

## Supporting Information

for

**Theoretical study on boron phosphide nanocages doped with superalkalis:**

**Novel electrides having significant nonlinear optical response**

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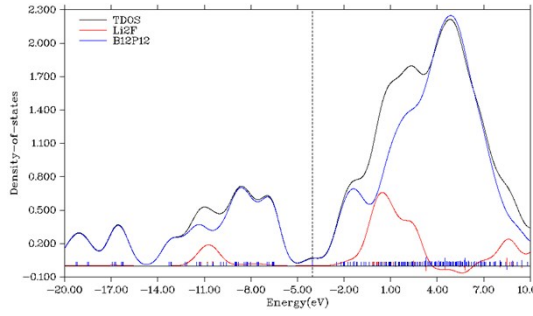
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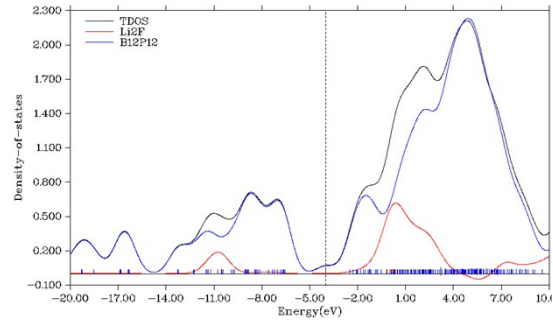
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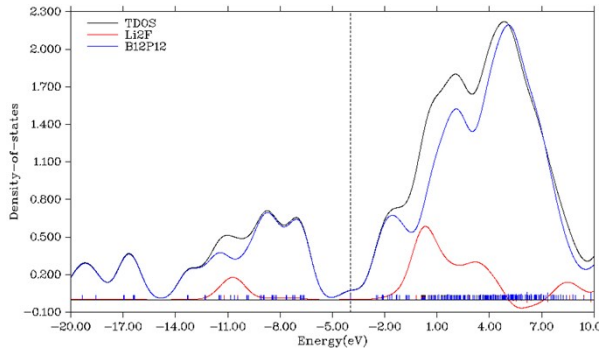
**E-mail:** mazhargilani@cuilahore.edu.pk (M. A. G.)



I

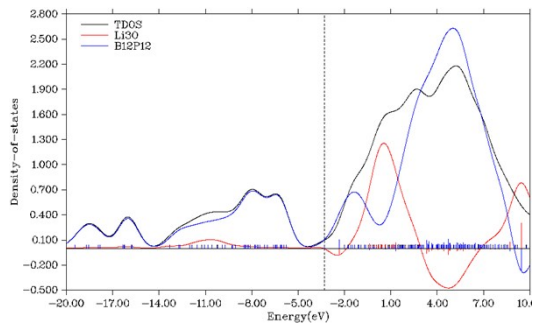


II

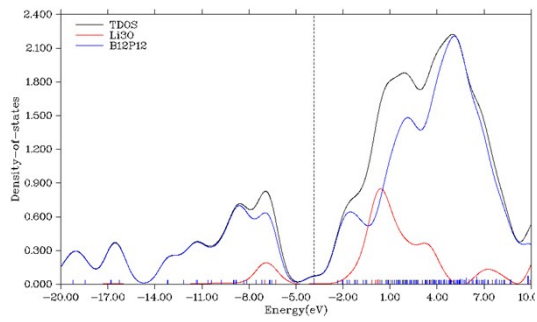


III

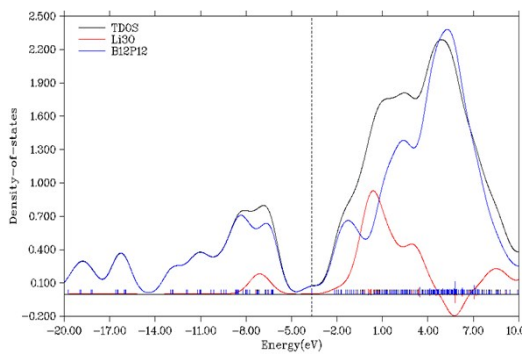
**SI. 1.** Total density of states (TDOS) and partial density of state (PDOS) of the  $\text{Li}_2\text{F}@B_{12}\text{P}_{12}$  isomers (I-III).



