

## **Effect of Co Doping on Mechanism and Kinetics of Ammonia Synthesis on Fe(111) Surface**

**Jin Qian<sup>1</sup>, Alessandro Fortunelli<sup>2</sup>, William A. Goddard III<sup>1,\*</sup>**

<sup>1</sup> Materials and Process Simulation Center (MSC), California Institute of Technology, Pasadena, California 91125, United States

<sup>2</sup>CNR-ICCOM, Consiglio Nazionale delle Ricerche, Pisa, 56124, Italy

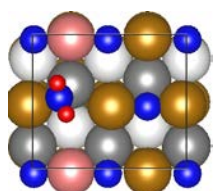
[\\*email: wag@caltech.edu](mailto:wag@caltech.edu); ORCID:0000-0003-0097-5716

### **Supplementary Materials**

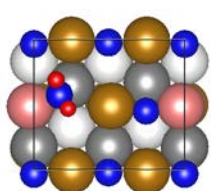
**SI Figure 1** Complete sampling of possible states.

**SI Figure 2** Pictorial illustration of reaction pathway for two sets of Co doped structures.

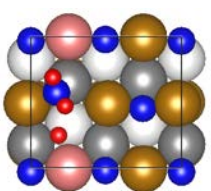
**CONTCAR** Atomic coordinates for all optimized structures



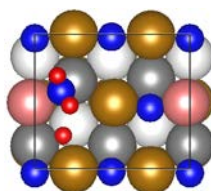
01\_3N.NH2/i



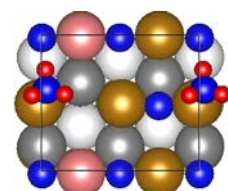
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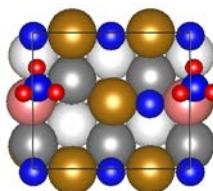
03\_3N.NH2/i.H



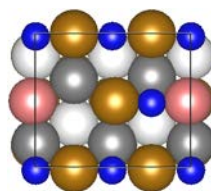
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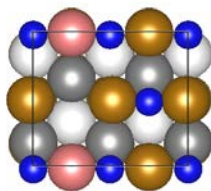
05\_3N.NH3/f



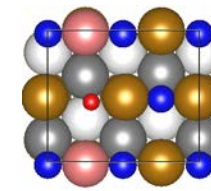
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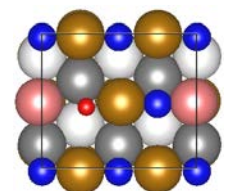
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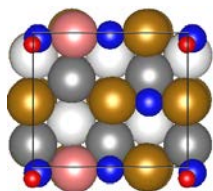
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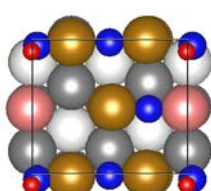
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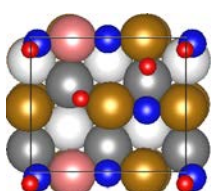
10\_3N.H/n



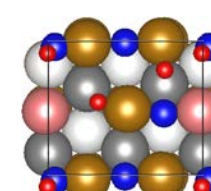
11\_2N\_z.V.NH\_b



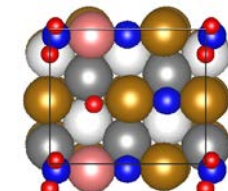
12\_2N\_z.V.NH\_c



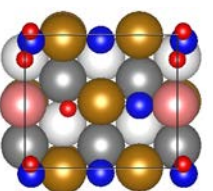
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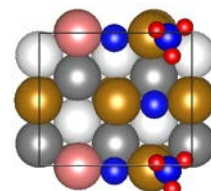
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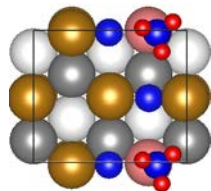
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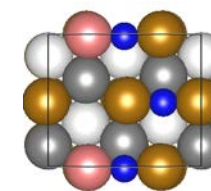
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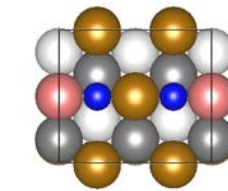
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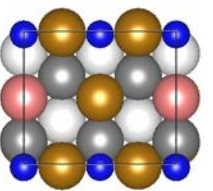
18\_2N.V.NH3\_a/n



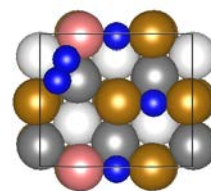
19\_2N\_z.2V\_b



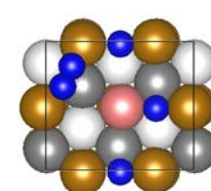
20\_2N\_l.2V\_b



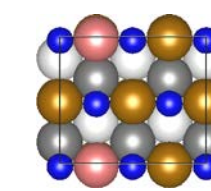
21\_2N\_l.2V\_a



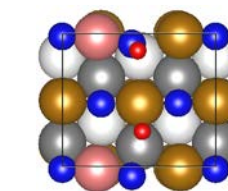
22\_2N\_diagonal.N2alpha\_c



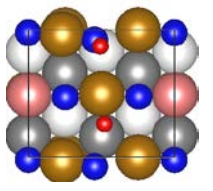
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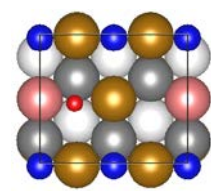
24\_4N



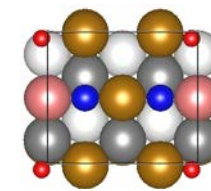
25\_3N.NH.H\_a/n



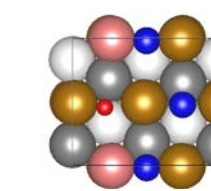
26\_3N.NH.H\_a/f



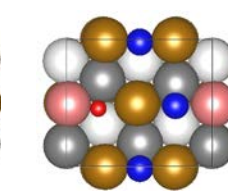
27\_2N\_l.H/n



28\_2N\_l.H/f

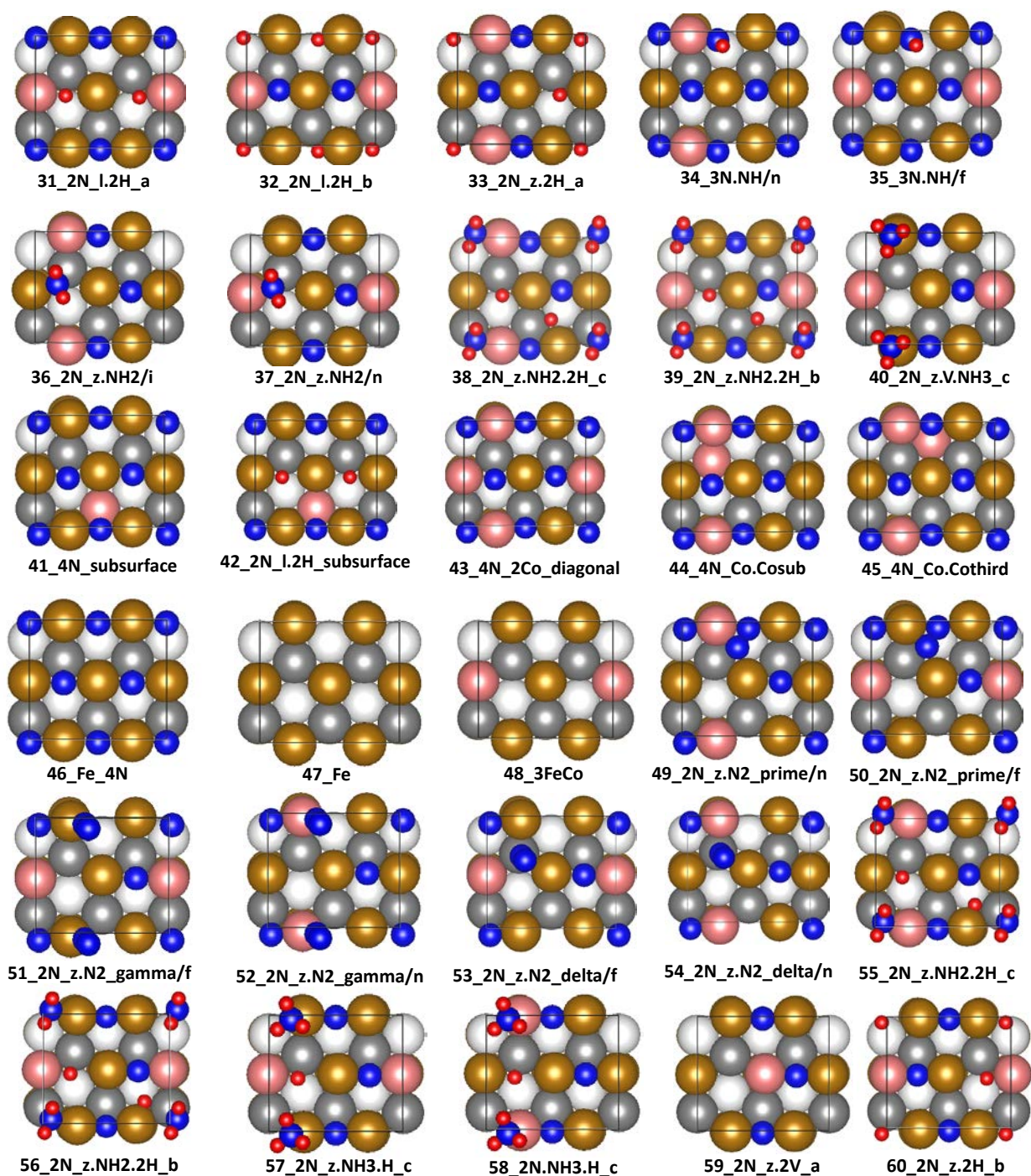


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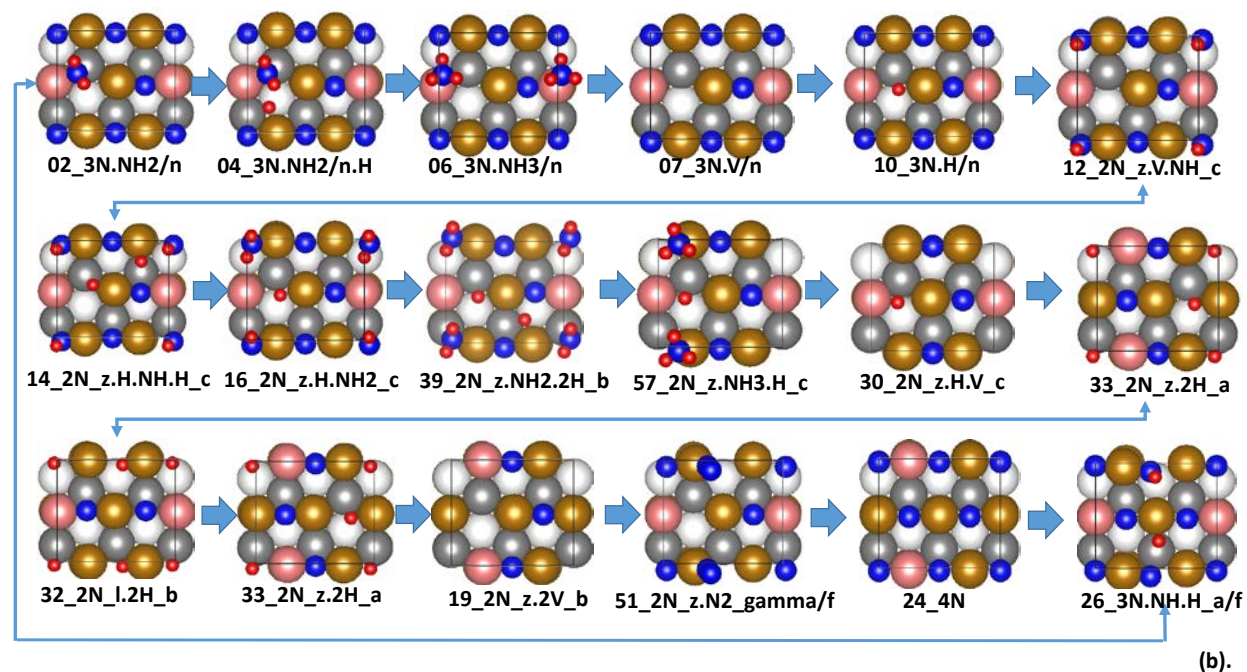
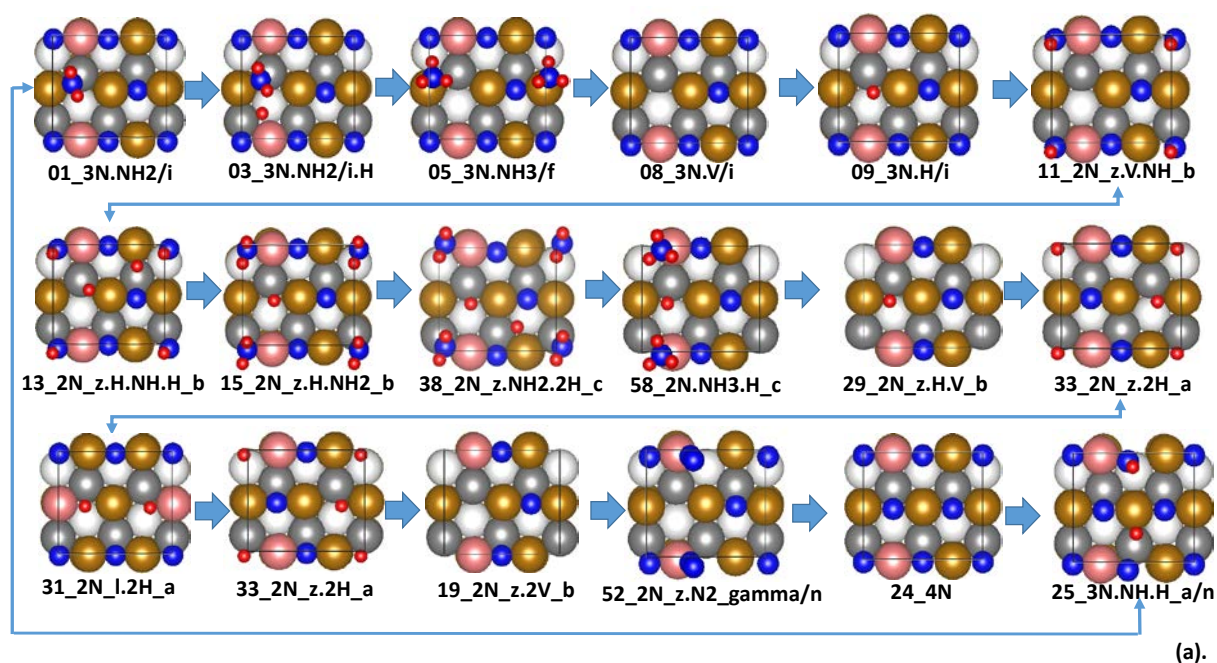


