Machine learning using structural representations for discovery of high temperature superconductors

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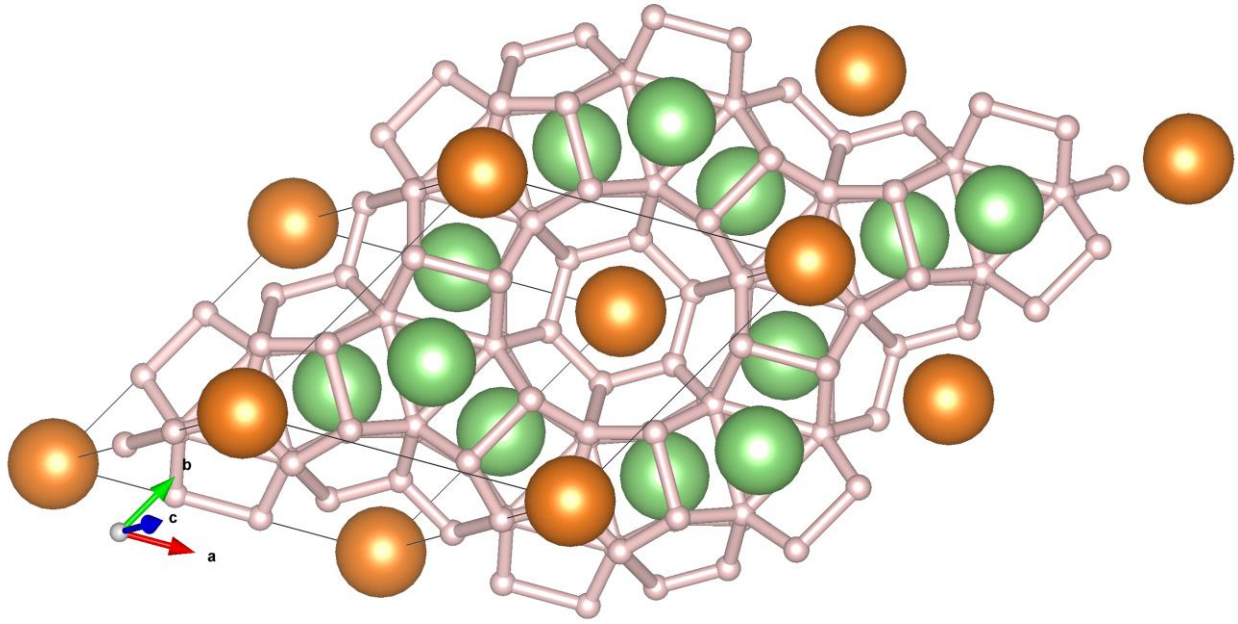

Fig S1. Fd-3m Li2MgH16 To show the clathrate structure all the H-H bonds were taken to be 1.6 A. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

Table S1: The crystallographic information for Fd-3m Li2MgH16 in a P1 representation. X: Labels sites part of random search detailed in the morphisms section in the main text.

```
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 X36 1 0.00000000 0.00000000 0.00000000 1
Mg X37 1 0.75000000 0.75000000 0.75000000 1

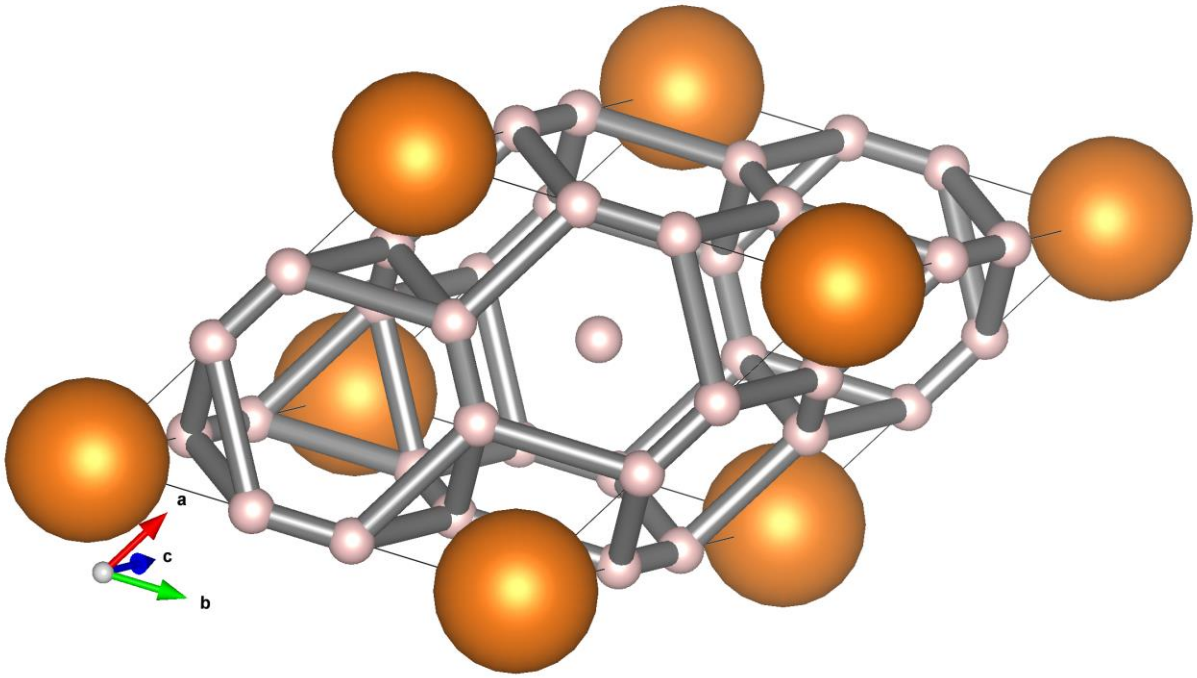

Fig S2. Fm-3m MgH13 To show the clathrate structure all the H-H bonds were taken to be 1.6 A. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

Table S2: The crystallographic information for Fm-3m MgH13 in a P1 representation. Atoms Mg (X1) and H (Y0) are replaced in variants.

