Electronic Supplementary Information

Computational design of species with the ultrashort Be-Be distances using planar hexacoordinate carbon structures as the templates

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Fig. S1. AdNDP view of chemical bonding in **1** and **4**–**9**.

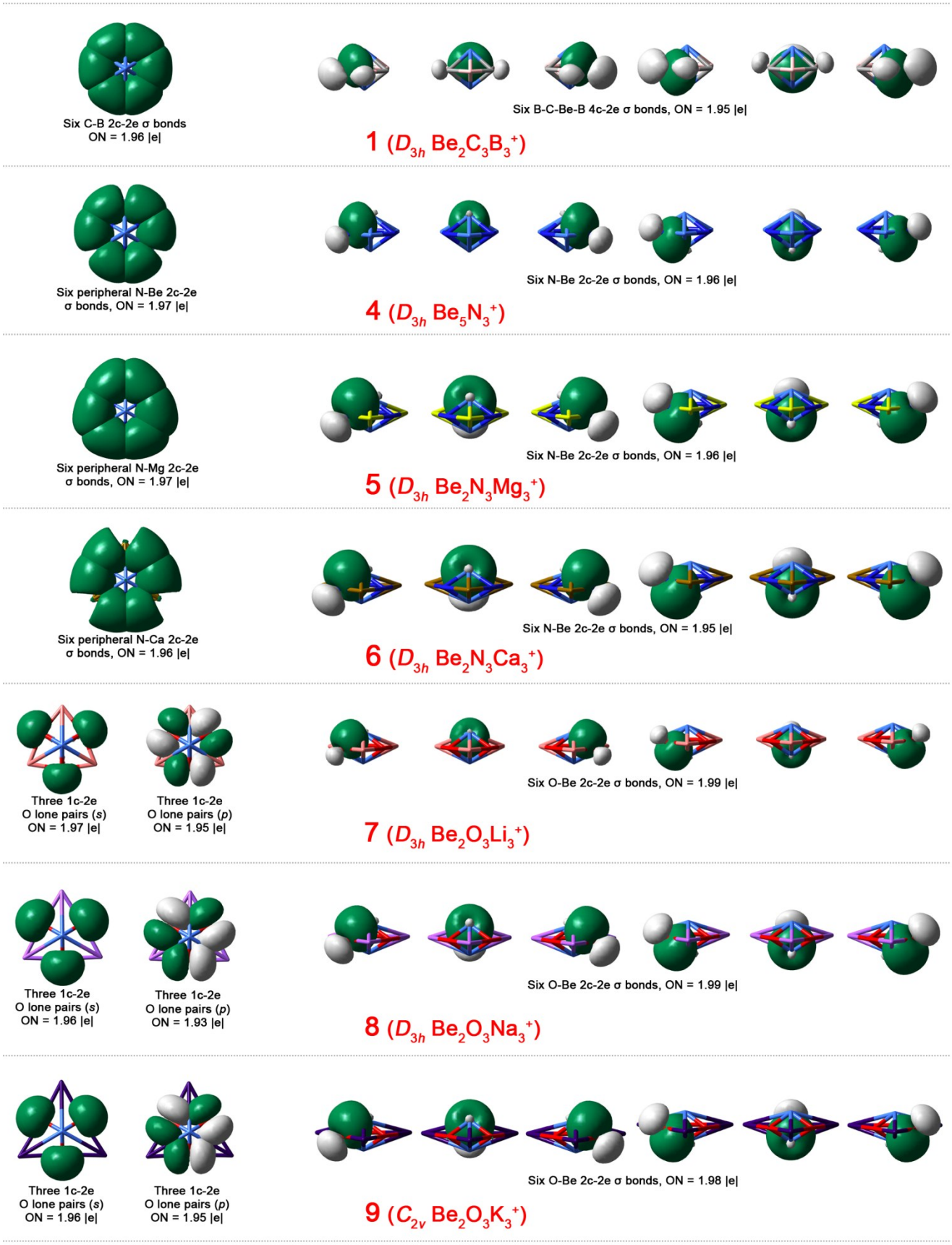
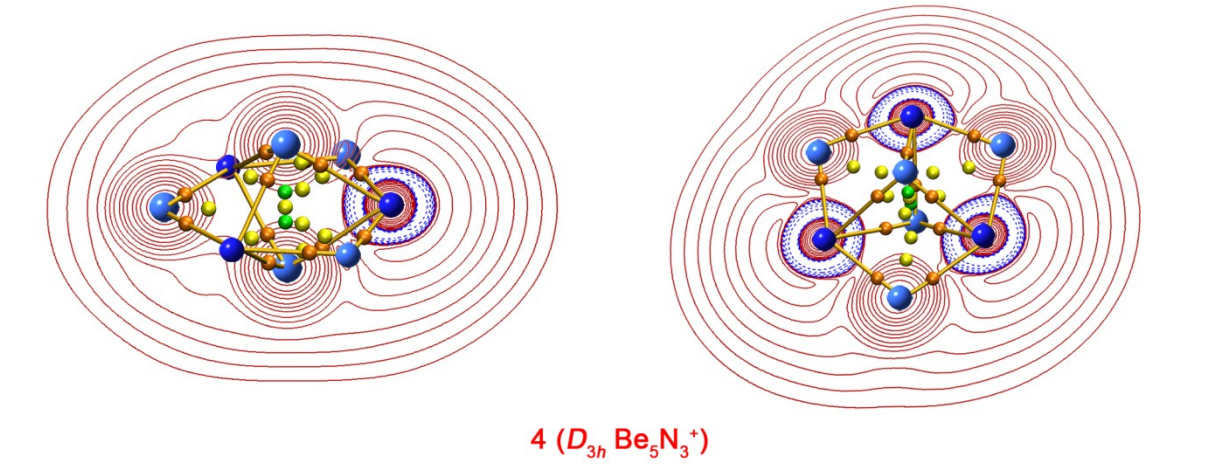
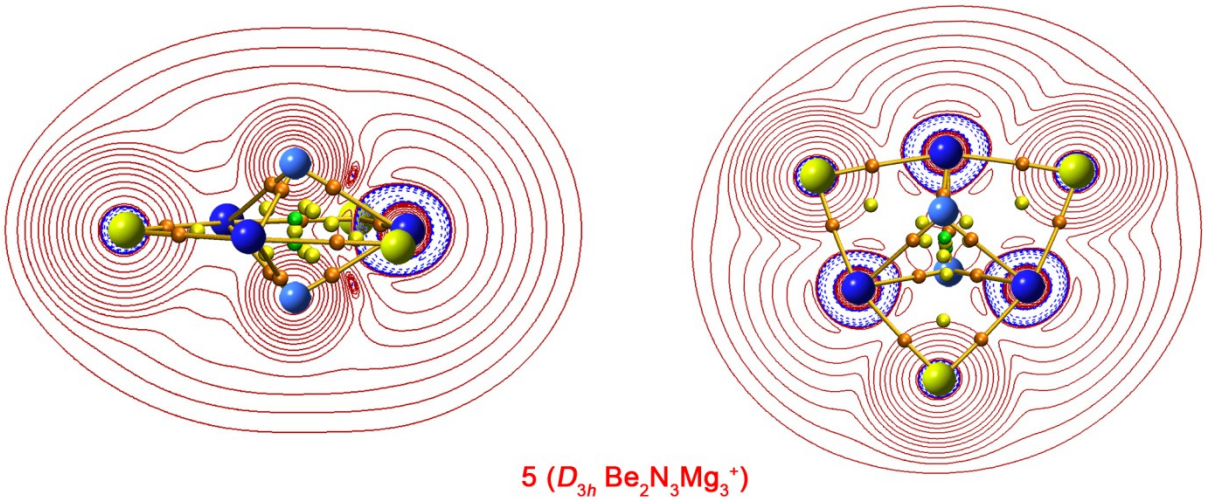


