

Electronic Supplementary Information (ESI) available for:

**Theoretical study on superalkali-doped nanocages: unique
inorganic electrides with high stability, deep-ultraviolet
transparency, and considerable nonlinear optical response**

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1. Figures and Table

Fig. S1. Structures of isolated M_3O ($M = \text{Li, Na, K}$) and $X_{12}Y_{12}$ ($X = \text{B, Al}$; $Y = \text{N, P}$) clusters.

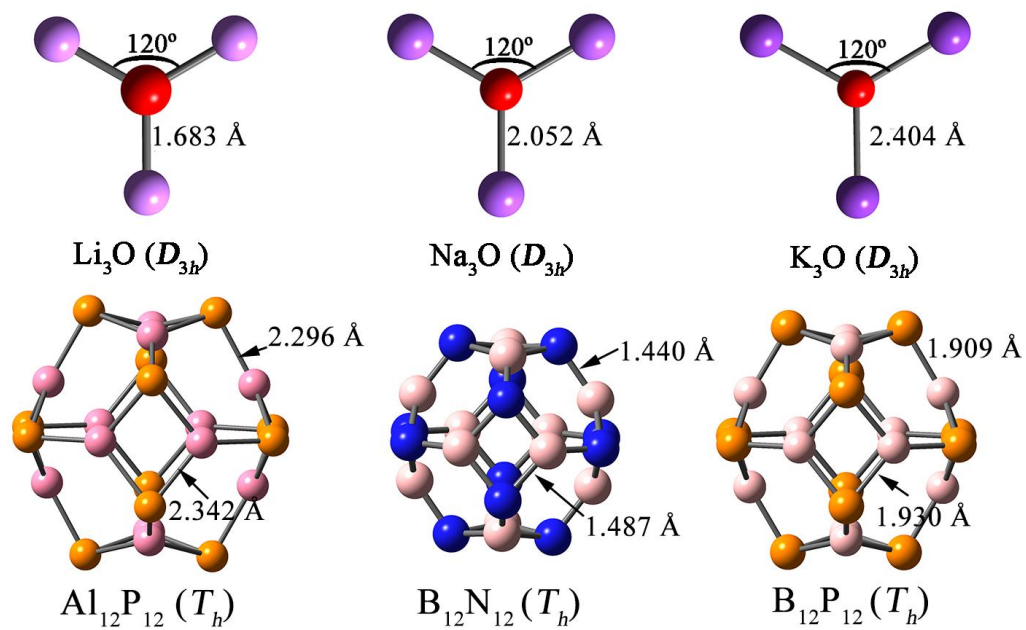


Fig. S2. The equilibrium geometries of $M_3O@Al_{12}N_{12}$ ($M = Na$ and K) and $Li_3O@X_{12}Y_{12}$ ($X = B, Al$; $Y = N, P$) compounds.