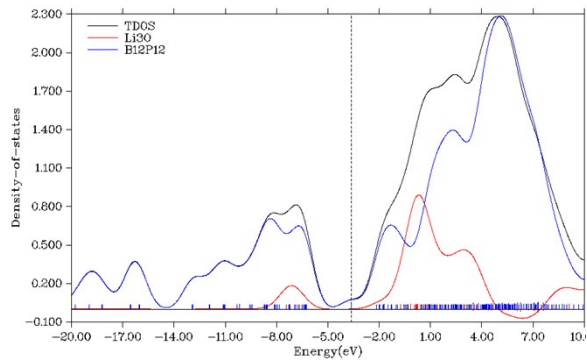
IV



V

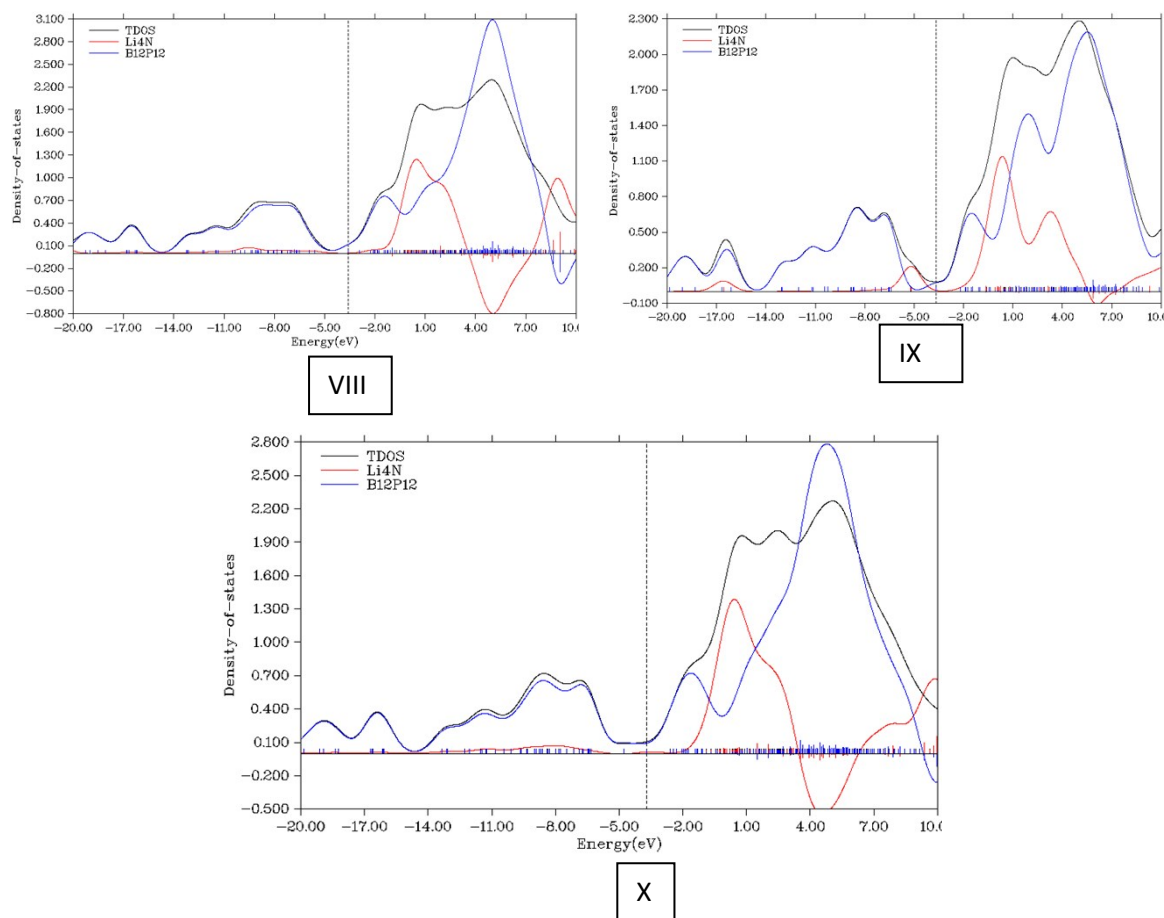


VI



VII

**SI. 2.** Total density of states (TDOS) and partial density of state (PDOS) of the  $\text{Li}_3\text{O}@B_{12}\text{P}_{12}$  isomers (IV-VII).



**SI. 3.** Total density of states (TDOS) and partial density of state (PDOS) of the Li<sub>4</sub>N@B<sub>12</sub>P<sub>12</sub> isomers (VIII-X).

### Cartesian Coordinates:

#### B<sub>12</sub>P<sub>12</sub>

B	2.0543380000	1.3049390000	1.1887820000
B	2.0543380000	1.3049390000	-1.1887820000
B	2.3081520000	-1.4171530000	0.0000000000
B	0.6374170000	-1.0035810000	2.4341460000
B	0.3014890000	-2.6907530000	0.0000000000

B	-2.0543300000	-1.3047170000	1.1889840000
B	-2.0543300000	-1.3047170000	-1.1889840000
B	0.6374170000	-1.0035810000	-2.4341460000
B	-0.6376270000	1.0034350000	-2.4340990000
B	-0.3009840000	2.6907350000	0.0000000000
B	-0.6376270000	1.0034350000	2.4340990000
B	-2.3082650000	1.4168590000	0.0000000000
P	1.2373070000	0.7859200000	2.8348330000
P	-1.2374980000	-0.7860670000	2.8353150000
P	1.5199280000	-2.3930460000	1.4659900000
P	3.1787330000	0.2823830000	0.0000000000
P	1.2373070000	0.7859200000	-2.8348330000
P	1.5199280000	-2.3930460000	-1.4659900000
P	-1.2374980000	-0.7860670000	-2.8353150000
P	-1.6067210000	-2.7568910000	0.0000000000