30\_2N\_z.H.V\_c





**SI Figure 1.** Complete sample of possible states. All structures are named based on our nomenclature in main text Table 1. Out of 60 structures, 40 (with name and energetics in main text Table 2) are used in studying the mechanism of Haber Bosch mechanism. Out of the remaining 20 cases, such as 41-38 are useful for studying stabilities of Co atoms and the stabilities of double dopants.



**SI Figure 2a) and 2b).** Pictorial illustration of reaction pathway for two sets of Co doped structures. Whereas figure a). has the initial surface species  $\text{NH}_2$  far from Co dopant and figure b). has the initial surface species  $\text{NH}_2$  near Co dopant. Energetics of the intermediate states along the pathway, including transition state is given in table 2) and figure 2) in main text.

01\_3N.NH2\_TfSDNH2.3N

0.9907000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
4 2 23 1

Selective dynamics

Direct

0.6114415767009485	0.0070096544833137	0.9741839200044370	T	T	T
0.6116076605046931	0.7477956275151159	0.4731494331571396	T	T	T
0.6114066723820853	0.4947680658024307	0.9762577792903373	T	T	T
0.6730356734405728	0.1902852062266371	0.5448235093711246	T	T	T
0.7016637353861797	0.2370372857036357	0.4200992894940510	T	T	T
0.7217107202146722	0.1837817343511174	0.6518653582018049	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5395098327833947	0.4954546862888064	0.1804420421829705	T	T	T
0.5342650731295485	0.7497289627742190	0.6768725339668900	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.5000284621712211	0.4928031755062285	0.8334224820361884	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4947876439290159	0.7509214925732817	0.3326538919656943	T	T	T
0.5988045725870301	0.7498624563567712	-0.0100201365320836	T	T	T
0.5979799449642492	0.5124747214538065	0.4937729933957533	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5410120843713390	0.0044920639336760	0.1813239900033096	T	T	T
0.5491449521696388	0.2481328048184024	0.6458559933872754	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4989154622920535	0.0052987103811985	0.8345575922509327	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4912417243877646	0.2499561577503888	0.3297961780080760	T	T	T
0.6038380086904147	0.9808409714953491	0.4941778652656780	T	T	T
0.5960248629395065	0.2508838555640528	0.9920950631881683	T	T	T



02\_3N.NH2\_TcSDNH2.3N

0.9906000000000000

14.8120002747000008 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.0120000420000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 6.9380002021999996

N H Fe Co  
4 2 23 1

Selective dynamics

Direct

0.6116424346691141	0.0038028804634393	0.9698160953837616	T	T	T
0.6107577260182034	0.7481134486043776	0.4749458572081796	T	T	T
0.6119888118745376	0.4978965276668555	0.9753169889770941	T	T	T
0.6719880925949782	0.1795005450492248	0.5512288944571042	T	T	T
0.7035961196152019	0.2289391421797934	0.4313419936248987	T	T	T
0.7193253037927203	0.1622862748452935	0.6594925696300873	T	T	T
0.3312200009999984	0.5000000000000000	0.83337999990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.33337999990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5384498992590568	0.4971316545190257	0.1784504287254409	T	T	T
0.5347199022007718	0.7504044948868057	0.6783750154048865	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4987989713573908	0.4935156433422278	0.8320175706416489	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4948000544552486	0.7502569963984165	0.3340068848176994	T	T	T
0.5990210789074419	0.7500046535126798	-0.0091669959264962	T	T	T
0.5977696595627616	0.5126627468208409	0.4926444117893403	T	T	T
0.3312200009999984	0.0000000000000000	0.83337999990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.33337999990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5409867240453912	0.0031348337986212	0.1798388287677984	T	T	T
0.5494601470904628	0.2470237447054617	0.6446906548276634	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4969066052423387	0.0045251175453550	0.8343589632602733	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F

0.4911091956617256	0.2506149928921241	0.3299403451414736	T	T	T
0.5981281215987676	0.2513387790962683	0.9933575659325677	T	T	T
0.6023952656301459	0.9782900940985612	0.4885473263444554	T	T	T

03\_3N.NH2.H\_TfSDNH2.3N.2H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
4	3	23	1

Selective dynamics

Direct

0.6103585873574634	0.0006358862634111	0.9630409749769816	T	T	T
0.6119085437819958	0.7464412430005344	0.4725884034779437	T	T	T
0.6107135076483534	0.4948123930804375	0.9726160057543930	T	T	T
0.6747759073143589	0.1851927362842019	0.5593827659761115	T	T	T
0.7076192215792597	0.2339629090731076	0.4404513504046288	T	T	T
0.7199091419228733	0.1772378988448078	0.6730816868712822	T	T	T
0.5954452843173981	0.1965793250229078	0.2341567263939398	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F

0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5403221835154320	0.4970491525685944	0.1802373092267748	T	T	T
0.5337519117741918	0.7489607942386606	0.6761031929167135	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4993129178696105	0.4920483901625811	0.8333455881259516	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4953185425642341	0.7512159581925001	0.3320232476285372	T	T	T
0.5986399783002183	0.7489829850144447	-0.0126803191825213	T	T	T
0.5977435578627919	0.5123899859650743	0.4967453514895667	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5436357842897952	0.0038295394933195	0.1797905948384895	T	T	T
0.5494947147119332	0.2479213751918323	0.6498717744194686	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4976127828052330	0.0045091959263907	0.8344471916411368	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4910454027928520	0.2515329453411835	0.3320969286177021	T	T	T
0.6049326745672305	0.9782930170681299	0.4986155066988484	T	T	T
0.5962244880894084	0.2502364214934607	0.9924993373012798	T	T	T



04\_3N.NH2.H\_TcSDNH2.3N.2H

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14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
4 3 23 1

Selective dynamics

Direct

0.6108423854497459	-0.0026986999893226	0.9602147990796449	T	T	T
0.6105849471319900	0.7476718352351963	0.4746646292888244	T	T	T
0.6114617971409592	0.4983864774650079	0.9725527697401740	T	T	T
0.6730995039964660	0.1696359967144983	0.5767083924955542	T	T	T
0.7113246626092251	0.2227520390206539	0.4681558176171575	T	T	T
0.7147112571083580	0.1434053859854581	0.6930005171289786	T	T	T
0.5951605855818983	0.1902370552370493	0.2408852352476414	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5390142533219446	0.4985011816946124	0.1783192714216616	T	T	T
0.5342455198477258	0.7499236314873603	0.6784841092627591	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4984180763966770	0.4929484294748735	0.8320526366564006	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
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0.5988409495191603	0.7491215734653855	-0.0106168956069999	T	T	T
0.5973494947686960	0.5134307725483767	0.4945456523470321	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5426619445055127	0.0021698540903248	0.1766330201581944	T	T	T
0.5490857530396076	0.2470422594456325	0.6488438118974962	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4960977314491796	0.0042045674383853	0.8342408236545805	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4911617839245548	0.2517851766295877	0.3322950151579120	T	T	T
0.5995760766932577	0.2519371633177408	0.9936788692640364	T	T	T
0.6013633771315181	0.9769947984701125	0.4934027667160089	T	T	T

05\_3N.NH3\_fCIF file

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
4	3	23	1

Selective dynamics

Direct

0.6133554430706919	0.0048921488829898	0.9727222165459509	T	T	T
0.6095608811553326	0.7463189164261164	0.4720682839771553	T	T	T
0.6121035857659621	0.4960714636682815	0.9746255291178096	T	T	T
0.7307530418381319	0.0357401138527224	0.5971625965495231	T	T	T
0.7205367081777615	0.0333403249005299	0.7459171356274568	T	T	T
0.7757059352885791	0.9424722406448731	0.5591311287506324	T	T	T
0.7574127921619358	0.1504080758124015	0.5599025202380564	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5396342373470822	0.4938912931963793	0.1778693027194267	T	T	T
0.5348142871340517	0.7508880131117747	0.6772475622611916	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4999512391574708	0.4951585509719100	0.8325474193413912	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4956481080364187	0.7515064338792690	0.3323371554219003	T	T	T
0.5982702401050987	0.7489796175045088	0.9912270541459840	T	T	T
0.5950031513755342	0.5098065109259408	0.4921914228929225	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5407215088851983	0.0056510583918640	0.1771420244456318	T	T	T
0.5440443762204700	0.2481264920152874	0.6525575203101621	T	T	T

0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4993453010997184	0.0040731214169096	0.8333332050020488	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4947485342421537	0.2491851193374336	0.3312378481056974	T	T	T
0.6009400145342819	0.9878668353528759	0.4895620139820708	T	T	T
0.5986377812415329	0.2512023565122264	0.9842362554267883	T	T	T

06\_3N.NH3\_cCIF file

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
4	3	23	1

Selective dynamics

Direct

0.6134190747568969	0.0030712726330903	0.9704730796165590	T	T	T
0.6108504683584010	0.7444890304134757	0.4752333070428496	T	T	T
0.6129157135548281	0.4977628111838114	0.9749255418792904	T	T	T
0.7270312368534533	0.0322549822929761	0.5939615210420168	T	T	T
0.7190046457548287	0.0257560527356848	0.7430455274898223	T	T	T
0.7714040271259962	0.9397496684945602	0.5509196105393754	T	T	T

0.7540756622341901	0.1470918961734845	0.5594504447161577	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5387284034678965	0.4962032753568187	0.1770356693882801	T	T	T
0.5354041432674814	0.7515189307964145	0.6786883931109187	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4997914246483817	0.4946610723288191	0.8316473827557538	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4969648183953858	0.7523750040463623	0.3345425609742178	T	T	T
0.5982067889892883	0.7486914945933109	0.9927746913872755	T	T	T
0.5944864858732963	0.5096761663771474	0.4922525038415507	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5415553288743542	0.0046820489618524	0.1786285286279338	T	T	T
0.5448977384534428	0.2454228310775320	0.6515006678844343	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4977292613671578	0.0032305311626467	0.8355896517145053	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4946511234267741	0.2499998798698669	0.3305746268402380	T	T	T
0.6003677813856726	0.2516369194932731	0.9900188810274133	T	T	T
0.5987081200280008	0.9845702135650279	0.4891346224399692	T	T	T



07\_3N\_holeCCIF file

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N Fe Co

3 23 1

Selective dynamics

Direct

0.6119482196623961	0.0021356531290819	0.9719443368473384	T	T	T
0.6111925147813194	0.7495248093149823	0.4771176361296379	T	T	T
0.6126210627794473	0.4974400295381136	0.9747033086652860	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5393199112408015	0.4954667193310640	0.1775480842493410	T	T	T
0.5354623382159459	0.7499399515703423	0.6795818282823017	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4996305736896340	0.4948394192572056	0.8322385020317301	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4958193632600460	0.7497943899840024	0.3333220333405905	T	T	T
0.5991549986643023	0.7493959700846929	-0.0079713336695558	T	T	T
0.5968412296166572	0.5128147695936406	0.4912767963380342	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5408736027522388	0.0049764558793759	0.1793482635580776	T	T	T
0.5453816499873609	0.2478298597988113	0.6518864741485116	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4981151921014706	0.0039289732966613	0.8343642548287078	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4948559888953880	0.2506768402200560	0.3315174981987667	T	T	T
0.6015560479337707	0.2499575582225730	0.9878188386744328	T	T	T
0.5919625272565398	0.9861069106657113	0.4927685201990155	T	T	T

