

Electronic Supplementary Information

Water Adsorption on the $\text{Fe}_3\text{O}_4(111)$ Surface: Dissociation and Network Formation

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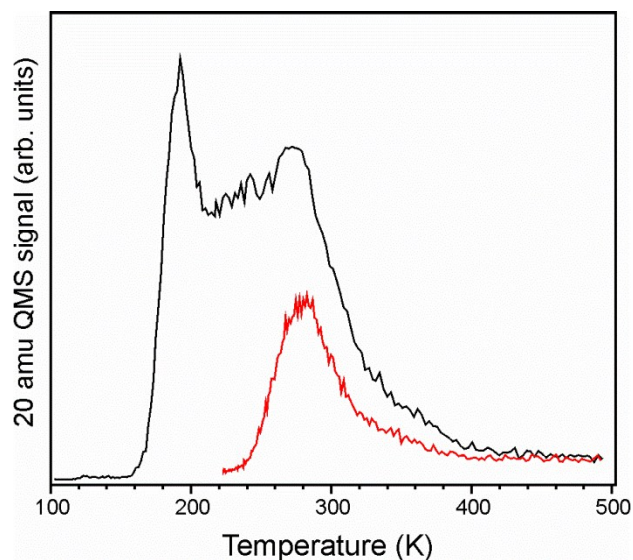


Figure S1. TPD spectra measured after IRAS experiments at 140 K (black line) and 250 K (red line) which show a similar desorption profiles as obtained in the TPD setup (Fig. 1 in the main text). Some deviation in the temperature readings originates from instrumental differences in the sample holders and thermocouples used in the two setups. In addition, the QMS used here had no differential pumping stage.

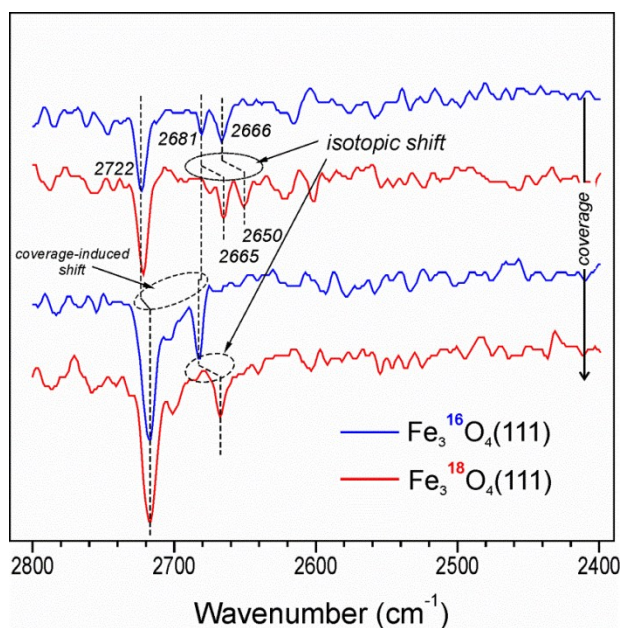


Figure S2. Selected IRA spectra of D₂O at low coverages adsorbed on Fe₃O₄(111) films prepared with ¹⁶O and ¹⁸O as indicated. It is clear that all the bands below 2700 cm⁻¹ exhibit isotopic effect.

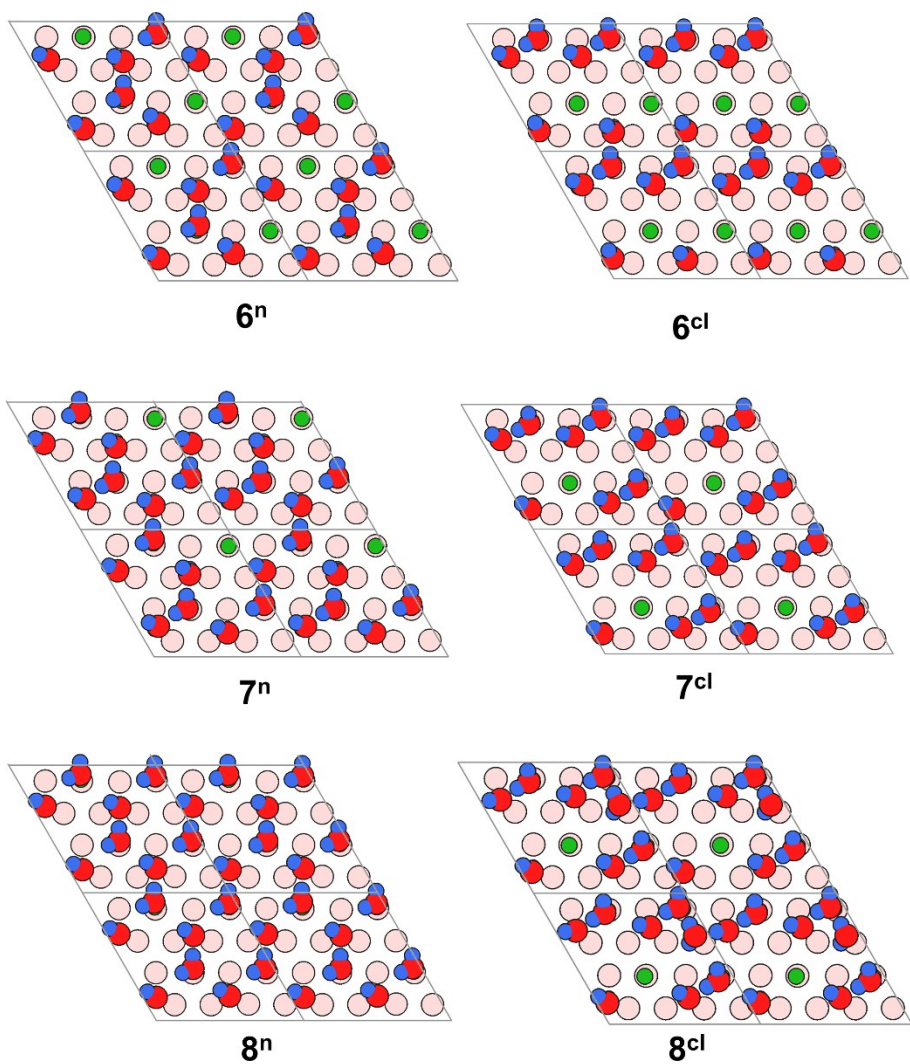


Figure S3. Top views of structures 6^n , 6^{cl} , 7^n , 7^{cl} , 8^n , and 8^{cl} . The (2x2) surface unit cells used for structure optimization are outlined.

Table S1. Scaled harmonic wavenumbers (in cm^{-1}) for stretching vibrations of terminal O_wD species in structures shown in Figures 9, 11, and 12.

	θ (ML)	$\nu(\text{Fe-O}_w\text{D})$	$\nu(\text{OD in non-diss. water})$	$\nu(\text{O}_s\text{D})$
1	0.25	2736		2699
2	0.5	2730, 2729		2698, 2697
2^{cl}	0.5	2735	2732	
3	0.75	2740,2737,2728		2704, 2698, 2694
3^{cl}	0.75	2731, 2730	2431 ^(p)	2710
4	1	2737,2735,2732,2731		2704,2703,2700, 2693
4^{cl}	1	2718, 2717	2713,2712	
5^{cl(1)}	1.25	2738, 2736, 2734, 2711		2714, 2700, 2699
5^{cl(2)}	1.25	2723, 2718, 2715	2711, 2708	2709
6ⁿ	1.5	2722, 2718, 2714, 2698	2713, 2678	2703, 2702
6^{cl}	1.5	2741, 2732, 2709, 2698	2426 ^(p)	2715
7ⁿ	1.75	2720, 2719, 2707, 2690	2714, 2693	2717
7^{cl}	1.75	2724, 2708, 2699, 2690	2715, 2702	2717
8ⁿ	2	2709, 2698, 2697 2685	2709, 2704, 2692, 2684	
8^{cl}	2	2723, 2709, 2689	2710, 2708, 2699	2712

^(p) Main component parallel to the surface.

