

D_{3h} CN_3Be_3^+ and CO_3Li_3^+ : Viable Planar Hexacoordinate Carbon Prototypes

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ESI 1: The Figures mentioned in the text.

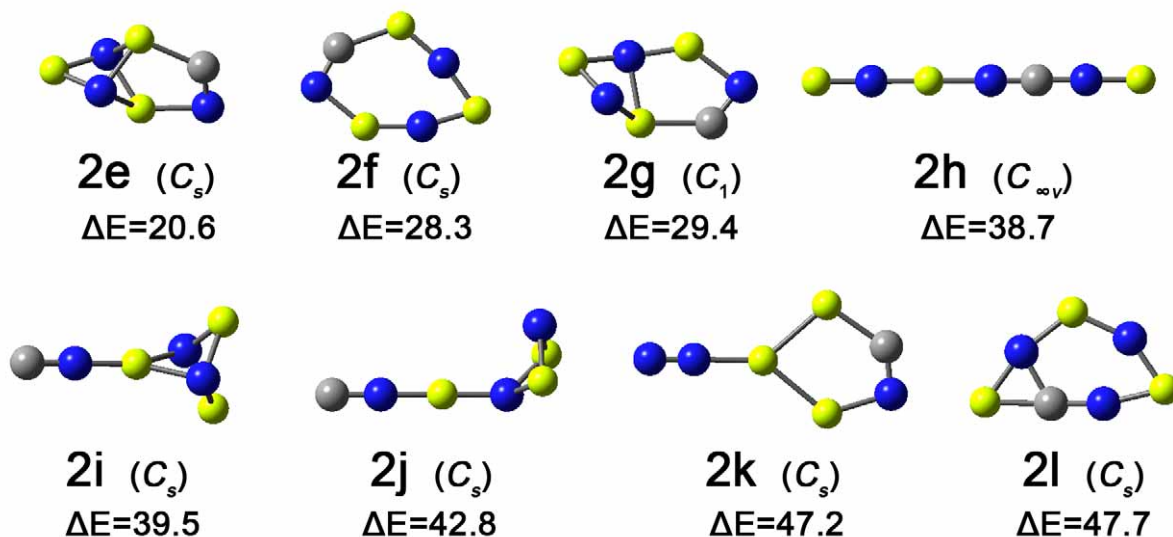


Fig. S1. The CCSD(T)/aug-cc-pVTZ optimized structures and relative energies (in Å, relative to **2a**) of higher lying isomers of CN_3Be_3^+ (within 50 kcal/mol).

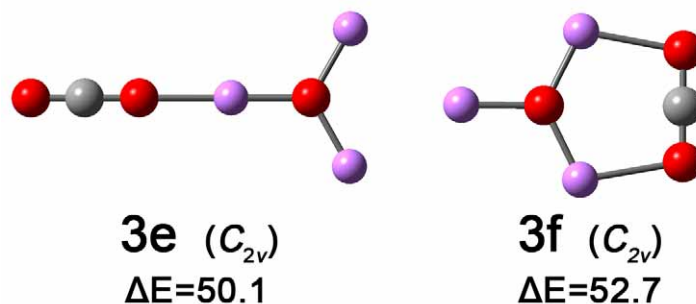


Fig. S2. The CCSD(T)/aug-cc-pVTZ optimized structures and relative energies (in Å, relative to **3a**) of higher lying isomers of CO_3Li_3^+ (within 100 kcal/mol).