08\_3N\_holefCIF file

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
3	23	1

Selective dynamics

Direct

0.6116686600319954	0.0042466906668248	0.9741928900062929	T	T	T
0.6106397825417114	0.7500008745692166	0.4746900817647085	T	T	T
0.6116698173024023	0.4957081243340152	0.9741978777922263	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5399379478817281	0.4931597276561455	0.1781171575891737	T	T	T
0.5349061229339681	0.7499944680727954	0.6782752625229362	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4997667030203887	0.4952224446861376	0.8328100708736944	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4952019181190289	0.7499965229199476	0.3323807862267124	T	T	T
0.5988851634870713	0.7499832267821507	0.9916037476699547	T	T	T
0.5969305102864779	0.5120988218046336	0.4913100448572996	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5399387891248809	0.0068219196344950	0.1781163841136505	T	T	T
0.5443856928389746	0.2499956763128264	0.6525527552869144	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4997666545229424	0.0047686818375281	0.8328114273569119	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4948031424957708	0.2499925926896892	0.3321224500305758	T	T	T
0.5969283005518334	0.9878930093488821	0.4913183547465770	T	T	T
0.5995310657426334	0.2499843533418303	0.9829343026212858	T	T	T

09\_3N.H\_fCIF file

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	1	23	1

Selective dynamics

Direct

0.6118333343471640	0.0039501964103181	0.9717355737968619	T	T	T
0.6116933167922708	0.7494589320321723	0.4741965244930895	T	T	T
0.6117721061316389	0.4960668390675391	0.9711332775664981	T	T	T
0.6097126138318508	0.2789490196018556	0.4526987787898691	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5394954864090321	0.4952405217134934	0.1744462388827644	T	T	T
0.5347819573704578	0.7495992349208384	0.6772814247766495	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4987723635595194	0.4958332614551542	0.8323362929937325	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4952936607676177	0.7498346769210020	0.3317975651858892	T	T	T
0.5994161495610395	0.7500475137219146	-0.0101178327295100	T	T	T
0.5967746181448351	0.5121874234998058	0.4903014831166742	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F

0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5394766311754929	0.0050112616807475	0.1748326403674200	T	T	T
0.5448505330058970	0.2502083848606525	0.6546990921459728	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4991609648296221	0.0039326416334019	0.8317892302907322	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4961417439250486	0.2500743668332926	0.3307475244726619	T	T	T
0.5971178875250738	0.9864352999296735	0.4896684000906688	T	T	T
0.5993238317612541	0.2499643049664306	0.9818377439928658	T	T	T

10\_3N.H\_cCIF file

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	1	23	1

Selective dynamics

Direct

0.6122921038346213	0.0016598594259365	0.9683965987211305	T	T	T
0.6125805147103938	0.7488884589684097	0.4768116595024706	T	T	T
0.6125804510334375	0.4978035562751049	0.9705895238811051	T	T	T
0.6085463044423828	0.2893282468770291	0.4507657511160372	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F



0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5389423350810637	0.4973198582107171	0.1732648216249989	T	T	T
0.5355228929608143	0.7495367093782792	0.6786736906764553	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4982429467415443	0.4955661011858838	0.8321201355870418	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4957980322837705	0.7497812404771970	0.3330062781099469	T	T	T
0.5998083775342372	0.7492432055810853	-0.0095066040627747	T	T	T
0.5957764739638322	0.5136617750707733	0.4903588536316321	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5406788538112814	0.0034425370767758	0.1753281405797907	T	T	T
0.5447603162901428	0.2490062364361547	0.6534981967246734	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4979673496889218	0.0034157403351107	0.8327411619016269	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4967888349383603	0.2502117849697317	0.3294973074492606	T	T	T
0.6018911726534403	0.2501073014247009	0.9841802817692760	T	T	T
0.5916778846859794	0.9826668083042859	0.4900923108592698	T	T	T

```

0.9906000000000000
  14.8120002747000008      0.0000000000000000      0.0000000000000000
    0.0000000000000000      8.0120000420000004      0.0000000000000000
    0.0000000000000000      0.0000000000000000      6.9380002021999996
  N      H      Fe      Co
    3      1      23      1
Selective dynamics
Direct
0.6114428279844285  0.7515425109044347  0.4768606642441091  T  T  T
0.6110829753937308  0.4977234621324608  0.9783015234401036  T  T  T
0.6196726622215525  0.0233906168617421  0.9574150693277483  T  T  T
0.6853043061651823  0.9971893276508673  0.9149869234158376  T  T  T
0.3312200009999984  0.5000000000000000  0.8333799990000017  F  F  F
0.3312200009999984  0.7500000000000000  0.3333799990000017  F  F  F
0.4282651369103760  0.7500000000000000  0.0001050071835991  F  F  F
0.4282651369103760  0.5000000000000000  0.5001050221835968  F  F  F
0.5381732587263978  0.4932496682183459  0.1836089815156956  T  T  T
0.5353844571412989  0.7521941601766287  0.6792405818796290  T  T  T
0.3810960778633330  0.5000000000000000  0.1667699372837745  F  F  F
0.4974347646607734  0.4959300869896716  0.8326762748227352  T  T  T
0.3810960778633330  0.7500000000000000  0.6667699072837721  F  F  F
0.4953544989453774  0.7511669099098677  0.3323341563014610  T  T  T
0.5948103639880488  0.7367385922076469  -0.0051869035951471  T  T  T
0.5963829409885772  0.5139921119029299  0.4932051776202005  T  T  T
0.3312200009999984  0.0000000000000000  0.8333799990000017  F  F  F
0.3312200009999984  0.2500000000000000  0.3333799990000017  F  F  F
0.4282651369103760  0.2500000000000000  0.0001050071835991  F  F  F
0.4282651369103760  0.0000000000000000  0.5001050221835968  F  F  F
0.5427658646406994  0.0039283660868937  0.1692903461998119  T  T  T
0.5458181549339237  0.2510417414412761  0.6518663050733319  T  T  T
0.3810960778633330  0.0000000000000000  0.1667699372837745  F  F  F
0.5000090192288240  0.0054895358545784  0.8295775084900245  T  T  T
0.3810960778633330  0.2500000000000000  0.6667699072837721  F  F  F
0.4944432099704240  0.2471439428452710  0.3325811899370383  T  T  T
0.5973313017203353  0.9883487925551383  0.4842911599981098  T  T  T
0.5970443911763571  0.2628222486088947  0.9833323050555843  T  T  T

```

12\_2N.NH\_f2N.NH

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
3 1 23 1

Selective dynamics

Direct

0.6121957636113293	0.7508857629713788	0.4793674542236609	T	T	T
0.6122788632216317	0.4986099168199256	0.9785624122888404	T	T	T
0.6200983636143372	0.0210867797431301	0.9548004961425247	T	T	T
0.6845577697069563	0.9918455386616649	0.9068925006673311	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5372996211634011	0.4954157468357338	0.1823374471396747	T	T	T
0.5357536037090503	0.7520400550224067	0.6800870727556779	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4978066820099884	0.4956388384886630	0.8316462775576984	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4955867588201078	0.7513115220938853	0.3329766194304025	T	T	T
0.5949927103647302	0.7373084517655554	-0.0043893620297162	T	T	T
0.5960722245982798	0.5150349500132141	0.4926163257528773	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5440431850934337	0.0027846780396526	0.1717255177383402	T	T	T
0.5465467122730719	0.2484917461191937	0.6516281091844438	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4986003800756466	0.0047183259604199	0.8312320103717441	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4948089988798489	0.2479718921934472	0.3322795506721766	T	T	T
0.5982634445893599	0.2623412057130673	0.9906140843910194	T	T	T
0.5915289800517370	0.9857396014524460	0.4879794655856296	T	T	T

13\_2N.NH\_c.2H2N.NH.2H

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N H Fe Co  
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Selective dynamics

Direct

0.6100191216304236	0.7508599938953642	0.4544608428725065	T	T	T
0.6103105340969633	0.4951721741024767	0.9837360071664336	T	T	T
0.6181052912227446	0.0366473344703741	0.9575442685337782	T	T	T
0.6807777442023379	0.9953148801045182	0.9114503741508596	T	T	T
0.6451305983866173	0.3158804520687124	0.5407502522969870	T	T	T
0.6438432629021187	0.7515987402878094	0.7792816616370108	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5369888967826295	0.4952618761970567	0.1871738414735949	T	T	T
0.5408317587829458	0.7529918043031103	0.6741930806241535	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4972218745146043	0.4964251819901531	0.8319654509196305	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4937746882428201	0.7516707589406587	0.3331522729342524	T	T	T
0.5939411602448555	0.7314822986624255	0.9933548413661175	T	T	T
0.6000979592422165	0.5127699567717051	0.4925067420250241	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F



0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5418011585414586	0.0020151241994582	0.1664333130733666	T	T	T
0.5490247258168869	0.2518823449146566	0.6477360825662166	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.5005294209521072	0.0057344095056016	0.8272893950202372	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4927460824276909	0.2461219937740525	0.3328602663419960	T	T	T
0.5994558759467389	0.9887136003245850	0.4782633202618531	T	T	T
0.5945830011044794	0.2659523091117045	0.9890620203815258	T	T	T

14\_2N.NH\_f.2H2N.NH.2H

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N H Fe Co

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Selective dynamics

Direct

0.6104821074687327

0.7506026699785091

0.4563858072129516

T T T

0.6110118930238231

0.4977917618604955

0.9846701002321324

T T T

0.6189230317867289	0.0365557118380559	0.9521131227711372	T	T	T
0.6800573490170985	0.9906822439630126	0.9022682703691821	T	T	T
0.6462613609961743	0.3248119483762070	0.5536380237110586	T	T	T
0.6440330876463365	0.7496634584088371	0.7797160247098525	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5360770831035451	0.4971764802366658	0.1865296879155817	T	T	T
0.5411052589359311	0.7525682026581669	0.6744630656186023	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4965388925683396	0.4967933123688349	0.8315546277327830	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4942992255103788	0.7520496571002612	0.3338928900100109	T	T	T
0.5941847727340723	0.7327499596047009	0.9936677675392396	T	T	T
0.6000681214535700	0.5145156961735754	0.4916773226765382	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5430234523595788	0.0017207453744470	0.1655757560439823	T	T	T
0.5494733560153151	0.2500292370049129	0.6483988778818971	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4989572909498707	0.0046013473610261	0.8275163510058177	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4935326612841007	0.2464945163111978	0.3325393888835119	T	T	T
0.5963614579495882	0.2666619739284699	0.9942337808590185	T	T	T
0.5921231456157494	0.9863588356075056	0.4795416452435813	T	T	T

15\_2N.NH2\_c.H\_fixN2N.NH.2H

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N H Fe Co  
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Selective dynamics

Direct

0.6118434035048463	0.7525383935589312	0.4814142863110081	T	T	T
0.6108215932008422	0.4991264543128545	0.9760743008634337	T	T	T
0.6710927402632546	0.0614835118769672	0.0418320016732001	T	T	T
0.7220665282455802	0.0728187663436628	0.1431712774847138	T	T	T
0.6086233881011532	0.2152180941348265	0.4561934920862670	T	T	T
0.6976923382754106	0.0113256528250526	0.9168073226708324	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5360970069874418	0.4950564207964304	0.1806181992207252	T	T	T
0.5366833230371930	0.7543311942760978	0.6867983435759579	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4958985727867607	0.4965441893634671	0.8333084777481504	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4977029302922297	0.7557294638722692	0.3320594105828757	T	T	T
0.5975441927979420	0.7349613371336843	-0.0027290480696815	T	T	T
0.5948531864417501	0.5155979432288464	0.4937021286099981	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5492593562400040	0.0035600589871339	0.1463140144144798	T	T	T
0.5460331525390579	0.2480976710262111	0.6620256724411293	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4909752047535099	0.0044529211658228	0.8299259093857856	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4964915346165426	0.2443126286137330	0.3310083044303093	T	T	T
0.5941170401750794	0.9879846955858860	0.4949627964222678	T	T	T
0.6038312626960476	0.2684174669334223	0.9863499185948882	T	T	T

16\_2N.NH2\_f.H\_fixN2N.NH.2H

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	3	23	1

Selective dynamics

Direct

0.6120320634813310	0.7513161094794767	0.4819124545563294	T	T	T
0.6119711974929990	0.4980844909679036	0.9745693391294291	T	T	T
0.6725534433650165	0.0530763433352213	0.0467095390408327	T	T	T
0.7230024034337569	0.0573805821384027	0.1499151661823753	T	T	T
0.6082334996318020	0.2893661828733167	0.4540937679231744	T	T	T
0.6984706078870898	0.0032656830733918	0.9207752641300815	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5357045097428524	0.4965352715915052	0.1793230869373786	T	T	T
0.5379226790626647	0.7527905398909845	0.6881167561733069	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4964536573030432	0.4949678960968451	0.8326072534665808	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4980001874228254	0.7545793480046961	0.3340978017460138	T	T	T
0.5977079400177484	0.7340167560034199	-0.0005787087145922	T	T	T
0.5949332089168528	0.5152884120270986	0.4929282782478550	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F



0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5487127327359389	0.0021004578065276	0.1509594777453744	T	T	T
0.5468016468292713	0.2483423782979258	0.6608712890577245	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4916626275242271	0.0044808582112317	0.8305156207739626	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4974824768738124	0.2446044498166014	0.3319519820672886	T	T	T
0.6047453057152851	0.2646667542913517	0.9942467687876518	T	T	T
0.5887487931002626	0.9851158980218642	0.5001407592244927	T	T	T

17\_2N.NH3\_f2N.NH2.H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	3	23	1

Selective dynamics

Direct

0.6125732616810307	0.7539182577871018	0.4836935853821466	T	T	T
0.6108468805016958	0.4932179126060105	0.9811533155031901	T	T	T
0.7328779619293093	0.8279388472565405	0.9479256763276280	T	T	T
0.7361498703848773	0.9513647259499808	-0.0066585003017378	T	T	T

0.7849823626541637	0.7597887926553938	0.0109693035425174	T	T	T
0.7404607039925447	0.8266883962511492	0.7988642134825947	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5374839419831096	0.4959563746122034	0.1845313729782498	T	T	T
0.5373918564023538	0.7556776778131806	0.6883927813250729	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4977298078130946	0.4982062498613513	0.8337519278559554	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4985464135698010	0.7538873055494555	0.3338773866586394	T	T	T
0.6019185712700745	0.7329609624387747	-0.0030825649271125	T	T	T
0.5944606143578443	0.5153793685315703	0.4956822847586269	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5459702108539702	0.0006299594329203	0.1542178098426378	T	T	T
0.5463133293191882	0.2489454795042892	0.6599522615461733	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4945568402536002	0.0058656157472106	0.8317101284838774	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4961736490728720	0.2433554760886197	0.3336786370651196	T	T	T
0.5966598508183129	0.9914214233484632	0.4885418783204869	T	T	T
0.5907685411977588	0.2583881449462984	0.9946285455316148	T	T	T

18\_2N.NH3\_c2N.NH2.H

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N H Fe Co  
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Selective dynamics

Direct

0.6111732456651020	0.7545876117297543	0.4766283794894866	T	T	T
0.6115714948138826	0.4919910997554251	0.9789348588634788	T	T	T
0.7282516337166176	0.8132284659563277	0.0235467509907934	T	T	T
0.7431409199355881	0.8335415473684977	0.1673867002531900	T	T	T
0.7730819855308343	0.7263983351862060	-0.0313031890407024	T	T	T
0.7357639497068790	0.9247416777612038	0.9504288444791302	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5374323921497286	0.4968001081784879	0.1834453409634635	T	T	T
0.5394780632800678	0.7556757486251831	0.6879243431670939	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4979104034378880	0.4977468289238737	0.8346904938805711	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4956800647935318	0.7532582298775752	0.3348091801019135	T	T	T
0.5956930053089379	0.2586705439020990	0.9916893230620828	T	T	T
0.5948770588281085	0.5140878495506398	0.4950731034790471	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5460226934951999	-0.0024930006628050	0.1548448280728789	T	T	T
0.5444327787836912	0.2490164312334727	0.6575549967478498	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4950273191969728	0.0065552728973601	0.8318990375911114	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4968891699809811	0.2436909369813452	0.3322628129833664	T	T	T
0.5962539886880212	0.9921598860101434	0.4915086091060826	T	T	T
0.5972997268822406	0.7310777142214520	-0.0045765429246510	T	T	T

19\_2N\_diagonalCIF file

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N Fe Co

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Selective dynamics

Direct

0.6112309566692327	0.7531360692696705	0.4820139322566866	T	T	T
0.6111257009694743	0.4970920518079925	0.9816051252220874	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5379330127832510	0.4940924585941647	0.1865830695748276	T	T	T
0.5373523417082049	0.7557721458734067	0.6866610519468087	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4972538553621774	0.4969368167212513	0.8337220262236341	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4981803305495668	0.7542324493008643	0.3328296294242588	T	T	T
0.5963887236772462	0.7336770051500093	-0.0038019832989415	T	T	T
0.5953021907782249	0.5145911446098148	0.4972497919383137	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5470709586227180	0.0025844568063861	0.1557824061368433	T	T	T
0.5458423360716855	0.2482614493340409	0.6601256937809166	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4953315262442157	0.0049207719489411	0.8330406509336201	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F

0.4957422086996564	0.2431733808096768	0.3335522929034347	T	T	T
0.5975262962353930	0.9904556118223309	0.4913087361702887	T	T	T
0.5915373647780856	0.2609987138628210	0.9931649412068307	T	T	T

20\_2N\_edge\_cCIF file

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
2	23	1

Selective dynamics

Direct

0.6124349544113856	0.2472777017778746	0.4803214203968305	T	T	T
0.6124348887426309	0.7527219996167789	0.4803264304264958	T	T	T
0.3312200009999984	0.5000000000000000	0.83337999990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.33337999990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5391971106647889	0.5000013343883416	0.1620634064441629	T	T	T
0.5412033038587895	0.7519596942366273	0.6844928824059096	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4941943155625736	0.5000014766055634	0.8309226244414343	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.5018366398055994	0.7511291379264933	0.3357193855885117	T	T	T
0.5933599847181651	0.7488195149765567	0.0014562091360871	T	T	T
0.6010636338801933	0.4999988117048338	0.4905254297979402	T	T	T

0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5412094026364663	-0.0000033442982809	0.1619599828217599	T	T	T
0.5412009517573361	0.2480405404541375	0.6844870139454919	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4941696850645122	-0.0000027025636504	0.8324672587358006	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.5018388068630721	0.2488718752255280	0.3357118596534295	T	T	T
0.5933543509507122	0.2511788453221403	0.0014612643165553	T	T	T
0.5982022302756723	0.0000019788697633	0.4911306095946750	T	T	T

21\_2N\_edge\_fCIF file

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
2	23	1

Selective dynamics

Direct

0.6124648212148945	-0.0000058167626730	0.9768885859207722	T	T	T
0.6134512669247295	0.5000085943209835	0.9806165035698962	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F

0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5404764259602661	0.5000010130794175	0.1836706313325909	T	T	T
0.5409809521200899	0.7535628020123909	0.6605869992312228	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.5023831159338920	0.5000013784814847	0.8345628040312584	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4932091619229323	0.7490398046972682	0.3310731215359741	T	T	T
0.6008475197837917	0.7499157014460057	-0.0078309912237606	T	T	T
0.5920250619777239	0.4999993655721479	0.5040186770504935	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5421523464524729	-0.0000008101588196	0.1852329411595170	T	T	T
0.5409799309424410	0.2464377981859742	0.6605837469526892	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4983263529574818	0.0000001660195517	0.8391901762046221	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4932086115287590	0.2509595501701197	0.3310681377875911	T	T	T
0.6008480287723570	0.2500863740363603	0.9921657788387589	T	T	T
0.5924926835845251	0.0000007166102719	0.5008676589204252	T	T	T

22\_2N\_diagonal.N2\_cCIF file

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co			
4	23	1			
Selective dynamics					
Direct					
0.6876071850250253	0.1710946855968899	0.8235244616080009	T	T	T
0.6731008684811970	0.1189141129595015	0.6624774543951706	T	T	T
0.6111107212422054	0.7479914735892533	0.4757260082073901	T	T	T
0.6091639624173897	0.5008486092594879	0.9767628511547455	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5362648244146144	0.4905314068826097	0.1812869116993875	T	T	T
0.5366981733124762	0.7553156178376249	0.6829485569920388	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4962298029991882	0.4948993593525858	0.8331589136829097	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4979771932811473	0.7563465042631916	0.3310275486974226	T	T	T
0.5938012679093820	0.7349563102667834	-0.0025103262013430	T	T	T
0.5927727526697556	0.5139970818365885	0.4908015582728718	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5473392868892026	0.0063613742451894	0.1565564168174692	T	T	T
0.5463356889575114	0.2448205623214843	0.6535027586487431	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4915088296182836	0.0037753624736507	0.8344158452724864	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4938639628161731	0.2432440479161797	0.3304734210937211	T	T	T
0.6067311083854477	-0.0170458963728123	0.4939151633941450	T	T	T
0.6008992772331176	0.2610085210480376	0.9876586214836802	T	T	T



23\_2N\_diagonal.N2\_fCIF file

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N

Fe

Co

4

23

1

Selective dynamics

Direct

0.6792959445462583

0.1736687666214335

0.8098454040071352

T

T

T

0.6766395927349242

0.1131210945637335

0.6496499999269696

T

T

T

0.6117039742163551

0.7472682493389335

0.4762333925070565

T

T

T

0.6099513799720151

0.5029287453092310

0.9786829211173871

T

T

T

0.3312200009999984

0.5000000000000000

0.8333799990000017

F

F

F

0.3312200009999984

0.7500000000000000

0.3333799990000017

F

F

F

0.4282651369103760

0.7500000000000000

0.0001050071835991

F

F

F

0.4282651369103760

0.5000000000000000

0.5001050221835968

F

F

F

0.5368796983072698

0.4927058471761845

0.1838666873677288

T

T

T

0.5372976901103391

0.7550268639569463

0.6830784996138334

T

T

T

0.3810960778633330

0.5000000000000000

0.1667699372837745

F

F

F

0.4969645231922538

0.4954714661637034

0.8337051704416284

T

T

T

0.3810960778633330

0.7500000000000000

0.6667699072837721

F

F

F

0.4981638272651654

0.7556255493071046

0.3320342019666371

T

T

T

0.6065446182024847

0.2631837882627036

0.0033162328866125

T

T

T

0.6066962362220397

-0.0191813965535912

0.4854030549568847

T

T

T

0.3312200009999984

0.0000000000000000

0.8333799990000017

F

F

F

0.3312200009999984

0.2500000000000000

0.3333799990000017

F

F

F

0.4282651369103760

0.2500000000000000

0.0001050071835991

F

F

F

0.4282651369103760

0.0000000000000000

0.5001050221835968

F

F

F

0.5449312144075544

0.0054584429661414

0.1565653545163364

T

T

T

0.5495914472657417

0.2468711780058765

0.6559357673886492

T

T

T

0.3810960778633330

0.0000000000000000

0.1667699372837745

F

F

F

0.4917606315671478

0.0040566679244333

0.8334857494497657

T

T

T

0.3810960778633330

0.2500000000000000

0.6667699072837721

F

F

F

0.4952851927174292

0.2431925670307927

0.3319662373161008

T

T

T

0.5941589100497050

0.7377745907679208

0.9970657234261306

T

T

T

0.5890112899107994

0.5166997886323933

0.4937078678946901

T

T

T

24\_4NN Fe  
 0.9906000000000000  
 14.8120002747000008 0.0000000000000000 0.0000000000000000  
 0.0000000000000000 8.0120000420000004 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 6.9380002021999996

N Fe Co  
 4 23 1

Selective dynamics

Direct

0.6117363974790221	0.0016140004070480	0.9707293714088350	T	T	T
0.6123397033195778	0.7500396332825499	0.4695947366572245	T	T	T
0.6117349077051193	0.4984448423353264	0.9707313822409367	T	T	T
0.6122977671709195	0.2500528915609598	0.4650926223304541	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5376869795277041	0.4987273282267510	0.1713778100216325	T	T	T
0.5367992443468910	0.7500268110560845	0.6697801113367980	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4988186631944188	0.4991525914620241	0.8313113366004751	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4976465383644278	0.7500207278194382	0.3309050073570578	T	T	T
0.6001059488237472	0.7500302569453178	-0.0137610034952583	T	T	T
0.6006692009197695	0.5004713894211749	0.4859002159943207	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5376871694299040	0.0013193990338782	0.1713739303148573	T	T	T
0.5387047886240729	0.2500298509732644	0.6693298989065541	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F

0.4988175587189071	0.0008868426005267	0.8313020267682566	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4971263928420150	0.2500188798525844	0.3320458224702185	T	T	T
0.6006688424039089	-0.0003805745798264	0.4858944203706140	T	T	T
0.5981013453330414	0.2500276083274622	0.9824388461728021	T	T	T

25\_3N.NH\_c.HNH.H.3N

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
4	2	23	1

Selective dynamics

Direct

0.6172216666220118	0.9843235102470289	0.9962629214130576	T	T	T
0.6113438931983434	0.7573969012218078	0.4714413026046826	T	T	T
0.6087126862252278	0.4185070223171887	0.8870316606080044	T	T	T
0.6115757699269483	0.2562794515773240	0.4689570730886970	T	T	T
0.6696603570171651	0.4714508830670314	0.8460182458268110	T	T	T
0.6486477415045028	0.5357385809853779	0.2306305577349178	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F

0.5484123116308990	0.4910193006668037	0.1345504996808710	T	T	T
0.5376405034795808	0.7511861076919180	0.6719713686215296	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4893797660099163	0.5105813074473206	0.8236313540908727	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4965721797392545	0.7411377581230281	0.3303120449832616	T	T	T
0.5946266693754606	0.7593363674452679	-0.0096002052570978	T	T	T
0.6014652605345151	0.5070950360729209	0.4590416647575069	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5343039250483121	-0.0058141469160935	0.1874592027677146	T	T	T
0.5463048108524274	0.2681319085742311	0.6860917538677290	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4969240202549522	0.0033424158869905	0.8334981118672522	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4983765229811613	0.2526831194691514	0.3355233420344590	T	T	T
0.5997749049887638	0.0066632067458533	0.4956532018618067	T	T	T
0.6011178378560796	0.2071052257474545	0.9969045860695762	T	T	T