P	-1.5198340000	2.3928400000	-1.4658240000
P	-1.5198340000	2.3928400000	1.4658240000
P	1.6072620000	2.7577010000	0.0000000000
P	-3.1790770000	-0.2824320000	0.0000000000

**I**

B	0.8416180000	-2.4893110000	-0.0161520000
B	-1.5401710000	-2.4387290000	0.0184800000
B	-0.2969070000	-1.1850260000	2.4151800000
B	2.0926340000	0.0006740000	1.1015020000
B	-0.2970680000	1.1874550000	2.4140350000
B	0.8413660000	2.4894770000	-0.0184100000
B	-1.5404910000	2.4386020000	0.0161510000
B	-2.7670180000	0.0004470000	1.2136320000

B	-2.8006520000	-0.0007090000	-1.1434900000
B	-0.3661690000	-1.1872800000	-2.4145280000
B	2.0649030000	-0.0004280000	-1.1741850000
B	-0.3662680000	1.1848630000	-2.4156410000
P	2.5139360000	-1.5161120000	-0.0414770000
P	2.5138190000	1.5164500000	-0.0429570000
P	1.1821780000	0.0014990000	2.7926240000
P	-0.3310750000	-2.8503670000	1.4725750000
P	-3.1953000000	-1.4745790000	0.0416690000
P	-1.7585740000	0.0013160000	2.8353100000
P	-3.1954910000	1.4742580000	0.0402380000
P	-0.3314620000	2.8519030000	1.4698660000
P	-1.8393540000	-0.0014590000	-2.7937420000
P	1.1013830000	-0.0013360000	-2.8357080000
P	-0.3736140000	-2.8513760000	-1.4695480000
P	-0.3739280000	2.8498200000	-1.4722300000
Li	4.9738900000	1.4756520000	-0.0007020000
Li	4.9739160000	-1.4756090000	0.0016160000
F	5.7933220000	-0.0000630000	0.0072320000