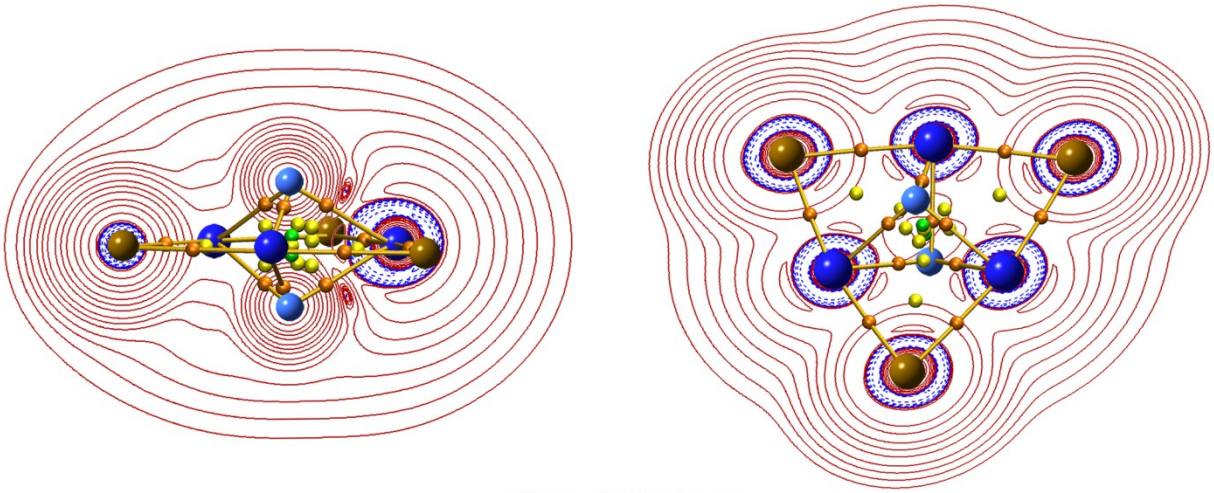
Fig. S2. QTAIM results of **4–6** concerning critical points and bond paths.