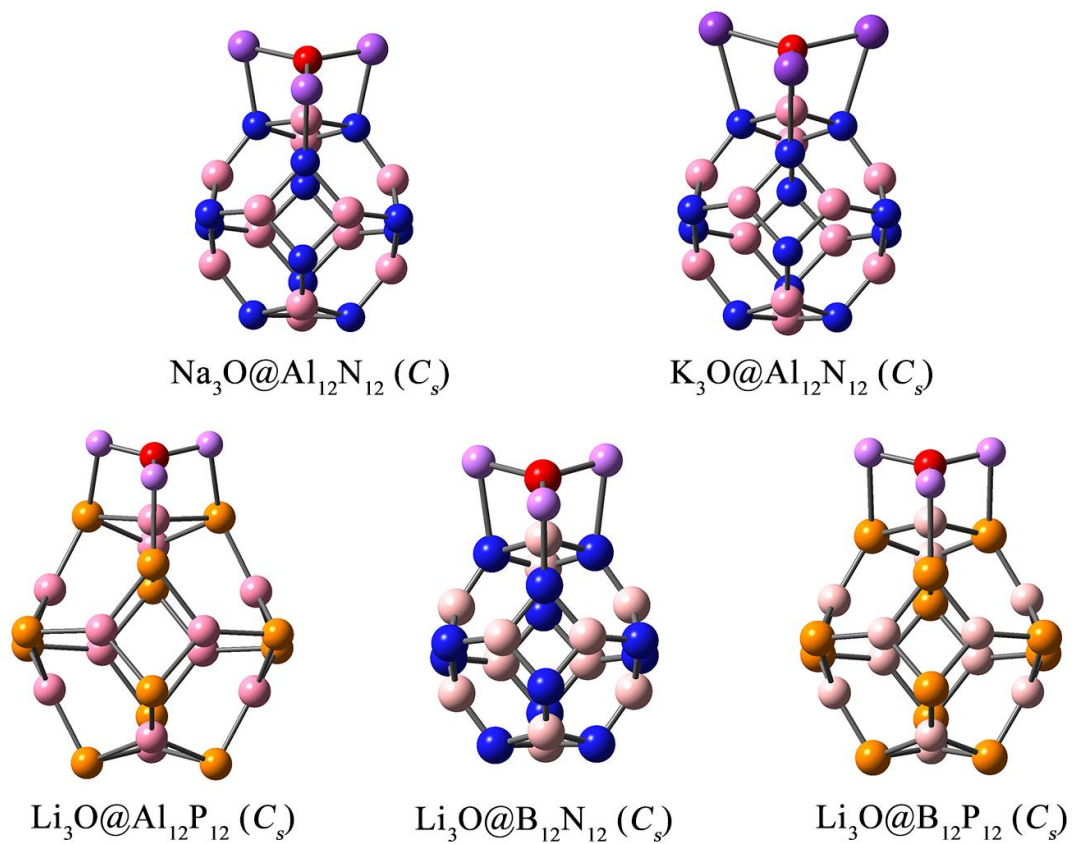


Fig. S3. The HOMOs of $M_3O@Al_{12}N_{12}$ ($M = Na$ and K) and $Li_3O@X_{12}Y_{12}$ ($X = B, Al$; $Y = N, P$) compounds.