## **II**

B	1.1319360000	-2.3026480000	-0.1719960000
B	-0.8259690000	-2.1944600000	-1.5209930000
B	-1.3793670000	-2.0397070000	1.4066960000
B	1.0615460000	-0.5223380000	2.2681240000
B	-1.8544190000	0.1268830000	2.2173680000
B	0.1669590000	2.2052720000	1.5253720000
B	-1.7954990000	2.2779670000	0.1539710000
B	-2.9673600000	-0.3867340000	-0.4999930000
B	-1.7194460000	0.5480250000	-2.2701020000

B	1.1957060000	-0.1468050000	-2.2179730000
B	2.2243480000	0.3725090000	0.5480510000
B	0.7199730000	2.0709790000	-1.4028430000
P	2.3052350000	-1.4973380000	1.1341770000
P	1.7379960000	1.2905570000	2.1735740000
P	-0.6178340000	-1.1632820000	2.9502930000
P	-0.5549010000	-3.1858570000	0.1148230000
P	-2.3833410000	-1.2580660000	-2.1263740000
P	-3.0442160000	-1.0714940000	1.2832810000
P	-2.9707010000	1.4488780000	-1.1116950000
P	-1.6777230000	2.0229100000	2.0632030000
P	-0.0282310000	1.1596630000	-2.9269490000
P	2.3794040000	1.0639040000	-1.2544000000
P	1.0253550000	-2.0454510000	-2.0900700000
P	-0.1128920000	3.2047100000	-0.1164620000
Li	4.7063930000	-0.9491290000	0.9444260000
Li	4.8633800000	1.0720580000	-1.1601260000
F	5.6251560000	0.0054990000	-0.1035930000

### III

B	-1.8428890000	0.9204570000	1.3194360000
B	-0.5563680000	2.5893700000	0.2316770000
B	0.8983130000	1.1274600000	2.3935690000
B	-0.3981090000	-1.5611980000	2.1014120000
B	2.3746950000	-0.5663610000	1.6369660000
B	1.1854320000	-2.5590630000	-0.2228510000
B	2.4858140000	-0.9110710000	-1.3183270000
B	2.2965150000	1.8259520000	-0.1394850000
B	1.0040580000	1.5531410000	-2.1016890000
B	-1.7489940000	0.5508800000	-1.6448250000

B	-1.6302950000	-1.7734100000	0.1542910000
B	-0.2777360000	-1.1408650000	-2.3966590000
P	-2.2080990000	-0.9017500000	1.8250340000
P	-0.3436190000	-3.0245140000	0.8457260000
P	1.0366290000	-0.6937610000	3.0307820000
P	-0.6643090000	2.2108450000	2.1236190000
P	0.9573930000	3.0324590000	-0.8524150000
P	2.6735950000	1.3431660000	1.6724720000
P	2.7962850000	0.9229640000	-1.7726140000
P	2.8957310000	-1.8518410000	0.3193400000
P	-0.4274260000	0.6808820000	-3.0320440000
P	-2.0793630000	-1.3621310000	-1.6783820000
P	-2.2764660000	1.8674900000	-0.3395810000
P	1.2869280000	-2.2052980000	-2.1217810000
Li	-4.1804530000	-1.4142800000	0.2132300000
Li	-4.7424730000	1.5067540000	-0.2276460000
F	-5.2102870000	-0.0923970000	-0.0362960000

#### IV

B	-0.7281650000	-0.4987270000	-2.4274240000
B	1.3804100000	0.5367080000	-2.4306770000
B	-0.7355590000	2.1800970000	-1.1699740000
B	-2.9638150000	-0.0003640000	0.0000700000
B	-0.7358750000	2.1718590000	1.1843820000
B	-0.7283260000	-0.5152780000	2.4242140000
B	1.3801560000	0.5201900000	2.4342570000
B	1.9828180000	2.1446660000	0.0073180000
B	3.0268270000	0.0157190000	0.0001710000
B	1.3964990000	-2.1842560000	-1.1932080000
B	-1.3001590000	-2.1415890000	-0.0073800000



