Supplementary Information for:

The Devil in the Details: Lessons from Li_6PS_5X for Robust High-Throughput Workflows

Asif Iqbal Bhatti[1,2], Sandeep Kumar[1,2], Catharina Jaeken[3], Michael Sluydts[3], Danny E.P. Vanpoucke[1,4], and Stefaan Cottenier*[1,2]

[1]Department of Electromechanical, Systems and Metal Engineering, Ghent University, Belgium

[2]Center for Molecular Modeling, Ghent University, Belgium

[3]ePotentia, Belgium

[4]Hasselt University and imec, Institute for Materials Research (imo-imomec), Quantum & Artificial inTelligence design Of Materials (QuATOMs), Belgium

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*Corresponding author: stefaan.cottenier@ugent.be

1 Supplementary Information

All data used in this paper are available at https://doi.org/10.5281/zenodo.13744522 (cif files as well as VASP input and output files). A selection of these data and some additional pictures are listed in this Supplementary Information file.

1.1 Isovalent crystals

Table S1: Isovalent analog crystals. ΔE_{hull} values in eV/atom when the crystal is kept to be cubic and when a random distortion followed by a full geometry optimization is applied.

Crystals	cubic	distorted	Crystals	cubic	distorted	Crystals	cubic	distorted
Li24Te2N1Y1S16S4Cl4	0.36	0.30	Li24Ir2Os1Mn1S16S4Cl4	0.20	0.19	Li24W2Sm1Pt1S16S4Cl4	0.18	0.14
Li24Se2Mn1Re1S16S4Cl4	0.15	0.13	Li24Se2Mo1Te1S16S4Cl4	0.15	0.11	Li24Mo2Ta1V1S16S4Cl4	0.13	0.12
Li24W2Mn1Hg1S16S4Cl4	0.13	0.11	Li24P2V1As1S16S4Cl4	0.04	0.02	Li24Re2Ge1Te1S16S4Cl4	0.13	0.11
Li24Ru2Be1Se1S16S4Cl4	0.23	0.15	Li24Mn2Ta1Ru1S16S4Cl4	0.14	0.14	Li24Se2Mn1Te1S16S4Cl4	0.14	0.11
Li24Mo2Mn1Pt1S16S4Cl4	0.15	0.13	Li24Ru2Mn1V1S16S4Cl4	0.18	0.17	Li24Se2Nb1W1S16S4Cl4	0.14	0.12
Li24Nb2Ru1Si1S16S4Cl4	0.14	0.11	Li24Cr2Ir1P1S16S4Cl4	0.12	0.10	Li24N2Mn1Ru1S16S4Cl4	0.40	0.36
Li24Nb2Os1Te1S16S4Cl4	0.15	0.13	Li24Pt2Mn1As1S16S4Cl4	0.14	0.12	Li24Nb2Ru1Bi1S16S4Cl4	0.16	0.14
Li24Os2Mn1Cr1S16S4Cl4	0.16	0.16	Li24Re2Ti1Cr1S16S4Cl4	0.13	0.12	Li24Mo2Pb1W1S16S4Cl4	0.14	0.13
Li24Ru2Ce1Pd1S16S4Cl4	0.22	0.19	Li24Ru2N1Cu1S16S4Cl4	0.44	0.39	Li24Se2Mn1Be1S16S4Cl4	0.16	0.10
Li24Ru2P1Tl1S16S4Cl4	0.17	0.14	Li24Ir2Pt1Os1S16S4Cl4	0.23	0.21	Li24Ru2W1Nd1S16S4Cl4	0.21	0.20
Li24Rh2Se1Mn1S16S4Cl4	0.18	0.16	Li24As2Se1V1S16S4Cl4	0.08	0.06	Li24Cr2Eu1Ta1S16S4Cl4	0.27	0.24
Li24W2Si1Se1S16S4Cl4	0.12	0.09	Li24Bi2Cr1Te1S16S4Cl4	0.14	0.10	Li_6PS_5Cl	0.09	0.02
Li24Se2Mn1Pt1S16S4Cl4	0.17	0.12	Li24Mn2W1Pb1S16S4Cl4	0.11	0.10			
Li24Re2P1Ta1S16S4Cl4	0.13	0.12	Li24Mo2Re1Ti1S16S4Cl4	0.15	0.13			
Li24Mo2Yb1W1S16S4Cl4	0.13	0.12	Li24Re2W1Ni1S16S4Cl4	0.16	0.14			
Li24Pt2C1Re1S16S4Cl4	0.20	0.17	Li24Sb2Re1Sn1S16S4Cl4	0.10	0.08			
Li24Sb2N1Ir1S16S4Cl4	0.35	0.31	Li24Os2Hf1Re1S16S4Cl4	0.19	0.18			
Li24Os2Ca1W1S16S4Cl4	0.21	0.17	Li24V2Mn1Mo1S16S4Cl4	0.11	0.09			
Li24Nb2Os1Ir1S16S4Cl4	0.17	0.16	Li24Cr2Re1Ru1S16S4Cl4	0.14	0.13			
Li24Se2Cr1Gd1S16S4Cl4	0.31	0.28	Li24Re2Ru1Ti1S16S4Cl4	0.17	0.16			
Li24Te2Cr1Zn1S16S4Cl4	0.13	0.08	Li24Mo2Re1Fe1S16S4Cl4	0.16	0.15			
Li24Ru2Cr1Pt1S16S4Cl4	0.20	0.18	Li24Te2Hf1Mo1S16S4Cl4	0.15	0.12			
Li24Ta2Se1Cr1S16S4Cl4	0.12	0.10	Li24Ir2W1Re1S16S4Cl4	0.20	0.18			
Li24Re2Se1Yb1S16S4Cl4	0.16	0.15	Li24Mo2N1Ru1S16S4Cl4	0.39	0.36			
Li24W2Rh1C1S16S4Cl4	0.16	0.14	Li24Mo2Ag1Bi1S16S4Cl4	0.14	0.10			
Li24Os2Pt1Zr1S16S4Cl4	0.21	0.19	Li24Te2Pd1Co1S16S4Cl4	0.17	0.11			
Li24Mn2Te1Cd1S16S4Cl4	0.15	0.11	Li24As2Bi1P1S16S4Cl4	0.11	0.03			
Li24W2Al1As1S16S4Cl4	0.08	0.05	Li24Cr2Rh1Re1S16S4Cl4	0.14	0.12			
Li24Cr2Hf1Ce1S16S4Cl4	0.16	0.10	Li24Co2W1Te1S16S4Cl4	0.16	0.14			
Li24W2Os1Te1S16S4Cl4	0.16	0.14	Li24Ru2Bi1Fe1S16S4Cl4	0.19	0.18			
Li24Re2Tb1Pt1S16S4Cl4	0.19	0.16	Li24Ta2Te1W1S16S4Cl4	0.13	0.11			
Li24Ta2Se1V1S16S4Cl4	0.11	0.09	Li24Mo2Ru1Zn1S16S4Cl4	0.18	0.13			
Li24Fe2Re1Mn1S16S4Cl4	0.16	0.15	Li24Te2Ba1Mo1S16S4Cl4	0.20	0.12			
Li24Te2Mn1Er1S16S4Cl4	0.14	0.11	Li24V2Os1W1S16S4Cl4	0.13	0.12			
Li24Mn2B1Pt1S16S4Cl4	0.15	0.12	Li24Mn2W1Cu1S16S4Cl4	0.13	0.10			
Li24Ta2Re1Ti1S16S4Cl4	0.12	0.11	Li24Rh2Te1Mo1S16S4Cl4	0.17	0.14			
Li24Re2W1Tm1S16S4Cl4	0.16	0.14	Li24Ru2Se1Ni1S16S4Cl4	0.21	0.19			
Li24N2W1Ta1S16S4Cl4	0.37	0.34	Li24Pt2Cr1Ru1S16S4Cl4	0.19	0.17			
Li24W2Mn1Os1S16S4Cl4	0.15	0.14	Li24Sb2Te1Pb1S16S4Cl4	0.11	0.08			
Li24Se2Nb1Ir1S16S4Cl4	0.17	0.14	Li24Se2Rh1Ru1S16S4Cl4	0.20	0.15			

