

Lithiation of phosphorus at the nanoscale: a computational study of Li_nP_m clusters

Supplementary Information

*Dmitry V. Rybkovskiy^{*1,2}, Sergey V. Lepeshkin^{1,3}, Anastasiia A. Mikhailova^{1,2}, Vladimir S. Baturin¹, Artem R. Oganov¹*

1. Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, 121205 Moscow, Russian Federation
 2. Prokhorov General Physics Institute, Russian Academy of Sciences, 38 Vavilov St., 119991 Moscow, Russian Federation
 3. Lebedev Physical Institute, Russian Academy of Sciences, 53, Lenin Ave., 119991 Moscow, Russian Federation
- *E-mail: rybkovskiyd@gmail.com

Section S1. Heat maps of $\Delta^2_{\text{min}}(n, m)$, $\Delta^2_{\text{ext}}(n, m)$ and $G_{\text{frag}}(n, m)$, calculated at $T = 300$ K	2
Section S2. Average number of P-P bonds per phosphorus atom in Li_nP_m clusters	3
Section S3. Stability of helical L_nP_n clusters	4
Table S1. Atomization energies per atom $E_{\text{at}} = (nE(\text{Li}) + mE(\text{P}) - E(\text{Li}_n, \text{P}_m)) / (n + m)$ of Li_nP_m clusters with $0 \leq n \leq 10$ and $0 \leq m \leq 20$	6
Table S2. Fragmentation energies and fission products of Li_nP_m clusters with $0 \leq n \leq 10$ and $0 \leq m \leq 20$	9
Section S4. Atomic coordinates and total energies of all calculated ground-state structures of L_nP_m clusters with $0 \leq n \leq 10$ and $0 \leq m \leq 20$ in the XYZ format.	13

Section S1. Heat maps of $\Delta^2_{\min}(n, m)$, $\Delta^2_{\text{ext}}(n, m)$ and $G_{\text{frag}}(n, m)$, calculated at $T = 300$ K

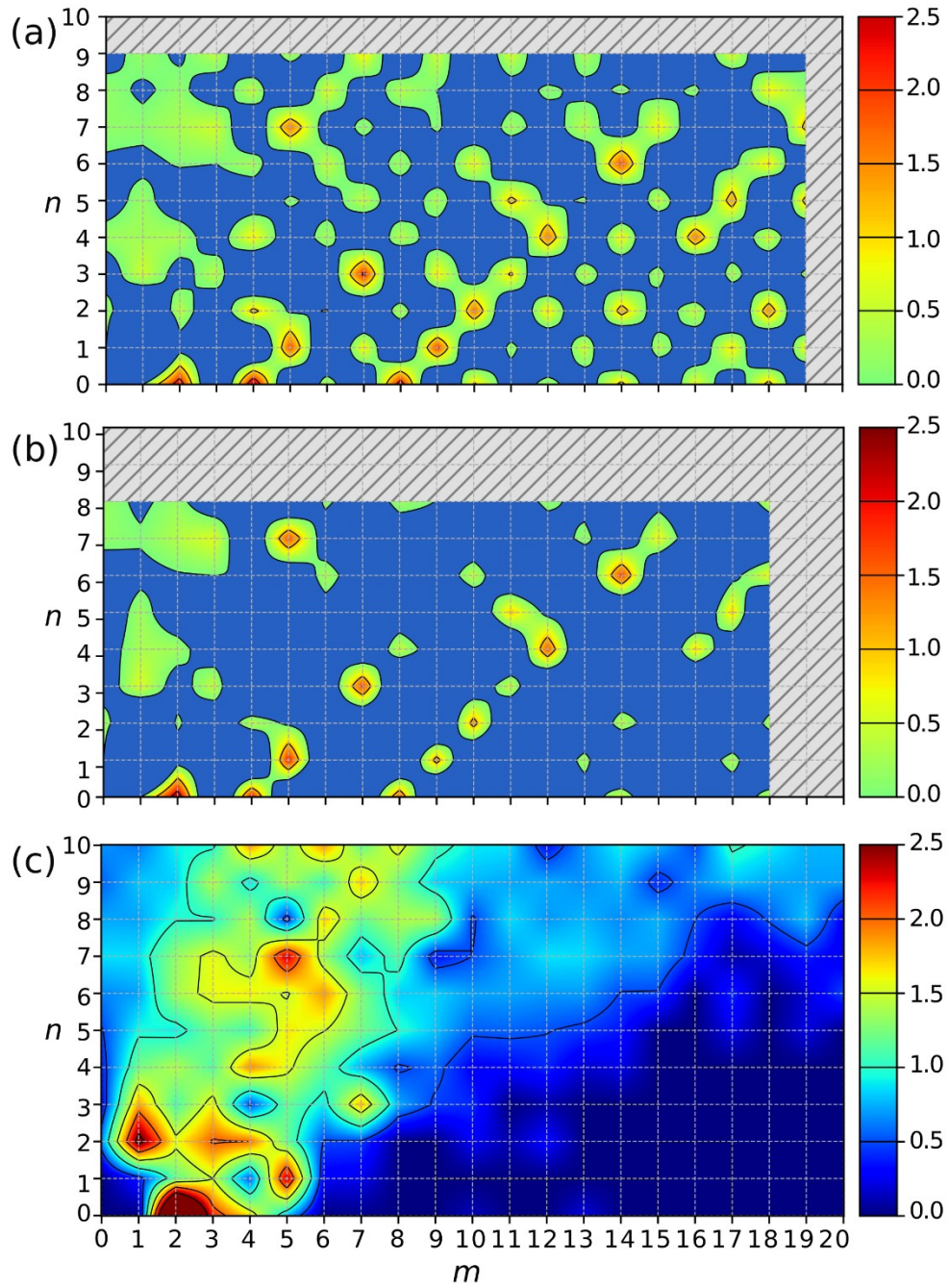


Figure S1. Interpolated heat maps of (a) $\Delta^2_{\min}$, (b) Δ^2_{ext} and (c) $G_{\text{frag}}(n, m)$ (in eV) for Li_nP_m clusters, calculated at $T = 300$ K.

Section S2.

Average number of P-P bonds per phosphorus atom in Li_nP_m clusters

To apply the Zintl-Klemm concept to the structure of Li_nP_m clusters, we used two approaches. The first approach was based on the calculation of average coordination numbers (ACN) of phosphorus atoms (considering only the phosphorus neighbors) for each obtained Li_nP_m ground state. The resulting ACN as a function of Li/P ratio are given in Fig. S2a. Most of the ACN values are located close to the 3 - Li/P line and are reduced from 3 (pure P clusters) to 0 (Li_nP_m clusters with $\text{Li/P} \geq 3$). The exceptions mainly correspond to clusters containing the P_5 pentagonal fragments, which are aromatic and have higher bond orders. To take the aromaticity into account, we also applied a second approach by calculating the average number of P-P bonds based on the Mayer bond orders [Ref. 1] between the P atoms. The bond orders were calculated using the ORCA software [Ref. 2] with the B3LYP hybrid functional and the def2TZVPP basis set. The resulting values as function of the Li/P ratio of the clusters are given in Fig. S2b. It can be clearly seen that the calculated average bond numbers follow the 3 - Li/P line more closely than in the case of the ACN values. This relation is generally better fulfilled for the clusters which are stable according to Δ^2_{ext} .

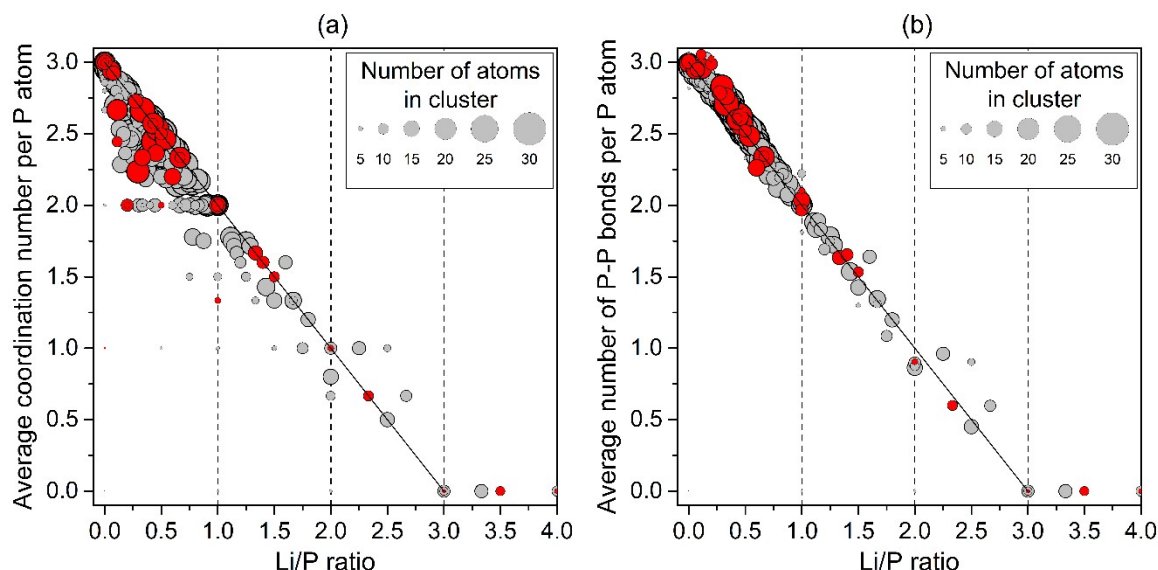


Figure S2. The calculated average coordination number (a) and average number of P-P bonds (b) per phosphorus atom for each Li_nP_m ground state as a function of Li/P ratio. Red and gray circles represent values for clusters with $\Delta^2_{\text{ext}} > 0$ and $\Delta^2_{\text{ext}} \leq 0$, respectively. The size of each circle is proportional to the total number of atoms in the cluster. The solid line depicts the 3 - Li/P relation.

Section S3.

Stability of helical Li_nP_n clusters

We investigated the impact of different exchange-correlation functionals and basis sets on the relative energies of our ground-state structures and the Li-P helices (see Fig. S3). Zero-point energy corrections have been included during this study. We found that, at the B3LYP level with the 6-311+G* basis set, the Li_5P_5 , Li_7P_7 and Li_8P_8 clusters have the ground state with helical geometry, whereas for other studied compositions the helices have higher energy. However, when using higher-quality basis sets, including the def2TZVPP basis used throughout this work, the helical configurations are higher in energy for all studied composition. We also considered the M06-2X functional (suggested in Ref.3) and ended up at the same conclusions - for high-quality basis sets the helical structures are higher in energy than the other structures suggested earlier (for $n=5,6$) and those found in this work (see Fig. S4).

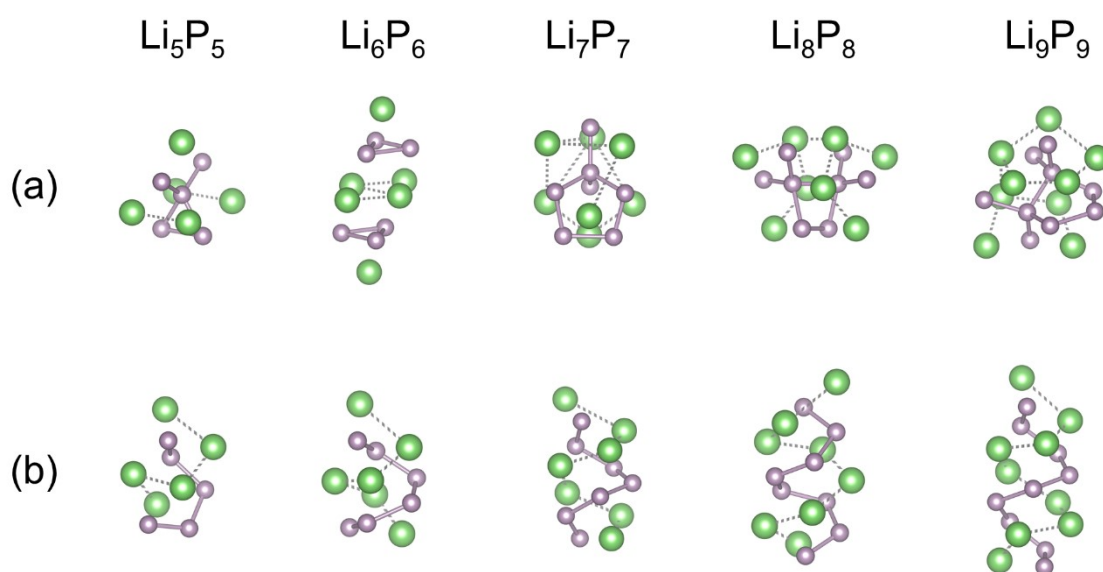


Figure S3. Structures of Li_nP_n clusters with $n = 5-9$. (a) Ground states. (b) Helical isomers.

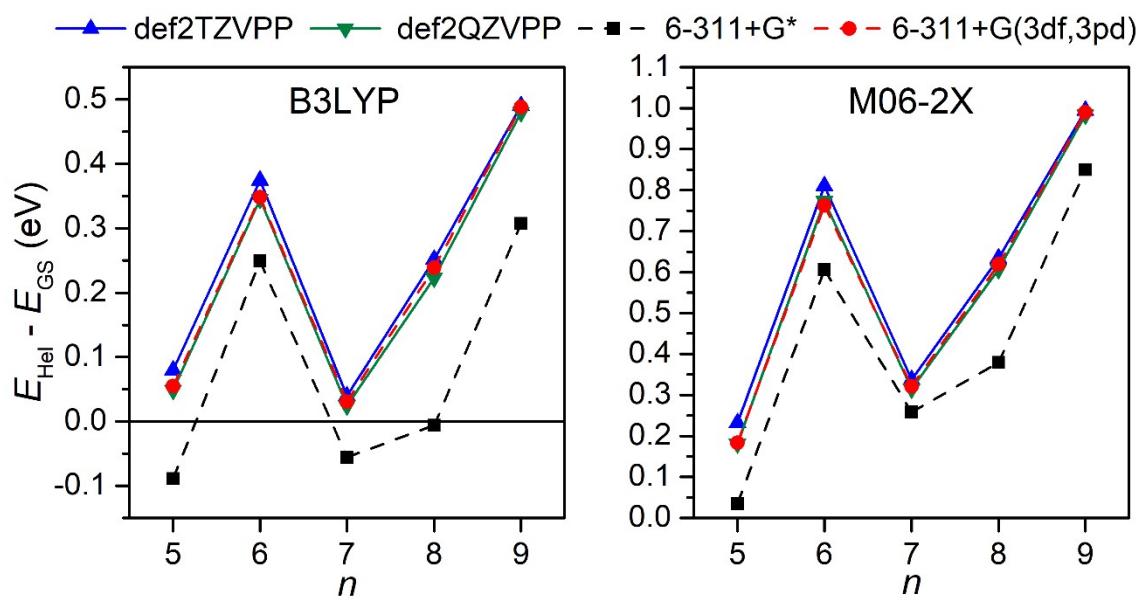


Figure S4. Differences between ZPE-corrected energies for helical (E_{HeI}) and ground state (E_{GS}) Li_nP_n clusters with $n = 5-9$, calculated with B3LYP and M06-2X functionals and different basis sets.

References:

- 1 I. Mayer, Chemical Physics Letters, 1983, 97, 270–274.
- 2 F. Neese, WIREs Comput Mol Sci, 2012, 2, 73–78.
- 3 A. K. Jissy and A. Datta, J. Phys. Chem. Lett., 2013, 4, 1018–1022.

Table S1. Atomization energies per atom $E_{\text{at}} = (nE(\text{Li}) + mE(\text{P}) - E(\text{Li}_n, \text{P}_m)) / (n + m)$ of Li_nP_m clusters with $0 \leq n \leq 10$ and $0 \leq m \leq 20$

Cluster	E_{at} , eV/atom	Cluster	E_{at} , eV/atom	Cluster	E_{at} , eV/atom
P ₂	2.51	LiP ₁₇	3.05	Li ₃ P ₁₀	2.86
P ₃	2.49	LiP ₁₈	3.02	Li ₃ P ₁₁	2.91
P ₄	3.04	LiP ₁₉	3.05	Li ₃ P ₁₂	2.89
P ₅	2.77	LiP ₂₀	3.03	Li ₃ P ₁₃	2.93
P ₆	2.89	Li ₂	0.44	Li ₃ P ₁₄	2.93
P ₇	2.90	Li ₂ P	1.28	Li ₃ P ₁₅	2.96
P ₈	3.04	Li ₂ P ₂	2.11	Li ₃ P ₁₆	2.93
P ₉	2.94	Li ₂ P ₃	2.36	Li ₃ P ₁₇	2.97
P ₁₀	3.03	Li ₂ P ₄	2.68	Li ₃ P ₁₈	2.96
P ₁₁	3.01	Li ₂ P ₅	2.70	Li ₃ P ₁₉	2.98
P ₁₂	3.04	Li ₂ P ₆	2.75	Li ₃ P ₂₀	2.97
P ₁₃	3.03	Li ₂ P ₇	2.79	Li ₄	0.62
P ₁₄	3.08	Li ₂ P ₈	2.85	Li ₄ P	1.51
P ₁₅	3.04	Li ₂ P ₉	2.86	Li ₄ P ₂	1.96
P ₁₆	3.08	Li ₂ P ₁₀	2.96	Li ₄ P ₃	2.18
P ₁₇	3.07	Li ₂ P ₁₁	2.91	Li ₄ P ₄	2.42
P ₁₈	3.10	Li ₂ P ₁₂	2.96	Li ₄ P ₅	2.50
P ₁₉	3.06	Li ₂ P ₁₃	2.94	Li ₄ P ₆	2.63
P ₂₀	3.10	Li ₂ P ₁₄	2.99	Li ₄ P ₇	2.68
LiP	0.32	Li ₂ P ₁₅	2.98	Li ₄ P ₈	2.76
LiP ₂	2.15	Li ₂ P ₁₆	3.00	Li ₄ P ₉	2.77
LiP ₃	2.35	Li ₂ P ₁₇	2.98	Li ₄ P ₁₀	2.81
LiP ₄	2.60	Li ₂ P ₁₈	3.03	Li ₄ P ₁₁	2.83
LiP ₅	2.90	Li ₂ P ₁₉	2.99	Li ₄ P ₁₂	2.92
LiP ₆	2.78	Li ₂ P ₂₀	3.03	Li ₄ P ₁₃	2.88
LiP ₇	2.90	Li ₃	0.46	Li ₄ P ₁₄	2.92
LiP ₈	2.86	Li ₃ P	1.51	Li ₄ P ₁₅	2.91
LiP ₉	2.98	Li ₃ P ₂	1.97	Li ₄ P ₁₆	2.95
LiP ₁₀	2.93	Li ₃ P ₃	2.30	Li ₄ P ₁₇	2.94
LiP ₁₁	2.97	Li ₃ P ₄	2.40	Li ₄ P ₁₈	2.95
LiP ₁₂	2.95	Li ₃ P ₅	2.57	Li ₄ P ₁₉	2.94
LiP ₁₃	3.01	Li ₃ P ₆	2.66	Li ₄ P ₂₀	2.99
LiP ₁₄	2.98	Li ₃ P ₇	2.84	Li ₅	0.66
LiP ₁₅	3.03	Li ₃ P ₈	2.78	Li ₅ P	1.48
LiP ₁₆	3.01	Li ₃ P ₉	2.86	Li ₅ P ₂	1.85

Cluster	E _{at} , eV/atom
Li ₃ P ₃	2.11
Li ₃ P ₄	2.31
Li ₃ P ₅	2.46
Li ₃ P ₆	2.56
Li ₃ P ₇	2.64
Li ₃ P ₈	2.67
Li ₃ P ₉	2.73
Li ₃ P ₁₀	2.76
Li ₃ P ₁₁	2.84
Li ₃ P ₁₂	2.84
Li ₃ P ₁₃	2.86
Li ₃ P ₁₄	2.86
Li ₃ P ₁₅	2.90
Li ₃ P ₁₆	2.90
Li ₃ P ₁₇	2.95
Li ₃ P ₁₈	2.91
Li ₃ P ₁₉	2.95
Li ₃ P ₂₀	2.94
Li ₆	0.75
Li ₆ P	1.42
Li ₆ P ₂	1.82
Li ₆ P ₃	2.09
Li ₆ P ₄	2.29
Li ₆ P ₅	2.39
Li ₆ P ₆	2.53
Li ₆ P ₇	2.56
Li ₆ P ₈	2.63
Li ₆ P ₉	2.66
Li ₆ P ₁₀	2.74
Li ₆ P ₁₁	2.75
Li ₆ P ₁₂	2.79
Li ₆ P ₁₃	2.82
Li ₆ P ₁₄	2.89
Li ₆ P ₁₅	2.86
Li ₆ P ₁₆	2.89

Cluster	E _{at} , eV/atom
Li ₆ P ₁₇	2.90
Li ₆ P ₁₈	2.92
Li ₆ P ₁₉	2.92
Li ₆ P ₂₀	2.95
Li ₇	0.81
Li ₇ P	1.39
Li ₇ P ₂	1.80
Li ₇ P ₃	2.08
Li ₇ P ₄	2.23
Li ₇ P ₅	2.43
Li ₇ P ₆	2.47
Li ₇ P ₇	2.54
Li ₇ P ₈	2.58
Li ₇ P ₉	2.65
Li ₇ P ₁₀	2.67
Li ₇ P ₁₁	2.73
Li ₇ P ₁₂	2.76
Li ₇ P ₁₃	2.80
Li ₇ P ₁₄	2.82
Li ₇ P ₁₅	2.86
Li ₇ P ₁₆	2.85
Li ₇ P ₁₇	2.87
Li ₇ P ₁₈	2.88
Li ₇ P ₁₉	2.93
Li ₇ P ₂₀	2.91
Li ₈	0.84
Li ₈ P	1.36
Li ₈ P ₂	1.75
Li ₈ P ₃	2.01
Li ₈ P ₄	2.19
Li ₈ P ₅	2.30
Li ₈ P ₆	2.44
Li ₈ P ₇	2.50
Li ₈ P ₈	2.57
Li ₈ P ₉	2.61

Cluster	E _{at} , eV/atom
Li ₈ P ₁₀	2.65
Li ₈ P ₁₁	2.68
Li ₈ P ₁₂	2.73
Li ₈ P ₁₃	2.76
Li ₈ P ₁₄	2.79
Li ₈ P ₁₅	2.81
Li ₈ P ₁₆	2.83
Li ₈ P ₁₇	2.84
Li ₈ P ₁₈	2.89
Li ₈ P ₁₉	2.90
Li ₈ P ₂₀	2.90
Li ₉	0.85
Li ₉ P	1.34
Li ₉ P ₂	1.70
Li ₉ P ₃	1.98
Li ₉ P ₄	2.12
Li ₉ P ₅	2.28
Li ₉ P ₆	2.37
Li ₉ P ₇	2.50
Li ₉ P ₈	2.52
Li ₉ P ₉	2.60
Li ₉ P ₁₀	2.61
Li ₉ P ₁₁	2.67
Li ₉ P ₁₂	2.68
Li ₉ P ₁₃	2.73
Li ₉ P ₁₄	2.75
Li ₉ P ₁₅	2.78
Li ₉ P ₁₆	2.79
Li ₉ P ₁₇	2.83
Li ₉ P ₁₈	2.84
Li ₉ P ₁₉	2.86
Li ₉ P ₂₀	2.87
Li ₁₀	0.88
Li ₁₀ P	1.31
Li ₁₀ P ₂	1.66

Cluster	E_{ats} eV/atom
Li_{10}P_3	1.94
Li_{10}P_4	2.13
Li_{10}P_5	2.24
Li_{10}P_6	2.36
Li_{10}P_7	2.44
Li_{10}P_8	2.52
Li_{10}P_9	2.54
$\text{Li}_{10}\text{P}_{10}$	2.59
$\text{Li}_{10}\text{P}_{11}$	2.63
$\text{Li}_{10}\text{P}_{12}$	2.66
$\text{Li}_{10}\text{P}_{13}$	2.69
$\text{Li}_{10}\text{P}_{14}$	2.73
$\text{Li}_{10}\text{P}_{15}$	2.75
$\text{Li}_{10}\text{P}_{16}$	2.77
$\text{Li}_{10}\text{P}_{17}$	2.80
$\text{Li}_{10}\text{P}_{18}$	2.83
$\text{Li}_{10}\text{P}_{19}$	2.83
$\text{Li}_{10}\text{P}_{20}$	2.86

Table S2. Fragmentation energies and fission products of Li_nP_m clusters with $0 \leq n \leq 10$ and $0 \leq m \leq 20$

Cluster	Fission products	Fragmentation energy, eV
P ₂	P + P	5.02
P ₃	P + P ₂	2.46
P ₄	P ₂ + P ₂	2.12
P ₅	P ₂ + P ₃	1.34
P ₆	P ₂ + P ₄	0.14
P ₇	P ₃ + P ₄	0.68
P ₈	P ₄ + P ₄	0
P ₉	P ₄ + P ₅	0.46
P ₁₀	P ₄ + P ₆	0.84
P ₁₁	P ₄ + P ₇	0.61
P ₁₂	P ₄ + P ₈	0.01
P ₁₃	P ₄ + P ₉	0.83
P ₁₄	P ₄ + P ₁₀	0.7
P ₁₅	P ₄ + P ₁₁	0.34
P ₁₆	P ₄ + P ₁₂	0.7
P ₁₇	P ₄ + P ₁₃	0.57
P ₁₈	P ₄ + P ₁₄	0.54
P ₁₉	P ₄ + P ₁₅	0.44
P ₂₀	P ₄ + P ₁₆	0.45
LiP	P + Li	0.65
LiP ₂	P ₂ + Li	1.44
LiP ₃	P ₃ + Li	1.92
LiP ₄	P ₄ + Li	0.83
LiP ₅	P ₂ + LiP ₃	2.98
LiP ₆	P ₄ + LiP ₂	0.87
LiP ₇	P ₂ + LiP ₅	0.78
LiP ₈	P ₄ + LiP ₄	0.63
LiP ₉	P ₄ + LiP ₅	0.23
LiP ₁₀	P ₄ + LiP ₆	0.58
LiP ₁₁	P ₄ + LiP ₇	0.31
LiP ₁₂	P ₄ + LiP ₈	0.45
LiP ₁₃	P ₄ + LiP ₉	0.23
LiP ₁₄	P ₄ + LiP ₁₀	0.27
LiP ₁₅	P ₄ + LiP ₁₁	0.6
LiP ₁₆	P ₄ + LiP ₁₂	0.68

