Electronic Supplementary Material (ESI) for Dalton Transactions

Superalkali Character of Alkali-Monocyclic (Pseudo)oxocarbons Clusters

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Table S1. Symmetry Point Group, the Lowest Vibrational Frequencies (υ_1, in cm^{-1}), HOMO–LUMO Gaps (in eV) of the $C_3X_3Li_3$ (X=O, S, Se, NCN, and $C(CN)_2$) species.

Species	Symmetry	υ_1(cm-1)	Gap(eV)
$C_3O_3Li_3$	C_{2v}	42.6	1.88
$C_3S_3Li_3$	D_{3h}	48.9	3.83
$C_3Se_3Li_3$	C_s	46.0	6.99
C_3NCN_3	C_s	39.2	1.58
C_3ONCN_2	C_s	43.6	4.64
C_3SNCN_2	C_s	42.5	1.97
C_3SeNCN_2	C_s	42.2	1.98
$C_3[C(CN)_2]_3Li_3$	C_s	47.1	6.10
$C_3NCN[C(CN)_2]_2Li_3$	C_s	56.6	6.29
$C_3O[C(CN)_2]_2Li_3$	C_{2v}	8.5	2.96
$C_3S[C(CN)_2]_2Li_3$	C_1	43.3	6.22
$C_3Se[C(CN)_2]_2Li_3$	C_1	39.7	6.30

Table S2. Dissociation Channels and Calculated Energies of Dissociation.

dissociation channel	⊿E (kcal/mol)
$C_3O_3Li_3^+ \rightarrow 3CO + Li_3^+$	102.8
$C_3O_3Li_3^+ \rightarrow C_3O_3^{2-} + 3Li^+$	481.4
$C_3S_3Li_3^+ \rightarrow C_3S_3 + Li_3^+$	162.3
$C_3S_3Li_3^+ \rightarrow C_3S_3^{2-} + 3Li^+$	417.0
$C_3Se_3Li_3^+ \rightarrow C_3Se_3 + Li_3^+$	161.3
$C_3Se_3Li_3^+ \rightarrow C_3Se_3^{2-} + 3Li^+$	407.4

Table S3. Dissociation Channels and Calculated Energies of Dissociation.

dissociation channel	⊿E (kcal/mol)
$C_3NCN_3Li_3^+ \rightarrow C_3NCN_3 + Li_3^+$	191.3
$C_3NCN_3Li_3^+ \rightarrow C_3NCN_3^{2-} + 3Li^+$	402.7
$C_3ONCN_2Li_3^+ \rightarrow C_3ONCN_2 + Li_3^+$	185.5
$C_3ONCN_2Li_3^+ \rightarrow C_3ONCN_2^{2-} + 3Li^+$	420.4
$C_3SNCN_2Li_3^+ \rightarrow C_3SNCN_2 + Li_3^+$	184.6
$C_3SNCN_2Li_3^+ \rightarrow C_3SNCN_2^{2-} + 3Li^+$	410.5
$C_3SeNCN_2Li_3^+ \rightarrow C_3SeNCN_2 + Li_3^+$	184.0
$C_3SeNCN_2Li_3^+ \rightarrow C_3SeNCN_2^{2-} + 3Li^+$	407.4

Table S4. Dissociation Channels and Calculated Energies of Dissociation.

dissociation channel	⊿E (kcal/mol)
$C_3[C(CN)_2]_3Li_3^+ \rightarrow C_3[C(CN)_2]_3 + Li_3^+$	220.7
$C_3[C(CN)_2]_3Li_3^+ \rightarrow C_3[C(CN)_2]_3^{2-} + 3Li^+$	417.5
$C_3NCN[C(CN)_2]_2Li_3^+ \rightarrow C_3NCN[C(CN)_2]_2 + Li_3^+$	210.1
$C_3NCN[C(CN)_2]_2Li_3^+ \rightarrow C_3NCN[C(CN)_2]_2^{2-} + 3Li^+$	411.2
$C_3O[C(CN)_2]_2Li_3^+ \rightarrow C_3O[C(CN)_2]_2 + Li_3^+$	187.7
$C_3O[C(CN)_2]_2Li_3^+ \rightarrow C_3O[C(CN)_2]_2^{2-} + 3Li^+$	406.2
$C_3S[C(CN)_2]_2Li_3^+ \rightarrow C_3S[C(CN)_2]_2 + Li_3^+$	190.7
$C_3S[C(CN)_2]_2Li_3^+ \rightarrow C_3S[C(CN)_2]_2^{2-} + 3Li^+$	404.1
$C_3Se[C(CN)_2]_2Li_3^+ \rightarrow C_3Se[C(CN)_2]_2 + Li_3^+$	190.7
$C_3Se[C(CN)_2]_2Li_3^+ \rightarrow C_3Se[C(CN)_2]_2^{2-} + 3Li^+$	402.7