1.2 Simulated XRD spectrum of $\beta-Li_3PS_4$ and $\beta'-Li_3PS_4$

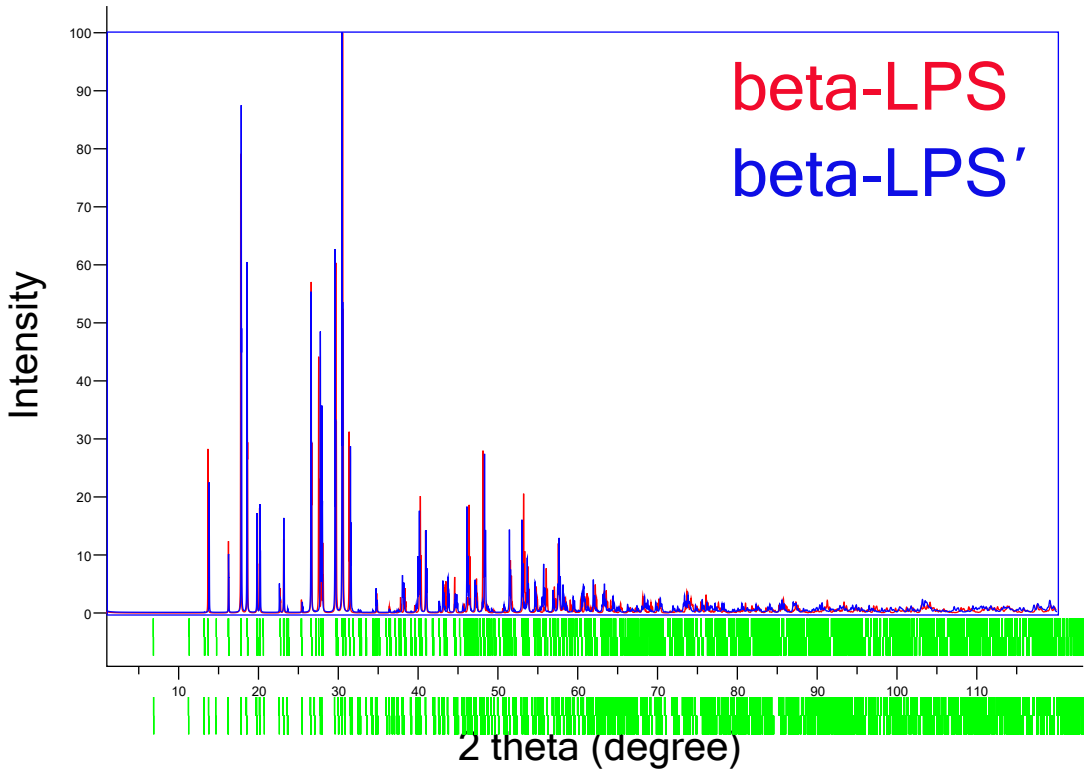

Figure S1: Simulated XRD spectrum generated using the VESTA software for geometry-optimized $\beta-Li_3PS_4$(cubic) as well as for the distorted β'-Li_3PS_4 phase (random kick on all atoms followed by a new geometry optimization). Although the differences between both crystals are meaningfull – for instance, the cubic crystal is dynamically unstable – the XRD spectra are very similar and experimentally hardly distinguishable.

1.3 Structures files for $x-Li_3PS_4$

CIF files for x-Li_3PS_4 ($x = \alpha, \beta, \gamma$) for the cubic as well as for the distorted crystals.

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#======================================================================

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   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
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   Li2        1.0     0.242377     0.815188     0.953769    Uiso  ? Li
   Li3        1.0     0.757623     0.815188     0.953769    Uiso  ? Li
   Li4        1.0     0.742377     0.184812     0.453769    Uiso  ? Li
   Li5        1.0     0.000000     0.649338     0.467183    Uiso  ? Li
   Li6        1.0     0.500000     0.350662     0.967183    Uiso  ? Li
   P1         1.0     0.000000     0.317662     0.955291    Uiso  ? P
   P2         1.0     0.500000     0.682338     0.455291    Uiso  ? P
   S1         1.0     0.222362     0.168727     0.065176    Uiso  ? S
   S2         1.0     0.277638     0.831273     0.565176    Uiso  ? S
   S3         1.0     0.722362     0.831273     0.565176    Uiso  ? S
   S4         1.0     0.777638     0.168727     0.065176    Uiso  ? S
   S5         1.0     0.000000     0.614396     0.070743    Uiso  ? S
   S6         1.0     0.500000     0.385604     0.570743    Uiso  ? S
   S7         1.0     0.000000     0.311377     0.618864    Uiso  ? S
   S8         1.0     0.500000     0.688623     0.118864    Uiso  ? S


#======================================================================
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   Li2        1.0     0.242397     0.821442     0.953760    Uiso  ? Li
   Li3        1.0     0.757617     0.821447     0.953776    Uiso  ? Li
   Li4        1.0     0.742384     0.191053     0.453777    Uiso  ? Li
   Li5        1.0     0.999995     0.655621     0.467173    Uiso  ? Li
   Li6        1.0     0.500005     0.356879     0.967172    Uiso  ? Li
   P1         1.0     0.000004     0.323929     0.955294    Uiso  ? P
   P2         1.0     0.499996     0.688571     0.455294    Uiso  ? P
   S1         1.0     0.222367     0.174984     0.065174    Uiso  ? S
   S2         1.0     0.277634     0.837517     0.565174    Uiso  ? S
   S3         1.0     0.722357     0.837511     0.565188    Uiso  ? S
   S4         1.0     0.777643     0.174988     0.065188    Uiso  ? S
   S5         1.0     0.000008     0.620676     0.070738    Uiso  ? S
   S6         1.0     0.499991     0.391824     0.570740    Uiso  ? S
   S7         1.0     0.999995     0.317656     0.618865    Uiso  ? S
   S8         1.0     0.500005     0.694843     0.118865    Uiso  ? S

#======================================================================
# CRYSTAL DATA
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_space_group_IT_number                 1