Cluster	Fission products	Fragmentation energy, eV
LiP ₁₇	P ₄ + LiP ₁₃	0.58
LiP ₁₈	P ₁₃ + LiP ₅	0.59
LiP ₁₉	P ₄ + LiP ₁₅	0.45
LiP ₂₀	P ₄ + LiP ₁₆	0.22
Li ₂	Li + Li	0.89
Li ₂ P	P + Li ₂	2.96
Li ₂ P ₂	Li + LiP ₂	1.98
Li ₂ P ₃	Li + LiP ₃	2.38
Li ₂ P ₄	P ₂ + Li ₂ P ₂	2.62
Li ₂ P ₅	Li + LiP ₅	1.47
Li ₂ P ₆	P ₂ + Li ₂ P ₄	0.94
Li ₂ P ₇	P ₄ + Li ₂ P ₃	1.14
Li ₂ P ₈	P ₄ + Li ₂ P ₄	0.29
Li ₂ P ₉	P ₄ + Li ₂ P ₅	0.38
Li ₂ P ₁₀	LiP ₅ + LiP ₅	0.76
Li ₂ P ₁₁	P ₄ + Li ₂ P ₇	0.56
Li ₂ P ₁₂	P ₄ + Li ₂ P ₈	0.82
Li ₂ P ₁₃	P ₄ + Li ₂ P ₉	0.51
Li ₂ P ₁₄	P ₄ + Li ₂ P ₁₀	0.06
Li ₂ P ₁₅	P ₄ + Li ₂ P ₁₁	0.63
Li ₂ P ₁₆	P ₄ + Li ₂ P ₁₂	0.3
Li ₂ P ₁₇	P ₄ + Li ₂ P ₁₃	0.35
Li ₂ P ₁₈	P ₄ + Li ₂ P ₁₄	0.59
Li ₂ P ₁₉	P ₄ + Li ₂ P ₁₅	0.03
Li ₂ P ₂₀	P ₄ + Li ₂ P ₁₆	0.56
Li ₃	Li + Li ₂	0.5
Li ₃ P	Li + Li ₂ P	2.21
Li ₃ P ₂	Li + Li ₂ P ₂	1.42
Li ₃ P ₃	Li + Li ₂ P ₃	2.04
Li ₃ P ₄	Li + Li ₂ P ₄	0.75
Li ₃ P ₅	Li + Li ₂ P ₅	1.65
Li ₃ P ₆	LiP ₂ + Li ₂ P ₄	1.45
Li ₃ P ₇	P ₄ + Li ₃ P ₃	2.45
Li ₃ P ₈	LiP ₅ + Li ₂ P ₃	1.39
Li ₃ P ₉	LiP ₅ + Li ₂ P ₄	0.89

Cluster	Fission products	Fragmentation energy, eV
Li ₃ P ₁₀	LiP ₅ + Li ₂ P ₅	0.92
Li ₃ P ₁₁	P ₄ + Li ₃ P ₇	0.17
Li ₃ P ₁₂	P ₄ + Li ₃ P ₈	0.58
Li ₃ P ₁₃	P ₄ + Li ₃ P ₉	0.33
Li ₃ P ₁₄	P ₄ + Li ₃ P ₁₀	0.41
Li ₃ P ₁₅	LiP ₅ + Li ₂ P ₁₀	0.24
Li ₃ P ₁₆	P ₄ + Li ₃ P ₁₂	0.23
Li ₃ P ₁₇	P ₄ + Li ₃ P ₁₃	0.36
Li ₃ P ₁₈	P ₄ + Li ₃ P ₁₄	0.24
Li ₃ P ₁₉	P ₄ + Li ₃ P ₁₅	0.22
Li ₃ P ₂₀	LiP ₅ + Li ₂ P ₁₅	0.37
Li ₄	Li ₂ + Li ₂	0.7
Li ₄ P	Li + Li ₃ P	1.48
Li ₄ P ₂	Li + Li ₃ P ₂	1.88
Li ₄ P ₃	Li + Li ₃ P ₃	1.45
Li ₄ P ₄	Li ₂ + Li ₂ P ₄	2.44
Li ₄ P ₅	Li + Li ₃ P ₅	1.97
Li ₄ P ₆	Li ₂ P ₂ + Li ₂ P ₄	1.77
Li ₄ P ₇	Li + Li ₃ P ₇	1.09
Li ₄ P ₈	Li ₂ P ₄ + Li ₂ P ₄	0.98
Li ₄ P ₉	Li ₂ P ₄ + Li ₂ P ₅	1.03
Li ₄ P ₁₀	P ₄ + Li ₄ P ₆	0.88
Li ₄ P ₁₁	P ₄ + Li ₄ P ₇	0.81
Li ₄ P ₁₂	LiP ₅ + Li ₃ P ₇	0.87
Li ₄ P ₁₃	P ₄ + Li ₄ P ₉	0.8
Li ₄ P ₁₄	LiP ₅ + Li ₃ P ₉	0.85
Li ₄ P ₁₅	P ₄ + Li ₄ P ₁₁	0.56
Li ₄ P ₁₆	P ₄ + Li ₄ P ₁₂	0.2
Li ₄ P ₁₇	P ₄ + Li ₄ P ₁₃	0.63
Li ₄ P ₁₈	P ₄ + Li ₄ P ₁₄	0.15
Li ₄ P ₁₉	P ₄ + Li ₄ P ₁₅	0.36
Li ₄ P ₂₀	P ₄ + Li ₄ P ₁₆	0.48
Li ₅	Li + Li ₄	0.81
Li ₅ P	Li + Li ₄ P	1.36
Li ₅ P ₂	Li + Li ₄ P ₂	1.19

Cluster	Fission products	Fragmentation energy, eV
Li ₅ P ₃	Li + Li ₄ P ₃	1.62
Li ₅ P ₄	Li + Li ₄ P ₄	1.42
Li ₅ P ₅	Li + Li ₄ P ₅	2.06
Li ₅ P ₆	Li + Li ₄ P ₆	1.83
Li ₅ P ₇	Li ₂ P ₄ + Li ₃ P ₃	1.79
Li ₅ P ₈	P ₂ + Li ₅ P ₆	1.54
Li ₅ P ₉	Li ₂ P ₂ + Li ₃ P ₇	1.42
Li ₅ P ₁₀	P ₄ + Li ₅ P ₆	1.09
Li ₅ P ₁₁	Li ₂ P ₄ + Li ₃ P ₇	0.98
Li ₅ P ₁₂	Li ₂ P ₅ + Li ₃ P ₇	1
Li ₅ P ₁₃	LiP ₅ + Li ₄ P ₈	0.92
Li ₅ P ₁₄	P ₄ + Li ₅ P ₁₀	0.92
Li ₅ P ₁₅	P ₄ + Li ₅ P ₁₁	0.36
Li ₅ P ₁₆	P ₄ + Li ₅ P ₁₂	0.46
Li ₅ P ₁₇	LiP ₅ + Li ₄ P ₁₂	0.72
Li ₅ P ₁₈	P ₄ + Li ₅ P ₁₄	0.42
Li ₅ P ₁₉	P ₄ + Li ₅ P ₁₅	0.72
Li ₅ P ₂₀	P ₄ + Li ₅ P ₁₆	0.33
Li ₆	Li ₂ + Li ₄	1.14
Li ₆ P	Li + Li ₅ P	1.02
Li ₆ P ₂	Li + Li ₅ P ₂	1.61
Li ₆ P ₃	Li + Li ₅ P ₃	1.91
Li ₆ P ₄	Li + Li ₅ P ₄	2.06
Li ₆ P ₅	Li + Li ₅ P ₅	1.79
Li ₆ P ₆	Li + Li ₅ P ₆	2.29
Li ₆ P ₇	Li + Li ₅ P ₇	1.6
Li ₆ P ₈	Li ₂ P ₄ + Li ₄ P ₄	1.41
Li ₆ P ₉	Li ₂ P ₄ + Li ₄ P ₅	1.42
Li ₆ P ₁₀	P ₄ + Li ₆ P ₆	1.35
Li ₆ P ₁₁	Li ₂ P ₄ + Li ₄ P ₇	1.2
Li ₆ P ₁₂	Li ₂ P ₄ + Li ₄ P ₈	1.07
Li ₆ P ₁₃	Li ₃ P ₆ + Li ₃ P ₇	1.24
Li ₆ P ₁₄	Li ₃ P ₇ + Li ₃ P ₇	0.96
Li ₆ P ₁₅	Li ₃ P ₇ + Li ₃ P ₈	0.97
Li ₆ P ₁₆	LiP ₅ + Li ₅ P ₁₁	0.62

Cluster	Fission products	Fragmentation energy, eV
Li ₆ P ₁₇	P ₄ + Li ₆ P ₁₃	0.95
Li ₆ P ₁₈	P ₄ + Li ₆ P ₁₄	0.18
Li ₆ P ₁₉	P ₄ + Li ₆ P ₁₅	0.8
Li ₆ P ₂₀	P ₄ + Li ₆ P ₁₆	0.94
Li ₇	Li + Li ₆	1.17
Li ₇ P	Li + Li ₆ P	1.21
Li ₇ P ₂	Li + Li ₆ P ₂	1.65
Li ₇ P ₃	Li + Li ₆ P ₃	2.02
Li ₇ P ₄	Li + Li ₆ P ₄	1.67
Li ₇ P ₅	Li + Li ₆ P ₅	2.86
Li ₇ P ₆	Li + Li ₆ P ₆	1.65
Li ₇ P ₇	P ₂ + Li ₇ P ₅	1.3
Li ₇ P ₈	P ₂ + Li ₇ P ₆	1.68
Li ₇ P ₉	P ₄ + Li ₇ P ₅	0.98
Li ₇ P ₁₀	P ₄ + Li ₇ P ₆	1.12
Li ₇ P ₁₁	Li ₃ P ₇ + Li ₄ P ₄	1.29
Li ₇ P ₁₂	Li ₃ P ₇ + Li ₄ P ₅	1.46
Li ₇ P ₁₃	Li ₃ P ₇ + Li ₄ P ₆	1.39
Li ₇ P ₁₄	Li ₃ P ₇ + Li ₄ P ₇	1.25
Li ₇ P ₁₅	Li ₃ P ₇ + Li ₄ P ₈	1.28
Li ₇ P ₁₆	P ₄ + Li ₇ P ₁₂	0.98
Li ₇ P ₁₇	P ₄ + Li ₇ P ₁₃	0.72
Li ₇ P ₁₈	P ₄ + Li ₇ P ₁₄	0.7
Li ₇ P ₁₉	LiP ₅ + Li ₆ P ₁₄	0.99
Li ₇ P ₂₀	P ₄ + Li ₇ P ₁₆	0.88
Li ₈	Li + Li ₇	1.03
Li ₈ P	Li + Li ₇ P	1.08
Li ₈ P ₂	Li + Li ₇ P ₂	1.28
Li ₈ P ₃	Li + Li ₇ P ₃	1.29
Li ₈ P ₄	Li + Li ₇ P ₄	1.77
Li ₈ P ₅	Li + Li ₇ P ₅	0.67
Li ₈ P ₆	Li + Li ₇ P ₆	2.18
Li ₈ P ₇	LiP ₂ + Li ₇ P ₅	1.78
Li ₈ P ₈	P ₂ + Li ₈ P ₆	1.94
Li ₈ P ₉	P ₂ + Li ₈ P ₇	1.97

Cluster	Fission products	Fragmentation energy, eV
Li ₈ P ₁₀	LiP ₅ + Li ₇ P ₅	1.08
Li ₈ P ₁₁	P ₄ + Li ₈ P ₇	1.42
Li ₈ P ₁₂	P ₄ + Li ₈ P ₈	1.27
Li ₈ P ₁₃	P ₄ + Li ₈ P ₉	1.33
Li ₈ P ₁₄	Li ₃ P ₇ + Li ₅ P ₇	1.3
Li ₈ P ₁₅	P ₄ + Li ₈ P ₁₁	1.35
Li ₈ P ₁₆	P ₄ + Li ₈ P ₁₂	1.13
Li ₈ P ₁₇	P ₄ + Li ₈ P ₁₃	0.86
Li ₈ P ₁₈	Li ₃ P ₇ + Li ₅ P ₁₁	1.2
Li ₈ P ₁₉	Li ₃ P ₇ + Li ₅ P ₁₂	1.49
Li ₈ P ₂₀	LiP ₅ + Li ₇ P ₁₅	0.95
Li ₉	Li + Li ₈	0.9
Li ₉ P	Li + Li ₈ P	1.2
Li ₉ P ₂	Li + Li ₈ P ₂	1.2
Li ₉ P ₃	Li + Li ₈ P ₃	1.68
Li ₉ P ₄	Li + Li ₈ P ₄	1.28
Li ₉ P ₅	Li ₂ + Li ₇ P ₅	1.9
Li ₉ P ₆	Li + Li ₈ P ₆	1.35
Li ₉ P ₇	Li ₂ P ₂ + Li ₇ P ₅	2.39
Li ₉ P ₈	Li + Li ₈ P ₈	1.65
Li ₉ P ₉	Li ₂ P ₄ + Li ₇ P ₅	1.46
Li ₉ P ₁₀	Li ₂ P ₄ + Li ₇ P ₆	1.45
Li ₉ P ₁₁	P ₄ + Li ₉ P ₇	1.24
Li ₉ P ₁₂	P ₄ + Li ₉ P ₈	1.35
Li ₉ P ₁₃	P ₄ + Li ₉ P ₉	1.2
Li ₉ P ₁₄	LiP ₅ + Li ₈ P ₉	1.35
Li ₉ P ₁₅	P ₄ + Li ₉ P ₁₁	1.1
Li ₉ P ₁₆	P ₄ + Li ₉ P ₁₂	1.27
Li ₉ P ₁₇	Li ₃ P ₇ + Li ₆ P ₁₀	1.37
Li ₉ P ₁₈	P ₄ + Li ₉ P ₁₄	1.34
Li ₉ P ₁₉	Li ₂ P ₄ + Li ₇ P ₁₅	1.29
Li ₉ P ₂₀	Li ₃ P ₇ + Li ₆ P ₁₃	1.3
Li ₁₀	Li + Li ₉	1.16
Li ₁₀ P	Li + Li ₉ P	0.97
Li ₁₀ P ₂	Li + Li ₉ P ₂	1.24

Cluster	Fission products	Fragmentation energy, eV
Li_{10}P_3	$\text{Li} + \text{Li}_9\text{P}_3$	1.4
Li_{10}P_4	$\text{Li} + \text{Li}_9\text{P}_4$	2.16
Li_{10}P_5	$\text{Li} + \text{Li}_9\text{P}_5$	1.59
Li_{10}P_6	$\text{Li} + \text{Li}_9\text{P}_6$	2.21
Li_{10}P_7	$\text{Li} + \text{Li}_9\text{P}_7$	1.42
Li_{10}P_8	$\text{Li}_3\text{P}_3 + \text{Li}_7\text{P}_5$	2.29
Li_{10}P_9	$\text{Li} + \text{Li}_9\text{P}_9$	1.48
$\text{Li}_{10}\text{P}_{10}$	$\text{P}_2 + \text{Li}_{10}\text{P}_8$	1.47
$\text{Li}_{10}\text{P}_{11}$	$\text{P}_4 + \text{Li}_{10}\text{P}_7$	1.55
$\text{Li}_{10}\text{P}_{12}$	$\text{Li}_3\text{P}_7 + \text{Li}_7\text{P}_5$	0.94
$\text{Li}_{10}\text{P}_{13}$	$\text{Li}_2\text{P}_4 + \text{Li}_8\text{P}_9$	1.31
$\text{Li}_{10}\text{P}_{14}$	$\text{LiP}_5 + \text{Li}_9\text{P}_9$	1.38
$\text{Li}_{10}\text{P}_{15}$	$\text{P}_4 + \text{Li}_{10}\text{P}_{11}$	1.39
$\text{Li}_{10}\text{P}_{16}$	$\text{LiP}_5 + \text{Li}_9\text{P}_{11}$	1.23
$\text{Li}_{10}\text{P}_{17}$	$\text{Li}_2\text{P}_4 + \text{Li}_8\text{P}_{13}$	1.62
$\text{Li}_{10}\text{P}_{18}$	$\text{P}_4 + \text{Li}_{10}\text{P}_{14}$	1.51
$\text{Li}_{10}\text{P}_{19}$	$\text{P}_4 + \text{Li}_{10}\text{P}_{15}$	1.33
$\text{Li}_{10}\text{P}_{20}$	$\text{Li}_3\text{P}_7 + \text{Li}_7\text{P}_{13}$	1.42

Section S4.

Atomic coordinates and total energies of all calculated ground-state structures of L_nP_m clusters with $0 \leq n \leq 10$ and $0 \leq m \leq 20$ in the XYZ format.

1
P1 E = -9286.7176 eV
P 0.000000 0.000000 0.000000

2
P2 E = -18578.4540 eV
P 0.000000 0.000000 0.944780
P 0.000000 0.000000 -0.944780

3
P3 E = -27867.6289 eV
P -0.000000 1.165621 -0.000000
P 1.127161 -0.582478 -0.000000
P -1.127161 -0.583143 0.000000

4
P4 E = -37159.0245 eV
P -0.816653 -0.817531 -0.697027
P 0.744072 -0.730900 0.856214
P -0.740160 0.890121 0.693500
P 0.812740 0.658310 -0.852687

5
P5 E = -46447.4252 eV
P 0.124031 -0.150219 1.474470
P 0.124031 1.560679 -0.000000
P 0.124031 -0.150219 -1.474470
P -1.555967 0.173316 -0.000000
P 1.183876 -1.433557 0.000000

6
P6 E = -55737.6231 eV
P 0.366652 1.613135 -0.000018
P -1.807246 -1.006116 -0.000018
P 1.440573 0.000006 1.106042
P -1.807207 1.006124 0.000012
P 0.366655 -1.613125 0.000022
P 1.440573 -0.000024 -1.106038

7
P7 E = -65027.3328 eV
P -1.161058 -0.966975 1.122790
P -1.160518 -0.967325 -1.122620
P -1.718166 0.843869 -0.000240
P 1.160922 -0.966991 1.122750
P 1.718094 0.843975 0.000110
P 1.160812 -0.967121 -1.122690
P -0.000087 2.180567 -0.000100

8

P8 E = -74318.0454 eV

P -4.072659 0.021580 0.052148
P -2.253289 -0.883273 0.904889
P -2.243698 1.229602 0.279197
P 2.298132 0.260902 1.253465
P -2.327869 -0.367912 -1.236244
P 2.244081 -1.196444 -0.398524
P 2.281921 0.963170 -0.835142
P 4.073381 -0.027624 -0.019788

9

P9 E = -83606.9080 eV

P 0.124554 1.128889 -1.433196
P 1.578926 -0.000059 1.563284
P 0.124557 -1.128761 -1.433296
P -0.663714 -0.000072 1.682444
P -1.263562 -1.588113 0.224294
P -1.263607 1.588087 0.224414
P 2.078634 1.139582 -0.281216
P 2.078647 -1.139548 -0.281316
P -2.794434 -0.000005 -0.265416

10

P10 E = -92897.4841 eV

P -1.714912 1.622100 0.036750
P -3.200101 -0.000052 -0.325660
P -1.992331 0.000029 1.541260
P -1.714830 -1.622110 0.036870
P -0.000010 -1.109869 -1.289220
P 0.000008 1.109871 -1.289220
P 1.714910 -1.622098 0.036750
P 3.200099 0.000054 -0.325660
P 1.992339 -0.000037 1.541260
P 1.714828 1.622112 0.036870

11

P11 E = -102186.9627 eV

P -2.094450 2.807615 0.000000
P -2.332956 0.942150 1.126330
P -2.332956 0.942150 -1.126330
P 2.026604 -1.844237 -1.140710
P -0.214060 0.480452 -1.706980
P -0.214060 -1.652251 -1.134130
P 0.901423 1.361938 0.000000
P 2.661968 -0.021778 0.000000
P -0.214060 -1.652251 1.134130
P 2.026604 -1.844237 1.140710
P -0.214060 0.480452 1.706980

12

P12 E = -111477.0780 eV
P -2.530557 -0.612369 -1.159169
P -2.530590 -0.697703 1.109769
P -2.530588 1.309965 0.049284
P -0.428250 -1.095972 1.743485
P -0.428268 2.057961 0.077466
P -0.428177 -0.961836 -1.820803
P 0.428171 -2.057876 -0.077440
P 0.428300 0.961879 1.820888
P 0.428234 1.096103 -1.743378
P 2.530611 0.612195 1.159128
P 2.530573 0.697719 -1.109796
P 2.530541 -1.310066 -0.049434

13
P13 E = -120766.7640 eV
P 0.806637 -0.001802 1.567123
P -2.629643 -1.625012 0.041893
P -2.629673 1.624858 0.045913
P -2.982933 -0.001922 1.528733
P -0.868333 -1.128152 -1.215797
P 0.800977 -1.691662 0.140753
P 2.961947 -0.002793 2.003013
P 3.868847 0.000137 -0.021967
P 0.800947 1.691458 0.144763
P 2.413387 1.113577 -1.306787
P -0.868403 1.131128 -1.213047
P 2.413377 -1.110293 -1.309547
P -4.087133 0.000478 -0.405047

14
P14 E = -130057.2074 eV
P -3.714394 -1.137693 0.179222
P -2.763724 -0.000003 1.863202
P -2.095764 -1.136283 -1.382478
P -3.714404 1.137687 0.179212
P -2.095764 1.136297 -1.382478
P -0.484804 1.696187 0.014692
P 1.248506 1.132787 -1.261458
P 1.248506 -1.132763 -1.261468
P -0.484794 -1.696193 0.014652
P 3.174946 -0.000003 1.612892
P 4.403416 -0.000003 -0.246808
P 2.922226 1.625247 0.109232
P -0.566154 -0.000013 1.452362
P 2.922206 -1.625253 0.109222

15
P15 E = -139346.3276 eV
P -2.458019 1.471808 1.111755
P -1.382999 -0.376288 1.764026
P 0.754469 0.348447 -1.759480

P 1.040017 1.669346 -0.001591
 P 0.754471 0.351784 1.758809
 P 3.832008 -0.287728 -1.134106
 P 3.831999 -0.285592 1.134638
 P 3.277427 1.575546 -0.001487
 P 1.890296 -1.424986 -1.138875
 P 1.890280 -1.422835 1.141569
 P -3.796920 -1.603135 0.001463
 P -1.601131 -1.693976 0.001640
 P -4.190889 0.587586 -0.000552
 P -2.458015 1.469694 -1.114547
 P -1.382994 -0.379672 -1.763263

16

P16 E = -148636.8071 eV

P -1.338007 -0.000023 -1.653637
 P -1.078256 -1.765923 -0.338757
 P 4.138593 -1.136221 -0.275607
 P 4.138593 1.136259 -0.275487
 P 2.207873 -1.141182 -1.432407
 P 2.207933 1.141178 -1.432327
 P 1.078264 -1.765912 0.338843
 P 1.338063 -0.000002 1.653683
 P 3.579853 -0.000071 1.581723
 P 1.078263 1.765958 0.338793
 P -2.207947 -1.141173 1.432413
 P -4.138607 -1.136224 0.275533
 P -3.579787 -0.000064 -1.581777
 P -2.207987 1.141197 1.432333
 P -4.138597 1.136266 0.275433
 P -1.078247 1.765937 -0.338757

17

P17 E = -157926.3631 eV

P -2.045422 0.209699 1.695354
 P -3.601302 -1.303461 1.116174
 P -2.104622 1.626719 -0.002616
 P -3.601312 -1.306941 -1.112116
 P -5.101962 -0.081661 0.000074
 P -2.045412 0.204309 -1.696086
 P -4.274422 1.980939 -0.002916
 P -0.352952 -1.119461 1.154554
 P -0.352912 -1.123071 -1.151046
 P 4.660908 0.083319 -1.138316
 P 1.425438 0.088599 -1.698936
 P 2.963578 -1.390801 -1.134036
 P 1.582248 1.521359 -0.002326
 P 3.798208 1.817169 -0.002776
 P 2.963568 -1.387331 1.138304
 P 4.660918 0.086789 1.138054
 P 1.425458 0.093829 1.698664

18

P18 E = -167216.7688 eV

P	0.000009	-1.156959	-1.214981
P	3.323139	-1.136187	-1.348761
P	1.827149	0.000032	1.503319
P	4.029229	0.000023	1.888069
P	4.959608	1.138893	0.191239
P	4.959599	-1.138917	0.191269
P	1.727640	-1.700038	0.069339
P	3.323148	1.136133	-1.348801
P	-1.727642	1.700040	0.069389
P	-3.323132	1.136210	-1.348751
P	-4.959601	-1.138911	0.191219
P	-4.029241	-0.000041	1.888069
P	-1.827161	-0.000050	1.503329
P	-4.959612	1.138889	0.191259
P	-3.323141	-1.136120	-1.348811
P	-1.727660	-1.700040	0.069269
P	1.727678	1.700032	0.069299
P	-0.000012	1.157011	-1.214961

19

P19 E = -176505.7944 eV

P	-5.603272	-1.217935	0.573788
P	-4.361642	-1.442515	-1.219242
P	-5.067962	0.580445	-0.564672
P	0.730858	-1.190815	0.907098
P	0.785778	-0.486775	-1.210862
P	1.269018	1.656445	-0.865962
P	-0.323672	2.191725	0.589138
P	-0.498692	0.335835	1.963398
P	-2.547062	-0.500095	1.515158
P	-1.940542	1.851565	-0.872532
P	-3.418422	1.381115	0.722098
P	-2.294982	-1.657315	-0.372452
P	-1.377672	-0.199925	-1.784222
P	2.982188	1.523125	0.539658
P	2.680618	-0.420885	1.645678
P	4.596218	1.022285	-0.901342
P	5.836628	-0.491775	0.165268
P	4.457468	-1.132675	-1.461212
P	4.095148	-1.801835	0.631218

20

P20 E = -185796.2858 eV

P	-5.788696	-1.140124	0.092618
P	-5.788946	1.139836	0.091939
P	-5.060905	-0.000579	-1.696859
P	-3.989584	1.135403	1.441408
P	-3.989274	-1.134807	1.442026
P	-2.827810	-0.000199	-1.565498
P	-2.568996	1.701897	-0.153086

P	-2.568851	-1.701723	-0.152587
P	-0.692205	-1.153135	0.887420
P	-0.692361	1.153595	0.887119
P	0.692224	-1.153300	-0.887301
P	0.692359	1.153440	-0.887385
P	2.568901	-1.701882	0.152637
P	2.568921	1.701728	0.152974
P	2.827760	-0.000116	1.565481
P	3.989569	-1.135098	-1.441723
P	3.989392	1.135102	-1.441683
P	5.060844	0.000004	1.696912
P	5.788871	-1.140001	-0.092192
P	5.788785	1.139959	-0.092219

1
Li1 E = -203.8894 eV
Li 0.000000 0.000000 0.000000

2
Li1P1 E = -9491.2549 eV
Li 0.000000 0.000000 -1.923033
P 0.000000 0.000000 0.384607

3
Li1P2 E = -18783.7816 eV
Li 1.916863 -0.378187 0.000000
P -0.000000 1.009369 -0.000000
P -0.383373 -0.933732 0.000000

4
Li1P3 E = -28073.4414 eV
Li 0.000030 -1.262618 1.548535
P -1.250524 -0.453343 -0.232570
P 1.250536 -0.453316 -0.232573
P -0.000018 1.159183 0.155436

5
Li1P4 E = -37363.7432 eV
Li -0.000285 2.465490 -0.000798
P -1.453006 0.518906 -0.000298
P -0.000000 -0.766230 -1.088168
P 1.452914 0.519115 -0.000408
P 0.000150 -0.764890 1.089032

6
Li1P5 E = -46654.8798 eV
Li -0.000607 -0.000285 1.721644
P 1.799478 0.158975 -0.068886
P 0.405061 1.760593 -0.068706
P -1.549305 0.929017 -0.069016
P -1.362458 -1.186106 -0.068856
P 0.707346 -1.662422 -0.068866

7

Li1P6 E = -55943.6805 eV

Li	0.877973	0.000275	1.887036
P	-0.360399	1.615734	-0.065099
P	-1.533293	-0.000300	1.082263
P	-1.475373	0.000390	-1.120148
P	1.777201	1.068573	-0.104423
P	1.777120	-1.068947	-0.104673
P	-0.360851	-1.615506	-0.065326

8

Li1P7 E = -65234.1168 eV

Li	1.071215	-0.004315	1.946533
P	-1.041312	1.154960	1.109799
P	0.852882	1.665389	-0.111575
P	-1.013899	1.151909	-1.141348
P	2.226311	-0.010020	-0.104274
P	0.837554	-1.673227	-0.110409
P	-1.051886	-1.144683	1.109846
P	-1.023893	-1.143465	-1.141346

9

Li1P8 E = -74523.4023 eV

Li	0.000924	0.000056	-2.248261
P	-0.005119	2.089296	-1.046261
P	1.756309	1.174105	-0.173621
P	1.125585	0.002814	1.618599
P	-1.762512	1.165717	-0.173751
P	-1.125766	-0.002922	1.618479
P	-1.756340	-1.174093	-0.173841
P	0.005158	-2.089204	-1.046351
P	1.762501	-1.165725	-0.173601

10

Li1P9 E = -83814.1298 eV

Li	-0.440218	-0.001813	-0.001511
P	2.131431	1.124407	-0.000851
P	2.131642	-1.125483	-0.000711
P	3.654312	-0.000332	1.109349
P	3.655222	-0.000462	-1.109671
P	-2.295388	-0.903074	1.562079
P	-2.300918	-1.764154	-0.375821
P	-2.298068	-0.186914	-1.793941
P	-2.293509	1.207026	1.341859
P	-2.296679	1.649346	-0.731991

11

Li1P10 E = -93103.2825 eV

Li	1.986832	-0.000438	-2.213929
P	2.781814	-1.084584	-0.081298
P	-0.318458	-1.148284	-1.323320

P	2.781530	1.084916	-0.081463
P	-0.318938	1.148866	-1.322922
P	-2.093411	-0.000490	1.397056
P	0.739232	1.702144	0.525031
P	0.113902	-0.000284	1.813337
P	0.739469	-1.702176	0.524617
P	-2.411114	-1.139310	-0.504489
P	-2.411393	1.139290	-0.503763

12

Li1P11 E = -102393.4562 eV

Li	-2.222287	-0.000922	2.629503
P	0.984102	-1.135476	-1.426820
P	-0.429361	-1.710002	0.159873
P	-2.407867	-1.128058	-0.786557
P	-3.611144	-0.000169	0.670380
P	-2.407952	1.128322	-0.786143
P	2.833559	1.136144	-0.136790
P	0.984027	1.135854	-1.426636
P	-0.060125	-0.000094	1.506252
P	2.155043	-0.000160	1.677216
P	-0.429308	1.710098	0.160337
P	2.833484	-1.136276	-0.137013

13

Li1P12 E = -111682.8764 eV

Li	-1.870236	-0.000551	1.815763
P	3.618332	0.000269	-0.010330
P	0.591130	-1.716821	0.116018
P	2.192500	-1.115630	-1.326738
P	2.192390	1.116610	-1.325983
P	0.590939	1.717019	0.116695
P	-1.181425	1.141510	-1.114265
P	-1.181166	-1.140810	-1.115200
P	0.629479	-0.000382	1.504630
P	-2.910388	-1.761253	0.119958
P	-3.986448	-0.000391	0.513197
P	-2.910838	1.761067	0.121196
P	2.729544	-0.001077	2.037670

14

Li1P13 E = -120973.3843 eV

Li	-2.654087	-2.743021	0.131785
P	-2.382874	1.775193	0.376605
P	-0.722735	1.373775	-1.061404
P	-3.790543	0.100639	-0.019902
P	-2.383727	0.002125	1.751973
P	-0.776632	-1.290584	0.889701
P	-0.822905	-0.837183	-1.279407
P	-2.946045	-1.151967	-1.653206
P	2.951632	-0.898659	-1.287680
P	0.953981	1.650688	0.381182

P	2.684812	1.288585	-0.960483
P	2.648267	-1.403719	0.859070
P	4.142559	0.146121	0.278363
P	0.975027	-0.206410	1.698830

15

Li1P14 E = -130262.5789 eV

Li	3.043403	1.904574	-2.045979
P	-1.396060	-1.664003	-0.367700
P	-2.142101	1.693210	-0.797915
P	-1.134379	-0.019645	-1.828763
P	-1.127555	-0.742390	1.630361
P	-3.586258	-1.494175	-0.329168
P	-2.150017	1.228879	1.373673
P	-3.914397	0.662335	0.112648
P	2.056805	-1.369097	-1.298933
P	1.011566	0.586955	-1.516724
P	2.108380	-1.717923	0.917576
P	1.008584	-0.027792	1.859192
P	1.344038	1.612756	0.408121
P	3.800304	-0.658042	-0.065397
P	3.512410	1.528018	0.312226

16

Li1P15 E = -139553.0804 eV

Li	-3.340545	2.773997	-0.388472
P	-1.629323	0.990308	1.324498
P	-2.439413	-1.908603	-0.368550
P	-1.333513	-1.204470	1.421346
P	-1.323879	1.406036	-0.822394
P	-3.802153	1.012006	1.223379
P	-2.382921	-0.238865	-1.873236
P	-4.113645	-0.441754	-0.444272
P	1.905313	0.024783	1.820591
P	0.812932	-1.594015	0.824529
P	1.902152	1.797618	0.384469
P	3.364759	-0.955232	-1.196185
P	0.830454	1.143507	-1.416205
P	1.129528	-1.055442	-1.309305
P	3.876515	-0.644223	0.971060
P	3.871302	1.113546	-0.462030

17

Li1P16 E = -148842.5777 eV

Li	-3.604064	1.950319	1.999606
P	-3.231453	-1.589214	-0.934017
P	-1.673067	-0.205730	-1.740182
P	-3.207924	-1.246314	1.284932
P	-1.862392	1.542203	-0.375042
P	-1.707807	0.396247	1.515208
P	-4.010546	1.885081	-0.378644
P	-4.712795	-0.202343	-0.030820

P	0.098920	-0.861310	1.356692
P	4.839855	-0.116213	0.045820
P	3.317405	-1.045916	1.392405
P	1.776189	0.575025	1.611506
P	4.039672	1.906921	-0.399458
P	1.865264	1.589644	-0.352456
P	3.323754	-1.534416	-0.780807
P	0.068401	-1.317538	-0.918485
P	1.797337	-0.166192	-1.696573

18

Li1P17 E = -158132.9895 eV

Li	-3.840975	-2.690660	0.889101
P	3.046323	1.770225	-0.014175
P	1.476995	1.010864	-1.367555
P	-0.257581	0.240927	1.655805
P	3.039158	0.340283	1.752451
P	1.589598	-1.172642	-0.947769
P	1.457882	-1.124390	1.275815
P	3.799365	-1.451631	-1.154298
P	4.700242	-0.842959	0.808259
P	-0.288603	1.661311	-0.189289
P	-2.098343	-1.215356	-1.015610
P	-1.972420	0.961574	-1.464115
P	-4.229406	-1.599107	-1.227250
P	-5.022644	0.095087	-0.013133
P	-2.008764	-1.018040	1.189749
P	-3.576777	0.501721	1.667847
P	-3.596860	1.789545	-0.174421
P	4.710030	0.590722	-0.960132

19

Li1P18 E = -167422.2341 eV

Li	-3.897946	-0.899882	-2.634426
P	0.925373	1.523353	-1.067931
P	3.889156	-1.622870	0.807387
P	2.697757	1.629176	0.261663
P	0.512801	-0.670854	-1.089938
P	4.270930	0.945614	-1.149522
P	5.582866	-0.366744	0.085698
P	-0.622267	2.216064	0.364164
P	-1.691149	-0.556954	-1.489504
P	-2.264431	1.601062	-0.976956
P	-4.625545	-1.919421	-0.522592
P	-3.781444	1.292366	0.601286
P	-2.778485	-0.333109	1.766823
P	-2.527493	-1.833941	0.155448
P	0.522193	-1.049081	1.118649
P	2.474105	-0.132852	1.654032
P	-0.716739	0.590278	1.992846
P	4.166847	-1.271634	-1.373942
P	-5.254886	0.139524	-0.610728

20

Li1P19 E = -176712.5530 eV

Li	-0.578583	-0.003068	3.032158
P	6.123117	0.000291	-0.545122
P	2.850357	1.125522	-1.158082
P	1.300867	1.650272	0.384788
P	4.687997	1.622481	-0.017522
P	1.449677	-0.000408	1.796298
P	5.112867	-0.000549	1.441818
P	-0.339403	1.144332	-1.070532
P	-2.153243	1.717572	0.072258
P	4.688077	-1.622429	-0.018952
P	2.850257	-1.124648	-1.158932
P	1.301117	-1.650468	0.383918
P	-0.339433	-1.144088	-1.070702
P	-5.424563	1.138602	-0.030132
P	-2.443603	0.000212	1.456588
P	-2.153073	-1.717308	0.072418
P	-3.659043	-1.139428	-1.427892
P	-4.652683	0.000102	1.741338
P	-5.424483	-1.138748	-0.030022
P	-3.659093	1.139302	-1.427962

21

Li1P20 E = -186001.8259 eV

Li	4.734724	-2.698644	1.043874
P	1.270214	-0.809998	-1.498994
P	5.122860	-0.532048	2.037014
P	5.992715	0.046371	0.067214
P	2.978771	-1.537301	-0.306070
P	4.601579	-0.651858	-1.561925
P	3.010596	-0.333697	1.552642
P	4.620870	1.498036	-0.902508
P	-0.457680	-1.632461	-0.389942
P	-2.106073	1.443851	-1.137366
P	-2.967859	-0.364919	1.621928
P	-3.446201	1.588801	0.631934
P	-2.102892	-0.826306	-1.643125
P	-5.423098	-0.992189	-0.783990
P	-0.683196	-0.310287	1.417990
P	1.307326	1.430145	-0.928830
P	2.943202	1.658371	0.562564
P	-0.473784	1.658594	0.353670
P	-3.430107	-1.722253	-0.099374
P	-5.431771	1.193095	-0.303418
P	-6.272417	-0.264218	1.101813

2

Li2 E = -408.6662 eV

Li	0.000000	0.000000	1.354990
Li	0.000000	0.000000	-1.354990

3

Li2P1 E = -9698.3389 eV

Li	1.762710	-1.005222	0.000000
Li	-1.762710	-1.005328	0.000000
P	-0.000000	0.402110	0.000000

4

Li2P2 E = -18989.6503 eV

Li	-0.000007	-2.043013	0.000033
Li	0.000090	2.043047	0.000033
P	-1.044678	0.000016	-0.000007
P	1.044662	-0.000022	-0.000007

5

Li2P3 E = -28279.7107 eV

Li	-2.018039	-0.369126	-0.000000
Li	2.018001	-0.369144	-0.000000
P	0.000002	1.267965	0.000000
P	0.000002	-0.560155	1.182290
P	0.000002	-0.560155	-1.182290

6

Li2P4 E = -37570.7206 eV

Li	0.000000	0.000000	1.913340
Li	0.000000	-0.000000	-1.913340
P	-0.000000	1.550110	0.000000
P	-0.000000	-1.550110	0.000000
P	1.550110	-0.000000	0.000000
P	-1.550110	0.000000	0.000000

7

Li2P5 E = -46860.2436 eV

Li	-0.000481	0.092270	1.722477
Li	0.003399	0.092531	-1.722003
P	-1.755256	-0.586576	-0.003893
P	-1.108061	1.523966	0.005267
P	-0.027397	-1.826282	0.000007
P	1.152964	1.490883	-0.005233
P	1.737166	-0.638952	0.003757

8

Li2P6 E = -56150.1183 eV

Li	-0.000008	-1.388337	1.589451
Li	0.000055	1.385962	1.590681
P	1.948583	-0.001020	1.075441
P	1.237515	1.097151	-0.695719
P	1.237252	-1.095809	-0.697819
P	-1.948457	-0.000585	1.075491
P	-1.237358	-1.096186	-0.697319
P	-1.237545	1.096924	-0.696099

9

Li2P7 E = -65439.8769 eV

Li	-0.397922	1.029191	-2.124724
Li	-0.402476	1.030880	2.124276
P	1.463377	-0.540384	-1.111714
P	-1.785516	-0.123202	-0.001074
P	-0.617819	-1.305002	-1.454894
P	1.461951	-0.539122	1.113776
P	-0.619447	-1.303475	1.455376
P	-0.947817	1.944585	-0.001444
P	1.205351	1.454586	0.000066

10

Li2P8 E = -74730.0359 eV

Li	2.969992	0.093193	-0.792718
Li	-0.590288	2.533755	0.951496
P	1.347243	1.787757	-0.213797
P	0.143571	-1.392442	-1.251354
P	-1.948694	0.865712	-0.337009
P	-0.082930	0.882227	-1.613408
P	-1.076965	0.070603	1.639661
P	1.647586	-1.625247	0.276516
P	1.202964	0.221719	1.400709
P	-1.708715	-1.335719	0.066926

11

Li2P9 E = -84019.6474 eV

Li	-1.905268	-2.394140	0.784247
Li	1.783647	1.407074	1.436828
P	-2.428231	-0.802549	-0.965770
P	-0.302546	-1.168479	-1.288346
P	-2.319389	0.802630	0.568686
P	-0.515204	0.336816	1.833901
P	0.372379	-1.439992	0.808259
P	-0.439181	1.920661	0.160090
P	0.530228	0.870945	-1.549279
P	2.521692	-0.927018	0.764381
P	2.604576	0.604399	-0.776138

12

Li2P10 E = -93310.5159 eV

Li	1.227904	-0.001298	-1.108980
Li	-1.228676	-0.001562	1.109496
P	-3.634284	1.065546	0.665338
P	2.174757	1.733077	0.704875
P	1.310899	-0.000400	1.560880
P	2.176979	-1.733283	0.705892
P	3.634130	1.064514	-0.666589
P	-1.309931	-0.001579	-1.559845
P	-2.173601	1.732713	-0.705430
P	-2.177540	-1.733707	-0.704847
P	-3.636754	-1.062644	0.665597

P 3.635501 -1.063666 -0.665974

13

Li2P11 E = -102599.4633 eV

Li -1.560365 0.152414 -1.064440

Li 0.631944 0.495133 1.108316

P 3.485212 1.075986 0.647186

P 1.842063 2.046997 -0.459199

P 0.925096 0.418849 -1.475705

P 2.020154 -1.390266 -0.843527

P 4.115855 -0.722225 -0.512385

P -4.143084 0.799481 -0.777237

P -3.798157 -1.300316 -0.803000

P -1.836256 0.071529 1.598615

P -2.907330 1.663124 0.700629

P -2.348242 -1.757670 0.661192

P 2.830373 -1.034998 1.254656

14

Li2P12 E = -111889.8762 eV

Li -1.838185 -0.001623 -1.046813

Li 0.283903 -0.001370 0.948848

P 1.727326 1.689739 -0.684094

P 0.653371 -0.000772 -1.515270

P -4.278763 1.064386 -0.852550

P -2.964980 1.730788 0.660089

P -4.279591 -1.063704 -0.852398

P 3.844648 -1.149129 -0.519763

P 1.729218 -1.690351 -0.684569

P 3.843436 1.150871 -0.519596

P 2.597458 1.153502 1.359173

P 2.598610 -1.153688 1.359076

P -2.193628 -0.000210 1.609113

P -2.966249 -1.730832 0.660382

15

Li2P13 E = -121179.1809 eV

Li 1.847325 -0.803327 -0.646181

Li 0.242407 2.257684 0.902498

P -1.088522 1.535166 -1.195320

P -3.017797 1.722326 -0.196406

P -2.054554 1.308271 1.733338

P -0.662180 -0.560628 -0.701602

P -4.065465 -0.233254 -0.720930

P -3.279644 -1.747589 0.683852

P -2.508470 -1.625946 -1.464319

P -1.364017 -0.752569 1.419019

P 3.014685 -0.434339 1.773687

P 4.145809 -1.626661 0.446265

P 4.406221 -0.556660 -1.372916

P 2.620295 1.370301 0.747357

P 3.435693 1.310711 -1.203288

16

Li2P14 E = -130469.5955 eV

Li	0.612902	0.548334	-0.000220
Li	-2.901305	0.804818	0.001460
P	-4.534807	-1.010968	-1.064020
P	0.053303	2.626807	-1.733730
P	-1.153709	2.657881	0.000530
P	0.053562	2.625646	1.734430
P	2.053698	2.643187	-1.061260
P	-1.329832	-1.335510	0.000420
P	-2.539441	-1.202554	-1.731150
P	-2.540943	-1.204472	1.731210
P	-4.535708	-1.012257	1.062470
P	2.053898	2.642407	1.061780
P	2.660299	-1.401910	1.113670
P	3.020370	-3.259460	-0.001180
P	4.537662	-1.639237	-0.000600
P	2.659330	-1.400189	-1.112820

17

Li2P15 E = -139759.1207 eV

Li	2.605523	0.227947	-0.971241
Li	0.733486	0.734115	1.937621
P	4.352822	1.290662	0.795696
P	4.555775	-1.629424	-1.012795
P	5.293430	0.358415	-0.847321
P	3.149438	-1.957930	0.527189
P	3.071642	-0.163698	1.644381
P	-0.191066	2.488420	0.389486
P	0.370818	1.312586	-1.333436
P	-1.343812	0.049969	-1.901859
P	-3.035088	1.311348	-1.164777
P	-3.845092	-1.031170	1.493642
P	-1.217004	-1.412764	-0.258732
P	-1.765180	-0.185729	1.564082
P	-2.251729	1.841185	0.838504
P	-4.485952	-0.277969	-0.531871
P	-3.326804	-2.186314	-0.395463

18

Li2P16 E = -149049.2016 eV

Li	3.598491	1.506585	-2.360515
Li	-3.597169	1.509678	2.359857
P	1.700477	0.172440	1.744808
P	4.001540	1.977730	-0.028731
P	4.763708	-0.112668	0.092466
P	3.299187	-1.464999	-0.961533
P	3.312365	-1.303728	1.279184
P	1.758017	0.038827	-1.562856
P	1.862100	1.581622	0.026643
P	-0.032922	-1.190931	-1.172329

P	-1.700509	0.171343	-1.744984
P	-3.299201	-1.464458	0.962382
P	-4.001548	1.977703	0.027617
P	-3.312419	-1.304499	-1.278418
P	-4.763730	-0.112789	-0.092263
P	-1.862129	1.581582	-0.027689
P	0.032889	-1.190196	1.173058
P	-1.758089	0.039767	1.562776

19

Li2P17 E = -158338.5537 eV

Li	-2.019835	2.583828	1.654440
Li	-5.142961	0.658599	-1.199208
P	-1.912898	-0.805619	1.282254
P	-4.302826	-1.780431	-0.933380
P	-5.191624	-0.809120	0.785406
P	-3.276834	1.982817	-0.375359
P	-3.616662	0.614847	1.387162
P	-0.335705	0.767390	1.218597
P	-2.039452	0.715512	-1.753845
P	-2.121007	-1.333262	-0.877535
P	3.056528	1.170017	1.333697
P	1.647287	-1.525161	-0.233377
P	1.567013	0.146491	-1.710394
P	-0.098288	1.432773	-0.948344
P	1.509202	-0.369625	1.665585
P	3.159363	1.448563	-0.917769
P	4.814439	-0.066764	-1.046510
P	3.855401	-1.892938	-0.177037
P	4.718623	-0.343976	1.209804

20

Li2P18 E = -167629.2120 eV

Li	-1.687100	-0.042076	1.367097
Li	-3.638880	0.004840	-0.912103
P	0.710822	2.565830	1.470457
P	-1.355607	0.985626	-0.985623
P	1.932151	1.364008	-1.638073
P	3.770913	0.958101	-0.445443
P	-0.812870	2.954269	-0.132653
P	0.496211	-0.113652	-0.797173
P	3.064938	0.192386	1.582127
P	0.867417	0.341751	1.336447
P	4.471886	-0.903345	-1.430453
P	3.285068	-2.644803	-0.704533
P	3.372813	-2.002062	1.426037
P	5.248444	-2.168209	0.231997
P	1.352108	3.240284	-0.571883
P	-5.368094	0.555859	1.086857
P	-4.088463	-2.483543	0.025167
P	-4.032813	-1.020122	1.555077
P	-5.531778	-1.839942	-1.376183

P -6.317950 0.025012 -0.723153

21

Li2P19 E = -176918.1800 eV

Li -1.292826 -0.318181 1.203048

Li -3.113979 -0.192091 -1.017513

P 1.002023 2.397608 1.574490

P -0.911032 0.924541 -1.067772

P 2.382284 1.444939 -1.554584

P 4.187774 1.017640 -0.319743

P -0.469523 2.845055 -0.059938

P 0.966904 -0.129566 -0.868973

P 3.431744 0.099316 1.624210

P 1.240789 0.193934 1.302961

P 4.986510 -0.752361 -1.394855

P 3.833211 -2.573826 -0.829032

P 3.820598 -2.069215 1.340246

P 5.743459 -2.098352 0.211999

P 1.700275 3.226844 -0.390968

P -3.615459 -1.264645 1.319266

P -5.791198 -1.451112 -1.275492

P -4.037852 -2.458375 -0.391257

P -6.908187 -0.455912 0.377924

P -5.058877 0.404605 1.267042

P -5.622083 0.800937 -0.902632

22

Li2P20 E = -186208.7860 eV

Li 2.249548 -0.117474 1.354685

Li 4.241813 -0.174255 -0.895105

P 5.976910 0.100979 1.151625

P 4.406864 -2.735192 -0.071915

P 4.474244 -1.344429 1.524035

P 5.938719 -2.185557 -1.418465

P -0.383749 3.574632 -0.502605

P 1.725907 3.032989 -0.046505

P -1.143267 1.806819 -1.638065

P -3.040056 1.527220 -0.510545

P 2.071545 1.042824 -0.956025

P 0.105016 0.157153 -0.819825

P -2.438587 0.618420 1.533935

P -0.238871 0.585887 1.324235

P 6.902845 -0.445614 -0.666085

P -3.891099 -0.185384 -1.615965

P -2.947047 -2.053019 -0.827455

P -2.915285 -1.534792 1.348815

P -5.778465 -0.541433 -0.484925

P 0.149320 2.774218 1.526765

P -5.138725 -1.437888 1.462665

P -5.134493 -2.699488 -0.405605

3

Li3 E = -613.0516 eV
 Li 1.674960 -0.734167 0.000000
 Li -1.674960 -0.734120 0.000000
 Li -0.000000 1.468287 0.000000

4
 Li3P1 E = -9904.4428 eV
 Li -0.273031 -1.154626 1.659460
 Li -0.273031 -1.154626 -1.659460
 Li 1.911217 0.713120 0.000000
 P -0.273031 0.319226 -0.000000

5
 Li3P2 E = -19194.9647 eV
 Li 0.000139 -1.339276 -1.480614
 Li -0.000061 -1.338276 1.481486
 Li 0.000137 2.052864 -0.000134
 P 1.137708 0.062455 -0.000044
 P -1.137752 0.062483 -0.000104

6
 Li3P3 E = -28485.6383 eV
 Li 0.264356 -1.267622 -1.322261
 Li 0.264413 -1.267743 1.322739
 Li -2.172720 1.652406 0.000289
 P 0.037636 0.822437 -0.000001
 P 1.909931 -0.063572 -0.000041
 P -1.618777 -0.582273 -0.000111

7
 Li3P4 E = -37775.3617 eV
 Li 0.000241 0.214898 -1.732386
 Li 0.000471 0.215088 1.733614
 Li 0.000391 2.584698 -0.000606
 P -1.625062 0.898322 0.000064
 P 1.625258 0.897975 -0.000026
 P -1.075323 -1.199456 -0.000106
 P 1.074907 -1.199777 -0.000056

8
 Li3P5 E = -47065.7782 eV
 Li 0.134763 -0.201601 -1.993229
 Li 0.698698 0.069948 1.861870
 Li -2.063974 0.015962 1.610270
 P 1.508723 1.107087 -0.156972
 P 1.571484 -1.033203 -0.083371
 P -0.500973 -1.641302 0.313152
 P -0.575715 1.632092 0.283669
 P -1.757417 -0.041535 -0.652260

9
 Li3P6 E = -56355.9566 eV

Li	1.208688	-0.000430	-1.837077
Li	-0.148186	-1.409020	1.755156
Li	-0.150378	1.412260	1.754214
P	-1.077711	-1.142658	-0.745731
P	1.036997	-1.768842	-0.264698
P	-1.996714	-0.000347	0.953192
P	1.897440	0.000555	0.734345
P	1.036211	1.768958	-0.265395
P	-1.078247	1.141772	-0.746171