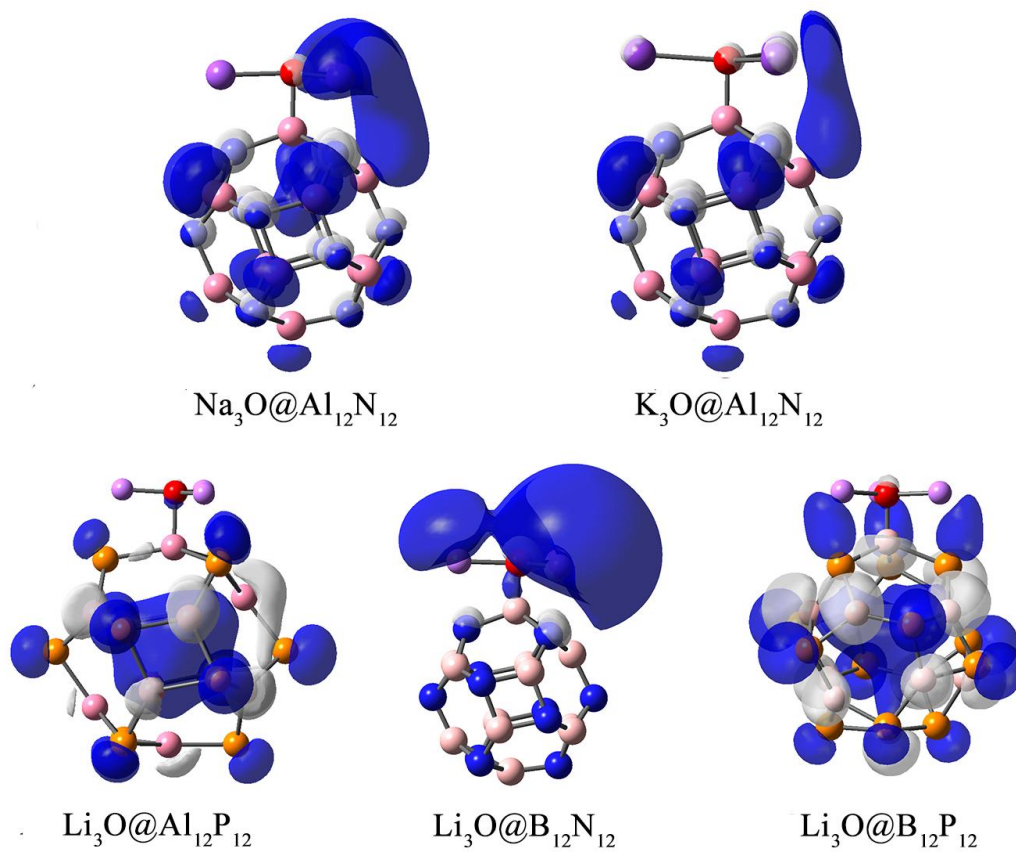
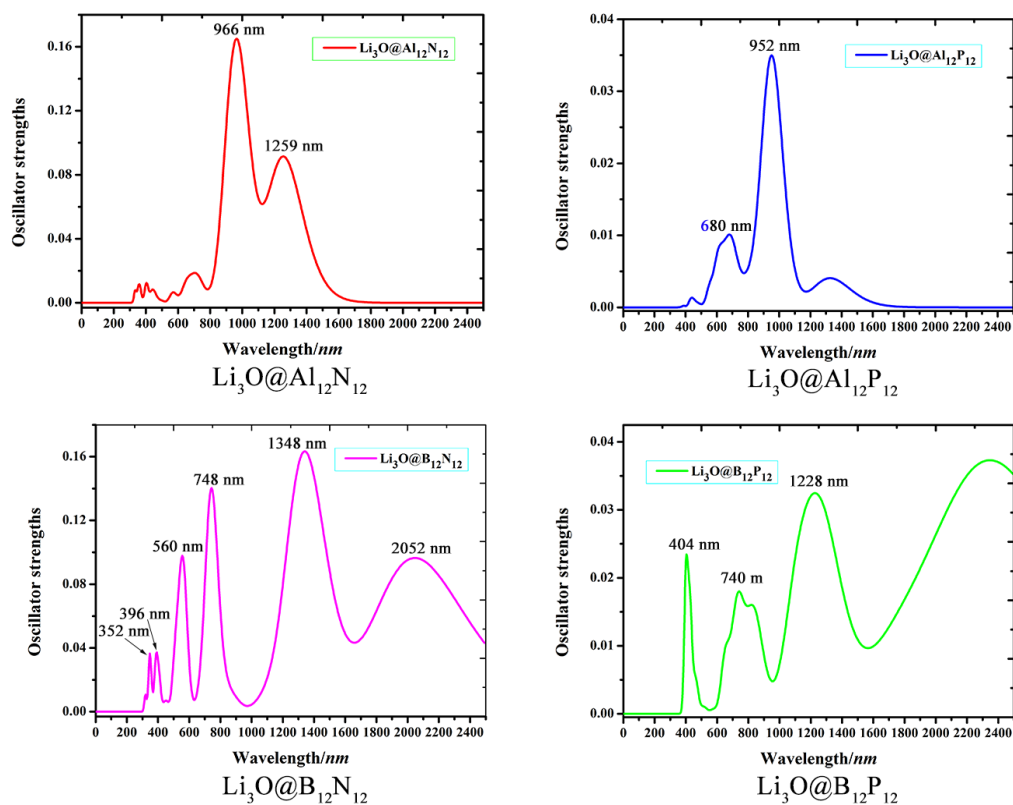


Fig. S4 The UV-VIS-IR spectra of $\text{Li}_3\text{O}@X_{12}Y_{12}$ ($X = \text{B}, \text{Al}; Y = \text{N}, \text{P}$) compounds.



