Machine learning using structural representations for discovery of high temperature  
superconductors  
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Fd-3m

data\_Li4Mg2H32

\_symmetry\_space\_group\_name\_H-M 'P 1'

\_cell\_length\_a 4.75000000

\_cell\_length\_b 4.75000000

\_cell\_length\_c 4.75000000

\_cell\_angle\_alpha 60.00000000

\_cell\_angle\_beta 60.00000000

\_cell\_angle\_gamma 60.00000000

\_symmetry\_Int\_Tables\_number 1

\_chemical\_formula\_structural Li4Mg2H32

\_chemical\_formula\_sum 'Li4 Mg2 H32'

\_cell\_formula\_units\_Z 1

loop\_

\_symmetry\_equiv\_pos\_site\_id

\_symmetry\_equiv\_pos\_as\_xyz

1 'x, y, z'

loop\_

\_atom\_site\_type\_symbol

\_atom\_site\_label

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_occupancy

H H0 1 0.16695000 0.16694500 0.49916000 1

H H1 1 0.25084000 0.58305500 0.58305000 1

H H2 1 0.16695000 0.49916000 0.16694500 1

H H3 1 0.58305500 0.58305500 0.58305000 1

H H4 1 0.16694500 0.16694500 0.16695000 1

H H5 1 0.58305500 0.25084000 0.58305500 1

H H6 1 0.49916000 0.16694500 0.16694500 1

H H7 1 0.58304500 0.58305500 0.25084000 1

H H8 1 0.12508000 0.74560000 0.38372000 1

H H9 1 0.36628000 0.62492000 0.00440000 1

H H10 1 0.74560000 0.38372000 0.74560000 1

H H11 1 0.00440000 0.00440000 0.62492000 1

H H12 1 0.74560000 0.12508000 0.74560000 1

H H13 1 0.62492000 0.36628000 0.00440000 1

H H14 1 0.38372000 0.74560000 0.12508000 1

H H15 1 0.00440000 0.00440000 0.36628000 1

H H16 1 0.74560000 0.38372000 0.12508000 1

H H17 1 0.62492000 0.00440000 0.36628000 1

H H18 1 0.38372000 0.74560000 0.74560000 1

H H19 1 0.00440000 0.62492000 0.00440000 1

H H20 1 0.12508000 0.74560000 0.74560000 1

H H21 1 0.36628000 0.00440000 0.62492000 1

H H22 1 0.74560000 0.12508000 0.38372000 1

H H23 1 0.00440000 0.36628000 0.00440000 1

H H24 1 0.38372000 0.12508000 0.74560000 1

H H25 1 0.00440000 0.36628000 0.62492000 1

H H26 1 0.74560000 0.74560000 0.38372000 1

H H27 1 0.62492000 0.00440000 0.00440000 1

H H28 1 0.74560000 0.74560000 0.12508000 1

H H29 1 0.00440000 0.62492000 0.36628000 1

H H30 1 0.12508000 0.38372000 0.74560000 1

H H31 1 0.36628000 0.00440000 0.00440000 1

Li X32 1 0.37500000 0.37500000 0.87500000 1

Li X33 1 0.87500000 0.37500000 0.37500000 1

Li X34 1 0.37500000 0.87500000 0.37500000 1

Li X35 1 0.37500000 0.37500000 0.37500000 1

Mg Y36 1 0.00000000 0.00000000 0.00000000 1

Mg Y37 1 0.75000000 0.75000000 0.75000000 1

data\_MgH13

\_symmetry\_space\_group\_name\_H-M 'P 1'

\_cell\_length\_a 3.46956

\_cell\_length\_b 3.46956

\_cell\_length\_c 3.46956

\_cell\_angle\_alpha 60.00000000

\_cell\_angle\_beta 60.00000000

\_cell\_angle\_gamma 60.00000000

\_symmetry\_Int\_Tables\_number 1

\_chemical\_formula\_structural MgH13

\_chemical\_formula\_sum 'Mg1 H13'

