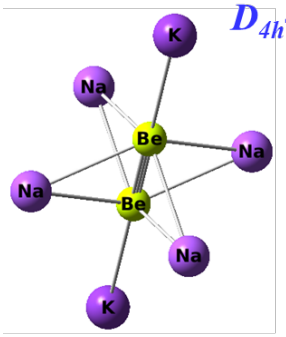


C_1-$Be_2Na_4Li_2$

NPA_{Be}= -1.68 |*e*|
NPA_{Li1}= 0.46 |*e*|
NPA_{Naa}= 0.58 |*e*|
NPA_{Nab}= 0.64 |*e*|

$WBI_{Be\text{-}Be}$= 2.305
$WBI_{Li1\text{-}Be}$= 0.307
$WBI_{Li2\text{-}Be}$= 0.394
$WBI_{Naa\text{-}Be}$= 0.413
$WBI_{Nab\text{-}Be}$= 0.244
$WBI_{Li1\text{-}Naa}$= 0.058
$WBI_{Na\text{-}Na}$ = 0.038
$WBI_{Na\text{-}Na}$ = 0.066

$R_{Be\text{-}Be}$ = 1.970 Å
$R_{Be\text{-}Li1}$ = 2.438 Å
$R_{Be\text{-}Li2}$ = 2.414Å
$R_{Be\text{-}Naa}$ = 2.720 Å
$R_{Be\text{-}Nab}$ = 2.790 Å
$R_{Li1\text{-}Naa}$ = 4.241 Å
$R_{Li\text{-}Li}$ = 3.025 Å
$R_{Nab\text{-}Nac}$ = 3.917Å
$A_{Be\text{-}Be\text{-}Naa}$= 159.36 °



D_{4h}-$Be_2Na_4K_2$

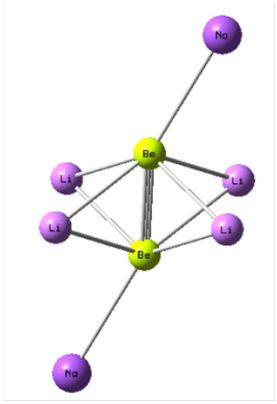
NPA_{Be}= -1.63 |*e*|
NPA_{K}= 0.67 |*e*|
NPA_{Na}= 0.48 |*e*|

$WBI_{Be\text{-}Be}$= 2.429
$WBI_{Be\text{-}Na}$= 0.289
$WBI_{Na\text{-}Na}$= 0.085
$WBI_{Be\text{-}K}$= 0.298

$R_{Be\text{-}Be}$ = 1.986 Å
$R_{Be\text{-}Na}$ = 2.819 Å
$R_{Na\text{-}Na}$ = 3.730 Å
$R_{Be\text{-}K}$ = 3.170 Å

Figure S2. The detailed structural parameters of ***C*$_{2h}$-Be$_2$Li$_6$**, ***C*$_{2h}$-Be$_2$Na$_6$**, ***C*$_{2h}$-Be$_2$Li$_4$Na$_2$**, ***C*$_{2h}$-Be$_2$Li$_4$K$_2$**, ***C*$_{2h}$-Be$_2$Na$_4$Li$_2$**, ***C*$_1$-Be$_2$Na$_4$Li$_2$** and ***D*$_{4h}$-Be$_2$Na$_4$K$_2$**, together with other parameters to describe the bonding nature inside.

SI4



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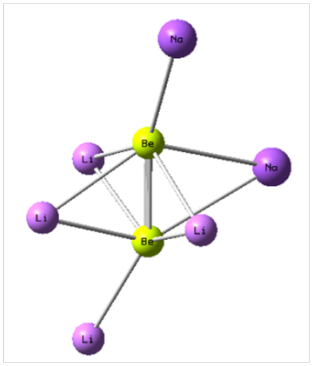
1a (C_{2h}, ^{1}A)



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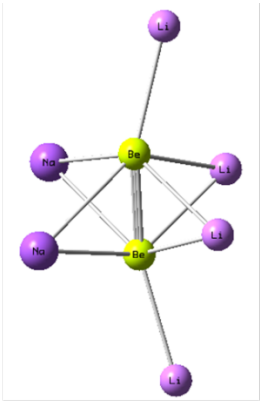

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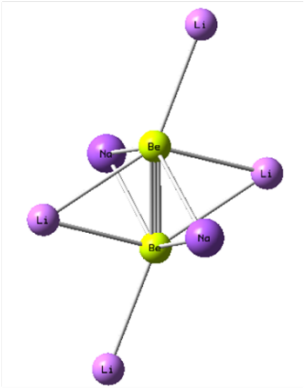

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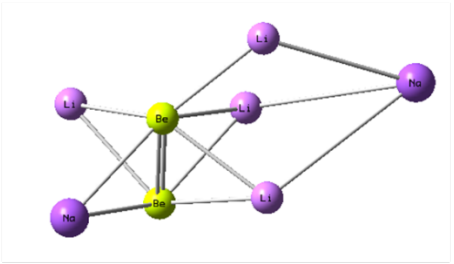

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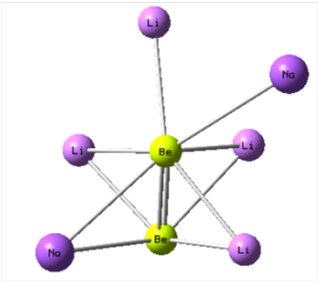

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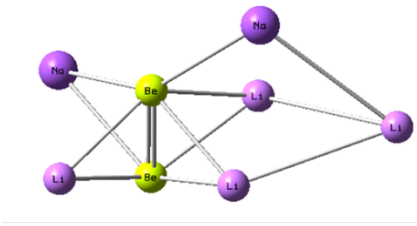

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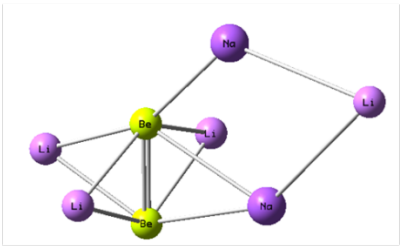

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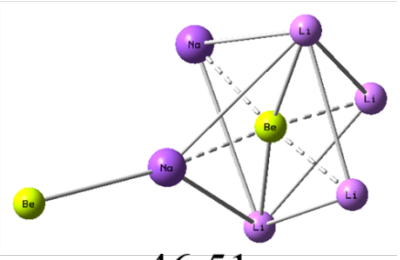

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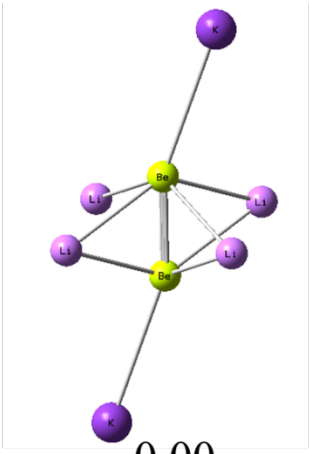
SI5



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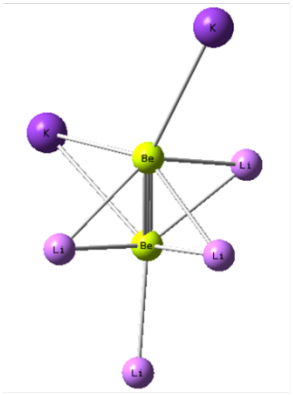

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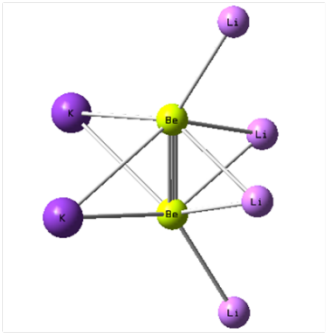

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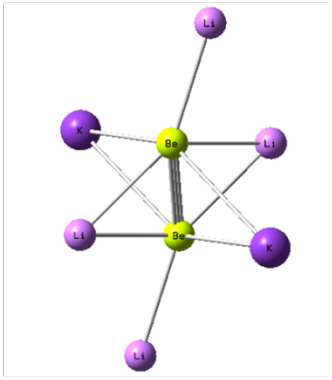

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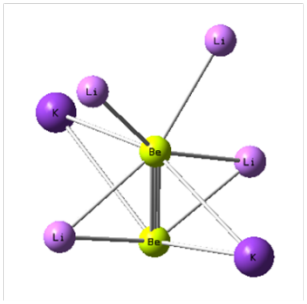

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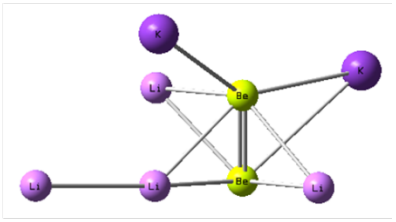

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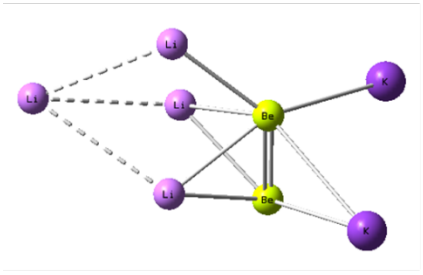

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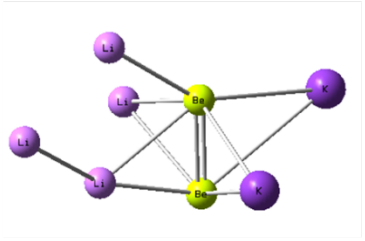

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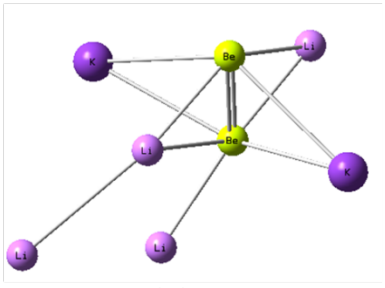

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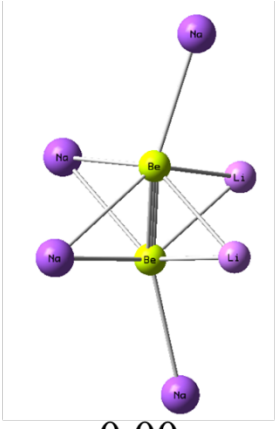

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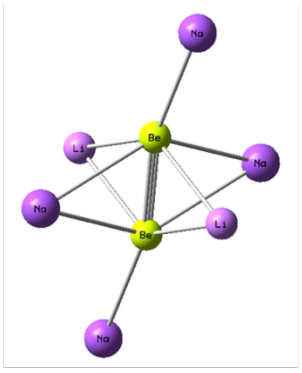