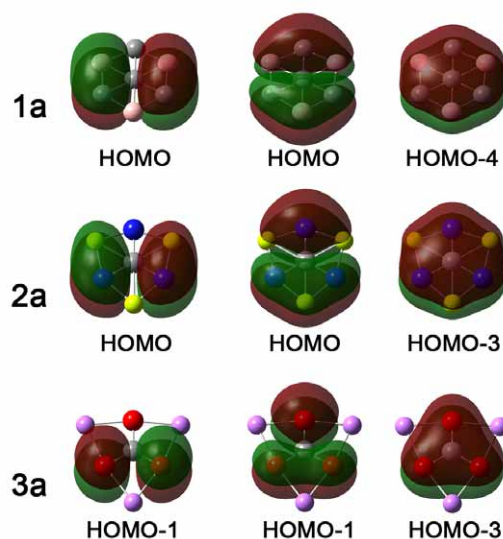
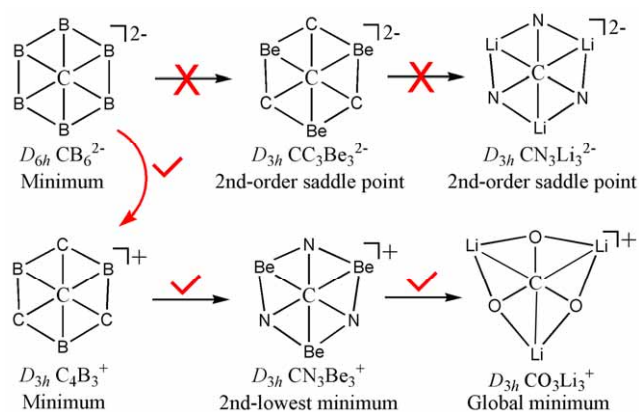


Fig. S3. The three occupied π MOs of **1a-3a**. Note the greater ionic character of the **3a** set.

ESI 2: The Scheme describing the designing idea of this work.



Scheme 1. Two ways to design the new species with phC. *: D_{3h} $\text{CN}_3\text{Li}_3^{2-}$ is studied at B3LYP/cc-pVTZ level.

ESI 3: The Cartesian coordinates of CCSD(T)/aug-cc-pVTZ optimized structures (in Cartesian coordinates) of species mentioned in the text and ESI. The CCSD(T)/aug-cc-pVTZ energies are given in the notation lines of .xyz format.

1a

CCSD(T)/aug-cc-pVTZ ENERGY=-225.82512591

C	0.0000000000	-0.0000023151	0.0000000000
C	0.0000000000	1.4545772675	0.0000000000
B	1.3382457021	0.7726385195	0.0000000000
C	1.2596951215	-0.7272933208	0.0000000000
B	0.0000000000	-1.5452653499	0.0000000000
C	-1.2596951215	-0.7272933208	0.0000000000
B	-1.3382457021	0.7726385195	0.0000000000

1b

CCSD(T)/aug-cc-pVTZ ENERGY=-225.88860987

C	0.0000000000	2.2689200793	-0.3601047293
C	0.0000000000	1.4167487332	0.6509242089
C	0.0000000000	-1.4167487332	0.6509242089
C	0.0000000000	-2.2689200793	-0.3601047293
B	0.0000000000	0.8202357569	-0.8481377205
B	0.0000000000	0.0000000000	1.0020564818
B	0.0000000000	-0.8202357569	-0.8481377205

2a

CCSD(T)/aug-cc-pVTZ ENERGY=-245.91168122

C	0.0000000000	0.0000000000	-0.0000125549
N	0.0000000000	0.0000000000	1.3780514673
N	0.0000000000	1.1934113459	-0.6890209649
N	0.0000000000	-1.1934113459	-0.6890209649
Be	0.0000000000	1.5167752142	0.8757128993
Be	0.0000000000	-1.5167752142	0.8757128993
Be	0.0000000000	0.0000000000	-1.7514227811

2b

CCSD(T)/aug-cc-pVTZ ENERGY=-245.92139539

C	-1.2485790479	-0.3715898665	0.0000000000
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N	1.3952778801	0.4152472591	0.0000000000
N	-0.7920419552	-1.5275824849	0.0000000000
N	-1.4984393204	0.8459183396	0.0000000000
Be	0.0019210688	1.2062090978	0.0000000000
Be	0.6611709898	-1.0088701854	0.0000000000
Be	2.7762863847	0.8262558402	0.0000000000

2c

CCSD(T)/aug-cc-pVTZ ENERGY=-245.90670794			
C	0.3282823566	1.0099511032	0.0000000000
N	-0.9633737530	0.9954165256	0.0000000000
N	1.4914967430	0.6634131646	0.0000000000
N	-0.3512122696	-1.5044974892	0.0000000000
Be	-0.9497995352	-0.4185892227	0.9539303588
Be	-0.9497995352	-0.4185892227	-0.9539303588
Be	1.0926739934	-0.9470198588	0.0000000000