B	1.3963360000	-2.1923260000	1.1785470000
P	-2.1788220000	-1.2677300000	-1.4788210000
P	-2.1789330000	-1.2775230000	1.4698180000
P	-2.2298660000	1.8966690000	0.0061030000
P	-0.3324400000	1.3459060000	-2.8503790000
P	2.8672220000	1.2635650000	-1.4677390000
P	0.3933810000	3.2180410000	0.0109500000
P	2.8670780000	1.2535380000	1.4764420000
P	-0.3326350000	1.3265050000	2.8591980000
P	2.8895430000	-1.8926610000	-0.0062430000
P	0.2667350000	-3.2349780000	-0.0109210000
P	0.9742600000	-1.3088460000	-2.8442780000
P	0.9741110000	-1.3281420000	2.8355070000
Li	-4.5089170000	-0.9267510000	-1.5365430000
Li	-4.5086040000	-0.9343340000	1.5326680000
Li	-4.5907140000	1.8051290000	0.0045800000
O	-4.4656940000	0.0086500000	0.0002300000

**V**

B	-1.7109360000	-0.0940570000	1.7110930000
B	-0.3745280000	-2.0372670000	1.6732750000
B	-1.7065770000	-1.4412240000	-0.9383730000
B	-1.7090800000	1.5281770000	-0.7800460000
B	-0.3695640000	-0.4326730000	-2.6016300000
B	1.0681450000	2.0185390000	-1.6600890000
B	2.4295990000	0.0806640000	-1.7178660000
B	1.0711370000	-2.4470500000	-0.9154740000
B	2.4273970000	-1.5273460000	0.7947540000
B	1.0640810000	0.4310200000	2.5790730000
B	-0.3772670000	2.4681550000	0.9265510000

B	2.4253870000	1.4525140000	0.9308120000
P	-2.1515670000	1.6814990000	1.1113840000
P	-0.4407830000	2.9639710000	-0.9429120000
P	-2.1456650000	0.1209110000	-2.0193430000
P	-2.1494340000	-1.8109420000	0.8989110000
P	1.1364990000	-2.9640290000	0.9494210000
P	-0.4348380000	-2.2993840000	-2.0971650000
P	2.8328560000	-1.6807390000	-1.0881500000
P	1.1386100000	0.6619050000	-3.0405180000
P	2.8274270000	-0.1014610000	2.0064200000
P	1.1310900000	2.3043420000	2.0944840000
P	-0.4426250000	-0.6668680000	3.0375590000
P	2.8298240000	1.7889710000	-0.9088850000
Li	-4.6796560000	-0.0324290000	-1.6389640000
Li	-4.6932340000	-1.4021840000	0.8455780000
Li	-4.6979690000	1.4387840000	0.7912700000
O	-5.1184120000	0.0021990000	-0.0027680000

## VI

B	-0.7573150000	-2.4787600000	0.1556040000
B	1.6016940000	-2.4373290000	-0.1558780000
B	0.0934370000	-1.1885980000	-2.3961060000
B	-2.1137190000	-0.0007330000	-0.8178120000
B	0.0930630000	1.1852290000	-2.3976750000
B	-0.7581900000	2.4785950000	0.1523100000
B	1.6009470000	2.4374100000	-0.1591100000
B	2.6838380000	-0.0007390000	-1.4870750000
B	2.9873250000	0.0009570000	0.8509680000
B	0.7197660000	-1.1841980000	2.4001530000
B	-1.8480050000	0.0009710000	1.4676360000