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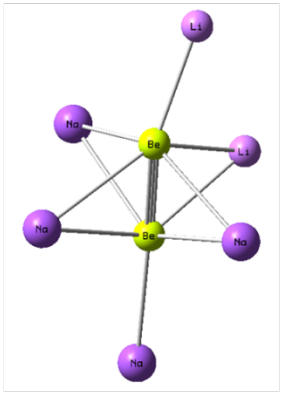

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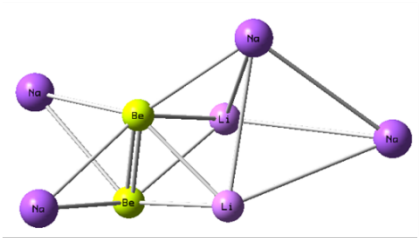

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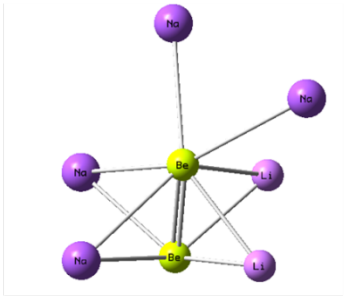

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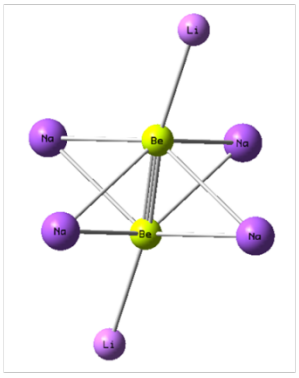

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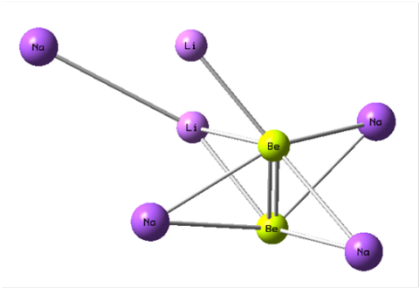

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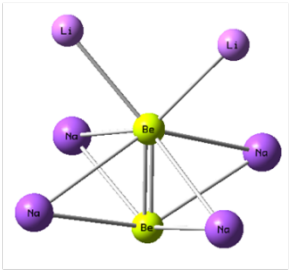

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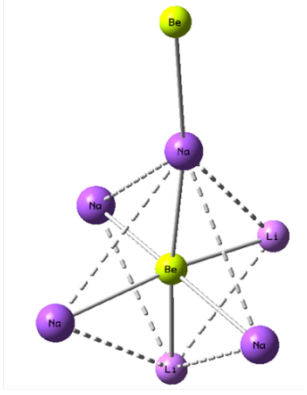

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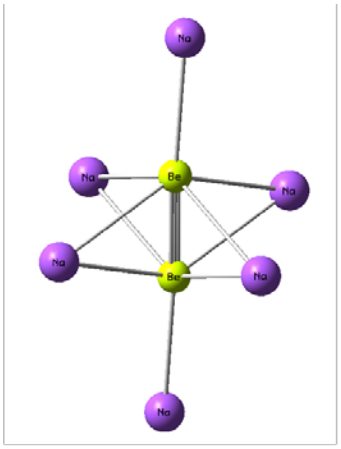
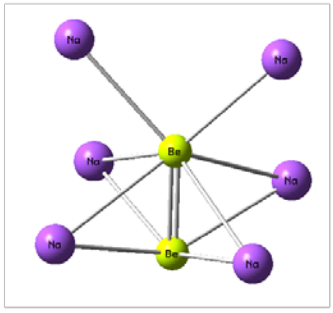


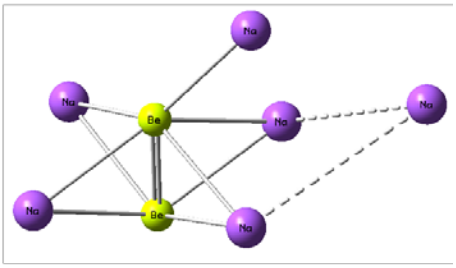
0.0

4a (C_{2h}, ^1A_g)



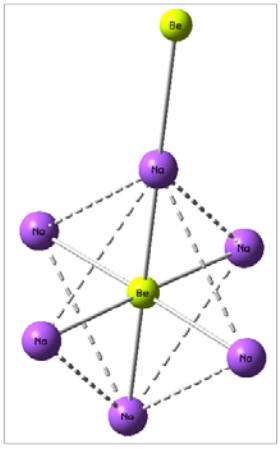
8.89

4b (C_2, ^1A)



13.65

4c (C_s, ^1A)



39.99

4d (C_{4v}, ^1A)

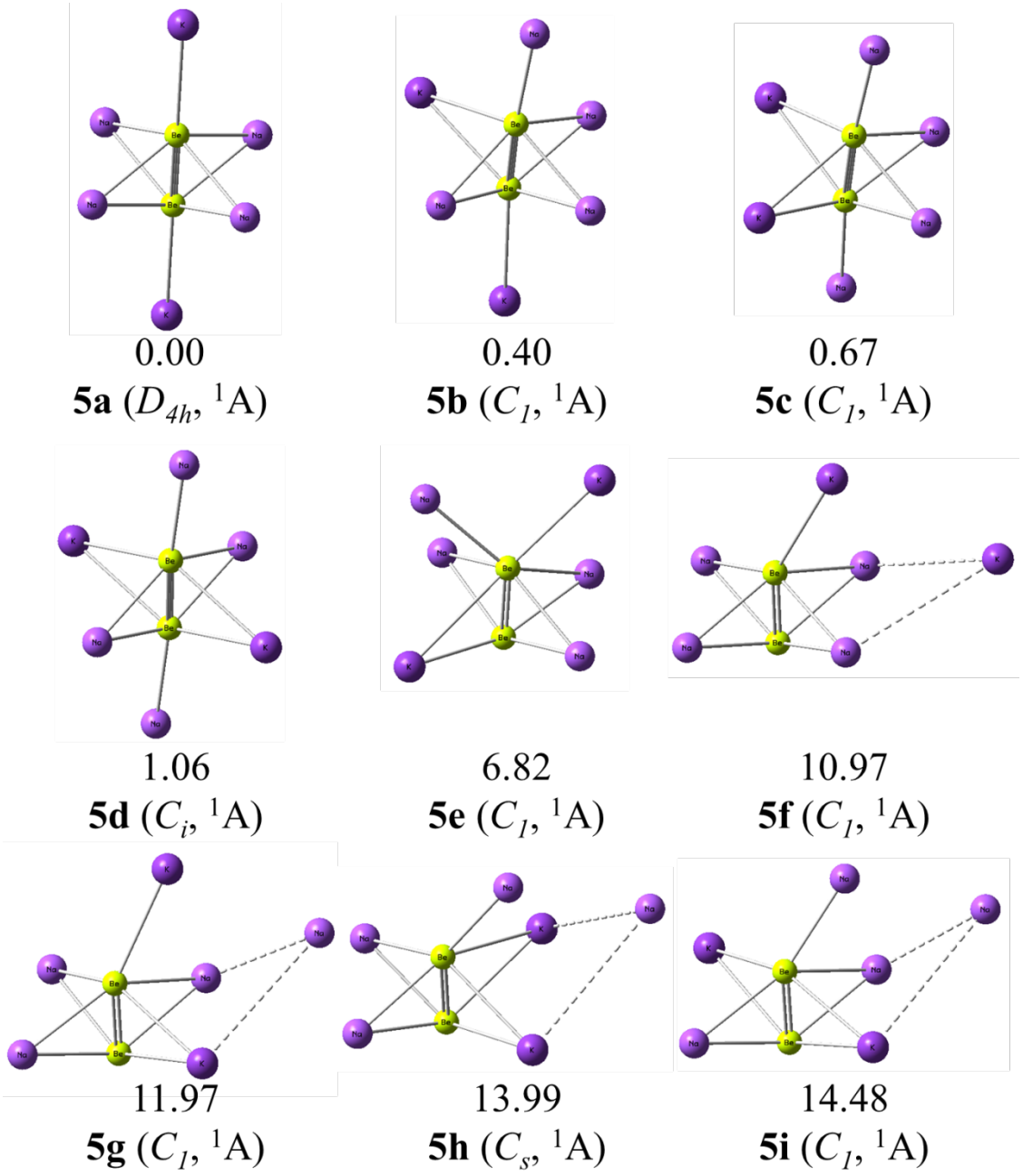


Figure S3. The global minimum structure and other low-energy structures of **(1)** $Be_2Li_4Na_2$, **(2)** $Be_2Li_4K_2$, **(3)** $Be_2Na_4Li_2$, **(4)** Be_2Na_6 and **(5)** $Be_2Na_4K_2$ with energy in kcal/mol. These structures are re-optimized and filtrated at the B3LYP/6-31G(d) level after searched by CALYPSO program.