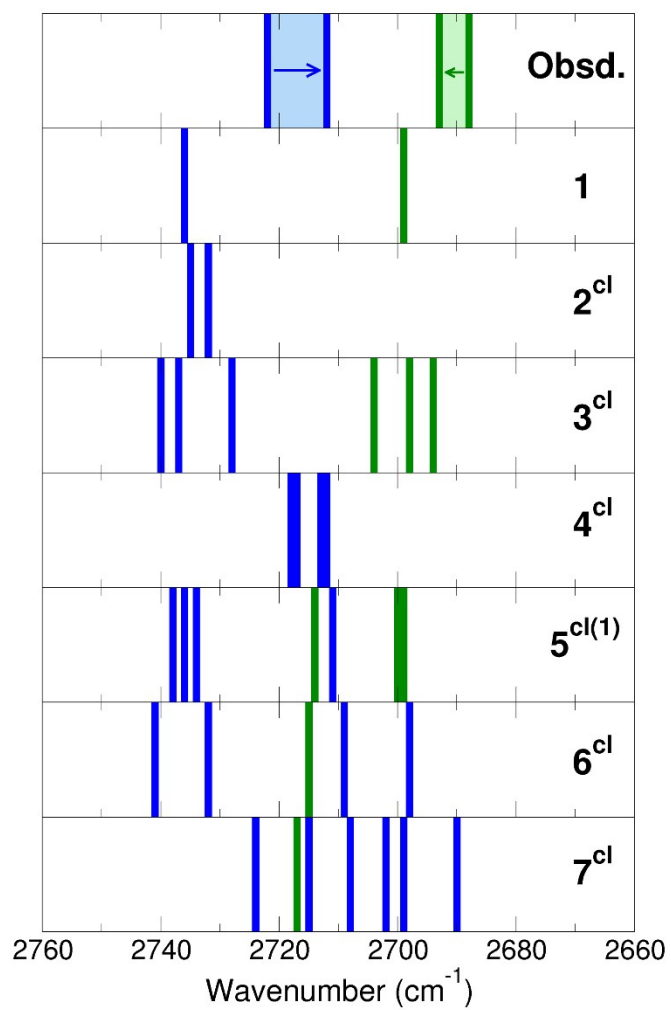


Figure S4. Stick representation of calculated wavenumbers (cm⁻¹) for the structures as indicated on the right-hand side. Topmost panel displays experimental results. Color code as in Fig. 13 of the main text.

Table S2. Total energies (PBE + U (=3.8)) of water structures adsorbed on a Fe₃O₄(111)-(2×2) slab model.

Structure	Total energy (eV)	Coordinates on page
H ₂ O (molecule)	-14.242	-
Fe ₄₈ O ₆₄ (clean)	-752.072	S8 – S10
Fe ₄₈ O ₆₅ H ₂ (monomer, 1)	-767,595	S10 – S12
Fe ₄₈ O ₆₆ H ₄ (dimer, 2^{cl})	-782.706	S12 – S14
Fe ₄₈ O ₇₀ H ₁₂ (6^{cl})	-843.013	S14 – S17
Fe ₄₈ O ₇₀ H ₁₂ (6ⁿ)	-842.819	S17 – S19
Fe ₄₈ O ₇₁ H ₁₄ (7^{cl})	-857.840	S19 – S22
Fe ₄₈ O ₇₁ H ₁₄ (7ⁿ)	-858.027	S22 – S24

Table S3 Dispersion effects after Grimme^a (D2-approach). Total energy contributions, contribution per water molecule, as well as total adsorption energies including dispersion calculated at PBE+U structures.

	θ	$\Delta D2^{\text{tot}}$	$\Delta D2/\text{per}$	$\Delta E^{\text{ads}+\text{D2}}^{\text{b}}$
1	0.25	-14.0	-14.0	-137.6
2	0.5	-24.2	-12.1	-124.2
2^{cl}	0.5	-31.6	-15.8	-135.3
3	0.75	-33.3	-11.1	-115.4
3^{cl}	0.75	-43.4	-14.5	-143.4
4	1	-44.4	-11.1	-122.4
4^{cl}	1	-56.7	-14.2	-148.9
5^{cl(1)}	1.25	-62.4	-12.5	-145.9
5^{cl(2)}	1.25	-66.1	-13.2	-150.0
6ⁿ	1.5	-78,2	-13.0	-163.3
6^{cl}	1.5	-82,3	-13.7	-170.6
7ⁿ	1.75	-96,2	-13.7	-182.5
7^{cl}	1.75	-98,0	-14.0	-181.7
8ⁿ	2	-112,0	-14.0	-197.8
8^{cl}	2	-111,1	-13.9	-191.6

^a Ref. [1].; ^b PBE+U+D2//PBE+U.

References

- [1] S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787.

Atomic Coordinates of Optimized Structures

(VASP POSCAR format)

Clean Surface

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12.0327997207999999 0.0000000000000000 0.0000000000000000
-6.0163998604000000 10.4207102367999997 0.0000000000000000
0.0000000000000000 0.0000000000000000 19.2106990814000014
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Fe O
48 64

Selective dynamics

Direct

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Fe O H
48 65 2

Selective dynamics

Direct

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0.1025258907731181	0.2065079366455881	0.1868154125888428	T	T	T
0.4368451929202295	0.3716831277483316	0.4328908311301437	T	T	T
0.1842399980000025	0.1273099929999972	0.0650599969999988	F	F	F
0.0156761167338095	0.2946109163210058	0.3174255544902623	T	T	T
0.4430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.2783149649059726	0.2927297863093921	0.3167052582101764	T	T	T
0.4371800119999989	0.8743600250000014	0.0673199969999985	F	F	F
0.2692079157089157	0.5379314173513693	0.3218011996868664	T	T	T
0.3641313760002076	0.7138835653740473	0.1918356009530531	T	T	T
0.1856879217368532	0.8684788244155305	0.4337997210641380	T	T	T
0.3644124711200322	0.9605577373580000	0.1920711166024020	T	T	T
0.1867546189550325	0.6236326145170964	0.4343182266261890	T	T	T
0.0967151092801647	0.9537521026569928	0.1890625729600882	T	T	T
0.4267168709831755	0.6196130064424309	0.4372559308496077	T	T	T
0.1842399980000025	0.8684700129999996	0.0650599969999988	F	F	F
0.0164875411146669	0.5297848822227798	0.3163796326836022	T	T	T
0.1030766457027541	0.7068175250191968	0.1866267196991842	T	T	T
0.4345617440275437	0.8703384687877260	0.4360337880440922	T	T	T
0.1842399980000025	0.6273099779999995	0.0650599969999988	F	F	F
0.0161233184781227	0.7945150441990412	0.3160588214026051	T	T	T
0.4430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.2794703343591606	0.7933655013774762	0.3162466186873528	T	T	T
0.9371799830000000	0.3743599949999989	0.0673199969999985	F	F	F
0.7706734394104728	0.0391021885888416	0.3219620683603734	T	T	T
0.8644692312793251	0.2145108442116373	0.1916572634395179	T	T	T
0.6932434174689501	0.3817164209132264	0.4382058164983198	T	T	T
0.8647326927638620	0.4603556344258650	0.1919478556775788	T	T	T
0.6889314707124217	0.1160202124913714	0.4372836208982963	T	T	T
0.5969548796513230	0.4536215881587629	0.1895583473958302	T	T	T
0.9286867609023086	0.1177383345317011	0.4382252323076347	T	T	T
0.6842399840000013	0.3684700129999996	0.0650599969999988	F	F	F

0.5140682646929420	0.0264327588201786	0.3188489752941118	T	T	T
0.6022257156186571	0.2058797286180531	0.1869779190259859	T	T	T
0.9359488907680532	0.3721953596168949	0.4327495035793798	T	T	T
0.6842399840000013	0.1273099929999972	0.0650599969999988	F	F	F
0.5161430411237646	0.2941344461798311	0.3175743519032970	T	T	T
0.9430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.7779323415045986	0.2924286783005186	0.3160409973396203	T	T	T
0.9371799830000000	0.8743600250000014	0.0673199969999985	F	F	F
0.7719485252685803	0.5396915454806182	0.3229124997583718	T	T	T
0.8644079214942654	0.7143752496873366	0.1916854805681814	T	T	T
0.6888288775334066	0.8791404951771933	0.4371303594300200	T	T	T
0.8647486792451130	0.9603449717370308	0.1918671975684467	T	T	T
0.6935259379776494	0.6180726305665241	0.4383091526140681	T	T	T
0.5966796155492740	0.9535827425580725	0.1896311987532268	T	T	T
0.9405494837340611	0.6239677419227407	0.4357940922533262	T	T	T
0.6842399840000013	0.8684700129999996	0.0650599969999988	F	F	F
0.5164214494475379	0.5296503140939391	0.3176421374767250	T	T	T
0.6021517831190933	0.7068055693330225	0.1870033146340020	T	T	T
0.9359445010290380	0.8705397754221248	0.4329686167924400	T	T	T
0.6842399840000013	0.6273099779999995	0.0650599969999988	F	F	F
0.5137734599364352	0.7951033633177377	0.3185931399261188	T	T	T
0.9430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.7780253241761430	0.7932448198016727	0.3160496960162438	T	T	T
0.1231563917565991	0.7113768142030884	0.5719975918561402	T	T	T
0.0811904220228850	0.7446993397577720	0.6016194442447440	T	T	T
0.4300397849681207	0.8671462158830259	0.4866683894140774	T	T	T