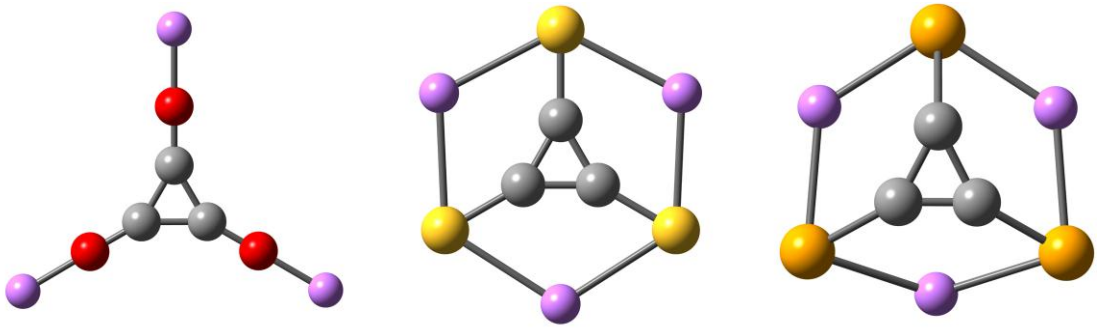

Figure S1. The minimum energy structures of three polynuclear superalkali species (**1A**)$C_3O_3Li_3$, (**1B**)$C_3S_3Li_3$, and (**1C**)$C_3Se_3Li_3$. For common atoms, grey color is for carbon, light purple for lithium, blue for nitrogen.

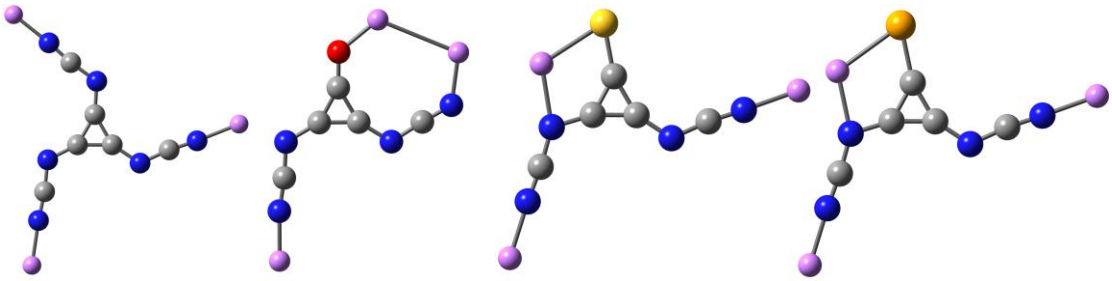

Figure S2. The minimum energy structures of four polynuclear superalkali species: (**2A**)$C_3NCN_3Li_3$, (**2B**)$C_3ONCN_2Li_3$, (**2C**)$C_3SNCN_2Li_3$ and (**2D**)$C_3SeNCN_2Li_3$. For common atoms, grey color is for carbon, light purple for lithium, blue for nitrogen.