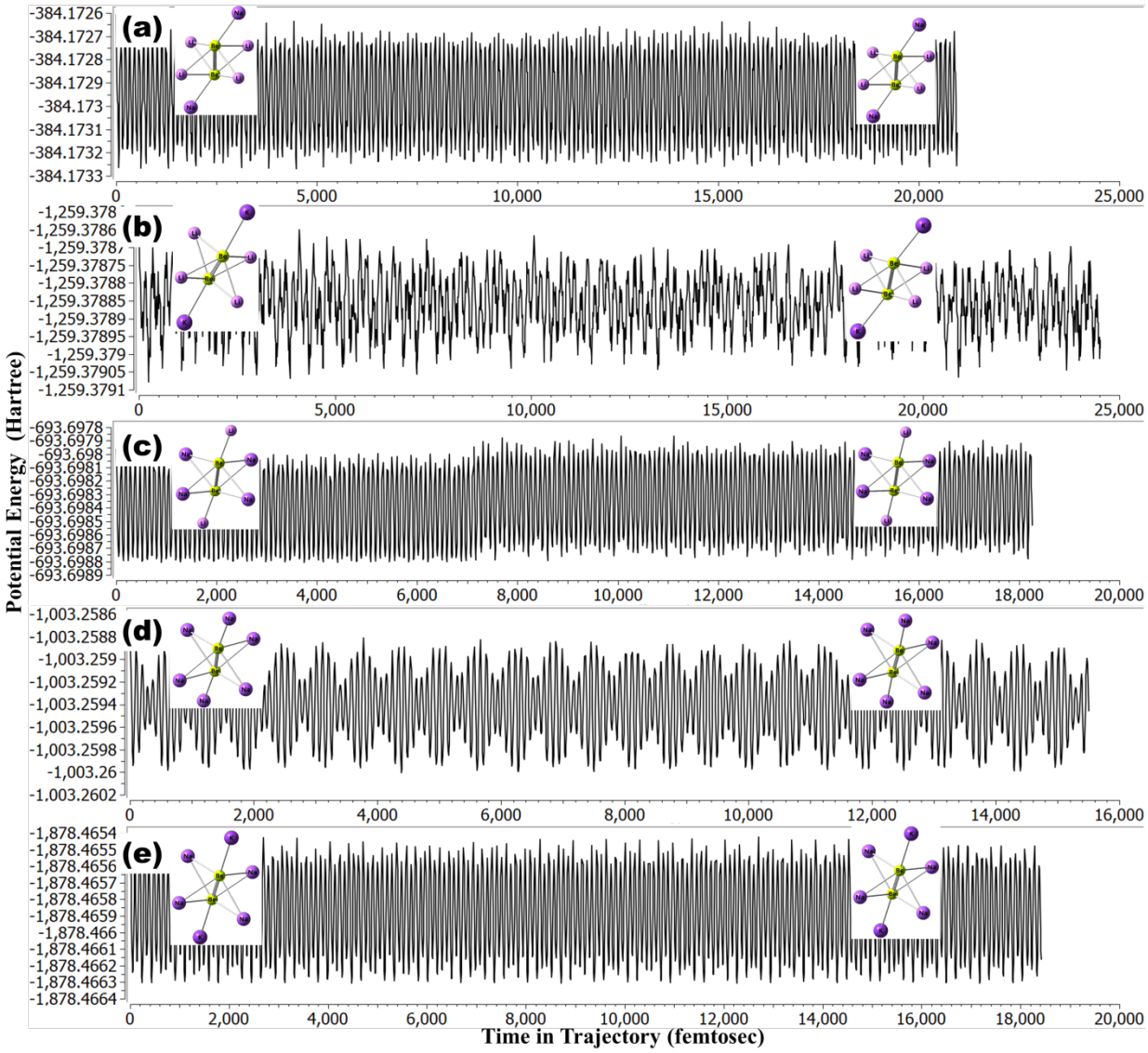


Figure S4. The BOMD results of **(a)** C_{2h}-$Be_2Li_4Na_2$, **(b)** C_{2h}-$Be_2Li_4K_2$, **(c)** C_{2h}-$Be_2Na_4Li_2$, **(d)** C_{2h}-Be_2Na_6 and **(e)** D_{4h}-$Be_2Na_4K_2$ at the B3LYP/6-31G (d) level. The molecular structure configuration of initial state and final state are also listed as insert.

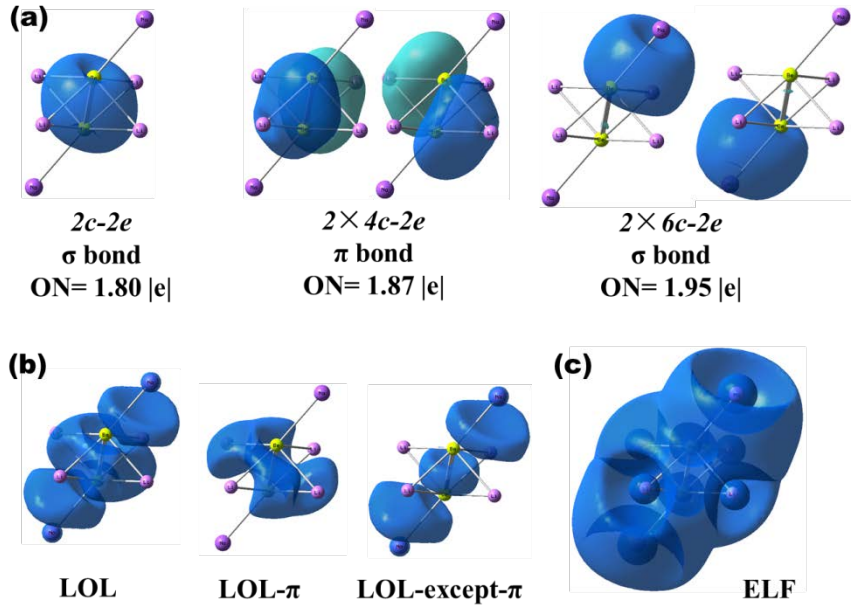


Figure S5. (a) AdNDP orbitals, **(b)** LOL profiles and **(c)** ELF profile of ***C*$_{2h}$-Be$_2$Li$_4$Na$_2$**. ON stands for the occupation number.

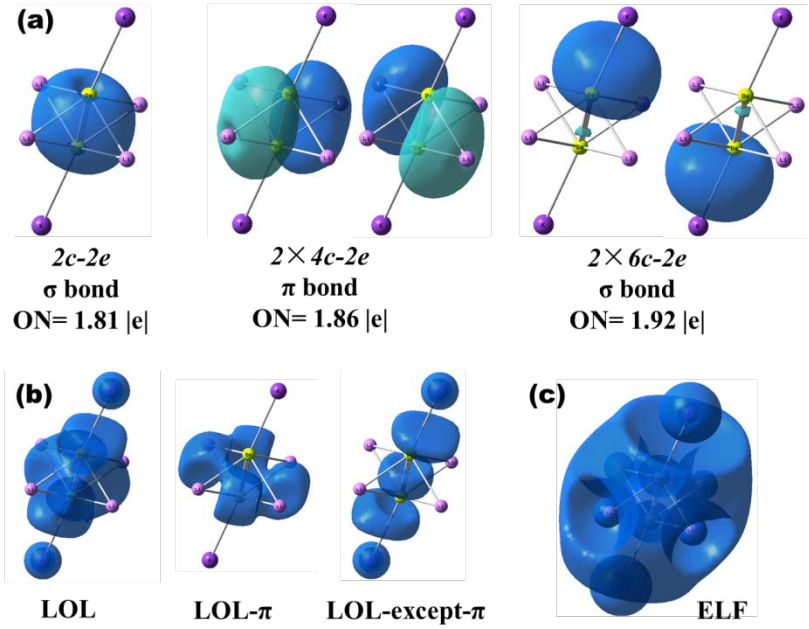


Figure S6. (a) AdNDP orbitals, **(b)** LOL profiles and **(c)** ELF profile of ***C*$_{2h}$-Be$_2$Li$_4$K$_2$**. ON stands for the occupation number.

SI11

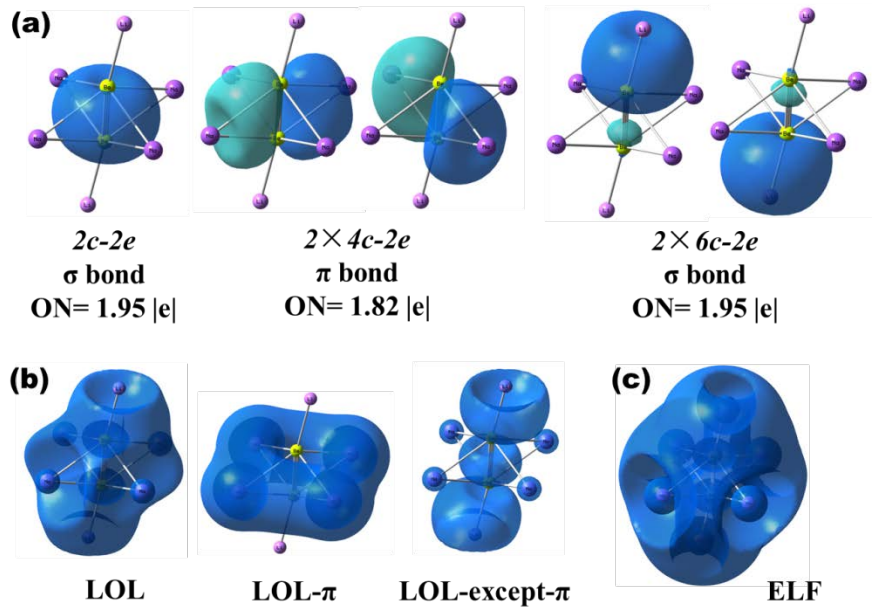


Figure S7. (a) AdNDP orbitals, **(b)** LOL profiles and **(c)** ELF profile of ***C*$_{2h}$-Be$_2$Na$_4$Li$_2$**. ON stands for the occupation number.

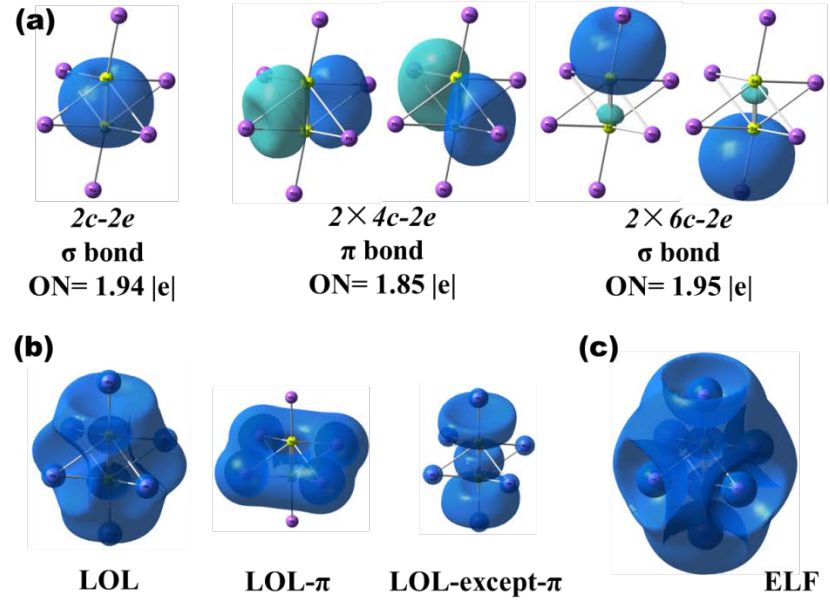


Figure S8. (a) AdNDP orbitals, **(b)** LOL profiles and **(c)** ELF profile of ***C*$_{2h}$-Be$_2$Na$_6$**. ON stands for the occupation number.