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   _atom_site_fract_z
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   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
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   Li2        1.0     0.257779     0.378121     0.523142    Uiso  ? Li
   Li3        1.0     0.732927     0.578588     0.032424    Uiso  ? Li
   Li4        1.0     0.214574     0.779595     0.531969    Uiso  ? Li
   Li5        1.0     0.755149     0.895530     0.953822    Uiso  ? Li
   Li6        1.0     0.747179     0.896722     0.513198    Uiso  ? Li
   Li7        1.0     0.308933     0.006572     0.008252    Uiso  ? Li
   Li8        1.0     0.712363     0.262409     0.528464    Uiso  ? Li
   Li9        1.0     0.257402     0.693817     0.040986    Uiso  ? Li
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   Li10       1.0     0.718975     0.580814     0.459979    Uiso  ? Li
   Li11       1.0     0.013726     0.147410     0.259222    Uiso  ? Li
   Li12       1.0     0.730800     0.261739     0.957820    Uiso  ? Li
   P1         1.0     0.972152     0.822484     0.235415    Uiso  ? P
   P2         1.0     0.014109     0.141598     0.742613    Uiso  ? P
   P3         1.0     0.473385     0.317860     0.236512    Uiso  ? P
   P4         1.0     0.503177     0.645239     0.745327    Uiso  ? P
   S1         1.0     0.291219     0.481764     0.243532    Uiso  ? S
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   S3         1.0     0.284609     0.568221     0.745672    Uiso  ? S
   S4         1.0     0.694762     0.397373     0.243534    Uiso  ? S
   S5         1.0     0.793459     0.991225     0.235824    Uiso  ? S
   S6         1.0     0.196083     0.985600     0.736433    Uiso  ? S
   S7         1.0     0.791077     0.066182     0.737016    Uiso  ? S
   S8         1.0     0.185470     0.910625     0.255974    Uiso  ? S
   S9         1.0     0.006185     0.283972     0.537744    Uiso  ? S
   S10        1.0     0.965535     0.701436     0.013209    Uiso  ? S
   S11        1.0     0.957141     0.697783     0.451335    Uiso  ? S
   S12        1.0     0.016589     0.267698     0.965553    Uiso  ? S
   S13        1.0     0.510424     0.769938     0.530378    Uiso  ? S
   S14        1.0     0.468215     0.206601     0.004690    Uiso  ? S
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   _atom_site_fract_z
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   Li2        1.0     0.254836     0.565647     0.454254    Uiso  ? Li
   Li3        1.0     0.709256     0.702638     0.037633    Uiso  ? Li
   Li4        1.0     0.224622     0.883522     0.518119    Uiso  ? Li
   Li5        1.0     0.754847     0.065654     0.019787    Uiso  ? Li
   Li6        1.0     0.758854     0.769859     0.537635    Uiso  ? Li
   Li7        1.0     0.213265     0.906840     0.954250    Uiso  ? Li
   Li8        1.0     0.743491     0.088972     0.455918    Uiso  ? Li
   Li9        1.0     0.243499     0.588974     0.018122    Uiso  ? Li
   Li10       1.0     0.713276     0.406847     0.519784    Uiso  ? Li
   Li11       1.0     0.209258     0.202634     0.436402    Uiso  ? Li
   Li12       1.0     0.724614     0.383520     0.955916    Uiso  ? Li
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   P2         1.0     0.965887     0.146508     0.731657    Uiso  ? P
   P3         1.0     0.502226     0.325987     0.231659    Uiso  ? P
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   P4         1.0     0.465886     0.646506     0.742379    Uiso  ? P
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   S3         1.0     0.280889     0.488411     0.740706    Uiso  ? S
   S4         1.0     0.687223     0.484083     0.233332    Uiso  ? S
   S5         1.0     0.777718     0.902457     0.251459    Uiso  ? S
   S6         1.0     0.190394     0.070038     0.722579    Uiso  ? S
   S7         1.0     0.780890     0.988415     0.733335    Uiso  ? S
   S8         1.0     0.187223     0.984080     0.240702    Uiso  ? S
   S9         1.0     0.952467     0.276558     0.522226    Uiso  ? S
   S10        1.0     0.005196     0.712010     0.021463    Uiso  ? S
   S11        1.0     0.015645     0.695935     0.451813    Uiso  ? S
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   _atom_site_fract_z
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   Li2        1.0     0.625633     0.967838     0.330123    Uiso  ? Li
   Li3        1.0     0.874367     0.967838     0.830123    Uiso  ? Li
   Li4        1.0     0.125633     0.032162     0.169877    Uiso  ? Li
   Li5        1.0     0.625633     0.532162     0.330123    Uiso  ? Li
   Li6        1.0     0.374367     0.467838     0.669877    Uiso  ? Li
   Li7        1.0     0.125633     0.467838     0.169877    Uiso  ? Li
   Li8        1.0     0.874367     0.532162     0.830123    Uiso  ? Li
   Li9        1.0     0.500000     0.000000    -0.000000    Uiso  ? Li
   Li10       1.0    -0.000000     0.000000     0.500000    Uiso  ? Li
   Li11       1.0     0.500000     0.500000    -0.000000    Uiso  ? Li
   Li12       1.0    -0.000000     0.500000     0.500000    Uiso  ? Li
   P1         1.0     0.143036     0.250000     0.912323    Uiso  ? P
   P2         1.0     0.856964     0.750000     0.087677    Uiso  ? P
   P3         1.0     0.643036     0.750000     0.587677    Uiso  ? P
   P4         1.0     0.356964     0.250000     0.412323    Uiso  ? P
   S1         1.0     0.803802     0.250000     0.902917    Uiso  ? S
   S2         1.0     0.196198     0.750000     0.097083    Uiso  ? S
   S3         1.0     0.303802     0.750000     0.597083    Uiso  ? S
   S4         1.0     0.696198     0.250000     0.402917    Uiso  ? S
   S5         1.0     0.276700     0.250000     0.061289    Uiso  ? S
```

```
   S6         1.0     0.723300     0.750000     0.938711    Uiso  ? S
   S7         1.0     0.776700     0.750000     0.438711    Uiso  ? S
   S8         1.0     0.223300     0.250000     0.561289    Uiso  ? S
   S9         1.0     0.262969     0.028569     0.847249    Uiso  ? S
   S10        1.0     0.737031     0.971431     0.152751    Uiso  ? S
   S11        1.0     0.762969     0.971431     0.652751    Uiso  ? S
   S12        1.0     0.237031     0.028569     0.347249    Uiso  ? S
   S13        1.0     0.737031     0.528569     0.152751    Uiso  ? S
   S14        1.0     0.262969     0.471431     0.847249    Uiso  ? S
   S15        1.0     0.237031     0.471431     0.347249    Uiso  ? S
   S16        1.0     0.762969     0.528569     0.652751    Uiso  ? S