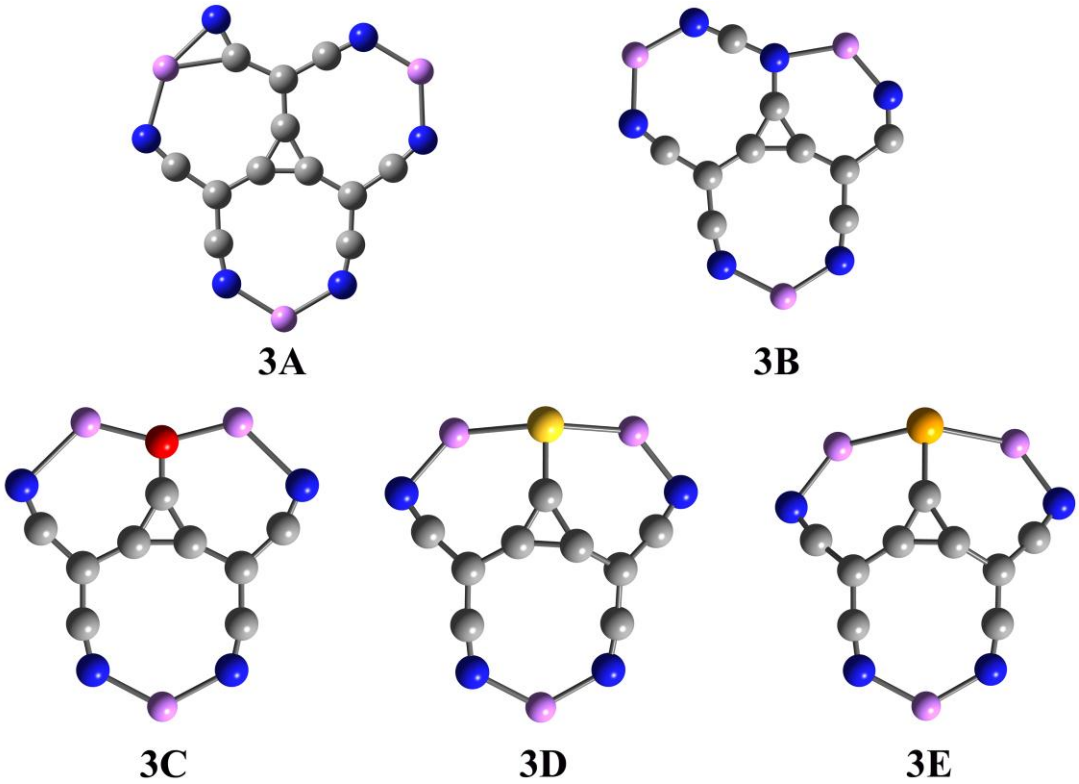

Figure S3. The minimum energy structures of five polynuclear superalkali species: (**3A**)$C_3[C(CN)_2]_3Li_3$, (**3B**)$C_3NCN[C(CN)_2]_2Li_3$, (**3C**)$C_3O[C(CN)_2]_2Li_3$, (**3D**)$C_3S[C(CN)_2]_2Li_3$ and (**3E**)$C_3Se[C(CN)_2]_2Li_3$. For common atoms, grey color is for carbon, light purple for lithium, blue for nitrogen.

Cartesian atomic coordinates and total energies of all calculated structures:

$1A^+$ -362.5955527

C	0.00000000	0.81131400	0.00000000
C	0.70261900	-0.40565700	0.00000000
C	-0.70261900	-0.40565700	0.00000000
O	-1.80551200	-1.04241300	0.00000000
O	0.00000000	2.08482600	0.00000000
O	1.80551200	-1.04241300	0.00000000
Li	0.00000000	3.74366400	0.00000000
Li	3.24210800	-1.87183200	0.00000000
Li	-3.24210800	-1.87183200	0.00000000

$1B^+$ -1331.4935467

C	0.00000000	0.80945500	0.00000000
C	0.70100900	-0.40472700	0.00000000
C	-0.70100900	-0.40472700	0.00000000
Li	-2.24827400	1.29804100	0.00000000
Li	2.24827400	1.29804100	0.00000000
Li	0.00000000	-2.59608300	0.00000000
S	0.00000000	2.49735500	0.00000000
S	-2.16277300	-1.24867800	0.00000000
S	2.16277300	-1.24867800	0.00000000

$1C^+$ -7341.4941978

C	0.00000000	0.80857500	0.00000000
C	0.70024600	-0.40428700	0.00000000
C	-0.70024600	-0.40428700	0.00000000
Li	-2.28862100	1.32133600	0.00000000
Li	2.28862100	1.32133600	0.00000000
Li	0.00000000	-2.64267200	0.00000000
Se	0.00000000	2.64876400	0.00000000
Se	2.29389700	-1.32438200	0.00000000
Se	-2.29389700	-1.32438200	0.00000000

$2A^+$ -579.73629

C	0.00000000	0.80393300	0.00000000
C	0.69622600	-0.40196600	0.00000000
C	-0.69622600	-0.40196600	0.00000000
N	1.80877100	-1.13518100	0.00000000
N	-1.88748100	-0.99885100	0.00000000
N	0.07871000	2.13403200	0.00000000
C	-2.04092200	-2.26419000	0.00000000
C	2.98130700	-0.63539600	0.00000000