4 (D_{3h} $Be_5N_3^+$)

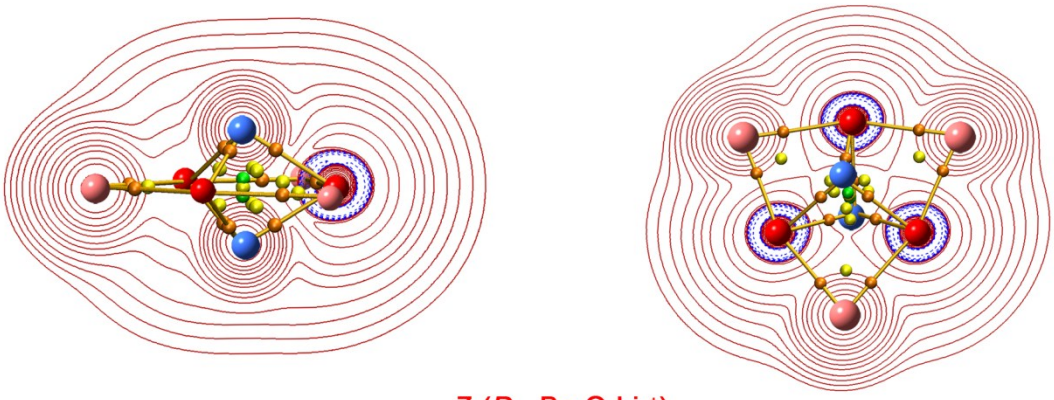


5 (D_{3h} $Be_2N_3Mg_3^+$)

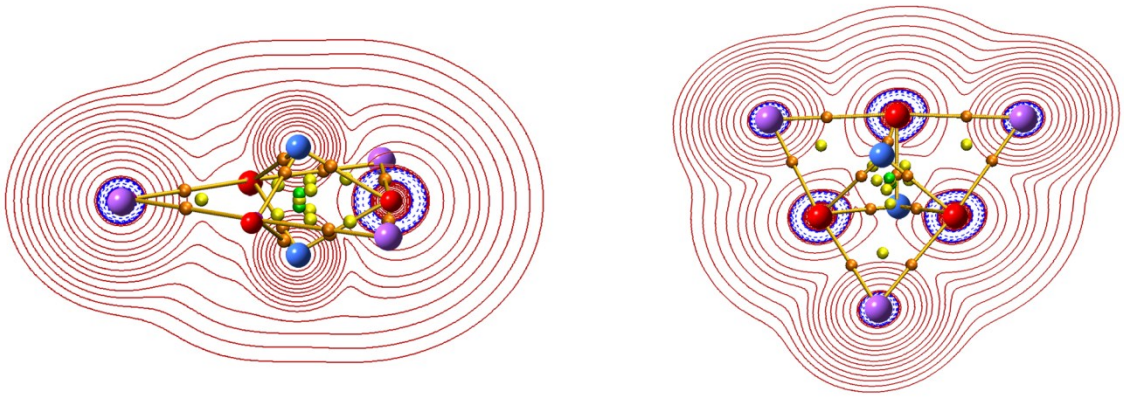


6 (D_{3h} $Be_2N_3Ca_3^+$)