Dimer (2cl)

1.0000000000000000		
12.0327997207999999	0.0000000000000000	0.0000000000000000
-6.0163998604000000	10.4207102367999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.2106990814000014

Fe O H
48 66 4

Selective dynamics

Direct

0.2720399642737013	0.0418629315949996	0.2235424750622637	T	T	T
0.1042213393469531	0.2060739469286969	0.4552699109713028	T	T	T
0.2705200019999978	0.0410300010000029	0.0319599990000015	F	F	F
0.1014453446078415	0.2053587271345931	0.2891857031721701	T	T	T
0.1038500000000013	0.2076999989999990	0.0000000000000000	F	F	F
0.4346453661315219	0.3721097955789440	0.2570345044044542	T	T	T
0.0205199999999977	0.0410199980000030	0.1278599950000014	F	F	F
0.3512427836213699	0.2032932012415729	0.3893069853305629	T	T	T
0.0205199999999977	0.2910299899999984	0.1278599950000014	F	F	F
0.3511385782450355	0.4559749344908268	0.3892347241415141	T	T	T
0.2705200019999978	0.2910299899999984	0.1278599950000014	F	F	F
0.1035902031779880	0.4569328291716941	0.3879413267653339	T	T	T
0.2720063283676901	0.5406193486197522	0.2234826625534621	T	T	T
0.1035314726772387	0.7051700682942885	0.4747959023252863	T	T	T
0.2705200019999978	0.5410299899999984	0.0319599990000015	F	F	F
0.1014374032863451	0.7054470271215260	0.2878259757198633	T	T	T
0.1038500000000013	0.7077000139999967	0.0000000000000000	F	F	F
0.4342420864051260	0.8719989465316779	0.2555366042452486	T	T	T
0.0205199999999977	0.5410299899999984	0.1278599950000014	F	F	F

0.3474431077208492	0.6978092322767023	0.3847450208923381	T	T	T
0.0205199999999977	0.7910299899999984	0.1278599950000014	F	F	F
0.3468560805048272	0.9571985340902213	0.3848400814432738	T	T	T
0.2705200019999978	0.7910299899999984	0.1278599950000014	F	F	F
0.1034651697686842	0.9549276289873178	0.3877410345294920	T	T	T
0.7728231591061302	0.0417043199108574	0.2239424400290602	T	T	T
0.6026724734663309	0.2068535551106322	0.4528394800318135	T	T	T
0.7705100180000031	0.0410199980000030	0.0319599990000015	F	F	F
0.6011974608190959	0.2046199299314079	0.2895540738009592	T	T	T
0.6038500069999984	0.2076999989999990	0.0000000000000000	F	F	F
0.9333600605868200	0.3717122820862411	0.2564900897857183	T	T	T
0.5205100180000031	0.0410300010000029	0.1278599950000014	F	F	F
0.8526604416024480	0.2040557773482190	0.3889878522153393	T	T	T
0.5205100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.8539807649100314	0.4595557454797125	0.3885626243059574	T	T	T
0.7705100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.6061338935847068	0.4576407552685443	0.3884891365052017	T	T	T
0.7725374056983102	0.5415679435061723	0.2245924383291258	T	T	T
0.6022481323809449	0.7042828919320364	0.4545894037461081	T	T	T
0.7705100180000031	0.5410299899999984	0.0319599990000015	F	F	F
0.6012604047086846	0.7056655606149321	0.2895188674767029	T	T	T
0.6038500069999984	0.7077000139999967	0.0000000000000000	F	F	F
0.9333079646624806	0.8715905232433178	0.2564519608187553	T	T	T
0.5205100180000031	0.5410299899999984	0.1278599950000014	F	F	F
0.8535928137479678	0.7031986420715541	0.3885986765985149	T	T	T
0.5205100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.8525335181232244	0.9569695824097917	0.3891142955310392	T	T	T
0.7705100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.6098146342430186	0.9588696547493251	0.3861573190579789	T	T	T
0.4371800119999989	0.3743599949999989	0.0673199969999985	F	F	F
0.2694504828995513	0.0389987773514428	0.3219454238046857	T	T	T
0.3645232197504585	0.2150510560551720	0.1919373621625808	T	T	T
0.1895474612682624	0.3819951814965568	0.4379096796298536	T	T	T
0.3647391739134336	0.4601513338001173	0.1920746009779669	T	T	T
0.1897895530141345	0.1155068451945409	0.4382509328694429	T	T	T
0.0966446221669922	0.4537385719495614	0.1890444033943975	T	T	T
0.4261392261371356	0.1142082018579941	0.4376632523637016	T	T	T
0.1842399980000025	0.3684700129999996	0.0650599969999988	F	F	F
0.0158551508141386	0.0295138138477047	0.3172393726643368	T	T	T
0.1024703819450519	0.2066726227759429	0.1867060117614288	T	T	T
0.4363129450242196	0.3722035603965849	0.4326844805474216	T	T	T
0.1842399980000025	0.1273099929999972	0.0650599969999988	F	F	F
0.0157136077120510	0.2954476107557973	0.3170930509849122	T	T	T
0.4430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.2780960062313938	0.2933172302481188	0.3164932144420430	T	T	T
0.4371800119999989	0.8743600250000014	0.0673199969999985	F	F	F
0.2691715346425727	0.5389925576742717	0.3218384661422418	T	T	T
0.3642651143433666	0.7141904999589471	0.1917203430695456	T	T	T
0.1850189972155164	0.8689265112327985	0.4332651075122952	T	T	T
0.3644348160116178	0.9607505623804277	0.1919009515389569	T	T	T
0.1859910011419391	0.6244175116102696	0.4336899912848225	T	T	T
0.0966999071197055	0.9538512649998042	0.1890317515016951	T	T	T
0.4262895775023496	0.6197574384182112	0.4371665416016795	T	T	T
0.1842399980000025	0.8684700129999996	0.0650599969999988	F	F	F
0.0159284706296912	0.5305483195747643	0.3162529637140158	T	T	T
0.1029196577698511	0.7069539368938287	0.1863879344782066	T	T	T
0.4337507650065914	0.8708768903573000	0.4357954213592279	T	T	T

0.1842399980000025	0.6273099779999995	0.0650599969999988	F	F	F
0.0157635043605221	0.7947445391371576	0.3159879298379711	T	T	T
0.4430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.2790233338647221	0.7938987236569164	0.3156149254350376	T	T	T
0.9371799830000000	0.3743599949999989	0.0673199969999985	F	F	F
0.7698658172806364	0.0393337432976715	0.3222279628769488	T	T	T
0.8644014087033064	0.2146255188349608	0.1916995970962987	T	T	T
0.6930132725223954	0.3826718880194658	0.4379960989553006	T	T	T
0.8645020334298690	0.4606321802621862	0.1918095389890252	T	T	T
0.6891755640589027	0.1174178157576023	0.4374006259435435	T	T	T
0.5968401123221025	0.4538050005791774	0.1895300811203338	T	T	T
0.9285779710853669	0.1185286446544825	0.4379111358016170	T	T	T
0.6842399840000013	0.3684700129999996	0.0650599969999988	F	F	F
0.5140558748701737	0.0273371541318608	0.3185759351191916	T	T	T
0.6022141743172056	0.2061557084762700	0.1869211866338265	T	T	T
0.9359361351726456	0.3731334416218203	0.4322676762648187	T	T	T
0.6842399840000013	0.1273099929999972	0.0650599969999988	F	F	F
0.5159533065092162	0.2947918181777690	0.3175027571972294	T	T	T
0.9430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.7778569425309025	0.2934087685546153	0.3158964283995830	T	T	T
0.9371799830000000	0.8743600250000014	0.0673199969999985	F	F	F
0.7717013615415532	0.5405196457552107	0.3229104988444597	T	T	T
0.8643083482245409	0.7145095787688152	0.1916492710472560	T	T	T
0.6892746857833872	0.8800255328935236	0.4374531355510911	T	T	T
0.8645562878472570	0.9605466716988522	0.1918450000393503	T	T	T
0.6929052322987685	0.6191185783672736	0.4383414084735310	T	T	T
0.5966749056716356	0.9537648104035299	0.1895579074886020	T	T	T
0.9390536217535695	0.6241034062332238	0.4364799802293525	T	T	T
0.6842399840000013	0.8684700129999996	0.0650599969999988	F	F	F
0.5161917486461601	0.5302095758805211	0.3175019259354432	T	T	T
0.6022184429469615	0.7069711144685901	0.1869265289487481	T	T	T
0.9360862017187428	0.8714548965178884	0.4325522749458574	T	T	T
0.6842399840000013	0.6273099779999995	0.0650599969999988	F	F	F
0.5139407190265424	0.7954959601732684	0.3184076931456175	T	T	T
0.9430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.7778548116594649	0.7935085954931242	0.3159965452598696	T	T	T
0.1362618919959175	0.7182635605476356	0.5709746655588889	T	T	T
0.3893179368046986	0.8430900883213145	0.5676890974475364	T	T	T
0.2929559389570552	0.7967996336895230	0.5756196498293383	T	T	T
0.0862092063615501	0.7390034614224124	0.6024687124378320	T	T	T
0.4214712396677793	0.8641198706167804	0.4894376272336504	T	T	T
0.4243732116010481	0.9225435951147050	0.5939506490549540	T	T	T