C	-0.94038500	2.89958500	0.00000000
N	-1.79411500	3.71169600	0.00000000
N	-2.31736500	-3.40959700	0.00000000
N	4.11148000	-0.30209900	0.00000000
Li	-3.10942900	4.91662400	0.00000000
Li	5.81263500	0.23453200	0.00000000
Li	-2.70320700	-5.15115600	0.00000000

$2B^+$ -507.3555936

C	0.00000000	0.43703200	0.00000000
C	0.81854000	-0.69416200	0.00000000
C	1.39421100	0.57361800	0.00000000
N	1.01426000	-2.01482300	0.00000000
N	-1.26231000	0.87580100	0.00000000
C	0.07585300	-2.87552600	0.00000000
C	-1.61571000	2.09571000	0.00000000
N	-2.08158300	3.18074100	0.00000000
N	-0.69182400	-3.77035300	0.00000000
Li	-2.93472700	4.74339900	0.00000000
Li	-1.83279500	-5.13848900	0.00000000
Li	3.99752100	1.87834600	0.00000000
O	2.42785600	1.30382900	0.00000000

$2C^+$ -830.3281354

C	0.00000000	0.62547600	0.00000000
C	0.29934600	-0.71826400	0.00000000
C	-1.03714400	-0.34291800	0.00000000
N	0.97224600	-1.89910900	0.00000000
N	0.45121300	1.86966500	0.00000000
C	2.25746500	-1.97570400	0.00000000
C	-0.32520200	2.88716200	0.00000000
N	-0.93270800	3.89294300	0.00000000
N	3.41718200	-2.14260000	0.00000000
Li	-1.94997400	5.37365500	0.00000000
Li	5.21988200	-2.31845800	0.00000000
Li	-0.95551900	-2.68931900	0.00000000
S	-2.59159300	-0.99990200	0.00000000

$2D^+$ -2833.6619544

C	0.68572900	-0.69373100	0.00000000
C	-0.69076400	-0.65416400	0.00000000
C	0.00000000	0.54563800	0.00000000
N	-1.99808700	-1.02235800	0.00000000
N	1.78364400	-1.42995500	0.00000000

C	-2.37690400	-2.25372600	0.00000000
C	2.95781400	-0.91839200	0.00000000
N	4.07909000	-0.56857300	0.00000000
N	-2.81332300	-3.34066700	0.00000000
Li	5.76078300	0.06699000	0.00000000
Li	-3.40810500	-5.05290300	0.00000000
Li	-2.39025500	1.01287700	0.00000000
Se	-0.31475800	2.36165400	0.00000000

3A^{+} -808.4536319

C	0.00000000	0.00000000	0.79926600
C	0.00000000	0.69223900	-0.39962600
C	0.00000000	-0.69223900	-0.39962600
C	0.00000000	0.00000000	2.20705300
C	0.00000000	1.91155100	-1.10351800
C	0.00000000	-1.91155100	-1.10351800
C	0.00000000	-1.25076800	2.83928700
C	0.00000000	1.25076800	2.83928700
C	0.00000000	3.08464600	-0.33650300
C	0.00000000	1.83370200	-2.50287700
C	0.00000000	-1.83370200	-2.50287700
C	0.00000000	-3.08464600	-0.33650300
N	0.00000000	3.93463600	0.45425300
N	0.00000000	2.36056200	3.17996900
N	0.00000000	-2.36056200	3.17996900
N	0.00000000	-3.93463600	0.45425300
N	0.00000000	-1.57393200	-3.63436000
N	0.00000000	1.57393200	-3.63436000
Li	0.00000000	4.14115300	2.39138300
Li	0.00000000	0.00000000	-4.78180900
Li	0.00000000	-4.14115300	2.39138300

3B^{+} -732.2143598

C	0.34708700	-0.85167700	0.00000000
C	-0.97481900	-0.48445100	0.00000000
C	0.00000000	0.49796200	0.00000000
C	1.24360500	-1.93287200	0.00000000
C	0.41664600	1.84106900	0.00000000
C	2.61194100	-1.64948900	0.00000000
C	0.52187600	-3.13974800	0.00000000
C	-0.60823000	2.79794900	0.00000000
C	1.80431100	2.04223600	0.00000000
N	-0.36246900	-3.89636100	0.00000000
N	3.67136500	-1.17364400	0.00000000