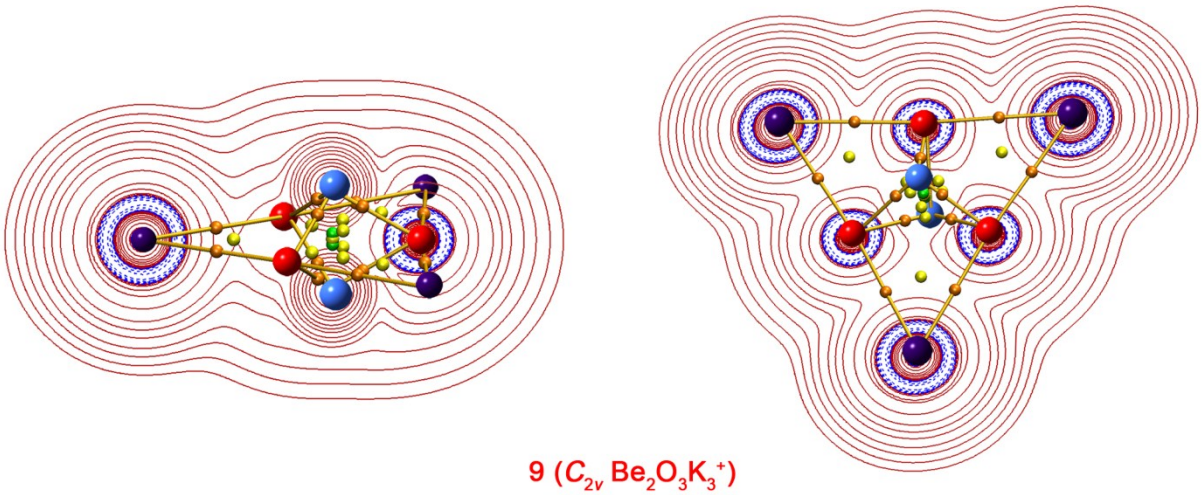
Fig. S3. QTAIM results of **7–9** concerning critical points and bond paths



7 (D_{3h} $Be_2O_3Li_3^+$)