Structure 6cl

1.0000000000000000		
12.0327997207999999	0.0000000000000000	0.0000000000000000
-6.0163998604000000	10.4207102367999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.2106990814000014

Fe O H

48 70 12

Selective dynamics

Direct

0.2719350921454788	0.0430925034504271	0.2209100643705919	T	T	T
0.1003642924337085	0.2017153068838725	0.4724741454738594	T	T	T
0.2705200019999978	0.0410300010000029	0.0319599990000015	F	F	F

0.1024367175233448	0.2041236185936336	0.2917871437422758	T	T	T
0.1038500000000013	0.2076999989999990	0.0000000000000000	F	F	F
0.4407960758932495	0.3772866006811184	0.2595142565958636	T	T	T
0.0205199999999977	0.0410199980000030	0.1278599950000014	F	F	F
0.3504241907312534	0.2007628147365186	0.3838877906624764	T	T	T
0.0205199999999977	0.2910299899999984	0.1278599950000014	F	F	F
0.3514148494387832	0.4607505222081750	0.3883932984854734	T	T	T
0.2705200019999978	0.2910299899999984	0.1278599950000014	F	F	F
0.1107910497056455	0.4602615418317720	0.3869950892666129	T	T	T
0.2714293048034666	0.5412544977947173	0.2237236070483452	T	T	T
0.1105278318666141	0.7114391502055876	0.4746425941812455	T	T	T
0.2705200019999978	0.5410299899999984	0.0319599990000015	F	F	F
0.1018924042674648	0.7055930339312551	0.2898208980101006	T	T	T
0.1038500000000013	0.7077000139999967	0.0000000000000000	F	F	F
0.4348353490745009	0.8721049056896517	0.2531677557097580	T	T	T
0.0205199999999977	0.5410299899999984	0.1278599950000014	F	F	F
0.3536127540080028	0.7038985903853893	0.3856479648556603	T	T	T
0.0205199999999977	0.7910299899999984	0.1278599950000014	F	F	F
0.3514382787003732	0.9573518774268087	0.3823085707569072	T	T	T
0.2705200019999978	0.7910299899999984	0.1278599950000014	F	F	F
0.1063418135797800	0.9569698037832242	0.3848449684790682	T	T	T
0.7706597729244786	0.0422346732216840	0.2208369567784908	T	T	T
0.5993585642523411	0.1984605517681906	0.4737109560357841	T	T	T
0.7705100180000031	0.0410199980000030	0.0319599990000015	F	F	F
0.6057200520550428	0.2048795024932164	0.2922911399099903	T	T	T
0.6038500069999984	0.2076999989999990	0.0000000000000000	F	F	F
0.9389674314329416	0.3755744715499542	0.2573873378820137	T	T	T
0.5205100180000031	0.0410300010000029	0.1278599950000014	F	F	F
0.8505499717090746	0.2010258980051664	0.3836193564632214	T	T	T
0.5205100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.8515527413162043	0.4604297651238338	0.3904765475702741	T	T	T
0.7705100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.6126466169390204	0.4593686046567981	0.3897251011660995	T	T	T
0.7717924786554043	0.5419312198112950	0.2253664070263310	T	T	T
0.6074910226318803	0.7117600608345707	0.4743734802227530	T	T	T
0.7705100180000031	0.5410299899999984	0.0319599990000015	F	F	F
0.6047266928414848	0.7073287697930004	0.2902415801851905	T	T	T
0.6038500069999984	0.7077000139999967	0.0000000000000000	F	F	F
0.9373322451986656	0.8729401495446547	0.2544558289208388	T	T	T
0.5205100180000031	0.5410299899999984	0.1278599950000014	F	F	F
0.8532508841527667	0.7018801083822667	0.3885984586264692	T	T	T
0.5205100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.8510799040041425	0.9567591756630888	0.3828051321312556	T	T	T
0.7705100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.6064364735606437	0.9573944412638714	0.3835008995575346	T	T	T
0.4371800119999989	0.3743599949999989	0.0673199969999985	F	F	F
0.2696055562150783	0.0406348191715611	0.3208771511915708	T	T	T
0.3594005585119440	0.2189924262512245	0.1898939288447509	T	T	T
0.1874355875478997	0.3733102024881994	0.4392815823900089	T	T	T
0.3580354895580918	0.4539003861641668	0.1895389789982904	T	T	T
0.1879255553856514	0.1228578017122818	0.4342373996850419	T	T	T
0.0990360707016093	0.4628145984392156	0.1928517610053232	T	T	T
0.4353765526996581	0.1224336383011438	0.4324008071620724	T	T	T
0.1842399980000025	0.3684700129999996	0.0650599969999988	F	F	F
0.0119439612793014	0.0214321634735410	0.3201850234901149	T	T	T
0.1068155292747467	0.2053296046480549	0.1833353451196034	T	T	T
0.4371201764593632	0.3735277338615948	0.4421247343891251	T	T	T

0.1842399980000025	0.1273099929999972	0.0650599969999988	F	F	F
0.0161542619945861	0.3033473279061780	0.3216517598992560	T	T	T
0.4430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.2896575828073574	0.3037991881930325	0.3220775519255052	T	T	T
0.4371800119999989	0.8743600250000014	0.0673199969999985	F	F	F
0.2718038677469537	0.5397537653216284	0.3244338945764904	T	T	T
0.3646774687905644	0.7110695768923582	0.1905209026553775	T	T	T
0.1893549246131766	0.8763663691077910	0.4340206271486376	T	T	T
0.3624985531562834	0.9649528369324146	0.1887218842318362	T	T	T
0.1894552785207726	0.6220584090077254	0.4373918326277342	T	T	T
0.1015953750047549	0.9551091410115178	0.1853370586603775	T	T	T
0.4368097267619429	0.6227206862083494	0.4390915112449360	T	T	T
0.1842399980000025	0.8684700129999996	0.0650599969999988	F	F	F
0.0157481145721273	0.5314800690531404	0.3224914540125218	T	T	T
0.0998197825929282	0.7067306965392759	0.1873764329776494	T	T	T
0.4365557087212407	0.8727832986124534	0.4373455947468627	T	T	T
0.1842399980000025	0.6273099779999995	0.0650599969999988	F	F	F
0.0139906483754391	0.7894316294128284	0.3224796001674503	T	T	T
0.4430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.2750300291626824	0.7891273426705556	0.3203679459602685	T	T	T
0.9371799830000000	0.3743599949999989	0.0673199969999985	F	F	F
0.7701253474582312	0.0401499623500439	0.3205680975705764	T	T	T
0.8515950223347697	0.2161091903555723	0.1929944478237334	T	T	T
0.6865883608331448	0.3713156723030647	0.4426141061601003	T	T	T
0.8620075006890326	0.4506275094155622	0.1892737825548101	T	T	T
0.6878590588147178	0.1219780490986604	0.4340543644083837	T	T	T
0.5893665590890724	0.4524687747246709	0.1884136612598974	T	T	T
0.9357775211155941	0.1226028332629531	0.4319888574677584	T	T	T
0.6842399840000013	0.3684700129999996	0.0650599969999988	F	F	F
0.5120818506341207	0.0222067836803192	0.3198189623436086	T	T	T
0.6036066906560670	0.2090326715553710	0.1825658300728956	T	T	T
0.9388425788577750	0.3728639679773987	0.4425651991279179	T	T	T
0.6842399840000013	0.1273099929999972	0.0650599969999988	F	F	F
0.5162739646102698	0.3035296747304524	0.3224224059404147	T	T	T
0.9430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.7897938529802109	0.3043917668103009	0.3236851968095327	T	T	T
0.9371799830000000	0.8743600250000014	0.0673199969999985	F	F	F
0.7718927140773267	0.5387511081416937	0.3299641664056058	T	T	T
0.8583225803861407	0.7196015218093071	0.1858577642067545	T	T	T
0.6885089007896098	0.8763066194340199	0.4334027041768987	T	T	T
0.8542537051388793	0.9554892400088757	0.1855674974951574	T	T	T
0.6876633516775185	0.6220582379620702	0.4398054654309253	T	T	T
0.6009101815097019	0.9546961177028122	0.1855433106805896	T	T	T
0.9385210939647576	0.6231546032846854	0.4423280229895729	T	T	T
0.6842399840000013	0.8684700129999996	0.0650599969999988	F	F	F
0.5170715740062294	0.5325006498474786	0.3211485929634275	T	T	T
0.6047574885162953	0.7069279486466928	0.1864259348839757	T	T	T
0.9364059578381639	0.8733899343188616	0.4388934221569880	T	T	T
0.6842399840000013	0.6273099779999995	0.0650599969999988	F	F	F
0.5153633542449273	0.7901258520507120	0.3212001006328637	T	T	T
0.9430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.7762983836711221	0.7894005585787631	0.3214492974893007	T	T	T
0.6434008536848935	0.7419850697706500	0.5698493926143751	T	T	T
0.9121956943243509	0.8926583797995343	0.5669901371650948	T	T	T
0.5709078856922932	0.1495050315128466	0.5681069667761353	T	T	T
0.0736604540071875	0.1610172814473388	0.5676118035980323	T	T	T
0.1544161084052005	0.7373726008275613	0.5696687444915929	T	T	T

