

Supplementary Information for:

Oxidation and De-Alloying of PtMn particle models: a DFT investigation

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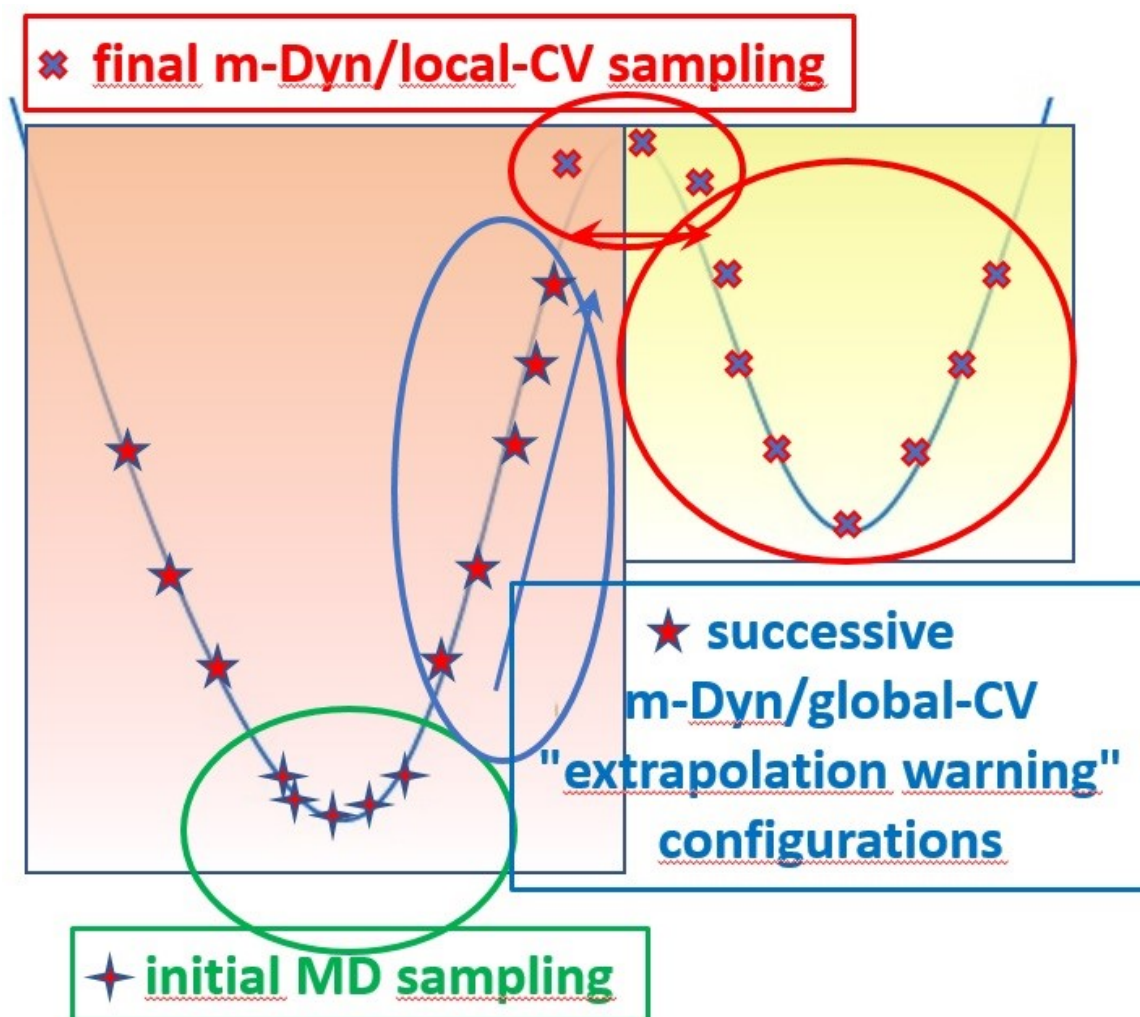


Figure S1. Schematic depiction of the strategy to incrementally sample the Potential Energy Surface (PES) of the system from snapshots of the initial MD simulations using the first NNPs to the

“extrapolation warning” configurations sequentially extracted from m-Dyn runs using global Collective Variables (CVs) and Neural Network Potentials (NNPs) of increasing quality, up to the final m-Dyn runs using local Collective Variables (CVs) and Neural Network Potentials (NNPs) of maximum quality, augmented with the results of DFT/NEB simulations, as described in the main text. See Ref.[M. Yang, L. Bonati, D. Polino and M. Parrinello, Catalysis Today, 2022, 387, 143-149] for a more comprehensive description of similar approaches.

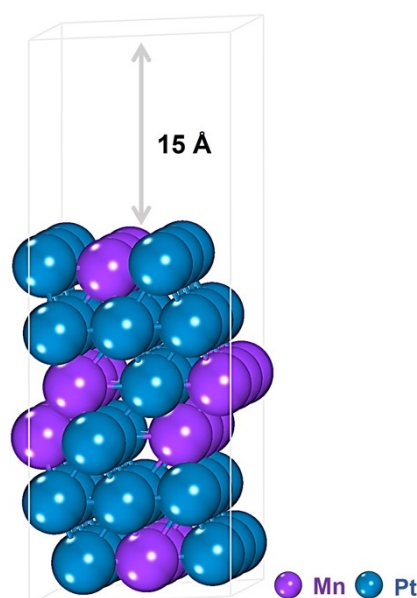


Figure S2. The optimized structure of a Pt₂Mn bulk built as a mixture of L1₂ and L1₀ chemical ordering.

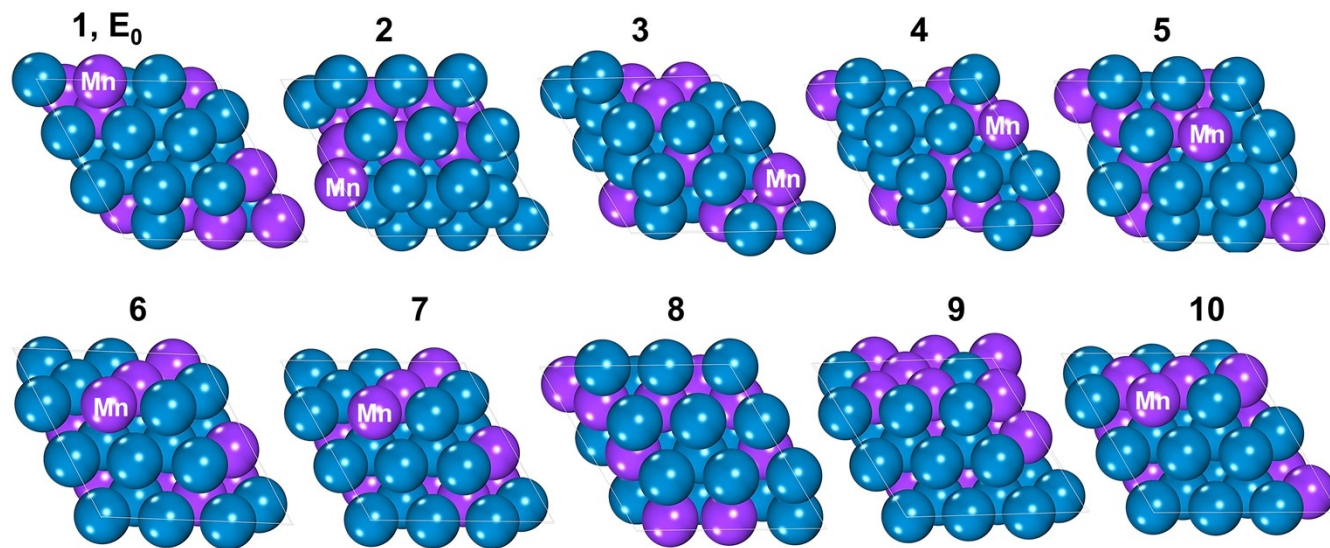


Figure S3. Ten lowest-energy structures of our Pt_2Mn (111) slab models.

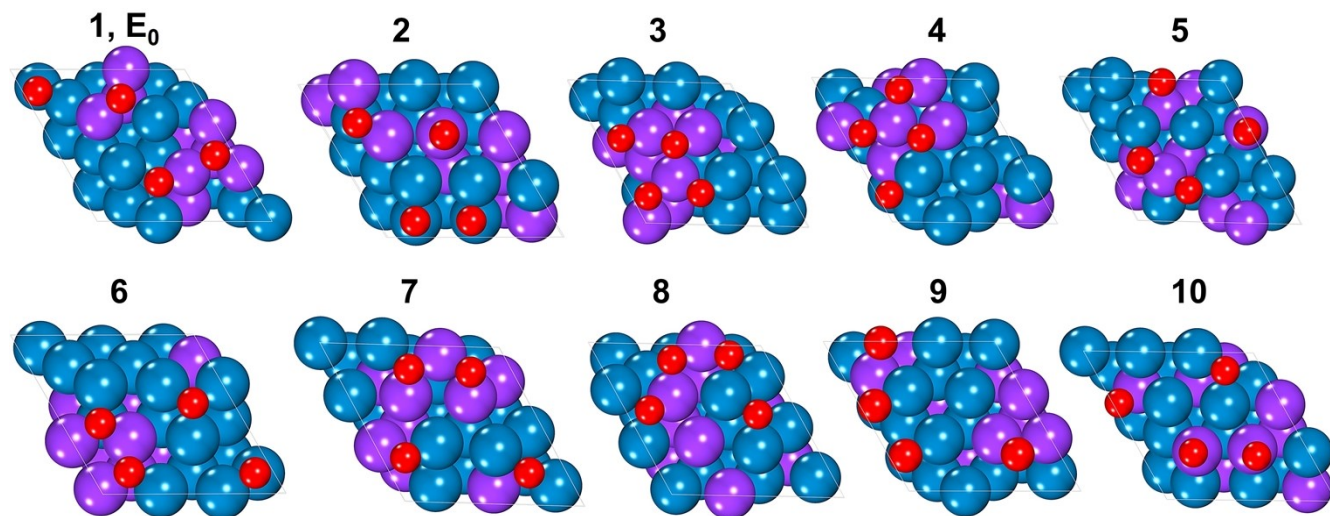


Figure S4. Ten lowest-energy structural models of oxygen adsorption onto the bare Pt_2Mn (111) configurations.

