

# Machine learning using structural representations for discovery of high temperature superconductors

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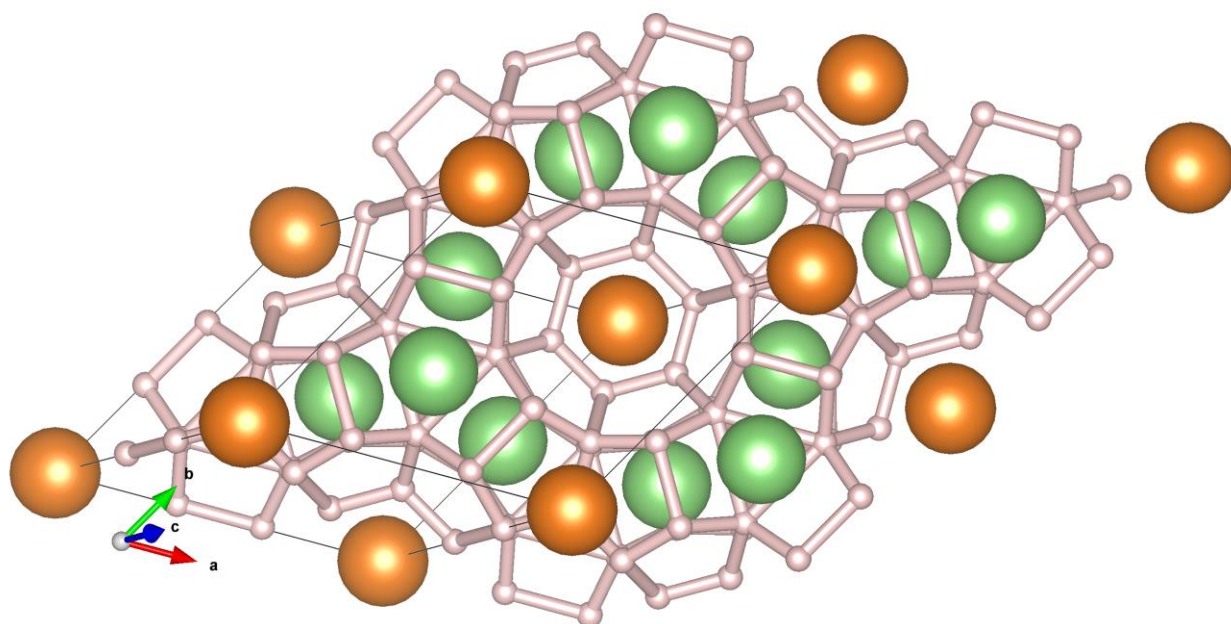


Fig S1. Fd-3m  $\text{Li}_2\text{MgH}_{16}$  To show the clathrate structure all the H-H bonds were taken to be 1.6 Å. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

Table S1: The crystallographic information for Fd-3m  $\text{Li}_2\text{MgH}_{16}$  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

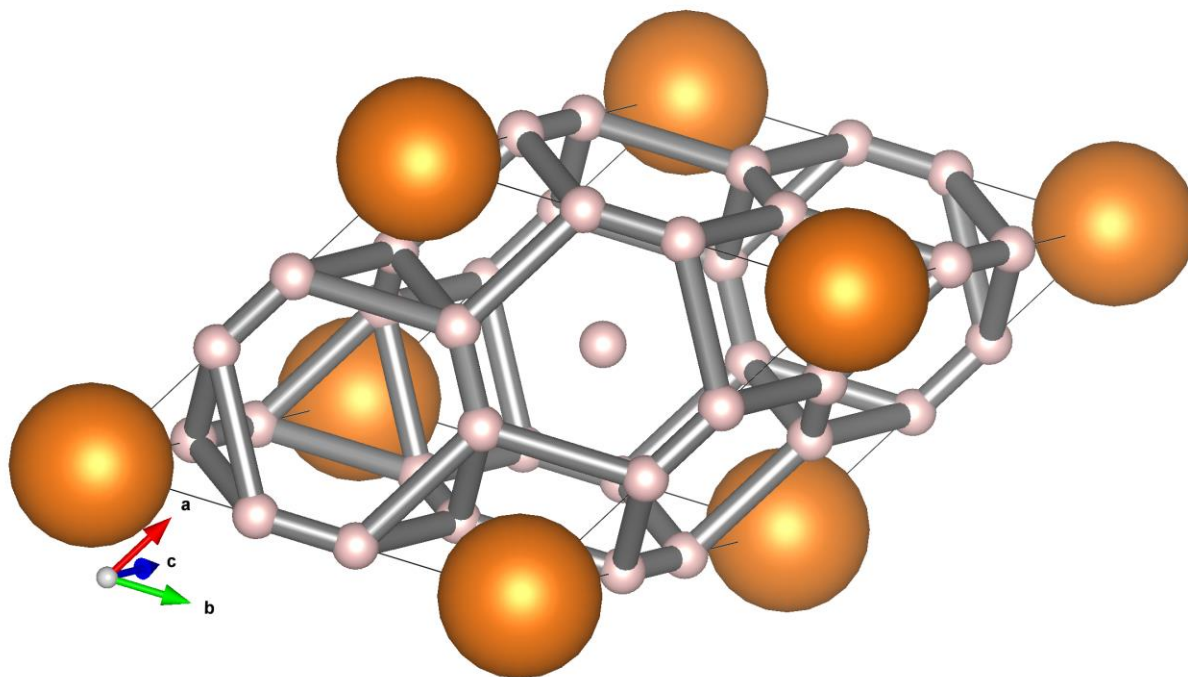


Fig S2. Fm-3m  $\text{MgH}_{13}$  To show the clathrate structure all the H-H bonds were taken to be 1.6 Å. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