```
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

Table S3: The crystallographic information for P-3m1 Li2MgH16 in a P1 representation as described in the results section of the main text.

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

Table S4: The crystallographic information for the Im-3m SeH3 variation of H3S in a P1 representation.

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

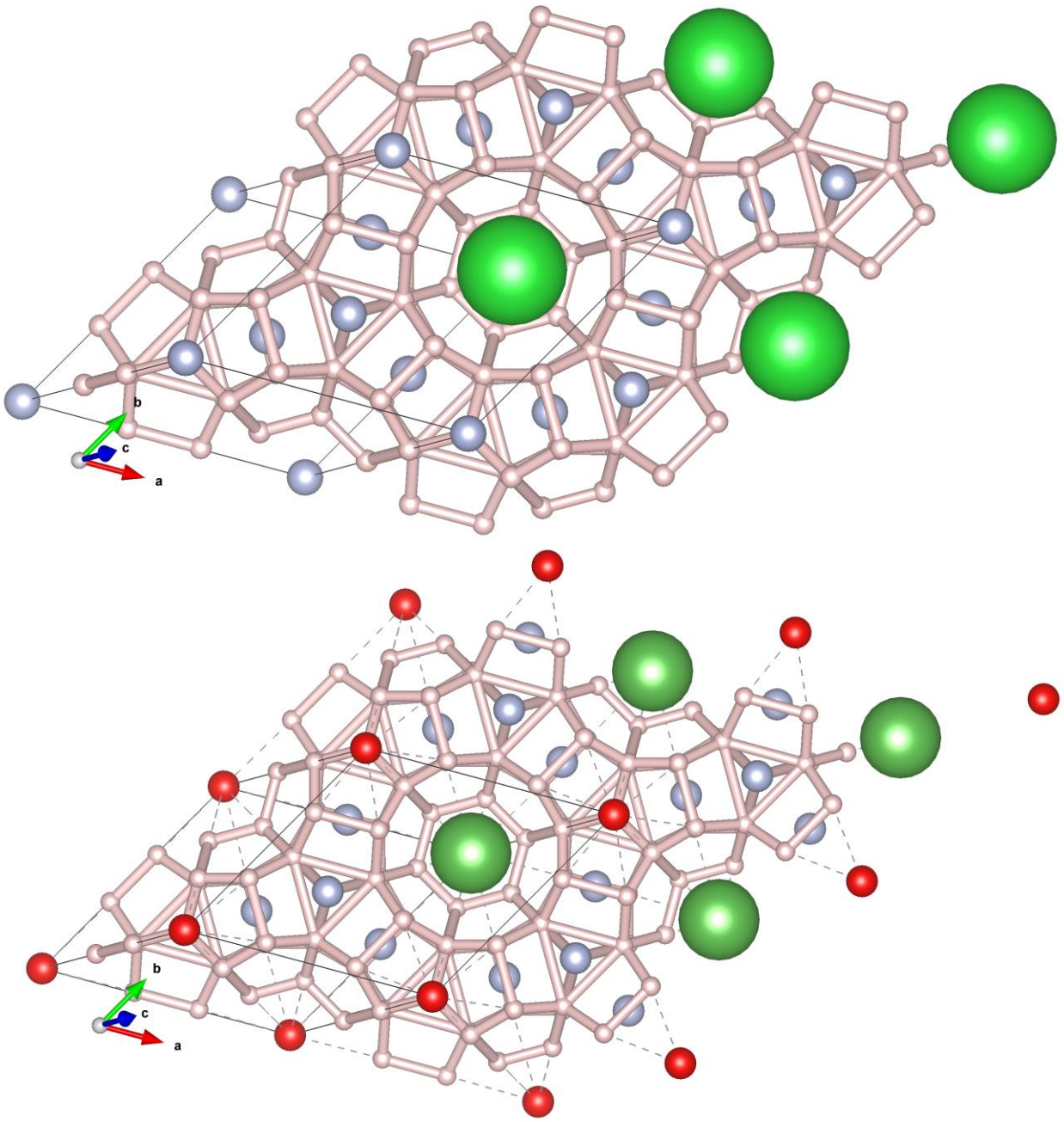

Fig S3. Fd-3m Li2MgH16 as BaH32N5 (top) and LaH32N4O (bottom) variants. To show the clathrate structure all the H-H bonds were taken to be 1.6 A. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

Table S5: The crystallographic information for Fd-3m LaH32N4O in a P1 representation. X: Labels sites part of random search detailed in the morphisms section in the main text.

```
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
```

Table S6: The crystallographic information for Fd-3m BaH32N5 in a P1 representation. X: Labels sites part of random search detailed in the morphisms section in the main text.

```
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