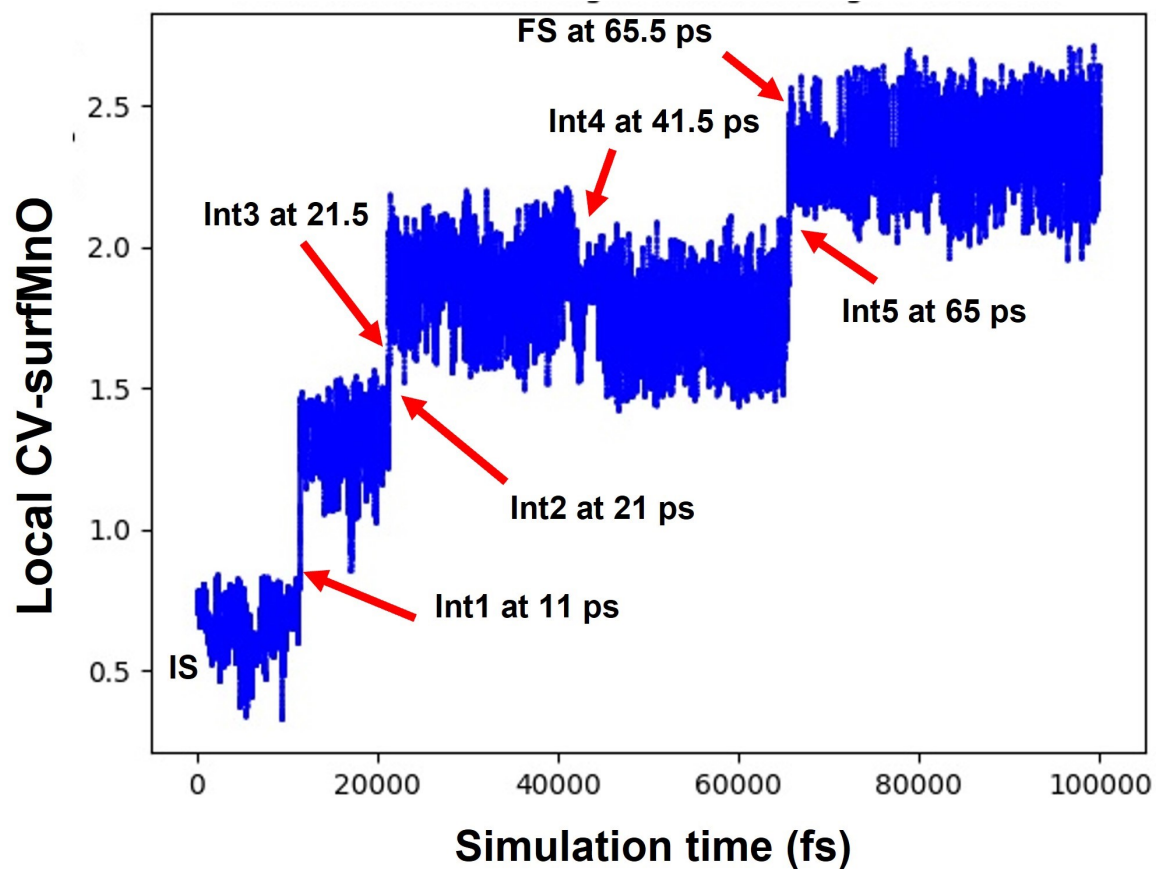


Figure S5. Time evolution of the local collective variable CV-SurfMnO corresponding to the m-Dyn simulation reported in Figure 4 of the main text.

S1. The NNP parameters

In this study, we use the neural network potentials (NNP) as a tool to construct the potentials to investigate the energy potential surface in the MD and m-Dyn simulations. The parameter in the input file for the NNP training was used as follows:

```
number_of_elements      3          # Number of elements.
elements                Pt Mn O    # Specification of elements.
remove_atom_energies
atom_energy             O -432.5084987
atom_energy             Mn -2860.910513    # Free atom reference energy (Mn).
atom_energy             Pt -2857.264696    # Free atom reference energy (Pt).
cutoff_type             2 0.0        # Cutoff type (optional argument: shift parameter alpha).
scale_symmetry_functions          # Scale all symmetry functions with min/max values.
scale_min_short         0.0         # Minimum value for scaling.
scale_max_short         1.0         # Maximum value for scaling.
center_symmetry_functions          # Center all symmetry functions, i.e. subtract mean value.
global_hidden_layers_short 2        # Number of hidden layers.
global_nodes_short       30 30      # Number of nodes in each hidden layer.
global_activation_short   t t l     # Activation function for each hidden layer and output layer.
#normalize_nodes          # Normalize input of nodes.
#####
# ADDITIONAL SETTINGS FOR DATASET TOOLS
#####
# These keywords are used only by some tools handling data sets:
# nnp-comp2, nnp-scaling, nnp-dataset, nnp-train.
use_short_forces          # Use forces.
random_seed              25708      # Random number generator seed.
#####
# ADDITIONAL SETTINGS FOR TRAINING
#####
# These keywords are solely used for training with nnp-train.
epochs                  200         # Number of training epochs.
updater_type            1          # Weight update method (0 = Gradient Descent, 1 = Kalman filter).
parallel_mode           0          # Training parallelization used (0 = Parallel (rank 0 update), 1 =
Parallel (all update)).
jacobian_mode           1          # Jacobian computation mode (0 = Summation to single gradient, 1
= Per-task summed gradient, 2 = Full Jacobian).
update_strategy         0          # Update strategy (0 = Combined, 1 = Per-element).
selection_mode          2          # Update candidate selection mode (0 = Random, 1 = Sort, 2 =
Threshold).
task_batch_size_energy  1          # Number of energy update candidates prepared per task for each
update (0 = Entire training set).
task_batch_size_force   1          # Number of force update candidates prepared per task for each
update (0 = Entire training set).
#memorize_symfunc_results          # Keep symmetry function results in memory.
test_fraction           0.0        # Fraction of structures kept for testing.
force_weight            10.0       # Weight of force updates relative to energy updates.
```

```

short_energy_fraction      1.000      # Fraction of energy updates per epoch.
short_force_fraction       0.05       # Fraction of force updates per epoch.
short_energy_error_threshold 0.00      # RMSE threshold for energy update candidates.
short_force_error_threshold 1.00      # RMSE threshold for force update candidates.
rmse_threshold_trials      3          # Maximum number of RMSE threshold trials.
#use_old_weights_short     # Restart fitting with old weight parameters.
weights_min               -1.0        # Minimum value for initial random weights.
weights_max               1.0        # Maximum value for initial random weights.
#precondition_weights      # Precondition weights with initial energies.
nguyen_widrow_weights_short # Initialize neural network weights according to Nguyen-
Widrow scheme.
main_error_metric          RMSEpa      # Main error metric for screen output
(RMSEpa/RMSE/MAEpa/MAE).
write_trainpoints          1          # Write energy comparison every this many epochs.
write_trainforces          1          # Write force comparison every this many epochs.
write_weights_epoch        1          # Write weights every this many epochs.
write_neuronstats          1          # Write neuron statistics every this many epochs.
write_trainlog             # Write training log file.
#####
# GRADIENT DESCENT #
#####
# This section is only used if "updater_type" is "0".
gradient_type              1          # Gradient descent type (0 = Fixed step size, 1 = Adam).
gradient_eta               1.0E-5     # Fixed step size gradient descent parameter eta.
gradient_adam_eta          1.0E-3     # Adam parameter eta.
gradient_adam_beta1        0.9        # Adam parameter beta1.
gradient_adam_beta2        0.999     # Adam parameter beta2.
gradient_adam_epsilon      1.0E-8     # Adam parameter epsilon.
#####
# KALMAN FILTER (STANDARD) #
#####
# This section is only used if "updater_type" is "1".
kalman_type                0          # Kalman filter type (0 = Standard, 1 = Fading memory).
kalman_epsilon             1.0E-2     # General Kalman filter parameter epsilon (sigmoidal: 0.01,
linear: 0.001).
kalman_q0                  0.01       # General Kalman filter parameter q0 ("large").
kalman_qtau                2.302      # General Kalman filter parameter qtau (2.302 => 1 order of
magnitude per epoch).
kalman_qmin                1.0E-6     # General Kalman filter parameter qmin (typ. 1.0E-6).
kalman_eta                 0.01       # Standard Kalman filter parameter eta (0.001-1.0).
kalman_etatau              2.302      # Standard Kalman filter parameter etatau (2.302 => 1 order of
magnitude per epoch).
kalman_etamax              1.0        # Standard Kalman filter parameter etamax (1.0+).
#####
### symmetry function definitions (all modes):
#####
symfunction_short Pt 9 O O  0.020  -1.000  1.000  6.000
symfunction_short Pt 9 Mn Mn 0.014  -1.000  4.000  6.000