26\_3N.NH\_f.HNH.H.3N  
0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000			
0.0000000000000000	8.0120000420000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	6.9380002021999996			
N	H	Fe	Co		
4	2	23	1		

Selective dynamics

Direct

0.6124265705713156	0.9976369652831658	0.9712317064072474	T	T	T
0.6111526485729732	0.7552345300413614	0.4757779762461757	T	T	T
0.6181859587912820	0.4639915248061207	0.9283315695447170	T	T	T
0.6113817090452921	0.2489870284177876	0.4715474638886886	T	T	T
0.6808477447782079	0.5011426726930278	0.8773294977072265	T	T	T
0.6502946682220355	0.5177151855921940	0.2606863462653792	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5490187271717041	0.5022266699735932	0.1549874116917163	T	T	T
0.5371721858553032	0.7496257772973884	0.6741727929756135	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4961441374433716	0.5010143291097876	0.8292280890078360	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4982430731388320	0.7478293872928021	0.3317228014219626	T	T	T
0.5975486577880966	0.7629336753067921	-0.0112874261221381	T	T	T
0.5998348113043488	0.5023281858267807	0.4774275787760038	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5365988684682150	-0.0004032548284174	0.1772307538514736	T	T	T
0.5377930251039258	0.2502439944042756	0.6719626376409032	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4937590823568828	-0.0007091961939389	0.8325030497553201	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4985166214059971	0.2527388493202023	0.3313099045279189	T	T	T
0.5974052213211680	0.2306299159931856	0.9851221841256842	T	T	T
0.5975196033373669	0.0007890740019767	0.4869953984319391	T	T	T

27\_2N\_edge\_f.H\_cCIF file

0.9906000000000000

14.8120002747000008 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.0120000420000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 6.9380002021999996

N H Fe Co  
2 1 23 1

Selective dynamics

Direct

0.6123183372755637	0.7522012609869883	0.4756840019103476	T	T	T
0.6120349237578011	0.2480091574862807	0.4769494789258872	T	T	T
0.6081705624518704	0.9825306063814692	0.9624353663152370	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5391328394042321	0.4984620225727708	0.1601293211231089	T	T	T
0.5412798585374791	0.7506107580547383	0.6803123517967828	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4945296292237054	0.5011101199037984	0.8303102338901954	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.5005975034061154	0.7511350090033788	0.3351385435769824	T	T	T
0.5929365716560601	0.7462842290524456	-0.0005195928881905	T	T	T
0.6012996108393146	0.4998776298530228	0.4863718074014112	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5417526743866304	0.0016813817886404	0.1619345612201948	T	T	T
0.5417845294157149	0.2495128738774610	0.6834117967134496	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4950493207507828	-0.0011430916240880	0.8309272429871548	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4992987387208637	0.2488843111045280	0.3388093428985458	T	T	T
0.5994109979919435	0.2550178338944939	0.9984743955872402	T	T	T
0.5981185121899206	0.0003232572165999	0.4878242436636599	T	T	T

28\_2N\_edge\_c.H\_fCIF file

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
2	1	23	1

Selective dynamics

Direct

0.6123115954383470	0.2480469365496721	0.4764866617824486	T	T	T
0.6123114321520216	0.7519426131075574	0.4764733503434547	T	T	T
0.6078583688899301	0.9995248826263320	0.9636200028613647	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5392630119158426	0.4999934650191151	0.1602483865070068	T	T	T
0.5411256905973388	0.7506321493216236	0.6809751796900435	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4951571525241943	0.4999942848466805	0.8309463503047088	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.5005594737076331	0.7508435162571113	0.3358653817648000	T	T	T
0.5929504031574697	0.7478507577913304	-0.0003026828917814	T	T	T
0.6012210850716150	0.4999911859803120	0.4870171838672657	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F

0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5410247315411553	-0.0000093618530872	0.1630582090609542	T	T	T
0.5411183539747084	0.2493506151528111	0.6809823918825109	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4954940791814146	-0.0000079434527760	0.8311020409962744	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.5005633854601932	0.2491415568119119	0.3358738279539480	T	T	T
0.5929475765306643	0.2521143681204537	0.9997236490930299	T	T	T
0.5982020160183821	-0.0000046926439477	0.4878619991150817	T	T	T

29\_2N\_diagonal.H\_f2N.2H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
2	1	23	1

Selective dynamics

Direct

0.6111095368598998	0.2476264795873644	0.4791623563611413	T	T	T
0.6120000145189739	0.5027932173901809	0.9811022166976803	T	T	T
0.6092678271931793	0.9676748798392770	0.9559785541426195	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F



0.5372043629103298	0.5052045988013736	0.1861551806844724	T	T	T
0.5468029520799430	0.7523409705381710	0.6538150961135504	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4983165920162428	0.5046919676683350	0.8322268471677468	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4950003024952408	0.7543915748906637	0.3329789011959756	T	T	T
0.5967381199031568	0.7391687121740961	-0.0064339877127179	T	T	T
0.5970242411563598	0.4845673858392042	0.4953794003250693	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5458384112403594	-0.0022349617972391	0.1612357556197383	T	T	T
0.5370961499419652	0.2456387376570787	0.6832059807021568	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4969908659022828	-0.0059063310397690	0.8313179239992491	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4967707477528815	0.2475230082490906	0.3332504076749495	T	T	T
0.5956011661619439	0.2656941240566947	0.9954349353451475	T	T	T
0.5923792730916381	0.0113958903538016	0.4908348786283906	T	T	T

40\_2N.NH3\_f22N.NH2.H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co				
3	3	23	1				
Selective dynamics							
Direct							
0.6116003849353246	0.7524809530222595	0.4820511591863939	T	T	T		
0.6111744089293477	0.4996088751255911	0.9820040261703348	T	T	T		
0.7357375732910743	0.1663461176025869	0.9651733687595583	T	T	T		
0.7610086881833318	0.1288530518175250	0.0972427949327958	T	T	T		
0.7797768517757666	0.2511776490962038	-0.0965070036438769	T	T	T		
0.7309628467558986	0.0622969223378371	0.8772459819123525	T	T	T		
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F		
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F		
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F		
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F		
0.5368097551047712	0.4929551697225927	0.1850271840290458	T	T	T		
0.5382257867810910	0.7554959658413521	0.6873439179533303	T	T	T		
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F		
0.4987190607660721	0.4940510104355978	0.8335755763435845	T	T	T		
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F		
0.4972081461396501	0.7526667201302271	0.3342306862523764	T	T	T		
0.5939209987950002	0.7361481740516975	-0.0010208888673665	T	T	T		
0.5954746501242894	0.5160210737168039	0.4951576535711070	T	T	T		
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F		
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F		
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F		
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F		
0.5452275115194183	0.0029542036839044	0.1592354394692851	T	T	T		
0.5481346799022743	0.2470514315629367	0.6567665996034983	T	T	T		
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F		
0.4954245051149264	0.0070267637733902	0.8328143358135182	T	T	T		
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F		
0.4957287027110008	0.2450179360571119	0.3336555337001176	T	T	T		
0.6033675608943816	0.2600026703853183	0.9927234709059645	T	T	T		
0.5910263024431042	0.9880063472325515	0.4916283280864601	T	T	T		

41_4N_subN	Fe	
0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
4	23	1

Selective dynamics

Direct

0.6126894184783590	0.0000151227017134	0.9745457602443419	T	T	T
0.6128165462259514	0.7507740775118718	0.4727505182034454	T	T	T
0.6118160817432814	0.5000270001390685	0.9704457845033537	T	T	T
0.6128138731120196	0.2493052824672823	0.4727400027084229	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5369227801395762	0.7500423547282604	0.6716920182015086	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.5007980806512892	0.5000218295302027	0.8322984281811101	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4992216198799080	0.7506669379984348	0.3321421236629631	T	T	T
0.6009034214972850	0.7488511524367685	-0.0126662517339961	T	T	T
0.6008956127146226	0.5000339305166781	0.4883762319880717	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5367127237662058	0.0000171243407669	0.1730006157516561	T	T	T
0.5369193722683978	0.2500125322253728	0.6716877412400106	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.5000764258746251	0.0000174071436191	0.8323835961194661	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4992193889205680	0.2493701452581025	0.3321326112671346	T	T	T
0.6007661399002283	0.0000388106154734	0.4886533576771156	T	T	T
0.6009011711255258	0.2511942328603280	0.9873248182274299	T	T	T
0.5359713423303131	0.5000250596357179	0.1724913025355796	T	T	T

42\_2N\_edge\_f.2H\_c\_sub2N.2H

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
2 2 23 1

Selective dynamics

Direct

0.6131883692998423	0.0000000483321135	0.9778389331999485	T	T	T
0.6123615600656004	0.5000012347258387	0.9742827032627751	T	T	T
0.6080451877613143	0.7625313632257724	0.4673190287404601	T	T	T
0.6080494154584045	0.2376096174214077	0.4673411157490103	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5400688722119131	0.7503526671673320	0.6633680901170026	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.5014185491506761	0.5000096393520160	0.8371894013425019	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4951753706719599	0.7510373318029264	0.3308609097517516	T	T	T
0.6014241597382215	0.7484373718269000	-0.0115270377761602	T	T	T
0.5919764855452612	0.5000056699340278	0.5017233902411689	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F

0.5404244584276562	0.0000043820617567	0.1807173871990054	T	T	T
0.5400631133216378	0.2496607687860809	0.6633807186619074	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.5009208589817568	0.0000063646697277	0.8370030638229069	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4951722982811153	0.2489647710124438	0.3308612446315264	T	T	T
0.6014219487838620	0.2515821612498840	0.9884711420234923	T	T	T
0.5925623350429151	0.0000271458984328	0.5007957438274468	T	T	T
0.5392129209629946	0.5000028455811784	0.1818715880332199	T	T	T

43\_4N\_2CoN      Fe

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N      Fe      Co

4      22      2

Selective dynamics

Direct

0.6115401765706373	0.0014856135981494	0.9651832151916074	T	T	T
0.6116005757241019	0.7513907825589673	0.4695467883262622	T	T	T
0.6116048013804342	0.4986285478227119	0.9695512592567814	T	T	T
0.6115444965500602	0.2485421796031853	0.4651907241284948	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F

0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5373957334795022	0.4987967598459447	0.1703318290522077	T	T	T
0.5373900841653283	0.7512124117107827	0.6703259483946300	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4977855124627551	0.4991174644575158	0.8305897729620212	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4977789395505266	0.7508885903274998	0.3305884488690207	T	T	T
0.6001091909004409	0.7495179043540642	-0.0150733851311509	T	T	T
0.6001122215645709	0.5005032273592999	0.4849389617194668	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5394284957693848	0.0009274174645970	0.1701846175756938	T	T	T
0.5394280318921851	0.2490812477140412	0.6701826102025507	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4973510203845547	0.0007213415758321	0.8318550232868274	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4973572449148244	0.2492864304490431	0.3318571456416161	T	T	T
0.5979344572086230	-0.0006394545504607	0.4817672773301453	T	T	T
0.5979352520972455	0.2506535381983519	0.9817666730077876	T	T	T

44\_4N\_Co.Cosub\_relax5N      Fe  
0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000			
0.0000000000000000	8.0120000420000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	6.9380002021999996			
N	Fe	Co			
4	22	2			

Selective dynamics

Direct

0.6104097790475220	0.0198300655956733	0.9517593889411412	T	T	T
0.6116216380320795	0.7517420222770311	0.4706452392915044	T	T	T
0.6120001026715592	0.5049133307307752	0.9719646693061328	T	T	T
0.6112568071616354	0.2517900962009492	0.4514335107602161	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4265582508601127	0.7510262549652749	0.0004363591924352	T	T	T
0.4264860529052411	0.5000421956175690	0.5007231143041939	T	T	T
0.5367754746773308	0.4976267565173900	0.1753260047335646	T	T	T
0.5368714578592422	0.7539142758749300	0.6746148457504545	T	T	T
0.3810213277549002	0.4997044488134242	0.1657368923618777	T	T	T
0.4963758192120374	0.4996615916691618	0.8337537180168664	T	T	T
0.3813934965362799	0.7501874131575752	0.6652891056340785	T	T	T
0.4960920633285341	0.7516741103231555	0.3340653383335027	T	T	T
0.5957178451088413	0.7494677993411712	-0.0055370947334028	T	T	T
0.5962422676290572	0.4999290757147626	0.4933154744680999	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4274166598481055	0.2496421157805802	0.0008457558433510	T	T	T
0.4284789239487785	0.0002992243209966	0.5003862338767644	T	T	T
0.5418679033596431	0.0056498969200523	0.1569906783285088	T	T	T
0.3820231602186388	0.0003910766780716	0.1654446003023867	T	T	T
0.4966148414498624	0.0025204510258876	0.8302047727473240	T	T	T
0.3818815920894818	0.2492860562310777	0.6658571212398081	T	T	T
0.4967242816691099	0.2480023558319258	0.3325992385622923	T	T	T
0.6035004891887291	0.0013144483430923	0.4735832311610284	T	T	T
0.5991770804863160	0.2598003185220009	0.9718683929044597	T	T	T
0.5408795689834431	0.2473416636119951	0.6584978281051714	T	T	T