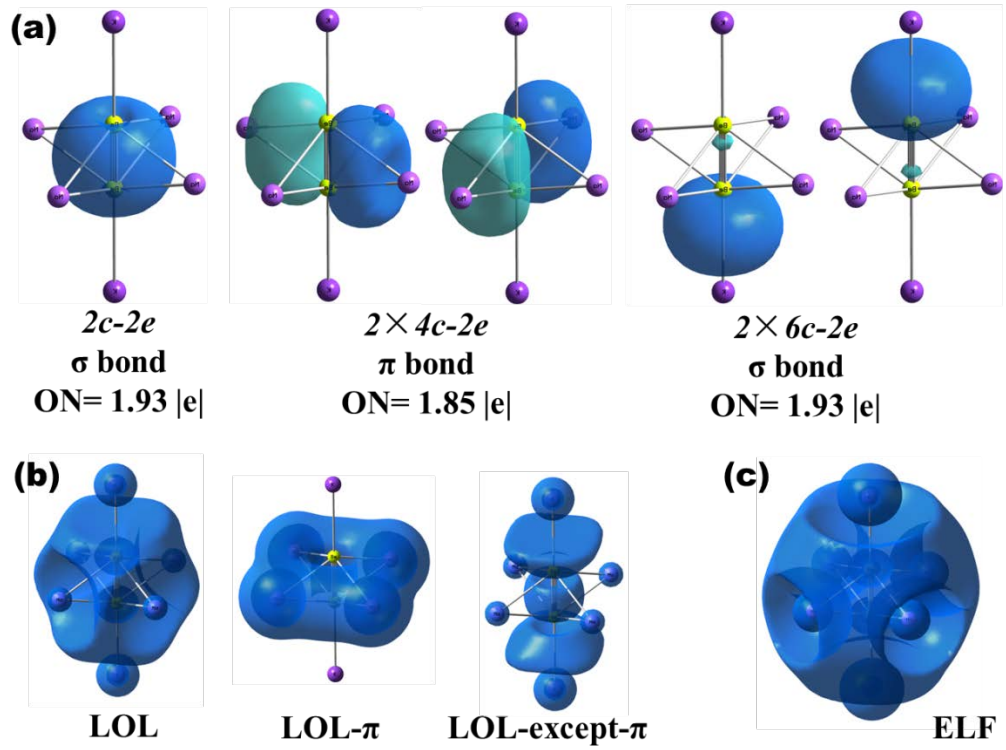


Figure S9. (a) AdNDP orbitals, **(b)** LOL profiles and **(c)** ELF profile of D_{4h}-$Be_2Na_4K_2$. ON stands for the occupation number.

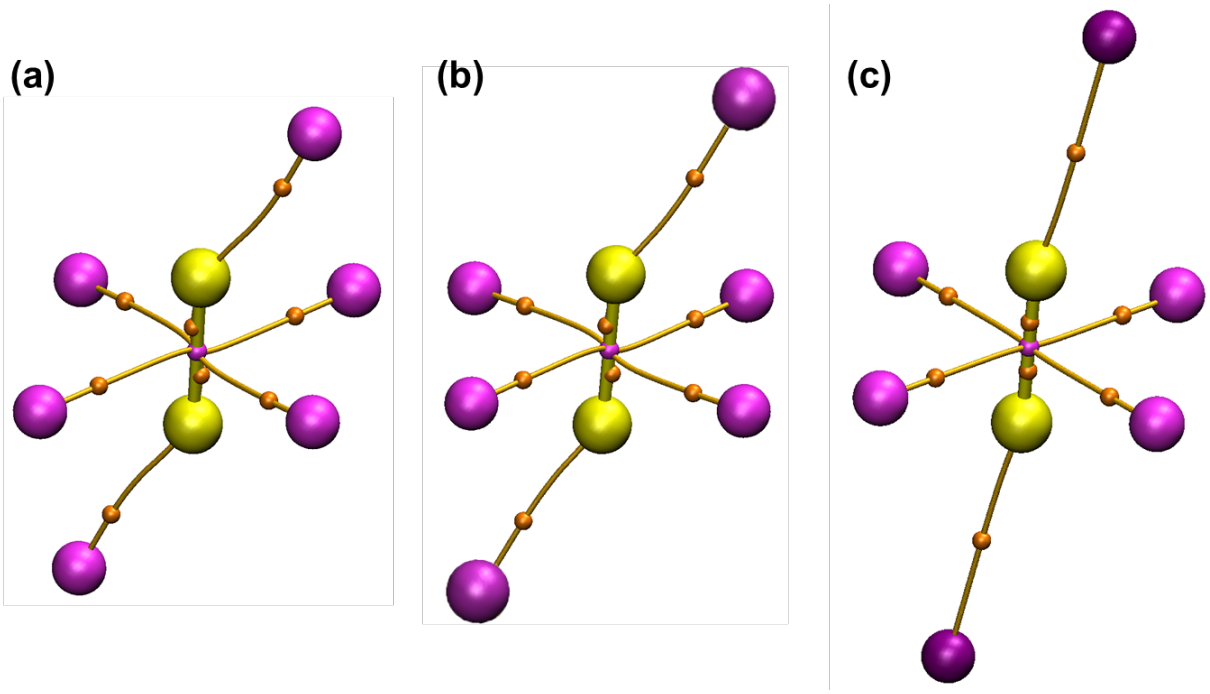


Figure S10. AIM (Please refer to R. F. W. Bader, Atoms in Molecules, Clarendon Press, Oxford, 1994) results of (**a**) C_{2h}-Be_2Li_6, (**b**) C_{2h}-$Be_2Li_4Na_2$ and (**c**) C_{2h}-$Be_2Li_4K_2$. Here the orange dots are bond critical points (BCP). The orange solid lines represent the path connected the BCP and nuclear critical points (NCP). It should note to be that there is a "Non-nuclear-attractor" (NNA, pink dot in centre) between two Be atoms. At NNA point, the corresponding real space function values are in turn: the density of all electrons is 0.060, 0.058, 0.060; Laplacian of electron density is -0.075, -0.068, -0.073; Electron localization function (ELF): 0.847, 0.814, 0.829; Localized orbital locator (LOL): 0.702, 0.677, 0.688; Ellipticity of electron density: 0.249, 0.282, 0.041. Unit: a.u..

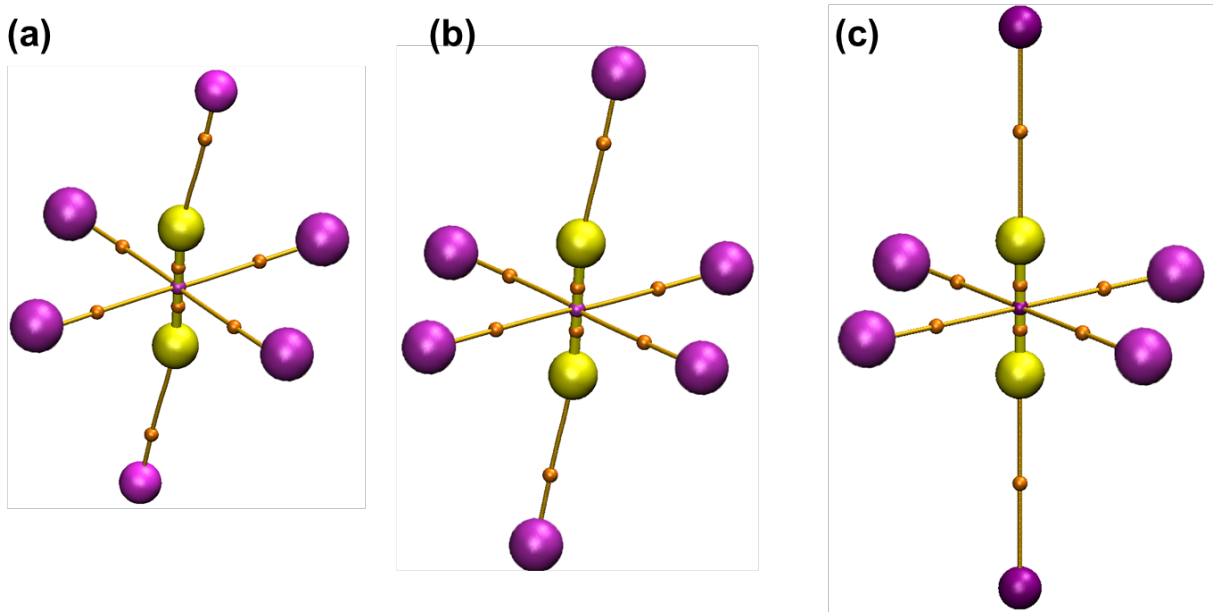


Figure S11. AIM results of (**a**) C_{2h}-$Be_2Na_4Li_2$, (**b**) C_{2h}-Be_2Na_6 and (**c**) D_{4h}-$Be_2Na_4K_2$. At NNA point, the corresponding real space function information are in turn: the density of all electrons is 0.066, 0.064, 0.063; Laplacian of electron density is -0.106, -0.100, -0.098; Electron localization function (ELF): 0.944, 0.926, 0.924; Localized orbital locator (LOL): 0.804, 0.780, 0.778; Ellipticity of electron density: 0.011, 0.008, 0.000. Unit: a.u..

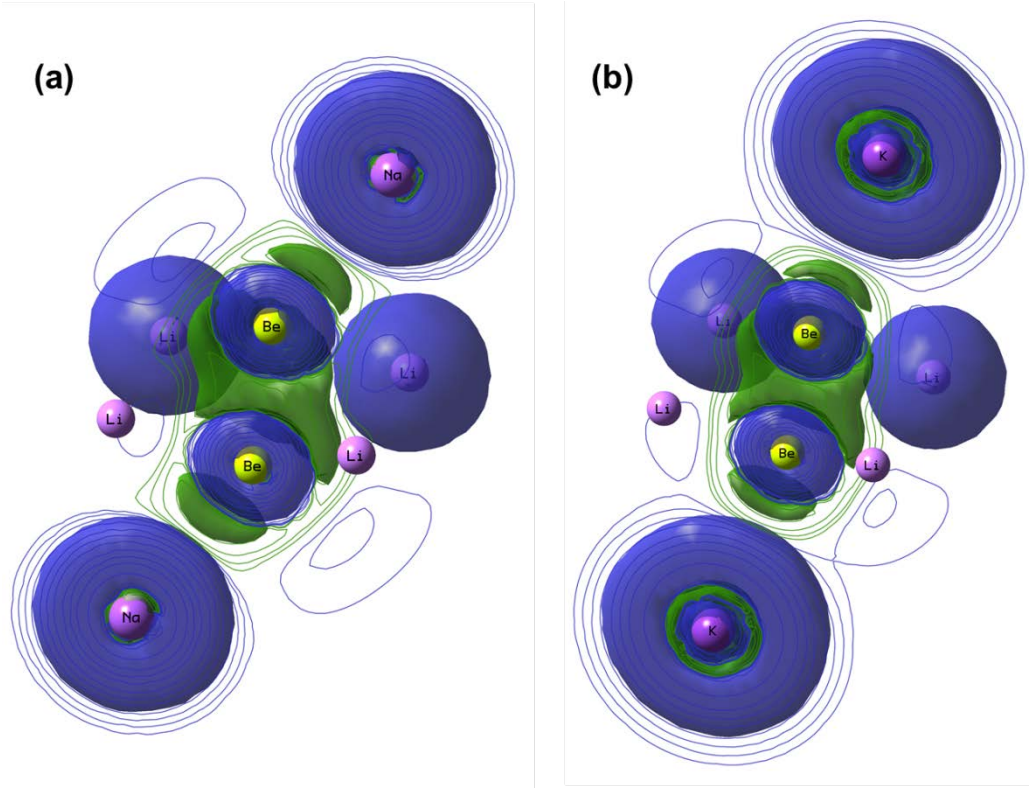


Figure S12. Laplacian electron density ($\nabla^2\rho(r)$) plots of (**a)** ***C*$_{2h}$-Be$_2$Li$_4$Na$_2$** and **(b**) ***C*$_{2h}$-Be$_2$Li$_4$K$_2$**. The green lines including corresponding region indicates the charge concentration ($\nabla^2\rho(r)<0$), while blue lines and region represent the charge depletion ($\nabla^2\rho(r)>0$).

