

Electronic Supplementary Information

Ammonia synthesis on BaTiO_{2.5}H_{0.5}: computational insights into the role of hydrides

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1. Details of the thermodynamic calculations

The change in Gibbs free energy corresponding to NH₃ desorption (ΔG_{des}) from the surface was approximated using the following equation

$$\Delta G_{des} = \Delta H_{des} - T\Delta S_{des} \approx (\Delta E_{elec} + \Delta E_{vib}) - T\Delta S_{des} \quad (S1)$$

where ΔE_{elec} is the change in electronic energy, ΔE_{vib} is the change in vibrational energy, T is temperature at 673 K, and ΔS_{des} is the change in entropy between the adsorbed state (initial state) and the desorbed state (final state). In this work, we approximated that the rotational and vibrational entropic contributions are much less than the translational entropic contribution such that

$$\Delta S_{des} = S_{NH_3} - S_{NH_3^*} = S_{NH_3} - (S_{NH_3} - S_{NH_3,trans}) = S_{NH_3,trans} \quad (S2)$$

where S_{NH_3} is the total entropy of gaseous NH_3 , $S_{\text{NH}_3^*}$ is the total entropy of adsorbed NH_3 , and $S_{\text{NH}_3,\text{trans}}$ is the translational entropy of gaseous NH_3 . The equation used to calculate E_{vib} in equation S1 is

$$E_{\text{vib}} = \sum_i \left\{ \frac{h\nu_i}{2} + \frac{h\nu_i e^{-\frac{h\nu_i}{kT}}}{1 - e^{-\frac{h\nu_i}{kT}}} \right\} \quad (\text{S3})$$

where h is the Planck's constant, ν_i is the vibrational frequency of mode i , T is the temperature at 673 K, and k is the Boltzmann constant. The Sackur-Tetrode equation (see A. Savara, J. Phys. Chem. C, 2013, **117**, 15710–15715) was used to calculate $S_{\text{NH}_3,\text{trans}}$ which approximately equals to ΔS_{des}

$$\Delta S_{\text{des}} \approx S_{\text{NH}_3,\text{trans}} = R \ln \left(\left(\frac{\sqrt{2\pi m k T}}{h} \right)^D \frac{L^D}{n N_A} \right) + \left(1 + \frac{D}{2} \right) R \quad (\text{S4})$$

where R is the ideal gas constant, m is the molecular mass of NH_3 , D is the number of dimensions NH_3 gas is confined to, L is the length of the box NH_3 is confined to, n is the total number of moles, and N_A is Avogadro's number. In this work, $D = 3$ such that L^D gives the volume of the box in which NH_3 is confined. The value of L was calculated by first solving for the volume (V) of the box using the ideal gas equation ($PV = nRT$), where $P = 1$ bar, and then taking the cube root of V . The value of n was set to 1.

2. Surface slab

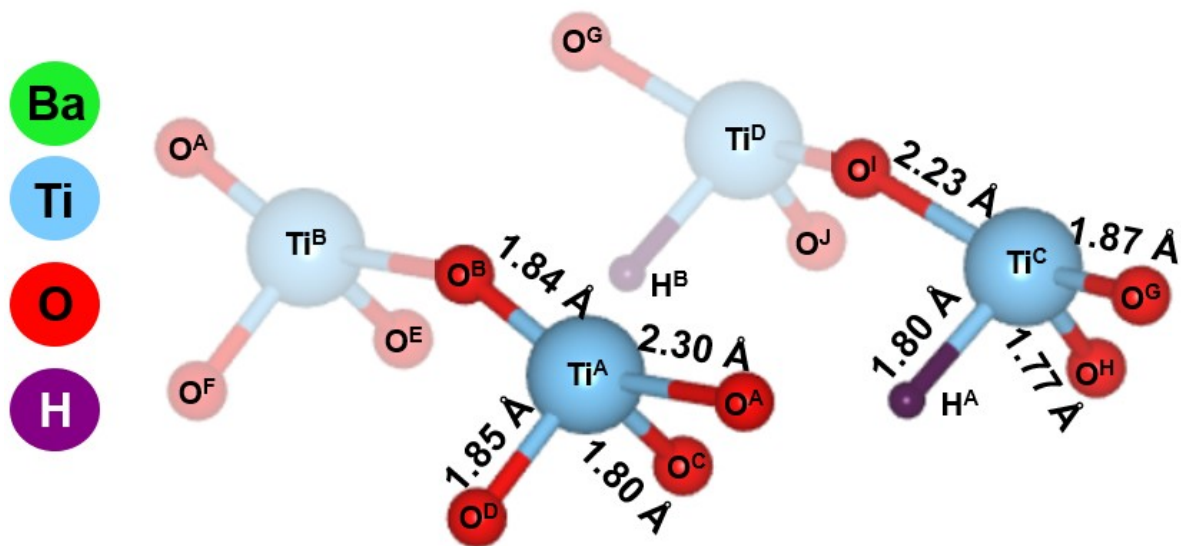


Fig. S1. The bond lengths between surface and subsurface atoms of the BTOH (210)-Ti₂O₂ surface. Since the slab model is a 2×2 supercell, the distances between atoms of the faded region are the same as the distances between atoms of the unfaded region.

3. H₂ dissociation over the (210)-Ti₂O₂ surface termination of BTOH

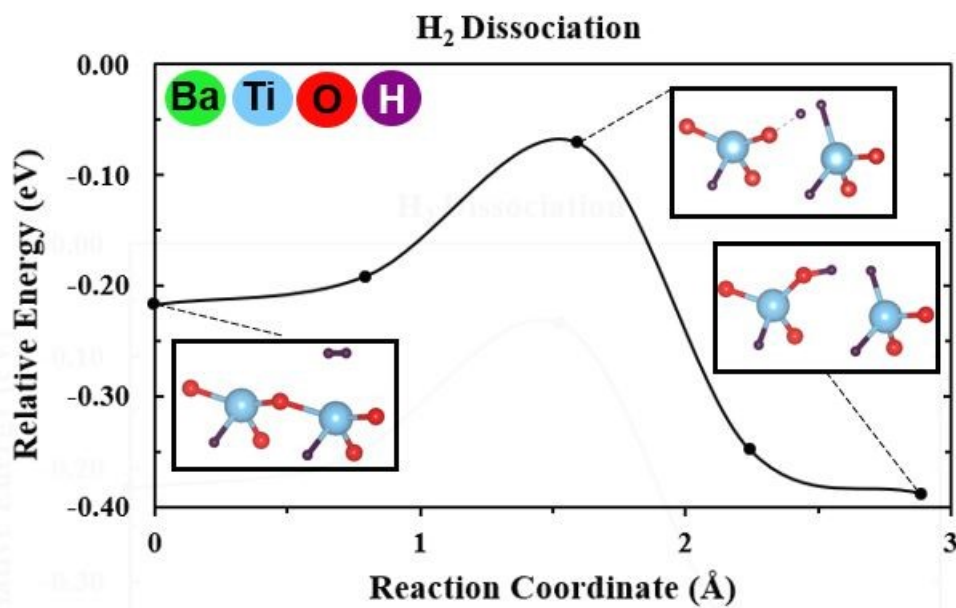


Fig. S2. Minimum energy path of H_2 dissociation across the surface Ti^C-O bond and the structures for the initial, transition, and final states.

4. N_2 dissociation over the (210)- Ti_2O_2 surface termination of BTOH

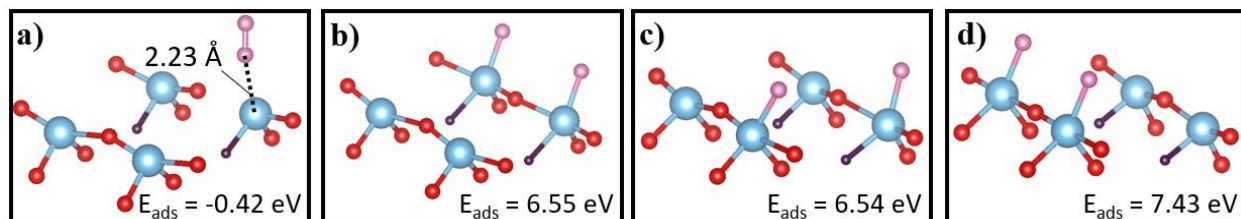


Fig. S3. The structures of N_2 adsorbed on a surface Ti site (a) and of dissociated N_2 adsorbed on different surface Ti sites (b)-(d). The adsorption energies are listed on the bottom of each panel.

5. Comparison of the two *NNH intermediates on the BTOH (210)-Ti₂O₂ surface

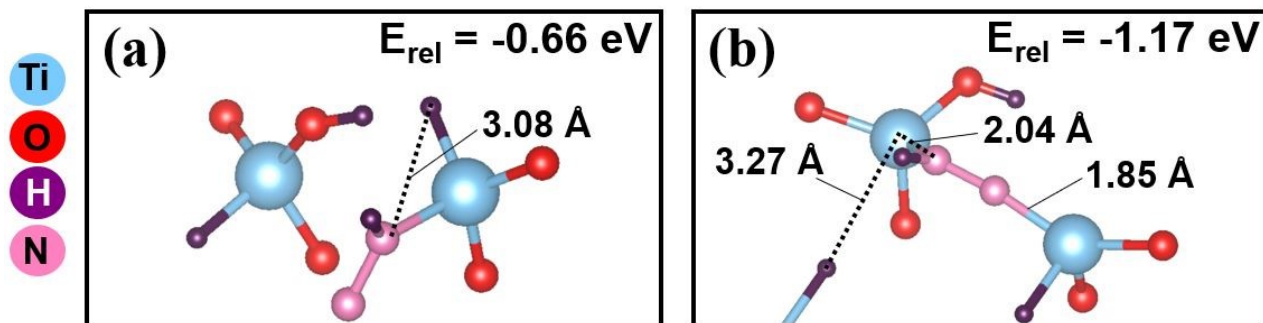


Fig. S4. Comparison of the two *NNH intermediates: (a) state 5 in the distal pathway (Fig. 5 in the main text), formed from reaction with a subsurface lattice hydride and adsorbed at the subsurface anion vacancy; (b) state 5 in the alternating pathway (Fig. 7 in the main text), formed from reaction with a surface hydride (from H₂ dissociation) and adsorbed on a surface Ti site.