0.4213904156914816	0.8828598541260372	0.5661943235429425	T	T	T
0.4357928740242182	0.3742497619489976	0.4927210529969741	T	T	T
0.4313611438725585	0.8751163899096683	0.4934544585730543	T	T	T
0.9283261344028995	0.8795660422517326	0.4942000320103253	T	T	T
0.5949033534636154	0.7746898729932373	0.5944605175483882	T	T	T
0.9400573204352709	0.3726183155349894	0.4931658984412711	T	T	T
0.8179891249713367	0.8511057338105815	0.5759246946145790	T	T	T
0.9547766864244519	0.9863385590626140	0.5765232212434157	T	T	T
0.5534396701711518	0.1991071782761231	0.6016801193746063	T	T	T
0.0758673780135640	0.2210410596151236	0.6020505222218784	T	T	T
0.1072993195526016	0.7662522577978876	0.5985137217089230	T	T	T
0.3272290998683789	0.8406144171029669	0.5759960233290994	T	T	T
0.4637652814342552	0.9769038729204632	0.5758272144707217	T	T	T

Structure 6n

1.0000000000000000		
12.0327997207999999	0.0000000000000000	0.0000000000000000
-6.0163998604000000	10.4207102367999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.2106990814000014

Fe O H
48 70 12

Selective dynamics

Direct

0.2694846935272310	0.0399977329269996	0.2232658362158078	T	T	T
0.1029917381830458	0.2062683906993190	0.4737284498265064	T	T	T
0.2705200019999978	0.0410300010000029	0.0319599990000015	F	F	F
0.1066301589285307	0.2095675917227251	0.2887591198354558	T	T	T
0.1038500000000013	0.2076999989999990	0.0000000000000000	F	F	F
0.4399804330717360	0.3789479337843061	0.2562086054057871	T	T	T
0.0205199999999977	0.0410199980000030	0.1278599950000014	F	F	F
0.3522867309832087	0.2046020322741048	0.3873307019513225	T	T	T
0.0205199999999977	0.2910299899999984	0.1278599950000014	F	F	F
0.3526026226335925	0.4622083542210567	0.3868211803185037	T	T	T
0.2705200019999978	0.2910299899999984	0.1278599950000014	F	F	F
0.1073836264272572	0.4590337159764009	0.3860927874301090	T	T	T
0.2696843253504446	0.5415755171721826	0.2234613205192478	T	T	T
0.1062376471929039	0.7086684388528331	0.4748194895484100	T	T	T
0.2705200019999978	0.5410299899999984	0.0319599990000015	F	F	F
0.1023160217515075	0.7035952000598165	0.2920809764849309	T	T	T
0.1038500000000013	0.7077000139999967	0.0000000000000000	F	F	F
0.4389652985196223	0.8791997345207330	0.2577623067849567	T	T	T
0.0205199999999977	0.5410299899999984	0.1278599950000014	F	F	F
0.3517270345777045	0.7052216730768736	0.3850967001396547	T	T	T
0.0205199999999977	0.7910299899999984	0.1278599950000014	F	F	F
0.3508730554608659	0.9627529111553162	0.3858000941012725	T	T	T
0.2705200019999978	0.7910299899999984	0.1278599950000014	F	F	F
0.1089912723559112	0.9605244935633191	0.3870990973408667	T	T	T
0.7683532736342323	0.0384830087276997	0.2226162212447134	T	T	T
0.6018151833253542	0.2108139180814691	0.4771241562946026	T	T	T
0.7705100180000031	0.0410199980000030	0.0319599990000015	F	F	F
0.6052088371878337	0.2122356347326835	0.2887586264366897	T	T	T
0.6038500069999984	0.2076999989999990	0.0000000000000000	F	F	F
0.9364834333308983	0.3707468076432229	0.2562257832400625	T	T	T
0.5205100180000031	0.0410300010000029	0.1278599950000014	F	F	F
0.8472825094704214	0.2010699715612351	0.3871742001228284	T	T	T
0.5205100180000031	0.2910299899999984	0.1278599950000014	F	F	F

0.8508814968311067	0.4623713331947669	0.3861964874211484	T	T	T
0.7705100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.6114023688658942	0.4637038016641706	0.3860140242235898	T	T	T
0.7700659161747463	0.5421569815999213	0.2226587592949249	T	T	T
0.6049565108666202	0.7101203393774056	0.4728411122099854	T	T	T
0.7705100180000031	0.5410299899999984	0.0319599990000015	F	F	F
0.6036187316953351	0.7125645284748315	0.2914294636871508	T	T	T
0.6038500069999984	0.7077000139999967	0.0000000000000000	F	F	F
0.9373543446492912	0.8744716959759512	0.2589781499517794	T	T	T
0.5205100180000031	0.5410299899999984	0.1278599950000014	F	F	F
0.8539972157792493	0.7054635642021954	0.3876543432708539	T	T	T
0.5205100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.8512256108984644	0.9621120617357060	0.3860966986779385	T	T	T
0.7705100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.6147070792094433	0.9680597515860555	0.3871969433472688	T	T	T
0.4371800119999989	0.3743599949999989	0.0673199969999985	F	F	F
0.2708178819598931	0.0433828821397676	0.3228418856565469	T	T	T
0.3553830533411546	0.2132139528901929	0.1895054431539905	T	T	T
0.1877929936903626	0.3755921952527894	0.4371498534116512	T	T	T
0.3480672903286386	0.4464253245755707	0.1925992451649832	T	T	T
0.1886908769084039	0.1248696875347242	0.4361899953690542	T	T	T
0.0978698044485202	0.4617924105624150	0.1921865974314642	T	T	T
0.4340944184042386	0.1248675775461968	0.4363930305176919	T	T	T
0.1842399980000025	0.3684700129999996	0.0650599969999988	F	F	F
0.0179938162266928	0.0342466680606054	0.3177557535079098	T	T	T
0.1046464372329366	0.2043081071001984	0.1869721342064358	T	T	T
0.4380219549827072	0.3764965362817418	0.4399274196202855	T	T	T
0.1842399980000025	0.1273099929999972	0.0650599969999988	F	F	F
0.0218186466539630	0.2994154001752560	0.3166279229557232	T	T	T
0.4430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.2816366188417777	0.2959020531122344	0.3201867271083495	T	T	T
0.4371800119999989	0.8743600250000014	0.0673199969999985	F	F	F
0.2718023225979752	0.5423748783845097	0.3233149431187244	T	T	T
0.3575232233036701	0.7162518658336789	0.1901701112515624	T	T	T
0.1888180581741678	0.8773467518731034	0.4365082449789240	T	T	T
0.3493349605723893	0.9474120066688531	0.1924459161502169	T	T	T
0.1882323744515278	0.6240284798507110	0.4347491253253238	T	T	T
0.0968698945036124	0.9552462102610525	0.1888414801463465	T	T	T
0.4366191667884049	0.6258313117133784	0.4364824612572016	T	T	T
0.1842399980000025	0.8684700129999996	0.0650599969999988	F	F	F
0.0097427994711221	0.5202508441118758	0.3212325272982190	T	T	T
0.1027218233722320	0.7078157453297368	0.1826374856966032	T	T	T
0.4372481363102645	0.8773571241021416	0.4406861546233241	T	T	T
0.1842399980000025	0.6273099779999995	0.0650599969999988	F	F	F
0.0171116584345570	0.8042790815198111	0.3212850348390358	T	T	T
0.4430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.2880623444876493	0.8037720764942924	0.3219070205700799	T	T	T
0.9371799830000000	0.3743599949999989	0.0673199969999985	F	F	F
0.7670998584058355	0.0346890335294835	0.3208647011558796	T	T	T
0.8492048499290243	0.2121492682722790	0.1923172899293658	T	T	T
0.6870154874840271	0.3767855111594071	0.4360590044076332	T	T	T
0.8608891919377186	0.4492975006491452	0.1881789031210162	T	T	T
0.6779255394601184	0.1213431051293828	0.4397526008799809	T	T	T
0.5891711604702418	0.4424918639796824	0.1906706174279399	T	T	T
0.9393914006357764	0.1230466411419701	0.4345291473251731	T	T	T
0.6842399840000013	0.3684700129999996	0.0650599969999988	F	F	F
0.5170304863578727	0.0363760650274015	0.3183512164529457	T	T	T