Cartesian coordinates

Isomer **A** of $\text{Li}_3\text{O@Al}_{12}\text{N}_{12}$ at the B3LYP/6-31+G(d) level

Al	-0.53383100	-1.43797500	-2.48016100
Al	0.55547900	0.81957500	-2.48247200
Al	-2.27216500	0.74878800	-1.25237100
Al	-2.18973900	-2.02796300	0.00000000
Al	-0.09208900	2.55919900	0.00000000
Al	-2.27216500	0.74878800	1.25237100
Al	-0.53383100	-1.43797500	2.48016100
Al	0.55547900	0.81957500	2.48247200
Al	0.07127900	-3.10266700	0.00000000
Al	2.24658700	1.44602400	0.00000000
Al	2.24299800	-1.37799000	-1.24969500
Al	2.24299800	-1.37799000	1.24969500
N	-1.22336000	0.29317400	-2.63579800
N	-1.13410200	-2.71323300	-1.36663300
N	1.16621500	2.14011600	-1.39412900
N	-2.98816200	-0.41493200	0.00000000
N	-1.89494500	2.10522000	0.00000000
N	-1.13410200	-2.71323300	1.36663300
N	1.16621500	2.14011600	1.39412900
N	-1.22336000	0.29317400	2.63579800
N	1.23854800	-0.89255600	2.65788800
N	1.23854800	-0.89255600	-2.65788800
N	2.96144400	-0.20291800	0.00000000
N	1.82107200	-2.68804700	0.00000000
O	-0.07505300	4.35848500	0.00000000
Li	-1.91032500	4.10506900	0.00000000
Li	1.01671700	4.11743000	-1.48481300
Li	1.01671700	4.11743000	1.48481300

Isomer **B** of $\text{Li}_3\text{O@Al}_{12}\text{N}_{12}$ at the B3LYP/6-31+G(d) level

Al	-0.34888600	-2.75770300	0.10173300
Al	-1.26775900	-1.37221700	-1.73044400
Al	-2.45712800	-0.37606200	0.90582000
Al	0.24061800	-1.05209400	2.49490000
Al	-1.79366500	1.99930500	-1.17506200
Al	-1.02007200	1.58629000	1.80163200
Al	1.99539500	1.34710800	1.76044000
Al	1.02536200	2.70385200	-0.10204800
Al	2.27250000	-1.62170900	1.13939000
Al	0.21481300	1.03438400	-2.45616400
Al	1.69974700	-1.60150500	-1.83294800
Al	2.83559000	0.45789700	-1.00533600

N	-2.01129800	-1.94729700	-0.11320700
N	0.71717200	-2.56962400	1.52189500
N	-1.52951500	0.33622100	-2.25487900
N	-1.30276700	-0.14374200	2.39603600
N	-2.33480200	1.56049100	0.52729500
N	1.95728900	-0.32182800	2.42028700
N	-0.06084800	2.59459300	-1.52784300
N	0.53509300	2.47701900	1.67867300
N	2.66992000	1.85344100	0.10252600
N	0.17049100	-2.52299400	-1.67217800
N	1.76846500	0.12146900	-2.49765500
N	2.95824100	-1.33317200	-0.50005700
O	-4.19800700	-0.41024900	0.33301500
Li	-4.25011000	1.37618700	0.71756400
Li	-3.59527200	0.13590700	-1.43944200
Li	-3.93220000	-2.16815500	0.07013200

Isomer C of $\text{Li}_3\text{O@Al}_{12}\text{N}_{12}$ at the B3LYP/6-31+G(d) level

Al	0.00000000	2.72352100	0.41322300
Al	1.35891300	1.14089900	1.84341300
Al	-1.66750400	0.60640400	1.84341300
Al	-2.33105000	1.34643300	-1.03014700
Al	0.30859100	-1.74730300	1.84341300
Al	-2.35863800	-1.36176000	0.41322300
Al	-1.33809300	-1.14000000	-2.46471800
Al	-0.00052000	-2.69196500	-1.03014700
Al	-0.31822300	1.72882300	-2.46471800
Al	2.35863800	-1.36176000	0.41322300
Al	2.33157000	1.34553200	-1.03014700
Al	1.65631600	-0.58882200	-2.46471800
N	-0.37895200	1.88569700	2.07000800
N	-1.04979200	2.69071400	-1.04042700
N	1.82253700	-0.61466700	2.07000800
N	-2.84238400	0.43191600	0.43451700
N	-1.44358500	-1.27103000	2.07000800
N	-1.78219900	0.59190800	-2.63265300
N	1.04714200	-2.67753500	0.43451700
N	-1.80533100	-2.25450400	-1.04042700
N	0.37849200	-1.83938400	-2.63265300
N	1.79524200	2.24561900	0.43451700
N	2.85512300	-0.43621100	-1.04042700
N	1.40370700	1.24747600	-2.63265300
O	0.00000000	0.00000000	4.51469800
Li	-1.26621200	-1.08922200	4.07922400