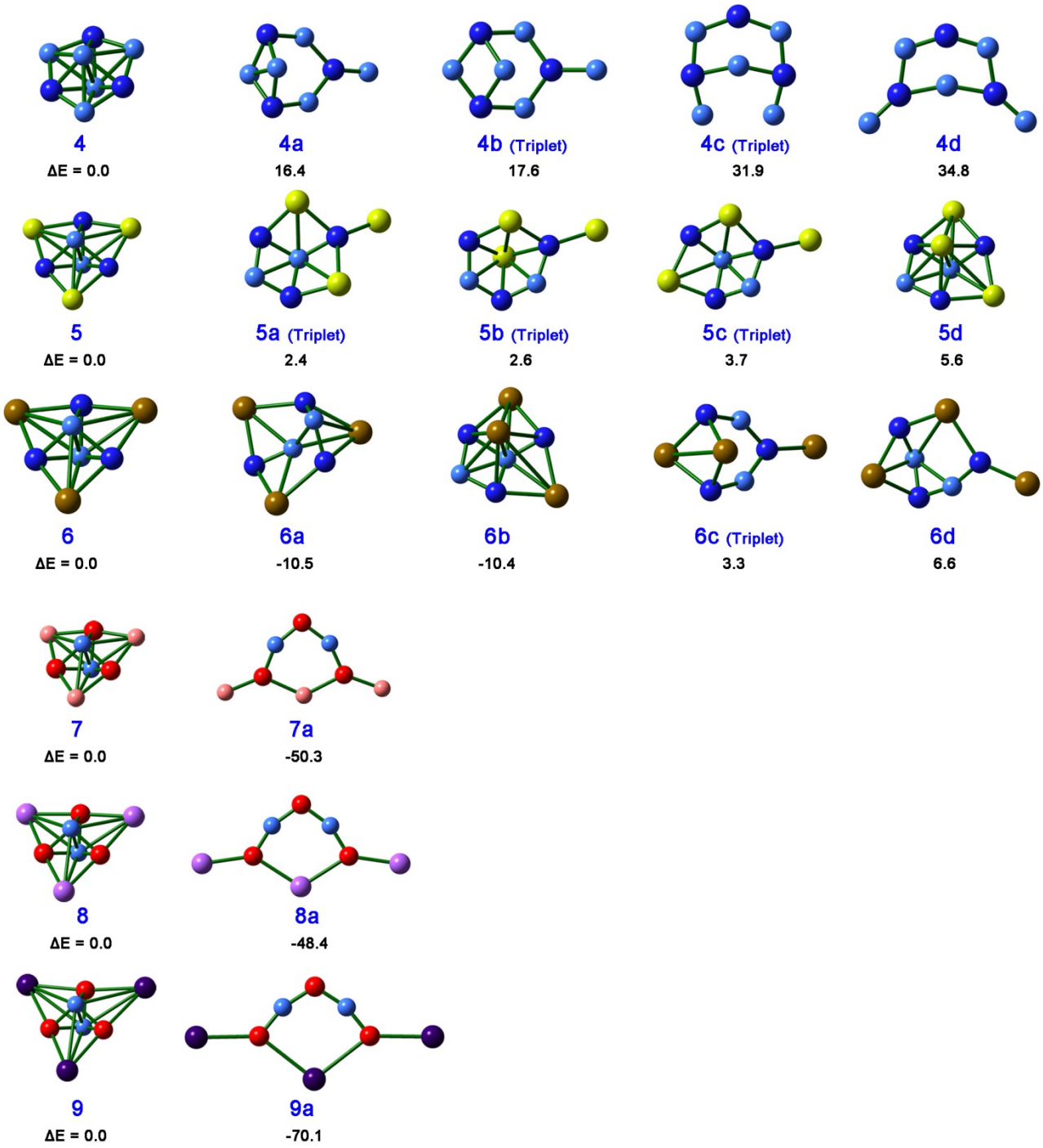
8 (D_{3h} $Be_2O_3Na_3^+$)



9 (C_{2v} $Be_2O_3K_3^+$)

Fig. S4. The structures and **4**–**9** and their lowest-lying isomers

The relative energies (ΔE, in kcal/mol) were compared at the CCSD(T)/BS1 level with the consideration of B3LYP/BS1 zero-point energy corrections.



Cartesian Coordinates for optimized structures of **1–9**.

B3LYP/BS1-optimized structures (in Cartesian coordinates) for **2** and **3**.

2

Be	-0.98674600	0.00000000	-0.01380500
Be	0.98674600	0.00000000	-0.01380500
C	0.00000000	0.00000000	-1.50065400
C	0.00000000	1.25210700	0.74392100
C	0.00000000	-1.25210700	0.74392100
Al	0.00000000	1.86085900	-1.09721700
Al	0.00000000	-1.86085900	-1.09721700
Al	0.00000000	0.00000000	2.20884300

3

Be	-1.05411000	0.00000000	-0.05257800
Be	1.05411000	0.00000000	-0.05257800
C	0.00000000	0.00000000	-1.57773300
C	0.00000000	1.12276600	0.76470000
C	0.00000000	-1.12276600	0.76470000
Ga	0.00000000	1.90607900	-1.22009900
Ga	0.00000000	-1.90607900	-1.22009900
Ga	0.00000000	0.00000000	2.46312100

CCSD(T)/BS1-optimized structures (in Cartesian coordinates) for **1** and **4**–**9**.

1

B	-1.30278194	0.75216637	0.00000000
B	0.00000000	-1.50432154	0.00000000
B	1.30278194	0.75216637	0.00000000
Be	0.00000000	-0.00000134	1.08089630
Be	0.00000000	-0.00000134	-1.08089630
C	0.00000000	1.45362664	0.00000000
C	1.25887181	-0.72681658	0.00000000
C	-1.25887181	-0.72681658	0.00000000

4

Be	0.00000000	0.00000318	0.93519508
Be	0.00000000	-1.71094913	0.00000000
Be	-1.48172718	0.85546982	0.00000000
Be	1.48172718	0.85546982	0.00000000
Be	0.00000000	0.00000318	-0.93519508
N	0.00000000	1.44665591	0.00000000
N	-1.25283858	-0.72332638	0.00000000
N	1.25283858	-0.72332638	0.00000000