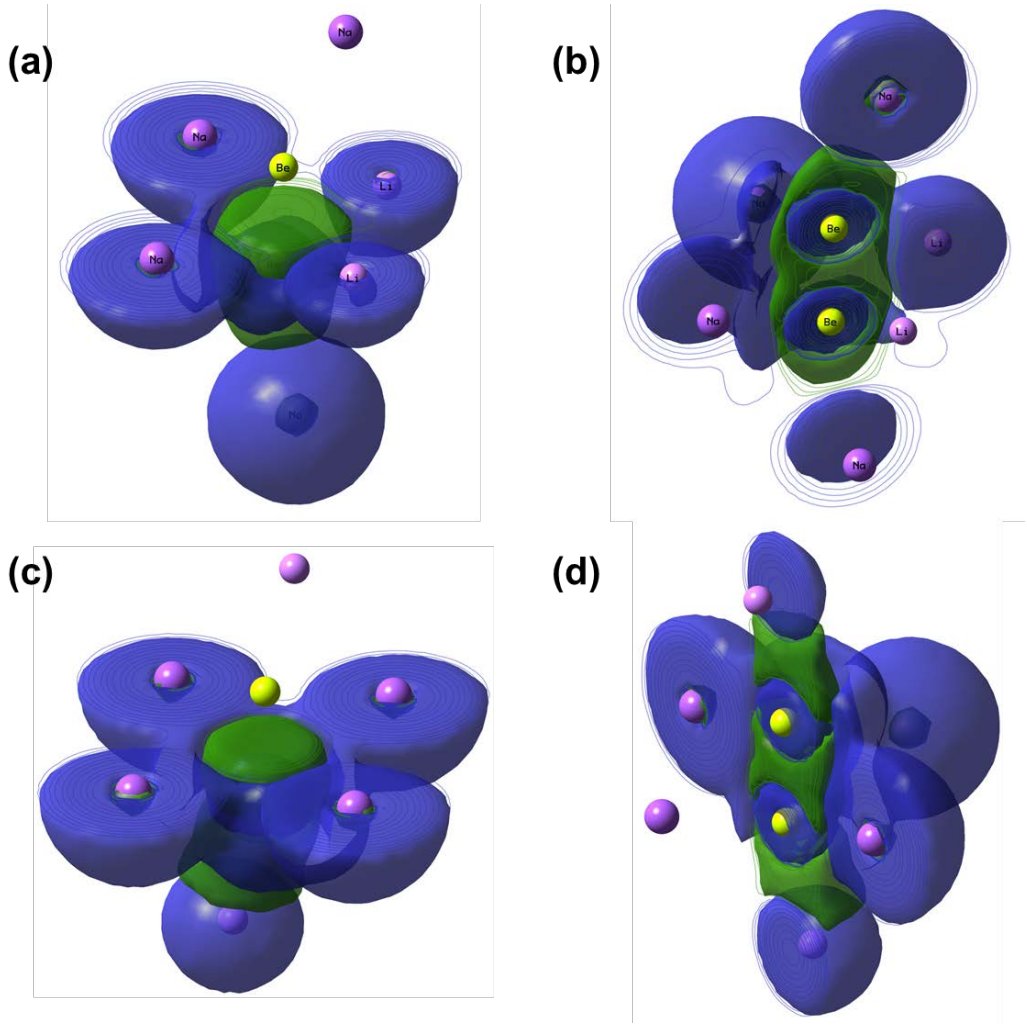


Figure S13. Laplacian electron density ($\nabla^2\rho(r)$) plots in two different view (**a)** Laplacian plot horizontal to Li_2Na_2 plane and **(b)** Laplacian plot along Be_2Na_3Li plane of ***C*$_1$-Be$_2$Na$_4$Li$_2$**, (**c)** Laplacian plot horizontal to Na_4 plane and (**d**) Laplacian plot along $Be_2Na_2Li_2$ of ***C*$_{2h}$-Be$_2$Na$_4$Li$_2$**. The green region indicates the areas of charge concentration ($\nabla^2\rho(r)<0$), while blue region represents the areas of charge depletion ($\nabla^2\rho(r)>0$).

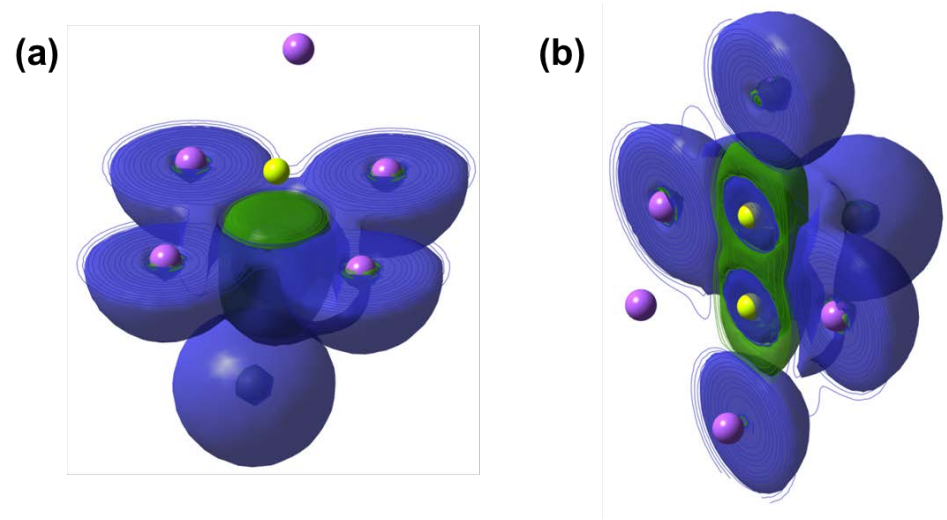


Figure S14. Laplacian electron density ($\nabla^2\rho(r)$) plot in two different view of ***C*$_{2h}$-Be$_2$Na$_6$**. (**a)** Laplacian plot horizontal to Na_4 plane and **(b)** Laplacian plot along Be_2Na_4 plane. The green region indicates the areas of charge concentration ($\nabla^2\rho(r)<0$), while blue region represents the areas of charge depletion ($\nabla^2\rho(r)>0$).

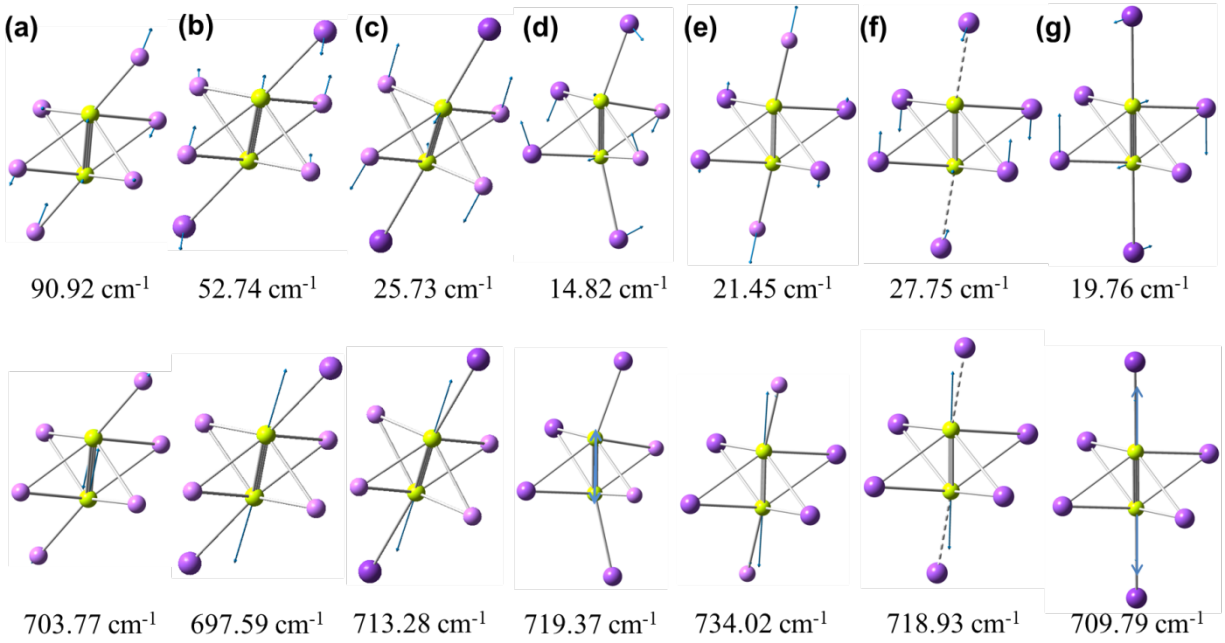
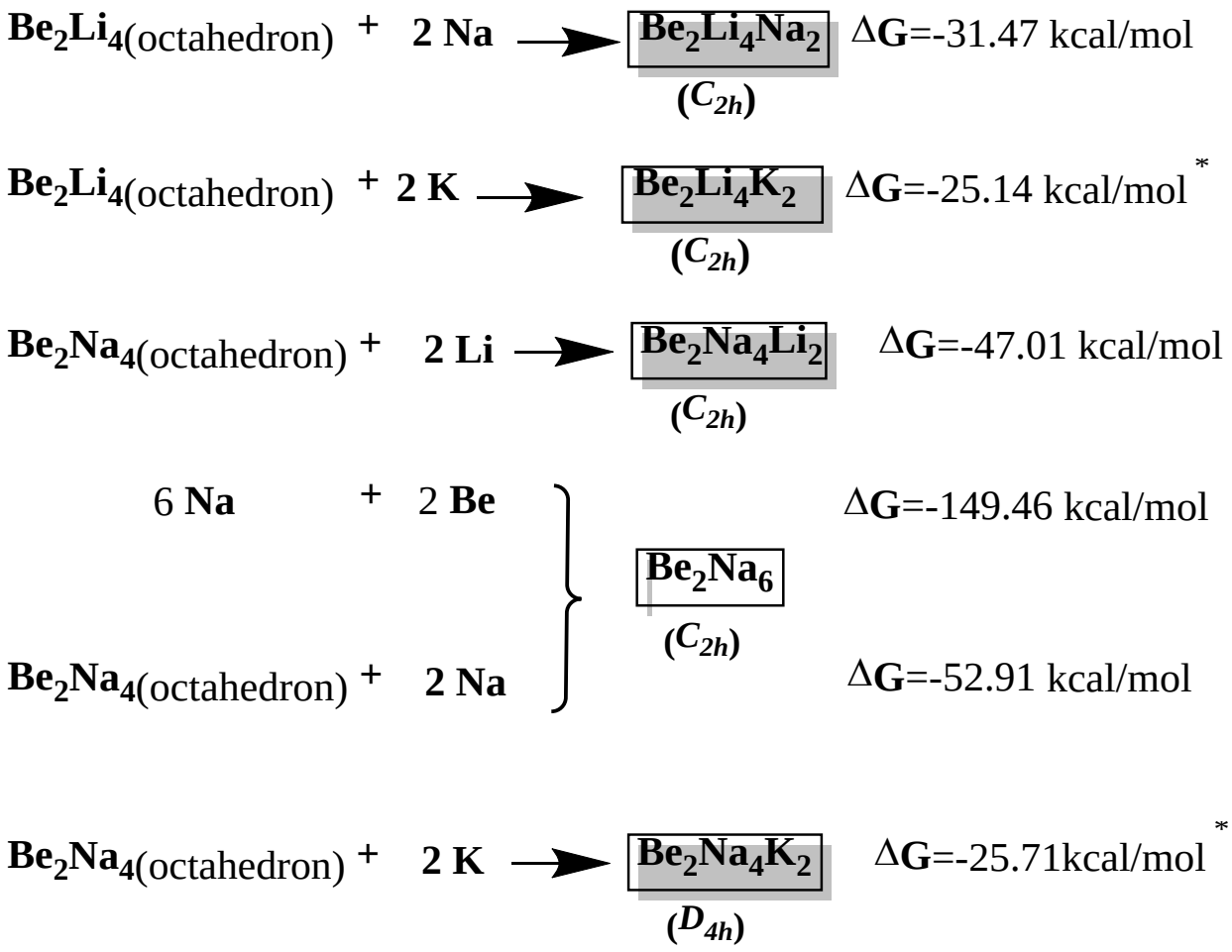