N	2.96311100	1.96872900	0.00000000
N	-1.60261300	3.39718600	0.00000000
N	-2.25545800	-0.91392400	0.00000000
C	-3.10808000	0.09144100	0.00000000
N	-3.80424600	1.02486300	0.00000000
Li	-3.51557500	2.94800500	0.00000000
Li	4.40605400	0.64431900	0.00000000
Li	-2.15510100	-2.96647600	0.00000000

3C$^+$ -659.8089595

C	0.00000000	0.69665900	0.21309500
C	0.00000000	0.00000000	1.40482900
C	0.00000000	-0.69665900	0.21309500
C	0.00000000	1.94947600	-0.42346700
C	0.00000000	-1.94947600	-0.42346700
C	0.00000000	1.94408000	-1.82064400
C	0.00000000	2.95042300	0.56405000
C	0.00000000	-2.95042300	0.56405000
C	0.00000000	-1.94408000	-1.82064400
N	0.00000000	3.43902800	1.62143000
N	0.00000000	1.65232200	-2.94544200
N	0.00000000	-1.65232200	-2.94544200
N	0.00000000	-3.43902800	1.62143000
Li	0.00000000	1.96203900	3.03634400
Li	0.00000000	-1.96203900	3.03634400
Li	0.00000000	0.00000000	-4.02120800
O	0.00000000	0.00000000	2.69454200

3D$^+$ -982.7874305

C	0.00000000	0.69191100	-0.02186700
C	0.00000000	0.00000000	1.17610700
C	0.00000000	-0.69191100	-0.02186700
C	0.00000000	1.93190600	-0.67622000
C	0.00000000	-1.93190600	-0.67622000
C	0.00000000	1.90774300	-2.07541300
C	0.00000000	2.98668800	0.25043200
C	0.00000000	-2.98668800	0.25043200
C	0.00000000	-1.90774300	-2.07541300
N	0.00000000	3.59353300	1.24291000
N	0.00000000	1.62765700	-3.20241200
N	0.00000000	-1.62765700	-3.20241200
N	0.00000000	-3.59353300	1.24291000
Li	0.00000000	2.50349100	2.89988600
Li	0.00000000	-2.50349100	2.89988600

Li	0.00000000	0.00000000	-4.30349700
S	0.00000000	0.00000000	2.88527400

$3E^+$ -2986.1212272

C	0.00000000	0.69227400	-0.47240500
C	0.00000000	0.00000000	0.72411800
C	0.00000000	-0.69227400	-0.47240500
C	0.00000000	1.92925900	-1.13104400
C	0.00000000	-1.92925900	-1.13104400
C	0.00000000	1.90098000	-2.53060300
C	0.00000000	2.99414600	-0.21634000
C	0.00000000	-2.99414600	-0.21634000
C	0.00000000	-1.90098000	-2.53060300
N	0.00000000	3.62233400	0.76234600
N	0.00000000	1.62273000	-3.65790500
N	0.00000000	-1.62273000	-3.65790500
N	0.00000000	-3.62233400	0.76234600
Li	0.00000000	2.63599800	2.47110200
Li	0.00000000	-2.63599800	2.47110200
Li	0.00000000	0.00000000	-4.76405400
Se	0.00000000	0.00000000	2.58421700

1A -362.7162128

C	0.00000000	0.00000000	0.81378800
C	0.00000000	0.70310200	-0.40406700
C	0.00000000	-0.70310200	-0.40406700
O	0.00000000	-1.80551100	-1.04123000
O	0.00000000	0.00000000	2.08710200
O	0.00000000	1.80551100	-1.04123000
Li	0.00000000	0.00000000	3.75748700
Li	0.00000000	3.24397300	-1.89058700
Li	0.00000000	-3.24397300	-1.89058700

1B -1331.6282528

C	0.00000000	0.80942000	0.00000000
C	0.70097800	-0.40471000	0.00000000
C	-0.70097800	-0.40471000	0.00000000
Li	-2.27723000	1.31475900	0.00000000
Li	2.27723000	1.31475900	0.00000000
Li	0.00000000	-2.62951800	0.00000000
S	0.00000000	2.49879300	0.00000000
S	-2.16401800	-1.24939600	0.00000000
S	2.16401800	-1.24939600	0.00000000

