Machine learning using structural representations for discovery of high temperature superconductors

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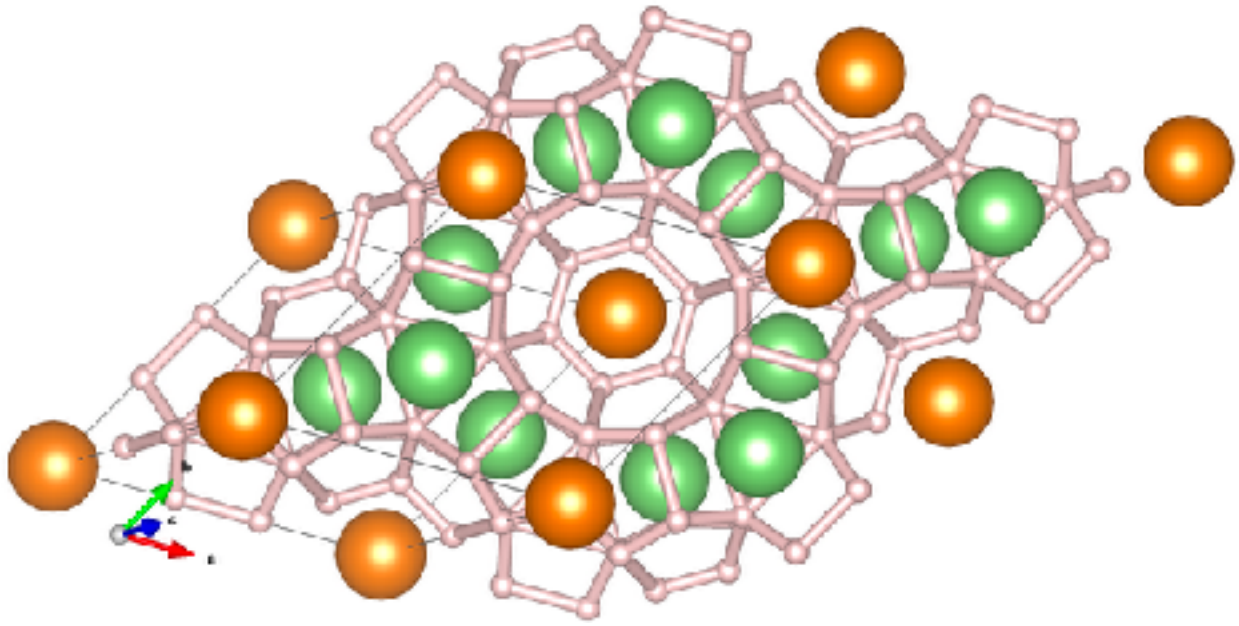

Fig 1. Fd-3m Li2MgH16 To show the clathrate structure all the H-H bonds were taken to be 1.6 A.

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_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'

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 _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

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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

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Mg Y37 1 0.75000000 0.75000000 0.75000000 1

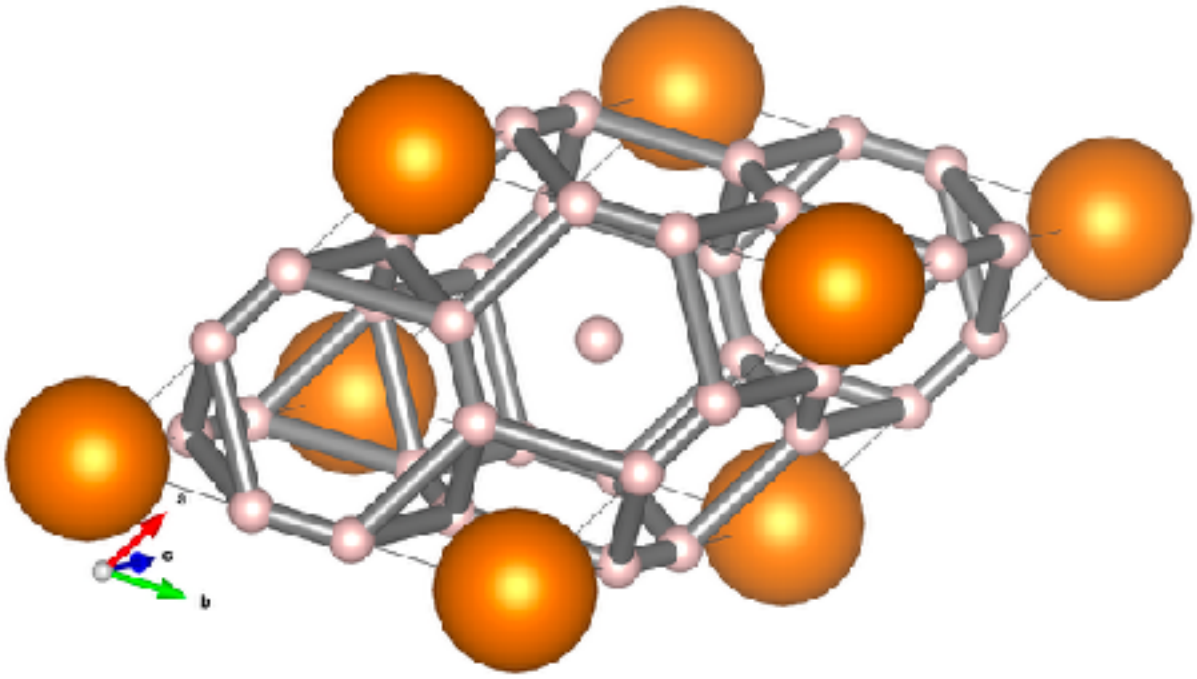

Fig 2. Fm-3m MgH13 Atoms Mg (X1) and H (Y0) are replaced in variants. To show the clathrate structure all the H-H bonds were taken to be 1.6 A.