```

symfunction_short Pt 9 Pt Mn	0.014	-1.000	4.000	6.000
symfunction_short Pt 9 O O	0.014	-1.000	1.000	6.000
symfunction_short Pt 9 Mn Mn	0.027	1.000	2.000	6.000
symfunction_short Pt 9 Pt Mn	0.056	-1.000	1.000	6.000
symfunction_short Pt 9 Pt Pt	0.014	-1.000	4.000	6.000
symfunction_short Pt 9 Pt Mn	0.027	-1.000	2.000	6.000
symfunction_short Pt 9 Pt Pt	0.056	-1.000	1.000	6.000
symfunction_short Pt 9 Pt Pt	0.027	-1.000	2.000	6.000
symfunction_short Pt 9 Pt Pt	0.014	1.000	2.000	6.000
symfunction_short Pt 9 Pt Pt	0.014	-1.000	2.000	6.000
symfunction_short Pt 9 Pt Pt	0.031	1.000	1.000	6.000
symfunction_short Pt 9 Pt Mn	0.014	-1.000	2.000	6.000
symfunction_short Pt 2 Mn	0.702	3.333	6.000	
symfunction_short Pt 9 Pt Mn	0.031	-1.000	1.000	6.000
symfunction_short Pt 9 Pt Pt	0.031	-1.000	1.000	6.000
symfunction_short Pt 9 Pt Pt	0.020	1.000	1.000	6.000
symfunction_short Pt 9 Pt Pt	0.014	1.000	1.000	6.000
symfunction_short Pt 2 Mn	0.002	0.000	6.000	
symfunction_short Pt 2 Mn	0.003	0.667	6.000	
symfunction_short Pt 2 Mn	0.010	2.000	6.000	
symfunction_short Pt 2 Mn	0.033	3.333	6.000	
symfunction_short Pt 2 Mn	0.008	2.000	6.000	
symfunction_short Pt 2 Mn	0.004	1.333	6.000	
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symfunction_short Pt 2 Mn	0.021	2.667	6.000	
symfunction_short Pt 9 Mn Mn	0.014	1.000	2.000	6.000
symfunction_short Pt 2 Mn	0.015	2.667	6.000	
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symfunction_short Pt 2 Mn	0.002	0.667	6.000	
symfunction_short Pt 2 Mn	0.702	2.000	6.000	
symfunction_short Pt 2 Mn	0.003	1.333	6.000	
symfunction_short Pt 9 Pt Pt	0.020	-1.000	1.000	6.000
symfunction_short Pt 2 Mn	0.003	6.000	6.000	
symfunction_short Pt 2 Mn	0.021	3.333	6.000	
symfunction_short Pt 2 Mn	0.010	2.667	6.000	
symfunction_short Pt 2 Mn	0.021	4.000	6.000	
symfunction_short Pt 2 Mn	4.000	2.667	6.000	
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symfunction_short Pt 2 Mn	0.002	6.000	6.000	
symfunction_short Pt 2 Mn	0.015	4.000	6.000	

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symfunction_short Pt 9 Mn Mn	0.056	1.000	1.000	6.000
symfunction_short Pt 2 Mn	0.002	2.000	6.000	
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symfunction_short Pt 2 Mn	0.002	3.333	6.000	
symfunction_short Pt 2 Mn	0.002	4.000	6.000	
symfunction_short Pt 9 Pt Mn	0.020	1.000	1.000	6.000
symfunction_short Pt 9 Mn Mn	0.027	-1.000	2.000	6.000
symfunction_short Pt 9 Mn O	0.020	-1.000	1.000	6.000
symfunction_short Pt 9 Mn Mn	0.056	-1.000	1.000	6.000
symfunction_short Pt 2 Mn	4.000	2.000	6.000	
symfunction_short Pt 9 Pt Mn	0.020	-1.000	1.000	6.000
symfunction_short Pt 2 O	4.000	2.000	6.000	
symfunction_short Pt 2 O	4.000	2.667	6.000	
symfunction_short Pt 9 Pt Mn	0.014	1.000	1.000	6.000
symfunction_short Pt 9 Pt Pt	0.014	-1.000	1.000	6.000
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symfunction_short O 2 O	0.010	2.000	6.000	
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symfunction_short O 2 O	0.008	4.000	6.000	
symfunction_short O 2 O	0.021	3.333	6.000	

symfunction_short O 2 O	0.002	2.000	6.000	
symfunction_short O 2 O	0.006	3.333	6.000	
symfunction_short O 2 O	0.004	2.667	6.000	
symfunction_short O 2 O	0.004	2.667	6.000	
symfunction_short O 2 O	0.003	4.000	6.000	
symfunction_short O 2 O	0.003	2.667	6.000	
symfunction_short O 2 O	0.004	3.333	6.000	
symfunction_short O 2 O	0.004	3.333	6.000	
symfunction_short O 2 O	0.002	4.000	6.000	
symfunction_short O 2 O	0.003	3.333	6.000	
symfunction_short O 2 O	0.002	2.667	6.000	
symfunction_short O 2 O	0.002	3.333	6.000	
symfunction_short O 9 Pt Pt	0.014	1.000	1.000	6.000
symfunction_short O 9 Pt Pt	0.027	-1.000	2.000	6.000
symfunction_short O 9 Mn O	0.031	-1.000	1.000	6.000
symfunction_short O 9 Pt O	0.014	1.000	1.000	6.000
symfunction_short O 9 Pt Pt	0.031	-1.000	1.000	6.000
symfunction_short O 9 Pt Mn	0.014	1.000	1.000	6.000
symfunction_short O 9 Pt O	0.020	-1.000	1.000	6.000
symfunction_short O 9 Pt Mn	0.031	-1.000	1.000	6.000
symfunction_short O 2 Mn	4.000	3.333	6.000	
symfunction_short O 9 Pt Pt	0.014	-1.000	2.000	6.000
symfunction_short O 9 Mn O	0.020	1.000	1.000	6.000
symfunction_short O 2 Mn	0.003	3.333	6.000	
symfunction_short O 2 Mn	0.002	3.333	6.000	
symfunction_short O 2 Mn	0.004	2.667	6.000	
symfunction_short O 2 Mn	0.004	2.667	6.000	
symfunction_short O 2 Mn	0.003	2.667	6.000	
symfunction_short O 2 Mn	0.002	2.667	6.000	
symfunction_short O 2 Mn	0.002	2.000	6.000	
symfunction_short O 9 Pt Mn	0.014	-1.000	2.000	6.000
symfunction_short O 9 Mn O	0.020	-1.000	1.000	6.000
symfunction_short O 2 O	0.702	0.667	6.000	
symfunction_short O 9 Mn O	0.014	1.000	1.000	6.000
symfunction_short O 2 O	4.000	3.333	6.000	
symfunction_short O 9 Mn O	0.014	-1.000	1.000	6.000
symfunction_short O 9 Pt Pt	0.020	-1.000	1.000	6.000
symfunction_short O 9 Pt O	0.014	-1.000	1.000	6.000
symfunction_short O 2 O	0.702	1.333	6.000	
symfunction_short O 2 Mn	4.000	2.667	6.000	
symfunction_short O 2 Pt	4.000	3.333	6.000	
symfunction_short O 9 Pt Mn	0.020	-1.000	1.000	6.000
symfunction_short O 2 Pt	0.702	1.333	6.000	
symfunction_short O 2 O	4.000	1.333	6.000	
symfunction_short O 2 Pt	0.106	4.000	6.000	
symfunction_short O 2 O	4.000	2.667	6.000	
symfunction_short O 2 O	4.000	2.000	6.000	
symfunction_short O 2 Mn	0.702	2.000	6.000	

symfunction_short O 2 Pt	0.235	4.000	6.000	
symfunction_short O 2 Mn	4.000	2.000	6.000	
symfunction_short O 2 Pt	0.002	3.333	6.000	
symfunction_short O 2 Pt	0.002	2.667	6.000	
symfunction_short O 9 Pt Pt	0.014	-1.000	1.000	6.000
symfunction_short O 2 Pt	4.000	2.667	6.000	
symfunction_short O 2 Mn	0.702	1.333	6.000	
symfunction_short O 9 Pt Mn	0.014	-1.000	1.000	6.000
symfunction_short O 2 Mn	4.000	1.333	6.000	
symfunction_short O 2 Pt	4.000	2.000	6.000	