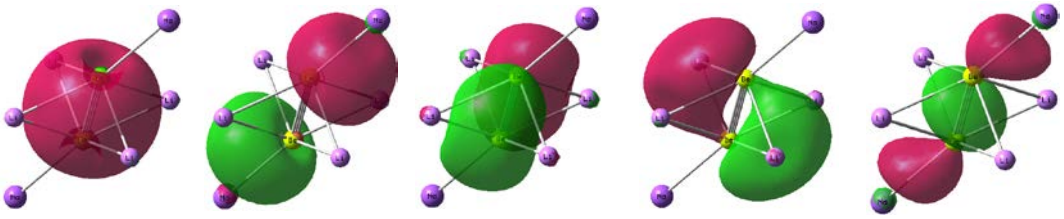
Figure S15. The lowest frequency and Be-Be stretching vibrational frequency accompany with their corresponding vibrational modes of (**a**) C_{2h}-Be_2Li_6, **(b)** C_{2h}-$Be_2Li_4Na_2$, **(c)** C_{2h}-$Be_2Li_4K_2$, **(d)** C_1-$Be_2Na_4Li_2$, **(e)** C_{2h}-$Be_2Na_4Li_2$, **(f)** C_{2h}-Be_2Na_6 and **(g)** D_{4h}-$Be_2Na_4K_2$.

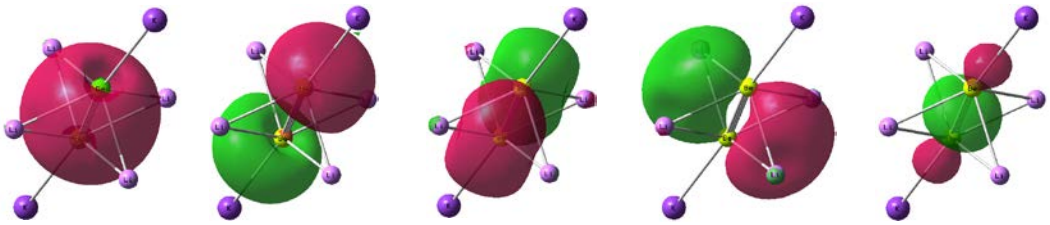
Scheme S1**.** Several potential reactions and thermodynamic values for the generation of ***C*$_{2h}$-$Be_2Li_4Na_2$**, ***C*$_{2h}$-$Be_2Li_4K_2$**, ***C*$_{2h}$-$Be_2Na_4Li_2$**, ***C*$_{2h}$-Be_2Na_6** and ***D*$_{4h}$-$Be_2Na_4K_2$**.

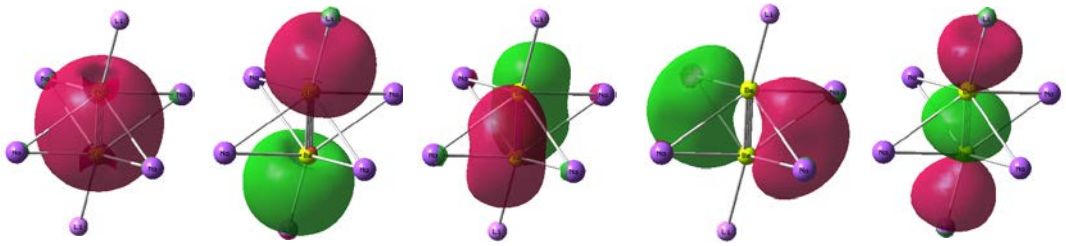


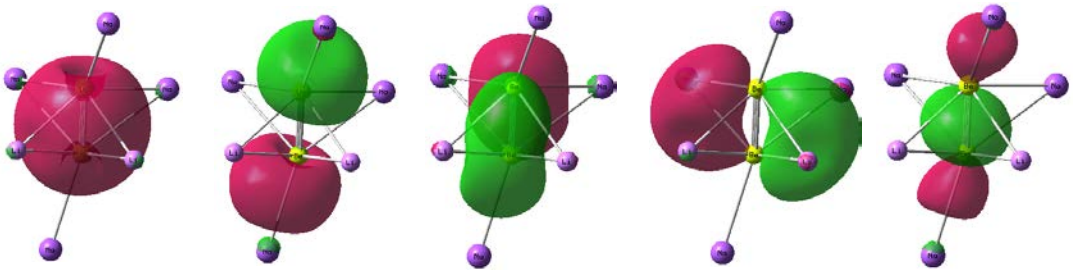
: This value is calculated at B3LYP/6-31G levels.

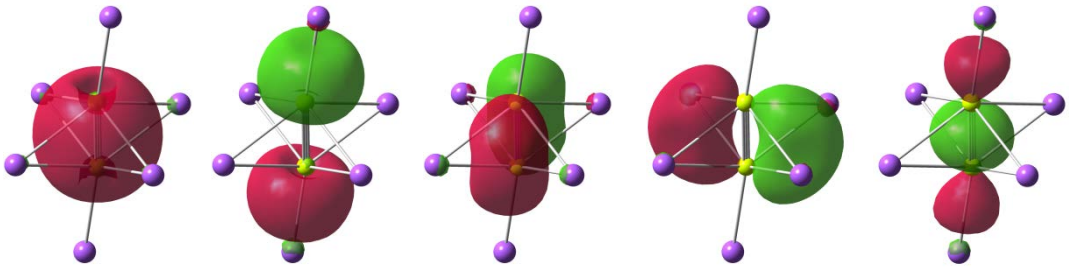
Table S1. The orbital composition of **(1)** ***C*$_{2h}$-$Be_2Li_4Na_2$**, **(2)** ***C*$_{2h}$-$Be_2Li_4K_2$**, **(3)** ***C*$_{2h}$-$Be_2Na_4Li_2$**, **(4)** ***C*$_1$-$Be_2Na_4Li_2$**, **(5)** ***C*$_{2h}$-Be_2Na_6** and **(6)** ***D*$_{4h}$-$Be_2Na_4K_2$**. The coefficient of each orbital is given by the contribution from the fragments.

(1) C_{2h}-**$Be_2Li_4Na_2$**	Occupied molecular orbitals				
	σ (HOMO-4)	σ* (HOMO-3)	π (HOMO-2)	π (HOMO-1)	σ (HOMO)
Diagram					
Energy(eV)	-11.11	-6.03	-4.90	-4.86	-4.01
Component (%)	Be_2©2s~52.2 Be_2©2p_z~7.0 Li_4©2s~29.0	Be_2©2s~63.6 Be_2©2p_z~3.8 Na_2©3s~18.8	Be_2©2p_x~17.1 Li_4©2s~67.0	Be_2©2s~60.0 Be_2©2p_y~5.7 Be_2©2p_z~3.4 Li_4©2s~24.1	Be_2©2p_z~11.2 Na_2©3s~72.2

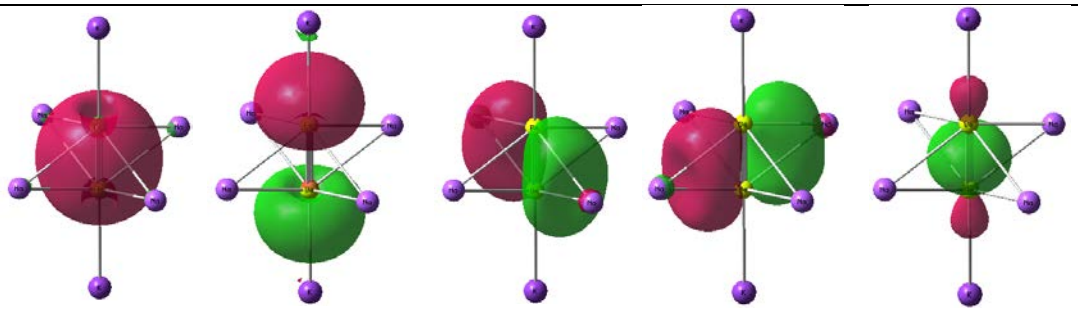
(2) C_{2h}-**$Be_2Li_4K_2$**	Occupied molecular orbitals				
	σ (HOMO-4)	σ* (HOMO-3)	π (HOMO-2)	π (HOMO-1)	σ (HOMO)
Diagram					
Energy(eV)	-10.86	-5.33	-4.66	-4.66	-3.33
Component (%)	Be_2©2s~50.1 Li_4©2s~28.9	Be_2©2s~72.6 K_2©4s~10.4	Be_2©2p_x~23.7 Li_4©2s~60.9	Be_2©2s~61.7 Be_2©2p_y~6.0 Li_4©2s~22.7	Be_2©2s~9.9 Be_2©2p_z~12.1 K_2©4s~54.6 Li_4©2s~4.9