#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------

_chemical_name_common                  beta-LPS (distorted)
_cell_length_a                         6.045046
_cell_length_b                         7.875972
_cell_length_c                         12.874979
_cell_angle_alpha                      89.999916
_cell_angle_beta                       89.999985
_cell_angle_gamma                      90.000008
_cell_volume                           612.985661
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Li1        1.0     0.632744     0.970213     0.663149    Uiso  ? Li
   Li2        1.0     0.403114     0.039522     0.325691    Uiso  ? Li
   Li3        1.0     0.132744     0.029789     0.833102    Uiso  ? Li
   Li4        1.0     0.903112     0.960480     0.170559    Uiso  ? Li
   Li5        1.0     0.369769     0.470207     0.333103    Uiso  ? Li
   Li6        1.0     0.599378     0.539524     0.670557    Uiso  ? Li
   Li7        1.0     0.869768     0.529793     0.163148    Uiso  ? Li
   Li8        1.0     0.099377     0.460475     0.825693    Uiso  ? Li
   Li9        1.0     0.557713     0.042879     0.003796    Uiso  ? Li
   Li10       1.0     0.057714     0.957119     0.492456    Uiso  ? Li
   Li11       1.0     0.444788     0.542879     0.992456    Uiso  ? Li
   Li12       1.0     0.944789     0.457124     0.503795    Uiso  ? Li
   P1         1.0     0.849054     0.749419     0.909704    Uiso  ? P
   P2         1.0     0.153446     0.249416     0.086547    Uiso  ? P
   P3         1.0     0.349053     0.250581     0.586547    Uiso  ? P
   P4         1.0     0.653445     0.750585     0.409703    Uiso  ? P
   S1         1.0     0.186160     0.743879     0.895754    Uiso  ? S
   S2         1.0     0.816338     0.243884     0.100495    Uiso  ? S
   S3         1.0     0.686160     0.256121     0.600495    Uiso  ? S
   S4         1.0     0.316338     0.756117     0.395753    Uiso  ? S
   S5         1.0     0.724097     0.756703     0.060410    Uiso  ? S
   S6         1.0     0.278404     0.256702     0.935842    Uiso  ? S
   S7         1.0     0.224094     0.243297     0.435841    Uiso  ? S
   S8         1.0     0.778401     0.743299     0.560410    Uiso  ? S
   S9         1.0     0.740034     0.971065     0.842441    Uiso  ? S
   S10        1.0     0.285108     0.031277     0.148278    Uiso  ? S
   S11        1.0     0.240034     0.028936     0.653811    Uiso  ? S
```

```
   S12        1.0     0.785109     0.968724     0.347973    Uiso  ? S
   S13        1.0     0.262474     0.471058     0.153812    Uiso  ? S
   S14        1.0     0.717384     0.531284     0.847971    Uiso  ? S
   S15        1.0     0.762475     0.528942     0.342440    Uiso  ? S
   S16        1.0     0.217384     0.468716     0.648280    Uiso  ? S
```

1.4 Cubic and distorted geometry-optimized crystal structures of Li_6PS_5X

The coordinates for the cubic and distorted coordinates of Li_6PS_5X are given below in CIF format.

```
#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
# CIF file created by FINDSYM, version 7.1.3

_chemical_name_common 'LPS-Cl (cubic)'

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a     10.0733160000
_cell_length_b     10.0733160000
_cell_length_c     10.0733160000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1022.1564511665

_symmetry_space_group_name_H-M "F -4 3 m"
_symmetry_Int_Tables_number 216
_space_group.reference_setting '216:F -4 2 3'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z
17 x,z,y
18 x,-z,-y
19 -x,z,-y
20 -x,-z,y
21 z,y,x
22 z,-y,-x
23 -z,y,-x
24 -z,-y,x
```

25 x,y+1/2,z+1/2
26 x,-y+1/2,-z+1/2
27 -x,y+1/2,-z+1/2
28 -x,-y+1/2,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/2,-x+1/2
31 -y,z+1/2,-x+1/2
32 -y,-z+1/2,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/2,-y+1/2
35 -z,x+1/2,-y+1/2
36 -z,-x+1/2,y+1/2
37 y,x+1/2,z+1/2
38 y,-x+1/2,-z+1/2
39 -y,x+1/2,-z+1/2
40 -y,-x+1/2,z+1/2
41 x,z+1/2,y+1/2
42 x,-z+1/2,-y+1/2
43 -x,z+1/2,-y+1/2
44 -x,-z+1/2,y+1/2
45 z,y+1/2,x+1/2
46 z,-y+1/2,-x+1/2
47 -z,y+1/2,-x+1/2
48 -z,-y+1/2,x+1/2
49 x+1/2,y,z+1/2
50 x+1/2,-y,-z+1/2
51 -x+1/2,y,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z,-x+1/2
55 -y+1/2,z,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x,-y+1/2
59 -z+1/2,x,-y+1/2
60 -z+1/2,-x,y+1/2
61 y+1/2,x,z+1/2
62 y+1/2,-x,-z+1/2
63 -y+1/2,x,-z+1/2
64 -y+1/2,-x,z+1/2
65 x+1/2,z,y+1/2
66 x+1/2,-z,-y+1/2
67 -x+1/2,z,-y+1/2
68 -x+1/2,-z,y+1/2
69 z+1/2,y,x+1/2
70 z+1/2,-y,-x+1/2
71 -z+1/2,y,-x+1/2
72 -z+1/2,-y,x+1/2
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/2,-z
75 -x+1/2,y+1/2,-z
76 -x+1/2,-y+1/2,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/2,-x
79 -y+1/2,z+1/2,-x
80 -y+1/2,-z+1/2,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/2,-y
83 -z+1/2,x+1/2,-y
84 -z+1/2,-x+1/2,y
85 y+1/2,x+1/2,z
86 y+1/2,-x+1/2,-z
87 -y+1/2,x+1/2,-z
88 -y+1/2,-x+1/2,z
89 x+1/2,z+1/2,y
90 x+1/2,-z+1/2,-y
91 -x+1/2,z+1/2,-y

```
92 -x+1/2,-z+1/2,y
93 z+1/2,y+1/2,x
94 z+1/2,-y+1/2,-x
95 -z+1/2,y+1/2,-x
96 -z+1/2,-y+1/2,x

loop_
_atom_type_symbol
Li
Cl
P
S

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1 Li  24 g  0.5232520000  0.2500000000  0.2500000000  1.0000000000 Dx,0,0
Cl1 Cl   4 a  0.0000000000  0.0000000000  0.0000000000  1.0000000000 0,0,0
P1  P    4 b  0.5000000000  0.5000000000  0.5000000000  1.0000000000 0,0,0
S1  S   16 e  0.3823810000  0.3823810000  0.3823810000  1.0000000000 Dx,Dx,Dx
S2  S    4 d  0.7500000000  0.7500000000  0.7500000000  1.0000000000 0,0,0

# end of cif

#=============================================================================
# CRYSTAL DATA
#-----------------------------------------------------------------------------
#
# Same structure as the one with space group 7, but here in P1 setting, without symmetry

_chemical_name_common                  'LPS-Cl (distorted, space group ITA=1)'
_cell_length_a                         9.832060
_cell_length_b                         9.609316
_cell_length_c                         9.609315
_cell_angle_alpha                      89.163658
_cell_angle_beta                       88.865364
_cell_angle_gamma                      88.865364
_cell_volume                           907.434388
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Li1        1.0     0.447003     0.718410     0.340692    Uiso  ? Li
   Li2        1.0     0.477583     0.168468     0.202390    Uiso  ? Li
   Li3        1.0     0.329044     0.868021     0.076003    Uiso  ? Li
   Li4        1.0     0.829044     0.250226     0.193798    Uiso  ? Li
   Li5        1.0     0.367842     0.000853     0.522347    Uiso  ? Li
   Li6        1.0     0.633430     0.916680     0.340212    Uiso  ? Li
```