30\_2N\_diagonal.H\_c2N.2H

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N

H

Fe

Co

2

1

23

1

Selective dynamics

Direct

0.6114421705043447

0.2463162164962643

0.4809942559688023

T

T

T

0.6112221346387638

0.5031894500060752

0.9795303449626660

T

T

T

0.6092953721186195

0.8014620655430330

0.4498009975781583

T

T

T

0.3312200009999984

0.5000000000000000

0.8333799990000017

F

F

F

0.3312200009999984

0.7500000000000000

0.3333799990000017

F

F

F

0.4282651369103760

0.7500000000000000

0.0001050071835991

F

F

F

0.4282651369103760

0.5000000000000000

0.5001050221835968

F

F

F

0.5367840682720347

0.5044065595574628

0.1838081620496523

T

T

T

0.5463066390601281

0.7522382888228372

0.6570502925327598

T

T

T

0.3810960778633330

0.5000000000000000

0.1667699372837745

F

F

F

0.4973501478856198

0.5038133500526970

0.8325338485413148

T

T

T

0.3810960778633330

0.7500000000000000

0.6667699072837721

F

F

F

0.4971962980978278

0.7553446214434217

0.3306748621108888

T

T

T

0.5978984322182521

0.7405526337404210

-0.0120634790590254

T

T

T

0.5955850511217214

0.4825955264821335

0.4960158010476838

T

T

T

0.3312200009999984

0.0000000000000000

0.8333799990000017

F

F

F

0.3312200009999984

0.2500000000000000

0.3333799990000017

F

F

F

0.4282651369103760

0.2500000000000000

0.0001050071835991

F

F

F

0.4282651369103760

0.0000000000000000

0.5001050221835968

F

F

F

0.5458881773226094

-0.0006385597144227

0.1574887929430818

T

T

T

0.5377362537791214

0.2435541900667232

0.6863957998625665

T

T

T

0.3810960778633330

0.0000000000000000

0.1667699372837745

F

F

F

0.4954161551189827

-0.0060131014168133

0.8330443921075696

T

T

T

0.3810960778633330

0.2500000000000000

0.6667699072837721

F

F

F

0.4971685285748053

0.2468454628230618

0.3335171754939619

T

T

T

0.5958665086292103

0.2647279205498738

0.9958808258190113

T

T

T

0.5938270268894702

0.0129585911000110

0.4903697975652982

T

T

T



3l\_2N\_edge\_f.2H\_c2N.2H

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
2 2 23 1

Selective dynamics

Direct

0.6124681729746486	0.0000170461805867	0.9704387405200495	T	T	T
0.6131568837784799	0.5000174437973526	0.9754224801110689	T	T	T
0.6071873978345054	0.7751321996481082	0.4593045489461090	T	T	T
0.6071896679233959	0.2248092035078627	0.4592746387320504	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5398171998402812	0.5000038934088994	0.1782689920510836	T	T	T
0.5410061687901401	0.7517096248345199	0.6617832835130023	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4998480165784612	0.4999982536614475	0.8346820163179937	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4956012995921706	0.7498295447212719	0.3307305008314159	T	T	T
0.6011668571602435	0.7494053346129433	-0.0131659946647722	T	T	T
0.5918487115887557	0.4999962234268952	0.5000524774522391	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5422473107915097	0.0000036783952772	0.1798508776291855	T	T	T
0.5410110954314732	0.2482800983537945	0.6617683233040157	T	T	T

0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4977012181313118	0.0000022855806566	0.8381992475900230	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4956027208361862	0.2501620978546234	0.3307285705644199	T	T	T
0.6011657551533700	0.2506232994571773	0.9868332975192815	T	T	T
0.5902425871322010	-0.0000133747414033	0.4990960387302096	T	T	T

32\_2N\_edge\_c.2H\_f2N.2H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
2	2	23	1

Selective dynamics

Direct

0.6122499071518976	0.2477934827196566	0.4753784040577795	T	T	T
0.6122481035014289	0.7522384616321377	0.4753288089791132	T	T	T
0.6073086850464474	0.5006470860520595	0.9656114682916702	T	T	T
0.6070003011340690	0.9992844950205559	0.9618073682135363	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5394390162600704	0.5000130317424898	0.1620674889460548	T	T	T

0.5408795209016596	0.7515572600406537	0.6799184764232548	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4948159952058687	0.5000096653626086	0.8299023695079782	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4999806782207462	0.7505945036251565	0.3363013781652701	T	T	T
0.5925814219289480	0.7498499615080739	0.0003088079000958	T	T	T
0.6009741373425740	0.5000111320500906	0.4855896518800372	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5411639215455489	0.0000008348300618	0.1631273363542867	T	T	T
0.5408682917992691	0.2484695519968852	0.6799400501363622	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4950071092355933	0.0000042411609745	0.8314593054634591	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4999873662476371	0.2494184569881747	0.3363034791625235	T	T	T
0.5925609427350407	0.2501577265322496	0.0003763169511356	T	T	T
0.5983336933936688	0.0000180538007940	0.4874647976488252	T	T	T

33\_2N\_diagonal.2H2N.2H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co	
2	2	23	1	
Selective dynamics				
Direct				
0.6116518177471009	0.2471800453907503	0.4787275701053649	T	T T
0.6121674033263457	0.5027713053569818	0.9783116983716774	T	T T
0.6091867700055338	0.8023165326107123	0.4476791755625649	T	T T
0.6091218588464961	0.9673733271994460	0.9522723143957051	T	T T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F F
0.5365821558960326	0.5039339740270858	0.1828309175327041	T	T T
0.5460742051080849	0.7521584443491722	0.6549411885381612	T	T T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F F
0.4973810252584285	0.5042255454569772	0.8317880219000714	T	T T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F F
0.4968002847503299	0.7548133873158981	0.3305380961102224	T	T T
0.5971350255393222	0.7389096620776096	-0.0103378357722732	T	T T
0.5960358595389575	0.4834987427567319	0.4946334238547212	T	T T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F F
0.5461567369420975	-0.0013902080251589	0.1582880457185659	T	T T
0.5369676809963843	0.2453158475123584	0.6830757385035703	T	T T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F F
0.4965866291078853	-0.0049875274776508	0.8311041239215428	T	T T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F F
0.4967048694320773	0.2474912375566827	0.3329520015658692	T	T T
0.5962295377674023	0.2659794927743416	0.9942376222454326	T	T T
0.5941311378029931	0.0138328073295133	0.4884528963805390	T	T T

34\_3N.NH\_cNH.H.3N

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
4 1 23 1

Selective dynamics

Direct

0.6115756053524621	0.0004879834646962	0.9747286049035252	T	T	T
0.6128627681210368	0.7488569658832787	0.4702072118004852	T	T	T
0.6207217656292244	0.4747325120154338	0.9529654875482567	T	T	T
0.6129057175345354	0.2516122356609867	0.4627894347979694	T	T	T
0.6848872106454464	0.5011584705103294	0.9015013167038811	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5414040814299876	0.5015540448448595	0.1624514977883479	T	T	T
0.5376607035881695	0.7492466330187495	0.6709905265544012	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4992186790208479	0.4990968924238631	0.8289661988303720	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4971671356798000	0.7484325346257219	0.3321487837889661	T	T	T
0.5964860362292230	0.7627798948223302	-0.0100247746938313	T	T	T
0.6010775702163329	0.5006717938889054	0.4800150176209982	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5360651716391761	0.0016035783169628	0.1770279746731430	T	T	T
0.5396063654612706	0.2488825437204612	0.6680054837909565	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4957155718354009	0.0004898154586078	0.8320734020722294	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4962402271832781	0.2523358028456245	0.3328506719900078	T	T	T
0.6007809833744062	-0.0007788512182699	0.4873987918598270	T	T	T
0.5962449148213119	0.2358329645088397	0.9807886557008862	T	T	T

35\_3N.NH\_fNH.H.3N

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
4	1	23	1

Selective dynamics

Direct

0.6121988147569210	-0.0005420282970232	0.9684433152641240	T	T	T
0.6122788571372486	0.7504385878222675	0.4711056401451226	T	T	T
0.6209498385349241	0.4878993961483964	0.9561986702327739	T	T	T
0.6122987067870631	0.2493822818788409	0.4697458302970334	T	T	T
0.6863973869589840	0.5051947351770032	0.9064924409811166	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5394271339628900	0.5011561332595655	0.1653893747235049	T	T	T
0.5381977062070105	0.7511241028169308	0.6718423454991839	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4984988229128980	0.4999930437025046	0.8290011003465155	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4982333346616032	0.7496726648186958	0.3327074878815146	T	T	T
0.5972375230321552	0.7598502473098495	-0.0104369322464030	T	T	T
0.6004186797838610	0.5000394112377750	0.4830231597922648	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F

0.5371681939794560	0.0000251637694151	0.1737527956198046	T	T	T
0.5381640372578351	0.2476854216977763	0.6705120121891035	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4948987974763421	-0.0002195073742735	0.8322087682074233	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4979879756752915	0.2504346952994880	0.3322686107414323	T	T	T
0.5977895404552004	0.2391176433378213	0.9868456985342773	T	T	T
0.5984906777484487	-0.0004336232747131	0.4835519517510965	T	T	T

36\_2N.NH2\_TfSDNH2.2N

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	2	23	1

Selective dynamics

Direct

0.6121001828777997	0.7514614980876944	0.4790632070802915	T	T	T
0.6111416351747927	0.4969044078764649	0.9828463085006237	T	T	T
0.6724295198524028	0.1975987314752948	0.5474757444676785	T	T	T
0.6974022482612627	0.2478336567507772	0.4209141437931507	T	T	T
0.7233568839647215	0.1935029923491414	0.6495190732505770	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F

0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5378014965309615	0.4957790758778822	0.1886991489816026	T	T	T
0.5360520937318288	0.7548728407731184	0.6832593441400869	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4978633508760195	0.4951420832747074	0.8340364201021518	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4979649551969221	0.7556204925027684	0.3326928087179446	T	T	T
0.5951714069194751	0.7338017826943589	-0.0058090823508942	T	T	T
0.5967789902620860	0.5154357943737038	0.5004932537083340	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5477834879343383	0.0026790484226523	0.1598090594010393	T	T	T
0.5489018623720276	0.2467154380324101	0.6531728049512034	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4960756333461634	0.0053064456941279	0.8342746978569550	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4917769017479067	0.2442492612351329	0.3310870147344762	T	T	T
0.6048268501368254	0.9849695569711814	0.4988330520330869	T	T	T
0.5886419146620882	0.2613372716429170	-0.0004294434215246	T	T	T



37\_2N.NH2\_TcSDNH2.2N

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
3 2 23 1

Selective dynamics

Direct

0.6106155615171786	0.7512335432028695	0.4780110628027434	T	T	T
0.6113027798138388	0.4976840181020573	0.9825376940001691	T	T	T
0.6706412869197503	0.1885008878350587	0.5424727384551160	T	T	T
0.6962899140481377	0.2420607827771623	0.4184324348403062	T	T	T
0.7220357557202395	0.1759005889937527	0.6425255845923840	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5368687781426408	0.4957004281984780	0.1873287426149097	T	T	T
0.5365284781080706	0.7565911015725304	0.6831117534911875	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4979493389806995	0.4947520807765603	0.8323068802164901	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4963244518696916	0.7539364269068465	0.3335718789035695	T	T	T
0.5945246977503915	0.7356776537536560	-0.0058112180377704	T	T	T
0.5965688796463124	0.5153402396923800	0.4985794398166875	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5458457779513067	0.0017833412150579	0.1612371482512504	T	T	T
0.5494721007507695	0.2448600757844488	0.6486590653171929	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4956971345780365	0.0060258205120063	0.8329323294144775	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4913884847452447	0.2453099479908733	0.3303326173406175	T	T	T
0.5936293461826770	0.2608476249180680	0.9938356022260810	T	T	T
0.6035749148522538	0.9817964688102454	0.4874101635913924	T	T	T

38\_2N.NH2.2H\_TfSDNH2.2N.2H

0.9906000000000000

14.8120002747000008 0.0000000000000000 0.0000000000000000

0.0000000000000000 8.0120000420000004 0.0000000000000000

0.0000000000000000 0.0000000000000000 6.9380002021999996

N H Fe Co  
3 4 23 1

Selective dynamics

Direct

0.6116633756741472	0.7514817889697868	0.4734488167692122	T	T	T
0.6112222262623452	0.5000874906365169	0.9789875401319522	T	T	T
0.6747175868668323	0.1908585860788226	0.5671189474794553	T	T	T
0.7060473047267036	0.2449855069206068	0.4493192118295835	T	T	T
0.7208747697838339	0.1834850107512311	0.6787985414450877	T	T	T
0.6079915380066259	-0.0435025953570215	-0.0460425883856612	T	T	T
0.6044218379904037	0.1727455107155166	0.2256935921739048	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5381261104432646	0.5003492887628700	0.1881782529070493	T	T	T
0.5353933965152357	0.7540950188482443	0.6789456406844044	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4980623205975551	0.4957824933526064	0.8333345958828241	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4959620965321313	0.7552548503338883	0.3332233050287713	T	T	T
0.5947000884673642	0.7350080570486053	-0.0087684415926187	T	T	T
0.5969071854125296	0.5168764484669992	0.5012189407806732	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5464027248064450	-0.0023103902565342	0.1595270679920285	T	T	T
0.5492166945173552	0.2484239032592177	0.6551803264416208	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4974437376764907	0.0059023172083158	0.8315724166779821	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4941214074982941	0.2465758344896141	0.3316701288292525	T	T	T