2d

CCSD(T)/aug-cc-pVTZ ENERGY=-245.88709826			
C	-0.0015186983	1.7857557224	0.0000000000
N	-0.0002859725	0.4504463704	0.0000000000
N	0.0019580412	-2.0631451024	0.0000000000
N	-0.0027195113	2.9531136140	0.0000000000
Be	0.9429861375	-0.7646399976	0.0000000000
Be	-0.9414435444	-0.7662715235	0.0000000000
Be	0.0023005478	-3.4939410833	0.0000000000

2e

CCSD(T)/aug-cc-pVTZ ENERGY=-245.87879516			
C	1.5377314090	0.6320444537	0.0001984135
N	-0.9328909087	-0.0221183175	0.9032161966
N	1.8191864222	-0.5134466708	0.0004892518
N	-0.9327843206	-0.0223485548	-0.9036053992
Be	-0.1804783996	1.1351719237	-0.0002665593
Be	0.1447771056	-0.9018483402	0.0000196906
Be	-2.1901333078	-0.2023264940	-0.0002355940

2f

CCSD(T)/aug-cc-pVTZ ENERGY=-245.86664024			
C	-1.6789229377	-0.0683329201	0.0000000000
N	0.8711967163	-1.1857219481	0.0000000000

N	-1.6347681488	1.1077361656	0.0000000000
N	1.2625708682	0.5274983898	0.0000000000
Be	-0.0059743917	1.3238968867	0.0000000000
Be	2.2579660680	-0.5911687165	0.0000000000
Be	-0.5963921742	-1.4203388573	0.0000000000

2g

CCSD(T)/aug-cc-pVTZ ENERGY=-245.86487338			
C	1.4609939382	-0.6875182509	-0.2624514950
N	2.0708548271	0.2035436676	0.2228562529
N	-1.4831416381	-0.7673930094	0.5152351466
N	-0.7636712161	0.7934496489	-0.2751100645
Be	-2.2465018949	0.3833324055	-0.1412651847
Be	-0.3231755991	-0.8664696263	-0.5051728566
Be	0.6614035829	1.0768671645	0.2289992012

2h

CCSD(T)/aug-cc-pVTZ ENERGY=-245.84996656			
C	-0.0426162905	1.3323871083	0.0000000000
N	0.0917531125	-2.8887463689	0.0000000000
N	-0.0030081739	0.1564505482	0.0000000000
N	-0.0843293779	2.5885169314	0.0000000000
Be	0.0464235885	-1.4269175358	0.0000000000
Be	-0.1311100034	3.9817913020	0.0000000000
Be	0.1384871447	-4.2924739853	0.0000000000

2i

CCSD(T)/aug-cc-pVTZ ENERGY=-245.84878194			
C	2.9545827040	-0.0000399983	-0.0001705343
N	-1.1926447072	0.9254363475	0.0001033492
N	-1.1927856828	-0.9253226461	0.0001630546
N	1.7666702195	-0.0001705630	-0.0003706330
Be	-1.7954669746	0.0001471144	1.1147217766
Be	0.2396477677	-0.0001197062	-0.0004073624
Be	-1.7965043266	0.0000774517	-1.1138886507

2j

CCSD(T)/aug-cc-pVTZ ENERGY=-245.84352555			
C	-0.0827820604	3.2790147885	0.0000000000
N	0.1106697884	2.1038552841	0.0000000000
N	0.6256425221	-0.9451619032	0.0000000000
N	-0.9814919967	-2.0517108530	0.0000000000

Be	0.1016664885	-1.9765095344	1.0790637663
Be	0.3532057698	0.6157257523	0.0000000000
Be	0.1016664885	-1.9765095344	-1.0790637663

