Machine learning using structural representations for discovery of high temperature superconductors

Lazar Novakovic,[1,2] Ashkan Salamat,[1,2,*] and Keith V. Lawler [2,†]
1 Department of Physics & Astronomy, University of Nevada, Las Vegas, Las Vegas, Nevada 89154, USA
2 Nevada Extreme Conditions Laboratory, University of Nevada, Las Vegas, Las Vegas, NV 89154, USA

* salamat@physics.unlv.edu
† keith.lawler@unlv.edu

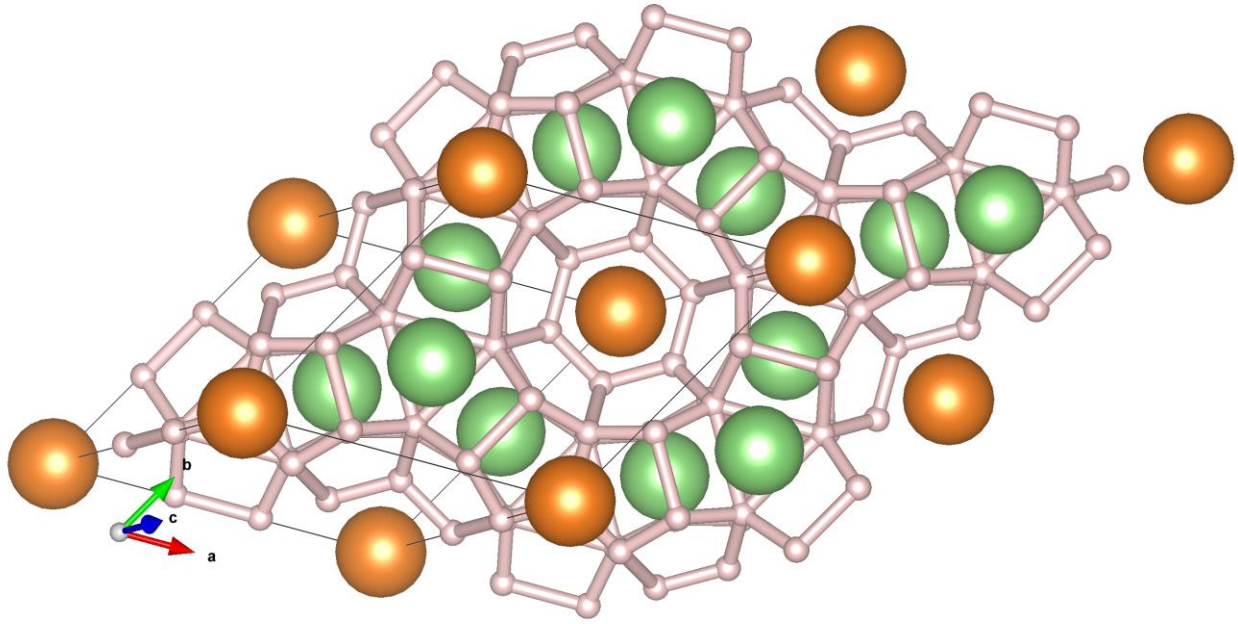

Fig 1. Fd-3m Li2MgH16 To show the clathrate structure all the H-H bonds were taken to be 1.6 A. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

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data_Li4Mg2H32
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_cell_length_c   4.75000000
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cell_angle_beta   60.00000000
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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
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
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H H12 1 0.74560000 0.12508000 0.74560000 1
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H H17 1 0.62492000 0.00440000 0.36628000 1
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H H25 1 0.00440000 0.36628000 0.62492000 1
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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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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