```
   Li7        1.0     0.447004     0.218409     0.840690    Uiso  ? Li
   Li8        1.0     0.633430     0.416679     0.840211    Uiso  ? Li
   Li9        1.0     0.183857     0.049849     0.316818    Uiso  ? Li
   Li10       1.0     0.183858     0.549850     0.816817    Uiso  ? Li
   Li11       1.0     0.329045     0.368022     0.576002    Uiso  ? Li
   Li12       1.0     0.367842     0.500851     0.022346    Uiso  ? Li
   Li13       1.0     0.947005     0.014916     0.544186    Uiso  ? Li
   Li14       1.0     0.133431     0.014432     0.742457    Uiso  ? Li
   Li15       1.0     0.683856     0.991044     0.875621    Uiso  ? Li
   Li16       1.0     0.829044     0.750227     0.693798    Uiso  ? Li
   Li17       1.0     0.867845     0.196570     0.826630    Uiso  ? Li
   Li18       1.0     0.977581     0.876613     0.994245    Uiso  ? Li
   Li19       1.0     0.133430     0.514434     0.242455    Uiso  ? Li
   Li20       1.0     0.947004     0.514915     0.044184    Uiso  ? Li
   Li21       1.0     0.867844     0.696571     0.326630    Uiso  ? Li
   Li22       1.0     0.477584     0.668468     0.702390    Uiso  ? Li
   Li23       1.0     0.977581     0.376614     0.494244    Uiso  ? Li
   Li24       1.0     0.683855     0.491044     0.375617    Uiso  ? Li
   Cl1        1.0     0.155752     0.676948     0.037724    Uiso  ? Cl
   Cl2        1.0     0.155753     0.176948     0.537725    Uiso  ? Cl
   Cl3        1.0     0.655752     0.711947     0.502724    Uiso  ? Cl
   Cl4        1.0     0.655752     0.211948     0.002725    Uiso  ? Cl
   P1         1.0     0.651289     0.704279     0.031760    Uiso  ? P
   P2         1.0     0.651290     0.204278     0.531761    Uiso  ? P
   P3         1.0     0.151289     0.705984     0.530053    Uiso  ? P
   P4         1.0     0.151289     0.205984     0.030054    Uiso  ? P
   S1         1.0     0.278009     0.069201     0.924429    Uiso  ? S
   S2         1.0     0.015208     0.086090     0.139912    Uiso  ? S
   S3         1.0     0.515209     0.814138     0.911866    Uiso  ? S
   S4         1.0     0.768650     0.839592     0.139667    Uiso  ? S
   S5         1.0     0.405140     0.951185     0.288657    Uiso  ? S
   S6         1.0     0.278008     0.569201     0.424428    Uiso  ? S
   S7         1.0     0.015208     0.586090     0.639912    Uiso  ? S
   S8         1.0     0.515210     0.314137     0.411866    Uiso  ? S
   S9         1.0     0.768651     0.339591     0.639667    Uiso  ? S
   S10        1.0     0.405140     0.451184     0.788656    Uiso  ? S
   S11        1.0     0.778009     0.098653     0.394978    Uiso  ? S
   S12        1.0     0.550568     0.070125     0.663761    Uiso  ? S
   S13        1.0     0.050569     0.837986     0.395901    Uiso  ? S
   S14        1.0     0.268651     0.813888     0.665369    Uiso  ? S
   S15        1.0     0.905140     0.962880     0.776961    Uiso  ? S
   S16        1.0     0.778008     0.598653     0.894978    Uiso  ? S
   S17        1.0     0.550566     0.570127     0.163761    Uiso  ? S
   S18        1.0     0.050570     0.337986     0.895901    Uiso  ? S
   S19        1.0     0.268650     0.313889     0.165370    Uiso  ? S
   S20        1.0     0.905139     0.462881     0.276959    Uiso  ? S

#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
# CIF file created by FINDSYM, version 7.1.3
#
# same structure as the one in P1 setting, but now with symmetry operations detected


_chemical_name_common                  'LPS-Cl (distorted, space group ITA=7)'

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a     6.8442224118
_cell_length_b     6.7450399522
_cell_length_c     11.8224808616
_cell_angle_alpha  90.0000000000
_cell_angle_beta   123.7654729061
_cell_angle_gamma  90.0000000000
_cell_volume       453.7172103539
```

```
_symmetry_space_group_name_H-M "P 1 c 1"
_symmetry_Int_Tables_number 7
_space_group.reference_setting '007:P -2yc'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,z+1/2

loop_
_atom_type_symbol
Li
Cl
P
S

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1 Li   2 a  0.4938955000  0.5465060000  0.5529960000  1.0000000000 Dx,Dy,Dz
Li2 Li   2 a  0.1515597500 -0.0418545000  0.5224177500  1.0000000000 Dx,Dy,Dz
Li3 Li   2 a  0.7269315000  0.1322047500  0.6709557500  1.0000000000 Dx,Dy,Dz
Li4 Li   2 a  0.1089572500  0.4457175000  0.6321567500  1.0000000000 Dx,Dy,Dz
Li5 Li   2 a  0.1096797500  0.3477545000  0.3665697500  1.0000000000 Dx,Dy,Dz
Li6 Li   2 a  0.4494785000  0.1911965000  0.8161435000  1.0000000000 Dx,Dy,Dz
Cl1 Cl   2 a  0.1295755000  0.2849997500  0.8442477500  1.0000000000 Dx,Dy,Dz
P1  P    2 a  0.6126725000  0.2517062500  0.3487107500  1.0000000000 Dx,Dy,Dz
S1  S    2 a  0.7283612500  0.7794512500  0.7219915000  1.0000000000 Dx,Dy,Dz
S2  S    2 a  0.7587885000 -0.0219532500 -0.0152087500  1.0000000000 Dx,Dy,Dz
S3  S    2 a  0.2520912500  0.2242972500  0.2313495000  1.0000000000 Dx,Dy,Dz
S4  S    2 a  0.3550195000  0.2616962500  0.5948602500  1.0000000000 Dx,Dy,Dz
S5  S    2 a  0.7155447500  0.5178600000  0.4494317500  1.0000000000 Dx,Dy,Dz

# end of cif


#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
# CIF file created by FINDSYM, version 7.1.3

_chemical_name_common                  'LPS-Br (cubic)'

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a     10.0833620000
_cell_length_b     10.0833620000
_cell_length_c     10.0833620000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1025.2176559925

_symmetry_space_group_name_H-M "F -4 3 m"
_symmetry_Int_Tables_number 216
_space_group.reference_setting '216:F -4 2 3'
```

```
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 y,x,z
14 y,-x,-z
15 -y,x,-z
16 -y,-x,z
17 x,z,y
18 x,-z,-y
19 -x,z,-y
20 -x,-z,y
21 z,y,x
22 z,-y,-x
23 -z,y,-x
24 -z,-y,x
25 x,y+1/2,z+1/2
26 x,-y+1/2,-z+1/2
27 -x,y+1/2,-z+1/2
28 -x,-y+1/2,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/2,-x+1/2
31 -y,z+1/2,-x+1/2
32 -y,-z+1/2,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/2,-y+1/2
35 -z,x+1/2,-y+1/2
36 -z,-x+1/2,y+1/2
37 y,x+1/2,z+1/2
38 y,-x+1/2,-z+1/2
39 -y,x+1/2,-z+1/2
40 -y,-x+1/2,z+1/2
41 x,z+1/2,y+1/2
42 x,-z+1/2,-y+1/2
43 -x,z+1/2,-y+1/2
44 -x,-z+1/2,y+1/2
45 z,y+1/2,x+1/2
46 z,-y+1/2,-x+1/2
47 -z,y+1/2,-x+1/2
48 -z,-y+1/2,x+1/2
49 x+1/2,y,z+1/2
50 x+1/2,-y,-z+1/2
51 -x+1/2,y,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z,-x+1/2
55 -y+1/2,z,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x,-y+1/2
59 -z+1/2,x,-y+1/2
60 -z+1/2,-x,y+1/2
61 y+1/2,x,z+1/2
62 y+1/2,-x,-z+1/2
```

