

Supporting Information

Direct Coupling of Two Inert CO₂ Molecules to Form C–C Bond on Cu⁰ Atomic Interfaces of the Nitrogen–Doped Graphene-Supported Cu₄ Cluster

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Table S1. Cu-Cu bond lengths in the Cu₄/N₃GN catalyst

	1	2	3	4	5
Cu ₁ -Cu ₂	2.398	2.390	2.316	2.413	2.037
Cu ₁ -Cu ₃	2.399	2.389		2.404	2.577
Cu ₁ -Cu ₄	2.405		1.897	2.636	2.540
Cu ₂ -Cu ₄	2.396	2.408	2.368	2.290	2.415
Cu ₂ -Cu ₃	2.382	2.279		2.326	2.338
Cu ₃ -Cu ₄	2.399	2.375	1.461		2.372

Table S2. Bader charges of Cu in the Cu₄/N₃GN catalyst

	atom	Bader charge transfer (e)
1	Cu ₁	-0.57
	Cu ₂	-0.01
	Cu ₃	+0.00
	Cu ₄	+0.00
2	Cu ₁	-0.45
	Cu ₂	-0.05
	Cu ₃	-0.45
	Cu ₄	+0.17
3	Cu ₁	-0.48
	Cu ₂	+0.08
	Cu ₃	+0.06
	Cu ₄	-0.12
4	Cu ₁	-0.56
	Cu ₂	+0.02
	Cu ₃	+0.12
	Cu ₄	-0.13
5	Cu ₁	-0.60
	Cu ₂	-0.30
	Cu ₃	+0.01
	Cu ₄	+0.02

Table S3. Cu-O, C-O, and C-C bond lengths for adsorption of two CO₂

	coupling *CO ₂	isolating *CO ₂
Cu ₂ -O ₁	1.985	2.118
Cu ₄ -O ₂	1.971	2.093
Cu ₃ -O ₃	1.900	1.973
Cu ₃ -C ₁		2.192
Cu ₃ -C ₂		2.249
C ₁ -C ