Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Mimicking the C_2 molecule: M_2B_2 and $M_3B_2^+$ Clusters (M = Li, Na) and the Reactivity of the N-Heterocyclic Carbene Bound Li_2B_2 Complex

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Table S1. Calculated C-C/B-B vibrational stretching frequencies (cm^{-1}) of the C_2, B_2^{2-}, M_2B_2 and $M_3B_2^+$ (M = Li, Na) clusters at the PBE0-D3/cc-pVTZ level.

	C_2	B_2^{2-} (S)	B_2^{2-} (T)	Li_2B_2	Na_2B_2	$Li_3B_2^+$	$Na_3B_2^+$
ν(C-C/B-B)	1901.1	1095.9	1037.3	1185.1	1131.2	1189.0	1134.8

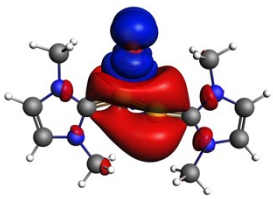
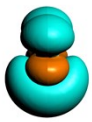
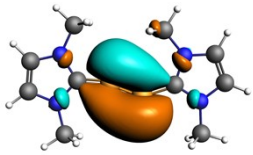
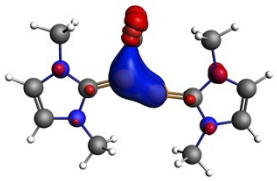
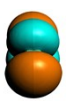
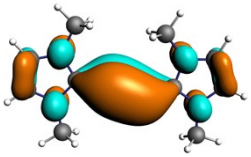
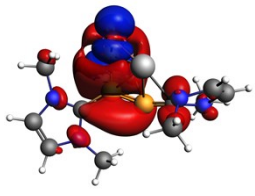
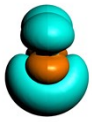
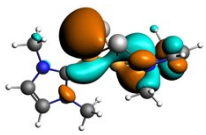
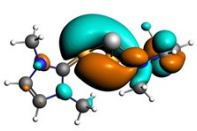
	Deformation density	CO_2		$B_2(NHC)_2$
$\Delta\rho_{(1)}$			←	
	$\Delta E_{orb(1)}$ = -140.9 kcal/mol $\lvert\nu_1\rvert$ = 1.17	ν = 0.97		ν = -0.91
$\Delta\rho_{(2)}$			→	
	$\Delta E_{orb(2)}$ = -3.9 kcal/mol $\lvert\nu_2\rvert$ = 0.18	ν = -0.01		ν = 0.01

Figure S1. Plot of the deformation densities, $\Delta\rho_{(1)-(2)}$ shown as the sum of α and β electronic charge corresponding to $\Delta E_{orb(1)-(2)}$ and the related interacting orbitals of CO_2-$B_2(NHC)_2$ at the PBE0/TZ2P-ZORA level using CO_2 (S) + $B_2(NHC)_2$ (S) as interacting fragments. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue. The isovalue for $\Delta\rho_{(1)-(2)}$ is 0.001 au.

	Deformation density	CO_2		$Li_2B_2(NHC)_2$	
$\Delta\rho_{(1)}$			←		
	$\Delta E_{orb(1)}$ = -279.1 kcal/mol $\lvert\nu_1\rvert$ = 1.51	ν = 1.31		ν = -0.97	ν = -0.30

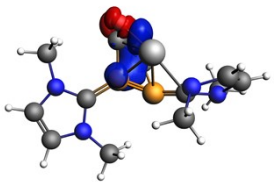
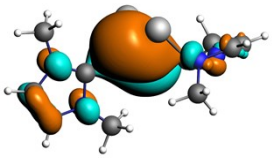
$\Delta\rho_{(2)}$			→	
	$\Delta E_{orb(2)}$ = -6.5 kcal/mol $\lvert\nu_2\rvert$ = 0.19	ν = -0.01		ν = 0.01

Figure S2. Plot of the deformation densities, $\Delta\rho_{(1)-(2)}$ shown as the sum of α and β electronic charge corresponding to $\Delta E_{orb(1)-(2)}$ and the related interacting orbitals of CO_2-$B_2(NHC)_2$ at the PBE0/TZ2P-ZORA level using CO_2 (S) + $Li_2B_2(NHC)_2$ (S) as interacting fragments. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue. The isovalue for $\Delta\rho_{(1)-(2)}$ is 0.001 au.

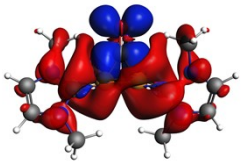
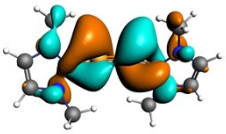
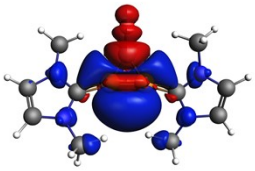
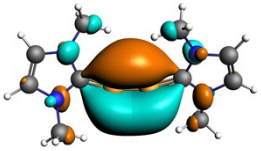
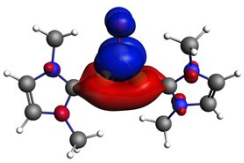
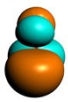
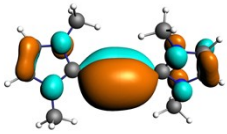
	Deformation density	CO		$B_2(NHC)_2$
$\Delta\rho_{(1)}$			←	
	$\Delta E_{orb(1)}$ = -197.7 kcal/mol $\lvert\nu_1\rvert$ = 1.48	ν = 0.81		ν = -1.37
$\Delta\rho_{(2)}$			→	
	$\Delta E_{orb(2)}$ = -187.8 kcal/mol $\lvert\nu_2\rvert$ =-1.11	ν = -1.21		ν = 0.78
$\Delta\rho_{(3)}$			←	
	$\Delta E_{orb(3)}$ = -52.6 kcal/mol $\lvert\nu_3\rvert$ = -0.65	ν = 0.31		ν = -0.36

Figure S3. Plot of the deformation densities, $\Delta\rho_{(1)-(3)}$ shown as the sum of α and β electronic charge corresponding to $\Delta E_{orb(1)-(2)}$ and the related interacting orbitals of CO-$B_2(NHC)_2$ at the PBE0/TZ2P-ZORA level using CO (S) + $B_2(NHC)_2$ (S) as interacting

fragments. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue. The isovalue for $\Delta\rho_{(1)-(3)}$ is 0.001 au. $\Delta E_{orb(1)}$ in Table 3 is the sum of $\Delta\rho_{(1)}$ and $\Delta\rho_{(3)}$.

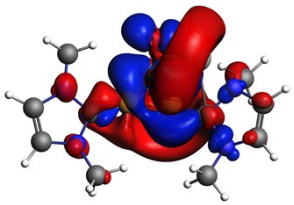
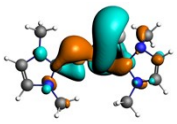
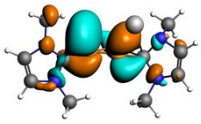
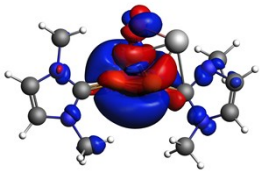
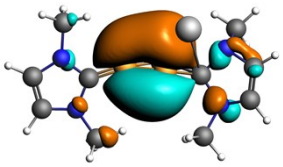
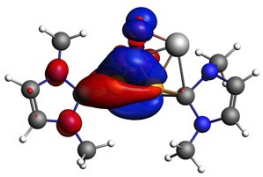
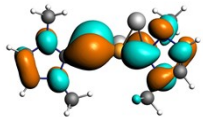
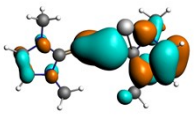
	Deformation density	CO		$Li_2B_2(NHC)_2$	
$\Delta\rho_{(1)}$			←		
	$\Delta E_{orb(1)}$ = -265.3 kcal/mol $\lvert\nu_1\rvert$ = 1.91	ν = 0.91		ν = -1.78	ν = 0.47
$\Delta\rho_{(2)}$			→		
	$\Delta E_{orb(2)}$ = -234.8 kcal/mol $\lvert\nu_2\rvert$ = 1.25	ν = -0.55		ν = 1.07	
$\Delta\rho_{(3)}$			←		
	$\Delta E_{orb(3)}$ = -51.4 kcal/mol $\lvert\nu_3\rvert$ = 0.68	ν = 0.29		ν = -0.18	ν = -0.07

Figure S4. Plot of the deformation densities, $\Delta\rho_{(1)-(3)}$ shown as the sum of α and β electronic charge corresponding to $\Delta E_{orb(1)-(2)}$ and the related interacting orbitals of CO-$Li_2B_2(NHC)_2$ at the PBE0/TZ2P-ZORA level using CO (S) + $Li_2B_2(NHC)_2$ (S) as interacting fragments. The eigenvalues ν indicate the size of the charge flow, and the

direction of charge flow is red→blue. The isovalue for $\Delta\rho_{(1)-(3)}$ is 0.001 au. $\Delta E_{orb(1)}$ in Table 3 is the sum of $\Delta\rho_{(1)}$ and $\Delta\rho_{(3)}$.

Coordinates and total energy of the singlet (S) and triplet (T) state of B_2^{2-}, M_2B_2, and $M_3B_2^+$ (M = Li, Na) determined by CASPT2(8,8)/cc-pVTZ optimization.

B_2^{2-} (S)
E = -49.14032899 a.u.

B	0.000000000	0.000000000	0.778994404
B	0.000000000	0.000000000	-0.778994404

B_2^{2-} (T)
E = -49.14716576 a.u.

B	0.000000000	0.000000000	0.808364794
B	0.000000000	0.000000000	-0.808364794

LiB_2^- (S)
E = -56.83945924 a.u.

B	0.776936791	0.000000000	-0.489098629
B	-0.776936791	0.000000000	-0.489098629
Li	0.000000000	0.000000000	1.530550984

LiB_2^- (T)
E = -56.84275391 a.u.

B	0.805427039	0.000000000	-0.519814933
B	-0.805427039	0.000000000	-0.519814933
Li	0.000000000	0.000000000	1.591983591

NaB_2^- (S)
E = -211.24127360 a.u.

B	0.000000000	0.783206082	-1.274952701
B	0.000000000	-0.783206082	-1.274952701
Na	0.000000000	0.000000000	1.194483402

NaB_2^- (T)
E = -211.25227297 a.u.

B	0.000000000	0.810585039	-1.263091271
B	0.000000000	-0.810585039	-1.263091271
Na	0.000000000	0.000000000	1.270760543

Li_2B_2 (S)

E = -64.34289223 a.u.

B	0.769547100	0.000000000	0.364124836
B	-0.769547100	0.000000000	0.364124836
Li	0.000000000	-1.791142494	-0.622727836
Li	0.000000000	1.791142494	-0.622727836

Li_2B_2 (T)

E = -64.33283056 a.u.

B	-0.793782120	0.000000000	0.000000000
B	0.793782120	0.000000000	0.000000000
Li	0.000000000	2.076013007	0.000000000
Li	0.000000000	-2.076013007	0.000000000

Na_2B_2 (S)

E = -373.15009157 a.u.

B	0.778147627	0.000000000	0.530712936
B	-0.778147627	0.000000000	0.530712936
Na	0.000000000	-2.042474027	-0.792270936
Na	0.000000000	2.042474027	-0.792270936

Na_2B_2 (T)

E = -373.14520007 a.u.

B	-0.800004227	0.000000000	0.000000000
B	0.800004227	0.000000000	0.000000000
Na	0.000000000	2.437328760	0.000000000
Na	0.000000000	-2.437328760	0.000000000

$Li_3B_2^+$ (S)

E = -71.69143840 a.u.

Li	0.000000000	2.131407941	0.000000000
B	0.000000000	0.000000327	0.765702582
Li	-1.845852972	-1.065703797	0.000000000
Li	1.845852972	-1.065703797	0.000000000
B	0.000000000	0.000000327	-0.765702582

$Li_3B_2^+$ (T)

E = -71.65169167 a.u.

Li	0.000000000	2.330035320	0.000000000
B	0.000000000	0.150068055	0.797090521
Li	-1.583542735	-1.315085215	0.000000000
Li	1.583542735	-1.315085215	0.000000000
B	0.000000000	0.150068055	-0.797090521

II-$Li_3B_2^+$ (T)

E = -71.66348921 a.u.

Li	0.000000000	0.000000000	-2.525246396
Li	2.157178363	0.000000000	0.571529113
B	0.000000000	0.000000000	-0.350901049
Li	-2.157178363	0.000000000	0.571529113
B	0.000000000	0.000000000	1.211844219

$Na_3B_2^+$ (S)

E = -534.92157369 a.u.

Na	0.000000000	2.498444600	0.000000000
B	0.000000000	-0.000000579	0.773108004
Na	-2.163718213	-1.249221221	0.000000000
Na	2.163718213	-1.249221221	0.000000000
B	0.000000000	-0.000000579	-0.773108004

$Na_3B_2^+$ (T)

E = -534.89366690 a.u.

Na	0.000000000	2.675843992	0.000000000
B	0.000000000	0.146322502	0.801095379
Na	-1.921721513	-1.484243998	0.000000000
Na	1.921721513	-1.484243998	0.000000000
B	0.000000000	0.146322502	-0.801095379

II-$Na_3B_2^+$ (T)

E = -534.89917526 a.u.

B	0.000000000	0.000000000	-1.483285984
Na	-2.512068462	0.000000000	-0.992002795
B	0.000000000	0.000000000	0.092057424
Na	0.000000000	0.000000000	2.601980778
Na	2.512068462	0.000000000	-0.992002795

Cartesian coordinates at the PBE0-D3(BJ)/def2-TZVPP level

$B_2Li_2(NHC)_2$

B -0.13427900 0.75378500 0.00000000
B 0.13427900 -0.75378500 0.00000000
Li 1.90933200 0.34003700 0.00000000
Li -1.90933200 -0.34003700 0.00000000
N 0.48468100 3.00997400 1.10327000
C 0.05726700 2.59586300 2.40456600
C 0.48468100 4.32465000 0.67210000
C 0.48468100 4.32465000 -0.67210000

N 0.48468100 3.00997400 -1.10327000
C 0.05726700 2.59586300 -2.40456600
H 0.56399400 5.14780500 1.36184400
H 0.56399400 5.14780500 -1.36184400
C 0.32277200 2.15759100 0.00000000
N -0.48468100 -3.00997400 1.10327000
C -0.05726700 -2.59586300 2.40456600
C -0.48468100 -4.32465000 0.67210000
C -0.48468100 -4.32465000 -0.67210000
N -0.48468100 -3.00997400 -1.10327000
C -0.05726700 -2.59586300 -2.40456600
H -0.56399400 -5.14780500 1.36184400
H -0.56399400 -5.14780500 -1.36184400
C -0.32277200 -2.15759100 0.00000000
H 0.28729300 3.37585700 3.13048900
H -1.02352700 2.38584900 2.40536800
H 0.56041100 1.67163200 2.68766400
H 0.28729300 3.37585700 -3.13048900
H 0.56041100 1.67163200 -2.68766400
H -1.02352700 2.38584900 -2.40536800
H -0.56041100 -1.67163200 2.68766400
H -0.28729300 -3.37585700 3.13048900
H 1.02352700 -2.38584900 2.40536800
H 1.02352700 -2.38584900 -2.40536800
H -0.28729300 -3.37585700 -3.13048900
H -0.56041100 -1.67163200 -2.68766400

$B_2Li_2(PPh_3)_2$

B 0.34194100 0.68281500 0.06230400
B -0.34194100 -0.68281500 0.06230400
Li -1.95587700 0.64824600 0.13376900
Li 1.95587700 -0.64824600 0.13376900
P 0.00234200 2.46228300 0.00071200
P -0.00234200 -2.46228300 0.00071200
C -1.77758700 2.90377100 -0.03725500
C -2.52266300 2.57953700 -1.19448300
C -2.49825200 3.12506500 1.15508700
C -3.90796100 2.52593000 -1.16184800
H -1.99891800 2.38624700 -2.12468800
C -3.88178800 3.06849200 1.17389000

H -1.95747000 3.35558200 2.06551100
C -4.60254600 2.77958400 0.01731000
H -4.45046900 2.29376300 -2.07111300
H -4.40680300 3.26403500 2.10186800
H -5.68363700 2.73708700 0.03864500
C 0.60926500 3.35447400 1.46007400
C 0.62990900 4.74526500 1.51020900
C 1.03024500 2.61944700 2.56264400
C 1.07016600 5.39295000 2.65546600
H 0.30652200 5.32579000 0.65508800
C 1.45474700 3.26768500 3.71122400
H 1.01913200 1.53569000 2.49239900
C 1.47970100 4.65604900 3.75697100
H 1.09379500 6.47573100 2.68671700
H 1.77123300 2.68981400 4.57152800
H 1.82231300 5.16374600 4.65082400
C 0.64873200 3.28331600 -1.48939900
C 1.70518800 2.70110500 -2.17926900
C 0.11885500 4.48979400 -1.94077200
C 2.22970600 3.31683600 -3.30379100
H 2.09238100 1.75370800 -1.81767400
C 0.64689600 5.10797700 -3.06355300
H -0.72440600 4.93379000 -1.42423000
C 1.70518800 4.52403000 -3.74512600
H 3.04899200 2.85265200 -3.84009600
H 0.22799100 6.04532100 -3.40990400
H 2.11763600 5.00779100 -4.62264900
C -0.60926500 -3.35447400 1.46007400
C -1.03024500 -2.61944700 2.56264400
C -0.62990900 -4.74526500 1.51020900
C -1.45474700 -3.26768500 3.71122400
H -1.01913200 -1.53569000 2.49239900
C -1.07016600 -5.39295000 2.65546600
H -0.30652200 -5.32579000 0.65508800
C -1.47970100 -4.65604900 3.75697100
H -1.77123300 -2.68981400 4.57152800
H -1.09379500 -6.47573100 2.68671700
H -1.82231300 -5.16374600 4.65082400
C -0.64873200 -3.28331600 -1.48939900
C -0.11885500 -4.48979400 -1.94077200
C -1.70518800 -2.70110500 -2.17926900
C -0.64689600 -5.10797700 -3.06355300
H 0.72440600 -4.93379000 -1.42423000
C -2.22970600 -3.31683600 -3.30379100

H -2.09238100 -1.75370800 -1.81767400
C -1.70518800 -4.52403000 -3.74512600
H -0.22799100 -6.04532100 -3.40990400
H -3.04899200 -2.85265200 -3.84009600
H -2.11763600 -5.00779100 -4.62264900
C 1.77758700 -2.90377100 -0.03725500
C 2.49825200 -3.12506500 1.15508700
C 2.52266300 -2.57953700 -1.19448300
C 3.88178800 -3.06849200 1.17389000
H 1.95747000 -3.35558200 2.06551100
C 3.90796100 -2.52593000 -1.16184800
H 1.99891800 -2.38624700 -2.12468800
C 4.60254600 -2.77958400 0.01731000
H 4.40680300 -3.26403500 2.10186800
H 4.45046900 -2.29376300 -2.07111300
H 5.68363700 -2.73708700 0.03864500

$B_2(NHC)_2$
B 0.00005100 0.72813600 -0.00002800
B -0.00005100 -0.72813600 -0.00002800
N 0.66452900 3.04880400 0.85508800
C 1.52705100 2.56551500 1.89504300
C 0.41878600 4.36222500 0.52965400
C 0.00002200 2.21077700 -0.00002300
H 2.51254400 2.30403600 1.50092400
H 1.63179500 3.32828500 2.66580500
H 1.08441000 1.66096900 2.31758700
C -0.41888500 4.36221700 -0.52962500
H 0.85585000 5.18029400 1.07468900
N -0.66452900 3.04878700 -0.85511000
H -0.85598300 5.18027200 -1.07465300
C -1.52709200 2.56547700 -1.89502000
H -2.51251200 2.30385100 -1.50081900
H -1.63199700 3.32829600 -2.66571200
H -1.08439400 1.66102200 -2.31769700
N -0.66452900 -3.04880400 0.85508800
C -1.52705100 -2.56551500 1.89504300
C -0.41878600 -4.36222500 0.52965400
C -0.00002200 -2.21077700 -0.00002300
H -1.08441000 -1.66096900 2.31758700
H -2.51254400 -2.30403600 1.50092400
H -1.63179500 -3.32828500 2.66580500
C 0.41888500 -4.36221700 -0.52962500

H -0.85585000 -5.18029400 1.07468900
N 0.66452900 -3.04878700 -0.85511000
H 0.85598300 -5.18027200 -1.07465300
C 1.52709200 -2.56547700 -1.89502000
H 2.51251200 -2.30385100 -1.50081900
H 1.63199700 -3.32829600 -2.66571200
H 1.08439400 -1.66102200 -2.31769700

CO2-$B_2(NHC)_2$
B -0.62545300 -0.51341000 0.50858300
B 0.74269800 -1.08437200 0.37774700
P -2.38230600 -0.19080500 0.12491300
P 2.28034400 -0.07568200 0.12010700
C -3.09970700 -1.58079500 -0.77272100
C -2.25620800 -2.60284500 -1.20188200
C -4.47124700 -1.64175900 -1.01906000
C -2.79674200 -3.68247800 -1.88643000
H -1.18947900 -2.57961000 -0.98934900
C -4.99412300 -2.71318500 -1.72104700
H -5.12909800 -0.86049800 -0.65751400
C -4.15552700 -3.73387500 -2.15408900
H -2.14126000 -4.48524500 -2.20009000
H -6.05773200 -2.75946900 -1.92081000
H -4.56992800 -4.57751400 -2.69326500
C -3.47604500 0.11462100 1.53899000
C -4.61763400 0.90506800 1.44007600
C -3.15718200 -0.50015500 2.74578000
C -5.44067800 1.06971500 2.54329000
H -4.85496900 1.40494600 0.50810100
C -3.98767400 -0.34021100 3.84290600
H -2.24748000 -1.08807500 2.81857300
C -5.12845100 0.44407400 3.74195200
H -6.32494400 1.69089600 2.46834200
H -3.73915100 -0.82187000 4.78055700
H -5.77233400 0.57541800 4.60317900
C -2.47580200 1.30261600 -0.88459400
C -2.16646400 2.52847000 -0.29644000
C -2.80182300 1.24082500 -2.23547500
C -2.19467300 3.68460500 -1.05734500
H -1.90781700 2.57494000 0.75482200
C -2.83990900 2.40462400 -2.98786000
H -3.03138200 0.28582800 -2.69181300
C -2.53937200 3.62499100 -2.40019500
H -1.94636300 4.63431800 -0.60028100

H -3.10679500 2.35654900 -4.03660700
H -2.56942800 4.53223700 -2.99143600
C 3.57643800 -0.89081900 -0.84526400
C 3.98589800 -2.16563500 -0.45241200
C 4.17467100 -0.27294600 -1.93915400
C 4.98818200 -2.80857900 -1.15800200
H 3.51750800 -2.65012500 0.39745700
C 5.17828000 -0.92572900 -2.63982100
H 3.85680200 0.71528000 -2.24695900
C 5.58455700 -2.19232500 -2.25003300
H 5.29869900 -3.80089200 -0.85530000
H 5.63995800 -0.44253000 -3.49238400
H 6.36570700 -2.70327400 -2.80020400
C 1.91936500 1.47134600 -0.74737300
C 2.40916100 2.69741700 -0.31250500
C 1.13060600 1.40927400 -1.89633500
C 2.11346700 3.85343200 -1.02200500
H 3.01384800 2.75131800 0.58400800
C 0.85256800 2.56233500 -2.60805200
H 0.72724700 0.45530500 -2.21488700
C 1.34213800 3.78620300 -2.17120900
H 2.49042500 4.80744500 -0.67366700
H 0.23823000 2.50787400 -3.49763500
H 1.11463600 4.68908600 -2.72530700
C 3.07178700 0.36435300 1.68533600
C 4.41806300 0.71973500 1.72671900
C 2.31687400 0.34675100 2.85261500
C 4.99862800 1.08120700 2.93117300
H 5.01246800 0.70088100 0.82073600
C 2.90500600 0.70652300 4.05498200
H 1.28141200 0.02926800 2.80477800
C 4.24096200 1.07708200 4.09461600
H 6.04584700 1.35618500 2.96373900
H 2.32043700 0.68235300 4.96645200
H 4.69911600 1.35074000 5.03759400
C 1.01564400 -2.73118700 0.68581800
O 0.68868300 -3.48511200 -0.22807200
O 1.58267200 -2.89264200 1.76838700