10

Li3P7 E = -65647.1127 eV

Li	-2.525124	0.392026	-0.208329
Li	0.922516	-2.381035	-0.215078
Li	1.601019	1.990473	-0.213118
P	-0.723041	1.863410	-0.741513
P	-0.002238	0.001021	-1.741581
P	-1.253591	-1.556147	-0.743037
P	-0.830088	-1.035027	1.367152
P	1.313545	-0.204222	1.364812
P	-0.477792	1.236531	1.367907
P	1.973522	-0.305859	-0.746434

11

Li3P8 E = -74935.9828 eV

Li	0.400489	0.009089	-2.429141
Li	-2.020223	-0.006147	2.187014
Li	2.685918	-0.004310	1.386529
P	-1.251204	1.139576	-0.906475
P	2.057089	1.089856	-0.793317
P	2.056523	-1.084732	-0.800727
P	0.362854	1.651240	0.597302
P	0.371897	-0.006677	2.049918
P	-1.251339	-1.133933	-0.913712
P	0.363168	-1.655285	0.586820
P	-2.922224	0.000230	-0.048689

12

Li3P9 E = -84226.4943 eV

Li	-0.850156	-0.000512	-1.036224
Li	4.057614	-0.000922	-1.650390
Li	1.325995	0.001516	1.259671
P	-2.008596	1.731651	0.663152
P	-1.238451	0.001190	1.611208
P	-2.006506	-1.730829	0.664463
P	-3.302620	-1.065024	-0.862378
P	-3.303900	1.063036	-0.863069
P	3.846635	-0.000076	0.815227
P	1.649773	0.000062	-1.307664
P	2.727827	-1.558443	-0.217189
P	2.729147	1.558417	-0.218363

13

Li3P10 E = -93516.0387 eV

Li	-1.256003	0.000150	1.089796
Li	1.120171	0.002286	-1.038926
Li	3.699728	-0.000365	1.547423
P	-1.395939	0.000140	-1.576582
P	-2.248282	-1.733020	-0.707856
P	-3.684015	-1.063804	0.687710
P	-2.249381	1.733120	-0.708547
P	-3.684634	1.063616	0.687325
P	2.117452	-1.795295	0.640372
P	2.122685	1.797185	0.637377
P	3.542608	-1.059661	-0.793563
P	3.546100	1.054439	-0.795463
P	1.220627	0.002866	1.609568

14

Li3P11 E = -102806.3079 eV

Li	-0.566612	0.004083	-0.379943
Li	3.329595	-2.204892	-0.151376
Li	3.335962	2.201667	-0.147374
P	-3.264824	0.001215	-1.193909
P	-4.658819	-1.111258	0.085138
P	-3.022362	0.002095	1.034563
P	-4.663801	1.107852	0.084804
P	1.084159	-1.721000	-0.784771
P	3.330235	-0.003176	1.419370
P	2.130788	0.001532	-1.739470
P	1.089107	1.725258	-0.781583
P	1.331679	-1.143611	1.335532
P	1.334958	1.143188	1.337694
P	4.089092	-0.002267	-0.661630

15

Li3P12 E = -112095.5849 eV

Li	-1.847237	0.017207	-1.031524
Li	0.206726	-0.218517	1.406655
Li	4.413956	-1.141169	0.419055
P	-2.356167	-0.046297	1.581105
P	-4.329385	-0.989360	-1.011617
P	-3.120021	-1.732439	0.552493
P	-4.282133	1.136153	-0.946763
P	-3.039215	1.731540	0.652592
P	2.354334	-1.376797	1.578062
P	2.882473	0.761777	1.543610
P	1.848260	-1.667306	-0.564248
P	3.765794	1.224368	-0.538749
P	0.672217	0.080609	-1.158555
P	1.653544	1.766307	-0.083903
P	3.395610	-0.620059	-1.762865

16

Li3P13 E = -121385.8524 eV

Li	0.466017	1.182597	1.029575
Li	-4.054075	2.227865	-0.095860
Li	2.196241	-0.659848	-0.625802
P	3.651927	1.601934	-0.815451
P	4.663250	-0.106368	-1.536964
P	-1.486865	1.144743	-1.198467
P	-0.286861	-0.623473	-0.705030
P	-1.872863	1.967754	0.850755
P	-3.502579	0.150325	-1.646175
P	-1.604291	-1.575076	0.700402
P	-2.710684	0.157751	1.756072
P	-4.487745	-0.191958	0.404234
P	3.044695	1.162013	1.164813
P	3.615362	-0.816418	1.660229
P	4.642762	-1.590279	-0.014830
P	-3.387744	-1.831070	-0.681169

17

Li3P14 E = -130675.4763 eV

Li	-0.691466	-0.677997	1.229921
Li	-2.623464	0.383800	-0.831246
Li	4.707953	0.627949	1.094674
P	-5.154483	1.172874	-0.387761
P	-4.018825	1.033653	1.387011
P	-3.224242	-0.928508	1.446236
P	-3.794611	-1.984190	-0.299077
P	-5.017078	-0.679309	-1.423537
P	1.841698	-0.954013	1.144288
P	2.240955	1.203097	1.543587
P	1.296011	-0.965830	-1.001888
P	3.106506	0.078188	-1.748491
P	3.064612	1.916658	-0.488042
P	0.933141	2.262580	0.063318
P	-0.156419	0.640377	-0.972320
P	4.709754	-1.083366	-0.727097
P	3.894376	-1.778962	1.165101

18

Li3P15 E = -139965.6328 eV

Li	0.526300	-1.945859	1.895298
Li	4.578296	0.438196	1.783716
Li	0.073965	2.792353	0.674706
P	1.997925	1.303352	0.633949
P	2.596123	-1.313174	-1.443050
P	4.482588	-0.298087	-0.827364
P	2.325726	-0.379629	2.030844
P	3.371353	-1.728002	0.647156
P	3.985396	1.741938	-0.158579
P	1.237819	0.422567	-1.270810
P	-0.752175	-0.602181	-1.192459
P	-2.183103	1.065252	-1.608830

P	-1.462170	-1.088648	0.825098
P	-3.368184	-1.964609	0.059945
P	-2.238648	2.278705	0.210026
P	-4.479741	-0.148217	0.849444
P	-3.995316	-0.281870	-1.300301
P	-2.553303	0.735665	1.674188

19

Li3P16 E = -149254.8417 eV

Li	0.770526	-2.185120	0.885437
Li	0.033429	1.157168	-2.144936
Li	4.577880	-1.512549	-1.572363
P	-4.188875	0.995934	0.683288
P	-3.594081	-1.904535	-1.396358
P	-2.928493	1.441458	-1.109951
P	-0.325790	1.214680	1.114569
P	-3.058748	-0.515427	1.867074
P	-1.215989	-0.781461	0.650774
P	4.835482	0.061508	0.655752
P	4.395150	0.883361	-1.340399
P	3.445699	-1.797645	0.872051
P	2.995706	0.189276	1.916241
P	2.258583	-1.838251	-0.976667
P	1.808787	1.381055	0.486767
P	2.277641	0.332271	-1.420617
P	-1.199950	2.569572	-0.435438
P	-4.644044	-1.189271	0.424600
P	-1.937444	-0.534424	-1.425314

20

Li3P17 E = -158545.2404 eV

Li	-5.107793	-0.703082	2.068164
Li	-2.960230	-2.590108	-1.676040
Li	-1.080451	1.872273	1.600599
P	-3.113760	0.621773	2.037082
P	-4.314966	-2.083015	0.273089
P	-1.849816	-0.525735	-1.028973
P	-3.471060	0.902238	-1.535673
P	-4.347698	1.500497	0.437356
P	-2.409598	-1.213904	1.021838
P	-5.197523	-0.274158	-0.724904
P	4.617376	-1.603532	-0.551731
P	1.725287	-0.520925	1.242935
P	1.413249	-1.054785	-0.904567
P	0.040796	0.573378	-1.526257
P	3.286904	-0.266596	-1.771674
P	2.184705	1.629637	0.994786
P	0.471667	2.321874	-0.167651
P	3.848949	1.495716	-0.462908
P	5.188764	0.170460	0.755558
P	3.756419	-1.388740	1.513149

21

Li3P18 E = -167834.7448 eV

Li	-1.642034	-0.058683	1.347157
Li	-3.565664	0.018324	-0.850880
Li	-6.233510	-1.701086	1.001862
P	1.429731	3.243554	-0.544877
P	-0.738688	2.955455	-0.120853
P	2.009957	1.375962	-1.625409
P	3.842638	0.955311	-0.429531
P	-1.281418	0.999491	-1.001986
P	0.565934	-0.106101	-0.806362
P	3.123837	0.174041	1.587252
P	0.927471	0.327769	1.333739
P	4.543245	-0.899186	-1.427559
P	3.349209	-2.644015	-0.722148
P	3.429517	-2.019228	1.413926
P	5.309758	-2.180570	0.226771
P	0.774801	2.550109	1.487240
P	-6.230430	0.138509	-0.801481
P	-3.944846	-1.003491	1.605348
P	-5.296319	0.686749	1.057836
P	-4.036679	-2.480796	-0.067124
P	-5.489476	-1.725274	-1.464410

22

Li3P19 E = -177124.8747 eV

Li	0.611447	1.184372	-1.961456
Li	2.274991	-0.585989	3.044764
Li	4.306508	2.917590	0.530003
P	5.191771	0.181031	0.705028
P	4.137788	-1.211720	-0.669382
P	3.661734	1.152397	2.018433
P	2.001474	1.289179	0.584737
P	-4.590287	1.533658	1.251505
P	-3.633447	-0.462158	1.631180
P	-1.529117	0.168762	1.480990
P	-5.150760	0.838719	-0.843422
P	-4.184513	-1.160531	-0.465002
P	2.873775	2.153516	-1.231314
P	-2.402907	-0.732361	-1.691757
P	-1.612764	1.017156	-0.585636
P	-0.898301	-2.261199	-1.086471
P	1.991746	-0.867186	-0.131595
P	1.350567	-2.196922	1.477871
P	-0.789160	-1.958405	1.151338
P	0.933704	-1.290177	-1.973728
P	-3.448568	2.279026	-0.521252
P	4.658676	0.824022	-1.424186

23

Li3P20 E = -186414.3680 eV

Li	-2.697792	1.132371	-1.860200
----	-----------	----------	-----------

Li	-5.245412	-2.830800	-0.742734
Li	-1.273680	0.184908	0.929811
P	5.097429	-1.103706	-1.352282
P	1.397181	0.230149	1.255263
P	1.227950	0.181897	-0.948892
P	4.553608	0.668038	-0.131385
P	2.935779	1.535890	-1.395179
P	3.543276	-2.445152	1.168536
P	3.517572	-0.280096	1.662995
P	1.549355	2.404215	1.753528
P	-0.428972	1.561617	-1.072622
P	0.287827	3.278681	0.121295
P	2.508057	3.286215	-0.074448
P	-3.809855	0.427488	1.346765
P	-4.792883	1.454324	-0.349144
P	-6.008846	-0.144172	-1.216172
P	-4.040205	-1.011662	-1.827122
P	-3.148838	-1.441551	0.194154
P	-4.926366	-1.482557	1.651311
P	-6.727298	-1.370188	0.452097
P	3.608417	-2.732751	-1.038990
P	5.500188	-2.713975	0.134916

4

Li4 E = -818.0293 eV

Li	-0.000021	-1.293005	0.000020
Li	2.728468	-0.000171	-0.000020
Li	0.000006	1.293335	0.000020
Li	-2.728452	-0.000159	-0.000020

5

Li4P1 E = -10109.8167 eV

Li	2.339909	-0.015455	-0.237191
Li	-2.036238	-0.063116	-0.930046
Li	-0.453771	1.614116	1.191734
Li	-0.450704	-1.444468	1.392748
P	0.120161	-0.018215	-0.283449

6

Li4P2 E = -19400.7381 eV

Li	0.000000	1.969170	-0.000237
Li	-0.000000	-1.969170	-0.000237
Li	-1.969230	0.000000	0.000023
Li	1.969230	-0.000000	0.000023
P	0.000000	-0.000000	-1.256027
P	-0.000000	0.000000	1.256113

7

Li4P3 E = -28690.9795 eV

Li	-0.126977	-1.274654	1.343743
Li	0.126781	-1.276251	-1.342702
Li	-2.128857	1.520701	0.844205

Li	2.129811	1.520294	-0.843617
P	1.792696	-0.466659	0.219518
P	0.000058	0.835147	-0.000407
P	-1.792906	-0.466507	-0.219437

8

Li4P4 E = -37981.8235 eV

Li	1.964015	0.000585	1.395491
Li	1.964075	-0.000035	-1.395489
Li	-1.325862	-2.234295	-0.000619
Li	-1.326478	2.234045	0.001491
P	1.043296	-1.774591	0.000391
P	1.042864	1.774789	-0.000309
P	-0.140405	-0.000008	-0.000179
P	-2.200905	-0.000250	-0.000079

9

Li4P5 E = -47271.6336 eV

Li	-1.446309	1.368698	1.632485
Li	0.692095	-0.514639	1.903827
Li	0.692561	0.513284	-1.903078
Li	-1.447274	-1.368785	-1.632457
P	0.562599	1.721116	0.198115
P	-1.395542	0.935415	-0.633666
P	0.561387	-1.721324	-0.198273
P	1.969693	-0.000649	0.000039
P	-1.396352	-0.934270	0.633630

10

Li4P6 E = -56562.1435 eV

Li	-0.429956	0.000431	-2.105385
Li	0.187032	1.405470	1.740004
Li	-2.849034	0.001285	-0.939874
Li	0.187276	-1.405220	1.740717
P	1.146425	1.167618	-0.718893
P	-1.041082	1.673061	-0.315649
P	2.071759	-0.000066	0.932077
P	-1.041042	-1.673039	-0.316307
P	-1.701411	-0.000456	1.050625
P	1.146288	-1.167512	-0.718945

11

Li4P7 E = -65852.0944 eV

Li	-2.306190	-0.487064	1.246338
Li	2.305930	-0.484966	1.247157
Li	-0.000924	2.987124	-0.808898
Li	0.000430	0.360711	-2.191881
P	1.727106	-0.888609	-1.091438
P	1.680042	1.250654	-0.408145
P	-1.726214	-0.889439	-1.091805
P	0.000549	-1.771762	0.016611
P	-0.000528	1.303056	1.103076

P -1.680768 1.249803 -0.408390
P -0.000035 -0.728865 1.981548

12

Li4P8 E = -75142.4226 eV

Li 0.000000 3.189710 -0.711178
Li -0.000000 -3.189710 -0.711178
Li -3.189650 0.000000 0.710042
Li 3.189650 -0.000000 0.710042
P 1.641100 -1.641250 0.000012
P -1.641100 1.641250 0.000012
P -1.641100 -1.641250 0.000012
P 1.641100 1.641250 0.000012
P 0.000000 1.184170 1.443062
P -0.000000 -1.184170 1.443062
P 1.184270 -0.000000 -1.442858
P -1.184270 0.000000 -1.442858

13

Li4P9 E = -84431.9908 eV

Li -1.361727 -0.004955 1.248268
Li -4.138140 0.003753 -1.625159
Li 3.603268 0.001333 1.331319
Li 0.755531 -0.004976 -0.962818
P -2.791501 1.558334 -0.212969
P -1.730530 -0.003802 -1.316359
P -3.899525 0.003847 0.835331
P -2.801813 -1.558476 -0.212276
P 1.143154 -0.001826 1.657706
P 1.949144 -1.795550 0.601473
P 1.943193 1.794350 0.601993
P 3.210184 -1.054804 -0.976982
P 3.205908 1.058896 -0.976239

14

Li4P10 E = -93722.0469 eV

Li 0.151780 3.242758 0.323137
Li -3.340052 0.453961 -1.302393
Li -1.235480 -2.845095 1.410830
Li 3.402809 -0.073436 1.246652
P -0.811597 -1.512417 -1.071517
P -2.559707 -1.178498 0.260904
P -1.810296 0.715383 1.187991
P -0.196406 0.549132 -1.888426
P -1.526538 1.882648 -0.692250
P 1.683974 1.569186 1.058798
P 1.921827 0.778739 -1.020252
P 2.528388 -1.315876 -0.612299
P 0.252001 0.084322 1.905454
P 0.722542 -1.728256 0.535952

15

Li4P11 E = -103011.9317 eV

Li	0.723887	-1.445973	0.853272
Li	-1.630312	-0.000036	-1.223692
Li	0.723538	1.445457	0.858863
Li	3.366028	0.001765	-2.103538
P	2.023714	-1.785539	-1.224334
P	-3.378302	1.726082	-0.064466
P	-1.882230	1.054342	1.263043
P	-3.383369	-1.724128	-0.067804
P	-4.323115	0.003060	-0.863946
P	-1.885418	-1.059868	1.261516
P	3.466957	-1.140976	0.385122
P	2.023042	1.787301	-1.220205
P	3.467595	1.139884	0.386867
P	0.804334	0.001256	-1.523582
P	2.430163	-0.001657	1.990806

16

Li4P12 E = -112302.8607 eV

Li	1.890671	0.028610	-0.946253
Li	-4.462981	-1.172003	0.878449
Li	-0.008217	-0.278122	1.357197
Li	-2.405047	0.769512	-2.567717
P	3.202429	1.691478	0.696546
P	4.359578	-0.988751	-1.120866
P	4.330467	1.134560	-0.998840
P	3.254441	-1.762755	0.503944
P	2.572783	-0.103175	1.630728
P	-1.594663	1.753974	-0.091236
P	-3.819094	1.225617	-0.283894
P	-0.595582	0.094076	-1.150138
P	-2.167376	-1.392774	1.513352
P	-2.671088	0.754022	1.649599
P	-1.978741	-1.586728	-0.693773
P	-3.896040	-0.689145	-1.399756

17

Li4P13 E = -121591.8105 eV

Li	-4.979377	1.075094	0.697680
Li	-2.783833	-1.429039	-2.262667
Li	1.390801	0.257660	-1.021738
Li	-0.407112	0.911141	1.135536
P	-4.414252	0.102919	-1.419387
P	-2.715597	1.708686	1.132008
P	-2.606859	1.362295	-1.060426
P	-1.039096	-0.211471	-1.161708
P	2.987232	2.072012	-0.278046
P	4.349521	0.603932	-1.202377
P	2.135233	0.989788	1.344386
P	-4.075799	-1.446399	0.130590
P	-2.943628	-0.377196	1.821236
P	-1.797635	-1.651962	0.329205

P	3.458444	-1.489109	-0.965348
P	5.037116	-0.781356	0.404836
P	2.981223	-1.045109	1.215269

18

Li4P14 E = -130882.2289 eV

Li	5.200619	-1.143635	0.969956
Li	0.726746	-0.267406	1.349028
Li	3.208298	0.722843	-2.560063
Li	-1.070309	-0.023331	-0.722677
P	2.340345	1.745962	-0.110805
P	4.570846	1.228269	-0.246466
P	2.894403	-1.367984	1.559745
P	3.383806	0.782547	1.670218
P	2.753563	-1.599758	-0.646409
P	4.680702	-0.704006	-1.327821
P	1.374107	0.065998	-1.170176
P	-1.813063	-0.142200	1.653476
P	-2.705884	1.626964	0.772575
P	-3.349181	-1.062978	-1.537575
P	-4.861486	-1.111573	0.133025
P	-2.809265	-1.738552	0.575143
P	-4.791671	1.181806	0.269298
P	-3.280292	1.237811	-1.401479

19

Li4P15 E = -140171.5194 eV

Li	0.067734	-1.323049	-0.581499
Li	4.870169	-1.165675	1.866550
Li	4.718875	0.902680	-2.159541
Li	1.107891	1.449645	0.809273
P	-4.512577	0.062370	1.541559
P	-5.320735	-0.351754	-0.476665
P	-3.424858	-0.772689	-1.673418
P	-2.399075	-0.781562	1.560050
P	-2.368505	-2.045094	-0.234191
P	-2.624888	1.262932	-1.153231
P	-1.289129	0.761218	0.501233
P	2.277974	-0.272111	-1.422489
P	2.943006	0.255325	2.042244
P	4.057319	-1.575771	-0.858602
P	4.240817	1.429538	0.672037
P	5.591871	-0.139545	-0.181087
P	2.356143	-1.324920	0.636144
P	2.824560	1.811440	-0.998022
P	-4.504856	1.707902	0.057483

20

Li4P16 E = -149462.0816 eV

Li	-2.263916	-1.230681	-0.374589
Li	1.051902	4.563663	-0.657632
Li	-2.286030	1.661828	0.355748

Li	2.178889	0.182864	-0.434625
P	-3.767502	-1.547771	1.826001
P	-4.298213	-2.649421	-1.387238
P	-3.750316	-3.250210	0.577952
P	-4.665278	-0.569878	-1.367421
P	-4.361316	0.091714	0.622159
P	0.294306	1.097827	1.569799
P	1.920326	2.600853	1.026141
P	-0.254485	0.236361	-0.385389
P	-1.115129	3.554664	-0.627857
P	-0.238643	3.311864	1.385656
P	0.035245	1.991041	-1.715870
P	2.136850	2.495197	-1.175083
P	5.894974	-1.841232	-0.180019
P	3.956493	-1.840604	-1.206920
P	4.100067	-1.324417	0.972463
P	4.376455	-3.391524	0.287848

21

Li4P17 E = -158751.4667 eV [Geometry 4]

Li	6.022967	-1.577388	1.256719
Li	4.636022	0.158470	-2.609597
Li	0.227554	0.597052	-1.248586
Li	1.803461	0.247248	1.215750
P	3.702786	-1.208979	1.708330
P	5.702052	-1.368540	-1.110906
P	2.644164	0.103080	-1.275338
P	3.913865	1.677285	-0.391411
P	4.649336	0.780982	1.564453
P	3.600878	-1.726975	-0.450076
P	5.980347	0.678175	-0.304720
P	-5.799275	-0.144067	-0.748839
P	-2.316236	-0.572627	-1.154473
P	-2.996444	1.532735	-1.185788
P	-1.260381	2.433145	-0.156751
P	-4.591958	1.402992	0.350316
P	-1.919163	-0.841094	1.008581
P	-0.638065	0.935407	1.277377
P	-3.880664	-0.177249	1.802328
P	-5.080006	-1.738525	0.715883
P	-4.249234	-1.650821	-1.371824

22

Li4P18 E = -168041.4003 eV

Li	-2.307488	3.051581	-0.911898
Li	-4.320415	-3.115658	-0.856968
Li	0.256424	-1.890633	-0.026829
Li	2.321630	4.180491	-1.080610
P	0.408394	3.940259	0.918861
P	0.845890	1.757546	-1.650497
P	0.328320	1.868973	1.802236
P	2.827162	-2.538563	0.058502

P	2.325036	2.690371	1.226348
P	4.501763	-1.730808	-1.090088
P	2.847427	1.861987	-0.749555
P	-0.010395	0.577183	0.029842
P	-0.028801	3.759877	-1.238387
P	-4.812746	-1.100829	0.928959
P	-2.729167	-0.882657	-1.700029
P	-2.895826	-2.307563	1.378983
P	-1.984270	-2.660913	-0.597179
P	-4.878953	-0.813978	-1.254925
P	-2.978386	-0.079272	1.698729
P	-2.234380	0.713405	-0.234254
P	4.598854	-1.807099	1.107980
P	4.680047	-3.693075	-0.060266

23

Li4P19 E = -177330.9080 eV

Li	-1.243902	2.701758	-0.128978
Li	-1.620017	-0.472861	0.316536
Li	-5.564033	1.758658	-0.920593
Li	-5.794272	-2.152977	1.196631
P	1.064386	3.220409	0.816066
P	1.667925	1.312880	1.745598
P	3.834820	1.135038	1.228547
P	0.899412	-0.102178	0.189262
P	3.842460	1.171787	-1.042460
P	1.720930	0.813121	-1.645845
P	3.890419	-1.002291	1.806045
P	3.466736	-2.500640	-1.015362
P	4.759334	-0.793157	-1.584891
P	5.280320	-1.890299	0.254303
P	1.003881	2.875127	-1.309900
P	-4.370603	0.417092	1.550256
P	-3.320197	1.405655	-0.140673
P	-3.474997	-1.612589	1.445189
P	-3.804464	-2.050359	-0.693791
P	-6.367315	0.101771	0.605700
P	-3.654824	-0.047230	-1.767695
P	-5.720516	-0.917514	-1.253794
P	2.126737	-1.903539	0.720725

24

Li4P20 E = -186621.5880 eV

Li	2.783382	0.875181	-1.654845
Li	5.217706	-3.030949	-0.656854
Li	1.194342	0.147395	0.956094
Li	6.510902	0.868914	1.231127
P	6.615881	-1.364544	0.358220
P	4.853015	-1.424081	1.686783
P	3.076983	-1.485435	0.258042
P	3.873146	-1.395369	-1.785360
P	5.719214	-0.235160	-1.356043

P	4.846273	1.548232	-0.358276
P	3.738395	0.508655	1.225755
P	-2.464483	3.291639	-0.174602
P	-0.245453	3.219025	0.024527
P	0.423286	1.454344	-1.128989
P	-1.536501	2.441898	1.684541
P	-3.584125	-0.188644	1.674502
P	-3.668288	-2.366461	1.247217
P	-2.940336	1.511029	-1.436982
P	-4.586641	0.732026	-0.153013
P	-1.270519	0.125854	-0.944480
P	-1.450723	0.251000	1.256878
P	-5.177082	-1.061774	-1.318747
P	-3.734508	-2.720536	-0.950317
P	-5.628800	-2.613806	0.215240

5

Li5 E = -1022.7260 eV

Li	0.008132	-1.678611	0.000000
Li	1.289274	1.076352	-0.000000
Li	-1.313670	0.610816	0.000000
Li	0.008132	-0.004279	2.566060
Li	0.008132	-0.004279	-2.566060

6

Li5P1 E = -10315.0645 eV

Li	-0.000000	2.292940	0.177056
Li	2.292940	-0.000000	0.177056
Li	0.000000	-2.292940	0.177056
Li	-2.292940	0.000000	0.177056
Li	0.000000	0.000000	-2.041054
P	0.000000	0.000000	0.266566

7

Li5P2 E = -19605.8145 eV

Li	-0.293825	1.441996	-1.323560
Li	0.727292	-1.335143	-1.459720
Li	-0.294480	1.441562	1.323960
Li	0.727104	-1.334372	1.460100
Li	-2.766053	0.866992	-0.000530
P	1.318683	0.369710	-0.000070
P	-0.938690	-0.585917	0.000020