S2. Source codes for selection of the symmetry function

```
import numpy as np
from scipy import linalg
from sklearn.metrics.pairwise import euclidean_distances, cosine_similarity

def div_mat(mat, n):
    split_mat = []
    div_1, mod_1 = divmod(mat.shape[0], n)
    div_2, mod_2 = divmod(mod_1, div_1)
    for i in range(mod_2):
        split_mat.append(mat[i*(n+div_2+1):(i+1)*(n+div_2+1),:])
    begin_index = mod_2 * (n+div_2+1)
    for i in range(div_1-mod_2):
        split_mat.append(mat[begin_index + i*(n+div_2):begin_index + (i+1)*(n+div_2),:])
    return split_mat

def read_symfunc(symfunc='function.data', emap=None):
    # define dict
    if emap == None:
        emap = {'Au':79, 'O':8, 'H':1}
    sfs = {}
    for key in emap.keys():
        sfs[key] = []

    # readlines
    with open(symfunc) as f:
        lines = f.readlines()
    i, j = 0, 0
    line_num = len(lines)
    while j < line_num:
        atoms_num = int(lines[j].rstrip())
        for k, line in enumerate(lines[j+1:j+atoms_num+1]):
            tmp_line = line.rstrip().split()
            for key, val in emap.items():
                if tmp_line[0] == str(val):
                    # element, image index, atom index, symmetry function values
                    sfs[key].append([int(tmp_line[0])] + [i] + [k] + list(map(float, tmp_line[1:])))
            j += (atoms_num+2)
            i += 1

    for key in sfs.keys():
        sfs[key] = np.asarray(sfs[key], dtype=float)
    for i, (key, val) in enumerate(emap.items()):
        print('No. {0} element: {1} Atomic number: {2} Center atoms number: {3} Symfunc number: {4}'.format(i+1, key, val, sfs[key].shape[0], sfs[key].shape[1]-3))
    return sfs
```

```

def CUR_decomposition(X, alpha=0.1, beta=0.1):
    # initialize W, W_T, Z, A_1, A_2, rho_1, rho_2, convergence criterion epsilon
    n, m = X.shape
    W = np.zeros((m,n))
    Z = A_1 = np.zeros((n,n)) # XW for maximizing distances between
    W_T = A_2 = np.zeros((n,m))
    rho_1 = rho_2 = 1E-6
    max_rho = 1E+10
    tau = 1.1
    epsilon = 1E-3
    k = 0

    # calculate theta_2, Q, T,
    theta_2, Q = linalg.eigh(X.T @ X)
    theta_2 = theta_2.reshape(-1,1)
    T = 1/(euclidean_distances(X) + 1E-6) # add a regularization term 0.001 # use Euclidean distance
    for reference structures selection
    obj_func = linalg.norm(X-X@W@X)**2 + alpha*np.sum(linalg.norm(W.T, axis=1)) +
    beta*linalg.norm(T*(X@W), ord=1)
    while True:
        # minimize W
        M = 2*X @ X.T + rho_1 * np.eye(n,n) #####
        theta_1, P = linalg.eigh(M)
        theta_1 = theta_1.reshape(1,-1)
        H = 2*X.T@X@X.T + rho_1*X.T@(Z-A_1/rho_1) + rho_2*(W_T-A_2/rho_2).T
        Y = Q.T@H@P / (theta_2@theta_1 + rho_2)
        W = Q@Y@P.T

        # minimize W_T
        S2 = W.T + A_2/rho_2
        W_T = np.zeros((n,m))
        S2_row_norm = linalg.norm(S2, axis=1)
        non_zero_indexs = np.where(S2_row_norm > alpha/rho_2)
        W_T[non_zero_indexs] = np.diag(1-alpha/(rho_2*S2_row_norm[non_zero_indexs])) @
        S2[non_zero_indexs]
        # minimize Z
        S1 = X@W + A_1/rho_1
        Z = np.maximum(np.abs(S1)-beta*T/rho_1, 0) * np.sign(S1)

        # updata multipliers and parameters
        A_1 = A_1 + rho_1*(X@W-Z)
        A_2 = A_2 + rho_2*(W.T - W_T)
        rho_1 = min(tau*rho_1, max_rho)
        rho_2 = min(tau*rho_2, max_rho)
        new_obj_func = linalg.norm(X-X@W@X)**2 + alpha*np.sum(linalg.norm(W.T, axis=1)) +
        beta*linalg.norm(T*(X@W), 1)

        # check the convergence conditions

```

```

        criteria = np.asarray([linalg.norm(X@W-Z, np.inf), linalg.norm(W.T-W_T, np.inf),
abs((new_obj_func-obj_func)/obj_func)], dtype=float)
        if np.all(criteria < epsilon):
            break
        obj_func = new_obj_func
        k += 1
        if k > 10000:
            break
    return W, criteria

def CUR_decomposition_col(X, alpha=0.1, beta=1000):
    # initialize W, W_T, Z, A_1, A_2, rho_1, rho_2, convergence criterion epsilon
    X = X.T
    n, m = X.shape
    W = np.zeros((m,n))
    Z = A_1 = np.zeros((n,n)) # XW for maximizing distances between
    W_T = A_2 = np.zeros((n,m))
    rho_1 = rho_2 = 1E-6
    max_rho = 1E+10
    tau = 1.1
    epsilon = 1E-3
    k = 0

    # calculate theta_2, Q, T,
    theta_2, Q = linalg.eigh(X.T @ X)
    theta_2 = theta_2.reshape(-1,1)
    T = cosine_similarity(X) # add a regularization term 0.001 # use Euclidean distance for reference
structures selection
    obj_func = linalg.norm(X-X@W@X)**2 + alpha*np.sum(linalg.norm(W.T, axis=1)) +
beta*linalg.norm(T*(X@W), ord=1)
    while True:
        # minimize W
        M = 2*X @ X.T + rho_1 * np.eye(n,n)
        theta_1, P = linalg.eigh(M)
        theta_1 = theta_1.reshape(1,-1)
        H = 2*X.T@X@X.T + rho_1*X.T@(Z-A_1/rho_1) + rho_2*(W_T-A_2/rho_2).T
        Y = Q.T@H@P / (theta_2@theta_1 + rho_2)
        W = Q@Y@P.T

        # minimize W_T
        S2 = W.T + A_2/rho_2
        W_T = np.zeros((n,m))
        S2_row_norm = linalg.norm(S2, axis=1)
        non_zero_indexs = np.where(S2_row_norm > alpha/rho_2)
        W_T[non_zero_indexs] = np.diag(1-alpha/(rho_2*S2_row_norm[non_zero_indexs])) @
S2[non_zero_indexs]

        # minimize Z

```

```

S1 = X@W + A_1/rho_1
Z = np.maximum(np.abs(S1)-beta*T/rho_1, 0) * np.sign(S1)

# updata multipliers and parameters
A_1 = A_1 + rho_1*(X@W-Z)
A_2 = A_2 + rho_2*(W.T - W_T)
rho_1 = min(tau*rho_1, max_rho)
rho_2 = min(tau*rho_2, max_rho)
new_obj_func = linalg.norm(X-X@W@X)**2 + alpha*np.sum(linalg.norm(W.T, axis=1)) +
beta*linalg.norm(T*(X@W), 1)

# check the convergence conditions
criteria = np.asarray([linalg.norm(X@W-Z, np.inf), linalg.norm(W.T-W_T, np.inf),
abs((new_obj_func-obj_func)/obj_func)], dtype=float)
if np.all(criteria < epsilon):
    break
obj_func = new_obj_func
k += 1
if k > 10000:
    break
return W, criteria

```

Cartesian Coordinates of IS structure from Figure 4 of the main text

Pt	0.0000009300	-2.2936900000	-5.3176100000	0	0	0
Pt	2.6878200000	-2.2937000000	-5.3176100000	0	0	0
Pt	-2.6878215400	-2.2937100000	-5.3176100000	0	0	0
Mn	-1.3439100000	-0.1263400000	-5.3155200000	0	0	0
Mn	1.3439100000	-0.1263300000	-5.3155100000	0	0	0
Mn	4.0317400000	-0.1263400000	-5.3155200000	0	0	0
Pt	-2.6878200000	2.1593800000	-5.1658100000	0	0	0
Pt	-0.0000000800	2.1593800000	-5.1658100000	0	0	0
Pt	2.6878200000	2.1593800000	-5.1658100000	0	0	0
Pt	1.3439100000	-3.1769440000	-2.9618100000	0	0	0
Pt	4.0317300000	-3.1769450000	-2.9618100000	0	0	0
Pt	-1.3439115400	-3.1769440000	-2.9618100000	0	0	0
Pt	0.0000002700	-0.7991600000	-3.0548200000	0	0	0
Pt	2.6878200000	-0.7991600000	-3.0548200000	0	0	0
Pt	-2.6878215400	-0.7991600000	-3.0548200000	0	0	0
Pt	-1.3439100000	1.4869400000	-2.8375600000	0	0	0
Pt	1.3439100000	1.4869500000	-2.8375600000	0	0	0
Pt	-4.0317315400	1.4869500000	-2.8375600000	0	0	0
Mn	-4.0317315400	2.9379500000	-0.6788000000	0	0	0
Mn	-1.3439100000	2.9379500000	-0.6788000000	0	0	0
Mn	1.3439100000	2.9379500000	-0.6788000000	0	0	0
Pt	-1.3439115400	-1.6788200000	-0.7468000000	0	0	0
Pt	1.3439100000	-1.6788200000	-0.7468000000	0	0	0
Pt	4.0317300000	-1.6788200000	-0.7468000000	0	0	0
Mn	-2.6878200000	0.9679900000	-0.7458000000	0	0	0
Mn	0.0000018100	0.9679900000	-0.7458000000	0	0	0
Mn	2.6878200000	0.9679900000	-0.7458000000	0	0	0
Mn	0.0556976180	-2.5868533090	1.3895463620			
Pt	-3.9034181139	2.9819027810	5.7502295440			
Pt	1.5233570280	-3.2510171900	3.4650150130			
Mn	2.4957747480	-2.4752061240	1.2793583990			
Mn	-1.3523570999	3.2346494670	6.3937618670			
Mn	4.2630353190	-3.1571668530	3.5730582260			
Pt	5.4343021650	-2.4233241680	1.4511122770			
Pt	1.4457949411	3.0163956560	5.6787319570			
Mn	-1.3429564630	-3.0817454410	3.4782754600			
Pt	-1.3825712860	0.0553459630	1.3669547980			
Pt	-1.2775022280	-1.6338605980	5.9020720420			
Pt	0.0074233200	-0.9083962300	3.4417760940			
Pt	1.3701046470	-0.0182091770	1.2491853810			
Pt	1.4395503800	-1.6799645430	5.7557390990			
Pt	2.9034833830	-0.9674264250	3.3490666330			
Pt	-4.0225924140	0.1217926760	1.2040942740			
Pt	4.0831717590	-1.7427261850	5.6705198010			
Mn	-2.5379114960	-1.0385864760	3.6180200140			
Mn	-2.7501035350	2.4583210710	1.1597497160			
Pt	-2.5783483360	0.6980522990	5.6783646750			
Mn	-1.2118956620	1.4878179590	3.5856348950			
Pt	-0.1318162220	2.4049382640	1.4038279480			
Pt	0.0586292030	0.7842841960	5.6197699250			
Pt	1.4358610840	1.5805699420	3.3764060240			
Mn	-5.2484967080	2.4285906430	1.2168153510			
Pt	2.8149261750	0.6596773580	5.6872259310			
Pt	-3.8450484430	1.4701317270	3.4632956640			
O	-2.0616909270	-0.3168725170	7.2758218280			
O	-1.1290646530	-3.3139819490	7.1859084810			
O	1.4804309220	-0.0758325260	7.0488724580			
O	-1.2082853440	2.9800251540	7.9066763960			