5

Be	-0.00000000	0.00000000	-0.86655858
N	0.00000000	1.49427530	-0.00000000
N	1.29408037	-0.74713765	-0.00000000
N	-1.29408037	-0.74713765	-0.00000000
Be	0.00000000	0.00000000	0.86655858
Mg	1.95686104	1.12979425	0.00000000
Mg	-1.95686104	1.12979425	0.00000000
Mg	0.00000000	-2.25958850	0.00000000

6

Be	0.00000000	-0.00000332	0.84908415
N	0.00000000	1.52383549	0.00000000
N	-1.31968094	-0.76191219	0.00000000
N	1.31968094	-0.76191219	0.00000000
Be	0.00000000	-0.00000332	-0.84908415
Ca	2.24522906	1.29628209	0.00000000
Ca	-2.24522906	1.29628209	0.00000000
Ca	0.00000000	-2.59256962	0.00000000

7

Be	-0.83923416	0.00000000	-0.00000888
Be	0.83923416	0.00000000	-0.00000888
O	0.00000000	0.00000000	1.38242966
O	0.00000000	1.19722175	-0.69121360
O	0.00000000	-1.19722175	-0.69121360
Li	0.00000000	0.00000000	-2.20452361
Li	0.00000000	1.90917637	1.10224995
Li	0.00000000	-1.90917637	1.10224995

8

Be	0.00000000	-0.00000000	-0.82417863
Be	0.00000000	-0.00000000	0.82417863
O	1.20963509	-0.69838315	-0.00000000
O	-1.20963509	-0.69838315	-0.00000000
O	-0.00000000	1.39676629	-0.00000000
Na	0.00000000	-2.65058886	-0.00000000
Na	2.29547729	1.32529443	-0.00000000
Na	-2.29547729	1.32529443	-0.00000000

9

Be	0.00000000	-0.02287190	0.81335442
Be	0.00000000	-0.02287190	-0.81335442
O	0.00000000	1.35866093	0.00000000

O	-1.20299723	-0.74232551	0.00000000
O	1.20299723	-0.74232551	0.00000000
K	0.00000000	-2.96945928	0.00000000
K	-2.63096052	1.57059660	0.00000000
K	2.63096052	1.57059660	0.00000000

Cartesian coordinates of structures shown in Fig. S2.

The geometries were optimized at the B3LYP/BS1 level. The total energies (E) were obtained by adding the B3LYP/BS1 zero-point energy corrections to the CCSD(T)/BS1 electronic energies (calculated using B3LYP/BS1 geometries).

4

E = -237.3363931 a.u.

Be	0.00000000	0.00000000	0.92755600
Be	0.00000000	-1.69278400	0.00000000
Be	-1.46599400	0.84639200	0.00000000
Be	1.46599400	0.84639200	0.00000000
Be	0.00000000	0.00000000	-0.92755600
N	0.00000000	1.43228000	0.00000000
N	-1.24039100	-0.71614000	0.00000000
N	1.24039100	-0.71614000	0.00000000

4a

E = -237.3102609 a.u.

Be	0.00706800	-1.35721500	0.90098100
Be	1.16404700	0.44511200	0.00000000
Be	0.00706800	-1.35721500	-0.90098100
Be	-1.11980500	0.40047500	0.00000000
Be	-0.10626600	2.96673900	0.00000000
N	-1.26059500	-1.10428400	0.00000000
N	0.00706800	1.54074100	0.00000000
N	1.28089100	-1.06382700	0.00000000

4b

E = -237.3082718 a.u.

Be	-0.25087500	-0.00007900	0.84489900
Be	2.79032600	0.00001500	0.22982400
Be	0.40066000	1.26132100	-0.48069100
Be	0.40063100	-1.26127900	-0.48089000
Be	-1.96649100	0.00004900	-0.15219900
N	-1.04014400	1.21733000	0.04834400
N	-1.04019200	-1.21730900	0.04808800
N	1.29505000	-0.00003600	-0.07411400

4c

E = -237.285579 a.u.