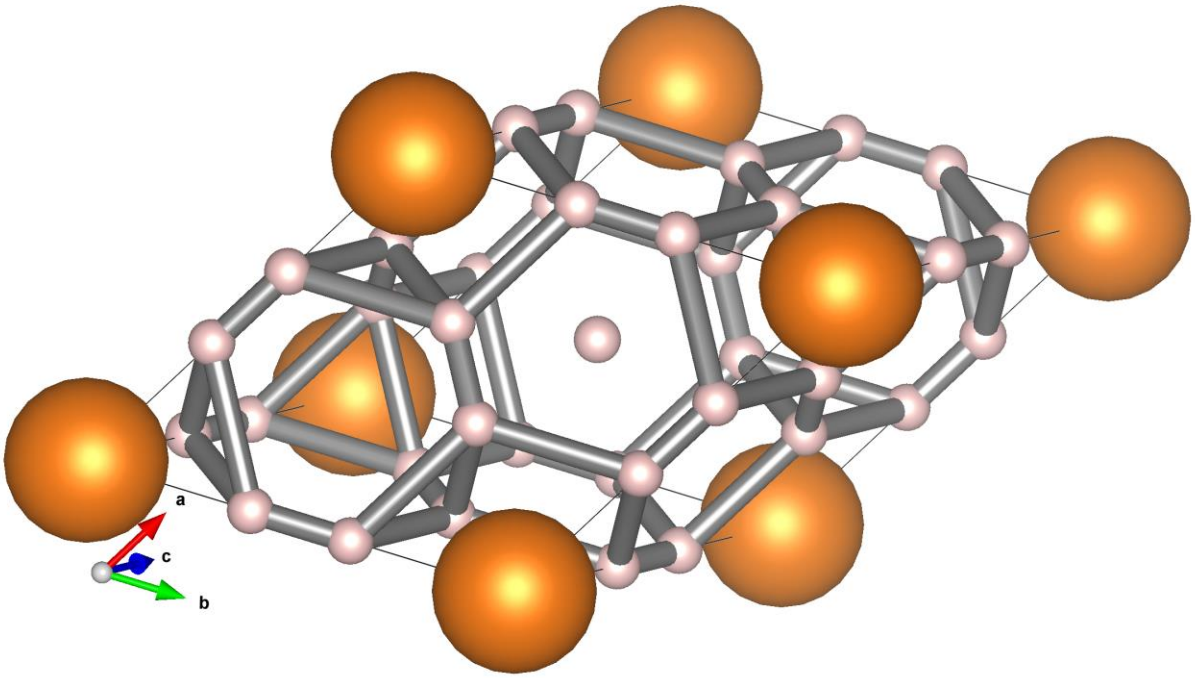

Fig 2. Fm-3m MgH13 Atoms Mg (X1) and H (Y0) are replaced in variants. To show the clathrate structure all the H-H bonds were taken to be 1.6 A. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

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_cell_angle_beta   60.00000000
_cell_angle_gamma   60.00000000
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 _atom_site_fract_x
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_atom_site_fract_z
_atom_site_occupancy
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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_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
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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
Mg Mg2 1 0.00000000 0.00000000 0.50000000 1
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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
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_cell_length_b 2.24900000
_cell_length_c 2.24900000
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_cell_angle_gamma 109.47121927
_symmetry_Int_Tables_number 1
_chemical_formula_structural SeH3
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loop_
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_atom_site_label
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
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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