Cartesian Coordinates of TS1 structure from Figure 4 of the main text

Pt	0.0000009300	-2.2936900000	-5.3176100000
Pt	2.6878200000	-2.2937000000	-5.3176100000
Pt	-2.6878215400	-2.2937100000	-5.3176100000
Mn	-1.3439100000	-0.1263400000	-5.3155200000
Mn	1.3439100000	-0.1263300000	-5.3155100000
Mn	4.0317400000	-0.1263400000	-5.3155200000
Pt	-2.6878200000	2.1593800000	-5.1658100000
Pt	-0.0000008000	2.1593800000	-5.1658100000
Pt	2.6878200000	2.1593800000	-5.1658100000
Pt	1.3439100000	-3.1769440000	-2.9618100000
Pt	4.0317300000	-3.1769450000	-2.9618100000
Pt	-1.3439115400	-3.1769440000	-2.9618100000
Pt	0.0000002700	-0.7991600000	-3.0548200000
Pt	2.6878200000	-0.7991600000	-3.0548200000
Pt	-2.6878215400	-0.7991600000	-3.0548200000
Pt	-1.3439100000	1.4869400000	-2.8375600000
Pt	1.3439100000	1.4869500000	-2.8375600000
Pt	-4.0317315400	1.4869500000	-2.8375600000
Mn	-4.0317315400	2.9379500000	-0.6788000000
Mn	-1.3439100000	2.9379500000	-0.6788000000
Mn	1.3439100000	2.9379500000	-0.6788000000
Pt	-1.3439115400	-1.6788200000	-0.7468000000
Pt	1.3439100000	-1.6788200000	-0.7468000000
Pt	4.0317300000	-1.6788200000	-0.7468000000
Mn	-2.6878200000	0.9679900000	-0.7458000000
Mn	0.0000018100	0.9679900000	-0.7458000000
Mn	2.6878200000	0.9679900000	-0.7458000000
Mn	0.0376902096	-2.5825064721	1.3858869730
Pt	-3.8320248767	3.0417514023	5.7930091836
Pt	1.4898499236	-3.2350137957	3.4198874832
Mn	2.5048594252	-2.4610369330	1.2731451094
Mn	-1.2964526216	3.4000476189	6.1616174498
Mn	4.2089427618	-3.1378899105	3.6057111788
Pt	5.4342559441	-2.4189783346	1.4553190925
Pt	1.4658808763	3.0707412878	5.7002182348
Mn	-1.3438757067	-3.0642309034	3.4696392377
Pt	-1.3860841951	0.0727547675	1.3253473594
Pt	-1.2787922080	-1.6145612633	5.7057208657
Pt	-0.0172729389	-0.8562688379	3.4207940446
Pt	1.3682652297	0.0100566547	1.2463031449
Pt	1.3752998757	-1.4856335909	5.5978852654
Pt	2.8726948834	-0.9300252435	3.3264801237
Pt	-4.0214750601	0.1093494778	1.1959072407
Pt	4.1074822066	-1.5780777857	5.6502195722
Mn	-2.5856538412	-1.0251552819	3.5858878012
Mn	-2.7392777013	2.4659291303	1.1856172474
Pt	-2.5485296411	0.7864958740	5.6379014946
Mn	-1.2196328878	1.5881409241	3.5387328825
Pt	-0.1109711160	2.4075686183	1.3884799030
Pt	0.0575898320	0.8995827242	5.6593487627
Pt	1.4103157648	1.6119150151	3.4326257939
Mn	-5.2574524345	2.4027622605	1.1878098620
Pt	2.8008442801	0.7713105929	5.6836992670
Pt	-3.8581492895	1.4943447619	3.4203976971
O	-1.2313951981	0.0677209594	7.0495000577
O	-1.1632416750	-3.2400721520	7.1492245332
O	2.6100682946	-1.7204292740	7.1317618406
O	-0.9357711880	2.7612567414	7.5398272279

Cartesian Coordinates of INT1 structure from Figure 4 of the main text

Pt	0.000000930	-2.293690000	-5.317610000	0	0	0
Pt	2.687820000	-2.293700000	-5.317610000	0	0	0
Pt	-2.687821540	-2.293710000	-5.317610000	0	0	0
Mn	-1.343910000	-0.126340000	-5.315520000	0	0	0
Mn	1.343910000	-0.126330000	-5.315510000	0	0	0
Mn	4.031740000	-0.126340000	-5.315520000	0	0	0
Pt	-2.687820000	2.159380000	-5.165810000	0	0	0
Pt	-0.000000080	2.159380000	-5.165810000	0	0	0
Pt	2.687820000	2.159380000	-5.165810000	0	0	0
Pt	1.343910000	-3.176944000	-2.961810000	0	0	0
Pt	4.031730000	-3.176945000	-2.961810000	0	0	0
Pt	-1.343911540	-3.176944000	-2.961810000	0	0	0
Pt	0.000000270	-0.799160000	-3.054820000	0	0	0
Pt	2.687820000	-0.799160000	-3.054820000	0	0	0
Pt	-2.687821540	-0.799160000	-3.054820000	0	0	0
Pt	-1.343910000	1.486940000	-2.837560000	0	0	0
Pt	1.343910000	1.486950000	-2.837560000	0	0	0
Pt	-4.031731540	1.486950000	-2.837560000	0	0	0
Mn	-4.031731540	2.937950000	-0.678800000	0	0	0
Mn	-1.343910000	2.937950000	-0.678800000	0	0	0
Mn	1.343910000	2.937950000	-0.678800000	0	0	0
Pt	-1.343911540	-1.678820000	-0.746800000	0	0	0
Pt	1.343910000	-1.678820000	-0.746800000	0	0	0
Pt	4.031730000	-1.678820000	-0.746800000	0	0	0
Mn	-2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.000001810	0.967990000	-0.745800000	0	0	0
Mn	2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.036781576	-2.561732935	1.397284374			
Pt	-3.967282054	3.039177276	5.705794206			
Pt	1.466319585	-3.209016961	3.441530932			
Mn	2.556312845	-2.450915506	1.340162395			
Mn	-2.769221604	3.921759853	7.588640826			
Mn	4.119814432	-3.081648058	3.445765666			
Pt	5.433661347	-2.424597948	1.436382883			
Pt	1.307459254	3.077673433	5.672117182			
Mn	-1.393237746	-3.037751503	3.501820486			
Pt	-1.384844427	0.055998342	1.340764229			
Pt	-1.310444464	-1.594713998	5.743045409			
Pt	-0.053378141	-0.857774797	3.473072637			
Pt	1.364977061	0.007177137	1.268472576			
Pt	1.415055901	-1.598915227	5.740125056			
Pt	2.814755789	-0.887427293	3.439309706			
Pt	-4.025050764	0.094870726	1.217137861			
Pt	4.017599183	-1.633868284	5.666691012			
Mn	-2.644214645	-0.948161772	3.521207456			
Mn	-2.742660603	2.491617145	1.196441466			
Pt	-2.626050878	0.824691807	5.636363236			
Mn	-1.299707599	1.542514433	3.510957660			
Pt	-0.107996317	2.389820893	1.381076270			
Pt	-0.002649900	0.888236124	5.690363814			
Pt	1.352020079	1.629470812	3.492876653			
Mn	-5.245969001	2.397889693	1.201391898			
Pt	2.714778229	0.743219781	5.733009444			
Pt	-3.918897477	1.526326648	3.414146452			
O	-1.307180819	0.216612834	7.054307430			
O	-2.815150747	-2.432111196	7.075506848			
O	0.343602733	-2.562805973	8.758274414			
O	-1.427655942	3.156524571	7.897569197			