Be	-0.23109700	1.80029800	1.23657200
Be	0.01572300	-1.11192100	1.47319000
Be	0.01572300	-1.11192100	-1.47319000
Be	-0.23109700	1.80029800	-1.23657200
Be	0.24464400	0.07887200	0.00000000

N	0.01572300	0.41078000	1.58263800
N	0.01572300	0.41078000	-1.58263800
N	0.07489900	-1.65334600	0.00000000

4d

E = -237.2809589 a.u.

Be	0.00000000	0.00000000	-0.18977000
Be	0.00000000	1.40911000	1.08088600
Be	0.00000000	-1.40911000	1.08088600
Be	0.00000000	2.67210100	-1.44910300
Be	0.00000000	-2.67210100	-1.44910300
N	0.00000000	0.00000000	1.51141400
N	0.00000000	-1.63957600	-0.49107800
N	0.00000000	1.63957600	-0.49107800

5

E = -792.2399081 a.u.

Be	0.00000000	0.00000000	0.85868700
N	0.00000000	1.47411000	0.00000000
N	-1.27661600	-0.73705500	0.00000000
N	1.27661600	-0.73705500	0.00000000
Be	0.00000000	0.00000000	-0.85868700
Mg	-1.94580800	1.12341300	0.00000000
Mg	1.94580800	1.12341300	0.00000000
Mg	0.00000000	-2.24682500	0.00000000

5a

E = -792.236107 a.u.

Be	0.28568400	0.94623900	0.00000000
Be	-1.01106300	2.37268200	0.00000000
Mg	-0.58018600	-0.27670200	1.72203000
Mg	1.86185600	-1.99451500	0.00000000
Mg	-0.58018600	-0.27670200	-1.72203000
N	0.37233000	-0.74434900	0.00000000
N	-0.58018600	1.60784100	1.25544100
N	-0.58018600	1.60784100	-1.25544100

5b

E = -792.2357953 a.u.

Be	-0.10597600	-1.01000900	-1.00886000
Be	2.33862800	-0.24476800	-0.58469400
Mg	-2.94313800	-0.15969600	0.06536000
Mg	0.16340800	1.56931700	-0.30580300

Mg	0.73502100	-0.66013600	1.09562400
N	1.35311000	-1.38990200	-0.78232400
N	1.88020400	0.88706100	0.36112700
N	-1.00389800	-0.06497400	-0.13422500

5c

E = -792.2339555 a.u.

Be	0.29105500	-1.28100400	0.79128100
Be	-0.35843300	-0.28793300	-0.66938100
Mg	0.29578900	1.62115600	0.40489000
Mg	-2.64157200	-0.32600100	-0.06308400
Mg	3.07857600	-0.42402100	-0.28398100
N	-1.10458700	-1.47042600	0.20165200
N	1.20046000	-0.15238500	0.18716900
N	-1.31358700	1.02597400	-0.55760800

5d

E = -792.2309866 a.u.

Be	0.79357600	0.15585100	0.00000000
Be	0.43002200	1.97189600	0.00000000
Mg	-1.31457400	0.37378600	0.00000000
Mg	0.28140300	-0.80299700	1.95834000
Mg	0.28140300	-0.80299700	-1.95834000
N	0.02674100	-1.27354200	0.00000000
N	0.28140300	1.08502200	1.28568400
N	0.28140300	1.08502200	-1.28568400

6

E = -2223.787451 a.u.

Be	0.00000000	0.00000000	0.84143300
N	0.00000000	1.50076800	0.00000000
N	-1.29970300	-0.75038400	0.00000000
N	1.29970300	-0.75038400	0.00000000
Be	0.00000000	0.00000000	-0.84143300
Ca	2.17332900	1.25477200	0.00000000
Ca	-2.17332900	1.25477200	0.00000000
Ca	0.00000000	-2.50954500	0.00000000

6a

E = -2223.804207 a.u.

Be	0.12522700	-0.12236600	0.00000000
Be	-1.16466300	1.17470800	0.00000000
N	0.15351400	-1.66394400	0.00000000

N	-0.32190600	0.91172900	1.28569800
N	-0.32190600	0.91172900	-1.28569800
Ca	-0.32190600	-1.25205800	-2.06538700
Ca	-0.32190600	-1.25205800	2.06538700
Ca	1.02330400	2.23781800	0.00000000

6b

E = -2223.80409 a.u.