```
63 -y+1/2,x,-z+1/2
64 -y+1/2,-x,z+1/2
65 x+1/2,z,y+1/2
66 x+1/2,-z,-y+1/2
67 -x+1/2,z,-y+1/2
68 -x+1/2,-z,y+1/2
69 z+1/2,y,x+1/2
70 z+1/2,-y,-x+1/2
71 -z+1/2,y,-x+1/2
72 -z+1/2,-y,x+1/2
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/2,-z
75 -x+1/2,y+1/2,-z
76 -x+1/2,-y+1/2,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/2,-x
79 -y+1/2,z+1/2,-x
80 -y+1/2,-z+1/2,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/2,-y
83 -z+1/2,x+1/2,-y
84 -z+1/2,-x+1/2,y
85 y+1/2,x+1/2,z
86 y+1/2,-x+1/2,-z
87 -y+1/2,x+1/2,-z
88 -y+1/2,-x+1/2,z
89 x+1/2,z+1/2,y
90 x+1/2,-z+1/2,-y
91 -x+1/2,z+1/2,-y
92 -x+1/2,-z+1/2,y
93 z+1/2,y+1/2,x
94 z+1/2,-y+1/2,-x
95 -z+1/2,y+1/2,-x
96 -z+1/2,-y+1/2,x

loop_
_atom_type_symbol
Li
P
S
Br

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1 Li  24 g  0.0234010000  0.2500000000  0.2500000000  1.0000000000 Dx,0,0
P1  P    4 b  0.5000000000  0.5000000000  0.5000000000  1.0000000000 0,0,0
S1  S   16 e  0.6175070000  0.6175070000  0.6175070000  1.0000000000 Dx,Dx,Dx
S2  S    4 c  0.2500000000  0.2500000000  0.2500000000  1.0000000000 0,0,0
Br1 Br   4 a  0.0000000000  0.0000000000  0.0000000000  1.0000000000 0,0,0

# end of cif

#=============================================================================
# CRYSTAL DATA
#-----------------------------------------------------------------------------
# CIF file created by FINDSYM, version 7.1.3

_chemical_name_common                  'LPS-Br (distorted)'
```

```
data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a     9.7279730000
_cell_length_b     9.8182750000
_cell_length_c     9.8849750000
_cell_angle_alpha  91.1095810000
_cell_angle_beta   90.8476870000
_cell_angle_gamma  90.0409010000
_cell_volume       943.8520649877

_symmetry_space_group_name_H-M "P 1"
_symmetry_Int_Tables_number 1
_space_group.reference_setting '001:P 1'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z

loop_
_atom_type_symbol
Li
P
S
Br

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1  Li   1 a  0.0329900000  0.3216400000  0.3189990000  1.0000000000 Dx,Dy,Dz
Li2  Li   1 a  0.4817160000  0.2083470000  0.2748180000  1.0000000000 Dx,Dy,Dz
Li3  Li   1 a  0.2882960000  0.1964580000  0.4762520000  1.0000000000 Dx,Dy,Dz
Li4  Li   1 a  0.1815940000  0.2166220000  0.0207000000  1.0000000000 Dx,Dy,Dz
Li5  Li   1 a  0.1884950000  0.0184450000  0.2128220000  1.0000000000 Dx,Dy,Dz
Li6  Li   1 a  0.3175010000  0.4602780000  0.1882270000  1.0000000000 Dx,Dy,Dz
Li7  Li   1 a  0.5172200000  0.2115000000  0.7111390000  1.0000000000 Dx,Dy,Dz
Li8  Li   1 a -0.0336200000  0.3353240000  0.6898960000  1.0000000000 Dx,Dy,Dz
Li9  Li   1 a  0.7019450000  0.2866660000 -0.0181610000  1.0000000000 Dx,Dy,Dz
Li10 Li   1 a  0.7222980000  0.2067940000  0.5252800000  1.0000000000 Dx,Dy,Dz
Li11 Li   1 a  0.8125980000  0.0431400000  0.8074700000  1.0000000000 Dx,Dy,Dz
Li12 Li   1 a  0.6910670000  0.4924320000  0.7969230000  1.0000000000 Dx,Dy,Dz
Li13 Li   1 a  0.5292780000  0.7092090000  0.1864180000  1.0000000000 Dx,Dy,Dz
Li14 Li   1 a -0.0109880000  0.7117760000  0.2887490000  1.0000000000 Dx,Dy,Dz
Li15 Li   1 a  0.7850340000  0.6958780000  0.4790490000  1.0000000000 Dx,Dy,Dz
Li16 Li   1 a  0.8099780000  0.8233260000  0.0377100000  1.0000000000 Dx,Dy,Dz
Li17 Li   1 a  0.7280550000  0.5148650000  0.2035010000  1.0000000000 Dx,Dy,Dz
Li18 Li   1 a  0.6950140000 -0.0374920000  0.3181380000  1.0000000000 Dx,Dy,Dz
Li19 Li   1 a  0.0174320000  0.7121980000  0.7164710000  1.0000000000 Dx,Dy,Dz
Li20 Li   1 a  0.4688580000  0.8325530000  0.6789570000  1.0000000000 Dx,Dy,Dz
Li21 Li   1 a  0.2041940000  0.7889660000 -0.0249030000  1.0000000000 Dx,Dy,Dz
Li22 Li   1 a  0.2164880000  0.6823490000  0.5249300000  1.0000000000 Dx,Dy,Dz
Li23 Li   1 a  0.3308050000  0.5416580000  0.8106860000  1.0000000000 Dx,Dy,Dz
Li24 Li   1 a  0.2005990000 -0.0140290000  0.7836630000  1.0000000000 Dx,Dy,Dz
P1   P    1 a  0.0080390000  0.5030060000 -0.0020340000  1.0000000000 Dx,Dy,Dz
P2   P    1 a  0.5009030000  0.5031200000  0.4946010000  1.0000000000 Dx,Dy,Dz
P3   P    1 a  0.5024640000  0.0011170000 -0.0008860000  1.0000000000 Dx,Dy,Dz
P4   P    1 a -0.0004980000  0.0039850000  0.5016090000  1.0000000000 Dx,Dy,Dz
S1   S    1 a  0.8870110000  0.1177080000  0.3675100000  1.0000000000 Dx,Dy,Dz
```