\_cell\_volume 19.09188309

\_cell\_formula\_units\_Z 1

loop\_

\_symmetry\_equiv\_pos\_site\_id

\_symmetry\_equiv\_pos\_as\_xyz

1 'x, y, z'

loop\_

\_atom\_site\_type\_symbol

\_atom\_site\_label

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_occupancy

H Y0 1 0.50000000 0.50000000 0.50000000 1

Mg X1 1 0.00000000 0.00000000 0.00000000 1

H H2 1 0.38369000 0.00000000 0.61631000 1

H H3 1 0.61631000 0.00000000 0.38369000 1

H H4 1 0.38369000 0.00000000 0.00000000 1

H H5 1 1.00000000 0.00000000 0.38369000 1

H H6 1 0.61631000 0.00000000 0.00000000 1

H H7 1 1.00000000 0.00000000 0.61631000 1

H H8 1 0.38369000 0.61631000 0.00000000 1

H H9 1 0.00000000 0.61631000 0.38369000 1

H H10 1 1.00000000 0.61631000 0.00000000 1

H H11 1 0.61631000 0.38369000 0.00000000 1

H H12 1 0.00000000 0.38369000 0.61631000 1

H H13 1 0.00000000 0.38369000 0.00000000 1

|  |
| --- |
| P3m1 |
|  | data\_Li2MgH16 |
|  | \_symmetry\_space\_group\_name\_H-M 'P 1' |
|  | \_cell\_length\_a 2.79596300 |
|  | \_cell\_length\_b 2.79596300 |
|  | \_cell\_length\_c 5.3130000 |
|  | \_cell\_angle\_alpha 90.00000000 |
|  | \_cell\_angle\_beta 90.00000000 |
|  | \_cell\_angle\_gamma 120.00000000 |
|  | \_symmetry\_Int\_Tables\_number 1 |
|  | \_chemical\_formula\_structural Li2MgH16 |
|  | \_chemical\_formula\_sum 'Li2 Mg1 H16' |
|  | \_cell\_volume 35.97204811 |
|  | \_cell\_formula\_units\_Z 1 |
|  | loop\_ |
|  | \_symmetry\_equiv\_pos\_site\_id |
|  | \_symmetry\_equiv\_pos\_as\_xyz |
|  | 1 'x, y, z' |
|  | loop\_ |
|  | \_atom\_site\_type\_symbol |
|  | \_atom\_site\_label |
|  | \_atom\_site\_symmetry\_multiplicity |
|  | \_atom\_site\_fract\_x |
|  | \_atom\_site\_fract\_y |
|  | \_atom\_site\_fract\_z |
|  | \_atom\_site\_occupancy |
|  | Li Li0 1 0.33333333 0.66666667 0.83626000 1 |
|  | Li Li1 1 0.66666667 0.33333333 0.16374000 1 |
|  | Mg Mg2 1 0.00000000 0.00000000 0.50000000 1 |
|  | H H3 1 0.82843000 0.17158000 0.92030000 1 |
|  | H H4 1 0.17157000 0.82842000 0.07970000 1 |
|  | H H5 1 0.34315000 0.17157000 0.92030000 1 |
|  | H H6 1 0.65685000 0.82843000 0.07970000 1 |
|  | H H7 1 0.82842000 0.65685000 0.92030000 1 |
|  | H H8 1 0.17158000 0.34315000 0.07970000 1 |
|  | H H9 1 0.66666667 0.33333333 0.42549000 1 |
|  | H H10 1 0.33333333 0.66666667 0.57451000 1 |
|  | H H11 1 0.33333333 0.66666667 0.39139000 1 |
|  | H H12 1 0.66666667 0.33333333 0.60861000 1 |
|  | H H13 1 0.32880000 0.16440000 0.76347000 1 |
|  | H H14 1 0.67120000 0.83560000 0.23653000 1 |
|  | H H15 1 0.83560000 0.67120000 0.76347000 1 |
|  | H H16 1 0.16440000 0.32880000 0.23653000 1 |
|  | H H17 1 0.83560000 0.16440000 0.76347000 1 |
|  | H H18 1 0.16440000 0.83560000 0.23653000 1 |

Im-3m

|  |  |
| --- | --- |
|  | # generated using pymatgen |
|  | data\_SeH3 |
|  | \_symmetry\_space\_group\_name\_H-M 'P 1' |
|  | \_cell\_length\_a 2.24900000 |
|  | \_cell\_length\_b 2.24900000 |
|  | \_cell\_length\_c 2.24900000 |
|  | \_cell\_angle\_alpha 109.47122200 |
|  | \_cell\_angle\_beta 109.47121927 |
|  | \_cell\_angle\_gamma 109.47121927 |
|  | \_symmetry\_Int\_Tables\_number 1 |
|  | \_chemical\_formula\_structural SeH3 |
|  | \_chemical\_formula\_sum 'Se1 H3' |
|  | \_cell\_volume 8.75682121 |
|  | \_cell\_formula\_units\_Z 1 |
|  | loop\_ |
|  | \_symmetry\_equiv\_pos\_site\_id |
|  | \_symmetry\_equiv\_pos\_as\_xyz |
|  | 1 'x, y, z' |
|  | loop\_ |
|  | \_atom\_site\_type\_symbol |
|  | \_atom\_site\_label |
|  | \_atom\_site\_symmetry\_multiplicity |
|  | \_atom\_site\_fract\_x |
|  | \_atom\_site\_fract\_y |
|  | \_atom\_site\_fract\_z |
|  | \_atom\_site\_occupancy |
|  | H H0 1 0.00000000 0.50000000 0.50000000 1 |
|  | H H1 1 0.50000000 0.50000000 0.00000000 1 |
|  | H H2 1 0.50000000 0.00000000 0.50000000 1 |
|  | Se X3 1 0.00000000 0.00000000 0.00000000 1 |

Fd-3m Li2MgH16 variants. X: Labels sites part of random search detailed in morphisms section.

# generated using pymatgen

data\_LaH32N4O

\_symmetry\_space\_group\_name\_H-M 'P 1'

\_cell\_length\_a 4.7500

\_cell\_length\_b 4.7500

\_cell\_length\_c 4.7500

\_cell\_angle\_alpha 60.00000000

\_cell\_angle\_beta 60.00000000

\_cell\_angle\_gamma 60.00000000

\_symmetry\_Int\_Tables\_number 1

\_chemical\_formula\_structural LaH32N4O

\_chemical\_formula\_sum 'La1 H32 N4 O1'

\_cell\_volume 21.06541812

\_cell\_formula\_units\_Z 1

loop\_

\_symmetry\_equiv\_pos\_site\_id

\_symmetry\_equiv\_pos\_as\_xyz

1 'x, y, z'

loop\_

\_atom\_site\_type\_symbol

\_atom\_site\_label

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_occupancy

H H0 1 0.16695000 0.16694500 0.49916000 1

H H1 1 0.25084000 0.58305500 0.58305000 1

H H2 1 0.16695000 0.49916000 0.16694500 1

H H3 1 0.58305500 0.58305500 0.58305000 1

H H4 1 0.16694500 0.16694500 0.16695000 1

H H5 1 0.58305500 0.25084000 0.58305500 1

H H6 1 0.49916000 0.16694500 0.16694500 1

H H7 1 0.58304500 0.58305500 0.25084000 1

H H8 1 0.12508000 0.74560000 0.38372000 1

H H9 1 0.36628000 0.62492000 0.00440000 1

H H10 1 0.74560000 0.38372000 0.74560000 1

H H11 1 0.00440000 0.00440000 0.62492000 1

H H12 1 0.74560000 0.12508000 0.74560000 1

H H13 1 0.62492000 0.36628000 0.00440000 1

H H14 1 0.38372000 0.74560000 0.12508000 1

H H15 1 0.00440000 0.00440000 0.36628000 1

H H16 1 0.74560000 0.38372000 0.12508000 1

H H17 1 0.62492000 0.00440000 0.36628000 1

H H18 1 0.38372000 0.74560000 0.74560000 1

H H19 1 0.00440000 0.62492000 0.00440000 1

H H20 1 0.12508000 0.74560000 0.74560000 1

H H21 1 0.36628000 0.00440000 0.62492000 1

H H22 1 0.74560000 0.12508000 0.38372000 1

H H23 1 0.00440000 0.36628000 0.00440000 1

H H24 1 0.38372000 0.12508000 0.74560000 1

H H25 1 0.00440000 0.36628000 0.62492000 1

H H26 1 0.74560000 0.74560000 0.38372000 1

H H27 1 0.62492000 0.00440000 0.00440000 1

H H28 1 0.74560000 0.74560000 0.12508000 1

H H29 1 0.00440000 0.62492000 0.36628000 1

H H30 1 0.12508000 0.38372000 0.74560000 1

H H31 1 0.36628000 0.00440000 0.00440000 1

N X32 1 0.37500000 0.37500000 0.87500000 1

N X33 1 0.87500000 0.37500000 0.37500000 1

N X34 1 0.37500000 0.87500000 0.37500000 1

N X35 1 0.37500000 0.37500000 0.37500000 1

O X36 1 0.00000000 0.00000000 0.00000000 1

La X37 1 0.75000000 0.75000000 0.75000000 1

# generated using pymatgen

data\_BaH32N5

\_symmetry\_space\_group\_name\_H-M 'P 1'

\_cell\_length\_a 4.75000

\_cell\_length\_b 4.75000

\_cell\_length\_c 4.75000

\_cell\_angle\_alpha 60.00000000

\_cell\_angle\_beta 60.00000000

\_cell\_angle\_gamma 60.00000000

\_symmetry\_Int\_Tables\_number 1

\_chemical\_formula\_structural BaH32N5

\_chemical\_formula\_sum 'Ba1 H32 N5'

\_cell\_volume 130.95122613

\_cell\_formula\_units\_Z 1

loop\_

\_symmetry\_equiv\_pos\_site\_id

\_symmetry\_equiv\_pos\_as\_xyz

1 'x, y, z'

loop\_

\_atom\_site\_type\_symbol

\_atom\_site\_label

\_atom\_site\_symmetry\_multiplicity

\_atom\_site\_fract\_x

\_atom\_site\_fract\_y

\_atom\_site\_fract\_z

\_atom\_site\_occupancy

H H0 1 0.16695000 0.16694500 0.49916000 1

H H1 1 0.25084000 0.58305500 0.58305000 1

H H2 1 0.16695000 0.49916000 0.16694500 1

H H3 1 0.58305500 0.58305500 0.58305000 1

H H4 1 0.16694500 0.16694500 0.16695000 1

H H5 1 0.58305500 0.25084000 0.58305500 1

H H6 1 0.49916000 0.16694500 0.16694500 1

H H7 1 0.58304500 0.58305500 0.25084000 1

H H8 1 0.12508000 0.74560000 0.38372000 1

H H9 1 0.36628000 0.62492000 0.00440000 1

H H10 1 0.74560000 0.38372000 0.74560000 1

H H11 1 0.00440000 0.00440000 0.62492000 1

H H12 1 0.74560000 0.12508000 0.74560000 1

H H13 1 0.62492000 0.36628000 0.00440000 1

H H14 1 0.38372000 0.74560000 0.12508000 1

H H15 1 0.00440000 0.00440000 0.36628000 1

H H16 1 0.74560000 0.38372000 0.12508000 1

H H17 1 0.62492000 0.00440000 0.36628000 1

H H18 1 0.38372000 0.74560000 0.74560000 1

H H19 1 0.00440000 0.62492000 0.00440000 1

H H20 1 0.12508000 0.74560000 0.74560000 1

H H21 1 0.36628000 0.00440000 0.62492000 1

H H22 1 0.74560000 0.12508000 0.38372000 1

H H23 1 0.00440000 0.36628000 0.00440000 1

H H24 1 0.38372000 0.12508000 0.74560000 1

H H25 1 0.00440000 0.36628000 0.62492000 1

H H26 1 0.74560000 0.74560000 0.38372000 1

H H27 1 0.62492000 0.00440000 0.00440000 1

H H28 1 0.74560000 0.74560000 0.12508000 1

H H29 1 0.00440000 0.62492000 0.36628000 1

H H30 1 0.12508000 0.38372000 0.74560000 1

H H31 1 0.36628000 0.00440000 0.00440000 1

N X32 1 0.37500000 0.37500000 0.87500000 1

N X33 1 0.87500000 0.37500000 0.37500000 1

N X34 1 0.37500000 0.87500000 0.37500000 1

N X35 1 0.37500000 0.37500000 0.37500000 1

N X36 1 0.00000000 0.00000000 0.00000000 1

Ba X37 1 0.75000000 0.75000000 0.75000000 1