Cartesian Coordinates of TS2 structure from Figure 4 of the main text

Pt	0.0000009300	-2.2936900000	-5.3176100000
Pt	2.6878200000	-2.2937000000	-5.3176100000
Pt	-2.6878215400	-2.2937100000	-5.3176100000
Mn	-1.3439100000	-0.1263400000	-5.3155200000
Mn	1.3439100000	-0.1263300000	-5.3155100000
Mn	4.0317400000	-0.1263400000	-5.3155200000
Pt	-2.6878200000	2.1593800000	-5.1658100000
Pt	-0.0000008000	2.1593800000	-5.1658100000
Pt	2.6878200000	2.1593800000	-5.1658100000
Pt	1.3439100000	-3.1769440000	-2.9618100000
Pt	4.0317300000	-3.1769450000	-2.9618100000
Pt	-1.3439115400	-3.1769440000	-2.9618100000
Pt	0.0000002700	-0.7991600000	-3.0548200000
Pt	2.6878200000	-0.7991600000	-3.0548200000
Pt	-2.6878215400	-0.7991600000	-3.0548200000
Pt	-1.3439100000	1.4869400000	-2.8375600000
Pt	1.3439100000	1.4869500000	-2.8375600000
Pt	-4.0317315400	1.4869500000	-2.8375600000
Mn	-4.0317315400	2.9379500000	-0.6788000000
Mn	-1.3439100000	2.9379500000	-0.6788000000
Mn	1.3439100000	2.9379500000	-0.6788000000
Pt	-1.3439115400	-1.6788200000	-0.7468000000
Pt	1.3439100000	-1.6788200000	-0.7468000000
Pt	4.0317300000	-1.6788200000	-0.7468000000
Mn	-2.6878200000	0.9679900000	-0.7458000000
Mn	0.0000018100	0.9679900000	-0.7458000000
Mn	2.6878200000	0.9679900000	-0.7458000000
Mn	0.0399265595	-2.5808622779	1.3863560900
Pt	-3.8986941658	3.0748240317	5.7201786811
Pt	1.5012147085	-3.2265815438	3.4254734255
Mn	2.5345224687	-2.4656735605	1.2939775060
Mn	-2.4639472184	4.0136122292	7.7179934451
Mn	4.1845669661	-3.1095775526	3.5300366647
Pt	-2.6165166421	-2.4170978610	1.4619838262
Pt	1.3748176210	3.1040383722	5.6626601687
Mn	-1.3948082742	-3.0509023230	3.5471521753
Pt	-1.3799524809	0.0613406861	1.3412327561
Pt	-1.3021101334	-1.6113619308	5.7275669178
Pt	-0.0076141474	-0.8796416929	3.4330450828
Pt	1.3712581619	0.0055094789	1.2505058778
Pt	1.4125004933	-1.5526389228	5.6544019645
Pt	2.8473489096	-0.9070088363	3.3705129663
Pt	-4.0159875797	0.1076118928	1.2055875377
Pt	4.0796054353	-1.6375107064	5.6677533520
Mn	-2.6289547537	-1.0194880609	3.6162275229
Mn	-2.7460330291	2.4711121646	1.1879000280
Pt	-2.6006272032	0.8013742640	5.6406450706
Mn	-1.2506490475	1.5482439627	3.5373621106
Pt	-0.1117893136	2.4035310038	1.3860350390
Pt	0.0116547709	0.9097597351	5.6758139710
Pt	1.3778307576	1.5979977383	3.4394587993
Mn	-5.2400656619	2.4057391178	1.1956581848
Pt	2.7472322058	0.8010568322	5.6804291661
Pt	-3.9010655526	1.5235064497	3.4232129350
O	-1.2622341818	0.0980939131	7.0369721481
O	2.6120575292	-1.5706103312	7.3746217873
O	-3.6009767035	4.2992388998	8.7642487931
O	-1.5385933048	2.7564470428	7.9326365022

Cartesian Coordinates of INT2 structure from Figure 4 of the main text

Pt	0.000000930	-2.293690000	-5.317610000	0	0	0
Pt	2.687820000	-2.293700000	-5.317610000	0	0	0
Pt	5.375640000	-2.293710000	-5.317610000	0	0	0
Mn	-1.343910000	-0.126340000	-5.315520000	0	0	0
Mn	1.343910000	-0.126330000	-5.315510000	0	0	0
Mn	4.031740000	-0.126340000	-5.315520000	0	0	0
Pt	-2.687820000	2.159380000	-5.165810000	0	0	0
Pt	-0.000000080	2.159380000	-5.165810000	0	0	0
Pt	2.687820000	2.159380000	-5.165810000	0	0	0
Pt	1.343910000	-3.176944000	-2.961810000	0	0	0
Pt	4.031730000	-3.176945000	-2.961810000	0	0	0
Pt	6.719550000	-3.176944000	-2.961810000	0	0	0
Pt	0.000000270	-0.799160000	-3.054820000	0	0	0
Pt	2.687820000	-0.799160000	-3.054820000	0	0	0
Pt	5.375640000	-0.799160000	-3.054820000	0	0	0
Pt	-1.343910000	1.486940000	-2.837560000	0	0	0
Pt	1.343910000	1.486950000	-2.837560000	0	0	0
Pt	4.031730000	1.486950000	-2.837560000	0	0	0
Mn	4.031730000	2.937950000	-0.678800000	0	0	0
Mn	-1.343910000	2.937950000	-0.678800000	0	0	0
Mn	1.343910000	2.937950000	-0.678800000	0	0	0
Pt	6.719550000	-1.678820000	-0.746800000	0	0	0
Pt	1.343910000	-1.678820000	-0.746800000	0	0	0
Pt	4.031730000	-1.678820000	-0.746800000	0	0	0
Mn	-2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.000001810	0.967990000	-0.745800000	0	0	0
Mn	2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.063296198	-2.573538222	1.362327371			
Pt	4.128866128	3.058481577	5.604191996			
Pt	1.579711057	-3.265257862	3.397370585			
Mn	2.533974537	-2.444708926	1.271460767			
Mn	1.730284607	-3.247792630	7.579402411			
Mn	4.252605757	-3.070159077	3.589314231			
Pt	5.451103365	-2.396112261	1.467058761			
Pt	1.361343199	3.036270704	5.643857168			
Mn	6.658856356	-3.059705634	3.538850564			
Pt	-1.377800907	0.081697940	1.335148927			
Pt	6.841883350	-1.635532708	5.749395810			
Pt	-0.016835032	-0.918206678	3.408081205			
Pt	1.376480523	-0.008869577	1.250433633			
Pt	1.426508899	-1.658748705	5.630122027			
Pt	2.879922608	-0.930861177	3.401931323			
Pt	4.042885676	0.094074605	1.203272589			
Pt	4.016420281	-1.698934485	5.815259722			
Mn	5.458746787	-0.937839561	3.672125014			
Mn	-2.745990249	2.473347846	1.166011281			
Pt	-2.581020417	0.846832770	5.760611897			
Mn	-1.262974774	1.437721574	3.604059124			
Pt	-0.115024212	2.424072855	1.394335409			
Pt	0.046704682	0.798993334	5.617145071			
Pt	1.410356755	1.601643667	3.378173036			
Mn	2.845354084	2.425811024	1.247923069			
Pt	2.732403674	0.719015853	5.678183765			
Pt	4.203741876	1.504518269	3.392738426			
O	5.555015734	-0.844743635	7.054993405			
O	3.241293728	-2.530239962	7.609127233			
O	0.763008722	-2.758642734	8.711431245			
O	-2.149677523	2.075674346	7.485932385			

Cartesian Coordinates of TS3 structure from Figure 4 of the main text

Pt	0.0000009300	-2.2936900000	-5.3176100000
Pt	2.6878200000	-2.2937000000	-5.3176100000
Pt	-2.6878215400	-2.2937100000	-5.3176100000
Mn	-1.3439100000	-0.1263400000	-5.3155200000
Mn	1.3439100000	-0.1263300000	-5.3155100000
Mn	4.0317400000	-0.1263400000	-5.3155200000
Pt	-2.6878200000	2.1593800000	-5.1658100000
Pt	-0.0000008000	2.1593800000	-5.1658100000
Pt	2.6878200000	2.1593800000	-5.1658100000
Pt	1.3439100000	-3.1769440000	-2.9618100000
Pt	4.0317300000	-3.1769450000	-2.9618100000
Pt	-1.3439115400	-3.1769440000	-2.9618100000
Pt	0.0000002700	-0.7991600000	-3.0548200000
Pt	2.6878200000	-0.7991600000	-3.0548200000
Pt	-2.6878215400	-0.7991600000	-3.0548200000
Pt	-1.3439100000	1.4869400000	-2.8375600000
Pt	1.3439100000	1.4869500000	-2.8375600000
Pt	-4.0317315400	1.4869500000	-2.8375600000
Mn	-4.0317315400	2.9379500000	-0.6788000000
Mn	-1.3439100000	2.9379500000	-0.6788000000
Mn	1.3439100000	2.9379500000	-0.6788000000
Pt	-1.3439115400	-1.6788200000	-0.7468000000
Pt	1.3439100000	-1.6788200000	-0.7468000000
Pt	4.0317300000	-1.6788200000	-0.7468000000
Mn	-2.6878200000	0.9679900000	-0.7458000000
Mn	0.0000018100	0.9679900000	-0.7458000000
Mn	2.6878200000	0.9679900000	-0.7458000000
Mn	0.0528214929	-2.5245034521	1.3436154643
Pt	-3.5134218290	2.7291700941	5.9600059885
Pt	1.4027538100	-3.2325941217	3.3931636886
Mn	2.5002894538	-2.4687051889	1.2488041321
Mn	-0.8264667076	2.6946813708	7.3088311957
Mn	3.7256769649	-3.6496674530	4.3623504244
Pt	-2.6725197811	-2.3301054133	1.5130108769
Pt	1.9155920010	3.0753072461	5.5804169252
Mn	-1.1607898850	-3.2789528394	3.2476943401
Pt	-1.3663596720	0.0777198328	1.3229713620
Pt	-1.0990387552	-1.5478154410	6.0574684294
Pt	-0.1310217285	-0.8806313112	3.5013703079
Pt	1.3578542624	-0.0517562542	1.3026840143
Pt	1.6084380610	-1.6825441628	5.6365858231
Pt	3.1250954705	-1.1984069642	3.4289575267
Pt	-4.0430166922	0.1047562634	1.1983595012
Pt	4.1808142911	-1.8356035826	6.2804994524
Mn	-2.6271925848	-1.9107839863	4.0485964648
Mn	-2.7479852743	2.4637960803	1.1739512947
Pt	-2.5458983513	0.3585656285	5.2764386584
Mn	-1.2459659584	1.5594965527	3.5441691159
Pt	-0.0840402282	2.4275321901	1.3898398193
Pt	0.1277691660	0.9063975332	5.6788783695
Pt	1.3988032544	1.5631227447	3.4174189047
Mn	-5.2991832708	2.4409774093	1.1937230486
Pt	2.9021107084	0.5614360550	5.6718098236
Pt	-3.9354126498	1.5048088424	3.3787405203
O	0.3786975518	-2.3931419627	7.0702769203
O	3.8345291265	-2.9135941446	7.9997789293
O	-2.4032097651	2.4069156067	7.6835535035
O	0.0339764019	1.3224402630	7.6931653160