6. Comparison of the distal and alternating pathways

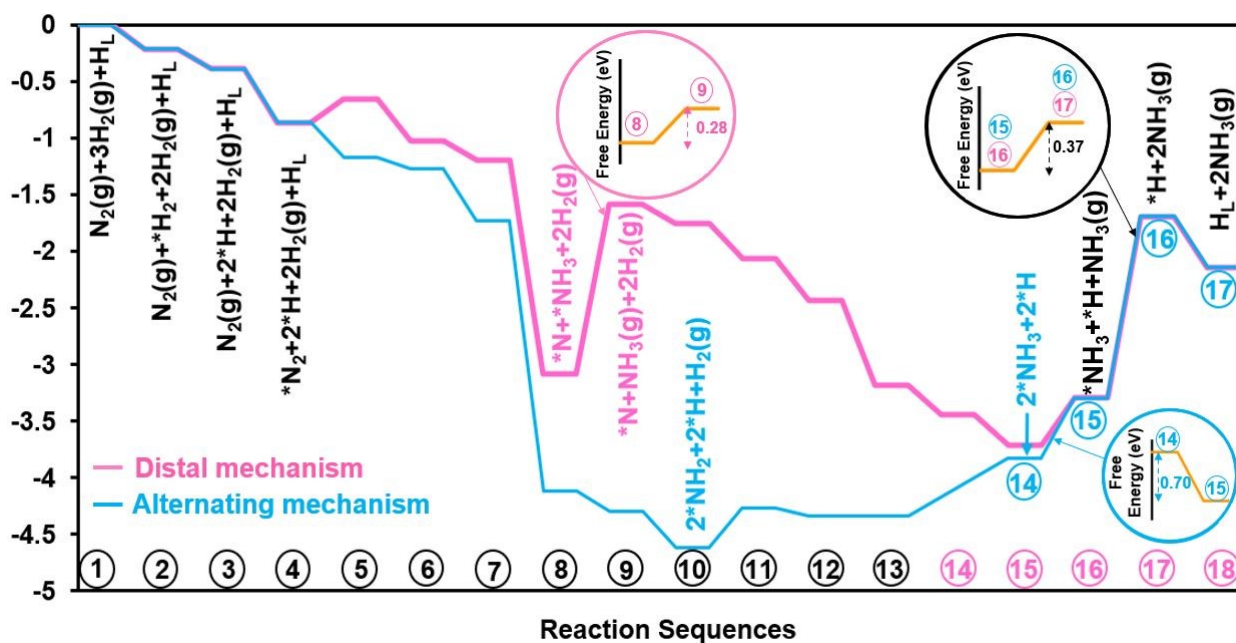


Fig. S5. Comparison of the energy profiles of the distal and alternating pathways. The intermediate states shared by the two pathways are labeled in black (in the beginning and the end).

7. Optimized geometries of intermediate states

This section lists the optimized geometries, in fractional coordinates, of all the intermediate states in both the distal and alternating mechanisms.

Distal mechanism: Clean (210)-Ti₂O₂ slab (state 1)

```
1.0000000000000000
 8.0600004195999997 0.0000000000000000 0.0000000000000000
 0.0000000000000000 11.3985996245999992 0.0000000000000000
 0.0000000000000000 0.0000000000000000 22.2077999115000004
Ba Ti O H
 8 12 30 6
Selective dynamics
Direct
0.0000000000000000 0.5000000000000000 0.0659599990000004 F F F
-0.0037941018790552 0.2540606864726686 0.1916155876061243 T T T
0.0000000000000000 0.0000000000000000 0.0659599990000004 F F F
-0.0004860342675610 0.7526339353338757 0.1896787239691944 T T T
0.5000000000000000 0.5000000000000000 0.0659599990000004 F F F
0.4962035717866282 0.2540583136029386 0.1916205646485058 T T T
0.5000000000000000 0.0000000000000000 0.0659599990000004 F F F
0.4995281703854711 0.7526243079003427 0.1896722240729709 T T T
0.2500000000000000 0.7461800230000009 0.0640000009999966 F F F
0.2387663565448006 0.4979077342512243 0.1872266022980883 T T T
0.2425039197184942 0.2595171522590658 0.3110385107113783 T T T
0.2500000000000000 0.2538199979999973 0.0679299979999968 F F F
0.2362552519436495 0.0152996018456535 0.1949679811848715 T T T
0.2588895348861243 0.7663364173385725 0.3133268454212547 T T T
0.7499999699999975 0.7461800230000009 0.0640000009999966 F F F
0.7387491694409042 0.4979172824879614 0.1872357451962299 T T T
0.7424986168328238 0.2595068703590096 0.3110191539519677 T T T
0.7499999699999975 0.2538199979999973 0.0679299979999968 F F F
0.7361967811861203 0.0153085203986151 0.1949670348738222 T T T
0.7588494679733415 0.7663238258611598 0.3133253035105685 T T T
0.2500000000000000 0.6249999790000018 0.0018099999999990 F F F
0.2500000000000000 0.3750000209999982 0.1301199910000008 F F F
0.2537458919156796 0.1354449082459454 0.2571787210391976 T T T
0.2500000000000000 0.8785200129999993 0.0036100000000019 F F F
0.2500000000000000 0.6285200129999993 0.1319299930000000 F F F
0.2553545864038563 0.3781459720282377 0.2577001871959758 T T T
0.0000000000000000 0.7535200339999975 0.0677699969999992 F F F
0.0071465258987316 0.5056520981944754 0.1948280942160031 T T T
0.0217036861041920 0.2576589148457055 0.3319278611791088 T T T
0.2500000000000000 0.3714799870000007 0.0000000000000000 F F F
0.2500000000000000 0.1214800070000024 0.1283199940000017 F F F
0.2512342158579459 0.8710635000798473 0.2543493060805284 T T T
0.0000000000000000 0.2464800070000024 0.0641599969999973 F F F
0.0078597356000254 -0.0007881115983847 0.1907755395110892 T T T
-0.0141795131270909 0.7515941404303713 0.3284988280085817 T T T
0.7499999699999975 0.6249999790000018 0.0018099999999990 F F F
0.7499999699999975 0.3750000209999982 0.1301199910000008 F F F
0.7537430186810440 0.1354628305842427 0.2571850052113361 T T T
```

0.7499999699999975	0.8785200129999993	0.0036100000000019	F	F	F
0.7499999699999975	0.6285200129999993	0.1319299930000000	F	F	F
0.7553797480987494	0.3781222597755282	0.2577137251120341	T	T	T
0.5000000000000000	0.7535200339999975	0.0677699969999992	F	F	F
0.5071131107802491	0.5056542086981535	0.1948231007986609	T	T	T
0.5217428690408586	0.2576834338155312	0.3319238736027079	T	T	T
0.7499999699999975	0.3714799870000007	0.0000000000000000	F	F	F
0.7499999699999975	0.1214800070000024	0.1283199940000017	F	F	F
0.7511917036286804	0.8710528300725885	0.2543435584068292	T	T	T
0.5000000000000000	0.2464800070000024	0.0641599969999973	F	F	F
0.5079586851675603	-0.0007987470493617	0.1907738107506634	T	T	T
0.4858093714192371	0.7516084369162140	0.3285010125296250	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000209999982	0.1301199910000008	F	F	F
0.2513855845780597	0.6452454026534463	0.2616531990464892	T	T	T
0.7499999699999975	0.1250000000000000	0.0018099999999990	F	F	F
0.7499999699999975	0.8750000209999982	0.1301199910000008	F	F	F
0.7513591988699516	0.6452194648731273	0.2616224422247638	T	T	T

Distal mechanism (state 2)

1.0000000000000000					
8.0600004195999997	0.0000000000000000	0.0000000000000000			
0.0000000000000000	11.3985996245999992	0.0000000000000000			
0.0000000000000000	0.0000000000000000	22.2077999115000004			

Ba Ti O H
8 12 30 8

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599990000004	F	F	F
0.9965740453520884	0.2543621784481268	0.1915456226096471	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599990000004	F	F	F
-0.0009226754655153	0.7523826041335686	0.1888854309801535	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599990000004	F	F	F
0.4960739858479422	0.2540549972918659	0.1916613189108332	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599990000004	F	F	F
0.5003540509422978	0.7525367760168660	0.1900860673256533	T	T	T
0.2500000000000000	0.7461800230000009	0.0640000009999966	F	F	F
0.2386699377978337	0.4984098952111142	0.1872976085424679	T	T	T
0.2424473051523427	0.2590701283757699	0.3111193559688526	T	T	T
0.2500000000000000	0.2538199979999973	0.0679299979999968	F	F	F
0.2357745309731908	0.0147342630060019	0.1950465551088426	T	T	T
0.2538519769293922	0.7632766409182135	0.3115131829198062	T	T	T
0.7499999699999975	0.7461800230000009	0.0640000009999966	F	F	F
0.7388011905816207	0.4980014227474382	0.1873107719688158	T	T	T
0.7431334743018072	0.2592384391957215	0.3110802172999501	T	T	T
0.7499999699999975	0.2538199979999973	0.0679299979999968	F	F	F
0.7370104928211816	0.0155897145946062	0.1949058210032288	T	T	T
0.7633909409655063	0.7632557810289397	0.3137901565302872	T	T	T
0.2500000000000000	0.6249999790000018	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000209999982	0.1301199910000008	F	F	F
0.2536205764571113	0.1348978918764893	0.2573424283627577	T	T	T
0.2500000000000000	0.8785200129999993	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200129999993	0.1319299930000000	F	F	F

0.2550290124318941	0.3776219626597073	0.2578624888650326	T	T	T
0.0000000000000000	0.7535200339999975	0.0677699969999992	F	F	F
0.0070595410893039	0.5054498503526816	0.1946859283427191	T	T	T
0.0215150608372646	0.2573387746495172	0.3322689963621423	T	T	T
0.2500000000000000	0.3714799870000007	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800070000024	0.1283199940000017	F	F	F
0.2505171655287369	0.8701946961145585	0.2530743002429523	T	T	T
0.0000000000000000	0.2464800070000024	0.0641599969999973	F	F	F
0.0071455446624335	-0.0007277362411175	0.1907510164354890	T	T	T
0.9944487634469815	0.7478144265621055	0.3272014406799146	T	T	T
0.7499999699999975	0.6249999790000018	0.0018099999999990	F	F	F
0.7499999699999975	0.3750000209999982	0.1301199910000008	F	F	F
0.7542555564082485	0.1352014185541976	0.2572559680882916	T	T	T
0.7499999699999975	0.8785200129999993	0.0036100000000019	F	F	F
0.7499999699999975	0.6285200129999993	0.1319299930000000	F	F	F
0.7555751218551385	0.3779272934032558	0.2578099565626562	T	T	T
0.5000000000000000	0.7535200339999975	0.0677699969999992	F	F	F
0.5072664677953953	0.5052973843091217	0.1948227127025947	T	T	T
0.5223358201919077	0.2572946048592877	0.3322205578626904	T	T	T
0.7499999699999975	0.3714799870000007	0.0000000000000000	F	F	F
0.7499999699999975	0.1214800070000024	0.1283199940000017	F	F	F
0.7525548530999807	0.8695619790024883	0.2559665847540925	T	T	T
0.5000000000000000	0.2464800070000024	0.0641599969999973	F	F	F
0.5089214593934360	-0.0011924130591189	0.1909343396635029	T	T	T
0.4783912112165239	0.7470987196795917	0.3280284588518651	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000209999982	0.1301199910000008	F	F	F
0.2492315592112157	0.6429178873922355	0.2590507307744782	T	T	T
0.7499999699999975	0.1250000000000000	0.0018099999999990	F	F	F
0.7499999699999975	0.8750000209999982	0.1301199910000008	F	F	F
0.7526617515663372	0.6429905818081346	0.2612897670839913	T	T	T
0.7801587679805295	0.7832997095097055	0.4141719397275329	T	T	T
0.6856757221430317	0.7831980620845672	0.4097347493964760	T	T	T

Distal mechanism (state 3)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H
8 12 30 8