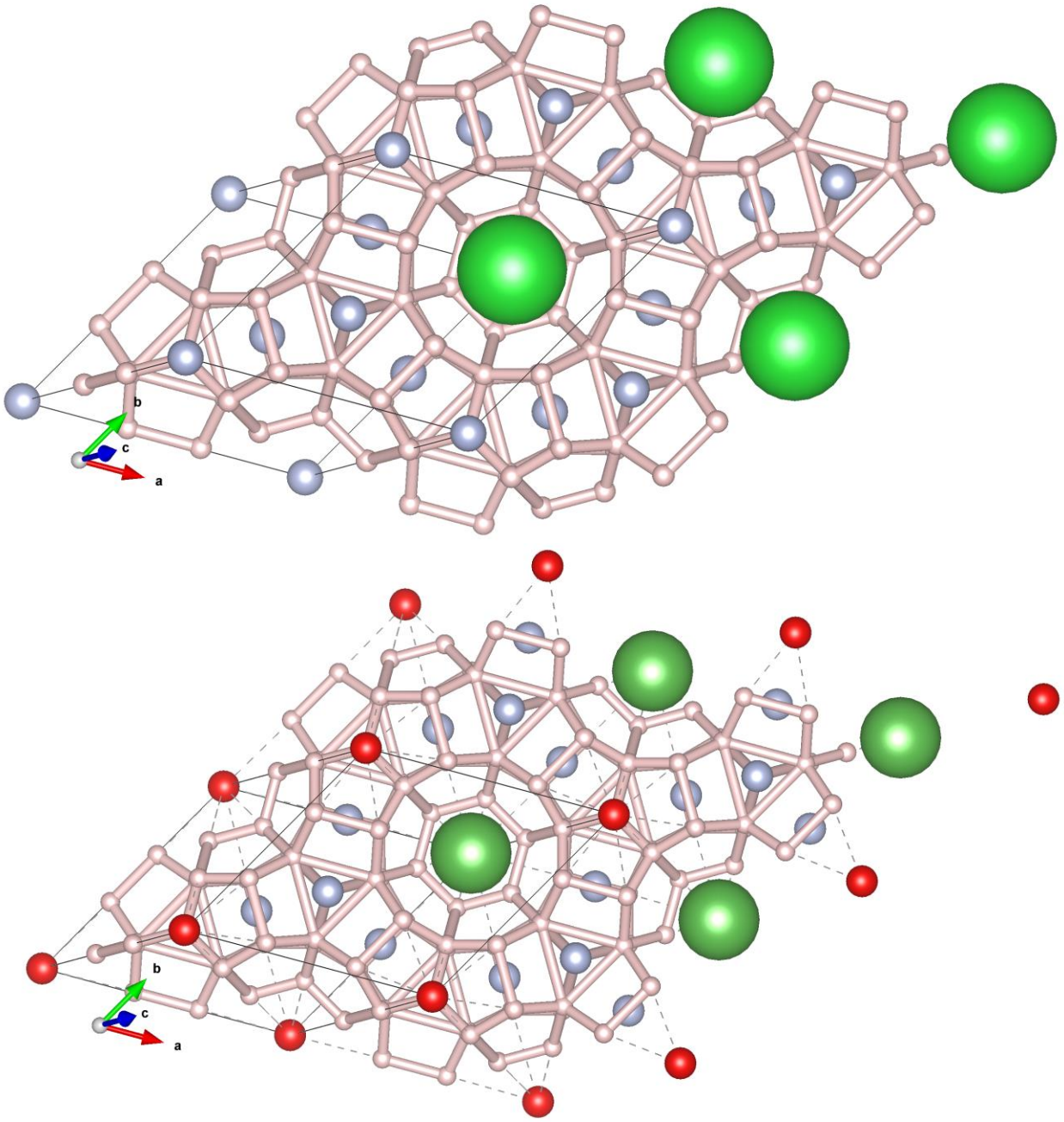

Fig 3. Fd-3m Li2MgH16 as BaH32N5 (top) and LaH32N4O (bottom) variants. X: Labels sites part of random search detailed in morphisms section. To show the clathrate structure all the H-H bonds were taken to be 1.6 A. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

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data_LaH32N4O
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_cell_length_b   4.7500
_cell_length_c   4.7500
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_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
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 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
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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
  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
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  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
```

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  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
  O  X36  1  0.00000000  0.00000000  0.00000000  1
  La X37  1  0.75000000  0.75000000  0.75000000  1

BaH32N5
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_cell_length_b   4.75000
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_symmetry_Int_Tables_number   1
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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
  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
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```

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H H13 1 0.62492000 0.36628000 0.00440000 1
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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
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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
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Ba X37 1 0.75000000 0.75000000 0.75000000 1