Be	-0.77246000	2.02816600	0.00000000
Be	-0.71957800	0.20423300	0.00000000
N	-0.45296000	1.20885200	1.29141200
N	-0.45296000	1.20885200	-1.29141200
N	0.03464300	-1.19153500	0.00000000
Ca	-0.45296000	-0.83383600	-2.16369700
Ca	-0.45296000	-0.83383600	2.16369700
Ca	1.50927300	0.79203300	0.00000000

6c

E = -2223.782156 a.u.

Be	0.36883900	0.00226000	-1.06711000
Be	0.36891400	0.00064800	1.06814600
N	-1.15238000	0.00033400	-1.32433600
N	1.47069700	0.00361100	0.00049300
N	-1.15259300	-0.00075500	1.32471600
Ca	3.59139500	-0.00063600	-0.00018400
Ca	-1.72293600	-1.66001300	-0.00042000
Ca	-1.72401400	1.65895100	0.00009100

6d

E = -2223.776893 a.u.

Be	1.34691000	-0.14776600	1.32396200
Be	-0.34919800	-0.99918100	0.35416500
N	0.96374200	-1.56539000	0.84149800
N	-1.41269400	0.03449400	-0.11815200
N	1.89472400	1.00601700	0.48868800
Ca	-3.29799800	-0.59046600	-0.12657500
Ca	0.04241000	1.85774600	-0.07941100
Ca	2.55002600	-0.85418300	-0.55385100

7

E = -277.3375228 a.u.

Be	-0.83415400	0.00000000	0.00000100
Be	0.83415400	0.00000000	0.00000100

O	0.00000000	0.00000000	1.37454300
O	0.00000000	1.19038500	-0.68726100
O	0.00000000	-1.19038500	-0.68726100
Li	0.00000000	0.00000000	-2.17090600
Li	0.00000000	1.88007200	1.08542300
Li	0.00000000	-1.88007200	1.08542300

7a

E = -277.4176313 a.u.

Be	0.00000000	1.12857700	0.78306300
Be	0.00000000	-1.12857700	0.78306300
O	0.00000000	-1.68691100	-0.54103800
O	0.00000000	1.68691100	-0.54103800
O	0.00000000	0.00000000	1.67411600
Li	0.00000000	-3.26328900	-1.15364700
Li	0.00000000	3.26328900	-1.15364700
Li	0.00000000	0.00000000	-1.35964900

8

E = -740.5416052 a.u.

Be	0.00000000	0.00000000	0.81949100
Be	0.00000000	0.00000000	-0.81949100
O	0.00000000	1.38798900	0.00000000
O	-1.20203400	-0.69399400	0.00000000
O	1.20203400	-0.69399400	0.00000000
Na	-2.25163400	1.29998100	0.00000000
Na	2.25163400	1.29998100	0.00000000
Na	0.00000000	-2.59996300	0.00000000

8a

E = -740.6187442 a.u.

Be	0.00000000	1.17129100	-1.11663400
Be	0.00000000	-1.17129100	-1.11663400
O	0.00000000	-1.91748100	0.09394300
O	0.00000000	1.91748100	0.09394300
O	0.00000000	0.00000000	-1.95981000
Na	0.00000000	3.96795600	0.39469800
Na	0.00000000	-3.96795600	0.39469800
Na	0.00000000	0.00000000	1.31137400

9

E = -2052.229119 a.u.

Be	0.00000000	0.00000000	0.81282600
Be	0.00000000	0.00000000	-0.81282600
O	0.00000000	1.39388802	0.00000000
O	-1.20694600	-0.69681498	0.00000000
O	1.20694600	-0.69681498	0.00000000
K	-0.00000000	-2.98293798	0.00000000
K	-2.58310900	1.49141002	0.00000000
K	2.58310900	1.49141002	0.00000000

9a

E = -2052.340785 a.u.

Be	0.00000000	1.21314900	-1.19701100
Be	0.00000000	-1.21314900	-1.19701100
O	0.00000000	2.10427300	-0.09809100
O	0.00000000	-2.10427300	-0.09809100
O	0.00000000	0.00000000	-1.98187600
K	0.00000000	4.49289300	-0.06237500
K	0.00000000	0.00000000	1.54583000
K	0.00000000	-4.49289300	-0.06237500