0.6052335075112634	0.9844932807315570	0.4972729399015973	T	T	T
0.5894889869322567	0.2688360341172572	0.0052740778955571	T	T	T

39\_2N.NH2.2H\_TcSDNH2.2N.2H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	4	23	1

Selective dynamics

Direct

0.6105129879571402	0.7504757033109938	0.4744628290844872	T	T	T
0.6114168291536853	0.5016284992186689	0.9780975455628462	T	T	T
0.6731150284148749	0.1751918976712302	0.5753410282296900	T	T	T
0.7075868824121011	0.2320068668924002	0.4634669540285168	T	T	T
0.7181639155258427	0.1542376069646521	0.6867726293510988	T	T	T
0.6074525005430353	-0.0357519208730771	-0.0469557009666875	T	T	T
0.6018265678321314	0.1728457646499885	0.2305091558036075	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F

0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5369080230526679	0.4997280311821959	0.1861703704219173	T	T	T
0.5358393702507117	0.7544357865144661	0.6803720168203927	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4974408112413234	0.4949234609833369	0.8315382313797646	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4960763376461648	0.7539501871762966	0.3335331641446592	T	T	T
0.5947140327719744	0.7372180391043046	-0.0067798907170561	T	T	T
0.5970211091807239	0.5160069496371160	0.4985518965181681	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5453593282439908	-0.0012668837776284	0.1586242725359695	T	T	T
0.5493037241476246	0.2459577922675405	0.6516019247916229	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4957851107204300	0.0053954549184876	0.8310132423067174	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4933038556566345	0.2470931993558874	0.3319480085526619	T	T	T
0.5945205465598199	0.2677620021370030	0.9982919843224469	T	T	T
0.6021094712141416	0.9806278862011530	0.4919947364679499	T	T	T

```

50_2N.N2_3fold_fN      Fe
0.9906000000000000
  14.8120002747000008    0.0000000000000000    0.0000000000000000
    0.0000000000000000    8.0120000420000004    0.0000000000000000
    0.0000000000000000    0.0000000000000000    6.9380002021999996

```

```

  N      Fe      Co
    4      23      1

```

Selective dynamics

Direct

0.6256515126016549	0.5087470989260297	0.9376505939273750	T	T	T
0.6277668150455613	0.4240147161770299	0.7701145312735629	T	T	T
0.6123661471911762	-0.0046103795136763	0.9731747169847981	T	T	T
0.6112417637366415	0.7513385124793257	0.4732210100956459	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5463155703119489	0.4951510462770892	0.1658275373154754	T	T	T
0.5341190037981600	0.7545069623841548	0.6763247959251436	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4888412003587956	0.4981218222328352	0.8333303158823124	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4968580974708279	0.7446245265124991	0.3304226575665943	T	T	T
0.5989505912714224	0.7554103446401973	-0.0150826410136979	T	T	T
0.5998667211175879	0.5168117920864640	0.5111474737503572	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5393525266961409	0.0019176702297722	0.1808668061525684	T	T	T
0.5470250152004472	0.2470560057027385	0.6579919480453267	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4963903842003944	0.0035527854502570	0.8343776939925160	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4973690292114262	0.2526932649912715	0.3333932733319814	T	T	T
0.6021056294643811	0.2343850631199314	0.9958383982659504	T	T	T
0.5916383014286126	0.9865582400747160	0.4917839126368893	T	T	T

```

49_2N.N2_3fold_1N      Fe
0.9906000000000000
  14.8120002747000008      0.0000000000000000      0.0000000000000000
    0.0000000000000000      8.0120000420000004      0.0000000000000000
    0.0000000000000000      0.0000000000000000      6.9380002021999996

```

```

  N      Fe      Co
    4      23      1

```

Selective dynamics

Direct

0.6237062596249777	0.5306065349158499	0.9410171600115120	T	T	T
0.6323722250362069	0.4199000304498763	0.7982003253811517	T	T	T
0.6123018199796744	-0.0036873090659273	0.9776341196812108	T	T	T
0.6106734773807873	0.7498404671260203	0.4721102797212055	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5500781122988740	0.4927680086199217	0.1661658669571470	T	T	T
0.5338165645233129	0.7540884750320658	0.6752797481750457	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4899333115095044	0.4988748042445932	0.8347814789607255	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4967685246914148	0.7435363556450274	0.3300608200026056	T	T	T
0.5981760472816239	0.7619635760282348	-0.0150753186450501	T	T	T
0.6031541161480561	0.5125841519776678	0.5124172632435613	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5385608188943994	0.0037917613876986	0.1815319185996311	T	T	T
0.5436767002921029	0.2509283480692521	0.6543408871361197	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4951631577473604	0.0039920663569357	0.8340722603048762	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4962515025868129	0.2525110997162282	0.3295829697088278	T	T	T
0.5969577443450947	0.9883469284147910	0.4902701369380946	T	T	T
0.6002322194537861	0.2257436779383755	0.9697329493428822	T	T	T

46_4NFeN	Fe		
0.9906000000000000			
14.8120002747000008	0.0000000000000000	0.0000000000000000	
0.0000000000000000	8.0120000420000004	0.0000000000000000	
0.0000000000000000	0.0000000000000000	6.9380002021999996	

N	Fe
4	24

Selective dynamics

Direct

0.6125645410718858	0.0000050613180150	0.9713194835524291	T	T	T
0.6125645175478500	0.7500335707123963	0.4713235248509199	T	T	T
0.6125636464142412	0.5000137551340691	0.9713245915354186	T	T	T
0.6125640494069980	0.2500387590888890	0.4713209035443591	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5370850778043887	0.5000138587919811	0.1712163253961110	T	T	T
0.5370868917320309	0.7500179836141132	0.6712170536092198	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4987168400136202	0.5000114783947983	0.8319512309421871	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4987170758873704	0.7500133259688595	0.3319514682098550	T	T	T
0.6006234985606788	0.7500095054275502	-0.0125042075436263	T	T	T
0.6006233483126735	0.5000327102932398	0.4874955090540141	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F

0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5370863090667685	0.0000097444448588	0.1712135223921930	T	T	T
0.5370862305340439	0.2500203679304131	0.6712163616810597	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4987164723954040	0.0000130068040356	0.8319445273217312	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4987168748176348	0.2500111056135084	0.3319448371294273	T	T	T
0.6006230793357170	0.0000356764154583	0.4874894418378202	T	T	T
0.6006241413700382	0.2500079259980354	0.9874893529977592	T	T	T

45\_4N\_Co.Cothird\_relax5N      Fe

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
4	22	2

Selective dynamics

Direct

0.6103299191431192	0.0019173281840716	0.9680462349799780	T	T	T
0.6114398429806202	0.7507919452983856	0.4679175403295348	T	T	T
0.6110111938883436	0.4980669921465582	0.9732979115044413	T	T	T
0.6112787595810735	0.2483257910554400	0.4635627119812852	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F



0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4266859939400681	0.7503874285197167	-0.0024835882953124	T	T	T
0.4255369084541128	0.5001391564912280	0.4998117721538132	T	T	T
0.5361189486402598	0.4987432247296739	0.1707748480412664	T	T	T
0.5349812330003445	0.7496525928215567	0.6672953725205213	T	T	T
0.3811343891850807	0.5004290413813033	0.1633762990711950	T	T	T
0.3799774176574168	0.7502023070820355	0.6644316270930996	T	T	T
0.4970153856415437	0.7495774360147928	0.3289142389396413	T	T	T
0.5983718890734939	0.7486425278558835	-0.0157820778511697	T	T	T
0.6000303341169108	0.5003284720169927	0.4825113155661653	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4245077266708869	0.2496175277440474	-0.0021997138471094	T	T	T
0.4261058697583283	-0.0004694580363510	0.4986093071402621	T	T	T
0.5368209000770543	0.0011984197065158	0.1689365133348642	T	T	T
0.5370046565780315	0.2503366771434355	0.6670340538062465	T	T	T
0.3806385694279119	-0.0004744100816372	0.1644657006639650	T	T	T
0.4980607781006984	0.0007305416680049	0.8284469366655512	T	T	T
0.3807550544066075	0.2494551467742638	0.6634465692590424	T	T	T
0.4963669169191930	0.2501311282184682	0.3298703491574417	T	T	T
0.5998982416907702	-0.0009352604052944	0.4827801536774794	T	T	T
0.5953633266874735	0.2512692844720510	0.9809281643144481	T	T	T
0.4986309372013841	0.4991637934562688	0.8274960298538313	T	T	T

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

Fe  
24

Selective dynamics

Direct

0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5428562388139559	0.4993456210498103	0.1661270396588996	T	T	T
0.5428584506119266	0.7506468321299652	0.6661224399160022	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4952526347815732	0.5007443195843677	0.8327165154270862	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4952528724545915	0.7492546890386940	0.3327132513713084	T	T	T
0.5941851765802869	0.7503543832138698	0.0002150014244177	T	T	T
0.5941844929458420	0.4996274902267474	0.5002110116171359	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5427880310000752	0.0005917934415535	0.1676051259653302	T	T	T
0.5427870945989249	0.2493990670751512	0.6676099892915767	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4948119499943313	-0.0007115893024071	0.8342989948580746	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4948124137873235	0.2507017105061851	0.3342971988549119	T	T	T
0.5976661108194086	0.0004764041651003	0.5005255462902852	T	T	T
0.5976664070740892	0.2495168537081867	0.0005224073026920	T	T	T

```

48_Fe3Co111N      Fe
0.990600000000000
  14.8120002747000008      0.0000000000000000      0.0000000000000000
    0.0000000000000000      8.0120000420000004      0.0000000000000000
    0.0000000000000000      0.0000000000000000      6.9380002021999996

```

```

Fe      Co
23      1

```

Selective dynamics

Direct

0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5433234765485330	0.4976470067990275	0.1648516931069519	T	T	T
0.5433536734232515	0.7499952097776821	0.6698744625695423	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4934734249417432	0.5003943811548152	0.8324229641124468	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4963113077934009	0.7499965998466914	0.3346372423422624	T	T	T
0.5973381656381320	0.7499909046498133	0.0077891631721136	T	T	T
0.5977059074244395	0.5018834399296925	0.4970744305121000	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5433240875451059	0.0023411506422990	0.1648495185948166	T	T	T
0.5440914465864821	0.2499952805680325	0.6675002059634352	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4934737081826526	-0.0004001534173908	0.8324261937170453	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4940095800556872	0.2499945288077677	0.3343960330615460	T	T	T
0.5977068963177785	0.9980990041802891	0.4970824831691505	T	T	T
0.5913511434764989	0.2499947483369329	-0.0013915554755999	T	T	T

51_2N.N2_gamma_fN	Fe	
0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
4	23	1

Selective dynamics

Direct

0.7107107930857220	0.3388586680579930	0.9429645205309447	T	T	T
0.7824486914873310	0.3894866807512273	0.9183988901209010	T	T	T
0.6110631802028018	0.0033457818504382	0.9791455750515707	T	T	T
0.6115500488424634	0.7467117846931213	0.4829076190710873	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5473823925097878	0.4946829526428727	0.1546479643311814	T	T	T
0.5375882746698298	0.7447574942930227	0.6873946139401436	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4944575599114048	0.4943103657280183	0.8312920295710585	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4987543668661285	0.7448254677198196	0.3328263249920888	T	T	T
0.5958436311299405	0.7672135105973233	-0.0040646430731454	T	T	T
0.5977276556545777	0.5106700250203923	0.4897593932984050	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5381222655585726	0.0075388085762477	0.1862043599696510	T	T	T
0.5486325269749431	0.2496488588939973	0.6593131421132137	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4961743786032073	0.0044614962938814	0.8356575616228209	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4956325771004880	0.2578250618181291	0.3336989939691488	T	T	T
0.6010250788273674	0.2376214936034572	0.9921776805265436	T	T	T
0.5901728723693659	0.9831431012016295	0.4974256605944657	T	T	T

52_2N.N2_gamma_cN	Fe	
0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
4	23	1

Selective dynamics

Direct

0.7137314346086937	0.3263507164120580	0.9621103074729629	T	T	T
0.7860578312694345	0.3770293606422159	0.9491929819350511	T	T	T
0.6111375054468641	0.0008741030612054	0.9794582233693093	T	T	T
0.6114222662966297	0.7475691806723398	0.4807472822234936	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5480331621067567	0.4926902678095466	0.1526103596341246	T	T	T
0.5371718007436533	0.7453072274436807	0.6858037427702969	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4936611703880870	0.4951821135373368	0.8308229530447120	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4979312873614770	0.7450494989841824	0.3319525198313048	T	T	T
0.5940619224457392	0.7669840191913005	-0.0033117131477900	T	T	T
0.5970933675845476	0.5110132127529505	0.4895108013309324	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5371325675933721	0.0096318727972284	0.1832717433322464	T	T	T
0.5473073787670353	0.2528277272519394	0.6598626474156056	T	T	T