0.6036758630259706	0.2094590647084120	0.1872630192018126	T	T	T
0.9387390112272513	0.3789872095684134	0.4421009696220417	T	T	T
0.6842399840000013	0.1273099929999972	0.0650599969999988	F	F	F
0.5134688353278324	0.2956017048150467	0.3197066448452309	T	T	T
0.9430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.7790209640233861	0.2975075637271239	0.3190728226759045	T	T	T
0.9371799830000000	0.8743600250000014	0.0673199969999985	F	F	F
0.7728397882282668	0.5453891307201993	0.3268759727467233	T	T	T
0.8633905308003452	0.7251769388017981	0.1894500358402908	T	T	T
0.6888400678577311	0.8782055327577845	0.4379227482192135	T	T	T
0.8601835912147452	0.9559117053334153	0.1889476686194784	T	T	T
0.6880823693762602	0.6265734417551060	0.4368889297297164	T	T	T
0.5950486701229177	0.9469497216455636	0.1922079266969141	T	T	T
0.9386676792770196	0.6263524545535090	0.4369082110261681	T	T	T
0.6842399840000013	0.8684700129999996	0.0650599969999988	F	F	F
0.5123174181978586	0.5250767291301963	0.3212163465014455	T	T	T
0.6057132963651746	0.7119128217187900	0.1832943727477150	T	T	T
0.9391416707567816	0.8783300232358006	0.4397942329672478	T	T	T
0.6842399840000013	0.6273099779999995	0.0650599969999988	F	F	F
0.5106352184386590	0.8020521339392314	0.3221811530710509	T	T	T
0.9430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.7886807177039802	0.8010072629185349	0.3216321333279692	T	T	T
0.6089182417288886	0.6926883626350600	0.5711276764373543	T	T	T
0.9407223297559558	0.9101640108700919	0.5713757626887671	T	T	T
0.4787360643517359	0.4302872891079260	0.5724222399436988	T	T	T
0.6049498992028949	0.2132546847452103	0.5728128868270721	T	T	T
0.0841761361832551	0.1726884451619293	0.5707098133758413	T	T	T
0.1156289108896546	0.7032535145650607	0.5701046454296643	T	T	T
0.4480622583655262	0.3902510310257723	0.4927659275230213	T	T	T
0.4362910788615463	0.8839034857866203	0.4911578116473745	T	T	T
0.9394887687698116	0.8877689337921513	0.4936433665140941	T	T	T
0.5692599500246466	0.7297978893938695	0.5998639541849997	T	T	T
0.9371750478517226	0.3843548271454725	0.4925892011218460	T	T	T
0.8523069734864093	0.8735799981577859	0.5874101918537054	T	T	T
0.9861316332385471	0.0058180721057419	0.5783812351499763	T	T	T
0.4000449249603188	0.3985593696899897	0.5992593029396764	T	T	T
0.5271369610960617	0.5264266367755009	0.5780821740494726	T	T	T
0.5823222337529669	0.2714219791851697	0.5956761510387953	T	T	T
0.0500218858657996	0.2156146465769106	0.5990173070138014	T	T	T
0.0784143429191933	0.7441220780913838	0.5978059556090853	T	T	T

Structure 7cl

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1.0000000000000000
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Fe O H
48 71 14

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Selective dynamics

Direct

0.2724238210611911	0.0425979502770599	0.2241585146151871	T	T	T
0.0963518614335266	0.1997877111431386	0.4748956432154871	T	T	T
0.2705200019999978	0.0410300010000029	0.0319599990000015	F	F	F
0.1023986437640263	0.2051146894754952	0.2895171249868182	T	T	T
0.1038500000000013	0.2076999989999990	0.0000000000000000	F	F	F

0.4346017709075198	0.3729195982588571	0.2604372714784123	T	T	T
0.0205199999999977	0.0410199980000030	0.1278599950000014	F	F	F
0.3490674042312263	0.2016721494870405	0.3880500028564252	T	T	T
0.0205199999999977	0.2910299899999984	0.1278599950000014	F	F	F
0.3509142400852535	0.4605050437854346	0.3903140047539235	T	T	T
0.2705200019999978	0.2910299899999984	0.1278599950000014	F	F	F
0.1120519918375539	0.4579529634585679	0.3892236575517653	T	T	T
0.2723887290922897	0.5419694775078550	0.2236675667493025	T	T	T
0.1054328639426737	0.7071218950266708	0.4736841517328661	T	T	T
0.2705200019999978	0.5410299899999984	0.0319599990000015	F	F	F
0.1020592300343651	0.7064357333007714	0.2899169605001153	T	T	T
0.1038500000000013	0.7077000139999967	0.0000000000000000	F	F	F
0.4318201661248259	0.8729175517472996	0.2588067444830952	T	T	T
0.0205199999999977	0.5410299899999984	0.1278599950000014	F	F	F
0.3545085937192353	0.6961694764957527	0.3886131150490005	T	T	T
0.0205199999999977	0.7910299899999984	0.1278599950000014	F	F	F
0.3499629712134812	0.9583659750817280	0.3875229576326903	T	T	T
0.2705200019999978	0.7910299899999984	0.1278599950000014	F	F	F
0.1064779701027150	0.9583097952839896	0.3863149743214495	T	T	T
0.7693345170295561	0.0411955985706996	0.2208607907024761	T	T	T
0.6045085388518944	0.2059904877785071	0.4720045183778845	T	T	T
0.7705100180000031	0.0410199980000030	0.0319599990000015	F	F	F
0.6036021831606223	0.2078594990740526	0.2907053159122938	T	T	T
0.6038500069999984	0.2076999989999990	0.0000000000000000	F	F	F
0.9394082720394720	0.3759719754447644	0.2586325642470730	T	T	T
0.5205100180000031	0.0410300010000029	0.1278599950000014	F	F	F
0.8497691323239580	0.2005551033221542	0.3841432512892342	T	T	T
0.5205100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.8514477742281140	0.4599950643941951	0.3868172198959386	T	T	T
0.7705100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.6073036026181895	0.4603830252197649	0.3865031646631333	T	T	T
0.7696196871513771	0.5396967822936588	0.2230172525521952	T	T	T
0.6117013808983228	0.7131071408117358	0.4754604625528580	T	T	T
0.7705100180000031	0.5410299899999984	0.0319599990000015	F	F	F
0.6030308856417499	0.7081212192674372	0.2917084016690814	T	T	T
0.6038500069999984	0.7077000139999967	0.0000000000000000	F	F	F
0.9362958274347616	0.8718045024176388	0.2553380788514365	T	T	T
0.5205100180000031	0.5410299899999984	0.1278599950000014	F	F	F
0.8528129885477043	0.7040560492974318	0.3870540691403118	T	T	T
0.5205100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.8509377532016330	0.9569190448442065	0.3824316210962749	T	T	T
0.7705100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.6051228351708390	0.9569591205277338	0.3851086293263517	T	T	T
0.4371800119999989	0.3743599949999989	0.0673199969999985	F	F	F
0.2693174445793312	0.0395944087649970	0.3243536928122707	T	T	T
0.3638929856517981	0.2159181392064407	0.1934202621547971	T	T	T
0.1800227023591225	0.3687109757014343	0.4403935903518371	T	T	T
0.3611441625676285	0.4560720349072261	0.1925857807013645	T	T	T
0.1869397124068662	0.1215438008149218	0.4384929834442496	T	T	T
0.0958268360377442	0.4539134242913517	0.1902849974331289	T	T	T
0.4345745168302902	0.1218543498667472	0.4389169919050851	T	T	T
0.1842399980000025	0.3684700129999996	0.0650599969999988	F	F	F
0.0190590480767277	0.0333248977323222	0.3210604693086506	T	T	T
0.0956142093738008	0.2022718417873935	0.1881610251538019	T	T	T
0.4385905600887206	0.3698567693173210	0.4450120101940878	T	T	T
0.1842399980000025	0.1273099929999972	0.0650599969999988	F	F	F
0.0171333384914234	0.2972900891631168	0.3186179370202906	T	T	T