1C **-7341.6724894**

C	-0.79796200	0.09502200	0.67154200
C	-0.79796200	0.09502200	-0.67154200
C	-0.18289100	1.25880000	0.00000000
Li	0.96269600	0.77638000	2.02442500
Li	-0.55083400	-2.08218400	0.00000000
Li	0.96269600	0.77638000	-2.02442500
Se	-0.79796200	-0.99184300	2.21870600
Se	-0.79796200	-0.99184300	-2.21870600
Se	1.78854800	1.77472100	0.00000000

2A **-579.8557455**

C	0.00000000	0.80407600	0.00000000
C	0.69618200	-0.40251100	0.00000000
C	-0.69685800	-0.40213500	0.00000000
N	1.81108600	-1.13459200	0.00000000
N	-1.88831700	-1.00160000	0.00000000
N	0.07678900	2.13562700	0.00000000
C	-2.01350200	-2.27511500	0.00000000
C	2.97656300	-0.60620900	0.00000000
C	-0.96319700	2.88123100	0.00000000
N	-1.83701200	3.66950300	0.00000000
N	-2.25847400	-3.42616100	0.00000000
N	4.09589200	-0.24286400	0.00000000
Li	-3.25500800	4.79502200	0.00000000
Li	5.77909300	0.42367500	0.00000000
Li	-2.52237200	-5.21716700	0.00000000

2B **-507.4953884**

C	0.00000000	0.32760700	0.00000000
C	0.48691100	-0.97377100	0.00000000
C	1.39142100	0.08849000	0.00000000
N	0.26998200	-2.30685500	0.00000000
N	-1.05987300	1.15278200	0.00000000
C	-0.88841700	-2.81266900	0.00000000
C	-0.80290700	2.41537400	0.00000000
N	-0.62365500	3.57999500	0.00000000
N	-1.92206500	-3.39300800	0.00000000
Li	1.01799100	4.46968900	0.00000000
Li	-3.56570800	-4.01021900	0.00000000
Li	3.12226100	2.23805400	0.00000000
O	2.56294900	0.55085500	0.00000000

2C **-830.4580287**

C	0.00000000	0.62300700	0.00000000
C	0.27845200	-0.73052600	0.00000000
C	-1.04919500	-0.32751700	0.00000000
N	0.92379600	-1.92157100	0.00000000
N	0.48215900	1.85278900	0.00000000
C	2.22048900	-2.00816000	0.00000000
C	-0.27762100	2.89067200	0.00000000
N	-0.85987600	3.90858000	0.00000000
N	3.37431100	-2.18234100	0.00000000
Li	-1.81438400	5.47410600	0.00000000
Li	5.24141600	-2.36589900	0.00000000
Li	-0.96264200	-2.64588700	0.00000000
S	-2.61679100	-0.97962600	0.00000000

2D -2833.7925174

C	0.69235200	-0.68039100	0.00000000
C	-0.69000500	-0.64805700	0.00000000
C	0.00000000	0.55152900	0.00000000
N	-1.99155900	-1.01795600	0.00000000
N	1.78412100	-1.42057400	0.00000000
C	-2.35487500	-2.26670700	0.00000000
C	2.96445900	-0.90739100	0.00000000
N	4.08528900	-0.56407200	0.00000000
N	-2.77329500	-3.35561500	0.00000000
Li	5.82484200	0.01965900	0.00000000
Li	-3.35679300	-5.14054500	0.00000000
Li	-2.37082500	0.95958300	0.00000000
Se	-0.34397500	2.37345700	0.00000000

3A -808.5683407

C	0.00000000	0.74878800	0.00000000
C	-0.69936600	-0.46463500	0.00000000
C	0.66673600	-0.47839300	0.00000000
C	-0.04761900	2.12753300	0.00000000
C	-1.94433500	-1.14432600	0.00000000
C	1.90516200	-1.18261300	0.00000000
C	1.18366500	2.78613800	0.00000000
C	-1.39279800	2.74512600	0.00000000
C	-3.10905000	-0.35766100	0.00000000
C	-1.90026400	-2.53568700	0.00000000
C	1.84867100	-2.57449500	0.00000000
C	3.06582200	-0.40534600	0.00000000
N	-3.94571200	0.44925200	0.00000000
N	-1.95420100	3.83129700	0.00000000