B	0.7194150000	1.1875900000	2.3985730000
P	-2.4121440000	-1.5078990000	0.3810040000
P	-2.4131150000	1.5080300000	0.3789280000
P	-1.4215670000	-0.0020130000	-2.6081300000
P	0.2321800000	-2.8539250000	-1.4607030000
P	3.2448580000	-1.4747700000	-0.3703500000
P	1.4967810000	-0.0018540000	-2.9841850000
P	3.2444200000	1.4750600000	-0.3723760000
P	0.2313190000	2.8518070000	-1.4644540000
P	2.2275750000	0.0020280000	2.6048770000
P	-0.6878230000	0.0019140000	2.9968680000
P	0.6162260000	-2.8473500000	1.4590780000
P	0.6153420000	2.8494280000	1.4552940000
Li	-4.8803620000	-1.3325460000	0.0626810000
Li	-7.6026600000	0.0000270000	-0.1672270000
Li	-4.8815990000	1.3317760000	0.0612520000
O	-5.9535270000	-0.0008230000	-0.0207260000

## VII

B	-0.9658200000	-0.5431130000	2.2783090000
B	-2.1434530000	0.4219530000	0.5758700000
B	-0.0217040000	2.1807350000	1.5704030000
B	1.9599230000	0.0456010000	2.2018830000
B	1.9212480000	2.2401300000	0.1819640000
B	3.0246170000	-0.4355630000	-0.5411630000
B	1.7747510000	0.5631280000	-2.2755370000
B	-0.6180300000	2.1198740000	-1.3504580000
B	-1.1521100000	-0.0644490000	-2.2026890000
B	-1.1083790000	-2.2599930000	-0.2010950000
B	1.4255350000	-2.0929980000	1.3532740000

B	0.8299550000	-2.1734200000	-1.5694150000
P	0.7054770000	-1.2336370000	2.9281880000
P	3.1111330000	-1.1595460000	1.2275850000
P	1.8238320000	1.9491830000	2.0884700000
P	-1.6027030000	1.2853270000	2.2143150000
P	-2.3013860000	1.1527000000	-1.2078830000
P	0.2575020000	3.2104660000	-0.0515810000
P	0.0927130000	1.2281180000	-2.9062260000
P	3.0622310000	1.4120990000	-1.1156610000
P	-1.0230220000	-1.9706360000	-2.1153220000
P	0.5583060000	-3.1944360000	0.0492160000
P	-2.2465940000	-1.4538050000	1.1326710000
P	2.4011280000	-1.2605100000	-2.1772280000
Li	-4.8034240000	1.0579890000	-0.9920980000
Li	-7.4555680000	-0.1103640000	-0.0507740000
Li	-4.6633640000	-0.8539840000	0.8553620000
O	-5.8056050000	0.0287260000	-0.0677970000

### VIII

B	-0.6830560000	-2.0839010000	-1.3616810000
B	1.4567510000	-2.4658690000	-0.3536030000
B	1.4861050000	-0.3505190000	-2.4494040000
B	-1.2676050000	0.7537840000	-1.9869440000
B	1.4908780000	1.8737710000	-1.6132110000
B	-0.6758740000	2.4711750000	0.3459770000
B	1.4647850000	2.0842500000	1.3554110000
B	3.1119960000	-0.0123410000	0.0190230000
B	2.0503390000	-0.7574870000	2.0079950000
B	-0.7047970000	-1.8678990000	1.6165890000
B	-3.1090910000	-0.0130520000	0.0128950000

B	-0.7019700000	0.3439820000	2.4459530000
P	-2.1262940000	-0.9348770000	-1.7313450000
P	-2.1246040000	1.8588920000	-0.6857170000
P	0.3398190000	1.1136200000	-2.9605720000
P	1.0493630000	-2.1892280000	-2.2154010000
P	2.9381380000	-1.8231480000	0.6688560000
P	2.9830560000	0.6591440000	-1.7670090000
P	2.9431750000	0.9231810000	1.7007830000
P	1.0600540000	3.1049410000	-0.2266670000
P	0.4473510000	-1.1177040000	2.9748830000
P	-2.1765400000	-0.6684990000	1.7846560000
P	-0.2725220000	-3.1045150000	0.2278970000
P	-0.2639520000	2.1877140000	2.2140160000
Li	-6.3817410000	0.0033650000	-0.0144140000
Li	-4.4754890000	-1.1723550000	-1.4715770000
Li	-4.4693300000	1.8479080000	-0.3099910000
Li	-4.5684580000	-0.6642340000	1.7836640000
N	-4.5518460000	-0.0094750000	0.0108920000