Li	1.57640000	-0.55196100	4.07922400
Li	-0.31018800	1.64118300	4.07922400

Isomer **D** of $\text{Li}_3\text{O@Al}_{12}\text{N}_{12}$ at the B3LYP/6-31+G(d) level

Al	-1.65427100	-0.43691900	-1.69233300
Al	-2.38914200	1.23437700	0.16985100
Al	-1.46067000	-1.73528000	0.98264100
Al	0.51247500	-2.51263000	-1.19162800
Al	-0.37817900	0.57525900	2.57115900
Al	0.87858500	-2.07438100	1.79316100
Al	2.98966800	-1.09168200	-0.16600700
Al	2.54792400	0.46292900	1.74242200
Al	1.23784000	-0.57618200	-2.58765600
Al	0.35216100	2.48789800	1.17511000
Al	-0.02135400	2.06125900	-1.76852800
Al	2.33950500	1.76363800	-0.99642600
N	-2.55278500	-0.75957600	-0.08364200
N	-0.38434700	-1.47220200	-2.43335800
N	-1.30941900	1.78260000	1.54971200
N	-0.10772400	-2.89421100	0.44627500
N	-0.59082800	-1.20948000	2.53052200
N	2.19200000	-1.83025000	-1.59553400
N	1.25156600	1.47028500	2.45598000
N	2.52931000	-1.39498800	1.60938100
N	3.33401500	0.71646500	0.07473700
N	-1.67013800	1.38565500	-1.59064400
N	0.98483800	2.90630200	-0.45278900
N	1.45166900	1.20075000	-2.52799300
O	-6.01754900	-0.11177200	-0.02157200
Li	-4.48940900	-0.94247200	-0.07045600
Li	-5.32827800	1.43830500	0.15896400
Li	-7.57090500	-0.65349400	-0.12814100

Isomer **E** of $\text{Li}_3\text{O@Al}_{12}\text{N}_{12}$ at the B3LYP/6-31+G(d) level

Al	-2.61996000	0.27723000	0.00000000
Al	-1.18647300	2.40471600	0.00000000
Al	-0.94548400	0.39172900	2.46883000
Al	-1.62698000	-2.29980200	1.24796700
Al	1.59772200	1.42492000	1.24564300
Al	0.93884700	-1.26032800	2.48533800
Al	1.04506100	-3.01301700	0.00000000
Al	2.68522500	-1.13371900	0.00000000
Al	-1.62698000	-2.29980200	-1.24796700
Al	1.59772200	1.42492000	-1.24564300

Al	-0.94548400	0.39172900	-2.46883000
Al	0.93884700	-1.26032800	-2.48533800
N	-1.98149600	1.33387900	1.36713800
N	-2.75329900	-1.52139100	0.00000000
N	0.72693700	2.52237400	0.00000000
N	-0.89445300	-1.46480000	2.65768000
N	0.89865200	0.59000500	2.66268200
N	-0.71656300	-3.34089000	0.00000000
N	2.73972200	0.66078100	0.00000000
N	1.99882500	-2.18592300	1.36711600
N	1.99882500	-2.18592300	-1.36711600
N	-1.98149600	1.33387900	-1.36713800
N	0.89865200	0.59000500	-2.66268200
N	-0.89445300	-1.46480000	-2.65768000
O	0.13279100	6.01869200	0.00000000
Li	0.71314400	7.56175500	0.00000000
Li	-1.43852900	5.35548100	0.00000000
Li	0.91934300	4.46705600	0.00000000