```
S2   S    1 a  0.1342240000  0.8805800000  0.3981880000  1.0000000000 Dx,Dy,Dz
S3   S    1 a  0.8990490000  0.3681980000  0.1121250000  1.0000000000 Dx,Dy,Dz
S4   S    1 a  0.1352790000  0.6162970000  0.1241080000  1.0000000000 Dx,Dy,Dz
S5   S    1 a  0.2485680000  0.2451240000  0.2490940000  1.0000000000 Dx,Dy,Dz
S6   S    1 a  0.3794670000  0.1295530000  0.8886720000  1.0000000000 Dx,Dy,Dz
S7   S    1 a  0.6226380000  0.8838190000  0.8740670000  1.0000000000 Dx,Dy,Dz
S8   S    1 a  0.3728430000  0.3899800000  0.6122940000  1.0000000000 Dx,Dy,Dz
S9   S    1 a  0.6086780000  0.6327330000  0.6235150000  1.0000000000 Dx,Dy,Dz
S10  S    1 a  0.7470460000  0.2647440000  0.7530200000  1.0000000000 Dx,Dy,Dz
S11  S    1 a  0.3868260000  0.6207140000  0.3657440000  1.0000000000 Dx,Dy,Dz
S12  S    1 a  0.6300440000  0.3815300000  0.3820810000  1.0000000000 Dx,Dy,Dz
S13  S    1 a  0.3807600000  0.8855990000  0.1206110000  1.0000000000 Dx,Dy,Dz
S14  S    1 a  0.6390970000  0.1070680000  0.1232240000  1.0000000000 Dx,Dy,Dz
S15  S    1 a  0.7569860000  0.7444100000  0.2514030000  1.0000000000 Dx,Dy,Dz
S16  S    1 a  0.8774320000  0.6284250000  0.8926900000  1.0000000000 Dx,Dy,Dz
S17  S    1 a  0.1310060000  0.3961620000  0.8668620000  1.0000000000 Dx,Dy,Dz
S18  S    1 a  0.8704940000  0.8897570000  0.6174590000  1.0000000000 Dx,Dy,Dz
S19  S    1 a  0.1081120000  0.1385290000  0.6246290000  1.0000000000 Dx,Dy,Dz
S20  S    1 a  0.2511190000  0.7573220000  0.7479270000  1.0000000000 Dx,Dy,Dz
Br1  Br   1 a  0.0222700000 -0.0070960000 -0.0092750000  1.0000000000 Dx,Dy,Dz
Br2  Br   1 a  0.5072360000  0.0358800000  0.5003390000  1.0000000000 Dx,Dy,Dz
Br3  Br   1 a  0.5199970000  0.4954120000  0.0116550000  1.0000000000 Dx,Dy,Dz
Br4  Br   1 a -0.0039390000  0.5274190000  0.5010350000  1.0000000000 Dx,Dy,Dz

# end of cif

#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
# CIF file created by FINDSYM, version 7.1.3

_chemical_name_common                  'LPS-I (cubic)'

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a     10.1157050000
_cell_length_b     10.1157050000
_cell_length_c     10.1157050000
_cell_angle_alpha  90.0000000000
_cell_angle_beta   90.0000000000
_cell_angle_gamma  90.0000000000
_cell_volume       1035.1146784284

_symmetry_space_group_name_H-M "F -4 3 m"
_symmetry_Int_Tables_number 216
_space_group.reference_setting '216:F -4 2 3'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x,-y,-z
3 -x,y,-z
4 -x,-y,z
5 y,z,x
6 y,-z,-x
7 -y,z,-x
8 -y,-z,x
9 z,x,y
10 z,-x,-y
11 -z,x,-y
12 -z,-x,y
13 y,x,z
14 y,-x,-z
15 -y,x,-z
```

16 -y,-x,z
17 x,z,y
18 x,-z,-y
19 -x,z,-y
20 -x,-z,y
21 z,y,x
22 z,-y,-x
23 -z,y,-x
24 -z,-y,x
25 x,y+1/2,z+1/2
26 x,-y+1/2,-z+1/2
27 -x,y+1/2,-z+1/2
28 -x,-y+1/2,z+1/2
29 y,z+1/2,x+1/2
30 y,-z+1/2,-x+1/2
31 -y,z+1/2,-x+1/2
32 -y,-z+1/2,x+1/2
33 z,x+1/2,y+1/2
34 z,-x+1/2,-y+1/2
35 -z,x+1/2,-y+1/2
36 -z,-x+1/2,y+1/2
37 y,x+1/2,z+1/2
38 y,-x+1/2,-z+1/2
39 -y,x+1/2,-z+1/2
40 -y,-x+1/2,z+1/2
41 x,z+1/2,y+1/2
42 x,-z+1/2,-y+1/2
43 -x,z+1/2,-y+1/2
44 -x,-z+1/2,y+1/2
45 z,y+1/2,x+1/2
46 z,-y+1/2,-x+1/2
47 -z,y+1/2,-x+1/2
48 -z,-y+1/2,x+1/2
49 x+1/2,y,z+1/2
50 x+1/2,-y,-z+1/2
51 -x+1/2,y,-z+1/2
52 -x+1/2,-y,z+1/2
53 y+1/2,z,x+1/2
54 y+1/2,-z,-x+1/2
55 -y+1/2,z,-x+1/2
56 -y+1/2,-z,x+1/2
57 z+1/2,x,y+1/2
58 z+1/2,-x,-y+1/2
59 -z+1/2,x,-y+1/2
60 -z+1/2,-x,y+1/2
61 y+1/2,x,z+1/2
62 y+1/2,-x,-z+1/2
63 -y+1/2,x,-z+1/2
64 -y+1/2,-x,z+1/2
65 x+1/2,z,y+1/2
66 x+1/2,-z,-y+1/2
67 -x+1/2,z,-y+1/2
68 -x+1/2,-z,y+1/2
69 z+1/2,y,x+1/2
70 z+1/2,-y,-x+1/2
71 -z+1/2,y,-x+1/2
72 -z+1/2,-y,x+1/2
73 x+1/2,y+1/2,z
74 x+1/2,-y+1/2,-z
75 -x+1/2,y+1/2,-z
76 -x+1/2,-y+1/2,z
77 y+1/2,z+1/2,x
78 y+1/2,-z+1/2,-x
79 -y+1/2,z+1/2,-x
80 -y+1/2,-z+1/2,x
81 z+1/2,x+1/2,y
82 z+1/2,-x+1/2,-y

```
83 -z+1/2,x+1/2,-y
84 -z+1/2,-x+1/2,y
85 y+1/2,x+1/2,z
86 y+1/2,-x+1/2,-z
87 -y+1/2,x+1/2,-z
88 -y+1/2,-x+1/2,z
89 x+1/2,z+1/2,y
90 x+1/2,-z+1/2,-y
91 -x+1/2,z+1/2,-y
92 -x+1/2,-z+1/2,y
93 z+1/2,y+1/2,x
94 z+1/2,-y+1/2,-x
95 -z+1/2,y+1/2,-x
96 -z+1/2,-y+1/2,x

loop_
_atom_type_symbol
Li
P
S
I

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1 Li  24 g  0.0236290000  0.2500000000  0.2500000000  1.0000000000 Dx,0,0
P1  P    4 b  0.5000000000  0.5000000000  0.5000000000  1.0000000000 0,0,0
S1  S   16 e  0.6171800000  0.6171800000  0.6171800000  1.0000000000 Dx,Dx,Dx
S2  S    4 c  0.2500000000  0.2500000000  0.2500000000  1.0000000000 0,0,0
I1  I    4 a  0.0000000000  0.0000000000  0.0000000000  1.0000000000 0,0,0