## IX

B	-1.1394440000	1.8582220000	1.8380670000
B	-2.4997190000	-0.0776380000	1.7203110000
B	-2.4997240000	1.5288860000	-0.7928560000
B	0.2999700000	2.5422930000	-0.6967810000
B	-1.1396690000	0.6628160000	-2.5282000000
B	1.6362400000	0.0649980000	-1.7172150000
B	0.2997810000	-1.8746640000	-1.8532940000
B	-2.5001690000	-1.4513480000	-0.9276690000
B	-1.1396640000	-2.5210650000	0.6903390000
B	0.3000680000	-0.6678120000	2.5500610000

B	1.6367530000	1.4552960000	0.9151980000
B	1.6356980000	-1.5195700000	0.8021850000
P	0.3666980000	2.8694560000	1.2094770000
P	2.0736240000	1.7777670000	-0.9562660000
P	-1.2081750000	2.4851060000	-1.8754460000
P	-2.9024730000	1.6971230000	1.0704660000
P	-2.9025190000	-1.7754360000	0.9343920000
P	-2.9025560000	0.0786450000	-2.0047680000
P	-1.2083420000	-2.8668350000	-1.2142510000
P	0.3665580000	-0.3871830000	-3.0894540000
P	0.3666570000	-2.4822450000	1.8801100000
P	2.0735330000	-0.0605800000	2.0175320000
P	-1.2080800000	0.3817300000	3.0896680000
P	2.0732960000	-1.7172710000	-1.0611950000
Li	7.1441630000	-0.0003020000	-0.0008250000
Li	4.6184400000	1.4846610000	-0.6488600000
Li	4.6159700000	-1.3038010000	-0.9613840000
Li	4.6172630000	-0.1810190000	1.6096700000
N	5.3912250000	-0.0006910000	-0.0000720000

## X

B	-0.4180920000	-2.7294880000	0.0036100000
B	-2.5603750000	-1.6166380000	0.0042580000
B	-0.9121240000	-1.0514330000	2.4196300000
B	1.8135650000	-1.1327380000	1.1359540000
B	0.1734030000	1.0626650000	2.4195770000
B	1.8398470000	1.6555440000	-0.0041830000
B	-0.3145590000	2.7227080000	-0.0034880000
B	-2.5533350000	1.1137900000	1.1801450000
B	-2.5555990000	1.1106990000	-1.1787900000

B	-0.9167080000	-1.0577090000	-2.4156390000
B	1.8120400000	-1.1356320000	-1.1374100000
B	0.1687670000	1.0564330000	-2.4233350000
P	1.5157820000	-2.7074120000	0.0016780000
P	2.8083840000	0.0207100000	-0.0027850000
P	0.9382760000	-0.6694830000	2.8065650000
P	-1.6697520000	-2.5148390000	1.4625440000
P	-3.6034000000	-0.0056280000	0.0031550000
P	-1.6752230000	0.6754060000	2.8152570000
P	-2.2295410000	2.6026180000	-0.0015600000
P	0.9268560000	2.5466120000	1.4698580000
P	-1.6806100000	0.6680820000	-2.8143910000
P	0.9328970000	-0.6766780000	-2.8072460000
P	-1.6726180000	-2.5186660000	-1.4534550000
P	0.9239950000	2.5427260000	-1.4787600000
Li	4.2868310000	-1.0185760000	1.5920950000
Li	4.2839050000	-1.0267360000	-1.5928340000
Li	4.3714140000	1.9923190000	-0.0034420000
Li	6.3370580000	0.0738240000	0.0116170000
N	4.5075080000	0.0706840000	-0.0052680000