$CO\text{-}B_2(NHC)_2$

B 0.01880100 0.78152300 0.25876400
B -0.01880100 -0.78152300 0.25876400
C 0.00000000 0.00000000 1.55077000

O 0.00000000 0.00000000 2.80189800
N -0.48856500 2.81581300 -1.29879600
C -0.91646600 2.05050800 -2.44126200
C -0.45791700 4.18367400 -1.20182300
C -0.06523700 2.24526100 -0.14189800
H -1.93288400 2.32610300 -2.72519900
H -0.24672500 2.21527100 -3.28705600
H -0.89183600 1.00143100 -2.14570800
C 0.00000000 4.47546700 0.03914100
H -0.76879100 4.82952900 -2.00453500
N 0.22563100 3.28518900 0.67716700
H 0.17110400 5.42491500 0.51549300
C 0.71318100 3.12488200 2.03343500
H 1.80096600 3.21201600 2.05469100
H 0.27743200 3.90393500 2.65839600
H 0.42602600 2.13695100 2.40603100
N 0.48856500 -2.81581300 -1.29879600
C 0.91646600 -2.05050800 -2.44126200
C 0.45791700 -4.18367400 -1.20182300
C 0.06523700 -2.24526100 -0.14189800
H 0.89183600 -1.00143100 -2.14570800
H 1.93288400 -2.32610300 -2.72519900
H 0.24672500 -2.21527100 -3.28705600
C 0.00000000 -4.47546700 0.03914100
H 0.76879100 -4.82952900 -2.00453500
N -0.22563100 -3.28518900 0.67716700
H -0.17110400 -5.42491500 0.51549300
C -0.71318100 -3.12488200 2.03343500
H -1.80096600 -3.21201600 2.05469100
H -0.27743200 -3.90393500 2.65839600
H -0.42602600 -2.13695100 2.40603100

N_2-$B_2(NHC)_2$
B -0.77347000 -0.17367000 0.31837000
B 0.77363100 -0.18700700 0.30753500
N -2.83880200 1.34185300 -0.05442900
C -2.12048600 2.58604900 -0.00382200
C -4.18644400 1.17981400 -0.24880400
C -2.23057200 0.12883300 0.06496900
H -1.11136200 2.40541600 -0.37463600
H -2.62064200 3.32475500 -0.62878100
H -2.05421500 2.96112500 1.02002000

C -4.42573600 -0.15320200 -0.25120200
H -4.85641000 2.01264700 -0.37431400
N -3.22758100 -0.78632700 -0.04774100
H -5.34618000 -0.69750100 -0.36948300
C -3.04872800 -2.20205500 0.19444600
H -3.20153500 -2.41160200 1.25522600
H -3.78527900 -2.75361200 -0.38947900
H -2.02001100 -2.53009600 -0.07728600
N 2.85119600 1.32848700 0.08210400
C 2.14030200 2.57064300 0.21509000
C 4.19469700 1.17804400 -0.15103100
C 2.23148100 0.11470100 0.06933100
H 1.31190800 2.42415900 0.90798300
H 2.81310000 3.33510400 0.60107600
H 1.73647300 2.89440000 -0.74764000
C 4.42332100 -0.14840900 -0.29332000
H 4.87071200 2.01471900 -0.18818300
N 3.22127700 -0.79170400 -0.14587900
H 5.34012100 -0.68481900 -0.46430600
C 3.04483300 -2.22436800 -0.03676400
H 3.70800200 -2.71763700 -0.74777100
H 3.30120200 -2.54715500 0.97452400
H 1.99118600 -2.51670300 -0.23116900
N -0.00991900 -1.44740100 0.21297100
N -0.02672500 -2.62920900 -0.13969300

CO_2-$Li_2B_2(NHC)_2$

B -0.69070900 -0.18503900 0.49314400
B 0.72760200 0.40994100 0.18880000
Li -1.02361200 1.03636000 -1.37241900
Li 0.07606200 1.61928800 1.99922900
N -3.27080300 -0.31666100 0.92573200
C -3.21345100 0.16675100 2.26481900
C -4.30867800 -0.01092300 0.06646400
C -3.90112600 -0.06381400 -1.20435100
N -2.50706000 -0.40179400 -1.25103300
C -2.27255100 -1.69754200 -1.89059100
H -5.29307900 0.21472700 0.44771000
H -4.47675900 0.03442600 -2.10991700
C -2.07555800 -0.33172300 0.15868700
N 3.28780900 0.16795400 -0.23617100
C 3.53610400 1.53474300 -0.63884200

C 4.24505900 -0.81283400 -0.17599900
C 3.62869600 -1.94434800 0.23111300
N 2.30376100 -1.63572600 0.40921000
C 1.28230400 -2.56171800 0.81569800
H 5.27395200 -0.62531500 -0.42726200
H 4.01563200 -2.93302100 0.40361500
C 2.07203600 -0.32529400 0.12628700
H -4.20190700 0.12828300 2.72358700
H -2.53259800 -0.45680600 2.84916500
H -2.84245000 1.20795600 2.30796900
H -2.60092200 -1.65423200 -2.93174000
H -1.20385300 -1.90994500 -1.86555100
H -2.81274300 -2.50376500 -1.37913100
H 3.28324100 2.22157000 0.16831100
H 4.59044800 1.63276100 -0.88880200
H 2.92837600 1.79115800 -1.50596100
H 0.59849800 -2.76381800 -0.00958000
H 1.75521900 -3.48476900 1.14771300
H 0.68792500 -2.11945400 1.61888300
C 0.65658900 2.01388800 -0.08915700
O 0.83262200 2.81281000 0.88995200
O 0.27946800 2.39084900 -1.23471600