# end of cif

#======================================================================
# CRYSTAL DATA
#----------------------------------------------------------------------
# CIF file created by FINDSYM, version 7.1.3

_chemical_name_common                  'LPS-I (distorted)'

data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a     9.9239540000
_cell_length_b     9.9537700000
_cell_length_c     10.0020930000
_cell_angle_alpha  89.0666960000
_cell_angle_beta   89.7256160000
_cell_angle_gamma  89.8113250000
_cell_volume       987.8667930249

_symmetry_space_group_name_H-M "P 1"
_symmetry_Int_Tables_number 1
_space_group.reference_setting '001:P 1'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
```

```
loop_
_atom_type_symbol
Li
P
S
I

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Li1  Li   1 a -0.0213460000  0.6814070000  0.3055050000  1.0000000000 Dx,Dy,Dz
Li2  Li   1 a  0.5314930000  0.7751440000  0.2649810000  1.0000000000 Dx,Dy,Dz
Li3  Li   1 a  0.7289310000  0.7818970000  0.4761260000  1.0000000000 Dx,Dy,Dz
Li4  Li   1 a  0.8179110000  0.7813000000  0.0249060000  1.0000000000 Dx,Dy,Dz
Li5  Li   1 a  0.7914040000 -0.0231190000  0.2267190000  1.0000000000 Dx,Dy,Dz
Li6  Li   1 a  0.7059000000  0.5280560000  0.1932650000  1.0000000000 Dx,Dy,Dz
Li7  Li   1 a  0.4888090000  0.7851700000  0.7222670000  1.0000000000 Dx,Dy,Dz
Li8  Li   1 a  0.0374930000  0.6889280000  0.7034230000  1.0000000000 Dx,Dy,Dz
Li9  Li   1 a  0.2994710000  0.7099460000 -0.0237370000  1.0000000000 Dx,Dy,Dz
Li10 Li   1 a  0.2840940000  0.7865790000  0.5244930000  1.0000000000 Dx,Dy,Dz
Li11 Li   1 a  0.2043050000 -0.0348100000  0.8077280000  1.0000000000 Dx,Dy,Dz
Li12 Li   1 a  0.2960250000  0.5147700000  0.7691350000  1.0000000000 Dx,Dy,Dz
Li13 Li   1 a  0.4912710000  0.2090010000  0.3009660000  1.0000000000 Dx,Dy,Dz
Li14 Li   1 a  0.0397500000  0.2071060000  0.2091960000  1.0000000000 Dx,Dy,Dz
Li15 Li   1 a  0.2148170000  0.2916800000  0.4723360000  1.0000000000 Dx,Dy,Dz
Li16 Li   1 a  0.3179380000  0.2720700000  0.0244300000  1.0000000000 Dx,Dy,Dz
Li17 Li   1 a  0.2859580000  0.4763840000  0.2237210000  1.0000000000 Dx,Dy,Dz
Li18 Li   1 a  0.2798880000  0.0181450000  0.2784050000  1.0000000000 Dx,Dy,Dz
Li19 Li   1 a -0.0048750000  0.2789840000  0.7255260000  1.0000000000 Dx,Dy,Dz
Li20 Li   1 a  0.5454890000  0.1854390000  0.6911010000  1.0000000000 Dx,Dy,Dz
Li21 Li   1 a  0.7932860000  0.2239230000 -0.0233150000  1.0000000000 Dx,Dy,Dz
Li22 Li   1 a  0.8026320000  0.3046840000  0.5226100000  1.0000000000 Dx,Dy,Dz
Li23 Li   1 a  0.7021430000  0.4652270000  0.8010740000  1.0000000000 Dx,Dy,Dz
Li24 Li   1 a  0.8061030000  0.0200120000  0.7836600000  1.0000000000 Dx,Dy,Dz
P1   P    1 a  0.0104180000  0.4957420000  0.0026040000  1.0000000000 Dx,Dy,Dz
P2   P    1 a  0.5105310000  0.4971480000  0.4985320000  1.0000000000 Dx,Dy,Dz
P3   P    1 a  0.5115870000 -0.0029800000 -0.0037730000  1.0000000000 Dx,Dy,Dz
P4   P    1 a  0.0088030000 -0.0046560000  0.5010680000  1.0000000000 Dx,Dy,Dz
S1   S    1 a  0.1171050000  0.8734230000  0.3750890000  1.0000000000 Dx,Dy,Dz
S2   S    1 a  0.8899420000  0.1217310000  0.3872690000  1.0000000000 Dx,Dy,Dz
S3   S    1 a  0.1226360000  0.6229350000  0.1173470000  1.0000000000 Dx,Dy,Dz
S4   S    1 a  0.8902110000  0.3812960000  0.1276000000  1.0000000000 Dx,Dy,Dz
S5   S    1 a  0.7605860000  0.7470540000  0.2492150000  1.0000000000 Dx,Dy,Dz
S6   S    1 a  0.6358160000  0.8750260000  0.8863610000  1.0000000000 Dx,Dy,Dz
S7   S    1 a  0.3944750000  0.1097190000  0.8677050000  1.0000000000 Dx,Dy,Dz
S8   S    1 a  0.6284080000  0.6127000000  0.6197830000  1.0000000000 Dx,Dy,Dz
S9   S    1 a  0.3977910000  0.3665680000  0.6142090000  1.0000000000 Dx,Dy,Dz
S10  S    1 a  0.2601860000  0.7448480000  0.7511330000  1.0000000000 Dx,Dy,Dz
S11  S    1 a  0.6316090000  0.3851020000  0.3754220000  1.0000000000 Dx,Dy,Dz
S12  S    1 a  0.3869040000  0.6185210000  0.3841980000  1.0000000000 Dx,Dy,Dz
S13  S    1 a  0.6237080000  0.1192150000  0.1165670000  1.0000000000 Dx,Dy,Dz
S14  S    1 a  0.3834260000  0.8822970000  0.1132040000  1.0000000000 Dx,Dy,Dz
S15  S    1 a  0.2656700000  0.2464290000  0.2507540000  1.0000000000 Dx,Dy,Dz
S16  S    1 a  0.1351750000  0.3739880000  0.8923420000  1.0000000000 Dx,Dy,Dz
S17  S    1 a  0.8876130000  0.6069070000  0.8778670000  1.0000000000 Dx,Dy,Dz
S18  S    1 a  0.1355900000  0.1071870000  0.6168900000  1.0000000000 Dx,Dy,Dz
S19  S    1 a  0.8936360000  0.8719570000  0.6223310000  1.0000000000 Dx,Dy,Dz
S20  S    1 a  0.7638410000  0.2464970000  0.7472940000  1.0000000000 Dx,Dy,Dz
I1   I    1 a -0.0048280000  0.0063380000  0.0041820000  1.0000000000 Dx,Dy,Dz
```

```
I2   I    1 a  0.5072000000 -0.0195480000  0.4889120000  1.0000000000 Dx,Dy,Dz
I3   I    1 a  0.4957670000  0.4987270000  0.0009440000  1.0000000000 Dx,Dy,Dz
I4   I    1 a  0.0173020000  0.4879060000  0.5104290000  1.0000000000 Dx,Dy,Dz

# end of cif
```