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

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_cell_angle_beta 60.00000000

_cell_angle_gamma 60.00000000

_symmetry_Int_Tables_number 1

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_chemical_formula_sum 'Mg1 H13'

_cell_volume 19.09188309

_cell_formula_units_Z 1

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_symmetry_equiv_pos_as_xyz

1 'x, y, z'

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_atom_site_type_symbol

_atom_site_label

_atom_site_symmetry_multiplicity

_atom_site_fract_x

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_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

P-3m1

data_Li2MgH16

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_cell_length_c 5.3130000

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_cell_angle_beta 90.00000000

_cell_angle_gamma 120.00000000

_symmetry_Int_Tables_number 1

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_chemical_formula_sum 'Li2 Mg1 H16'

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_cell_formula_units_Z 1

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_symmetry_equiv_pos_as_xyz
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_atom_site_label
_atom_site_symmetry_multiplicity
_atom_site_fract_x
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_atom_site_occupancy
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Li Li1 1 0.66666667 0.33333333 0.16374000 1
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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
data_SeH3
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_atom_site_symmetry_multiplicity
_atom_site_fract_x
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_atom_site_fract_z
_atom_site_occupancy
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H H2 1 0.50000000 0.00000000 0.50000000 1
Se X3 1 0.00000000 0.00000000 0.00000000 1

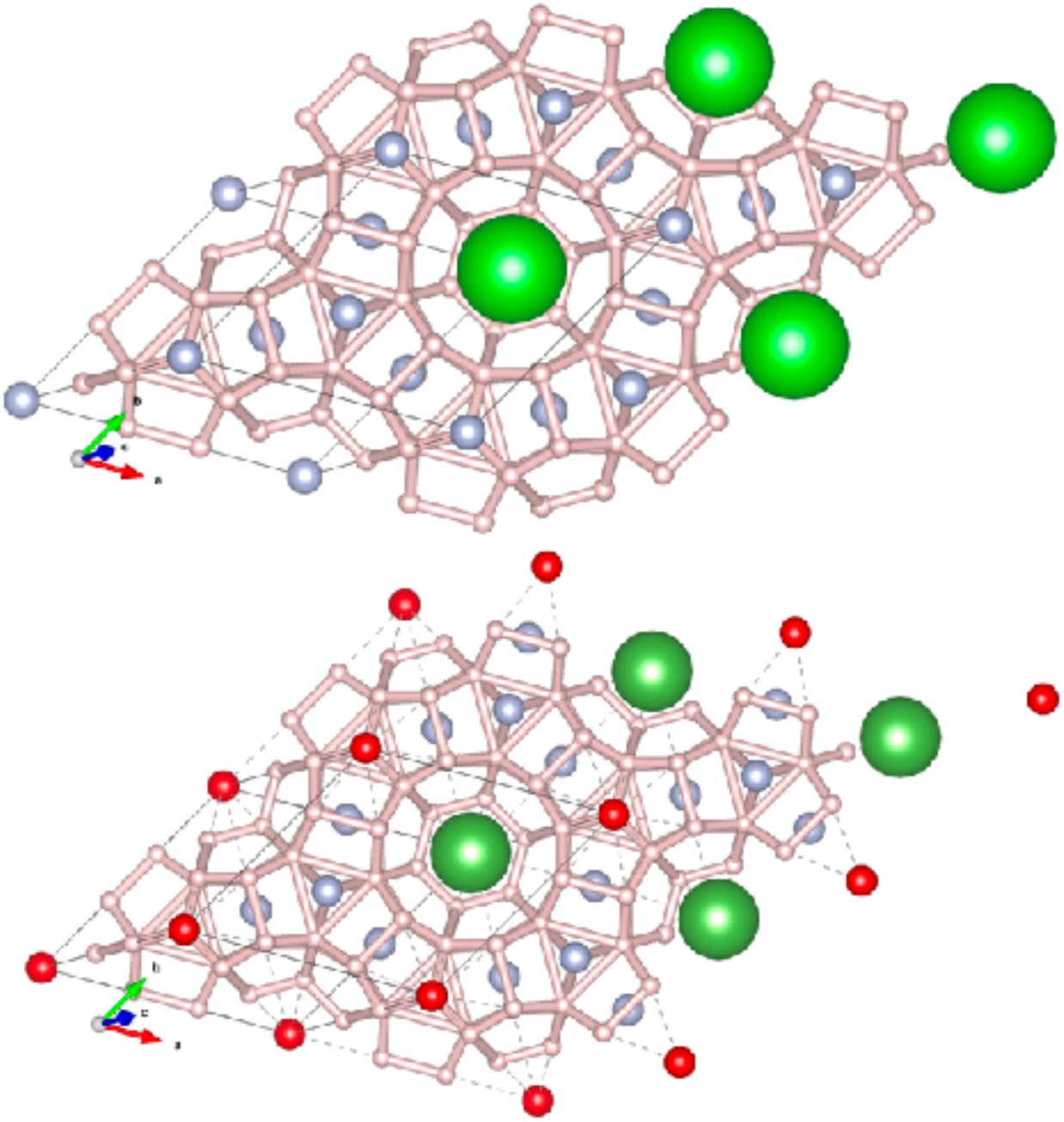

Fig 3. Fd-3m Li2MgH16 variants. X: Labels sites part of random search detailed in morphisms section. To show the clathrate structure all the H-H bonds were taken to be 1.6 A.

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_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

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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

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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

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La X37 1 0.75000000 0.75000000 0.75000000 1

BaH32N5

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_cell_length_b 4.75000

_cell_length_c 4.75000

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 _atom_site_occupancy
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  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
```

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H H5 1 0.58305500 0.25084000 0.58305500 1

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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

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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