8

Li5P3 E = -28896.4892 eV

Li	-1.623253	1.752957	-0.841240
Li	-1.622211	-1.752853	-0.841706
Li	-0.000111	-0.002638	1.843430
Li	1.624409	-1.750229	-0.845207
Li	1.622087	1.753839	-0.839342
P	-1.946524	-0.000316	0.527980
P	-0.000116	0.000396	-0.751499

P 1.946456 -0.000295 0.528332

9

Li5P4 E = -38187.1324 eV

Li 1.922891 1.100819 -1.175299

Li 1.547248 0.776990 1.498808

Li 0.000138 -2.495745 0.475499

Li -1.922109 1.099507 -1.177260

Li -1.548712 0.777334 1.497702

P 0.000053 -0.132952 -0.394340

P 1.895629 -1.074474 0.017471

P -0.000072 2.030127 0.135265

P -1.895501 -1.074483 0.017713

10

Li5P5 E = -47477.5853 eV

Li 0.369213 2.014934 1.580735

Li -2.863118 0.004750 0.000905

Li 0.363476 -2.015909 1.580825

Li 0.363066 -2.015199 -1.581535

Li 0.369862 2.015454 -1.580205

P -0.244946 0.000095 -0.000245

P 1.643265 -0.002489 1.163135

P -1.384161 -1.863203 -0.000185

P -1.378323 1.867060 -0.000115

P 1.643665 -0.002269 -1.162735

11

Li5P6 E = -56767.8612 eV

Li 2.050819 0.000543 -1.444592

Li -0.032537 0.000452 2.297487

Li -1.047475 -2.105629 0.844049

Li -3.441778 -0.001146 -0.827453

Li -1.048225 2.106131 0.843500

P 1.612948 -1.108502 0.752507

P 1.611886 1.109738 0.752022

P 0.359518 -1.707004 -0.994050

P -2.159509 -0.000115 1.080735

P -1.079221 -0.000693 -0.938879

P 0.358217 1.706506 -0.994933

12

Li5P7 E = -66058.1462 eV

Li 2.828559 -0.606733 0.000733

Li -1.020866 0.406191 -1.873067

Li -1.021528 0.407326 1.872413

Li -4.219438 0.040625 0.001563

Li -0.293847 2.512061 -0.000647

P 1.049313 -0.848274 1.726783

P 1.537305 1.196675 1.079073

P -0.050767 -1.718410 0.001193

P 1.536725 1.195309 -1.080557

P 1.049446 -0.850665 -1.725807
P -2.302057 1.351044 -0.000757
P -2.074541 -0.877572 -0.000127

13

Li5P8 E = -75347.8545 eV

Li -0.000202 1.139698 1.745194
Li 0.000278 -1.747792 1.503993
Li 3.313836 -0.012322 -0.782737
Li -3.313684 -0.013938 -0.782885
Li -0.000547 3.333701 -0.003565
P 1.806898 -1.746203 -0.107862
P 1.755865 1.652146 -0.058981
P 2.051297 -0.095350 1.338469
P -2.051333 -0.095898 1.338429
P -1.756715 1.651641 -0.059100
P -0.000281 1.060009 -1.345214
P 0.000245 -1.219375 -1.334061
P -1.805912 -1.746838 -0.107681

14

Li5P9 E = -84638.1837 eV

Li 3.111270 -0.000127 -1.165534
Li -0.558053 -2.961960 -0.459424
Li -3.477283 0.000399 1.418901
Li -0.557262 2.962120 -0.458774
Li -3.373968 -0.000206 -1.417453
P 1.925758 1.148921 1.082529
P 1.925895 -1.148529 1.083168
P 1.481413 1.731199 -1.042726
P 0.252540 -0.000548 -1.650430
P 1.481601 -1.731581 -1.042127
P -2.513445 1.751792 0.057796
P 0.183848 0.000252 1.825422
P -2.513857 -1.751578 0.058366
P -1.252692 0.000025 0.044460

15

Li5P10 E = -93927.9804 eV

Li -0.004007 -2.717542 0.038812
Li 3.710277 -0.017492 -0.075408
Li 0.000715 0.129241 0.525994
Li -3.710443 -0.011472 -0.071933
Li 0.003004 3.070021 -0.041479
P 2.012524 -1.622881 -0.836798
P -2.017186 -1.618728 -0.839954
P 2.030763 -1.245626 1.351334
P -1.192454 0.213158 -1.785902
P 1.191056 0.208721 -1.786736
P 2.011487 1.741128 -0.410631
P -2.031277 -1.246341 1.349087
P -2.090609 0.867349 1.646657

P -2.008343 1.744194 -0.405465
P 2.094131 0.868475 1.643212

16

Li5P11 E = -103218.8105 eV

Li -2.375926 0.810884 -2.489958
Li -4.150589 -1.191492 1.054559
Li 2.043058 0.091465 -1.120901
Li 0.366450 -0.353322 1.209077
Li 5.306411 -0.095024 1.166920
P -2.327289 0.725426 1.720548
P -3.627996 1.212263 -0.114616
P -1.397924 1.759647 -0.075042
P -1.817814 -1.413030 1.512482
P -3.767655 -0.685927 -1.252879
P -1.791374 -1.570395 -0.705313
P -0.460009 0.130719 -1.231428
P 3.692617 1.545086 0.207478
P 2.885091 -0.163576 1.310958
P 4.611879 0.156100 -1.195542
P 3.762592 -1.548816 -0.140584

17

Li5P12 E = -112508.3582 eV

Li 4.542534 -1.145441 0.880936
Li 2.468379 0.754500 -2.557406
Li -1.813649 0.031052 -0.861422
Li -4.900826 -0.050569 1.083850
Li 0.040351 -0.353648 1.374232
P 2.256894 -1.375521 1.530730
P 3.899486 1.224261 -0.301193
P 3.969957 -0.700516 -1.400471
P 2.055470 -1.591206 -0.672965
P 0.667529 0.083875 -1.132883
P 1.673354 1.752016 -0.095612
P -4.215716 1.187412 -1.062597
P -4.281524 -0.914599 -1.257438
P -3.240542 -1.840020 0.384590
P -3.126689 1.732503 0.711602
P -2.481493 -0.178071 1.668797
P 2.755917 0.772687 1.643401

18

Li5P13 E = -121798.2188 eV

Li -1.301206 0.453909 -1.060045
Li 2.905320 -1.140164 -2.396151
Li 5.009288 0.924990 0.925110
Li 0.400434 0.865444 1.146996
Li -4.419382 1.537679 1.288138
P -3.284058 -1.599936 -0.886665
P -3.026645 2.039215 -0.547538
P -4.252316 0.410778 -1.306872

P	4.527227	0.244309	-1.318385
P	2.720986	1.481452	-0.876703
P	1.134777	-0.037715	-1.227868
P	1.817612	-1.660429	0.101398
P	2.916047	-0.602880	1.780596
P	4.105851	-1.477215	0.014452
P	2.745556	1.554717	1.344645
P	-2.858849	-0.997845	1.238372
P	-2.106146	1.056871	1.303605
P	-4.958933	-0.939694	0.400154

19

Li5P14 E = -131087.9258 eV

Li	3.899101	0.489885	-2.346057
Li	0.949306	-0.135624	1.003885
Li	-0.771285	0.642487	-1.099214
Li	-5.273823	1.358816	-0.775285
Li	-3.427016	-1.366555	2.236354
P	3.166138	0.649983	1.927447
P	3.342662	-1.467970	1.224544
P	1.751869	0.527581	-1.327614
P	2.570758	-1.479226	-0.925553
P	4.783459	-1.144290	-0.436645
P	2.991762	1.767221	0.043520
P	-2.414688	-1.694214	-0.350231
P	-4.868250	0.322230	1.345578
P	-1.539476	-0.353266	1.170485
P	-4.659160	-1.247175	-0.206371
P	-3.383327	-0.294503	-1.863753
P	-2.946382	1.750628	-1.153908
P	-2.927567	1.381203	1.038685
P	5.056946	1.083996	-0.290122

20

Li5P15 E = -140378.1945 eV

Li	-5.414542	1.597247	-0.312555
Li	-3.777208	-2.191034	1.320907
Li	-0.831553	1.077301	-0.555550
Li	3.231241	2.974292	0.771394
Li	0.596258	-0.922632	1.530254
P	-5.163028	-0.248452	1.195943
P	-2.570353	-1.407449	-1.032730
P	-3.211523	0.789601	1.508718
P	-1.818356	-0.851803	0.964440
P	-3.432092	0.523649	-1.857526
P	-4.828999	-1.008007	-0.860872
P	-3.068219	2.057436	-0.310499
P	4.879840	0.505990	-0.378857
P	3.505848	1.857719	-1.366630
P	1.689069	0.975174	-0.497835
P	3.934744	-0.041054	1.671410
P	3.185622	-1.989457	0.817237

P	2.061187	1.070609	1.707291
P	1.950994	-1.260033	-0.924135
P	4.124427	-1.480958	-1.186843

21

Li5P16 E = -149667.8426 eV

Li	-4.400884	-1.870014	1.662352
Li	-0.954402	-0.398487	-1.036545
Li	-4.616789	2.282109	-0.178368
Li	0.142959	2.428659	-0.604969
Li	0.421661	-2.003023	1.193368
P	-4.924136	0.452922	1.348471
P	-3.261569	-1.759026	-0.935792
P	-2.708890	0.611952	1.457080
P	-2.135765	-1.474912	0.947712
P	-3.372587	0.344038	-1.884721
P	-5.120008	-0.463586	-0.663192
P	-2.307449	1.663885	-0.462068
P	1.862276	2.396541	1.197258
P	4.041379	-2.141680	0.215177
P	2.037511	-2.473029	-0.707690
P	3.895140	-0.400702	1.618054
P	2.692564	2.727383	-0.784137
P	3.147129	0.746590	-1.680645
P	4.782079	-0.114540	-0.418844
P	1.479403	-0.404319	-0.788757
P	1.774415	0.200634	1.334926

22

Li5P17 E = -158958.4566 eV

Li	-0.284888	2.327599	0.024485
Li	3.211704	-0.353970	-0.044052
Li	-0.806721	-2.319580	0.317917
Li	-4.104083	0.538194	2.093072
Li	-4.966528	-1.658925	-1.712122
P	1.713551	2.984370	1.720668
P	3.031480	-2.313713	1.776924
P	1.727059	-2.546661	0.132750
P	0.567910	4.637097	1.071998
P	1.632031	2.991915	-1.758670
P	2.363554	2.014533	-0.037195
P	2.787725	-2.433174	-1.689135
P	4.965097	-2.079671	0.954277
P	0.517392	4.642103	-1.050744
P	4.815994	-2.148361	-1.162909
P	-2.013723	0.550826	0.208905
P	-5.344830	-0.605501	0.404941
P	-4.068151	0.777320	-0.750608
P	-2.437676	-0.553144	-1.712663
P	-3.795252	-2.135204	0.940489
P	-2.879414	-2.600351	-1.035821
P	-2.192644	-0.889047	1.850930

23

Li5P18 E = -168247.3663 eV

Li	0.260519	-2.314698	0.765688
Li	-0.080433	1.031925	-1.560699
Li	-1.686058	1.130304	1.307609
Li	-3.411294	-2.580288	-1.151379
Li	-6.225508	0.532858	0.452786
P	4.969255	-0.673289	-0.262905
P	3.998593	-2.674492	0.060107
P	3.488330	0.446788	-1.504694
P	3.246656	2.364368	-0.383994
P	2.047345	-2.712603	-1.018204
P	1.648235	-0.604730	-0.891784
P	2.181866	1.820949	1.583803
P	1.859964	-0.337815	1.306810
P	0.295648	2.605543	0.694220
P	1.272662	3.116090	-1.171303
P	3.903031	-1.122904	1.671748
P	-4.194390	1.020309	1.641590
P	-3.851457	1.573669	-0.459667
P	-4.060720	-1.189894	1.474840
P	-4.647506	-0.179450	-1.716518
P	-5.421378	-1.633927	-0.245104
P	-2.412345	-0.021409	-1.223953
P	-2.095235	-1.357224	0.482208

24

Li5P19 E = -177537.9378 eV

Li	2.411063	0.333511	0.590399
Li	-3.234515	-1.171281	-0.682561
Li	0.800338	0.865037	-1.919650
Li	-3.273658	1.354804	0.936984
Li	-0.398906	4.936733	0.083291
P	-0.174632	0.748471	0.961413
P	4.835955	-2.921690	0.057668
P	5.015905	0.095128	1.182645
P	2.790187	-2.266634	-0.375204
P	3.718383	-1.759875	1.635455
P	4.691053	0.448708	-1.037539
P	6.129247	-1.073786	-0.392874
P	-5.854306	-0.615207	-0.789783
P	-5.376292	-2.531012	-1.538875
P	-4.023707	-2.303888	1.615066
P	-4.254909	-3.569285	-0.059228
P	2.883567	-0.550691	-1.696358
P	-2.283413	3.575510	0.688352
P	-0.651595	2.739104	1.912271
P	1.112208	2.609819	0.471026
P	0.406949	3.303993	-1.493182
P	-1.729505	2.726600	-1.297061
P	-1.450656	0.584008	-0.810393

P -5.045302 -0.503033 1.164909

25

Li5P20 E = -186827.2013 eV

Li -0.307187 1.886469 -0.633023
Li -3.322851 0.620033 1.440853
Li -0.379975 -2.730544 -0.389461
Li -4.886527 -3.107138 -0.843455
Li 0.793239 -0.988813 2.316585
P 3.897196 -1.736881 -1.840926
P 2.802401 -2.411256 1.391749
P 4.316079 -0.855682 1.642540
P 5.256987 -0.698819 -0.430067
P 2.744135 0.672022 1.636533
P -1.468743 -1.115699 1.320124
P -1.731849 -0.381284 -0.726288
P -2.612972 -3.805026 -0.448140
P -2.546307 -2.161228 -1.913309
P -4.763152 -1.356046 0.799132
P 1.993206 0.413478 -0.405805
P 3.890370 0.537436 -1.655983
P -2.450380 3.667221 -1.039491
P 0.666318 4.303696 0.272318
P -2.366431 2.970858 0.951370
P -0.452788 3.324745 1.770055
P -0.555266 4.502206 -1.451625
P -3.962294 -0.536305 -1.085249
P -3.054962 -2.645711 1.403093
P 2.019114 -1.823727 -0.568333

6

Li6 E = -1227.8337 eV

Li -0.000000 2.504020 0.000000
Li 2.504020 -0.000000 0.000000
Li 0.000000 -2.504020 0.000000
Li -2.504020 0.000000 0.000000
Li 0.000000 0.000000 1.269630
Li 0.000000 -0.000000 -1.269630

7

Li6P1 E = -10519.9773 eV

Li -1.290032 -1.353391 -0.732255
Li -1.289307 1.350689 -0.737370
Li 2.229132 -1.363904 0.465179
Li 2.225567 1.367936 0.462455
Li -3.852446 0.000991 0.499388
Li -0.711103 0.002810 1.650093
P 0.537638 -0.001026 -0.321498

8

Li6P2 E = -19811.3188 eV

Li 3.136750 1.633540 0.178481

Li	-0.354914	-1.280610	-0.720541
Li	-0.054990	-0.002186	1.520468
Li	-0.355290	1.282269	-0.716194
Li	-3.848903	0.003919	-0.903951
Li	3.136903	-1.633240	0.175613
P	1.706372	0.000417	-0.217186
P	-2.038284	-0.001156	0.310411

9

Li6P3 E = -29102.2924 eV

Li	4.434090	-0.002051	0.001963
Li	0.954480	-1.983008	-0.000427
Li	0.245610	-0.000087	-1.403237
Li	0.953791	1.983632	-0.000997
Li	0.245620	0.000413	1.403443
Li	-3.460250	-0.000401	0.002963
P	2.232430	0.000673	-0.000117
P	-1.453713	1.115969	-0.000267
P	-1.453386	-1.116341	-0.000357

10

Li6P4 E = -38393.0855 eV

Li	-2.175863	1.404033	-0.375593
Li	-1.746031	-1.022979	1.907167
Li	2.177896	1.400687	-0.375574
Li	1.744718	-1.026468	1.906970
Li	-0.001208	-2.386303	-0.735916
Li	-0.001340	0.265672	-1.756072
P	0.001501	2.137660	0.004297
P	-1.820384	-0.947174	-0.371829
P	1.818806	-0.949035	-0.372271
P	0.000442	0.031620	0.625607

11

Li6P5 E = -47683.2612 eV

Li	-0.361036	-0.001400	-1.290030
Li	-0.146849	-2.074136	0.280636
Li	3.634405	-0.000063	0.377270
Li	-0.148896	2.074884	0.279034
Li	-1.056647	0.000883	1.705373
Li	-4.189711	-0.000465	-0.789574
P	1.456182	-0.000747	1.272854
P	1.838864	-1.117931	-0.687936
P	1.838682	1.119079	-0.687439
P	-2.339539	-1.112476	-0.005493
P	-2.340443	1.112134	-0.004528

12

Li6P6 E = -56974.0362 eV

Li	0.000843	0.003044	-1.567863
Li	0.761656	1.984218	0.002450
Li	-3.971086	0.827082	0.002044

Li	-0.761471	-1.981313	-0.002747
Li	0.000077	-0.001551	1.568055
Li	3.971761	-0.827119	-0.001412
P	1.661567	-1.299311	-0.002261
P	2.390024	0.527681	-1.135088
P	-2.390340	-0.524835	-1.136699
P	-2.389738	-0.527266	1.135640
P	-1.661502	1.299117	0.001112
P	2.389633	0.523742	1.137190

13

Li6P7 E = -66263.6347 eV

Li	0.666748	1.836278	1.600546
Li	1.557871	-2.014171	0.035405
Li	-1.697649	-1.837048	1.854685
Li	-3.203592	1.418230	-0.025304
Li	-1.696928	-1.903110	-1.787832
Li	0.666978	1.778478	-1.663691
P	0.371258	-0.642911	1.724298
P	2.366494	0.032556	1.125044
P	-2.831018	-0.925308	0.016098
P	-1.007405	2.276347	-0.039926
P	-0.895518	0.114209	-0.002102
P	0.371087	-0.703498	-1.700477
P	2.366416	-0.007126	-1.125696

14

Li6P8 E = -75553.9550 eV

Li	0.886709	-1.381351	-1.485561
Li	0.923888	-2.397953	1.213817
Li	-3.103140	-0.728032	0.475333
Li	1.574767	0.138806	1.672522
Li	-0.007401	1.530508	-1.692527
Li	4.405349	-0.019947	-0.744442
P	-1.002654	-0.739133	1.802632
P	-1.116613	-2.027540	-0.032852
P	2.701782	-1.339323	0.084647
P	-1.591143	-0.692733	-1.652337
P	2.158947	0.651073	-0.818846
P	1.059810	2.135049	0.430562
P	-2.207841	1.197283	-0.760311
P	-0.938323	1.386917	1.058676

15

Li6P9 E = -84843.7692 eV

Li	0.233454	-0.590969	2.132914
Li	1.203631	-2.327015	-0.350814
Li	1.325197	-0.023364	-1.993135
Li	-3.166786	-1.298574	-0.700089
Li	3.087115	1.394357	-0.449975
Li	-0.933821	2.127791	1.207254
P	-1.123315	-2.019799	0.520770

P	2.461408	-0.563701	1.121583
P	-0.883231	-1.293824	-1.576452
P	-1.112701	0.936558	-1.445240
P	3.218942	-1.021291	-0.781340
P	0.642410	2.117937	-0.691779
P	1.436323	1.425957	1.312972
P	-2.235762	-0.479448	1.533960
P	-2.753833	1.041166	0.036295

16

Li6P10 E = -94134.4098 eV

Li	3.629160	0.000374	-0.043097
Li	-0.000290	0.039776	2.729385
Li	-3.630120	-0.000113	-0.044180
Li	-0.000319	2.689523	0.351732
Li	0.000199	0.006615	0.255978
Li	0.000426	-2.675387	0.429884
P	1.933931	1.118687	1.442503
P	1.933467	-1.075100	1.474819
P	1.980557	-1.717316	-0.676914
P	-1.980213	-1.717672	-0.676136
P	-1.182894	-0.029402	-1.880449
P	1.182976	-0.028576	-1.880506
P	-1.978182	1.696096	-0.728578
P	-1.934049	1.119102	1.441907
P	-1.933563	-1.074538	1.475292
P	1.978158	1.696561	-0.727877

17

Li6P11 E = -103424.0135 eV

Li	-0.651439	-1.018534	2.181409
Li	3.674105	0.596782	1.431761
Li	-0.329851	1.486562	0.161378
Li	2.608139	-1.799829	-1.926723
Li	-1.841354	-0.553579	-1.196582
Li	-5.148429	0.496726	0.944995
P	1.940399	2.164857	0.561076
P	1.242148	0.530087	1.941193
P	3.398076	-1.690468	0.419089
P	-2.938036	-0.546292	1.246240
P	-2.958324	1.377708	0.225182
P	2.130545	1.102195	-1.396596
P	1.241314	-1.289394	0.654848
P	0.611022	-0.515708	-1.324693
P	-4.185286	0.493515	-1.351521
P	-4.148573	-1.427825	-0.328883
P	4.004480	-0.040300	-0.965183

18

Li6P12 E = -112714.2168 eV

Li	3.833325	2.203350	-0.277179
Li	-0.147557	-0.183126	2.508553

Li	-1.361775	-1.043409	-0.576909
Li	-1.035894	1.803783	-0.199083
Li	-5.095802	0.336791	0.308786
Li	3.364743	-2.315314	-1.045911
P	-3.294579	1.835216	0.571971
P	-2.269155	0.105707	1.511647
P	-3.412249	-1.658039	0.816908
P	1.102904	-1.514819	-0.974881
P	1.458773	1.886533	-0.414351
P	4.209902	-0.066040	-0.968122
P	1.673805	-1.329240	1.124095
P	-3.822867	-1.160172	-1.222039
P	3.732535	-0.377077	1.170904
P	1.905856	0.934768	1.500421
P	2.145702	0.271481	-1.770280
P	-3.342033	0.911265	-1.489924

19

Li6P13 E = -122004.3086 eV

Li	0.348866	-1.952808	0.286030
Li	-1.440545	0.377888	1.590002
Li	3.928012	-0.147042	-2.246632
Li	2.467707	2.359117	1.138633
Li	-4.679998	-1.531669	-0.273887
Li	-1.163694	0.660249	-1.291428
P	3.119085	-0.264095	1.875900
P	3.161726	1.824820	-1.096451
P	3.843893	-1.503986	0.146826
P	1.389155	0.487244	-0.908489
P	1.109602	0.383454	1.284785
P	4.484140	0.711832	0.286577
P	2.206856	-1.533653	-1.321079
P	-2.073357	-1.725328	-0.019985
P	-3.974916	0.943276	-1.179907
P	-4.196207	0.793931	1.087627
P	-2.644537	2.095270	0.178890
P	-2.976417	-0.959361	-1.858474
P	-3.341093	-1.206551	1.683236

20

Li6P14 E = -131295.1824 eV

Li	3.642855	2.526037	0.525882
Li	5.338891	-1.302811	-0.966208
Li	-0.800225	1.163976	-0.304608
Li	-3.643261	-2.525858	0.525942
Li	-5.338407	1.302900	-0.966238
Li	0.800350	-1.164347	-0.304748
P	3.405605	-1.668291	0.923562
P	1.704315	1.273465	-0.093258
P	2.513702	0.273022	1.700262
P	4.764635	0.156988	1.262922
P	3.083950	0.495341	-1.655338

P	5.041813	1.061250	-0.742508
P	2.999312	-1.688530	-1.246588
P	-2.513838	-0.273273	1.700242
P	-4.764811	-0.156870	1.262782
P	-5.041939	-1.061022	-0.742728
P	-1.704490	-1.273736	-0.093258
P	-3.405421	1.668239	0.923702
P	-3.083916	-0.495213	-1.655378
P	-2.998958	1.688649	-1.246418

21

Li6P15 E = -140584.0652 eV

Li	1.219372	-0.188087	-1.188483
Li	5.668818	-1.338179	-1.187222
Li	-0.380429	0.240466	1.310912
Li	4.102836	0.609429	2.484151
Li	-3.408166	1.278614	-2.155243
Li	-4.849908	-1.586089	1.969130
P	2.119415	0.105016	1.244058
P	3.132814	1.727667	0.144990
P	-1.276544	0.202777	-1.257566
P	-2.446412	-1.463802	-0.289664
P	-3.347249	1.286007	1.300128
P	-1.839289	2.005279	-0.201822
P	-5.003800	1.009628	-0.228445
P	-2.618176	-0.731909	1.774288
P	-6.108621	-0.868341	0.036055
P	3.316505	-1.386034	-1.597410
P	5.368894	-0.915467	1.150284
P	3.958581	0.723081	-1.718423
P	5.324923	1.039255	0.104583
P	3.330144	-1.649003	0.609866
P	-4.381689	-0.887384	-1.317572

22

Li6P16 E = -149874.3148 eV

Li	-1.133206	-0.509901	-1.167929
Li	0.225034	-2.237285	1.029262
Li	-4.478090	-1.742816	1.591219
Li	0.042422	2.366069	-0.974254
Li	4.012227	2.203723	0.788593
Li	-0.619591	1.777139	1.998433
P	2.115604	-2.610465	-0.650416
P	-4.827885	0.638955	1.430939
P	-3.446646	-1.783033	-0.903825
P	-2.646219	0.637282	1.297036
P	-2.184500	-1.514453	0.885002
P	-3.547586	0.340948	-1.894444
P	-5.200269	-0.275562	-0.508741
P	-2.306491	1.615321	-0.642653
P	1.597687	2.317878	1.118428
P	4.062525	-2.106445	0.325312

P	3.704743	-0.372484	1.666353
P	2.463574	2.664114	-1.030152
P	2.986206	0.640644	-1.725327
P	4.660170	-0.087648	-0.422087
P	1.382548	-0.596817	-0.851962
P	1.576779	0.120379	1.253472

23

Li6P17 E = -159164.2785 eV

Li	-5.261907	-1.782808	-0.771448
Li	-2.634534	1.587448	1.183598
Li	-0.797524	-2.644660	-0.103489
Li	0.035090	1.870948	-0.938390
Li	0.703448	0.010137	2.303487
Li	3.207194	0.097919	-0.560124
P	-1.496881	-0.076397	-0.771979
P	-4.673128	0.017038	0.716404
P	-3.679106	0.380808	-1.209510
P	-2.753770	-1.644161	-1.845467
P	-3.421376	-1.654651	1.484110
P	-1.459662	-0.685168	1.322167
P	-3.282232	-3.059302	-0.245755
P	1.538226	3.839140	-1.528412
P	2.412652	2.421247	-0.168697
P	-0.327551	4.404895	-0.774701
P	1.140856	2.336224	1.593526
P	-0.708506	3.361090	1.058779
P	1.835062	-2.346338	-0.293342
P	3.409124	-2.466454	-1.690495
P	5.154361	-1.796189	-0.693062
P	4.665794	-1.254084	1.294137
P	2.595783	-1.605495	1.529570