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599990000004	F	F	F
0.9969423114919864	0.2535856863462506	0.1914800945673623	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599990000004	F	F	F
-0.0013171989282641	0.7517225738225650	0.1862867612498650	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599990000004	F	F	F
0.4957531187175336	0.2536215416692721	0.1916101602707549	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599990000004	F	F	F
0.5007569018888648	0.7521904085439918	0.1886973831998753	T	T	T
0.2500000000000000	0.7461800230000009	0.0640000009999966	F	F	F
0.2388054658619986	0.4972179145593740	0.1874839156402523	T	T	T

0.2421968243049863	0.2593228530326684	0.3111156315380919	T	T	T
0.2500000000000000	0.2538199979999973	0.0679299979999968	F	F	F
0.2369663939470814	0.0150182668268876	0.1952022281264343	T	T	T
0.2288002290153552	0.7657215688269753	0.3132882207224859	T	T	T
0.7499999699999975	0.7461800230000009	0.0640000009999966	F	F	F
0.7389871163979798	0.4959982003011204	0.1873367005559465	T	T	T
0.7428196444680949	0.2596595984223511	0.3110403914990709	T	T	T
0.7499999699999975	0.2538199979999973	0.0679299979999968	F	F	F
0.7368956273221292	0.0161767689090269	0.1950489296826381	T	T	T
0.7833844026274274	0.7756336062325353	0.3173939407066363	T	T	T
0.2500000000000000	0.6249999790000018	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000209999982	0.1301199910000008	F	F	F
0.2536684419377983	0.1350672036286786	0.2571577484000654	T	T	T
0.2500000000000000	0.8785200129999993	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200129999993	0.1319299930000000	F	F	F
0.2549203658792005	0.3775521054852445	0.2573587498854356	T	T	T
0.0000000000000000	0.7535200339999975	0.0677699969999992	F	F	F
0.0065430321455476	0.5068462376391331	0.1952440281340275	T	T	T
0.0214894523711164	0.2575667161948751	0.3313284142875271	T	T	T
0.2500000000000000	0.3714799870000007	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800070000024	0.1283199940000017	F	F	F
0.2573635312441497	0.8705430669785998	0.2546481276806147	T	T	T
0.0000000000000000	0.2464800070000024	0.0641599969999973	F	F	F
0.0083123695863889	-0.0024860740900098	0.1910608293472106	T	T	T
0.0034102700687042	0.7513726502776098	0.3319766725890791	T	T	T
0.7499999699999975	0.6249999790000018	0.0018099999999990	F	F	F
0.7499999699999975	0.3750000209999982	0.1301199910000008	F	F	F
0.7541001181083710	0.1360376951116171	0.2568183384982204	T	T	T
0.7499999699999975	0.8785200129999993	0.0036100000000019	F	F	F
0.7499999699999975	0.6285200129999993	0.1319299930000000	F	F	F
0.7560548132648947	0.3782535336150856	0.2573584338222087	T	T	T
0.5000000000000000	0.7535200339999975	0.0677699969999992	F	F	F
0.5071650620256674	0.5060914271718042	0.1950722223579677	T	T	T
0.5223283214878407	0.2580798634216546	0.3311404228774087	T	T	T
0.7499999699999975	0.3714799870000007	0.0000000000000000	F	F	F
0.7499999699999975	0.1214800070000024	0.1283199940000017	F	F	F
0.7528752636235788	0.8735137202189034	0.2565394202441560	T	T	T
0.5000000000000000	0.2464800070000024	0.0641599969999973	F	F	F
0.5086690393604519	0.9981379700505951	0.1906942818773698	T	T	T
0.3901676661285159	0.7532454554757505	0.3700643749483060	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000209999982	0.1301199910000008	F	F	F
0.2546713403838990	0.6420649362862358	0.2627964100060539	T	T	T
0.7499999699999975	0.1250000000000000	0.0018099999999990	F	F	F
0.7499999699999975	0.8750000209999982	0.1301199910000008	F	F	F
0.7344245783184198	0.6480691142763353	0.2719449709501204	T	T	T
0.6732819753377847	0.8214273125526430	0.3824302899481626	T	T	T
0.5017504041389765	0.7883773402343762	0.3795843014869322	T	T	T

Distal mechanism (state 4)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000

0.0000000000000000 0.0000000000000000 22.2077999115000004

Ba Ti O H N

8 12 30 8 2

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9956564025596943	0.2538886319319698	0.1919154484938272	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.9989367765753385	0.7522884175476873	0.1863686389153629	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4962455137022144	0.2536466928728748	0.1914864220803664	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5010536315488539	0.7528936356890225	0.1886265814151865	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2388819009945382	0.4971779115005658	0.1874356553153756	T	T	T
0.2428211950839954	0.2599821435795580	0.3110132900577354	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2364793277425640	0.0156469557606202	0.1953053480800403	T	T	T
0.2299591942679949	0.7689767891492211	0.3135033416097205	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7388391133434634	0.4975012117529155	0.1874515386259807	T	T	T
0.7400149866932284	0.2602107697856323	0.3114768215866685	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7363541866842129	0.0151594251708145	0.1958287733725493	T	T	T
0.7830489043043155	0.7688851936144938	0.3161607607205242	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2531655367913788	0.1358211730643759	0.2568690774859550	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2553605223046905	0.3785359114901182	0.2572623473646458	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0070438422376411	0.5066135798326284	0.1951187847833636	T	T	T
0.0225210595889842	0.2584649984845870	0.3313528457341055	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2581600711480270	0.8716646246644874	0.2539494555882424	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0078448109926639	0.9979774897295478	0.1913104808919855	T	T	T
0.0052140944359532	0.7526758373377441	0.3310939052421370	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7530471164946667	0.1367325887469965	0.2572387101389457	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7546188079643238	0.3789598409241425	0.2579231337104080	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5072346131951091	0.5064979831841310	0.1950890102383715	T	T	T
0.5185566816349954	0.2581590667795787	0.3308946655695322	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7501890222909537	0.8715767278093745	0.2562143637798240	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F

0.5083252805532147	0.9989513483046770	0.1907292121698266	T	T	T
0.3913918227200266	0.7602368631418011	0.3706490688319470	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2576605901890486	0.6438518365699705	0.2642243412425293	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7459256521846256	0.6475609523505809	0.2623331533759021	T	T	T
0.6777394973023535	0.8268501315032223	0.3793915189603685	T	T	T
0.5029231439074270	0.7968998727241662	0.3783914265993816	T	T	T
0.7220175581971707	0.5989217163160201	0.3653616247560266	T	T	T
0.7068935568556375	0.5088743469314952	0.3847349736777772	T	T	T

Distal mechanism (state 5)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9914092060067535	0.2591043867332947	0.1927642932353746	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.9961679458005189	0.7492017115764836	0.1891752014973579	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4997538670350167	0.2579503933754614	0.1920292021304329	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5037024726772804	0.7524932301358900	0.1937939418527441	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2442093878842378	0.4957266876223233	0.1870899103615848	T	T	T
0.2425598363583571	0.2584165214003812	0.3117528779110255	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2349863065644162	0.0169784660368768	0.1955674327012137	T	T	T
0.2281298660982816	0.8042879153508360	0.3231680845235381	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7372548962760734	0.5092294865403644	0.1947939010696388	T	T	T
0.7378953954699450	0.2551978466542523	0.3133486357648972	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7360944526736799	0.0161471083080890	0.1961302709908194	T	T	T
0.8183851960000869	0.8257806768290180	0.3298997487196403	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2523774154191745	0.1356727009579781	0.2566778300481826	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2544447160962334	0.3775124505832420	0.2587954000377213	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0120462627247546	0.5040822710066862	0.1947999948050333	T	T	T
0.0222461126515886	0.2561943702877272	0.3326722786411255	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F

0.2618198669591718	0.8772862210694538	0.2529546205050231	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0085788140874115	-0.0009369387181432	0.1902363738853020	T	T	T
0.0294461377383887	0.8514431459743442	0.3577063187706800	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7531010542511936	0.1329755489579417	0.2580917881238414	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7500448527571237	0.3711862591046885	0.2599264490538059	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4926824174379247	0.5055298286274664	0.1944322572840940	T	T	T
0.5155848470304892	0.2530776124320827	0.3325388782682144	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7600278525118545	0.8813466571725279	0.2569604424129857	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5097663553119087	0.9991623098638542	0.1901885924581382	T	T	T
0.4048310937269986	0.7882154661444759	0.3716885724992076	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2055616515327626	0.6653282101532448	0.2872789355670364	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.8815345949127317	0.5939196100612891	0.3338387126860453	T	T	T
0.6768619977594527	0.8575537508571941	0.3882294984051868	T	T	T
0.5221963447776257	0.8165857674874490	0.3798113261113316	T	T	T
0.7516612243352020	0.6167796140203951	0.2599543962537148	T	T	T
0.8137977635708091	0.6559779231630313	0.3100429218492198	T	T	T

Distal mechanism (state 6)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9916915209745275	0.2566575770781140	0.1918435362147041	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
-0.0044300997152217	0.7532669270613205	0.1878229181599331	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4985458210137197	0.2555409712314769	0.1918221028662580	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5029354614004183	0.7550016995860526	0.1950443157292765	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2389670950347794	0.5003041230249001	0.1884295062384055	T	T	T
0.2402167816796572	0.2605655352439925	0.3117033505598319	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2338923335911974	0.0142000006444311	0.1978697488867628	T	T	T
0.2324673231861284	0.7607359060771955	0.3081418701100825	T	T	T

0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7343240950140799	0.5099459539818600	0.1940771535716010	T	T	T
0.7399207318420116	0.2577396056198190	0.3125060161975960	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7350629523259472	0.0105465226983930	0.2000607768814956	T	T	T
0.7969733070372191	0.7666857138801592	0.3168330233223891	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2512755528473070	0.1364831898461543	0.2573458855017175	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2539537113023692	0.3789296123078945	0.2586780937173968	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0101200461640286	0.5033674639218053	0.1925703907814079	T	T	T
0.0197545606560611	0.2587411330717161	0.3320428230273405	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2518766082241689	0.8732459642481583	0.2488313214240456	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0075131234542319	0.0010964405911364	0.1898093190455570	T	T	T
0.0142855021259427	0.7537579762083203	0.3392449194457597	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7518782415707053	0.1358806657545806	0.2578229949399252	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7539687202057032	0.3760251841548930	0.2591605017503992	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4999635580068094	0.5036845877077566	0.1933218213837455	T	T	T
0.5192070021807046	0.2581979904593719	0.3320718807499028	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7580555035440427	0.8785187019904543	0.2540107765504908	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5084093068996592	0.0001160025559493	0.1905758242035038	T	T	T
0.4244500787274861	0.7189575292532496	0.3346000311007657	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2291090434613285	0.6405289307961901	0.2532296054407784	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.5828326391208275	0.5910767172957343	0.3330863532220429	T	T	T
0.7748277684952590	0.5237224387961215	0.3386915655447346	T	T	T
0.7020599906772420	0.7967406195637560	0.3841588200211725	T	T	T
0.7461090573054838	0.6268302071035606	0.2636946228708066	T	T	T
0.7082570153578734	0.5944487465191182	0.3237860003045845	T	T	T

Distal mechanism (state 7)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004
Ba	Ti	O H N