Cartesian Coordinates of INT3 structure from Figure 4 of the main text

Pt	0.000000930	-2.293690000	-5.317610000	0	0	0
Pt	2.687820000	-2.293700000	-5.317610000	0	0	0
Pt	5.375640000	-2.293710000	-5.317610000	0	0	0
Mn	-1.343910000	-0.126340000	-5.315520000	0	0	0
Mn	1.343910000	-0.126330000	-5.315510000	0	0	0
Mn	4.031740000	-0.126340000	-5.315520000	0	0	0
Pt	-2.687820000	2.159380000	-5.165810000	0	0	0
Pt	-0.000000080	2.159380000	-5.165810000	0	0	0
Pt	2.687820000	2.159380000	-5.165810000	0	0	0
Pt	1.343910000	-3.176944000	-2.961810000	0	0	0
Pt	4.031730000	-3.176945000	-2.961810000	0	0	0
Pt	6.719550000	-3.176944000	-2.961810000	0	0	0
Pt	0.000000270	-0.799160000	-3.054820000	0	0	0
Pt	2.687820000	-0.799160000	-3.054820000	0	0	0
Pt	5.375640000	-0.799160000	-3.054820000	0	0	0
Pt	-1.343910000	1.486940000	-2.837560000	0	0	0
Pt	1.343910000	1.486950000	-2.837560000	0	0	0
Pt	4.031730000	1.486950000	-2.837560000	0	0	0
Mn	4.031730000	2.937950000	-0.678800000	0	0	0
Mn	-1.343910000	2.937950000	-0.678800000	0	0	0
Mn	1.343910000	2.937950000	-0.678800000	0	0	0
Pt	6.719550000	-1.678820000	-0.746800000	0	0	0
Pt	1.343910000	-1.678820000	-0.746800000	0	0	0
Pt	4.031730000	-1.678820000	-0.746800000	0	0	0
Mn	-2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.000001810	0.967990000	-0.745800000	0	0	0
Mn	2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.049396566	-2.533722909	1.335836326			
Pt	-3.212489391	2.368667996	5.925939732			
Pt	1.539432495	-3.220943648	3.363750848			
Mn	2.524581727	-2.464656764	1.229791768			
Mn	-0.799257774	2.144315833	7.472698341			
Mn	-0.610982433	3.004904297	5.023750143			
Pt	5.395055789	-2.364667878	1.562082750			
Pt	1.897055490	2.734635432	5.664052156			
Mn	6.957017808	-3.245507529	3.317933805			
Pt	-1.375078635	0.049924784	1.316796553			
Pt	-0.936664908	-1.973433495	5.823125307			
Pt	-0.046783500	-0.900936066	3.466796567			
Pt	1.355563503	-0.048018447	1.276741942			
Pt	1.842223242	-1.911531127	5.716878485			
Pt	3.136164939	-1.142224289	3.397189144			
Pt	4.026891826	0.117191964	1.195388716			
Pt	4.423813727	-1.981010435	6.491222867			
Mn	5.116776476	-2.391934912	4.110213775			
Mn	-2.745635782	2.471434963	1.155174421			
Pt	5.682742395	-0.027670098	4.972541486			
Mn	-1.054162584	1.641688605	3.679841848			
Pt	-0.087734269	2.389858013	1.406382484			
Pt	0.309056761	0.530816040	5.757026438			
Pt	1.490551186	1.493497739	3.392509040			
Mn	2.781070742	2.446937492	1.210565830			
Pt	3.120045759	0.334470325	5.702709878			
Pt	4.219181167	1.518715438	3.393617725			
O	0.503151674	-2.760143333	6.964919419			
O	3.877031013	-3.385703700	7.957125695			
O	-2.386643202	1.914582141	7.827317680			
O	0.137785331	0.803173965	7.805997753			

Cartesian Coordinates of TS4 structure from Figure 4 of the main text

Pt	2.0000009300	-2.2936900000	-5.3176100000
Pt	4.6878200000	-2.2937000000	-5.3176100000
Pt	-0.6878215400	-2.2937100000	-5.3176100000
Mn	0.6560900000	-0.1263400000	-5.3155200000
Mn	3.3439100000	-0.1263300000	-5.3155100000
Mn	-2.0317215400	-0.1263400000	-5.3155200000
Pt	-0.6878200000	2.1593800000	-5.1658100000
Pt	1.9999999200	2.1593800000	-5.1658100000
Pt	-3.3756415400	2.1593800000	-5.1658100000
Pt	3.3439100000	-3.1769440000	-2.9618100000
Pt	-2.0317315400	-3.1769450000	-2.9618100000
Pt	0.6560884600	-3.1769440000	-2.9618100000
Pt	2.0000002700	-0.7991600000	-3.0548200000
Pt	-3.3756415400	-0.7991600000	-3.0548200000
Pt	-0.6878215400	-0.7991600000	-3.0548200000
Pt	0.6560900000	1.4869400000	-2.8375600000
Pt	-4.7195515400	1.4869500000	-2.8375600000
Pt	-2.0317315400	1.4869500000	-2.8375600000
Mn	-2.0317315400	2.9379500000	-0.6788000000
Mn	0.6560900000	2.9379500000	-0.6788000000
Mn	-4.7195515400	2.9379500000	-0.6788000000
Pt	0.6560884600	-1.6788200000	-0.7468000000
Pt	3.3439100000	-1.6788200000	-0.7468000000
Pt	-2.0317315400	-1.6788200000	-0.7468000000
Mn	-0.6878200000	0.9679900000	-0.7458000000
Mn	2.0000018100	0.9679900000	-0.7458000000
Mn	-3.3756415400	0.9679900000	-0.7458000000
Mn	2.0219354215	-2.5352436889	1.3206176314
Pt	-1.5601899853	2.6327036136	5.7068295715
Pt	3.5021335959	-3.1895085153	3.3329249409
Mn	4.5060701647	-2.4749660036	1.2157357258
Mn	1.8089208897	3.0239439333	7.7987504307
Mn	-2.9719566369	-4.0111636175	5.3459183474
Pt	-0.6869927894	-2.3589383706	1.6257519031
Pt	-4.5051627284	2.6921687910	5.9588373871
Mn	0.8959833947	-3.3152869266	3.3614145873
Pt	0.5911541261	0.0715551146	1.3003285557
Pt	0.8616660465	-1.9675874018	5.8947054297
Pt	1.7596085527	-0.9872526723	3.4389450618
Pt	3.3168377102	-0.0616009457	1.3500335537
Pt	3.6691991879	-1.8105905353	5.6805562877
Pt	-2.8330548069	-1.2086319992	3.3669288434
Pt	-2.0732548597	0.1043814177	1.1599490495
Pt	-1.8517962060	-1.7168943351	6.5337802260
Mn	-1.1267798729	-2.6827634055	4.1995857492
Mn	-0.7458681159	2.4747065830	1.1357877605
Pt	-0.5043169340	0.0104036887	4.9608835670
Mn	0.9082685112	1.7386076318	3.7575685074
Pt	1.9035755220	2.3866930699	1.4088950967
Pt	2.0837013763	0.5216424724	5.6259992092
Pt	-4.6285653264	1.6320234371	3.4549515353
Mn	-3.3125364303	2.4691440145	1.2132189256
Pt	-3.1383566691	0.4518530207	5.5061301482
Pt	-1.8497581313	1.5144999506	3.3035149405
O	2.4054869656	-2.7187606435	7.0075731951
O	-2.3786389219	-2.4148756812	8.4214445753
O	0.5567463244	2.0294156887	8.0021805163
O	3.3535497577	2.4146018244	8.0145572952