24

Li6P18 E = -168454.3876 eV

Li	3.141739	-0.000532	0.438527
Li	-1.120695	2.062328	-0.263486
Li	-5.764798	1.321728	-0.475652
Li	-1.516674	-0.681050	0.250911
Li	-5.361952	-3.095401	-0.543313
Li	2.659543	4.481190	0.596243
P	1.413234	1.138662	-1.563275
P	3.440516	2.295759	1.162897
P	3.243210	2.399902	-1.039708
P	1.200381	3.399143	-1.418956
P	1.284976	2.106796	1.703278
P	0.372069	3.802067	0.587920
P	-6.109020	-0.925316	-1.213887
P	-4.136702	0.320864	1.530774
P	-3.932333	-0.767464	-1.693603
P	-3.399448	0.989942	-0.438899
P	-3.952064	-1.937457	1.478936

P	-5.976503	-0.948751	0.999261
P	-3.073232	-2.425714	-0.486548
P	4.674801	-3.895116	-0.320678
P	4.771428	-1.809320	-0.997813
P	0.746403	0.389384	0.400890
P	4.566747	-2.299467	1.181830
P	6.458106	-2.651569	0.126935

25

Li6P19 E = -177743.8937 eV

Li	-0.276055	0.416107	2.051926
Li	-2.058748	2.221351	-0.747014
Li	1.550422	-2.762422	-0.097804
Li	2.619307	1.879974	-0.955852
Li	-0.563281	-1.442948	-1.441528
Li	5.870981	-1.132985	0.397322
P	-2.531715	4.905045	-0.517648
P	-2.451891	3.912380	1.345643
P	1.889123	-0.126104	0.920353
P	4.857181	0.724990	-0.744173
P	3.983513	0.658210	1.278300
P	3.475631	-1.567641	1.662520
P	-0.718542	4.552417	-1.566593
P	3.806382	-1.018862	-1.657086
P	4.082720	-2.642418	-0.158241
P	1.731993	-0.410475	-1.246301
P	0.481223	3.351060	-0.327604
P	-3.859413	-2.067380	1.720596
P	-1.873264	-1.260614	1.143284
P	-2.484051	-0.164422	-0.646559
P	-2.428269	-3.681651	-1.048527
P	-4.409209	-3.072633	-0.146161
P	-0.922085	-3.103995	0.436322
P	-3.480933	-1.772400	-1.744860
P	-0.576918	2.948678	1.455326

26

Li6P20 E = -187034.2779 eV

Li	-1.220412	3.786195	-1.376463
Li	-4.832113	-2.932031	1.275646
Li	-2.698022	1.179441	2.124127
Li	-0.065124	-1.476129	0.163642
Li	3.817758	-0.842750	-0.285116
Li	3.574042	3.864914	-1.309124
P	-4.020954	-2.800881	-0.985175
P	-5.397323	-0.250445	1.203513
P	-2.558850	-1.584971	0.091503
P	-3.521400	-1.066491	2.021637
P	-4.917798	0.674740	-0.809244
P	-5.715038	-1.410779	-0.795945
P	-2.784026	0.231916	-1.191770
P	-1.866452	1.912199	-0.014515

P	0.205716	1.102539	0.056460
P	3.093558	2.555776	1.252404
P	3.395685	1.554444	-0.709661
P	1.430145	1.892936	-1.641622
P	5.372876	-2.681254	0.949780
P	1.603031	4.231856	0.815556
P	1.187107	4.072194	-1.354195
P	0.945417	2.302578	1.766389
P	2.087610	-2.813568	0.195083
P	3.125034	-3.087609	-1.623619
P	5.179573	-3.019962	-1.136126
P	3.440864	-2.531145	1.791004

7

Li7 E = -1432.8941 eV

Li	0.000619	0.000364	1.367704
Li	-2.098720	-1.499093	0.000744
Li	0.776991	-2.458703	-0.000136
Li	2.579141	-0.021128	-0.000466
Li	0.816820	2.446147	0.000354
Li	-2.074440	1.532633	-0.000566
Li	-0.000409	-0.000220	-1.367636

8

Li7P1 E = -10725.0767 eV

Li	-1.759546	1.358175	-0.683573
Li	1.992200	1.282253	-0.001478
Li	1.991550	-1.282457	-0.003795
Li	-1.759346	-1.356004	-0.687179
Li	-4.270868	-0.001759	0.695089
Li	-1.166159	-0.002048	1.663701
Li	4.682520	-0.001371	0.554524
P	0.057930	0.000642	-0.307458

9

Li7P2 E = -20016.8623 eV

Li	-1.941640	-2.135361	-0.000256
Li	3.963051	0.935168	-0.000986
Li	0.000091	-0.461361	-1.358356
Li	1.941560	-2.135431	-0.000156
Li	0.000081	1.680009	0.000014
Li	-0.000109	-0.461321	1.358504
Li	-3.963089	0.935109	-0.000206
P	1.893201	0.164299	0.000334
P	-1.893189	0.164339	-0.000046

10

Li7P3 E = -29308.2017 eV

Li	-0.307223	0.000170	-1.359861
Li	2.660767	-0.000042	-1.452991
Li	-1.046484	-2.001799	0.000039
Li	-4.507793	0.000053	0.000339

Li	-1.046582	2.001921	0.000099
Li	-0.307753	0.000050	1.359679
Li	2.660407	0.000198	1.453269
P	1.344288	1.233489	-0.000001
P	1.344367	-1.233521	0.000059
P	-2.309723	-0.000079	-0.000171

11

Li7P4 E = -38598.6413 eV

Li	-0.385856	-1.605173	0.004902
Li	0.624030	0.006638	1.758790
Li	4.001980	-0.000313	0.001368
Li	0.624451	-0.005651	-1.758437
Li	-3.219245	-1.402811	0.005271
Li	-3.218104	1.404159	-0.004644
Li	-0.385663	1.604395	-0.006438
P	2.007116	-1.120313	0.003964
P	-1.811332	-0.004706	-1.216662
P	-1.811497	0.004512	1.216708
P	2.007395	1.120258	-0.004173

12

Li7P5 E = -47890.0152 eV

Li	0.979535	-2.448958	0.694802
Li	2.311141	0.004045	-0.004837
Li	0.976100	1.829757	1.771283
Li	0.967367	0.621629	-2.472315
Li	-1.570552	-0.546617	2.162798
Li	-1.577937	-1.602193	-1.545020
Li	-1.580703	2.140643	-0.605757
P	0.788384	-0.505909	2.012893
P	0.779184	1.999592	-0.570296
P	0.781573	-1.490991	-1.447961
P	-2.330081	-0.002567	0.005130
P	-0.120050	0.000213	0.000044

13

Li7P6 E = -57179.5763 eV

Li	-1.558949	-0.035846	-2.062294
Li	-1.343289	-1.825645	0.005776
Li	1.411876	-2.552928	0.007396
Li	2.289348	0.139400	2.034366
Li	-1.560352	-0.022320	2.062526
Li	2.290881	0.128674	-2.033784
Li	0.602064	2.889647	-0.005574
P	-2.985878	0.158099	-0.000824
P	0.436292	-1.324846	-1.782814
P	0.434718	-1.314301	1.789876
P	0.595332	0.014762	-0.000364
P	-1.273135	1.397792	-0.004574
P	2.366355	1.324298	-0.002984

14

Li7P7 E = -66469.7728 eV

Li	-2.076730	2.052400	-1.270806
Li	-2.936565	-0.155673	1.744479
Li	-1.822204	-1.540998	-2.024993
Li	0.372794	-2.115993	1.416399
Li	1.623887	0.037822	-2.106231
Li	0.305485	2.040620	1.453569
Li	1.815783	-0.010401	1.989387
P	-0.895480	-0.037576	0.073949
P	-2.973907	-0.028957	-0.625183
P	0.285734	-1.710397	-0.894050
P	0.237482	1.675511	-0.891739
P	-0.625051	-0.055631	2.266028
P	2.234613	1.262579	-0.059220
P	2.280119	-1.167084	-0.110146

15

Li7P8 E = -75759.7101 eV

Li	1.482692	-2.015403	-0.419456
Li	2.006998	-0.727122	2.068624
Li	-2.007370	0.729131	2.066654
Li	2.882999	1.534737	0.764274
Li	-1.481734	2.014382	-0.420296
Li	0.000204	-0.001341	-2.109016
Li	-2.884351	-1.534508	0.766534
P	0.305293	1.104699	1.479744
P	-0.305555	-1.100860	1.482064
P	3.480118	-0.737974	0.132044
P	-0.903099	-1.775429	-0.527046
P	2.356344	0.266586	-1.355036
P	0.903597	1.775047	-0.530766
P	-2.356436	-0.269877	-1.354756
P	-3.480150	0.737833	0.130284

16

Li7P9 E = -85050.0207 eV

Li	-0.552867	2.681106	1.185275
Li	-0.133034	0.000677	-2.415911
Li	-0.294243	0.000830	0.124869
Li	-2.773113	0.002156	-1.440174
Li	-0.931381	-0.003081	2.390724
Li	3.281955	-0.002913	0.591056
Li	-0.556316	-2.682474	1.183713
P	1.287731	1.756463	-0.518780
P	2.148686	-0.001341	-1.592876
P	-1.192517	1.955761	-1.078377
P	-2.385450	1.212917	0.614611
P	-2.387212	-1.210563	0.613891
P	1.416145	1.189620	1.617391
P	1.284674	-1.757537	-0.518620
P	1.414188	-1.190450	1.617760

P -1.194445 -1.954129 -1.078910

17

Li7P10 E = -94339.7200 eV

Li 0.404559 -1.747068 2.224651
Li 0.494468 -2.469678 -1.161237
Li 0.043135 -0.193727 0.348112
Li -3.698834 -0.489246 -0.073957
Li 3.664787 0.465344 0.005606
Li 0.082826 1.496027 2.380136
Li -0.438581 2.959300 -0.323396
P -1.855952 -1.599123 1.184386
P 2.177577 -1.591532 0.540233
P 2.313887 -0.830124 -1.563843
P -1.803521 -1.664728 -1.081378
P 2.098563 0.247333 1.878638
P -2.060555 0.555788 1.662991
P 1.690937 1.920814 0.351909
P -1.270707 0.373497 -1.769517
P 1.011343 0.999170 -1.579413
P -2.412044 1.584715 -0.303989

18

Li7P11 E = -103630.2287 eV

Li 3.465895 -0.041989 2.392092
Li 4.750512 1.079145 0.376730
Li -2.523064 -2.720754 -0.210014
Li 2.104138 -0.945795 0.232194
Li 0.149223 0.815832 1.154435
Li -3.771514 1.484678 -1.281818
Li 0.977341 2.543049 -0.748128
P 4.615048 -1.426383 0.767182
P 4.163083 -0.765775 -1.166391
P -1.849534 -0.817371 1.760172
P -0.513605 -1.458237 0.121065
P 2.424841 1.593765 0.981150
P 2.847850 1.001995 -1.106890
P -1.395186 -0.322521 -1.571338
P -3.853465 -0.423006 0.747972
P -3.540201 -0.897222 -1.395547
P -1.457175 1.731281 -0.723095
P -2.472164 1.340641 1.202622

19

Li7P12 E = -112920.2033 eV

Li -0.788816 2.265372 -0.262267
Li -4.928856 0.705361 -0.165722
Li -1.130792 -0.330106 -2.323972
Li 0.155202 -1.431835 0.095404
Li 3.457558 1.003599 2.061882
Li -1.210639 0.025402 2.079327
Li -4.644908 -2.062777 0.200484

P	-2.996839	1.652017	0.896808
P	-3.341950	-0.833743	-1.536605
P	-2.373448	-1.709628	0.285488
P	-2.938034	1.360068	-1.288201
P	1.516574	1.429700	-0.210327
P	1.223776	-0.080177	-1.773174
P	-3.520846	-0.387945	1.690828
P	2.588913	-1.606562	-1.056528
P	4.203778	-0.407553	-0.064316
P	3.689787	1.698976	-0.234994
P	1.206413	0.270913	1.678385
P	2.560127	-1.421069	1.275609

20

Li7P13 E = -122210.6433 eV

Li	4.325845	-0.532887	1.962289
Li	1.387240	-0.298276	-1.039690
Li	4.765886	1.660835	0.396211
Li	0.521616	2.039832	0.724291
Li	-0.310959	-1.369982	1.088177
Li	-4.413907	0.977387	1.736017
Li	-2.826556	1.017866	-2.425824
P	2.629068	1.839612	-0.620201
P	3.799448	0.181587	-1.624487
P	2.078887	-0.954272	1.348110
P	3.410617	-1.677553	-0.321653
P	5.389275	-0.646731	-0.294026
P	2.646409	1.223602	1.553241
P	-3.002760	-1.525398	-1.308327
P	-3.736987	1.907566	-0.381722
P	-1.197740	-0.281421	-1.232635
P	-4.697268	-0.050807	-0.758288
P	-3.802031	-1.514952	0.793417
P	-2.402445	-0.305551	1.979568
P	-1.804306	1.105362	0.378710

21

Li7P14 E = -131500.4554 eV

Li	0.407042	-0.571146	-1.838772
Li	4.953505	-1.852636	-0.352117
Li	3.752877	2.622133	-0.122323
Li	-0.410376	1.503327	0.534599
Li	-4.590982	1.085149	-1.779169
Li	-3.194386	-2.594353	0.303877
Li	1.007387	-0.763177	1.192231
P	-3.216676	-0.323600	1.915848
P	-3.929786	1.512061	0.836382
P	-4.046044	-1.246416	-1.500555
P	-2.053497	-0.291504	-1.235242
P	-2.523652	1.834875	-0.818922
P	1.754390	1.432648	-0.942977
P	5.054895	0.575744	-0.293399

P	3.418344	0.150308	-1.719707
P	-4.942264	-0.517120	0.390319
P	3.880577	0.146481	1.546300
P	3.080514	-1.893639	1.170026
P	2.099169	1.500395	1.277261
P	2.506187	-1.765840	-0.987580
P	-1.467170	-1.000252	0.774581

22

Li7P15 E = -140790.8148 eV

Li	-0.085592	1.630577	1.626460
Li	0.216884	-1.439355	-0.690202
Li	-0.714348	2.311856	-1.359512
Li	3.262678	2.668647	0.906810
Li	4.439649	-1.858486	1.488373
Li	-4.271280	-0.744073	2.381178
Li	-4.935941	0.006897	-2.056546
P	-2.914534	1.201138	-1.597502
P	-3.915777	1.427643	0.366566
P	-1.979310	-1.277561	0.793114
P	-3.921459	-1.923244	-0.208958
P	-5.343988	-0.293943	0.285061
P	1.146257	2.905494	-0.079475
P	2.353275	-2.261400	0.400091
P	3.308520	0.437156	-1.787069
P	4.956193	0.156285	-0.286819
P	-2.402451	0.628751	1.774119
P	4.089021	0.497026	1.722399
P	2.046614	-0.279547	1.324884
P	1.475533	0.802043	-0.549815
P	3.816094	-1.641554	-1.177440
P	-2.296398	-0.893498	-1.438469

23

Li7P16 E = -150080.2075 eV

Li	-4.703890	1.184214	1.717274
Li	-4.626402	-2.283266	-1.155428
Li	0.142312	-1.842613	-0.411653
Li	0.030797	1.313178	1.812924
Li	4.373537	-1.696812	1.935835
Li	3.001032	2.752853	0.778991
Li	-1.093560	3.168450	-0.927192
P	-2.761766	-0.308116	-1.814041
P	-4.787074	0.473315	-1.019454
P	-2.806759	1.405967	-0.369143
P	-2.325344	-2.059352	-0.571137
P	-5.291771	-0.877589	0.666746
P	-3.223375	-1.412914	1.351147
P	-2.378438	0.611468	1.616304
P	4.086306	0.646043	1.497886
P	4.975788	-0.218501	-0.320162
P	2.043997	-0.167138	1.254090

P	2.298519	-2.327373	0.901827
P	0.671319	3.416187	0.677751
P	3.834360	-2.195734	-0.709029
P	3.379863	-0.346597	-1.887271
P	1.530789	0.294243	-0.856503
P	1.328822	2.546892	-1.169160

24

Li7P17 E = -159370.3838 eV

Li	0.031956	1.990188	0.558496
Li	3.394422	-2.978454	1.228753
Li	5.242869	0.957473	-0.772504
Li	-1.340688	-1.591150	1.205117
Li	0.054452	-1.935565	-1.362619
Li	-4.796238	1.664509	1.694665
Li	-3.670273	0.721332	-2.512693
P	-5.519843	0.324644	-0.546951
P	-3.033675	0.069140	2.017450
P	-2.345309	1.057423	0.155725
P	-4.749161	-1.015916	1.175974
P	-4.173936	2.081629	-0.594076
P	1.018975	-2.263708	1.104205
P	2.010026	3.409807	-0.056266
P	3.339034	0.316742	1.700071
P	1.360367	-0.098557	0.865862
P	4.685836	-1.031842	0.496388
P	-4.188657	-1.518659	-0.943706
P	3.741250	2.296387	0.682140
P	3.423646	-1.543271	-1.308529
P	2.054917	-3.184637	-0.764813
P	2.925277	1.982903	-1.454167
P	1.856750	0.022936	-1.305700
P	-2.188796	-0.670688	-1.231449

25

Li7P18 E = -168660.1800 eV

Li	0.232205	-2.806665	-0.212778
Li	-1.395859	-0.482130	-1.012007
Li	-4.363643	-2.322194	1.530198
Li	2.783705	1.380475	-0.804841
Li	4.824288	-2.869726	-0.234092
Li	-0.232662	0.498278	2.369161
Li	-3.192152	1.545626	-0.044020
P	1.599619	-0.734078	1.195282
P	2.565774	-3.558501	-0.673144
P	2.613883	-2.758196	1.376805
P	3.840066	-0.788751	1.257924
P	2.714358	-1.650694	-1.821627
P	4.420598	-0.589948	-0.859053
P	1.089561	-0.469984	-0.913473
P	-3.668985	-0.045145	-1.989771
P	-2.313463	-0.593152	1.576815

P	-3.743026	-2.114267	-1.228731
P	-2.246231	-2.460035	0.440049
P	-5.159330	-0.529220	-0.416262
P	-4.379030	0.079652	1.616652
P	2.047114	3.517725	1.084619
P	1.939038	4.024635	-0.961567
P	0.113702	2.934870	1.677416
P	-0.030507	3.694123	-1.668707
P	-1.134317	3.052235	-0.011550

26

Li7P19 E = -177951.0519 eV

Li	-1.383148	-2.628468	-0.417899
Li	-4.915544	-0.100544	-2.096142
Li	0.345272	-1.632492	1.661818
Li	2.812335	-2.601138	-2.405334
Li	-2.443773	1.813815	1.453491
Li	-0.000013	1.132592	-1.081021
Li	3.903310	1.162538	0.303477
P	-2.310940	0.060760	-0.791035
P	-4.705741	-2.191854	-0.348048
P	-3.154417	-1.710983	-1.835772
P	-3.920462	-1.561893	1.674406
P	-5.319829	-0.164071	0.602885
P	-1.951109	-0.698549	1.260822
P	3.771194	-0.567639	-1.575243
P	3.778206	-2.190160	1.602411
P	1.825050	-0.538054	-0.515126
P	2.467801	-0.436070	1.602160
P	2.882136	-3.647858	0.133392
P	4.654068	-2.256054	-0.469277
P	1.119088	-2.635821	-0.695265
P	-0.230994	3.775755	-1.209423
P	-0.497433	3.401836	0.868010
P	1.843370	3.795418	-1.545621
P	1.355593	3.241506	1.826752
P	2.802105	3.540641	0.320372
P	-4.071376	1.353829	-0.390076

27

Li7P20 E = -187240.1077 eV

Li	-0.016340	0.207385	2.188914
Li	-3.012195	-3.886798	1.342717
Li	1.112203	-2.547122	-0.906901
Li	3.224829	1.724033	-0.056338
Li	0.068361	1.753094	-0.940370
Li	5.726801	-2.121952	-0.038160
Li	-4.488603	0.665343	1.827779
P	-0.254597	2.686700	1.711944
P	-3.887287	-1.689225	1.756380
P	-1.830135	-1.187707	1.147196
P	-1.187325	-2.990710	0.074505

P	2.087048	-0.597076	1.117748
P	5.165222	0.183234	-0.393584
P	4.309052	-0.410555	1.544789
P	3.319034	-2.482521	1.185973
P	-1.186065	4.244849	-1.341647
P	-1.962187	3.403335	0.529659
P	3.750031	-0.868025	-1.762284
P	1.810996	-0.151184	-1.001573
P	-2.139073	0.216269	-0.582214
P	-2.857806	-3.085123	-1.380848
P	-4.668882	-2.223594	-0.249349
P	-3.547796	-1.004845	-1.780321
P	0.884570	4.390689	-1.090124
P	1.468498	3.474785	0.726927
P	3.661135	-2.938773	-0.940470
P	-3.457446	1.870682	0.043766

8

Li8 E = -1637.8171 eV

Li	-1.797010	1.640010	0.523266
Li	1.797010	-1.640010	0.523266
Li	-1.797010	-1.640010	0.523266
Li	1.797010	1.640010	0.523266
Li	-0.000000	0.000000	2.420086
Li	0.000000	-1.643700	-2.167194
Li	0.000000	1.643700	-2.167194
Li	0.000000	-0.000000	-0.178764

9

Li8P1 E = -10930.0430 eV

Li	1.333642	0.001331	1.261981
Li	-2.628238	0.001002	1.364141
Li	3.121695	2.223502	0.000511
Li	0.066575	2.187344	-0.001309
Li	1.334862	-0.000159	-1.261849
Li	0.067818	-2.187656	-0.000479
Li	3.121058	-2.223158	0.001051
Li	-2.632768	0.000182	-1.359299
P	-0.756928	-0.000477	-0.000949

10

Li8P2 E = -20222.0304 eV

Li	-2.748852	-1.061233	1.774521
Li	0.301661	0.165099	1.349035
Li	0.177160	-1.545272	-0.640385
Li	3.480688	-1.336973	0.797749
Li	2.604318	1.971459	0.463837
Li	-2.146985	1.947035	0.861799
Li	0.102420	1.029358	-1.165546
Li	-3.320927	-0.124530	-1.649573
P	-1.735808	-0.138836	-0.040000
P	2.045911	-0.070152	-0.318287

11

Li8P3 E = -29513.3848 eV

Li	-2.810750	-0.189222	1.455701
Li	0.141828	0.068790	1.355091
Li	-2.811166	-0.188270	-1.455239
Li	0.141308	0.068803	-1.354439
Li	1.068407	-1.885287	-0.000279
Li	3.825495	-0.448475	1.389071
Li	0.668911	2.178572	-0.000299
Li	3.827066	-0.448233	-1.387579
P	-1.598396	1.158661	0.000241
P	-1.376414	-1.292409	-0.000309
P	2.164589	0.302412	-0.000339

12

Li8P4 E = -38804.3043 eV

Li	-2.907874	-0.805138	-1.554862
Li	0.043430	-0.066360	-1.137111
Li	3.092746	-0.583605	1.467782
Li	3.198228	0.869314	-1.249403
Li	-0.043215	2.379935	-0.216092
Li	-3.467040	0.369025	1.154045
Li	-0.354134	0.371519	1.453977
Li	0.261127	-2.229684	0.226556
P	1.805369	1.095993	0.582237
P	2.155903	-1.051056	-0.591986
P	-2.036238	1.067244	-0.512913
P	-1.889687	-1.173181	0.493684

13

Li8P5 E = -48094.5737 eV

Li	1.570722	0.262867	-2.142275
Li	-0.143809	2.827587	-0.005935
Li	3.751331	0.106181	0.002215
Li	-1.971936	0.128229	1.996205
Li	1.566252	0.274220	2.143205
Li	-1.970695	0.121981	-1.997195
Li	1.584795	-1.951421	0.003695
Li	-1.188241	-2.461857	0.004215
P	1.709922	1.366504	-0.002315
P	-0.110513	-1.322481	-1.781185
P	-0.165611	0.058254	-0.000375
P	-1.962578	1.352187	-0.002435
P	-0.110904	-1.316022	1.785485

14

Li8P6 E = -57385.6502 eV

Li	-0.087872	2.433496	1.300642
Li	3.529994	0.001198	-0.176852
Li	-0.085035	-2.433244	1.299134
Li	0.084928	2.434952	-1.298696

Li	0.086311	-2.435149	-1.299079
Li	1.491577	0.001068	1.691520
Li	-3.529718	-0.000381	0.176792
Li	-1.490222	-0.000850	-1.691446
P	1.996853	1.811107	0.069549
P	1.998593	-1.809923	0.069725
P	0.896498	0.000086	-0.684199
P	-0.896341	-0.000369	0.683969
P	-1.998207	1.809821	-0.070044
P	-1.997388	-1.810939	-0.069403

15

Li8P7 E = -66675.5740 eV

Li	-1.449424	0.112321	1.796410
Li	1.949265	1.859088	1.683033
Li	-3.841960	-0.050458	-0.075302
Li	0.041853	-2.225906	0.978852
Li	2.723394	0.156107	-1.988053
Li	-0.507977	-2.211876	-1.739332
Li	2.750241	-1.477347	1.173414
Li	-0.312420	2.838815	-0.775916
P	0.969392	-0.232764	2.170795
P	1.743430	-1.756283	-0.970313
P	0.958857	0.092066	-0.027821
P	1.904983	1.942284	-0.683370
P	-1.310206	0.101493	-0.687680
P	-2.190803	-1.771316	-0.019984
P	-2.346248	1.824372	0.007752