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9956721357368579	0.2526301190212627	0.1901713949576700	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0009251475025687	0.7546477647631369	0.1873365943164498	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.5009006301192177	0.2541583884993117	0.1914708596331952	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5014769109112585	0.7537793442107182	0.1899268409099955	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2535199472584395	0.4980361460796285	0.1864148856277047	T	T	T
0.2381753480243911	0.2576345238430582	0.3117195243573756	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2369045682451223	0.0147863772118232	0.1949619030607602	T	T	T
0.2372525969871949	0.7696874121849596	0.3126971067020682	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7648283729374801	0.5043154574762220	0.1903087895585313	T	T	T
0.7497454304056089	0.2520464411408295	0.3113503017551218	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7365315522637991	0.0114641255101798	0.1951964879535179	T	T	T
0.7737065581169035	0.7612546772816463	0.3128466574656008	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.25399699787778850	0.1356583957530674	0.2577097892289108	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2493676938955809	0.3783576979985162	0.2601129260206381	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
-0.0014978931748815	0.5072532648173336	0.1946000407494972	T	T	T
0.0167150934030246	0.2536695462229972	0.3331531849652253	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2515206149198945	0.8725722748219140	0.2520079848720004	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0085276571799590	-0.0008272920060855	0.1902050780572519	T	T	T
0.0024182208066317	0.7542423271674157	0.3324361360656738	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7548077387719350	0.1290526255956911	0.2576007224326037	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7576805614444116	0.3696068327708737	0.2570616350549977	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4867098570291894	0.5016480975255327	0.1962802124202782	T	T	T
0.5299168234710322	0.2598249269069639	0.3341841808563026	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7536570298903537	0.8685715179559417	0.2531718419294671	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5077660650647873	-0.0018447361904081	0.1904870073387095	T	T	T
0.4454028081306065	0.7471867476500126	0.3409710053081767	T	T	T

0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2446667334668547	0.6462359022372621	0.2615614214338323	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.5173914327306094	0.6127123930940472	0.3311051305860228	T	T	T
0.5114368052827964	0.5127945921869976	0.2728905893372081	T	T	T
0.6389754835584880	0.4839814238867619	0.3303878334491094	T	T	T
0.7156299151780439	0.6149870521659935	0.2710592775996945	T	T	T
0.5892564097623195	0.5516974063513714	0.3057063346797801	T	T	T

Distal mechanism (state 8)

1.0000000000000000
8.0600004195999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.3985996245999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9917721472796548	0.2572034095328815	0.1915124406374031	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0008644855407513	0.7549660395455438	0.1873509590486318	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.5014095462732555	0.2577149964831367	0.1915515237513711	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5032765259784664	0.7525540827955689	0.1913538839135651	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2581628300935606	0.4994771143646828	0.1886478331314104	T	T	T
0.2390451198141354	0.2597711597085340	0.3118254988103816	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2346543160956639	0.0146231140794980	0.1980851863307878	T	T	T
0.2233362106629606	0.7684525688075301	0.3122237397899701	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7643566812387197	0.5150698379713499	0.1979951917749308	T	T	T
0.7389312466560521	0.2583538116992319	0.3126855283864873	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7336870159933053	0.0111452106178728	0.1999475666867314	T	T	T
0.7811280552374652	0.7540191873283953	0.3108126121400371	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2513813851410967	0.1362797497913219	0.2574914430745994	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2480504388433380	0.3777791841508725	0.2586495446127450	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0001935501906102	0.5066663490258200	0.1941532827780156	T	T	T
0.0189986989251573	0.2567256502697163	0.3333245111186662	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2556724838416099	0.8744965888187498	0.2503584362163007	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F

0.0073812463307551	0.0000235228956036	0.1908059435505341	T	T	T
0.0013018807576218	0.7538481331381450	0.3331231197041530	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7511095468395345	0.1354756158194670	0.2580796115722369	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7505647793716150	0.3748957892052376	0.2592105504875049	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4872550162124385	0.5047699281202034	0.1941708019213999	T	T	T
0.5176695517673809	0.2576955950671810	0.3331394257154482	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7466944714258018	0.8787566016855417	0.2564973212461127	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5078278122906718	0.0005465063457861	0.1902662460169866	T	T	T
0.3719049791528589	0.7699516711439196	0.3681797101925946	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2564433281565446	0.6404452135897837	0.2616580077876484	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.5418970135005209	0.7269125079367814	0.3925531883688759	T	T	T
0.6726184255254668	0.6103717717991016	0.3962540435788556	T	T	T
0.7244832279988436	0.7311740369556088	0.4329009481591303	T	T	T
0.7485932457576389	0.6319411430938613	0.2607008790126685	T	T	T
0.6693089069474838	0.7000237678481664	0.3947151074493705	T	T	T

Distal mechanism (state 9)

1.0000000000000000
8.0600004195999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.3985996245999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9914045419585995	0.2580417970050686	0.1919151092365551	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0003657533612681	0.7552364074407591	0.1894499171284663	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.5017411601400646	0.2583187528313907	0.1917263938794826	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5027745446808889	0.7525888647278203	0.1932218220380712	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2577047675130326	0.4994205704009265	0.1881952858725250	T	T	T
0.2398973709924364	0.2594303359485214	0.3115763805064596	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2344049987820408	0.0160178402682352	0.1970519943082455	T	T	T
0.2444326110251333	0.7687450223235236	0.3119644867923566	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7643549200477927	0.5155830756401872	0.1977366785652977	T	T	T

0.7379516951622969	0.2581573111581486	0.3126581878419905	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7345451740773428	0.0115404618394519	0.1991430179419200	T	T	T
0.7689151829000472	0.7557819158503132	0.3108127013320630	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2521684919130266	0.1354505838124224	0.2570827047647472	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2479861670091175	0.3775147530953302	0.2583423021837115	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0001882941997314	0.5058249720060229	0.1938983723770407	T	T	T
0.0202388958020328	0.2555458085175359	0.3328624756920137	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2490923584531560	0.8732440180071133	0.2508807248051273	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0076080612867391	0.0013275865892003	0.1901010669813493	T	T	T
0.0030601623042338	0.7567333892836151	0.3304927496719130	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7514147702865592	0.1352100948301878	0.2579232366187776	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7498530060388358	0.3747564064219029	0.2591873060297942	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4870231648680189	0.5051408144488639	0.1945285650661879	T	T	T
0.5162278662866199	0.2561198798451724	0.3323729684933564	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7529878536421947	0.8769366810642414	0.2548870779411666	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5080400732540860	0.9997655987439765	0.1906022786481743	T	T	T
0.4608335133295727	0.7549251036548928	0.3321747297071720	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2446397319306203	0.6466165926920235	0.2597382384788177	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7530087296474398	0.6335755461290336	0.2604278220291049	T	T	T

Distal mechanism (state 10)

1.0000000000000000
8.0600004195999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.3985996245999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9914251586324166	0.2580023856251144	0.1918909074332744	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F

0.0003412475624226	0.7554021240201461	0.1889278021231471	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.5020067821126150	0.2583562995031283	0.1917096154064272	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5038292341343759	0.7525731144557402	0.1935081244722974	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2580970458792184	0.4994063816778547	0.1882416672906179	T	T	T
0.2399516980621361	0.2598831764929507	0.3115720201115003	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2344274119670042	0.0162175140770086	0.1970376569668217	T	T	T
0.2418059602844344	0.7683383830623205	0.3111288518084012	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7647417940801574	0.5151712840369483	0.1977128443894062	T	T	T
0.7379290371731477	0.2586224056733465	0.3127473601423407	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7345312222287343	0.0114731954218791	0.1995210894458016	T	T	T
0.7735167264905073	0.7551792741951825	0.3111458608347770	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2520760702947228	0.1359342891153658	0.2571474863002177	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2482683198036561	0.3780742496733203	0.2583747136119500	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0002120646152879	0.5059054493658173	0.1937871938415058	T	T	T
0.0202936706639079	0.2563979399478470	0.3330103668008061	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2494667219067028	0.8733929328776379	0.2502028121563622	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0075892005252844	0.0014634989039455	0.1901109419220030	T	T	T
0.0045883751435012	0.7560729262255267	0.3311122565817419	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7513194625578236	0.1356100959232949	0.2581465161984097	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7499671419881089	0.3751833896953723	0.2592541855643243	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4873294403615728	0.5052361752968472	0.1944523520646330	T	T	T
0.5161527510562047	0.2567996897914442	0.3325065552072016	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7530870331963343	0.8774637692932143	0.2552712349325605	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5081091002613439	-0.0000745430040394	0.1906522824309147	T	T	T
0.4533766295956683	0.7540085571193790	0.3343802648012699	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2450523597176720	0.6458620472136781	0.2587463650816693	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7493818144217188	0.6921833683316627	0.4056497781463834	T	T	T

0.6574622435565937 0.6980306524146808 0.3965840181861793 T T T
 0.7539115996157302 0.6330147968633842 0.2608697118666324 T T T

Distal mechanism (state 11)

1.0000000000000000
 8.0600004195999997 0.0000000000000000 0.0000000000000000
 0.0000000000000000 11.3985996245999992 0.0000000000000000
 0.0000000000000000 0.0000000000000000 22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000 0.5000000000000000 0.0659599970000002 F F F
 0.9910766337046737 0.2587698352254800 0.1920154196850982 T T T
 0.0000000000000000 0.0000000000000000 0.0659599970000002 F F F
 0.0010416770767852 0.7548181962691761 0.1869725001751134 T T T
 0.5000000000000000 0.5000000000000000 0.0659599970000002 F F F
 0.5019838410512351 0.2598040303732377 0.1917865799757824 T T T
 0.5000000000000000 0.0000000000000000 0.0659599970000002 F F F
 0.5039227001574357 0.7522055899357339 0.1911694418398431 T T T
 0.2500000000000000 0.7461799980000023 0.0640000029999968 F F F
 0.2565647533315685 0.4989665297250419 0.1884685956682645 T T T
 0.2397069044747687 0.2602454738684086 0.3118079108894480 T T T
 0.2500000000000000 0.2538200019999977 0.0679299979999968 F F F
 0.2366400250921058 0.0165918851413389 0.1976585436121578 T T T
 0.2246827950251830 0.7666837258111842 0.3134571349755941 T T T
 0.7500000000000000 0.7461799980000023 0.0640000029999968 F F F
 0.7629751427918335 0.5176033883706406 0.2000248943319370 T T T
 0.7376007405447514 0.2590708123015412 0.3129541687320959 T T T
 0.7500000000000000 0.2538200019999977 0.0679299979999968 F F F
 0.7333418600089411 0.0131530600511333 0.1992787506819021 T T T
 0.7847657204202905 0.7596234337037310 0.3100365979755464 T T T
 0.2500000000000000 0.6250000000000000 0.0018099999999990 F F F
 0.2500000000000000 0.3750000000000000 0.1301199939999975 F F F
 0.2524836852466958 0.1362163317463980 0.2571235312838903 T T T
 0.2500000000000000 0.8785200120000027 0.0036100000000019 F F F
 0.2500000000000000 0.6285200120000027 0.1319299939999965 F F F
 0.2481645689856581 0.3777853312345492 0.2581923673234970 T T T
 0.0000000000000000 0.7535200120000027 0.0677699969999992 F F F
 0.0009233022283532 0.5077403486547604 0.1947617988211840 T T T
 0.0199562477567106 0.2563019202554515 0.3322260794063779 T T T
 0.2500000000000000 0.3714799879999973 0.0000000000000000 F F F
 0.2500000000000000 0.1214800030000021 0.1283199940000017 F F F
 0.2604407745531758 0.8731944074017138 0.2542813947951854 T T T
 0.0000000000000000 0.2464800030000021 0.0641599969999973 F F F
 0.0102516144455002 -0.0007284130467772 0.1910164615452661 T T T
 0.0071971900283201 0.7547460887334476 0.3331975971922241 T T T
 0.7500000000000000 0.6250000000000000 0.0018099999999990 F F F
 0.7500000000000000 0.3750000000000000 0.1301199939999975 F F F
 0.7509232642071449 0.1362488250926341 0.2577386470647670 T T T
 0.7500000000000000 0.8785200120000027 0.0036100000000019 F F F
 0.7500000000000000 0.6285200120000027 0.1319299939999965 F F F
 0.7502070935651535 0.3754220424620372 0.2593055967669075 T T T