(3) C_{2h}-**$Be_2Na_4Li_2$**	Occupied molecular orbitals				
	σ (HOMO-4)	σ* (HOMO-3)	π (HOMO-2)	π (HOMO-1)	σ (HOMO)
Diagram					
Energy(eV)	-10.35	-5.99	-4.19	-4.19	-4.17
Component (%)	Be_2©2s~53.4 Na_4©3s~28.4	Be_2©2s~49.8 $Li_{2\text{-}z}$©3s~34.8	Be_2©2p_y~12.0 Na_4©3s~74.9	Be_2©2p_x~10.9 Na_4©3s~73.0	Be_2©2p_s~17.8 $Li_{2\text{-}z}$©2s~58.5 Na_4©3s~8.0

(4) C_1-**$Be_2Na_4Li_2$**	Occupied molecular orbitals				
	σ (HOMO-4)	σ* (HOMO-3)	π (HOMO-2)	π (HOMO-1)	σ (HOMO)
Diagram					
Energy (eV)	-10.80	-5.80	-4.62	-4.58	-3.91
Component (%)	Be_2©2s~52.9 $Na_{2\text{-}xy}$©3s~10.6 $Li_{2\text{-}XY}$©2s~18.0	Be_2©2s~54.9 $Na_{2\text{-}z}$©3s~29.4	Be_2©2p_y~14.7 $Na_{2\text{-}xy}$©3s~36.1 $Li_{2\text{-}xy}$©2s~28.4	Be_2©2p_x~12.0 Be_2©2s~13.3 $Na_{2\text{-}XY}$©3s~33.6 $Li_{2\text{-}XY}$©2s~27.7	Be_2©2p_z~12.5 $Na_{2\text{-}z}$©3s~57.8 $Na_{2\text{-}XY}$©3s~13.6 $Li_{2\text{-}XY}$©2s~1.9

(5) C_{2h}-**Be_2Na_6**	Occupied molecular orbitals				
	σ (HOMO-4)	σ* (HOMO-3)	π (HOMO-2)	π (HOMO-1)	σ (HOMO)
Diagram					
Energy(eV)	-10.40	-5.62	-4.25	-4.15	-3.90
Component (%)	Be_2©2s~53.6 Na_4©3s~26.9	Be_2©2s~55.1 $Na_{2\text{-}z}$©3s~30.5	Be_2©2p_y~13.6 Na_4©3s~73.7	Be_2©2p_x~10.7 Na_4©3s~72.7	Be_2©2p_z~13.0 $Na_{2\text{-}z}$©3s~62.1 Na_4©3s~9.5

$Na_{2\text{-}z}$ represents two vertex Na atoms. Na_4 represents four Na atoms on the equatorial plane.

(6) D_{4h}-**$Be_2Na_4K_2$**	Occupied molecular orbitals				
	σ (HOMO-3)	σ* (HOMO-2)	Degenerated-π (HOMO-1)		σ (HOMO)
Diagram					
Energy(eV)	-10.28	-5.11	-4.10		-3.33
Component (%)	Be_2©2s~52.3 Na_4©3s~25.7	Be_2©2s~39.3 Be_2©2p_z~35.8 $K_{2\text{-}z}$©4s~13.2	Be_2©2p_y~16.8 Na_{2y}©3s~72.4	Be_2©2p_x~16.8 Na_{2x}©3s~72.4	Be_2©2p_z~20.6 $K_{2\text{-}z}$©4s~44.8 Na_4©3s~22.7

SI23

Coordinates of **(1)** $Be_2Li_4Na_2$, **(2)** $Be_2Li_4K_2$, **(3)** $Be_2Na_4Li_2$, **(4)** Be_2Na_6 and **(5)** $Be_2Na_4K_2$. All of them are obtained at the B3LYP/6-31G(d) level.

Part A----- $Be_2Li_4Y_2$

$Be_2Li_4Na_2$--(1)

1a

Be	-0.36329605	-0.90378785	0.00000000
Be	0.36329605	0.90378785	0.00000000
Li	1.43283389	-0.67478587	1.53946245
Li	-1.43283389	0.67478587	-1.53946245
Li	1.43283389	-0.67478587	-1.53946245
Li	-1.43283389	0.67478587	1.53946245
Na	0.11424508	3.56434214	0.00000000
Na	-0.11424508	-3.56434214	0.00000000

1b

Be	-0.23858500	-0.45727400	-0.30150400
Be	1.61273700	-0.51644700	0.34508400
Na	0.76209500	2.07210100	0.02356200
Na	-2.90634800	-0.31315500	-0.13717700
Li	0.73119700	-2.65631200	0.02887600
Li	3.85955700	-1.38343400	0.26409500
Li	-0.12414500	-0.50788400	2.07897200
Li	1.56344900	-0.60354200	-2.01346100

1c

Be	0.47177400	0.58085700	-0.86613500
Be	-0.47320800	0.58702300	0.86316600

Na	1.76788800	-1.11969600	0.78302500
Na	-1.76495000	-1.12886600	-0.77476900
Li	-1.36318700	2.14327400	-0.64607700
Li	1.35735600	2.15357300	0.62870000
Li	-2.20212000	1.20447500	2.43448500
Li	2.19909000	1.18623300	-2.44342000

1d

Be	-0.03726999	0.90798494	-0.41872405
Be	0.03726999	-0.90798494	0.41872405
Na	-2.52807111	-0.09341876	0.00282900
Na	2.52807111	0.09341876	-0.00282900
Li	0.04094077	-1.07806712	-1.93260699
Li	-0.04094077	1.07806712	1.93260699
Li	0.20605453	-3.29652806	0.48784208
Li	-0.20605453	3.29652806	-0.48784208

1e

Be	-1.22604100	0.68691400	-1.23372600
Be	-0.83540600	0.35539500	0.66279200
Na	3.80179900	-0.29642000	-0.09970600
Na	-3.21474000	-0.82401600	0.05872300
Li	0.39460800	-1.17647300	-0.78709800
Li	1.28061600	-0.10472000	1.80897700
Li	-2.03359500	2.43679500	0.36717500
Li	0.95441600	1.56291400	-0.47754000

1f

Be	-0.01738700	0.24015500	-0.16105400

Be	1.19345000	0.59308600	1.38792400
Na	2.63305000	-0.76437400	-0.52259400
Na	-2.79330100	-0.67183100	-0.27670800
Li	1.43053200	2.31561000	-0.20829400
Li	-1.28030700	1.76015800	-1.58428000
Li	-1.05048800	1.53788600	1.52913100
Li	-0.08023200	-1.45855900	1.55839000

1g

Be	1.08594800	1.53041000	-0.14696800
Be	0.30321600	-0.16388300	0.45895200
Na	-2.28487100	-1.14199100	0.38171400
Na	2.86531300	-0.58500900	-0.46629300
Li	-0.51085200	0.48211700	-1.74820100
Li	-3.72542800	1.26775600	-1.26635500
Li	-1.21358100	1.73606100	0.65620400
Li	1.46935300	1.02436400	2.25249500

1h

Be	2.22699000	0.89886200	0.04541800
Be	1.18044200	-0.77663400	-0.02970100
Na	-1.54487200	-1.46006100	-0.02766300
Na	-0.52730800	1.56702400	0.01185800
Li	1.64659300	-0.08582700	2.23087600
Li	3.59085000	-1.15205600	0.01161000
Li	1.74469200	0.04796200	-2.22118300
Li	-3.92738700	0.63475200	0.01569300

1i

Be	0.84409817	0.66289381	0.00000000
Be	-4.71647883	-0.72597519	0.00000000
Na	-1.73243083	0.21943281	0.00000000
Na	1.64520817	-1.81473619	0.00000000
Li	0.97926806	0.84144138	-2.32267503
Li	0.97926806	0.84144138	2.32267503
Li	3.05440717	1.31269681	0.00000000
Li	0.46502917	2.93464081	0.00000000

$Be_2Li_4K_2$--(2)

2a

Be	0.12555200	0.96487000	0.00000000
Be	-0.12555200	-0.96487000	0.00000000
K	-1.56249500	-3.74218300	0.00000000
K	1.56249500	3.74218300	0.00000000
Li	-1.56249500	0.16964400	1.55385300
Li	1.56249500	-0.16964400	1.55385300
Li	1.56249500	-0.16964400	-1.55385300
Li	-1.56249500	0.16964400	-1.55385300

2b

Be	0.16434200	0.60593600	-0.21189700
Be	-1.44473900	1.58429600	0.32065400
Li	-1.12960200	1.64939100	-2.03281200
Li	-2.89379000	3.47736900	0.10178300
Li	0.46328700	2.98235600	0.11940300
Li	-0.05463700	0.84875400	2.18680300

K	-2.30705900	-1.47330000	-0.01053000
K	3.14736500	-0.40220200	-0.07160500

2c

Be	0.97729306	0.04474473	1.00218112
Be	-0.97729306	-0.04474473	1.00218112
Li	0.07051381	-1.44623248	2.63779779
Li	-0.07051381	1.44623248	2.63779779
Li	-3.07171613	-0.26825147	2.15211141
Li	3.07171613	0.26825147	2.15211141
K	-0.04730265	2.38130894	-0.96376278
K	0.04730265	-2.38130894	-0.96376278

2d

Be	0.44699520	-0.87755399	0.00000000
Be	-0.44699520	0.87755399	0.00000000
Li	1.90536794	1.13613119	0.00000000
Li	-0.49312534	3.31477988	0.00000000
Li	-1.90536794	-1.13613119	0.00000000
Li	0.49312534	-3.31477988	0.00000000
K	-0.00000000	-0.00000000	3.04895324
K	-0.00000000	-0.00000000	-3.04895324

2e

Be	0.00000000	0.00000000	0.53533585
Be	0.00000000	-0.00000000	-1.45984216
Li	-2.22033951	0.00000000	-0.53274565
Li	-1.50242518	0.00000000	2.42709954
Li	1.50242518	0.00000000	2.42709954

Li	2.22033951	0.00000000	-0.53274565
K	0.00000000	3.09030519	-0.20248820
K	0.00000000	-3.09030519	-0.20248820

2f

Be	-1.06826600	1.92041700	0.04327400
Be	-0.15330800	0.15382100	0.04903300
Li	-0.52436300	1.01062100	2.27476800
Li	4.49041500	2.28003700	-0.14422400
Li	1.40653300	2.08322400	0.08500500
Li	-0.39520400	1.05784400	-2.17416800
K	-3.35296700	-0.42231500	-0.03572800
K	2.82423800	-1.02990200	0.00976100

2g

Be	0.54001895	0.94370387	0.00000000
Be	-1.42853402	0.60486570	0.00000000
Li	-0.66964530	2.53692257	1.38889208
Li	-0.66964530	2.53692257	-1.38889208
Li	1.79309177	3.02173196	0.00000000
Li	-0.09969644	5.36874278	0.00000000
K	0.06555495	-1.21883675	2.34639141
K	0.06555495	-1.21883675	-2.34639141