Table S2: The crystallographic information for Fm-3m  $\text{MgH}_{13}$  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 Li<sub>2</sub>MgH<sub>16</sub> 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 SeH<sub>3</sub> variation of H<sub>3</sub>S 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

```

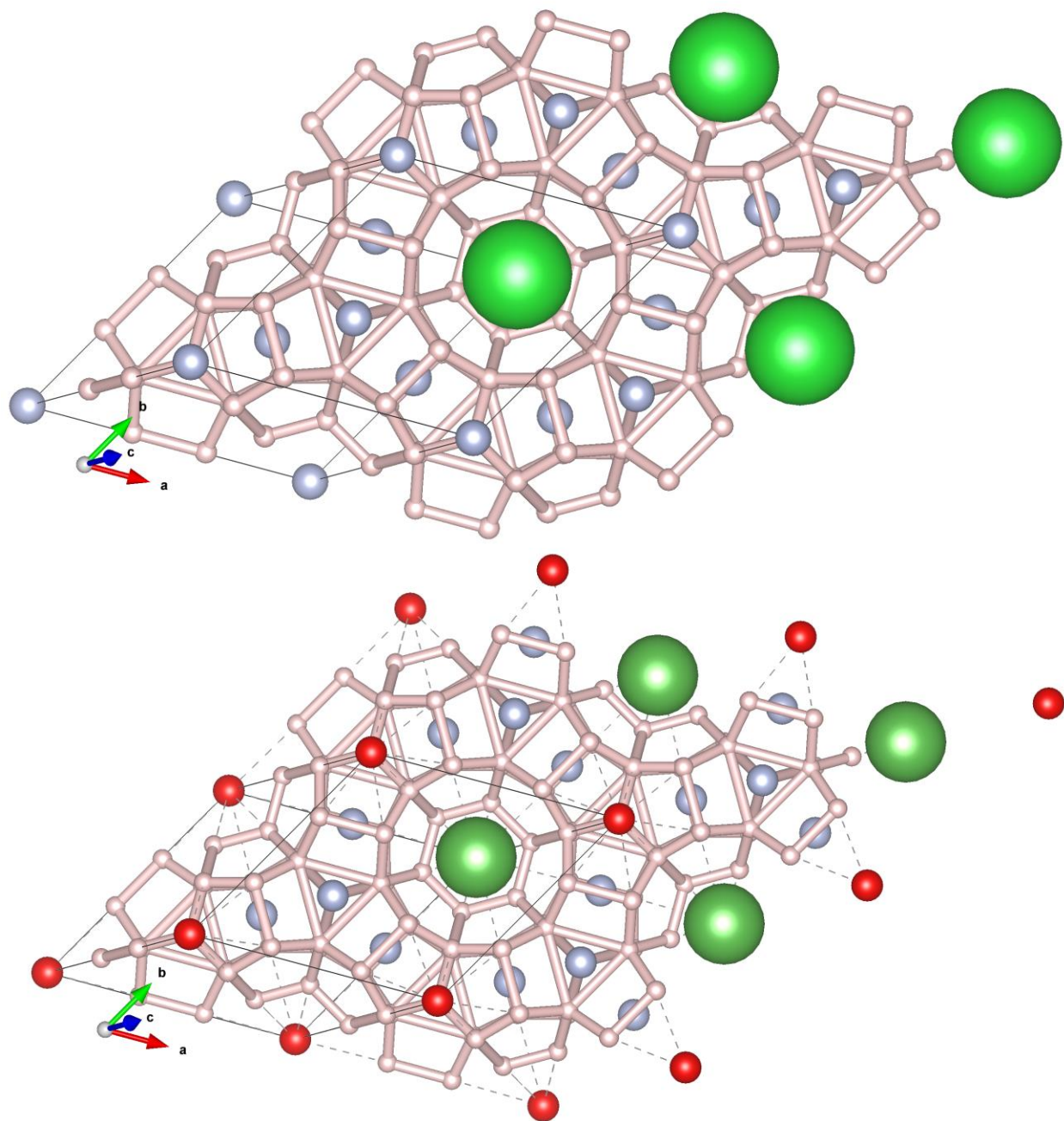


Fig S3.  $\text{Fd-}3\text{m}$   $\text{Li}_2\text{MgH}_{16}$  as  $\text{BaH}_{32}\text{N}_5$  (top) and  $\text{LaH}_{32}\text{N}_4\text{O}$  (bottom) variants. To show the clathrate structure all the H-H bonds were taken to be 1.6 Å. Below is crystallographic information for the above structure with all atoms present in the primitive unit cell (ie. a P1 representation).

Table S5: The crystallographic information for Fd-3m LaH<sub>32</sub>N<sub>4</sub>O 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 BaH<sub>32</sub>N<sub>5</sub> 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