CO-$Li_2B_2(NHC)_2$
B -0.91350000 -0.30481700 0.15016700
B 0.70189000 -0.12367600 -0.18034900
Li 0.60809100 -0.16840600 1.82899200
Li 1.73022800 -1.90174700 -0.99731300
C -0.10799400 -1.44776800 -0.30450500
O 0.05840600 -2.63199900 -0.77480800
N -2.93356100 1.33349200 0.06716800
C -2.16455400 2.54869300 0.10685600
C -4.30512400 1.24474800 0.00821300
C -2.37286700 0.09320400 0.08154100
H -2.45775100 3.21085000 -0.70885000
H -2.30477000 3.06767400 1.05825100
H -1.11663900 2.27244100 -0.00719200
C -4.61141800 -0.07114400 -0.02162400
H -4.93910700 2.11346200 -0.02363600
N -3.42653100 -0.76429200 0.00980600
H -5.56509700 -0.56614300 -0.07726000
C -3.28166500 -2.20049600 0.02432800
H -3.29309300 -2.57671000 1.05036500

H -4.10407800 -2.64798800 -0.53256000
H -2.32874600 -2.47055400 -0.43097800
N 2.84465100 1.40101700 0.11654300
C 2.11128100 2.58686700 -0.20702400
C 4.04971400 1.13657600 -0.49814100
C 2.11371900 0.15539000 0.13959700
H 1.38038300 2.80112100 0.57576900
H 2.79103500 3.43705500 -0.28070000
H 1.55802700 2.47161900 -1.15273100
C 4.26076000 -0.18104000 -0.60761400
H 4.69219900 1.94333800 -0.82052300
N 3.16128100 -0.89133600 -0.00354200
H 5.13830100 -0.70061700 -0.95771800
C 3.57113700 -1.46710800 1.27992000
H 4.38311000 -2.18288200 1.12442000
H 3.91543000 -0.69479400 1.98062400
H 2.72782400 -2.00865400 1.71795500

N_2-$Li_2B_2(NHC)_2$
B -0.87945000 -0.20434300 0.27023900
B 0.68661300 -0.02326600 -0.14985200
Li 0.63572000 0.24569600 1.88821700
Li 1.66883300 -1.77554000 -1.13820800
N -2.95570300 1.31945100 0.08844100
C -2.23884200 2.54988900 0.25313900
C -4.31997400 1.16942300 -0.02251200
C -2.34237600 0.10151600 0.09125200
H -1.31407200 2.50133200 -0.32300800
H -2.85089400 3.37960500 -0.09692400
H -1.97940400 2.71213800 1.30498800
C -4.56233800 -0.15610400 -0.11506600
H -4.99039400 2.01042300 -0.05414700
N -3.34969700 -0.80162700 -0.06422500
H -5.48877800 -0.69009900 -0.23349700
C -3.15756300 -2.23297000 0.01250300
H -3.24974400 -2.56715800 1.05068700
H -3.92104100 -2.72580300 -0.58901200
H -2.16283400 -2.50725500 -0.36801100
N 2.90943000 1.36730400 0.08280400
C 2.26236900 2.56285000 -0.37514200
C 4.14350100 1.01216900 -0.43199700
C 2.11846900 0.16063300 0.09552200
H 1.47080600 2.85423000 0.31805000

H 2.98423200 3.37878200 -0.42912700
H 1.79482700 2.41024000 -1.36074900
C 4.27913000 -0.31568000 -0.49978300
H 4.85829600 1.77089000 -0.71484600
N 3.08998100 -0.94829400 0.00217500
H 5.14409400 -0.89694800 -0.77581600
C 3.33000000 -1.61959200 1.28048300
H 4.08035200 -2.40337900 1.15118300
H 3.68734100 -0.91813400 2.04719400
H 2.40445100 -2.09310200 1.61536600
N -0.11959400 -1.32254900 -0.28980400
N -0.07312800 -2.45442600 -0.83720300