0.4430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.2761312331048070	0.2885691188935458	0.3191522749230872	T	T	T
0.4371800119999989	0.8743600250000014	0.0673199969999985	F	F	F
0.2668492071447652	0.5414403024176166	0.3222741435866957	T	T	T
0.3606497102752034	0.7158181231297395	0.1916063109525294	T	T	T
0.1873341822399482	0.8749974223005332	0.4372637720171843	T	T	T
0.3632942283528044	0.9601078378888604	0.1931427265327909	T	T	T
0.1876902061899685	0.6220382607940499	0.4368929382828943	T	T	T
0.0981495570144404	0.9546825603894716	0.1886648179574995	T	T	T
0.4435679263415732	0.6319155985399432	0.4424852554436708	T	T	T
0.1842399980000025	0.8684700129999996	0.0650599969999988	F	F	F
0.0152943554523421	0.5300816945995929	0.3198670053854237	T	T	T
0.0961618164271742	0.7050565391743027	0.1883873465918253	T	T	T
0.4343955002325016	0.8717369098765776	0.4398871331521114	T	T	T
0.1842399980000025	0.6273099779999995	0.0650599969999988	F	F	F
0.0184985690732830	0.7936296798533187	0.3228799453229567	T	T	T
0.4430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.2765328633488436	0.7955653943226757	0.3189936190101457	T	T	T
0.9371799830000000	0.3743599949999989	0.0673199969999985	F	F	F
0.7687424018303464	0.0398364768090620	0.3200670561532438	T	T	T
0.8579461604348256	0.2173710587595863	0.1902725198343314	T	T	T
0.6878691111860207	0.3738600409829864	0.4355272730354826	T	T	T
0.8578769547767022	0.4525172569861835	0.1906334617982187	T	T	T
0.6870742768935139	0.1228160486804909	0.4339219664449537	T	T	T
0.5953674565071883	0.4528174533580109	0.1908953548964339	T	T	T
0.9329604109496021	0.1216739881544153	0.4321955142296909	T	T	T
0.6842399840000013	0.3684700129999996	0.0650599969999988	F	F	F
0.5083184088635737	0.0231750813512735	0.3223491908498163	T	T	T
0.6076893215118986	0.2096080520629864	0.1831762096817132	T	T	T
0.9361761964698057	0.3720700759180783	0.4384159235827753	T	T	T
0.6842399840000013	0.1273099929999972	0.0650599969999988	F	F	F
0.5084679428607143	0.2960701634623342	0.3239541044535594	T	T	T
0.9430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.7887163734034491	0.2998575644306855	0.3195637973068254	T	T	T
0.9371799830000000	0.8743600250000014	0.0673199969999985	F	F	F
0.7713743358921035	0.5400840497994379	0.3229877949993366	T	T	T
0.8545649710443176	0.7088200470835372	0.1861879204747708	T	T	T
0.6887714364956905	0.8767861079892719	0.4327107914311450	T	T	T
0.8548880401511527	0.9561019975198364	0.1864136255081652	T	T	T
0.6897220352785194	0.6227574035919027	0.4377305003875391	T	T	T
0.5943252415918976	0.9533312013450135	0.1903795872481918	T	T	T
0.9362807939859443	0.6216971298188213	0.4381686996934878	T	T	T
0.6842399840000013	0.8684700129999996	0.0650599969999988	F	F	F
0.5143117293642738	0.5233024067364115	0.3228656946990410	T	T	T
0.6046802369230438	0.7085966577012438	0.1829574282427486	T	T	T
0.9373152953690709	0.8748216335717327	0.4391642103378466	T	T	T
0.6842399840000013	0.6273099779999995	0.0650599969999988	F	F	F
0.5081375380814623	0.7966084454745066	0.3206491618723088	T	T	T
0.9430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.7873891466961287	0.7952719479540717	0.3215307547891174	T	T	T
0.6512597943363451	0.7432648780717366	0.5708309198525071	T	T	T
0.9158567492373521	0.8957858056330810	0.5665492649342589	T	T	T
0.8942509678217605	0.3391985982210643	0.5717051455980950	T	T	T
0.6341562133068190	0.2111614911568797	0.5695326560040541	T	T	T
0.0627625198189599	0.1606834720068535	0.5702166189876327	T	T	T
0.1347177356048657	0.7171779650683198	0.5710523052949358	T	T	T
0.3959734160776565	0.8428840749169941	0.5733392744107417	T	T	T

0.4396258943919478	0.3699221035717004	0.4955724565540635	T	T	T
0.4249390283331766	0.8640582450183750	0.4931322539065686	T	T	T
0.9300477970094277	0.8822399603444113	0.4952487260091943	T	T	T
0.5950374917710077	0.7631837152209245	0.5978662771210302	T	T	T
0.9257187421292040	0.3635101701653115	0.4915973340993865	T	T	T
0.8215748955644039	0.8529173555148150	0.5762417852272876	T	T	T
0.9577145322861742	0.9903102098212037	0.5755251722090841	T	T	T
0.7978295113373745	0.2931602511631655	0.5770850639373041	T	T	T
0.9279491890938811	0.4213537776529170	0.5954117815464571	T	T	T
0.5949134431030312	0.2468163520315851	0.5996086532644221	T	T	T
0.0254910328980426	0.2062183808448741	0.5936429675593956	T	T	T
0.0977381666776297	0.7603555794038340	0.59701711133993127	T	T	T
0.2997129944204337	0.7978897899539356	0.5789940229180897	T	T	T
0.4307832778779403	0.9261153904951945	0.5959507822453352	T	T	T

Structure 7n

1.0000000000000000		
12.0327997207999999	0.0000000000000000	0.0000000000000000
-6.0163998604000000	10.4207102367999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.2106990814000014

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Selective dynamics

Direct

0.2690329882592519	0.0391245564185371	0.2237667270655909	T	T	T
0.1071458648463610	0.2123027041298851	0.4743971083715034	T	T	T
0.2705200019999978	0.0410300010000029	0.0319599990000015	F	F	F
0.1044596702449860	0.2075599959898287	0.2886024185801294	T	T	T
0.1038500000000013	0.2076999989999990	0.0000000000000000	F	F	F
0.4391600342345856	0.3768814510907538	0.2556346006595396	T	T	T
0.0205199999999977	0.0410199980000030	0.1278599950000014	F	F	F
0.3504413730578053	0.2028789446115419	0.3863002454476789	T	T	T
0.0205199999999977	0.2910299899999984	0.1278599950000014	F	F	F
0.3506537602525057	0.4600617099172497	0.3840571774294852	T	T	T
0.2705200019999978	0.2910299899999984	0.1278599950000014	F	F	F
0.1069209198891206	0.4609437859713130	0.3838362195172660	T	T	T
0.2696845368185800	0.5418466677633859	0.2223549850667522	T	T	T
0.1027886736156601	0.7063969212754443	0.4725639048117986	T	T	T
0.2705200019999978	0.5410299899999984	0.0319599990000015	F	F	F
0.1017997388199872	0.7047508070642557	0.2913637868426127	T	T	T
0.1038500000000013	0.7077000139999967	0.0000000000000000	F	F	F
0.4396817709422629	0.8792248398512498	0.2584200318629676	T	T	T
0.0205199999999977	0.5410299899999984	0.1278599950000014	F	F	F
0.3520254375094493	0.7059229984444749	0.3861921584583951	T	T	T
0.0205199999999977	0.7910299899999984	0.1278599950000014	F	F	F
0.3512269518461327	0.9600536218016743	0.3860805794601065	T	T	T
0.2705200019999978	0.7910299899999984	0.1278599950000014	F	F	F
0.1074735219554652	0.9605136033545464	0.3873765341059607	T	T	T
0.7678950716337561	0.0390531296020004	0.2246278563545367	T	T	T
0.6025062164640572	0.2061989805846075	0.4729826312526859	T	T	T
0.7705100180000031	0.0410199980000030	0.0319599990000015	F	F	F
0.6037945055795524	0.2094519847985616	0.2885593507027298	T	T	T
0.6038500069999984	0.2076999989999990	0.0000000000000000	F	F	F
0.9347469697866870	0.3702511064379490	0.2552327189643645	T	T	T