Na₃O@Al₁₂N₁₂ at the B3LYP/6-31+G(d) level

Al	0.52930800	-1.84348700	2.48470800
Al	-0.53913300	0.42285300	2.46480600
Al	2.23685400	0.34374200	1.24322700
Al	2.17842500	-2.43463600	0.00000000
Al	0.09183500	2.35249500	0.00000000
Al	2.23685400	0.34374200	-1.24322700
Al	0.52930800	-1.84348700	-2.48470800
Al	-0.53913300	0.42285300	-2.46480600
Al	-0.08448900	-3.50108700	0.00000000
Al	-2.14889500	1.01495900	0.00000000
Al	-2.24392600	-1.77124600	1.24906500
Al	-2.24392600	-1.77124600	-1.24906500
N	1.22992800	-0.12340100	2.65405500
N	1.12106200	-3.12088000	1.36697200
N	-1.14293700	1.74494200	1.39070300
N	2.97417300	-0.82478600	0.00000000
N	1.84896300	1.68097200	0.00000000
N	1.12106200	-3.12088000	-1.36697200
N	-1.14293700	1.74494200	-1.39070300
N	1.22992800	-0.12340100	-2.65405500
N	-1.23928600	-1.28960100	-2.65564000
N	-1.23928600	-1.28960100	2.65564000
N	-2.95501000	-0.59304300	0.00000000
N	-1.83367700	-3.08764900	0.00000000

O	0.11227400	4.12105900	0.00000000
Na	-1.19310000	4.06386400	-1.80768800
Na	-1.19310000	4.06386400	1.80768800
Na	2.31873500	3.98930100	0.00000000

K₃O@Al₁₂N₁₂ at the B3LYP/6-31+G(d) level

Al	0.53216100	-2.22557400	2.48718300
Al	-0.53896000	0.03939700	2.45329800
Al	2.21029700	-0.02658800	1.23767900
Al	2.17902800	-2.80668100	0.00000000
Al	0.07415900	2.06414700	0.00000000
Al	2.21029700	-0.02658800	-1.23767900
Al	0.53216100	-2.22557400	-2.48718300
Al	-0.53896000	0.03939700	-2.45329800
Al	-0.07875900	-3.88410000	0.00000000
Al	-2.11462000	0.61537000	0.00000000
Al	-2.23913000	-2.16038400	1.24819100
Al	-2.23913000	-2.16038400	-1.24819100
N	1.22905500	-0.50699100	2.66433700
N	1.12566100	-3.50200200	1.36740400
N	-1.14357100	1.36132100	1.39062100
N	2.96700100	-1.19500900	0.00000000
N	1.80661700	1.29851400	0.00000000
N	1.12566100	-3.50200200	-1.36740400
N	-1.14357100	1.36132100	-1.39062100
N	1.22905500	-0.50699100	-2.66433700
N	-1.23776200	-1.67771600	-2.65627200
N	-1.23776200	-1.67771600	2.65627200
N	-2.94954900	-0.98282900	0.00000000
N	-1.83018400	-3.48018900	0.00000000
O	0.10398900	3.81802600	0.00000000
K	-1.34062600	4.00041600	-2.13946600
K	-1.34062600	4.00041600	2.13946600
K	2.66717200	3.91370100	0.00000000

Li₃O@Al₁₂P₁₂ at the B3LYP/6-31+G(d) level

P	-2.38474700	2.70855400	0.00000000
P	-3.87368600	-0.50987700	0.00000000
P	-1.64173100	0.46099900	3.46672000
P	1.44750600	2.85305200	1.82518700
P	3.89570900	-0.00840000	0.00000000
P	1.64111900	-0.98825700	3.46085000
P	2.42547000	-3.26780500	0.00000000
P	-1.39306800	-3.41156800	1.78882700