Cartesian Coordinates of INT4 structure from Figure 4 of the main text

Pt	2.0000009300	-2.2936900000	-5.3176100000	0	0	0
Pt	4.6878200000	-2.2937000000	-5.3176100000	0	0	0
Pt	7.3756400000	-2.2937100000	-5.3176100000	0	0	0
Mn	0.6560900000	-0.1263400000	-5.3155200000	0	0	0
Mn	3.3439100000	-0.1263300000	-5.3155100000	0	0	0
Mn	6.0317400000	-0.1263400000	-5.3155200000	0	0	0
Pt	-0.6878200000	2.1593800000	-5.1658100000	0	0	0
Pt	1.9999999200	2.1593800000	-5.1658100000	0	0	0
Pt	4.6878200000	2.1593800000	-5.1658100000	0	0	0
Pt	3.3439100000	-3.1769440000	-2.9618100000	0	0	0
Pt	6.0317300000	-3.1769450000	-2.9618100000	0	0	0
Pt	8.7195500000	-3.1769440000	-2.9618100000	0	0	0
Pt	2.0000002700	-0.7991600000	-3.0548200000	0	0	0
Pt	4.6878200000	-0.7991600000	-3.0548200000	0	0	0
Pt	7.3756400000	-0.7991600000	-3.0548200000	0	0	0
Pt	0.6560900000	1.4869400000	-2.8375600000	0	0	0
Pt	3.3439100000	1.4869500000	-2.8375600000	0	0	0
Pt	6.0317300000	1.4869500000	-2.8375600000	0	0	0
Mn	6.0317300000	2.9379500000	-0.6788000000	0	0	0
Mn	0.6560900000	2.9379500000	-0.6788000000	0	0	0
Mn	3.3439100000	2.9379500000	-0.6788000000	0	0	0
Pt	8.7195500000	-1.6788200000	-0.7468000000	0	0	0
Pt	3.3439100000	-1.6788200000	-0.7468000000	0	0	0
Pt	6.0317300000	-1.6788200000	-0.7468000000	0	0	0
Mn	-0.6878200000	0.9679900000	-0.7458000000	0	0	0
Mn	2.0000018100	0.9679900000	-0.7458000000	0	0	0
Mn	4.6878200000	0.9679900000	-0.7458000000	0	0	0
Mn	2.0474825800	-2.5509639800	1.3778742800			
Pt	6.0584369300	3.1235215900	5.7154634300			
Pt	3.4543189400	-3.2075203300	3.3873313500			
Mn	4.5642957700	-2.4500489700	1.3106246800			
Mn	6.6200072200	-1.8826087000	7.1743053600			
Mn	0.7443670900	3.0792824300	5.5498016000			
Pt	7.4328077700	-2.4638517800	1.4182012000			
Pt	7.3358259400	-3.7525311300	5.6134039700			
Mn	8.8360583900	-3.1592564200	3.3605800100			
Pt	0.6567624800	0.0498348800	1.2996062500			
Pt	0.6382101900	-1.4849631900	5.8171053200			
Pt	2.0252164600	-0.8415099500	3.4725742500			
Pt	3.3792434400	0.0069685400	1.2461944600			
Pt	3.4419449900	-1.5264786600	5.7658406400			
Pt	4.8001085100	-0.9194056600	3.5352436000			
Pt	6.0475820400	0.0823124300	1.2381856200			
Pt	7.4190778700	-0.9202240400	3.6032999300			
Mn	5.9721341900	-3.2523844400	3.5569326400			
Mn	-0.7375306600	2.4724107600	1.1693900600			
Pt	-0.5414314300	0.9314323100	5.7488438700			
Mn	0.8529143400	1.6034801500	3.6564267700			
Pt	1.8897050900	2.3832544700	1.3818520900			
Pt	2.0587699200	0.8891309800	5.7631232100			
Pt	3.4300559600	1.6058379600	3.4549939500			
Mn	4.8784404800	2.4086043000	1.2843247800			
Pt	4.7255901300	0.7630136500	5.7825108400			
Pt	6.1177537500	1.5632095100	3.4470728100			
O	2.0578570100	-2.3445703000	7.1034511900			
O	6.1682650700	-0.1871420100	6.9814781300			
O	5.0362453700	-2.6283929500	6.7948675100			
O	7.1150171200	-2.2478013100	8.6006568100			

Cartesian Coordinates of TS5 structure from Figure 4 of the main text

Pt	0.0000009300	-2.2936900000	-5.3176100000
Pt	2.6878200000	-2.2937000000	-5.3176100000
Pt	-2.6878215400	-2.2937100000	-5.3176100000
Mn	-1.3439100000	-0.1263400000	-5.3155200000
Mn	1.3439100000	-0.1263300000	-5.3155100000
Mn	4.0317400000	-0.1263400000	-5.3155200000
Pt	-2.6878200000	2.1593800000	-5.1658100000
Pt	-0.0000008000	2.1593800000	-5.1658100000
Pt	2.6878200000	2.1593800000	-5.1658100000
Pt	1.3439100000	-3.1769440000	-2.9618100000
Pt	4.0317300000	-3.1769450000	-2.9618100000
Pt	-1.3439115400	-3.1769440000	-2.9618100000
Pt	0.0000002700	-0.7991600000	-3.0548200000
Pt	2.6878200000	-0.7991600000	-3.0548200000
Pt	-2.6878215400	-0.7991600000	-3.0548200000
Pt	-1.3439100000	1.4869400000	-2.8375600000
Pt	1.3439100000	1.4869500000	-2.8375600000
Pt	-4.0317315400	1.4869500000	-2.8375600000
Mn	-4.0317315400	2.9379500000	-0.6788000000
Mn	-1.3439100000	2.9379500000	-0.6788000000
Mn	1.3439100000	2.9379500000	-0.6788000000
Pt	-1.3439115400	-1.6788200000	-0.7468000000
Pt	1.3439100000	-1.6788200000	-0.7468000000
Pt	4.0317300000	-1.6788200000	-0.7468000000
Mn	-2.6878200000	0.9679900000	-0.7458000000
Mn	0.0000018100	0.9679900000	-0.7458000000
Mn	2.6878200000	0.9679900000	-0.7458000000
Mn	0.0154548245	-2.5280866666	1.3628073569
Pt	-4.0486200488	3.2456137122	5.6808674386
Pt	1.3941915678	-3.1525273630	3.4084412996
Mn	2.5405111578	-2.4511493929	1.3290741163
Mn	4.4065165739	-2.2338313200	7.5234923425
Mn	-1.3658075353	3.1872295392	5.5957914060
Pt	5.4130947567	-2.4669554944	1.4186620742
Pt	1.2769834901	3.3261340816	5.5848087826
Mn	-1.2218541302	-3.1414067311	3.3410662594
Pt	-1.3676475626	0.0551095787	1.2917531430
Pt	-1.2909902888	-1.4001565157	5.8574965456
Pt	-0.0291686582	-0.8137685410	3.4916870576
Pt	1.3480349836	0.0158030963	1.2543024101
Pt	1.3949685532	-1.4695013810	5.7829750213
Pt	2.7589249227	-0.8688126035	3.4883816534
Pt	-4.0386019211	0.0919250754	1.2338061770
Pt	-2.6870316522	-0.9286120118	3.5874960011
Mn	3.8927023727	-3.2052111589	3.5366780095
Mn	-2.7548815673	2.4954890849	1.1696385080
Pt	-2.6351403097	0.9971725185	5.7678571068
Mn	-1.2016697452	1.6915301353	3.6714908674
Pt	-0.1436277117	2.3845264850	1.3876836693
Pt	0.0089937164	0.9819793403	5.7279482582
Pt	1.4059459745	1.6688642411	3.4581671741
Mn	-5.2211417210	2.4318590240	1.2841293588
Pt	2.7315947234	0.8537530088	5.8123224169
Pt	-3.9549304177	1.5605976518	3.4174153993
O	2.6064846573	-0.6631066667	7.1426981636
O	5.1020960251	-2.7126222928	8.8373863876
O	3.0601232496	-3.3040033470	7.2152705826
O	-2.8578160403	-0.7745683590	6.9906149729

Cartesian Coordinates of FS structure from Figure 4 of the main text

Pt	0.000000930	-2.293690000	-5.317610000	0	0	0
Pt	2.687820000	-2.293700000	-5.317610000	0	0	0
Pt	5.375640000	-2.293710000	-5.317610000	0	0	0
Mn	-1.343910000	-0.126340000	-5.315520000	0	0	0
Mn	1.343910000	-0.126330000	-5.315510000	0	0	0
Mn	4.031740000	-0.126340000	-5.315520000	0	0	0
Pt	-2.687820000	2.159380000	-5.165810000	0	0	0
Pt	-0.000000080	2.159380000	-5.165810000	0	0	0
Pt	2.687820000	2.159380000	-5.165810000	0	0	0
Pt	1.343910000	-3.176944000	-2.961810000	0	0	0
Pt	4.031730000	-3.176945000	-2.961810000	0	0	0
Pt	6.719550000	-3.176944000	-2.961810000	0	0	0
Pt	0.000000270	-0.799160000	-3.054820000	0	0	0
Pt	2.687820000	-0.799160000	-3.054820000	0	0	0
Pt	5.375640000	-0.799160000	-3.054820000	0	0	0
Pt	-1.343910000	1.486940000	-2.837560000	0	0	0
Pt	1.343910000	1.486950000	-2.837560000	0	0	0
Pt	4.031730000	1.486950000	-2.837560000	0	0	0
Mn	4.031730000	2.937950000	-0.678800000	0	0	0
Mn	-1.343910000	2.937950000	-0.678800000	0	0	0
Mn	1.343910000	2.937950000	-0.678800000	0	0	0
Pt	6.719550000	-1.678820000	-0.746800000	0	0	0
Pt	1.343910000	-1.678820000	-0.746800000	0	0	0
Pt	4.031730000	-1.678820000	-0.746800000	0	0	0
Mn	-2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.000001810	0.967990000	-0.745800000	0	0	0
Mn	2.687820000	0.967990000	-0.745800000	0	0	0
Mn	0.029650610	-2.541640133	1.369988296			
Pt	0.009546083	-3.838312166	5.671153819			
Pt	1.433726659	-3.201304303	3.392184482			
Mn	2.540318447	-2.468987067	1.306774328			
Mn	4.097696846	-2.101714946	7.502199892			
Mn	2.677991648	-3.889038342	5.574958290			
Pt	5.429229693	-2.479018129	1.420548126			
Pt	5.305211121	-3.686176410	5.647149449			
Mn	6.856730256	-3.170607279	3.352515390			
Pt	-1.351475873	0.046535639	1.295134187			
Pt	-1.239186465	-1.505582575	5.851095582			
Pt	0.018038607	-0.853516656	3.476507958			
Pt	1.367588752	0.010518971	1.256371430			
Pt	1.430181398	-1.558720280	5.730395749			
Pt	2.811105205	-0.914458941	3.476533587			
Pt	4.037190246	0.079772734	1.225118582			
Pt	5.424589763	-0.946577895	3.580173792			
Mn	3.934648655	-3.249859615	3.580192153			
Mn	-2.750093119	2.478043938	1.169635792			
Pt	-2.607404853	0.887460475	5.753257422			
Mn	-1.171679193	1.628759376	3.664051725			
Pt	-0.124720459	2.376706542	1.391596469			
Pt	0.056771688	0.899203376	5.720768928			
Pt	1.428908010	1.639176874	3.476221284			
Mn	2.852715649	2.420422430	1.283954632			
Pt	2.749405941	0.763319208	5.793128925			
Pt	4.128188293	1.527414985	3.407526825			
O	2.766898314	-0.952944068	7.181608245			
O	4.497963063	-2.296727503	8.997304518			
O	3.040979112	-3.551166453	7.214832145			
O	5.280420649	-0.861477766	6.938289748			