2k

CCSD(T)/aug-cc-pVTZ ENERGY=-245.83639208			
C	0.7699101655	-2.4349238313	0.0000000000
N	-0.3776506124	-2.7195650809	0.0000000000
N	-0.2147789788	2.2733315550	0.0000000000
N	-0.3561834716	3.3678161837	0.0000000000
Be	-1.0810989359	-1.2075772664	0.0000000000
Be	-0.0022007194	0.5616743151	0.0000000000
Be	1.5840035525	-0.8136528753	0.0000000000

2l

CCSD(T)/aug-cc-pVTZ ENERGY=-245.83562157			
C	0.0014792457	0.9871189449	0.0000000000
N	-1.3405795963	0.4700676651	0.0000000000
N	1.0029261389	0.1800332103	0.0000000000
N	0.5173928219	-1.4393465028	0.0000000000
Be	1.9420059805	-1.0240362357	0.0000000000
Be	-1.2735548290	1.9693713026	0.0000000000
Be	-0.9706337617	-1.0524773844	0.0000000000

3a

CCSD(T)/aug-cc-pVTZ ENERGY=-285.92309032			
C	0.0000000000	-0.0000156457	0.0000000000
O	0.0000000000	1.2915911393	0.0000000000
O	1.1185290290	-0.6457882358	0.0000000000
O	-1.1185290290	-0.6457882358	0.0000000000
Li	1.9155840219	1.1059728765	0.0000000000
Li	0.0000000000	-2.2119437752	0.0000000000
Li	-1.9155840219	1.1059728765	0.0000000000

3b

CCSD(T)/aug-cc-pVTZ ENERGY=-285.87153990			
C	0.2753890868	0.0834519873	0.0000000000
O	-1.0848296646	0.1570000409	0.0000000000
O	0.9435613918	1.1307432639	0.0000000000
O	0.6887136550	-1.1480252651	0.0000000000
Li	-0.6742900257	-1.3161231177	1.3639335632

Li	-0.6742900257	-1.3161231177	-1.3639335632
Li	-0.6719464176	2.1009052084	0.0000000000

3c

CCSD(T)/aug-cc-pVTZ ENERGY=-285.86423978			
C	0.1747052337	-0.3250809895	0.0000000000
O	0.4152686536	-0.7958460846	1.1375967341
O	0.4152686536	-0.7958460846	-1.1375967341
O	-0.4258597744	0.9510101535	0.0000000000
Li	0.3999918447	0.8868690344	1.8669317608
Li	-2.2030584558	0.5830609363	0.0000000000
Li	0.3999918447	0.8868690344	-1.8669317608

3d

CCSD(T)/aug-cc-pVTZ ENERGY=-285.86731347			
C	0.0000000000	0.0000000000	0.0685888599
O	0.0000000000	1.0920666604	-0.6568518535
O	0.0000000000	0.0000000000	1.3261169413
O	0.0000000000	-1.0920666604	-0.6568518535
Li	-1.3344512101	0.0000000000	-1.5960468186
Li	1.3344512101	0.0000000000	-1.5960468186
Li	0.0000000000	0.0000000000	3.0289715430

3e

CCSD(T)/aug-cc-pVTZ ENERGY=-285.84320939			
C	0.0000000000	0.0000000000	2.1336301311
O	0.0000000000	0.0000000000	-2.7429219352
O	0.0000000000	0.0000000000	3.2870506455
O	0.0000000000	0.0000000000	0.9567897108
Li	0.0000000000	0.0000000000	-1.0186090640
Li	0.0000000000	1.4831575705	-3.5750927441
Li	0.0000000000	-1.4831575705	-3.5750927441

3f

CCSD(T)/aug-cc-pVTZ ENERGY=-285.83916702			
C	0.0018860858	-1.2623155471	0.0000000000
O	0.0020185249	-1.2673099474	1.1674157820
O	0.0020185249	-1.2673099474	-1.1674157820
O	-0.0024633922	1.6118235433	0.0000000000
Li	-0.0113490169	3.3228574394	0.0000000000
Li	0.0016856368	0.8528312296	1.5514887270
Li	0.0016856368	0.8528312296	-1.5514887270

ESI 4: The full form of references 17 and 18.

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