P	1.64111900	-0.98825700	-3.46085000
P	-1.64173100	0.46099900	-3.46672000
P	1.44750600	2.85305200	-1.82518700
P	-1.39306800	-3.41156800	-1.78882700
Al	2.39061400	1.71008200	0.00000000
Al	0.55922800	0.99396300	2.85841600
Al	-0.56153100	-1.55205100	2.84476200
Al	2.58685200	-1.39118800	1.39985500
Al	2.58685200	-1.39118800	-1.39985500
Al	0.55922800	0.99396300	-2.85841600
Al	-0.56153100	-1.55205100	-2.84476200
Al	0.13678800	-3.42562900	0.00000000
Al	-2.59407400	0.84389200	1.41921200
Al	-2.59407400	0.84389200	-1.41921200
Al	-0.09092300	3.26350100	0.00000000
Al	-2.43625500	-2.30985300	0.00000000
O	-0.15461700	5.11597400	0.00000000
Li	0.80050900	5.18716000	1.53106600
Li	-1.95910500	5.11001100	0.00000000
Li	0.80050900	5.18716000	-1.53106600

Li₃O@B₁₂N₁₂ at the B3LYP/6-31+G(d) level

N	-1.01195300	0.04305100	2.10641500
N	0.91255600	1.51661500	1.14504500
N	-0.88676900	-2.37245600	1.12436800
N	-1.51940300	1.50592300	0.00000000
N	-2.39228600	-0.57653400	0.00000000
N	0.91255600	1.51661500	-1.14504500
N	-0.88676900	-2.37245600	-1.12436800
N	-1.01195300	0.04305100	-2.10641500
N	1.01907400	-0.90998800	-2.11981200
N	1.01907400	-0.90998800	2.11981200
N	1.46397200	-2.35780100	0.00000000
N	2.37997800	-0.30343500	0.00000000
B	-0.07907400	2.14318700	0.00000000
B	1.65958400	0.95363500	0.00000000
B	0.41339000	0.44050600	1.94423400
B	-1.78431900	0.39357100	0.94508800
B	-0.39942300	-1.30684000	1.96339000
B	-1.69185700	-1.83205000	0.00000000
B	0.05282900	-2.63817000	0.00000000
B	1.78778300	-1.26595100	0.95840400
B	1.78778300	-1.26595100	-0.95840400
B	0.41339000	0.44050600	-1.94423400

B	-1.78431900	0.39357100	-0.94508800
B	-0.39942300	-1.30684000	-1.96339000
O	-0.09364200	3.55902200	0.00000000
Li	-1.88437600	3.48845900	0.00000000
Li	1.08900000	3.59306800	1.41068600
Li	1.08900000	3.59306800	-1.41068600

Li₃O@B₁₂P₁₂ at the B3LYP/6-31+G(d) level

B	-2.18858800	-1.39579300	1.18589200
B	-2.18858800	-1.39579300	-1.18589200
B	-2.14130300	1.30049700	0.00000000
B	-0.50682200	0.72824200	2.42587300
B	0.00017400	2.96416700	0.00000000
B	2.17620200	0.73501500	1.17736100
B	2.17620200	0.73501500	-1.17736100
B	-0.50682200	0.72824200	-2.42587300
B	0.52817200	-1.38034900	-2.43245900
B	0.01507500	-3.02680600	0.00000000
B	0.52817200	-1.38034900	2.43245900
B	2.14436400	-1.98316700	0.00000000
P	-1.31870100	-0.97388200	2.83997600
P	1.33637600	0.33222300	2.85499400
P	-1.27201300	2.17910400	1.47427400
P	-3.23519400	-0.26597700	0.00000000
P	-1.31870100	-0.97388200	-2.83997600
P	-1.27201300	2.17910400	-1.47427400
P	1.33637600	0.33222300	-2.85499400
P	1.89701400	2.22903300	0.00000000
P	1.25798200	-2.86734500	-1.47208000
P	1.25798200	-2.86734500	1.47208000
P	-1.89323800	-2.88897800	0.00000000
P	3.21823900	-0.39403900	0.00000000
O	0.00935900	4.46595100	0.00000000
Li	-0.93101000	4.50915700	-1.53413000
Li	-0.93101000	4.50915700	1.53413000
Li	1.80612100	4.58975700	0.00000000