0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4862970348370836	0.5057674293508775	0.1945523105481909	T	T	T
0.5159481917992396	0.2569874732316053	0.3317698376137609	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7495548209658484	0.8801919968337576	0.2551056555598341	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5070361476586196	0.0005702336977899	0.1902310559414992	T	T	T
0.3716946636792646	0.7421397521962533	0.3729412278845227	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2487583356555969	0.6438191390493397	0.2617172398517745	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.6585392470531731	0.7639937950754050	0.3752123498052092	T	T	T
0.4971948287966760	0.7531218868898620	0.3759009310748355	T	T	T
0.745443325523263	0.6337317451679398	0.2612531759446902	T	T	T

Distal mechanism (state 12)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9942634256868984	0.2555610076590147	0.1917803933695101	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0026620420387317	0.7529746681400529	0.1859559323675608	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.5000371598968313	0.2569809460639559	0.1918394293153695	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5017705403335760	0.7506325700110604	0.1916464037689999	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2584190041438650	0.4969773605354336	0.1873444132133694	T	T	T
0.2397379247958268	0.2587809226013592	0.3114703338075089	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2367833015230681	0.0159556774661631	0.1957477707305316	T	T	T
0.2236561381252173	0.7706791519978240	0.3168129575815723	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7632703011219677	0.5070766193553743	0.1907618514577081	T	T	T
0.7394426264211168	0.2565210789621436	0.3121216331403016	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7343979292288882	0.0140470427457184	0.1961925076053076	T	T	T
0.7961066503673959	0.7649106645867529	0.3096309817683312	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2528050784489373	0.1353867573768036	0.2570795550338754	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2475801183990482	0.3774989704255750	0.2581435748010245	T	T	T

0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
-0.0027097896230743	0.5048818958723047	0.1930546406424297	T	T	T
0.0193358848107601	0.2552106085630509	0.3324637473412828	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2543522096343619	0.8714761659196910	0.2560222509012929	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0096356168101978	0.9984908087328347	0.1906659398353641	T	T	T
0.0100895817690180	0.7654832895980616	0.3442638889722565	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7522280181899094	0.1340195282561413	0.2572671761614398	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7514787107532925	0.3746234887331415	0.2591108830413484	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4881725888723085	0.5036205168754411	0.1936430195409272	T	T	T
0.5177666591557453	0.2556151129576686	0.3319673472262285	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7517267322341888	0.8754548701859751	0.2534713547047088	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5068200015971006	-0.0015344371595757	0.1905387736935283	T	T	T
0.3907475361458015	0.7562537961784233	0.3724068053533430	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2405440540268450	0.6448698947700361	0.2670023638640664	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.5088969661414892	0.7788684815075823	0.3715113426280880	T	T	T
0.7466925812470999	0.5600349857420814	0.2977347644310446	T	T	T
0.7441058542321415	0.6264061740885605	0.2658118053625348	T	T	T

Distal mechanism (state 13)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9962257059380963	0.2537350528528764	0.1916362705452676	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0005710077191676	0.7529131605197428	0.1887745886476059	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4988291014468281	0.2540660235353662	0.1916068504856151	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5026032508251527	0.7527429921995351	0.1909959289737908	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2596913132591312	0.4975839847330813	0.1870896726713035	T	T	T
0.2404269783045515	0.2584057653611534	0.3111441982199536	T	T	T

0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2361186586961741	0.0149276422672019	0.1949099204318754	T	T	T
0.2523781673413134	0.7720416097978617	0.3136514983106591	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7614237493768797	0.5010324594853386	0.1877466598434689	T	T	T
0.7395501615147870	0.2542329507454409	0.3116286689028833	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7370579499436211	0.0135812504932788	0.1948934196177164	T	T	T
0.7738854714124660	0.7733212850650788	0.3171967832522567	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2524572250685767	0.1349792887751965	0.2570215879875084	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2488052005992674	0.3779372483630640	0.2581835887566357	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.9948265234611163	0.5056205377987536	0.1947413980518428	T	T	T
0.0195300956408025	0.2559619445198006	0.3326828217100441	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2511662809361409	0.8719053790594465	0.2518682860031797	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0075769257199538	-0.0009696968201475	0.1901800234995636	T	T	T
0.0019284976024864	0.7623306268797772	0.3337457607539088	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7534354334670732	0.1303244485603925	0.2582338739703726	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7505800721262113	0.3702694866536799	0.2573272799111174	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4915118379913251	0.5052209147631305	0.1949797033771990	T	T	T
0.5172610079061114	0.2551121818285907	0.3321364775704017	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7546850924957031	0.8696573735082801	0.2541763902721015	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5088089359811485	-0.0020609500070033	0.1905751657461922	T	T	T
0.4707124981833110	0.7580338895949327	0.3323840203774845	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2460915945078440	0.6472125989425895	0.2636637198082847	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.6403669945704212	0.5733354647680088	0.2933045970154787	T	T	T
0.8431218096596690	0.5611969772957047	0.2939464431534904	T	T	T
0.7474838149518699	0.6110798563597397	0.2770812830634338	T	T	T

Distal mechanism (state 14)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9966017571011958	0.2538569010245763	0.1914771652492634	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0006273479276758	0.7527169053289489	0.1891469622474685	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4983305875942241	0.2542208873635753	0.1916435607796371	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5017233953975123	0.7526863192213550	0.1905519457426001	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2595236091231522	0.4977784637140413	0.1871113482988237	T	T	T
0.2399286850566799	0.2578225263321330	0.3112700724326908	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2359100282385266	0.0147664648605619	0.1947869023977526	T	T	T
0.2522420280024485	0.7714448615854042	0.3133543786113254	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7614619384099475	0.5008653744088986	0.1875728305648686	T	T	T
0.7404005728455617	0.2538272245550895	0.3116343488175640	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7370780261330572	0.0142785402732068	0.1943708281392927	T	T	T
0.7662508873566114	0.7729896745951838	0.3172525404976974	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2523097233382883	0.1347800952917444	0.2571338741550293	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2485208056394141	0.3774682758567167	0.2584547329161019	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.9947935180369490	0.5054176135592044	0.1947230429652721	T	T	T
0.0187062651128737	0.2548897866489702	0.3330354257015259	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2513583491620049	0.8722001376739400	0.2520168155005946	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0071108719785301	0.9988131624934787	0.1902494020434471	T	T	T
-0.0007378401362209	0.7605581806327250	0.3310647307431570	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7536941151157684	0.1298879812734005	0.2581136957254683	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7505723024746096	0.3701240808754506	0.2574755638370544	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4915516130460088	0.5050808713517011	0.1951357363205032	T	T	T
0.5183342813600263	0.2540277576552072	0.3327036423523441	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7534011845801406	0.8683713645832959	0.2543579164135040	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5087866578437049	0.9981534154973410	0.1904736637955840	T	T	T

0.4746736118728503	0.7576557095862670	0.3320143089397525	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2471206402435338	0.6468262723886039	0.2631247373495793	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.6380157307184243	0.5737150571108639	0.2916557995479269	T	T	T
0.8411493769851720	0.5608161808899604	0.2945331199674461	T	T	T
0.7792158230273630	0.8602346345002267	0.4049140663336433	T	T	T
0.6847064268320672	0.8566793931187811	0.3997655947037689	T	T	T
0.7469695852230210	0.6111031626231039	0.2769870568732389	T	T	T

Distal mechanism (state 15)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9968587905471548	0.2534942248837998	0.1913973653456661	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0001209469180085	0.7521530401439590	0.1861628383403312	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4982135324672468	0.2538445956872947	0.1914893852432700	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5020991097727916	0.7524013657429576	0.1881944289315822	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2593107947585845	0.4968040478678525	0.1873288819874896	T	T	T
0.2397165062622710	0.2583075722775912	0.3111822837326426	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2373653594337274	0.0152498447743858	0.1948682611796072	T	T	T
0.2313596636591491	0.7682890018510181	0.3136344156875768	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7603473093593002	0.4991295163442809	0.1878164488393946	T	T	T
0.7399589659324296	0.2549551626425123	0.3115045472480133	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7369991727160360	0.0147041866798194	0.1946861538060116	T	T	T
0.7856746717158638	0.7752961363421397	0.3181455172554486	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2523758176049924	0.1349320594899472	0.2569984680097315	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2486305926778630	0.3775626337710857	0.2578429159194173	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.9933472723365004	0.5068858928181155	0.1955522428616754	T	T	T
0.0185551905232700	0.2559913871758048	0.3319053616439893	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2594766355688287	0.8713791079422761	0.2544581777663073	T	T	T

0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0083527460237644	0.9965620470985537	0.1909876217537369	T	T	T
0.0061314237735854	0.7583213922352742	0.3338845247450902	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7532739699148021	0.1319574269868064	0.2573339415152401	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7509620485736545	0.3725012108851946	0.2575415208853577	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4916259761917093	0.5055817036903121	0.1952553692297081	T	T	T
0.5182133588336066	0.2555679982727888	0.3315294192853377	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7501217811748975	0.8702432833916511	0.2559092269710255	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5083934703060413	0.9975579366964297	0.1903304516478341	T	T	T
0.3981089559358762	0.7511181509801346	0.3683607461659957	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2508362442982093	0.6434447846179365	0.2639685410428841	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.6160757085668254	0.5827952238875104	0.2913173307450369	T	T	T
0.8131257254170715	0.5564394429178148	0.3000646697726489	T	T	T
0.6791559478587840	0.8254302052600921	0.3828019812904187	T	T	T
0.5070830164647842	0.7884593322985500	0.3790409582006137	T	T	T
0.7319240038037201	0.6158086781706715	0.2813985754100769	T	T	T

Distal mechanism (state 16)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
-0.0008208390514189	0.2543296917136372	0.1913223897808286	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0000694863446853	0.7535260340298583	0.1872643947405380	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4957924698961260	0.2525579079567579	0.1916917957061865	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4998001089055330	0.7557229464159663	0.1899069217723192	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2598647097834536	0.4981919105044839	0.1873379525331826	T	T	T
0.2378935110651399	0.2602539716667427	0.3113708426826133	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2354248619920499	0.0152626881848843	0.1953436016977913	T	T	T
0.2381657948156705	0.7741784940584588	0.3131214410893198	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F