2h

Be	0.01586700	0.92549200	-0.43854600
Be	-0.29407200	0.67359100	1.51970900
Li	4.53500600	2.24962200	-0.42221000
Li	1.75536300	2.15526200	-1.60574800

Li	-0.90052300	2.90453700	0.56753700
Li	1.85686600	1.79485100	1.06059600
K	1.91680300	-1.54691900	0.02415400
K	-3.00245100	-0.22724700	-0.18863700

2i

Be	0.13162000	-0.25358600	0.75441800
Be	0.23563200	-0.99092700	-1.09824700
Li	-1.90841400	3.94139100	-0.19536600
Li	0.48333200	-2.68204200	0.76346200
Li	-0.20982400	1.45116000	-1.09417900
Li	-0.45715200	1.98247800	1.54970100
K	-2.94371800	-0.51639800	-0.04516400
K	3.19672700	0.03740200	-0.04407500

Part B-----$Be_2Na_4Y_2$

$Be_2Na_4Li_2$--(3)

3a

Be	0.94904979	-0.34264273	0.00934959
Be	-0.94222454	0.00277934	-0.35611765
Na	0.53862045	2.34913405	-0.25709787
Na	-0.55231394	-0.20028335	2.34465472
Na	-3.50505206	-0.44676194	-0.85534937
Na	3.51112815	-0.86984627	-0.40993681
Li	-0.42358410	-2.30766604	-0.24352041
Li	0.44241421	-0.29073859	-2.30911461

3b

Be	0.28998386	0.93468815	0.00000000
Be	-0.28998386	-0.93468815	0.00000000
Na	0.00000000	0.00000000	2.54091400
Na	0.09492680	3.58938658	0.00000000
Na	0.00000000	0.00000000	-2.54091400
Na	-0.09492680	-3.58938658	0.00000000
Li	2.09352068	-0.75148115	0.00000000
Li	-2.09352068	0.75148115	0.00000000

3c

Be	-1.47637336	0.18873912	-0.17491836
Be	0.46672005	-0.07526268	-0.36915360
Na	-0.23638050	0.01257027	2.29445574
Na	-0.26654585	2.59379752	-0.36666265
Na	-0.97961962	-2.44798718	-0.38504428
Na	3.10609968	-0.35330197	-0.44988282
Li	-3.76350083	0.45539829	-0.85228072
Li	-0.84332495	0.10801142	-2.42946537

3d

Be	1.47885560	1.16144287	0.00000000
Be	-0.44233353	0.68756630	0.00000000
Na	0.03199281	2.65765976	1.88294694
Na	0.87704268	-3.88185777	0.00000000
Na	-1.81284224	-1.69295498	0.00000000
Na	0.03199281	2.65765976	-1.88294694
Li	0.88923802	-0.76418616	1.41370098
Li	0.88923802	-0.76418616	-1.41370098

3e

Be	1.31421507	0.60018476	-1.38518912
Be	-0.09211059	0.32799324	0.00478057
Na	2.18456172	1.67503006	1.02017597
Na	-1.44379738	-1.91394775	0.83462139
Na	1.89412353	-1.81472772	-0.43200692
Na	-2.83700572	1.14422545	0.01354148
Li	-0.13618385	2.47182773	-1.23572935
Li	-0.75219002	-0.37485855	-2.19027634

3f

Be	0.11053788	0.98669195	0.00000000
Be	-0.11053788	-0.98669195	0.00000000
Na	-1.79743774	0.16066642	1.80378136
Na	1.79743774	-0.16066642	1.80378136
Na	1.79743774	-0.16066642	-1.80378136
Na	-1.79743774	0.16066642	-1.80378136
Li	0.59440022	3.34475163	0.00000000
Li	-0.59440022	-3.34475163	0.00000000

3g

Be	0.64568638	0.09766923	0.61604296
Be	1.10017737	-0.08774739	-1.32677877
Na	-4.16353396	0.47524360	0.11482371
Na	-0.84063902	-1.97348334	-0.37256005
Na	3.03668883	-1.25341515	0.42087828
Na	2.01684117	2.31004704	-0.14052383
Li	-1.05331629	1.06318949	-0.91518464

Li	-1.45547779	0.54281017	1.77989926

3h

Be	0.00000000	0.00000000	-1.21077243
Be	0.00000000	0.00000000	0.76218616
Na	-1.89590485	1.79622423	-0.31313712
Na	1.89590485	-1.79622423	-0.31313712
Na	1.89590485	1.79622423	-0.31313712
Na	-1.89590485	-1.79622423	-0.31313712
Li	0.00000000	1.56825538	2.59542805
Li	0.00000000	-1.56825538	2.59542805

3i

Be	-0.54645610	5.06575783	0.00000000
Be	0.37506279	-0.60621028	0.00000000
Na	0.19399167	2.03243586	0.00000000
Na	-2.20514846	-1.15678214	0.00000000
Na	0.55875196	-0.78616521	2.60961152
Na	0.55875196	-0.78616521	-2.60961152
Li	2.70844552	-0.46530277	0.00000000
Li	0.79476041	-2.90892013	0.00000000

Be_2Na_6--(4)

4a

Be	-0.98773927	0.04977411	0.00000000
Be	0.98773927	-0.04977411	0.00000000
Na	-0.00000000	0.00000000	2.54774393
Na	-0.10588406	-2.54478925	0.00000000

Na	0.10588406	2.54478925	0.00000000
Na	-0.00000000	0.00000000	-2.54774393
Na	3.62219474	0.02511650	0.00000000
Na	-3.62219474	-0.02511650	0.00000000

4b

Be	-0.00000000	0.00000000	1.75596471
Be	0.00000000	0.00000000	-0.22766120
Na	1.38191065	2.21810430	0.96080296
Na	-1.38191065	-2.21810430	0.96080296
Na	-2.29768467	1.24338865	0.96184815
Na	2.29768467	-1.24338865	0.96184815
Na	0.48053193	-1.81663674	-2.19883788
Na	-0.48053193	1.81663674	-2.19883788

4c

Be	-0.55963085	-0.89162007	0.00000000
Be	1.36449420	-1.49683692	0.00000000
Na	0.96650808	0.67266204	1.74612319
Na	0.19018177	4.06093499	0.00000000
Na	-0.22018474	-2.99001703	-1.78943680
Na	0.96650808	0.67266204	-1.74612319
Na	-1.97890403	1.43538382	0.00000000
Na	-0.22018474	-2.99001703	1.78943680

4d

Be	0.00000000	0.00000000	-5.47453595
Be	0.00000000	0.00000000	0.28647305
Na	0.00000000	0.00000000	-2.36623795

Na	0.00000000	2.64723600	0.32664505
Na	0.00000000	-2.64723600	0.32664505
Na	2.64723600	0.00000000	0.32664505
Na	-2.64723600	-0.00000000	0.32664505
Na	0.00000000	0.00000000	2.94541205

$Be_2Na_4K_2$--(5)

5a

Be	0.00000000	0.00000000	0.98728200
Be	0.00000000	0.00000000	-0.98728200
Na	0.00000000	2.57403700	0.00000000
Na	2.57403700	0.00000000	0.00000000
Na	-2.57403700	0.00000000	0.00000000
Na	0.00000000	-2.57403700	0.00000000
K	0.00000000	0.00000000	4.10466800
K	0.00000000	0.00000000	-4.10466800

5b

Be	1.34538860	-0.47305345	0.13415161
Be	-0.58075279	-0.08590406	-0.06096712
Na	0.56264303	-0.51209517	-2.51361635
Na	0.04975074	-0.29480981	2.59077482
Na	3.93723562	-1.00601710	0.08515801
Na	-0.14791529	-2.83153922	0.10084709
K	-3.70250441	0.09326112	-0.14478334
K	0.99316766	2.71331279	-0.02298177

5c

Be	-0.97506026	-0.05010186	0.36008350
Be	0.99419721	0.05184145	0.30916253
Na	0.15058559	-1.73828966	2.26902914
Na	-3.60507450	-0.17188349	0.60707491
Na	3.63129609	0.17555142	0.45754381
Na	-0.02806495	1.75277697	2.26289136
K	0.07957877	-2.28948494	-1.68680733
K	-0.16972153	2.27860779	-1.69418823

5d

Be	0.03070464	-0.96475075	0.21484807
Be	-0.03070464	0.96475075	-0.21484807
Na	-0.01096041	0.59456196	2.49449324
Na	0.11649140	-3.60970289	0.38879205
Na	0.01096041	-0.59456196	-2.49449324
Na	-0.11649140	3.60970289	-0.38879205
K	-3.09053315	-0.08571911	0.00326777
K	3.09053315	0.08571911	-0.00326777

5e

Be	-0.10969343	0.08178979	0.09600017
Be	0.91691862	-1.51902196	0.71733804
Na	-1.65280803	-1.91035845	1.63662972
Na	0.83819882	0.33455663	2.75567022
Na	0.51067950	2.77326425	0.06910140
Na	-0.19599745	-2.08968188	-1.74034344
K	3.19251836	-0.03752314	-0.87664031
K	-3.07302899	0.85664643	-0.86993811

5f

Be	1.41333547	0.29649360	-0.00906858
Be	2.05340387	-1.62364991	0.04897825
Na	-0.09452997	-1.15359820	1.80412919
Na	3.54477163	-0.00926359	1.78438157
Na	-0.07692347	-1.24502071	-1.75652908
Na	3.55707218	-0.12053671	-1.77187227
K	-3.89050317	-0.73942232	0.01573393
K	-0.85166797	2.48264530	-0.05893614

5g

Be	-1.04593712	-0.24942638	-0.32183475
Be	-1.90177942	0.77107263	1.21155776
Na	3.84851247	0.19282387	0.75363593
Na	0.46752708	-0.50230176	2.04894428
Na	-2.83915318	-1.89027531	1.09671322
Na	-3.53176247	0.82938415	-1.06585779
K	0.44375480	2.58491550	-0.32655534
K	1.36648222	-1.90136421	-1.50116487

5h

Be	0.67579041	-1.09889879	0.00000000
Be	-1.24465654	-1.74430138	0.00000000
Na	2.19771703	1.14828790	0.00000000
Na	0.44233493	-3.26669672	1.74808952
Na	0.44233493	-3.26669672	-1.74808952
Na	0.51269088	4.11262295	0.00000000
K	-0.98031852	0.66793305	-2.22367256

K	-0.98031852	0.66793305	2.22367256

5i

Be	-1.14209297	0.86168495	1.29168578
Be	-0.60742765	0.29359158	-0.57849600
Na	0.57945960	-1.33427448	1.44846731
Na	-2.47913025	2.38575455	-0.66288114
Na	1.15729883	-1.28966751	-1.88058942
Na	4.00184001	-1.58389349	0.02183907
K	1.79316545	2.22103033	0.30736284
K	-3.31190585	-1.40935747	0.16379752