16

Li8P8 E = -75966.0473 eV

Li	-3.350902	-1.336487	-0.630466
Li	-0.949550	-2.191092	1.154088
Li	-1.952289	2.098994	1.045529
Li	0.363591	0.156908	-2.599216
Li	3.349618	-1.337657	0.632097
Li	1.953546	2.097251	-1.048638
Li	0.949966	-2.192903	-1.153926
Li	-0.364116	0.160777	2.599671
P	-2.460145	-0.245677	1.299695
P	-1.346845	-1.554830	-1.887735
P	-1.085466	-0.048706	-0.399648
P	2.460001	-0.248157	-1.299422
P	1.085459	-0.048339	0.399748
P	1.346629	-1.551035	1.891044
P	0.643769	2.103424	0.950729
P	-0.643376	2.102161	-0.954238

17

Li8P9 E = -85255.9957 eV

Li	-1.689298	-3.333733	-0.223902
Li	1.838942	-2.040165	1.160114

Li	-0.312677	-0.016000	2.684874
Li	-0.276565	0.045040	-2.681801
Li	-1.338285	3.488438	0.210509
Li	-2.466257	1.072946	-1.053289
Li	-2.579034	-0.810383	1.035502
Li	2.057601	1.908537	-1.095878
P	-0.530195	-2.249751	1.592133
P	1.601789	-1.312745	-1.315961
P	-0.334950	-1.110145	-0.258988
P	1.722582	1.121014	1.331477
P	-1.910299	1.565387	1.516201
P	-0.274718	2.292977	-1.592855
P	-0.216014	1.136901	0.258004
P	-2.053829	-1.359392	-1.530874
P	2.948748	-0.147182	-0.006362

18

Li8P10 E = -94545.9713 eV

Li	-1.418054	0.064568	-0.486861
Li	-1.334808	0.991470	1.882103
Li	-3.849787	-0.066372	1.536757
Li	-0.949438	-2.591637	-0.551897
Li	-1.301594	2.611496	-1.114306
Li	0.518836	-0.975441	1.197000
Li	2.912861	2.141387	-0.337767
Li	2.775252	0.151343	-2.242478
P	-3.839773	0.347728	-0.967936
P	-3.218913	-1.618211	-0.261892
P	-1.879630	-1.503731	1.467826
P	0.911097	-1.052352	-1.414860
P	-3.077643	1.896323	0.293933
P	1.055937	1.516632	1.011623
P	2.694148	-1.505269	-0.106021
P	2.819966	0.172837	1.450103
P	4.270656	0.067438	-0.246989
P	0.793501	1.213243	-1.202297

19

Li8P11 E = -103836.0180 eV

Li	-0.917542	-2.224446	0.027080
Li	-0.819115	0.071828	2.282370
Li	-0.907932	2.251837	-0.088163
Li	-4.763301	0.023722	0.295385
Li	-4.096796	-0.067844	-2.421847
Li	0.531279	-0.031621	-1.116661
Li	3.555578	-1.331601	1.501725
Li	3.556368	1.406563	1.428389
P	-2.931564	1.149221	1.327522
P	-2.941050	-1.056102	1.398668
P	-3.110905	-1.655080	-0.758875
P	-3.085096	1.607855	-0.865546
P	-1.894874	-0.064145	-1.767098

P	2.857986	-1.177499	-1.115776
P	2.858847	1.113038	-1.177696
P	1.431451	1.759887	0.452321
P	1.430201	-1.736128	0.546241
P	1.562708	0.049803	1.914814
P	4.594588	-0.010538	-0.336230

20

Li8P12 E = -113126.3390 eV

Li	-4.081096	1.384226	1.120722
Li	-0.655953	-0.071604	-0.988026
Li	-3.943554	-1.347426	1.448026
Li	0.510689	2.305784	-0.227872
Li	0.620477	-2.425201	0.640999
Li	0.179751	0.772282	2.303764
Li	4.605053	0.845308	0.684016
Li	4.016916	0.284898	-1.932542
P	-2.115237	0.200923	2.016755
P	-1.847560	1.774175	0.425753
P	-1.673197	-1.652319	0.825161
P	-4.782685	-0.248206	-0.620825
P	-3.013442	0.917891	-1.318554
P	-2.895626	-1.356464	-1.049647
P	2.645347	-0.942052	1.224869
P	2.411791	1.271693	1.466311
P	2.845037	2.008960	-0.616817
P	4.308598	-1.506257	-0.164752
P	1.655113	0.565296	-1.865281
P	2.211406	-1.383294	-0.932790

21

Li8P13 E = -122416.3515 eV

Li	0.804821	-0.885938	1.210326
Li	-0.936569	1.211354	0.644110
Li	-3.668014	-2.322914	0.932813
Li	-5.056712	0.986486	-1.517943
Li	-3.297564	0.107904	2.216331
Li	4.361531	-1.395471	-1.804636
Li	-0.437350	-1.922727	-0.947863
Li	3.837185	2.555027	0.333251
P	-1.570490	-1.201025	1.109543
P	-4.524598	-1.336195	-1.018753
P	-2.761892	1.605575	-0.900002
P	-2.429557	-0.594881	-0.922955
P	-4.286191	1.762327	0.711998
P	-5.355646	-0.174637	0.703386
P	2.093713	-1.480937	-1.040102
P	1.701078	1.502695	0.596019
P	2.270433	0.704366	-1.396374
P	3.312728	-1.689374	0.791830
P	4.482500	0.953987	-1.335881
P	4.891595	-0.052259	0.595986

P 3.054863 0.333613 1.892026

22

Li8P14 E = -131706.5583 eV

Li 3.428578 1.989953 1.606465
Li 4.059589 2.134694 -0.998348
Li 4.323451 -2.171699 0.864669
Li 0.514390 -1.228933 -2.015679
Li 0.724944 1.211739 1.560626
Li -0.819925 -1.209691 0.782022
Li -4.223648 -0.602634 -2.109142
Li -0.306993 2.679925 -1.144943
P 4.836204 0.191850 0.579133
P 3.867912 -0.262798 -1.376102
P 1.679434 -1.042189 0.553568
P 1.795683 0.675363 -1.027812
P 1.866855 2.660718 -0.156870
P 2.743211 -2.167810 -1.049197
P 3.143781 -0.389385 2.051593
P -3.174764 -1.961142 -0.055189
P -1.914379 -0.876157 -1.501471
P -1.786982 1.025387 1.404813
P -2.240789 1.204232 -0.739117
P -4.825068 -0.372967 0.468832
P -3.110315 -0.625733 1.891158
P -4.420859 1.379960 -0.752471

23

Li8P15 E = -140996.3969 eV

Li -0.377809 -2.085040 -0.063182
Li 3.946018 -1.575603 -2.208357
Li 1.098718 0.203343 0.487414
Li 5.168576 0.619150 1.737476
Li 0.120279 1.501849 -2.035516
Li -3.319926 2.803049 -0.911791
Li 1.031218 3.087190 0.768204
Li -5.015917 -1.635182 -1.085556
P 3.077418 1.726467 1.050182
P 5.218257 -0.561302 -0.387779
P 3.907774 1.142044 -0.941440
P 2.173321 0.095264 -1.871959
P 3.688961 -1.680760 0.769101
P 2.856999 -0.176205 2.191087
P 2.013099 -1.824675 -0.708542
P -2.786966 -2.278054 -0.531733
P -2.453659 -0.317287 -1.487771
P -4.437621 0.670010 -1.355349
P -1.358388 0.651764 0.200055
P -2.840058 0.412813 1.858733
P -4.817820 0.368400 0.807715
P -3.719815 -1.574125 1.379378
P -1.051732 2.761895 -0.309418

24

Li8P16 E = -150286.4980 eV

Li	2.264923	2.571636	1.341231
Li	2.680835	3.236057	-1.770919
Li	-0.698662	2.466345	1.371743
Li	5.899878	-0.606386	0.343712
Li	0.529098	-1.316349	-0.632069
Li	-1.375405	-0.482186	1.387080
Li	-1.012623	2.289607	-1.713032
Li	-4.078498	-1.925475	-1.914927
P	4.307929	1.102602	0.952512
P	2.880268	-2.138510	0.404089
P	3.177908	-1.198480	-1.629600
P	3.393172	0.973232	-1.034661
P	1.006360	0.397314	1.494147
P	3.013117	-0.433450	1.883778
P	1.182194	1.192087	-0.626297
P	0.742836	3.370158	-0.436686
P	-4.941823	0.295876	-1.556494
P	-3.975239	-0.175653	1.853200
P	-2.829624	0.703769	-1.146426
P	-2.908159	1.464304	0.912905
P	-3.338638	-2.095011	0.659513
P	-5.317485	-0.914565	0.211239
P	-1.976749	-1.354279	-0.905819
P	4.742026	-2.436043	-0.717964

25

Li8P17 E = -159576.2329 eV

Li	-0.221233	0.760347	-2.301645
Li	0.033766	1.980957	0.826837
Li	-3.196154	1.331218	0.216894
Li	-1.228909	-0.789267	0.963280
Li	-3.943939	-2.665482	-1.600060
Li	0.714129	-2.695019	0.106233
Li	2.778643	2.041210	0.489334
Li	5.308349	-1.952809	0.324392
P	-1.803196	3.444885	0.030218
P	-0.358311	4.329778	1.363178
P	-0.267978	3.070525	-1.441040
P	1.185633	3.972008	-0.121544
P	-4.170747	-0.269186	-1.538773
P	-2.057505	-0.757818	-1.573087
P	-4.877381	-1.074930	0.445535
P	-3.430571	-0.528180	2.042043
P	-3.308336	-2.552604	1.166443
P	-1.803211	-2.684280	-0.551295
P	1.807581	-0.367072	-1.268550
P	4.529651	0.257386	0.871635
P	4.038724	-0.070072	-1.251630
P	3.136765	-2.198638	-1.355424

P	2.980496	-1.020433	1.830996
P	3.149729	-2.945933	0.719570
P	1.199728	-0.207669	0.826672

26

Li8P18 E = -168867.1223 eV

Li	-0.127114	0.986065	2.091773
Li	-4.131384	-1.725742	2.175098
Li	3.632165	-1.874521	-2.451641
Li	0.595871	-2.158931	1.043883
Li	-1.021336	-2.171157	-1.227703
Li	-2.905727	2.277996	-0.435920
Li	0.419552	2.076509	-0.874960
Li	3.405294	1.928004	0.483310
P	-3.631905	-2.779008	-0.299860
P	-2.044723	-0.113240	0.904241
P	-5.033309	-0.912009	-0.221062
P	-4.139896	0.484677	1.221021
P	-2.029494	-2.314118	1.153005
P	-1.855338	0.135093	-1.283640
P	-3.542852	-1.109551	-1.886901
P	4.161426	0.059173	-1.138697
P	1.988688	-0.074427	-0.758942
P	2.035387	-0.133590	1.449440
P	4.786097	-1.687067	0.046964
P	3.026475	-3.191846	-0.070530
P	3.349198	-1.847067	1.766483
P	1.522343	-2.172319	-1.321482
P	0.108949	3.330133	1.453493
P	-1.131982	4.039386	-0.156178
P	1.850189	3.881774	0.311864
P	0.607285	4.536361	-1.329987

27

Li8P19 E = -178156.9595 eV

Li	-4.376734	-1.752585	2.069165
Li	-1.294098	-2.064413	-1.369457
Li	-2.876502	2.371019	-0.088375
Li	-0.122221	0.643856	2.184322
Li	3.397870	-2.199115	-2.527734
Li	0.274319	-2.522421	0.881358
Li	0.744947	1.991817	-0.721027
Li	3.657844	1.126969	0.936467
P	1.229958	-2.329277	-1.476809
P	-3.928252	-2.576992	-0.502955
P	-2.158141	-0.166817	0.966273
P	-5.188233	-0.630968	-0.239555
P	-4.211192	0.536732	1.346464
P	-2.314131	-2.377411	0.994367
P	-1.933659	0.293315	-1.183290
P	-3.698111	-0.762984	-1.911962
P	4.142261	-0.533175	-0.971944

P	1.957176	-0.392768	-0.661189
P	1.899490	-0.711945	1.525714
P	4.468581	-2.474428	0.012037
P	2.527959	-3.688094	-0.323118
P	2.961114	-2.612919	1.671656
P	2.440025	3.311002	0.899724
P	0.443054	3.000037	1.734703
P	-0.928741	3.917997	0.307713
P	2.217456	4.169704	-1.048291
P	0.192300	4.509965	-1.412483

28

Li8P20 E = -187446.6465 eV

Li	3.405430	-2.491166	-2.552971
Li	1.079906	1.683912	-0.414601
Li	3.671451	0.903543	0.870026
Li	-4.400631	-2.084632	2.042191
Li	0.247689	-2.785600	0.819583
Li	-0.105432	0.313353	2.136345
Li	-2.923736	2.144847	0.146025
Li	-1.303322	-2.183760	-1.415332
P	1.219754	-2.553264	-1.531097
P	4.201631	-0.881784	-0.960691
P	2.026450	-0.679184	-0.656134
P	1.935553	-1.037084	1.518038
P	4.448356	-2.856060	-0.022655
P	2.462369	-3.987315	-0.403776
P	2.924390	-2.979550	1.622076
P	2.486777	3.103161	1.045252
P	2.096816	4.361043	-0.673922
P	0.140692	3.756163	-1.731567
P	-4.226530	0.243664	1.468474
P	-2.184752	-0.456226	1.017544
P	-1.974413	0.152084	-1.095089
P	-5.231382	-0.809700	-0.182279
P	-3.989621	-2.741095	-0.590553
P	-3.757082	-0.845385	-1.874018
P	-2.360527	-2.660626	0.902796
P	-0.804199	3.616845	0.337410
P	0.441998	2.665214	1.808717
P	0.209447	5.489000	-0.324778

9

Li9 E = -1842.6098 eV

Li	2.403011	0.422040	-1.230168
Li	1.760417	-1.233604	1.286352
Li	-1.233240	-1.760018	1.286652
Li	1.234562	1.760334	1.285292
Li	0.000061	0.000257	-0.225558
Li	-2.404128	-0.422799	-1.228948
Li	-1.759464	1.233379	1.286852
Li	-0.423721	2.402234	-1.229868

Li 0.422503 -2.401823 -1.230608

10

Li9P1 E = -11135.1293 eV

Li 1.463808 0.504455 -1.251748

Li 1.701598 -2.015675 0.001582

Li 1.461818 0.504721 1.252602

Li 1.771432 3.313272 -0.000628

Li 4.191028 -0.262284 0.002482

Li -2.133019 -0.597957 1.325152

Li -4.310221 1.128348 0.003192

Li -2.137261 -0.598805 -1.322368

Li -0.834588 1.621575 -0.001978

P -0.234919 -0.719530 -0.001658

11

Li9P2 E = -20427.1197 eV [Geometry 15]

Li -2.243024 2.283374 -0.001072

Li -3.278212 -0.824940 1.663679

Li -0.010860 0.648403 1.319771

Li -0.165154 -1.661812 0.000858

Li 3.645702 -0.441149 -1.405199

Li 3.645060 -0.439694 1.406241

Li 2.415501 1.996167 -0.000990

Li -0.010900 0.646914 -1.320685

Li -3.278719 -0.827397 -1.662248

P -1.961888 -0.018098 -0.000088

P 1.818010 -0.257875 0.000017

12

Li9P3 E = -29718.9498 eV

Li -3.977608 -2.279630 0.038764

Li -0.001281 -2.246284 0.486257

Li -1.411709 0.627340 1.344668

Li -0.000285 -0.285516 -0.880539

Li -2.071461 1.115290 -0.986808

Li 0.001051 4.289276 0.294367

Li 3.977352 -2.279884 0.039562

Li 2.072199 1.113147 -0.987767

Li 1.413521 0.626723 1.344452

P -2.116797 -1.118826 -0.053492

P 0.001079 2.103740 -0.031350

P 2.115363 -1.121006 -0.053750

13

Li9P4 E = -39009.4755 eV

Li -0.806151 -1.288797 1.320441

Li -0.806318 1.287993 1.320012

Li -4.721842 0.001079 0.418735

Li -1.634299 2.058762 -0.923323

Li 3.064733 1.526208 0.417588

Li -0.399762 0.000100 -1.070963

Li	3.065355	-1.524872	0.417836
Li	2.093055	-0.000073	-1.566528
Li	-1.632927	-2.059259	-0.923537
P	-2.540479	-0.000510	0.033484
P	0.858428	1.895098	-0.408065
P	1.178819	0.000095	0.900607
P	0.858863	-1.894912	-0.408077

14

Li9P5 E = -48300.5816 eV

Li	2.415464	-2.204143	-0.114342
Li	2.415510	2.204297	-0.114135
Li	1.771054	-0.000047	1.614266
Li	-1.015008	0.000009	1.343017
Li	-1.102705	1.299898	-1.324825
Li	-2.269835	2.045287	0.769914
Li	-2.269660	-2.045423	0.769948
Li	-1.102590	-1.300122	-1.324892
Li	-5.071617	0.000873	-1.014911
P	0.215113	-1.903829	0.675251
P	2.989457	0.000054	-0.596289
P	0.799172	0.000047	-0.586635
P	0.215037	1.903851	0.675268
P	-2.972902	-0.000250	-0.288402

15

Li9P6 E = -57590.8936 eV

Li	-0.423263	-1.864600	-1.048456
Li	2.813814	-2.171315	0.410259
Li	2.847354	2.066275	-0.820377
Li	2.365498	0.411254	1.506644
Li	-0.475411	0.464074	1.657234
Li	-1.548851	2.607393	0.647687
Li	-1.841462	-1.640295	1.102884
Li	-4.615614	0.385517	-0.891140
Li	-0.915358	0.838311	-1.276445
P	3.369192	-0.201959	-0.708255
P	0.652443	-1.585267	1.178804
P	0.731591	2.029286	0.249071
P	1.185378	-0.126876	-0.510267
P	-2.860819	0.558482	0.615721
P	-2.719126	-0.892988	-1.082733

16

Li9P7 E = -66882.0580 eV

Li	-0.049221	2.197148	1.079247
Li	-3.779781	-0.000353	0.059562
Li	-1.562812	-0.001214	1.730776
Li	-0.555505	2.324820	-1.632325
Li	-0.556149	-2.320560	-1.635139
Li	2.675446	0.000858	-1.965971
Li	2.624246	-1.566120	1.340216

Li	-0.048365	-2.200462	1.078234
Li	2.622254	1.565740	1.343164
P	-2.222204	1.794872	0.071819
P	-2.221606	-1.794888	0.071203
P	-1.272354	0.000435	-0.841291
P	1.764586	-1.891655	-0.836497
P	0.917126	0.000081	-0.064509
P	1.765318	1.892745	-0.834470
P	0.995112	-0.001562	2.154192

17

Li9P8 E = -76171.5905 eV

Li	-2.345081	-0.270719	1.326203
Li	2.923630	1.212385	-0.700799
Li	0.649224	3.153301	1.155072
Li	-1.925487	2.115517	0.245624
Li	-1.288308	1.528971	-2.373377
Li	0.067414	-1.123457	2.315361
Li	1.049566	-2.674757	-0.111864
Li	1.144567	-0.183224	-2.105485
Li	-3.271321	-2.039461	-0.645914
P	-2.867129	0.278643	-1.090452
P	0.376574	0.736136	0.388489
P	0.742681	2.279592	-1.135120
P	-0.596425	1.382798	2.201580
P	2.982877	-1.268539	-0.909312
P	2.170833	-0.534131	0.933645
P	-0.931500	-0.780243	-0.814519
P	-1.278752	-2.437966	0.604724

18

Li9P9 E = -85462.1920 eV

Li	-0.371443	-0.035256	2.707804
Li	2.166202	-0.495595	2.048654
Li	3.059789	0.974172	0.116897
Li	0.794091	3.594558	0.091120
Li	-1.438838	2.157864	1.211573
Li	0.475420	-2.460226	-1.385630
Li	-3.325905	-1.836540	0.217876
Li	-2.694191	0.809708	-0.890282
Li	-0.525946	0.342090	-2.686916
P	2.439488	-1.544544	-0.132579
P	1.810645	0.023433	-1.626379
P	-0.847675	2.500524	-1.255913
P	-2.503317	-0.047828	1.580867
P	0.569265	-2.089864	1.163300
P	1.239400	1.768204	1.633210
P	-1.809120	-1.500173	-1.610694
P	-0.941573	-0.769486	0.245452
P	0.415051	1.049580	-0.283483

19

Li9P10 E = -94751.7519 eV

Li	-2.114243	-3.185501	0.632816
Li	-2.703419	0.860307	-1.373863
Li	-1.429782	3.413861	-0.927379
Li	-0.934708	0.825371	2.639734
Li	-2.988440	-0.395725	1.101295
Li	1.899844	0.163932	-1.885384
Li	1.447263	-0.948748	1.916976
Li	-0.694780	-0.780049	-2.660727
Li	1.787105	2.613699	-0.727020
P	-2.482494	-1.564756	-1.141339
P	-0.714273	-1.120609	0.037482
P	-0.086565	1.740068	-2.094716
P	-2.251990	2.016944	0.817452
P	1.217982	1.616636	1.397993
P	-0.440443	1.168334	-0.007693
P	-0.956168	-1.648412	2.120404
P	0.964384	-2.032140	-1.091389
P	3.019756	0.709233	0.426463
P	2.876043	-1.398728	-0.207947

20

Li9P11 E = -104042.3239 eV

Li	3.633368	2.190219	1.302508
Li	3.848845	0.009823	-2.497589
Li	4.950035	-0.001747	0.093538
Li	1.121678	1.764299	-1.154373
Li	-3.562914	2.275053	-0.090995
Li	0.978324	-0.006425	1.989968
Li	3.629748	-2.203261	1.285200
Li	1.119225	-1.754757	-1.162754
Li	-3.567184	-2.274580	-0.103953
P	3.348564	-0.009177	2.104478
P	3.495806	1.812586	-1.020753
P	2.584285	0.000167	-0.024822
P	-2.481330	0.002637	-1.731641
P	-1.376563	1.736691	-0.907561
P	-1.303651	1.141173	1.192180
P	-3.242692	-0.001401	1.590463
P	-4.264345	0.001847	-0.376562
P	3.493674	-1.804706	-1.035531
P	-1.305496	-1.144775	1.189484
P	-1.378476	-1.734767	-0.912044

21

Li9P12 E = -113331.9655 eV

Li	0.042244	0.189419	0.041809
Li	-4.685111	0.546168	0.059570
Li	-0.887699	2.184836	1.666496
Li	-0.604482	2.450789	-1.439936
Li	3.699399	2.126893	0.099757
Li	-1.182294	-1.308957	2.207659

Li	0.270315	-0.071024	-2.478958
Li	-1.214943	-1.957301	-0.808356
Li	3.123771	-2.620078	0.368980
P	2.297759	-0.019343	1.748765
P	-2.820976	0.604768	1.723529
P	-2.680740	1.918010	-0.123903
P	1.749069	1.729969	-1.302799
P	1.463665	1.920144	1.020423
P	-3.318928	-1.387599	0.928767
P	-3.474640	-1.176514	-1.282231
P	-1.976581	0.413694	-1.621739
P	3.989838	-0.308098	0.342666
P	2.741030	-0.280568	-1.494582
P	1.312774	-1.959179	-1.099314
P	1.005491	-1.763432	1.217013

22

Li9P13 E = -122622.4183 eV

Li	-4.326787	-1.366889	1.579891
Li	0.209395	-2.674006	0.477732
Li	-0.854790	-1.146752	-1.445356
Li	1.030622	0.563329	-1.114553
Li	4.822928	1.766392	-0.057957
Li	3.523458	0.049525	-1.902480
Li	3.917786	-2.343088	-0.594175
Li	0.465826	3.060687	-0.480036
Li	0.490367	0.425070	2.135905
P	-1.857796	0.301427	1.337554
P	-3.512580	-1.456809	-1.010388
P	-4.663906	0.473521	-0.332259
P	-2.140540	-1.813676	0.684532
P	-3.907002	1.009767	1.636135
P	-2.979843	0.660813	-1.802766
P	-1.296030	1.252898	-0.561211
P	4.232689	-0.429687	1.270576
P	5.460595	-0.531834	-0.432360
P	2.440051	1.352962	0.954813
P	2.675810	2.278585	-0.989876
P	1.675746	-1.745480	-1.262356
P	2.017046	-1.019339	0.787812

23

Li9P14 E = -131912.2222 eV

Li	4.610458	-2.274725	-0.133592
Li	3.539147	1.681881	-1.817605
Li	1.003877	0.349072	-1.168666
Li	3.777685	1.940082	1.122161
Li	-1.032429	0.417710	1.208127
Li	-4.886692	-1.670014	1.090102
Li	-0.310855	-2.056008	-0.394601
Li	-3.624355	1.157514	-2.391677
Li	-0.300376	3.111355	0.232357

P	2.172307	-1.816719	-0.384918
P	5.045710	0.065706	-0.711684
P	4.629921	-0.329120	1.423317
P	2.437025	-0.685958	1.498247
P	3.462508	-0.841436	-1.860406
P	1.921582	2.524524	-0.391166
P	1.388281	1.238339	1.307346
P	-2.423323	-1.888297	0.950027
P	-3.026355	-1.457731	-1.156343
P	-4.920064	-0.318565	-0.942442
P	-1.525206	0.151676	-1.561632
P	-4.149995	1.103031	0.580395
P	-2.341060	1.909577	-0.441224
P	-3.226623	-0.186400	2.141163

24

Li9P15 E = -141202.4507 eV

Li	-0.141996	2.216394	1.751066
Li	-1.051388	-0.615560	1.391901
Li	-4.821153	1.640431	0.534811
Li	0.555977	-0.612865	-2.192586
Li	0.949755	-1.943393	0.058177
Li	5.143689	-1.591253	-0.694374
Li	3.130561	3.025826	-1.399921
Li	-0.589991	2.601253	-1.303771
Li	2.858291	2.106071	1.504851
P	1.340560	0.088462	1.547139
P	-4.458280	0.553655	-1.586145
P	-3.642569	-0.424942	1.823223
P	-2.370640	0.865149	-1.014053
P	-2.523591	1.365023	1.165703
P	-4.932663	-0.943135	-0.081580
P	-3.059358	-2.114809	0.302824
P	-1.589404	-1.204529	-0.996343
P	4.613049	0.510107	0.590933
P	3.206381	-2.641126	0.179294
P	2.885078	-1.502737	-1.813029
P	3.396997	0.587312	-1.234051
P	3.305454	-0.983198	1.621446
P	1.261234	3.325762	0.036157
P	1.361003	1.153624	-0.471548

25

Li9P16 E = -150492.2635 eV

Li	3.624305	-3.020419	-1.116017
Li	5.004246	0.469861	1.820722
Li	0.975247	-0.226962	0.274426
Li	0.310240	1.907614	1.729957
Li	0.131742	0.220251	-2.326891
Li	-0.865714	-2.282962	0.493681
Li	-1.952285	2.601122	-0.177366
Li	-4.795908	-0.874458	-1.829216