0.5205100180000031	0.0410300010000029	0.1278599950000014	F	F	F
0.8500678044757319	0.1995481797802944	0.3880581584154052	T	T	T
0.5205100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.8491150955768401	0.4602062218106837	0.3850132111248988	T	T	T
0.7705100180000031	0.2910299899999984	0.1278599950000014	F	F	F
0.6073486617550682	0.4605315768584535	0.3874150037545016	T	T	T
0.7697207432905940	0.5428520641904101	0.2223519635187604	T	T	T
0.5944793671638525	0.6976433409439721	0.4780895860378640	T	T	T
0.7705100180000031	0.5410299899999984	0.0319599990000015	F	F	F
0.6057319211481355	0.7094498896979959	0.2913557647104111	T	T	T
0.6038500069999984	0.7077000139999967	0.0000000000000000	F	F	F
0.9373219088215929	0.8765386302796860	0.2601185873079243	T	T	T
0.5205100180000031	0.5410299899999984	0.1278599950000014	F	F	F
0.8486106039292740	0.7024517685132674	0.3865893325295922	T	T	T
0.5205100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.8474117592921917	0.9593630711991351	0.3912011201062425	T	T	T
0.7705100180000031	0.7910299899999984	0.1278599950000014	F	F	F
0.6137734382382019	0.9541429332469558	0.3906672423292214	T	T	T
0.4371800119999989	0.3743599949999989	0.0673199969999985	F	F	F
0.2694445105711490	0.0407786834958229	0.3234760465824990	T	T	T
0.3552459495095948	0.2122097196031250	0.1892162671172530	T	T	T
0.1856624370817227	0.3754227541424344	0.4315288053944080	T	T	T
0.3482085186844101	0.4463013178966813	0.1921899959154350	T	T	T
0.1873877597641302	0.1243429785465829	0.4367212180025959	T	T	T
0.0969709382663503	0.4607695648548494	0.1923904303081964	T	T	T
0.4350964019244415	0.1241611502180649	0.4355903761674811	T	T	T
0.1842399980000025	0.3684700129999996	0.0650599969999988	F	F	F
0.0220710723328767	0.0351131252560374	0.3185234986569795	T	T	T
0.1041921148386988	0.2041792770020953	0.1869314171237025	T	T	T
0.4338280514924321	0.3725803202083450	0.4381906930746746	T	T	T
0.1842399980000025	0.1273099929999972	0.0650599969999988	F	F	F
0.0125432086908700	0.2924700111879127	0.3173434174000379	T	T	T
0.4430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.2797663595253939	0.2929503438500800	0.3181430249561857	T	T	T
0.4371800119999989	0.8743600250000014	0.0673199969999985	F	F	F
0.2693647876168409	0.5426530947680345	0.3216194293647119	T	T	T
0.3583127615383217	0.7167056693382272	0.1899205695332733	T	T	T
0.1879641683124134	0.8763421207605707	0.4383017739632332	T	T	T
0.3490729521462432	0.9468812903619518	0.1924282451297025	T	T	T
0.1855641473873094	0.6231563483896158	0.4345731954759290	T	T	T
0.0965288689111899	0.9549403504241275	0.1891527597008805	T	T	T
0.4314537904997566	0.6209991102992795	0.4345292504296709	T	T	T
0.1842399980000025	0.8684700129999996	0.0650599969999988	F	F	F
0.0081802198408460	0.5207724468384110	0.3196074036090146	T	T	T
0.1026309887047331	0.7076203637896787	0.1826190637500652	T	T	T
0.4370190814465513	0.8774314760038967	0.4407041538631035	T	T	T
0.1842399980000025	0.6273099779999995	0.0650599969999988	F	F	F
0.0147232987204461	0.8033360547778913	0.3225285801213896	T	T	T
0.4430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.2870327428661283	0.8022319535265516	0.3218618888933102	T	T	T
0.9371799830000000	0.3743599949999989	0.0673199969999985	F	F	F
0.7669466817485526	0.0423771635442439	0.3233778248764322	T	T	T
0.8478868396721992	0.2112908583888641	0.1919633686408829	T	T	T
0.6859107310885995	0.3740692747113128	0.4372248974647649	T	T	T
0.8597652129473443	0.4489786896802068	0.1880511683670583	T	T	T
0.6871049878657066	0.1227697522933697	0.4372937245213863	T	T	T
0.5890123810134443	0.4417365807883973	0.1907479504072334	T	T	T

0.9384668577702436	0.1299490901205127	0.4401183832888436	T	T	T
0.6842399840000013	0.3684700129999996	0.0650599969999988	F	F	F
0.5135580797934983	0.0352723412717530	0.3177811003326312	T	T	T
0.6035030850835891	0.2089845808277101	0.1870889873938748	T	T	T
0.9359545510204040	0.3739711024216666	0.4376326109893685	T	T	T
0.6842399840000013	0.1273099929999972	0.0650599969999988	F	F	F
0.5128497469087944	0.2938945284203216	0.3194350709901267	T	T	T
0.9430699939999982	0.1273099929999972	0.0650599969999988	F	F	F
0.7784635205772941	0.2954441254928256	0.3195373555997870	T	T	T
0.9371799830000000	0.8743600250000014	0.0673199969999985	F	F	F
0.7686554886105543	0.5421716121608746	0.3270293354745859	T	T	T
0.8636322418077961	0.7258783832323558	0.1899082118283265	T	T	T
0.6772480921414296	0.8663432879920052	0.4460171912764868	T	T	T
0.8597764732182701	0.9564289313976980	0.1899183950113206	T	T	T
0.6851340268302871	0.6229180214975747	0.4378238729194957	T	T	T
0.5953806203728264	0.9467635785092444	0.1927356231107574	T	T	T
0.9359725088297044	0.6239336057371345	0.4357290276840457	T	T	T
0.6842399840000013	0.8684700129999996	0.0650599969999988	F	F	F
0.5094234735126112	0.5230307120118406	0.3203134678435807	T	T	T
0.6070476194275468	0.7116739757649813	0.1831630974673102	T	T	T
0.9399844318080790	0.8723565350283601	0.4444152441158038	T	T	T
0.6842399840000013	0.6273099779999995	0.0650599969999988	F	F	F
0.5118331580293878	0.8009165320798863	0.3229656070909436	T	T	T
0.9430699939999982	0.6273099779999995	0.0650599969999988	F	F	F
0.7875398971753739	0.8008620016015180	0.3221134260845189	T	T	T
0.5648267748617534	0.6472528503247660	0.5723589198125648	T	T	T
0.4155326553171310	0.3835158528595075	0.5669896212042806	T	T	T
0.5927888243387490	0.1878172974178937	0.5710834487962916	T	T	T
0.1491253066286215	0.2400395622493561	0.5695876499924157	T	T	T
0.0904579499545545	0.6755609261461855	0.5700214031278615	T	T	T
0.9506383192923080	0.4128524786660119	0.5706232080453515	T	T	T
0.4560958372887559	0.9262191017171635	0.5736393929114396	T	T	T
0.4271323899958114	0.3751979431151355	0.4942550853690148	T	T	T
0.4415981032387224	0.8906185241739999	0.4936990112286161	T	T	T
0.9398573973087261	0.8697860294075542	0.4949521522651265	T	T	T
0.5459575632755236	0.6987487368162908	0.6039388895008874	T	T	T
0.9397786529396844	0.3836023313707687	0.4910520956191426	T	T	T
0.3213461444290295	0.3425125612422159	0.5764058605141530	T	T	T
0.4591663791449537	0.4777156945109949	0.5773574343469997	T	T	T
0.5511521192178168	0.2297456029833632	0.5938703968156728	T	T	T
0.1007193327651003	0.2688721183485685	0.5973804129710406	T	T	T
0.0524044058550240	0.7144256336861249	0.5985958561276351	T	T	T
0.8647499354121321	0.3800413065744954	0.5896905770268863	T	T	T
0.9981125546124707	0.5088550164255418	0.5766256455963505	T	T	T
0.3717437903383958	0.8941194268260279	0.5944439953601808	T	T	T
0.5035721540328729	0.0223794202138469	0.5793426626255734	T	T	T