0.7579294924896234	0.4947412743686400	0.1852319832944948	T	T	T
0.7404180011201936	0.2606011257046191	0.3111295321090047	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7397880480386017	0.0164806626115486	0.1942931608868435	T	T	T
0.7863906722613943	0.8004095946470143	0.3307922328322950	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2508441233755495	0.1366261110406949	0.2573472002475421	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2495320054681731	0.3787978990516411	0.2577013620511662	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.9907811257005897	0.5087367142829013	0.1963603484367563	T	T	T
0.0160856584777100	0.2597121182564093	0.3317386391388518	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2517930659298283	0.8736522897720738	0.2505757741330767	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0041887227341483	-0.0000688009359547	0.1912479270352571	T	T	T
0.0065755851436064	0.7738836775807656	0.3412057349569438	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7529748571348678	0.1398114231952496	0.2560154752617508	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7489710676706618	0.3863866901125796	0.2602145571615658	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.4958335377671523	0.5094328300220226	0.1967975404219882	T	T	T
0.5201272176171343	0.2596116450626316	0.3321152274486496	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7550055412321230	0.8569830830072840	0.2569980110400795	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5106807219952106	0.9991093720474931	0.1915350677854486	T	T	T
0.4372625503097252	0.7585799624004456	0.3442372620896545	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2397966598324725	0.6466424306676629	0.2637207686392009	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7220351486581786	0.5505785652348302	0.3136674276204488	T	T	T
0.7471973641319414	0.5899398309202276	0.3840381934937568	T	T	T
0.7472175740046334	0.9115734189256527	0.3809067741505086	T	T	T
0.5755345556344382	0.6349653072052081	0.3475334021835804	T	T	T
0.7027027932472242	0.6187650614223406	0.3434443942573702	T	T	T

Distal mechanism (state 17)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9972122515950627	0.2522501151560921	0.1918228737828581	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
-0.0013264612505202	0.7552652634136335	0.1932125741867328	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4949518679454508	0.2535317772279849	0.1919801545316297	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4996803341083398	0.7538476245585937	0.1886950556940540	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2381912982234594	0.4985281518074331	0.1874521306845020	T	T	T
0.2414499723895579	0.2604974346908355	0.3111178873635414	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2371768955645909	0.0150529097253987	0.1956504597356959	T	T	T
0.2791498463804999	0.7667642629132692	0.3138334440126374	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7406421073576087	0.4942389450043808	0.1859591581305536	T	T	T
0.7428052133534961	0.2600264361761322	0.3109539901335662	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7343195767627827	0.0149068553628805	0.1953846329366541	T	T	T
0.7506103479095456	0.8108772184334451	0.3242087265291334	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2535429965586422	0.1367077480122611	0.2572299449770356	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2548042419921744	0.3789498125215251	0.2574149090768319	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0052871185498546	0.5077430733187223	0.1955525912648606	T	T	T
0.0207535110593530	0.2589119603744047	0.3311006238054578	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2543859456197501	0.8729993905514003	0.2555006962400381	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0090567681527090	-0.0006642010309872	0.1909741111739266	T	T	T
-0.0439749380500576	0.7501036583466515	0.3269118900014841	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7524829598315134	0.1375642349647612	0.2562353284768160	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7569643603273718	0.3801479715727989	0.2577016057458746	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5099799503977239	0.5076202439532872	0.1958862738520979	T	T	T
0.5224585192098093	0.2593241601402684	0.3310892752403606	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7473910900679257	0.8714099698962914	0.2488434506002349	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5055660457840713	0.0009624922602829	0.1902014868922850	T	T	T
0.5046124246975219	0.7559187132301844	0.3287087793921072	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F

0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2575486027610918	0.6427692623040878	0.2629536887101755	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7713631066276814	0.9326578451330968	0.3694273536736815	T	T	T

Distal mechanism (state 18)

Same as state 1 of distal mechanism

Alternating mechanism (state 1-4)

Same as state 1-4 of distal mechanism

Alternating mechanism (state 5)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba	Ti	O	H	N
8	12	30	8	2

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9964289108591922	0.2548704249478851	0.1913309089827162	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0051123074702680	0.7529369739361939	0.1914757518003276	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4927304090302011	0.2568797366298936	0.1931389006910173	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4933201194204018	0.7507798462114544	0.1971268919473885	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2337153195589948	0.5050458415709461	0.1902009798733547	T	T	T
0.2332715560309367	0.2568423796039795	0.3125103705534902	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2349404752368747	0.0152502762996736	0.1958423372926237	T	T	T
0.2155702126131674	0.8509129381177885	0.3336116826489696	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7390992243147987	0.4981294654615700	0.1875093108718906	T	T	T
0.7446163322338368	0.2588758203396130	0.3110032223607724	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7337121542594981	0.0144456159972579	0.1960278610955068	T	T	T
0.7745186672753900	0.7821454078300606	0.3165705300793671	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2500442777446176	0.1368822410897341	0.2565868577188590	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2504492800801719	0.3760828554049145	0.2605090873849244	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0032344336794270	0.5063642868169020	0.1944189465693018	T	T	T
0.0106754480645539	0.2562705333239372	0.3313110767590007	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2501019174731273	0.8786934160459786	0.2537950226730549	T	T	T

0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0080688368942466	0.0006101926643878	0.1896935590385181	T	T	T
0.0027449630915409	0.7938453304222370	0.3437088853073222	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7532302717374202	0.1350722436918336	0.2564397013181286	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7544411051080693	0.3779044741699747	0.2574635538908804	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5106480610881980	0.5051911569319703	0.1947065547651808	T	T	T
0.5253087379348750	0.2537291180801754	0.3327481963009969	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7561580567970204	0.8757423610934850	0.2509176343788285	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5059456667897708	-0.0001326452066634	0.1904929012325558	T	T	T
0.2655206474433530	0.9884420995239944	0.3753981673009811	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2538520601220133	0.6181270180787615	0.2483570727072791	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7720475965028523	0.6530889502296685	0.2680110117380531	T	T	T
0.3763506627926040	0.0211466697833252	0.3690570288435328	T	T	T
0.3762728189096681	0.6515836670515621	0.3651086860799266	T	T	T
0.5598848417354013	0.7554939026926224	0.3429351321689736	T	T	T
0.4032796105838354	0.7375374581122801	0.3538412531599378	T	T	T

Alternating mechanism (state 6)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9977449801624014	0.2548879071307221	0.1908486557410372	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0056550097016499	0.7538033512882635	0.1922692569279205	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4920566512602001	0.2561384781464227	0.1931550482973009	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4940474411742275	0.7520291810448453	0.1970523347940752	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2341673399744891	0.5056386490418479	0.1901559854153179	T	T	T
0.2323151910467232	0.2551904388830362	0.3124561007937809	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2340733247751220	0.0152622045119490	0.1946509334506809	T	T	T
0.2544189584498884	0.8713433326907962	0.3338779917714164	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F

0.7402518343597501	0.4948356759772343	0.1859956314488720	T	T	T
0.7461967193414618	0.2572964635895158	0.3105356081925570	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7360833997934381	0.0140673954107665	0.1945518024906109	T	T	T
0.8051709623178570	0.8422173232897867	0.3307234644283849	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2475311650044868	0.1374708520546351	0.2553612156197845	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2498714962063059	0.3756265563629160	0.2610750011897439	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0012273833085805	0.5088822101672432	0.1960966870975896	T	T	T
0.0096070057231703	0.2541688136987147	0.3317151889874557	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2550027040194677	0.8809828595873558	0.2517738945053729	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0064469931201591	-0.0006689542246412	0.1893345610436491	T	T	T
0.0332224541577798	0.8305999832276859	0.3513772204853888	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7567991441174002	0.1346031185219739	0.2561041108086912	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7549227368587089	0.3788173642515553	0.2578875194401841	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5118849803620072	0.5065922724469062	0.1961982490684116	T	T	T
0.5259570655174924	0.2483280121151060	0.3320312598742990	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7579139629882431	0.8725581267128817	0.2527515213402686	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5085547313701088	-0.0005233643058489	0.1906254945484566	T	T	T
0.3221841470110903	0.0120828152739314	0.3677295573791660	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2549970733190139	0.6187928628669045	0.2487538590572465	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.4198600629212141	0.0548698028490174	0.3529484481856694	T	T	T
0.4126672788445893	0.6730383309097869	0.3448599949072653	T	T	T
0.6179340332480132	0.7393761498055840	0.4109054862300852	T	T	T
0.6047572354507458	0.7774596102699555	0.3691406351550511	T	T	T
0.4402650951759324	0.7610146827199981	0.3485227314852004	T	T	T

Alternating mechanism (state 7)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H N
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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9955944983235472	0.2535188235390368	0.1920683542927063	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0062104544252331	0.7538111970517021	0.2006460505867660	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4933418168021881	0.2563894723854587	0.1923779662981622	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4929373454618365	0.7508960468517856	0.1936385364250074	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2318216753661323	0.5043526471730828	0.1897202949726269	T	T	T
0.2394462251735435	0.2613525666992574	0.3123784042413009	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2357672233854439	0.0123909223963419	0.1991162746160638	T	T	T
0.2868385944666926	0.8284280279525030	0.3352881734618545	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7376662555137119	0.5024894391921799	0.1891873067650499	T	T	T
0.7406279962778469	0.2576978264199418	0.3119078492501964	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7314304410423531	0.0130825193424638	0.1969398128919476	T	T	T
0.7330858213476361	0.8049603186628260	0.3213725421588087	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2516764737771004	0.1378070510752467	0.2580685520836222	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2517098683961023	0.3801923924337149	0.2597586866210922	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0020900187743825	0.5073961620969960	0.1952855773033805	T	T	T
0.0184407490107344	0.2580234644302650	0.3324919847976178	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2564057323839200	0.8798961710427918	0.2546949083858910	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0094096473152659	0.0000429573596100	0.1905052523468856	T	T	T
-0.0766349092752660	0.8326069409994733	0.3550681064517356	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7508390300887069	0.1346544140086439	0.2572931225471415	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7547848160973873	0.3755178157739382	0.2585406273108533	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5105059636287173	0.5029445996164157	0.1932529571107583	T	T	T
0.5197192559951236	0.2582533183416731	0.3321794186149561	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7484921061425431	0.8749341011858890	0.2461952074569256	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5043418132441639	0.0019716296470019	0.1893244277278896	T	T	T
0.5155038795959426	0.8425689323009917	0.3501307753013241	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F

0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2706172736039730	0.6157119807212890	0.2421369580128863	T	T	T
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2537333948511254	0.5900167465777030	0.3319436138252395	T	T	T
0.6391794557134615	0.5866281029591737	0.2989021575799220	T	T	T
0.8392924040105210	0.5872420144578490	0.3024115188641604	T	T	T
0.7414072259874056	0.6315438580650375	0.2832192506262927	T	T	T
0.2485829406618316	0.6790432318400567	0.3364416459729342	T	T	T

Alternating mechanism (state 8)

1.0000000000000000					
8.0600004195999997	0.0000000000000000	0.0000000000000000			
0.0000000000000000	11.3985996245999992	0.0000000000000000			
0.0000000000000000	0.0000000000000000	22.2077999115000004			