0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4968555066967500	0.0055506809442261	0.8350755557177764	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4946516148682122	0.2569209578128646	0.3338221701349555	T	T	T
0.5941770814492892	0.9853128618513537	0.4949416360256609	T	T	T
0.6028901249995737	0.2361545795029900	0.9829047618107640	T	T	T

53\_2N.N2\_delta\_fN      Fe

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
4	23	1

Selective dynamics

Direct

0.6668579560614977	0.3010385957049767	0.5968773992394111	T	T	T
0.7242966640846229	0.3901554552882187	0.5311627508779085	T	T	T
0.6096004035396931	0.0010472535253315	0.9760984870430941	T	T	T
0.6118997739901809	0.7530717243186520	0.4778427543988604	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5436160115991577	0.4977159431249096	0.1584354191274723	T	T	T

0.5379954470609855	0.7456549395734438	0.6843359847990235	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4955078005214197	0.4953477954864841	0.8319756831137156	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4983674198113766	0.7452524768811111	0.3335687171091700	T	T	T
0.5957604083335554	0.7622581960441396	-0.0033657180923082	T	T	T
0.6072140095435329	0.5187954021817958	0.4852279278430002	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5381060227997135	0.0056117923993952	0.1852413547672777	T	T	T
0.5474165857810068	0.2502855097532676	0.6538655330764096	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4958859191290998	0.0021475358584247	0.8338482973869046	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4939461609630573	0.2563222825364475	0.3302967082863660	T	T	T
0.5970424569190953	0.2413349102392978	-0.0050124581416872	T	T	T
0.5910097623561233	0.9833551978185452	0.4951592815609162	T	T	T

54\_2N.N2\_delta\_2N      Fe

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N      Fe      Co  
       4       23       1  
 Selective dynamics  
 Direct

0.6653742526837927	0.2934346537088626	0.5854172059250691	T	T	T
0.7218134928717380	0.3836628982312972	0.5164585548294712	T	T	T
0.6106480681682194	0.0015191293842358	0.9795883397383837	T	T	T
0.6113771615618147	0.7542045032470078	0.4765456308352646	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5466441507318003	0.4970181649186770	0.1560314796385613	T	T	T
0.5369806529873199	0.7466183360064762	0.6830120333225516	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4952632021102029	0.4964474816872763	0.8318988505791051	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4984136482742434	0.7449108924736180	0.3315396036325292	T	T	T
0.5962643373666004	0.7647384429323956	-0.0049270272826769	T	T	T
0.6075896744718624	0.5194150285497482	0.4861570299636846	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5374878176209787	0.0048294960391438	0.1853629135630239	T	T	T
0.5466771565869574	0.2515139793032162	0.6552744241998772	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4963946499017637	0.0019157087080254	0.8354075820042812	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4932996474309382	0.2565719734982158	0.3303047538165131	T	T	T
0.5965018837869838	0.9884318297540127	0.4974542211033225	T	T	T
0.5899218904241620	0.2387447693856921	0.9967325385318949	T	T	T



55\_2N.NH2\_c.2H2N.NH.2H

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
3 4 23 1

Selective dynamics

Direct

0.6158134580237291	0.7501868721219284	0.4957417017513712	T	T	T
0.6115438689039332	0.4975184574001706	0.9732027337658450	T	T	T
0.6762764830252327	0.0875629777856874	0.0439705218361261	T	T	T
0.7240482756807675	0.1058901945929628	0.1505386088496551	T	T	T
0.6083337807167881	0.2118459091953981	0.4551389268910505	T	T	T
0.7060774349322956	0.0267603120001036	0.9291676557732180	T	T	T
0.6009487071254774	0.8273547637322322	0.2044215909935325	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5371302237357847	0.4955458837925855	0.1820362335128918	T	T	T
0.5346374908588208	0.7538252871794755	0.6860750909838208	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4943727930651434	0.4960966768865432	0.8331288463635317	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4978734412394399	0.7572963209437542	0.3308083955120573	T	T	T
0.5981342453017932	0.7279051910991133	0.9876972190090226	T	T	T
0.5942642063642158	0.5154600114459149	0.4974075815849416	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5562465281641875	0.0083664595858924	0.1391635933929754	T	T	T
0.5452278022384528	0.2474426583862499	0.6589810476153828	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4919812214750343	0.0041100106563708	0.8308076775153204	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4966200770087997	0.2424583528548142	0.3284985389226662	T	T	T
0.5942872428182879	0.9865785049840570	0.4994045287332113	T	T	T
0.6012449153793200	0.2721794939806789	0.9787910186401139	T	T	T

56\_2N.NH2\_f.2H2N.NH.2H

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co

3 4 23 1

Selective dynamics

Direct

0.6154334164211662	0.7518062485656999	0.4973815038187807	T	T	T
0.6114838405781549	0.4979543307368743	0.9718894148178497	T	T	T
0.6779735965113188	0.0737319062131680	0.0394583420730985	T	T	T
0.7263828825248408	0.0818063651565203	0.1467226850425503	T	T	T
0.6088206181549700	0.1965481788014671	0.4536828216956210	T	T	T
0.7048495711518757	0.0129785506609101	0.9213648330362537	T	T	T
0.5981340420158383	0.8228345761446232	0.2075018789280091	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5369184019796601	0.4966001856680344	0.1819633908514453	T	T	T
0.5351810589733645	0.7548318400570043	0.6879068260605432	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4951783813741744	0.4941076462887745	0.8321120459799111	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4976570485057765	0.7566654114237269	0.3327959910257237	T	T	T

0.5979047558855093	0.7289594669275703	0.9882864941619884	T	T	T
0.5943437866561070	0.5171605625668320	0.4981441342130880	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5545885098056018	0.0067538248640334	0.1430718887265087	T	T	T
0.5462268477483868	0.2478128053242246	0.6587551494552619	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4921273708886355	0.0054398001381486	0.8306667024176160	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4977692791653648	0.2428370363668327	0.3292228484007803	T	T	T
0.6049134604469315	0.2688975111787543	0.9855419497438860	T	T	T
0.5918714259288107	0.9858067813288978	0.4998923022182882	T	T	T

58\_2N.NH3\_c.H2N.NH2.H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
3	4	23	1

# Selective dynamics

## Direct

0.6122757388363416	0.7529524642527793	0.4807828081204058	T	T	T
0.6119343831341097	0.5021160297289379	0.9787320270485420	T	T	T
0.7289474887966743	0.1740861953541948	0.9616843344179772	T	T	T
0.7543759704396534	0.1371480447232436	0.0938399262063158	T	T	T
0.7720464213851074	0.2615126977092793	0.9018262812802853	T	T	T
0.7262110181700896	0.0701522621992081	0.8731918742180251	T	T	T
0.6098598609713612	0.2143181514770890	0.4551502935234642	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5364135855862150	0.4931809917782566	0.1804129386196174	T	T	T
0.5375611300365661	0.7551816803066052	0.6867069557701120	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4970527676587561	0.4958033664259991	0.8344288953900824	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4978435685457309	0.7549470070426103	0.3325409896348922	T	T	T
0.5945572246043790	0.7357740564099212	0.9973579922616815	T	T	T
0.5940412696681125	0.5161886189343846	0.4938554789720692	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5457335085990569	0.0046217544392931	0.1525792570636445	T	T	T
0.5469604137046267	0.2476569678296380	0.6617913007541948	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4940585796932566	0.0044010545594409	0.8312403496682217	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4965694795110179	0.2443122074677627	0.3318669984638036	T	T	T
0.5958951505396288	0.9881371376689603	0.4903041477782241	T	T	T
0.5994846266527519	0.2642718414744529	0.9886724969787800	T	T	T

57\_2N.NH3\_f.H2N.NH2.H

0.9906000000000000

14.8120002747000008

0.0000000000000000

0.0000000000000000

0.0000000000000000

8.0120000420000004

0.0000000000000000

0.0000000000000000

0.0000000000000000

6.9380002021999996

N H Fe Co  
3 4 23 1

Selective dynamics

Direct

0.6118772759478093	0.7533415809170362	0.4810464664961899	T	T	T
0.6109923054747993	0.5000002139940007	0.9795146108464415	T	T	T
0.7348274339794532	0.1633341714180145	0.9607937681281165	T	T	T
0.7597090741223714	0.1210783259731054	0.0913405654983190	T	T	T
0.7800487855095117	0.2474602444931091	0.9017784949415956	T	T	T
0.7284573175051181	0.0617126099805706	0.8694843481114746	T	T	T
0.6105014892853292	0.1964452221382204	0.4508983939457977	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5362818827402568	0.4940956202287990	0.1824986332294853	T	T	T
0.5379836145212895	0.7563298079099948	0.6866896150974420	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4977986077838299	0.4947115693423755	0.8331101374377834	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4971023203064690	0.7528183758531547	0.3339152143102694	T	T	T
0.5941616495168771	0.7362454687285680	0.9976564980740363	T	T	T
0.5947350064039951	0.5173920363363310	0.4949363682057510	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5452216980670652	0.0021357684702723	0.1566398421971577	T	T	T
0.5472949872573474	0.2475479094747561	0.6579857587395805	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4949590048891417	0.0062999526883525	0.8322589557258478	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4973477600797270	0.2446080003590101	0.3313581639445577	T	T	T
0.6034839088368618	0.2607859371839207	0.9892432212892022	T	T	T
0.5934698091527902	0.9861431692524778	0.4887819302883107	T	T	T

59\_2N\_diagonalCIF file

0.9906000000000000

14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	Fe	Co
2	23	1

Selective dynamics

Direct

0.6114382350954436	0.7526590651587558	0.4828491693056924	T	T	T
0.6107835266250123	0.4968107482049176	0.9793126556871636	T	T	T
0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5389434000360955	0.4935981628506698	0.1879041909994733	T	T	T
0.5378228864814498	0.7556527233962220	0.6871796188384447	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4966095360856731	0.4963507557896563	0.8346139304683829	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4980201799037364	0.7534408243956927	0.3336041428073048	T	T	T
0.5956703150167836	0.7355246540391134	0.9971562890479765	T	T	T

0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5444859963279135	0.0015442185742324	0.1580677087453716	T	T	T
0.5469934548936205	0.2508253280328601	0.6563469505699977	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4964826793352500	0.0067684744481038	0.8327596478104704	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4954901048863161	0.2433105162872994	0.3332268994558014	T	T	T
0.5975587914915090	0.9889191935079875	0.4910040937410292	T	T	T
0.5975948799242078	0.2590067797573913	0.9917888549489123	T	T	T
0.5909160026103480	0.5162579881942747	0.4989439308265367	T	T	T

60\_2Ndiagonal\_2H\_COMiddle2N.2H

0.9906000000000000		
14.8120002747000008	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0120000420000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	6.9380002021999996

N	H	Fe	Co
2	2	23	1

Selective dynamics

Direct

0.6127056846588034	0.2472364361628721	0.4798531204195333	T	T	T
0.6114239576524051	0.5027667172220021	0.9745645949859232	T	T	T
0.6090201736685208	0.7902489433403206	0.4494034724226508	T	T	T
0.6102293481486242	0.9714056070292871	0.9554208919817837	T	T	T

0.3312200009999984	0.5000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.7500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.7500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.5000000000000000	0.5001050221835968	F	F	F
0.5383892664461503	0.5041145049252548	0.1836323188895651	T	T	T
0.5461914340657658	0.7501739027227773	0.6553553795147223	T	T	T
0.3810960778633330	0.5000000000000000	0.1667699372837745	F	F	F
0.4965921290688590	0.5033287900307207	0.8326864832474317	T	T	T
0.3810960778633330	0.7500000000000000	0.6667699072837721	F	F	F
0.4974470466434500	0.7549386154829755	0.3300954395730596	T	T	T
0.5979703440767477	0.7399243323570022	0.9890792202133898	T	T	T
0.3312200009999984	0.0000000000000000	0.8333799990000017	F	F	F
0.3312200009999984	0.2500000000000000	0.3333799990000017	F	F	F
0.4282651369103760	0.2500000000000000	0.0001050071835991	F	F	F
0.4282651369103760	0.0000000000000000	0.5001050221835968	F	F	F
0.5447716488539874	0.9989373407684061	0.1569033287432413	T	T	T
0.5370878382004843	0.2458578085626917	0.6832804491824378	T	T	T
0.3810960778633330	0.0000000000000000	0.1667699372837745	F	F	F
0.4968816862067392	0.9942416356742508	0.8303076237241145	T	T	T
0.3810960778633330	0.2500000000000000	0.6667699072837721	F	F	F
0.4980022268928349	0.2465783434643194	0.3326220756568779	T	T	T
0.5966639973296571	0.2645624949514818	0.9944216154742016	T	T	T
0.5975235967589645	0.0123292421428427	0.4905162530858113	T	T	T
0.5913715176296458	0.4814034888023284	0.4956142366960656	T	T	T