N	2.23202000	3.31220900	0.00000000
N	3.91627800	0.39026400	0.00000000
N	1.61379100	-3.71641200	0.00000000
N	-1.67665500	-3.68100800	0.00000000
Li	-3.38749000	2.44853300	0.00000000
Li	-0.04918000	-4.68255300	0.00000000
Li	3.85053900	2.33875400	0.00000000

3B **-732.3481733**

C	0.31565300	-0.94724900	0.00000000
C	-1.00203700	-0.48936500	0.00000000
C	0.00000000	0.43387800	0.00000000
C	1.18624700	-2.01509900	0.00000000
C	0.46868900	1.77832100	0.00000000
C	2.53500600	-1.68007700	0.00000000
C	0.61070400	-3.41978600	0.00000000
C	-0.49363800	2.78732300	0.00000000
C	1.85162300	1.97555100	0.00000000
N	-0.58428600	-3.67528600	0.00000000
N	3.64212100	-1.29695800	0.00000000
N	3.01608800	1.96685000	0.00000000
N	-1.42217500	3.49254400	0.00000000
N	-2.33033300	-0.79985500	0.00000000
C	-3.11615500	0.23677400	0.00000000
N	-3.81045300	1.18140200	0.00000000
Li	-3.28998300	3.00478000	0.00000000
Li	4.26344300	0.47554000	0.00000000
Li	-2.21122400	-2.82782100	0.00000000

3C **-659.9376174**

C	0.00000000	0.69375600	0.19998900
C	0.00000000	0.00000000	1.39462100
C	0.00000000	-0.69375600	0.19998900
C	0.00000000	1.95735300	-0.42849000
C	0.00000000	-1.95735300	-0.42849000
C	0.00000000	1.96049100	-1.81850300
C	0.00000000	2.99317200	0.53244600
C	0.00000000	-2.99317200	0.53244600
C	0.00000000	-1.96049100	-1.81850300
N	0.00000000	3.46282600	1.60461300
N	0.00000000	1.71301500	-2.95923800
N	0.00000000	-1.71301500	-2.95923800
N	0.00000000	-3.46282600	1.60461300
Li	0.00000000	1.87966800	3.15770700

Li	0.00000000	-1.87966800	3.15770700
Li	0.00000000	0.00000000	-3.86154900
O	0.00000000	0.00000000	2.67626600

3D -982.9298641

C	0.11618100	-0.74072900	0.97794200
C	1.16620400	0.22871500	0.66047200
C	-0.09475800	0.65967800	0.61884200
C	-0.27401700	-1.96780600	0.21028300
C	-0.98439600	1.69036300	0.17841000
C	-1.60758500	-2.17280600	-0.06961000
C	0.77772600	-2.68274900	-0.32492000
C	-0.31477400	2.79489300	-0.34928200
C	-2.34779500	1.43772600	0.08140700
N	1.81465300	-3.11659000	-0.67457000
N	-2.77011400	-2.19650200	-0.22914500
N	-3.45837100	1.08210600	0.01806200
N	0.46205500	3.58331400	-0.72907900
Li	3.05386000	-1.67240900	-0.55497200
Li	2.16253500	2.61284700	-0.60839100
Li	-3.98977900	-0.75444200	-0.27024900
S	2.83511700	0.53075000	0.23141800

3E -2986.2640569

C	0.45328400	-0.75872200	-0.96352200
C	-0.74838100	0.01607600	-0.64696600
C	0.41888500	0.65643400	-0.59882000
C	1.06009400	-1.89695400	-0.20315200
C	1.13007600	1.81523600	-0.15820400
C	2.41838600	-1.88072300	0.03264300
C	0.16480500	-2.76841600	0.38204100
C	0.30393700	2.79222100	0.39808200
C	2.51888600	1.79022400	-0.08806800
N	-0.76113200	-3.37177900	0.78647800
N	3.57396200	-1.71977700	0.15789200
N	3.67404700	1.62552100	-0.05029100
N	-0.57044800	3.45029600	0.81124800
Li	-2.27258200	-2.22298000	0.76538900
Li	-2.13457600	2.28384800	0.77657100
Li	4.53121700	-0.08964600	0.19109000
Se	-2.59138300	0.04718400	-0.17825500