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9960951931066830	0.2537891350386812	0.1914426070773630	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.0016433658668822	0.7530294125507303	0.1905994215674373	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4961257942792748	0.2540028855146050	0.1915582546635444	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4988670666613720	0.7527277049169409	0.1890003696274575	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2381079389250292	0.5003812159631988	0.1877957953409170	T	T	T
0.2420887085151610	0.2540493013595934	0.3116616323248197	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2365946253283777	0.0137424883693865	0.1946536361446746	T	T	T
0.2755633511975756	0.7803109405735026	0.3182896426421543	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7382370470460223	0.5007064360109745	0.1875156789936643	T	T	T
0.7426918053520307	0.2531759185594639	0.3115817884034501	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7360939764967533	0.0134005755864381	0.1943493151540742	T	T	T
0.7577595000079715	0.7778272775110062	0.3162362284256969	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2534617166152635	0.1313742198506916	0.2577113155779288	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2545441348768171	0.3722030602427508	0.2583616912426308	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0058939465410767	0.5045696496792486	0.1949384941213225	T	T	T
0.0200557372446775	0.2540528848590871	0.3329353125885531	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2550042751142387	0.8722173769724539	0.2536062623792463	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0083378578202660	-0.0027003073820117	0.1901496146071590	T	T	T

0.9773284725737453	0.7715963496072709	0.3352976847946139	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7539806749947262	0.1296852095232296	0.2578057349104740	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7542436453335192	0.3708755407068687	0.2581099801112208	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5055863993417169	0.5047533100033276	0.1949471812316626	T	T	T
0.5208750776190658	0.2534446233617595	0.3329465636829996	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7517321155383510	0.8682139491815924	0.2505583614530744	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5076226218421733	-0.0019036089380317	0.1899343658436195	T	T	T
0.5030260933055618	0.7730135288936862	0.3359469914107770	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.3482103616220249	0.5644164604011462	0.2932245926712980	T	T	T
0.6454648802005011	0.5732902366447229	0.2931115163843089	T	T	T
0.8463525418652046	0.5654589262411541	0.2938061847626756	T	T	T
0.1482342819217451	0.5767082499626704	0.2962739520487624	T	T	T
0.7499261663339241	0.6136086427538217	0.2765100175654829	T	T	T
0.2520189418864029	0.6161827644695030	0.2785555642988779	T	T	T

Alternating mechanism (state 9)

1.0000000000000000
8.0600004195999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.3985996245999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9964825761828093	0.2543469170819956	0.1913663693280870	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
-0.0009826331785285	0.7524858416037989	0.1889087947334789	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4957223249611635	0.2540049577770540	0.1914862625838635	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5014286898407253	0.7531089830202773	0.1906650616912607	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2384453073148631	0.5007843497021643	0.1874625525714543	T	T	T
0.2419409762903006	0.2532276182697529	0.3116942746973297	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2357602899142474	0.0134677650211866	0.1942598660965218	T	T	T
0.2558756022776879	0.7780828446073937	0.3159885019079016	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7386231652895404	0.5001578102263924	0.1875651997159565	T	T	T
0.7424979118914021	0.2541791825312556	0.3116685074192959	T	T	T

0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7370076489402041	0.0144720165122371	0.1944187811653163	T	T	T
0.7739602958153313	0.7798987816798177	0.3189687636216492	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2534853212148003	0.1298866662779060	0.2579250910970092	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2538073655119548	0.3708621012651077	0.2582995340675061	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0053577776955086	0.5046246572831178	0.1949103661356335	T	T	T
0.0199832677742297	0.2537561106931918	0.3332894545563625	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2514599056359680	0.8687857795445616	0.2503837103862646	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0070175993394733	0.9980506026855553	0.1899512097928094	T	T	T
0.0030886368380798	0.7723792648312691	0.3351323824687638	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7538862696363590	0.1314326155911290	0.2576688445041592	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7544783378806029	0.3724109570702017	0.2584370016473128	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5060764575134994	0.5046968433101017	0.1950913984759134	T	T	T
0.5207407185259941	0.2539068817870535	0.3332410851968102	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7552119203062598	0.8708742599776864	0.2542806703152461	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5087968190771218	0.9974531160595584	0.1902805932686230	T	T	T
0.4760499933532275	0.7714079980932100	0.3358893767742266	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.3470657132999818	0.5665507369292180	0.2932612642101480	T	T	T
0.6474989111221979	0.5777455198169048	0.2955235900368743	T	T	T
0.8478163374047355	0.5642429598126540	0.2936486987739563	T	T	T
0.1463730033884047	0.5720598432694005	0.2926980966542865	T	T	T
0.6676690146767373	0.7867905939625432	0.4120699946886073	T	T	T
0.7593584896751036	0.7859376354867724	0.4217238330078116	T	T	T
0.7528460644387921	0.6169723587606125	0.2789396838888529	T	T	T
0.2496032019966752	0.6136471611904902	0.2760021366958183	T	T	T

Alternating mechanism (state 10)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9969734300890211	0.2536218579639054	0.1911984667858451	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
-0.0009858582194091	0.7519380864073797	0.1864660827851882	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4957401476553240	0.2538454012180380	0.1913857019950259	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.5010816638510190	0.7523619931486234	0.1882301739413389	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2387911845960453	0.4997317096302759	0.1876088499034915	T	T	T
0.2416848876906478	0.2539809004548418	0.3115898675225951	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2374278939551820	0.0139862038754899	0.1943905643675437	T	T	T
0.2321017432035921	0.7774533120342804	0.3174691681910434	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7397559956092167	0.4979972625436126	0.1875566418831041	T	T	T
0.7427520978209211	0.2554364457972934	0.3114376235869714	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7367599897218808	0.0151424513961414	0.1944335333162151	T	T	T
0.7886544174120608	0.7849256829673333	0.3201032632064624	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2534495231164924	0.1309294104157722	0.2575964906531091	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2536184131051534	0.3719126781945684	0.2579807614372800	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0051570375271291	0.5062069541026030	0.1955384627100804	T	T	T
0.0199888372795175	0.2548232183124250	0.3323762985149875	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2608200404591409	0.8692292393877837	0.2532733555670060	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0082918827596812	0.9959884410556360	0.1908026422976875	T	T	T
0.0082135110367902	0.7750027676917871	0.3387910962977901	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7537925373538483	0.1332642264081015	0.2569572130104671	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7563486284632711	0.3748377237726614	0.2583341314958750	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5068027311524721	0.5051961860513401	0.1955772547737019	T	T	T
0.5213489459230810	0.2560022596338548	0.3319774591737775	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7500778321376492	0.8728524487400939	0.2555854777857796	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5082475144522749	0.9973242312178346	0.1900684224779669	T	T	T
0.3899388099964020	0.7836480880974764	0.3758741093079807	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F

0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.3555330286578798	0.5701364071384549	0.2933109959979966	T	T	T
0.6304805906817705	0.5851909339554384	0.2958988079463538	T	T	T
0.8275077674230839	0.5625378910505967	0.3010812361574096	T	T	T
0.1568331573263204	0.5649869577738734	0.2946611709420751	T	T	T
0.5038293257071247	0.8176518747347401	0.3816021928000473	T	T	T
0.6785057044378678	0.8409813821619786	0.3824582565973986	T	T	T
0.7427872260252809	0.6224039323885949	0.2851606697667389	T	T	T
0.2530617883211932	0.6141291067299659	0.2775675368644234	T	T	T

Alternating mechanism (state 11)

1.0000000000000000					
8.0600004195999997	0.0000000000000000	0.0000000000000000			
0.0000000000000000	11.3985996245999992	0.0000000000000000			
0.0000000000000000	0.0000000000000000	22.2077999115000004			

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Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
-0.0007988793480576	0.2536476395917889	0.1913410788068633	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
-0.0000047037341055	0.7549444165202929	0.1872017277909120	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4942624374815400	0.2529125796641835	0.1916606127257547	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4994484835547203	0.7547090016012722	0.1893570897454942	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2382936050282380	0.5009638820410234	0.1877329720761118	T	T	T
0.2413894848319088	0.2558958573828655	0.3116310851079588	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2365116166510147	0.0138003909546729	0.1950471106171670	T	T	T
0.2414388148299604	0.7800739463243535	0.3163694516127100	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7422862923275250	0.4945021809643730	0.1855349127794012	T	T	T
0.7435346524292678	0.2604349017820954	0.3112413871758021	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7395759936886731	0.0166242515927219	0.1942722915781961	T	T	T
0.7904677000264776	0.8150749352406986	0.3328402275940824	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2527488896551506	0.1321977626978201	0.2578231781663340	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2535080959564722	0.3728767331325658	0.2573660335380992	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0016537821986780	0.5085413718125926	0.1957852661564148	T	T	T
0.0197466087175961	0.2577227962497966	0.3323936882856582	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2521603446092484	0.8701431796047288	0.2495627112048969	T	T	T

0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0046823403332448	-0.0008947945927068	0.1911951170124704	T	T	T
0.0101578280404103	0.7893725912719765	0.3445595531888135	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7536872400217710	0.1397760207647560	0.2558653374692519	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7584088761135147	0.3870100287673482	0.2609284962557411	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5105429311844946	0.5092043490045083	0.1978552514590333	T	T	T
0.5224899363340394	0.2602250713734373	0.3320359619666354	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7563967774198734	0.8587683212932168	0.2571019730424450	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5105021167731684	0.9979668797859614	0.1913608345591493	T	T	T
0.4375344011405268	0.7788417650988834	0.3510033397481084	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.3375335707354464	0.5665848627257686	0.2945970715393312	T	T	T
0.5752035411112094	0.6595813385482858	0.3556145671453239	T	T	T
0.7465974896515566	0.6042119190956364	0.3892599511812363	T	T	T
0.1373932501216840	0.5711347547488826	0.2912163182301598	T	T	T
0.7512320485281766	0.9333754319019487	0.3783792630043843	T	T	T
0.7095152517950218	0.5684787626618857	0.3189632722889725	T	T	T
0.7001821543906682	0.6360381337489696	0.3495785059833770	T	T	T
0.2418352735369201	0.6149148587681079	0.2768884475244067	T	T	T

Alternating mechanism (state 12)

1.0000000000000000
8.0600004195999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.3985996245999992 0.0000000000000000
0.0000000000000000 0.0000000000000000 22.2077999115000004

Ba Ti O H N
8 12 30 12 2

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9990609574017705	0.2536329675840600	0.1913660494979484	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.9997304794550723	0.7549509766647404	0.1872346873340412	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4942045262866085	0.2529513510521134	0.1916944134325222	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4990235477683357	0.7546701505936244	0.1892297920850444	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2382614379644466	0.5009301113263840	0.1877322473190378	T	T	T
0.2412555380044752	0.2560136947574972	0.3116201306655131	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2363864469295065	0.0139069397428818	0.1950023400069264	T	T	T