Li	2.525164	4.044168	-0.062730
P	3.006280	1.662852	-0.071732
P	3.761903	-0.043215	-1.389688
P	4.804088	-1.235682	0.146224
P	2.010631	-1.334185	-1.845245
P	1.627275	-2.520277	0.129240
P	3.040825	-1.510740	1.513758
P	2.605659	0.673211	1.940952
P	-3.837668	1.254086	-1.281074
P	-3.370335	-0.193068	1.978337
P	-2.102129	-0.119699	-1.139833
P	-1.488817	0.215869	0.957871
P	-4.912562	0.513197	0.488854
P	0.989890	2.159484	-0.997783
P	-4.359875	-1.744763	0.677238
P	-2.957436	-2.158039	-0.968709
P	0.190863	3.813326	0.100275

26

Li9P17 E = -159782.8900 eV

Li	-3.614172	1.800503	-0.900113
Li	-2.171589	2.955002	1.397932
Li	-0.053729	0.981897	1.903643
Li	-3.333761	-2.832709	-1.890183
Li	0.021417	0.944295	-1.724218
Li	-1.061863	5.374294	0.559054
Li	2.418191	2.250741	0.811292
Li	0.972313	-2.384053	0.189873
Li	4.719728	-0.574018	-2.227112
P	-3.977586	-0.530496	-1.721208
P	-1.922975	-0.421605	-0.894277
P	-2.351954	0.444752	1.095036
P	-4.894862	-1.617217	-0.035171
P	-3.186966	-2.941640	0.853677
P	-3.785881	-1.005308	1.833651
P	-0.642922	3.143443	-0.657659
P	0.286825	3.510241	1.225158
P	-2.518492	4.061352	-0.807304
P	1.923105	-0.290301	1.229446
P	3.965151	1.343038	-0.993898
P	2.208333	-0.010298	-0.941005
P	5.269573	0.140887	0.303860
P	2.963875	-2.025661	-1.469099
P	4.611843	-2.077378	-0.012027
P	3.935182	-0.904122	1.791664
P	-1.461557	-2.522877	-0.424878

27

Li9P18 E = -169072.5913 eV

Li	3.678852	1.302066	-0.539656
Li	2.114012	2.367685	1.770513
Li	-0.040101	0.605343	2.097866

Li	3.157454	-3.127754	-2.057684
Li	0.013355	0.845781	-1.545310
Li	0.832370	5.177835	1.260207
Li	-2.378316	2.034829	1.121368
Li	-1.160781	-2.599580	0.007741
Li	-4.735412	-0.325631	-2.263257
P	3.901414	-0.877427	-1.689176
P	1.831542	-0.750998	-0.899442
P	2.244855	-0.054525	1.160023
P	4.736109	-2.133943	-0.074597
P	2.956566	-3.439104	0.680807
P	3.616582	-1.610530	1.813241
P	0.623511	2.995373	-0.368581
P	-0.192029	3.114464	1.680198
P	2.786990	3.714001	-0.254274
P	-2.015185	-0.590097	1.259965
P	-3.920537	1.392742	-0.799246
P	-2.232988	-0.045527	-0.866892
P	-5.314308	0.116677	0.322434
P	-3.071913	-1.943054	-1.647599
P	-4.757598	-2.080589	-0.239793
P	-4.069774	-1.161095	1.701909
P	1.277088	-2.859371	-0.597190
P	1.303388	4.956888	-1.152144

28

Li9P19 E = -178362.8219 eV

Li	-0.184087	0.474544	-2.234875
Li	-4.190702	-2.512189	-1.880985
Li	3.777376	-1.862164	2.458749
Li	0.617005	-2.529107	-0.860746
Li	-0.945475	-2.116292	1.378617
Li	-3.027744	2.083160	-0.257066
Li	0.373461	5.604941	-0.466437
Li	0.303116	1.693125	0.705896
Li	3.370498	1.654134	-0.854184
P	-3.495357	-2.999391	0.719236
P	-2.156266	-0.564336	-1.119223
P	-5.010631	-1.264243	0.361273
P	-4.298262	-0.155200	-1.395742
P	-2.005311	-2.765456	-0.898028
P	-1.873970	0.140596	0.946771
P	-3.423846	-1.029728	1.934723
P	4.255887	-0.070676	0.937757
P	2.071097	-0.234187	0.688248
P	1.987692	-0.514007	-1.498680
P	4.811083	-1.938419	-0.085354
P	3.050750	-3.408667	0.265146
P	3.295077	-2.247890	-1.712541
P	1.611096	-2.255384	1.479052
P	1.884910	3.681167	-0.823272
P	0.021238	2.727674	-1.545967

P	-1.495711	4.041856	-0.601270
P	1.413660	4.094948	1.301678
P	-0.661826	4.263311	1.448399

29

Li9P20 E = -187652.7169 eV

Li	2.050051	1.521134	-1.620764
Li	-2.271605	-2.279505	1.087648
Li	-2.466581	2.393431	-0.280920
Li	-0.210473	-1.775591	-1.582426
Li	-6.273293	-0.355756	-0.139538
Li	0.528503	1.077780	1.184150
Li	1.889629	-3.863001	2.167969
Li	4.038867	-0.136450	0.193905
Li	3.088608	4.804650	0.890203
P	-1.976327	0.193662	1.025265
P	-4.878038	1.596258	-0.046244
P	-4.080783	0.367027	1.635475
P	-4.759853	-1.701474	1.147211
P	1.258687	4.435651	-1.164184
P	-4.206013	0.383557	-1.755374
P	-4.137460	-1.796863	-0.962275
P	-2.263396	-0.494001	-1.027888
P	0.480135	3.896228	0.911681
P	-0.047677	2.662860	-0.877465
P	2.139603	2.925856	2.038216
P	3.423155	-2.116306	1.611001
P	1.546930	-1.297585	0.756002
P	0.229364	-3.074764	0.604210
P	3.374779	3.680611	-1.224519
P	3.497285	2.281119	0.449522
P	2.131717	-1.030202	-1.355517
P	1.593522	-4.398957	-0.510912
P	3.723528	-3.748670	0.162874
P	2.876102	-3.041344	-1.797127

10

Li10 E = -2047.6628 eV

Li	1.761389	2.049310	-1.344736
Li	3.814201	-0.000821	0.000170
Li	1.131361	0.734752	1.118429
Li	1.760703	-2.049195	1.345871
Li	-1.131988	-1.119582	0.736868
Li	-3.814099	0.000593	0.001688
Li	-1.762540	-1.347676	-2.046600
Li	1.131271	-0.735453	-1.121444
Li	-1.132000	1.119966	-0.737877
Li	-1.758298	1.348106	2.047631

11

Li10P1 E = -11339.9920 eV

Li	-1.008085	0.905868	0.925280
----	-----------	----------	----------

Li	1.009655	0.905638	-0.925400
Li	1.640824	-0.151374	1.422280
Li	1.336866	2.989232	0.927320
Li	-1.640686	-0.149650	-1.421560
Li	2.066232	-1.733243	-0.859310
Li	-2.068478	-1.733101	0.857820
Li	-3.934967	0.821156	0.217950
Li	-1.334864	2.989984	-0.926050
Li	3.936333	0.818300	-0.220330
P	-0.000566	-1.132562	0.000400

12

Li10P2 E = -20632.2525 eV

Li	2.529946	-0.103293	2.219289
Li	3.519997	-1.899448	-0.259359
Li	3.522332	1.913908	-0.085687
Li	0.563768	0.081925	-1.771645
Li	-5.674618	-0.049214	1.059231
Li	-2.424426	-0.078144	1.677298
Li	0.307491	1.303648	0.565702
Li	-3.352740	1.385465	-0.502378
Li	0.307251	-1.349900	0.443479
Li	-3.352043	-1.333305	-0.629086
P	2.288144	0.003740	-0.076556
P	-1.477536	0.021932	-0.466813

13

Li10P3 E = -29924.2387 eV

Li	3.232859	-2.478727	-0.000290
Li	1.967038	0.000113	1.256280
Li	-1.056401	-1.771048	1.276660
Li	-0.056262	-0.000098	-0.000840
Li	1.968028	0.000183	-1.256010
Li	3.232457	2.479193	0.000050
Li	-1.056771	-1.771978	-1.276210
Li	-4.559762	-0.000060	-0.000180
Li	-1.056772	1.771282	1.276540
Li	-1.057142	1.771562	-1.276460
P	1.018999	-2.035118	0.000090
P	1.018688	2.035232	-0.000010
P	-2.349142	-0.000199	0.000010

14

Li10P4 E = -39215.5285 eV

Li	1.624003	-1.154210	1.482578
Li	1.221327	2.401677	-0.000712
Li	4.817951	0.537286	0.006108
Li	-1.284901	-3.452275	0.000878
Li	-1.112133	0.781705	1.974968
Li	1.623017	-1.156393	-1.484152
Li	0.249300	0.233856	-0.000442
Li	-2.386697	-0.209162	0.000928

Li	-1.113615	0.781726	-1.974832
Li	-2.442800	4.004696	0.000208
P	2.633212	0.429449	-0.002322
P	-0.806141	-1.566761	1.226148
P	-0.807300	-1.566879	-1.225422
P	-1.258862	2.150410	0.000488

15

Li10P5 E = -48506.0572 eV

Li	2.425667	0.592274	0.686866
Li	1.818624	4.453662	0.139172
Li	-0.013917	0.991227	1.642860
Li	-1.317877	2.522288	-0.273005
Li	-1.285903	-1.425980	1.386936
Li	-4.197664	0.087888	-0.771090
Li	-0.028520	0.119039	-0.654423
Li	2.063737	1.061292	-1.812000
Li	2.916801	-2.633655	0.653089
Li	-0.014214	-2.362955	-0.755917
P	1.009808	2.426538	-0.162371
P	-2.250637	-1.108213	-0.847142
P	-2.435593	0.551384	0.649012
P	1.131825	-1.321318	1.265683
P	2.071250	-1.229406	-0.953679

16

Li10P6 E = -57796.9964 eV

Li	-2.385160	-2.028526	-0.403111
Li	-1.806109	-0.000221	1.605004
Li	0.452705	-2.210287	1.406335
Li	0.454159	2.210353	1.406997
Li	2.903516	-0.000978	1.842364
Li	-2.385118	2.028194	-0.402810
Li	-5.641104	0.001666	0.275705
Li	-1.419127	-0.000177	-1.609008
Li	2.230918	-1.870815	-1.595260
Li	2.230527	1.871155	-1.595030
P	0.888172	0.000007	-0.040367
P	-0.000279	-1.908701	-0.896910
P	0.581795	-0.000442	2.225732
P	-3.470969	-0.000249	-0.101865
P	-0.000390	1.908959	-0.896280
P	3.074629	0.000353	-0.476548

17

Li10P7 E = -67087.3708 eV

Li	1.026451	1.319450	-2.351186
Li	-2.080796	-0.264998	-1.749605
Li	-1.010667	-1.761844	0.166333
Li	-5.360125	0.199544	-0.112810
Li	-0.815928	1.595446	0.046317
Li	1.280549	1.717392	2.062108

Li	2.262845	-1.607079	2.075855
Li	3.753938	1.292311	-0.201735
Li	2.335442	-1.983518	-1.713113
Li	-2.157315	-0.019577	1.816472
P	-3.258877	1.111900	-0.075072
P	0.279729	-0.856043	-1.785198
P	1.581728	2.205156	-0.238258
P	1.395959	-0.041163	-0.013374
P	3.395265	-0.991911	0.125662
P	-3.488668	-1.110840	0.086831
P	0.247985	-0.414525	1.891682

18

Li10P8 E = -76377.9406 eV

Li	3.321053	-1.447730	0.210533
Li	3.124119	1.208441	-1.468157
Li	0.798399	1.339322	2.295773
Li	-0.780636	2.562564	0.179833
Li	-0.798053	-1.332479	2.300103
Li	0.412513	1.383616	-2.113557
Li	-0.413822	-1.390094	-2.109207
Li	-3.318818	1.452492	0.204033
Li	-3.124657	-1.214664	-1.461947
Li	0.783213	-2.559224	0.184493
P	1.601823	2.252151	-0.024357
P	1.728548	-0.973633	1.882043
P	1.187013	0.106674	0.060363
P	-1.729161	0.980501	1.878783
P	-1.187524	-0.106346	0.060653
P	-1.985137	0.886072	-1.744677
P	-1.600829	-2.252733	-0.016037
P	1.984605	-0.893134	-1.741147

19

Li10P9 E = -85667.5565 eV

Li	-1.975268	-2.932258	0.907648
Li	-3.255251	-1.380012	-1.562234
Li	0.723639	-2.123644	1.036591
Li	-2.188471	1.359544	1.643408
Li	-1.260593	2.574304	-0.856924
Li	1.496624	3.251669	-0.573454
Li	0.473051	0.559460	2.709784
Li	3.132301	0.384478	-1.242885
Li	1.230105	-1.445427	-1.835931
Li	-1.098621	0.190074	-2.458506
P	-2.874907	0.780594	-0.727140
P	-1.375746	-1.048076	2.183829
P	-1.033902	-2.246803	-1.217776
P	-1.284378	-0.491054	0.083841
P	0.081395	2.598960	1.237182
P	2.334677	-0.162972	1.083221
P	0.635856	0.902633	0.009557

P 1.055783 1.367427 -2.081176
P 3.005719 -1.788347 -0.125038

20

Li10P10 E = -94957.8688 eV

Li 2.163970 2.275852 0.054870
Li 1.466985 0.962560 -2.347286
Li 0.255750 -3.188280 -0.423053
Li 2.520469 0.137553 1.862898
Li 2.826100 -1.592296 -2.216422
Li -0.460792 -0.216792 2.844030
Li -2.676403 2.249188 -0.962612
Li -1.964377 -1.877983 -1.042525
Li -1.350024 0.339179 -2.308824
Li -0.162158 3.661858 0.880301
P 3.211191 0.146413 -0.619560
P 0.406502 -1.476347 -2.218762
P 1.009200 -1.939414 1.431660
P 1.227719 -0.670729 -0.348735
P -2.149438 0.034314 0.833606
P -0.143132 1.062724 0.359539
P 0.762932 1.891868 2.153296
P -0.220169 2.526717 -1.264414
P -3.395265 -0.004813 -0.943256
P -1.233443 -2.120901 1.348350

21

Li10P11 E = -104247.9440 eV

Li 2.633283 -2.395528 0.846982
Li 1.686733 -1.605964 -1.906899
Li 3.961160 0.328071 1.310098
Li 0.938142 2.167890 1.501407
Li -0.851864 -0.296124 2.482120
Li 0.984750 2.202045 -1.476513
Li -0.175108 0.043122 -0.124638
Li -3.692026 1.838736 -0.561738
Li -2.273611 -2.281388 0.724712
Li 4.493188 1.161406 -1.332090
P 0.196739 -2.218081 1.203652
P -0.510188 -2.221959 -0.973555
P 3.824704 -1.074034 -0.829662
P 2.937781 2.349211 0.041476
P 1.491980 -0.364953 1.790162
P 2.186158 0.303671 -0.282774
P -1.473727 1.528132 -1.581432
P -1.502604 2.069745 0.610065
P -2.901625 0.621648 1.531763
P -3.723629 -0.575199 -0.162902
P -2.066519 -0.650634 -1.639482

22

Li10P12 E = -113538.0719 eV

Li	-0.311963	0.527028	-2.289029
Li	0.785378	1.682231	2.308304
Li	0.421444	2.625530	-0.482466
Li	0.243572	0.033037	0.390704
Li	4.175734	1.638170	-1.376213
Li	1.316867	-1.748148	-1.360935
Li	-3.158457	-2.624937	-0.260027
Li	-3.761722	2.053235	0.503107
Li	1.095694	-2.020999	1.779330
Li	4.685505	-0.029095	0.852009
P	-1.877569	1.999655	-0.979643
P	-1.482303	1.654835	1.308134
P	3.111308	-1.729513	0.500533
P	3.562510	-0.732213	-1.436905
P	2.618870	1.797349	0.483742
P	2.594275	0.061952	1.912585
P	1.981744	0.860542	-1.497834
P	-4.049114	-0.371471	0.216190
P	-2.377100	-0.373901	1.671977
P	-2.783126	0.034383	-1.564399
P	-1.283634	-1.641067	-1.463648
P	-1.114273	-1.987761	0.836311

23

Li10P13 E = -122828.0229 eV

Li	0.913984	-0.837019	1.037395
Li	4.512480	-1.324242	-1.562288
Li	3.177188	-0.112506	2.336637
Li	-3.503581	2.209823	1.074610
Li	-3.962332	1.772056	-1.520575
Li	-4.188018	-2.039077	1.222465
Li	-0.295346	-1.581037	-1.662414
Li	-0.824476	1.575539	1.359725
Li	0.569520	2.628554	-0.757972
Li	3.915146	2.319191	1.047935
P	2.126291	-1.251255	-1.080560
P	4.578461	1.021923	-0.821894
P	2.352269	0.944007	-0.799306
P	5.020444	-0.516437	0.733052
P	3.376802	-1.993186	0.608849
P	1.685983	1.530444	1.285680
P	-4.776544	0.177231	0.421900
P	-3.677700	-0.629285	-1.340921
P	-1.574715	-0.879754	0.806693
P	-1.655416	0.462255	-1.120018
P	-1.862141	2.576752	-0.708880
P	-2.508069	-2.367242	-0.562190
P	-3.148579	0.002291	2.062491

24

Li10P14 E = -132118.4539 eV

Li	0.291033	-0.675892	1.636048
----	----------	-----------	----------

Li	-4.224586	1.081327	2.192345
Li	-4.839410	-0.920155	-1.792662
Li	-0.271108	-2.334371	-0.914063
Li	0.069356	2.644201	-0.015635
Li	3.436936	-1.677156	1.927025
Li	4.492959	1.507772	-0.674929
Li	3.724281	-2.741191	-0.511993
Li	2.325244	1.118898	-2.344071
Li	3.485504	3.030640	1.381709
P	-4.196854	1.510062	-0.627871
P	-2.126437	1.467275	0.327679
P	-3.546818	-1.491237	0.844502
P	-2.163598	-0.089109	1.857821
P	-5.272968	-0.122526	0.421073
P	-2.657608	-1.657154	-1.180534
P	-2.414853	0.465612	-1.664582
P	1.574255	-2.499296	0.569576
P	3.978902	-0.698165	-1.677848
P	3.846019	0.647934	1.701072
P	5.101999	-0.687536	0.249305
P	1.967246	0.957872	0.534448
P	1.886373	-0.844725	-0.860890
P	2.326302	2.834181	-0.670506

25

Li10P15 E = -141408.3615 eV

Li	-6.365850	-0.224859	-0.421190
Li	0.262083	-0.945982	-1.602584
Li	-3.162259	3.343265	0.096114
Li	-2.559804	0.937646	1.392992
Li	0.317849	0.847448	1.631675
Li	1.105274	2.584466	-0.821534
Li	1.643383	-1.327621	0.626182
Li	-2.543256	-2.380590	-0.689353
Li	5.130046	1.353318	1.619402
Li	-2.893576	-1.687225	1.940571
P	-1.375165	0.610594	-0.802421
P	-4.799797	1.505916	0.277994
P	-3.583908	0.741833	-1.395233
P	-4.451985	-1.267002	-1.655778
P	-4.916330	-0.203815	1.732146
P	-4.873632	-1.970479	0.437236
P	-0.935493	-1.121085	0.631735
P	5.336640	1.279634	-0.778795
P	4.050280	-1.092612	1.664910
P	3.150846	1.203867	-0.637469
P	2.819762	0.730342	1.527953
P	5.710035	-0.697617	0.041075
P	-0.975178	2.479327	0.342588
P	3.971770	-2.007735	-0.496324
P	2.685378	-0.691142	-1.644071

26

Li10P16 E = -150698.4324 eV

Li	0.140969	2.491380	1.176423
Li	0.157672	-2.738443	-0.796258
Li	4.206809	2.330023	-0.652469
Li	4.266909	-2.280646	0.646840
Li	-0.414434	2.703749	-1.958914
Li	-1.090361	0.003861	0.638359
Li	-4.470243	-2.393943	0.331409
Li	-0.922203	-0.269995	-2.057929
Li	-0.267267	-2.117493	2.282688
Li	-4.509744	2.333710	-0.398562
P	1.832062	-2.414145	1.113954
P	1.772056	2.420754	-1.064571
P	3.222774	-0.803080	-1.612153
P	2.560258	2.834151	1.062519
P	3.226684	0.813702	1.600804
P	4.600794	0.022078	-0.020250
P	1.374939	-0.265388	1.102471
P	1.353986	0.257922	-1.107216
P	2.592696	-2.824313	-1.030240
P	-3.595314	0.300185	1.633908
P	-2.393946	2.015463	0.805497
P	-2.489453	1.608526	-1.491498
P	-5.068894	-0.030649	-0.001424
P	-2.538052	-1.658673	1.544077
P	-3.588796	-0.325888	-1.624637
P	-2.281415	-1.963085	-0.753559

27

Li10P17 E = -159988.6876 eV

Li	3.507031	-2.815539	-1.893486
Li	-4.841936	-0.244642	-2.129674
Li	-1.125973	-2.600884	-0.432631
Li	0.633333	-1.472107	1.479925
Li	0.020393	1.102370	-1.741005
Li	2.023500	3.117063	1.352686
Li	-0.263178	1.423308	1.651821
Li	3.554969	1.971409	-0.988480
Li	-2.475438	3.135546	0.471744
Li	0.984700	5.500156	0.316703
P	1.475144	-2.580513	-0.621000
P	3.088584	-2.988177	0.835235
P	-3.823606	1.384136	-0.697153
P	-2.130006	-0.004870	-0.985459
P	-3.102759	-1.852296	-1.739313
P	-5.058208	0.105010	0.590454
P	-3.661763	-1.220842	1.752572
P	-4.595162	-2.061137	-0.122966
P	-1.680674	-0.601864	1.092893
P	1.933664	-0.434829	-1.009296
P	4.817010	-1.583166	0.159039

P	4.057093	-0.502248	-1.601992
P	3.509365	-1.007642	1.894623
P	2.119223	0.434765	1.020694
P	-0.348068	3.797059	1.313937
P	2.486126	4.090545	-0.835991
P	0.510557	3.202733	-0.663798

28

Li10P18 E = -169278.9932 eV

Li	-2.127548	2.426191	1.258874
Li	0.392383	1.168528	1.888655
Li	-0.272953	-1.875924	1.436859
Li	-3.158403	-3.217536	-1.968392
Li	-4.193353	1.486971	-0.845104
Li	-0.059213	1.016603	-1.682873
Li	2.227385	3.288346	0.599769
Li	4.903969	0.261705	-2.134367
Li	1.510871	-2.625067	-0.599969
Li	-1.722454	4.940726	0.662061
P	-3.881493	-0.977632	-1.492873
P	-3.165656	-1.647680	1.939957
P	-1.747208	-0.762697	-0.972417
P	-1.898598	-0.081792	1.113982
P	-2.622316	-3.516534	0.733799
P	-4.485604	-2.228343	0.215062
P	-1.105372	-2.880513	-0.748947
P	0.063497	3.599356	1.653813
P	-2.099614	3.216562	-1.370098
P	3.738945	1.640094	-0.557910
P	2.217117	0.082772	-0.934056
P	3.386283	-1.573777	-1.836696
P	5.152354	0.427357	0.598836
P	3.959227	-1.143027	1.679867
P	4.936675	-1.721806	-0.268594
P	1.901431	-0.716379	1.105458
P	-0.144999	3.164032	-0.483669
P	-3.704806	3.745900	-0.098617

29

Li10P19 E = -178568.7162 eV

Li	-0.253019	0.377394	2.125654
Li	0.761260	-3.023861	-0.211984
Li	5.312866	-2.710710	0.080148
Li	-0.968762	-1.228713	-1.488721
Li	-3.798622	-3.438587	1.361082
Li	-0.021862	1.637329	-0.872177
Li	3.096244	1.392947	-0.593123
Li	-2.626885	2.842347	0.206339
Li	0.741587	5.679946	-0.300399
Li	1.169628	4.665364	2.224289
P	1.775086	-0.823952	1.129638
P	4.813475	-0.469448	-0.612028

P	3.997874	-0.701142	1.422354
P	2.946228	-2.764593	1.428607
P	3.305978	-1.637039	-1.754062
P	3.173836	-3.552599	-0.616904
P	1.470272	-0.648698	-1.032171
P	-4.392294	-1.138928	1.759717
P	-2.274335	-0.863987	1.271838
P	-2.379157	0.478968	-0.474815
P	-3.295083	-2.840753	-1.257390
P	-5.067961	-1.705628	-0.232817
P	-1.733066	-2.808401	0.304552
P	-3.773044	-0.642533	-1.731009
P	-1.146299	4.465529	-1.126909
P	0.844406	3.798144	-1.775796
P	0.223980	2.695193	1.493052
P	1.887888	3.428469	0.180214
P	-1.060272	4.492708	1.117709

30

Li10P20 E = -187859.1765 eV

Li	0.162796	0.024905	-2.220029
Li	4.185820	-2.808532	-1.805347
Li	-3.867386	-2.107740	2.444465
Li	-0.497955	-2.834374	-0.621234
Li	0.967356	-2.015161	1.588853
Li	3.156185	1.854218	-0.796676
Li	-1.503436	1.924497	0.858807
Li	-3.505235	1.129362	-1.266264
Li	-0.472397	4.881224	-1.897832
Li	1.076277	2.402730	1.042721
P	3.816593	-2.978917	0.899421
P	2.179241	-0.823425	-1.038079
P	5.227796	-1.276108	0.144402
P	4.260410	-0.411241	-1.632639
P	2.138353	-2.976200	-0.546911
P	2.097267	0.084776	0.972367
P	3.826746	-0.912952	1.860246
P	-4.487178	-0.611168	0.668089
P	-2.296224	-0.487694	0.578409
P	-2.005007	-1.010783	-1.549267
P	-4.707056	-2.650720	-0.122350
P	-2.794211	-3.793490	0.519438
P	-3.053894	-2.917020	-1.615207
P	-1.600414	-2.307648	1.638873
P	-2.034509	3.200681	-1.274901
P	-0.092976	2.123632	-1.155462
P	1.430665	3.733792	-1.059385
P	0.493728	5.016795	0.615789
P	-1.752293	4.670486	0.465029
P	-0.587441	3.836977	2.166645