0.2407250595427635	0.7806598703532480	0.3163149971353207	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7422098186399587	0.4944329082679394	0.1855803170486193	T	T	T
0.7434484029290004	0.2604146307785883	0.3112332269282953	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7393407406062024	0.0166696693713426	0.1942424134193018	T	T	T
0.7883321806728599	0.8163255271027030	0.3325562585268038	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2525584116829572	0.1322789030830795	0.2578119731175978	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2534695694755226	0.3730719005034770	0.2573847660921278	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0016699345525247	0.5085378426074149	0.1958442735206719	T	T	T
0.0196466898242258	0.2578010399255498	0.3323446271059155	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2519896031345342	0.8701431357465153	0.2494537123524250	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0044916315560948	0.9991400724431126	0.1912105553433441	T	T	T
0.0080664624732461	0.7901895020532289	0.3436451558959113	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7535944693841000	0.1397388599200159	0.2558871790706226	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7582937237203808	0.3868582864237385	0.2608820805420604	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5104535597440928	0.5092646414312172	0.1978784040325013	T	T	T
0.5223810607120886	0.2602494669301577	0.3320016628958617	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7546600425172421	0.8588939711805142	0.2566929009483155	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5100651884013095	0.9982456993431588	0.1913501516209146	T	T	T
0.4364308489534712	0.7809131564119752	0.3512162105234504	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.3374181367343868	0.5668669914077954	0.2948095578580763	T	T	T
0.5730228958351345	0.6620623235529373	0.3571342409570286	T	T	T
0.7059266847046120	0.5702337888963344	0.3202860061889796	T	T	T
0.1373099390495090	0.5715855244909810	0.2913326263445522	T	T	T
0.7525643982329232	0.9359245473279817	0.3775810166021181	T	T	T
0.7454036005982076	0.6067221393279822	0.3903854744867387	T	T	T
0.0565299043626425	0.8200839024313730	0.4526460231524774	T	T	T
0.0953505187796673	0.8180310084160047	0.4834666322099783	T	T	T
0.6977756219117953	0.6380141406773906	0.3507840745389231	T	T	T
0.2418823320211502	0.6153354279590399	0.2770820470064856	T	T	T

Alternating mechanism (state 13)

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1.0000000000000000
 8.060000419599997  0.000000000000000  0.000000000000000
 0.000000000000000  11.398599624599992  0.000000000000000
 0.000000000000000  0.000000000000000  22.207799911500004
Ba Ti O H N
 8 12 30 12 2
Selective dynamics
Direct
0.000000000000000 0.500000000000000 0.0659599970000002 F F F
0.9986118672544638 0.2532614088890545 0.1908314887927154 T T T
0.000000000000000 0.000000000000000 0.0659599970000002 F F F
0.0036127965823032 0.7557798001670061 0.1904691325764100 T T T
0.500000000000000 0.500000000000000 0.0659599970000002 F F F
0.4943932489871228 0.2535081294006748 0.1918324267432522 T T T
0.500000000000000 0.000000000000000 0.0659599970000002 F F F
0.4971820736322211 0.7540137439700144 0.1880906207577910 T T T
0.250000000000000 0.7461799980000023 0.0640000029999968 F F F
0.2373868695188715 0.5013141248126995 0.1881065478350451 T T T
0.2389577607037103 0.2557853470202635 0.3119822854624507 T T T
0.250000000000000 0.2538200019999977 0.0679299979999968 F F F
0.2365172030239025 0.0147779605571467 0.1951207278316844 T T T
0.2755837072292026 0.7825470760466351 0.3179771980901581 T T T
0.750000000000000 0.7461799980000023 0.0640000029999968 F F F
0.7417930879271549 0.4950337976100427 0.1850652498812949 T T T
0.7463186690716226 0.2585433169726084 0.3109978281760530 T T T
0.750000000000000 0.2538200019999977 0.0679299979999968 F F F
0.7373276077851877 0.0147444318722892 0.1942133275774312 T T T
0.7387680982002294 0.7924118291368321 0.3230651557890795 T T T
0.250000000000000 0.625000000000000 0.0018099999999990 F F F
0.250000000000000 0.375000000000000 0.1301199939999975 F F F
0.2524593310453009 0.1335406453016220 0.2579461507831032 T T T
0.250000000000000 0.8785200120000027 0.0036100000000019 F F F
0.250000000000000 0.6285200120000027 0.1319299939999965 F F F
0.2530418870718735 0.3728433042166133 0.2581128457014120 T T T
0.000000000000000 0.7535200120000027 0.0677699969999992 F F F
0.0022393752559679 0.5087319192209178 0.1960985961535425 T T T
0.0167386669263809 0.2579031665168529 0.3324132094793794 T T T
0.250000000000000 0.3714799879999973 0.000000000000000 F F F
0.250000000000000 0.1214800030000021 0.1283199940000017 F F F
0.2539072281153140 0.8743554403589208 0.2530410996606943 T T T
0.000000000000000 0.2464800030000021 0.0641599969999973 F F F
0.0064932126529043 -0.0011093428809063 0.1909187428939882 T T T
-0.0087863554399396 0.7647422155655157 0.3339025047652315 T T T
0.750000000000000 0.625000000000000 0.0018099999999990 F F F
0.750000000000000 0.375000000000000 0.1301199939999975 F F F
0.7538827377433083 0.1380768048027713 0.2557595606668756 T T T
0.750000000000000 0.8785200120000027 0.0036100000000019 F F F
0.750000000000000 0.6285200120000027 0.1319299939999965 F F F
0.7602132066650027 0.3849892641707486 0.2601632646313686 T T T
0.500000000000000 0.7535200120000027 0.0677699969999992 F F F
0.5107233053501650 0.5081986839205813 0.1975189861171902 T T T
0.5268977566009269 0.2603000136624253 0.3324997431455989 T T T
0.750000000000000 0.3714799879999973 0.000000000000000 F F F

```

0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7508642984536056	0.8605823479490829	0.2508079702033597	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5082642452881369	-0.0005832728244736	0.1908166726232177	T	T	T
0.5034632612004721	0.7685424060158391	0.3288875801143891	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.3462078652306361	0.5639115454461197	0.2930495626976903	T	T	T
0.6375723248480983	0.5795239857007769	0.3643143137416171	T	T	T
0.7548427515784955	0.5275148951815052	0.3100542759804678	T	T	T
0.1453036250641383	0.5742988365640747	0.2961809455704192	T	T	T
0.7545500352814211	0.8999765263295716	0.3768279542506568	T	T	T
0.8435570477374303	0.5863547502412305	0.3697080838729420	T	T	T
0.2267353623870477	0.8506008046458255	0.3868615069447572	T	T	T
0.0216481724764072	0.8218842399910010	0.3656348737709123	T	T	T
0.7448678847086168	0.5955305770458584	0.3409919445956587	T	T	T
0.2486150398232553	0.6150256838690881	0.2790064812277075	T	T	T

Alternating mechanism (state 14)

1.0000000000000000		
8.0600004195999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	11.3985996245999992	0.0000000000000000
0.0000000000000000	0.0000000000000000	22.2077999115000004

Ba Ti O H N
8 12 30 12 2

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.9967443060644902	0.2518350644158638	0.1915593948994747	T	T	T
0.0000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
-0.0007391649903767	0.7587062134544366	0.1903725627277884	T	T	T
0.5000000000000000	0.5000000000000000	0.0659599970000002	F	F	F
0.4967288224276080	0.2518007505215135	0.1915663660318677	T	T	T
0.5000000000000000	0.0000000000000000	0.0659599970000002	F	F	F
0.4992581860159350	0.7587136325474577	0.1903966215178604	T	T	T
0.2500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.2408532999282539	0.4957622031158039	0.1852117899255498	T	T	T
0.2427417296503160	0.2623672148029424	0.3114258109946436	T	T	T
0.2500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.2377286769356983	0.0148984415899886	0.1956123032564608	T	T	T
0.2673402535090247	0.8043089868327850	0.3245440973925733	T	T	T
0.7500000000000000	0.7461799980000023	0.0640000029999968	F	F	F
0.7408784333109265	0.4957541183733183	0.1852121666053179	T	T	T
0.7427421096295053	0.2623896568149603	0.3114288811573753	T	T	T
0.7500000000000000	0.2538200019999977	0.0679299979999968	F	F	F
0.7378006507732978	0.0149513142281042	0.1955968797357113	T	T	T
0.7677226985072979	0.8041919830719776	0.3245669200722391	T	T	T
0.2500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.2523781955023837	0.1419225762974310	0.2563941727258995	T	T	T
0.2500000000000000	0.8785200120000027	0.0036100000000019	F	F	F

0.2500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.2585767142541532	0.3881102206385448	0.2604050109117242	T	T	T
0.0000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.0077029501269580	0.5114666207294610	0.1978694461910706	T	T	T
0.0219673552066603	0.2641477936582075	0.3322373850921296	T	T	T
0.2500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.2500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.2504426574291561	0.8676178902012238	0.2495540808133456	T	T	T
0.0000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.0061093699381824	0.0030860733023963	0.1916856489012657	T	T	T
-0.0108495688166107	0.7783125377347025	0.3287913646118181	T	T	T
0.7500000000000000	0.6250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.3750000000000000	0.1301199939999975	F	F	F
0.7523980526199209	0.1419435970718610	0.2563875205802095	T	T	T
0.7500000000000000	0.8785200120000027	0.0036100000000019	F	F	F
0.7500000000000000	0.6285200120000027	0.1319299939999965	F	F	F
0.7585813116586896	0.3881303098587867	0.2604478520541786	T	T	T
0.5000000000000000	0.7535200120000027	0.0677699969999992	F	F	F
0.5077596766786272	0.5115432373348817	0.1979156878688204	T	T	T
0.5219591446322608	0.2641239089692857	0.3322152943655307	T	T	T
0.7500000000000000	0.3714799879999973	0.0000000000000000	F	F	F
0.7500000000000000	0.1214800030000021	0.1283199940000017	F	F	F
0.7505436358914306	0.8675192366186874	0.2495873458558692	T	T	T
0.5000000000000000	0.2464800030000021	0.0641599969999973	F	F	F
0.5061856025950988	0.0030601587385305	0.1916916612688191	T	T	T
0.4888337176721432	0.7786797427179070	0.3288684693411399	T	T	T
0.2500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.2500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.7500000000000000	0.1250000000000000	0.0018099999999990	F	F	F
0.7500000000000000	0.8750000000000000	0.1301199939999975	F	F	F
0.2686972721494889	0.5914453344650652	0.3846394110589778	T	T	T
0.5927149705787672	0.6131488040699810	0.3456555406489494	T	T	T
0.7517753859640177	0.5404428283404169	0.3154885779618131	T	T	T
0.0940392006272571	0.6119457692678093	0.3462219627074046	T	T	T
0.7568477907893706	0.9138061267610019	0.3773403333203364	T	T	T
0.7658372024897332	0.5914013212246804	0.3847811868522603	T	T	T
0.2531024027734390	0.5405293639655977	0.3153946327939942	T	T	T
0.2563326588098336	0.9138858828751094	0.3773122899326174	T	T	T
0.7198504925508618	0.6101718053242862	0.3428948797408277	T	T	T
0.2211016015651258	0.6100066735396257	0.3429610496143257	T	T	T

Alternating mechanism (state 15)

Same as state 16 of distal mechanism

Alternating mechanism (state 16)

Same as state 17 of distal mechanism

Alternating mechanism (state 17)

Same as state 1 of distal mechanism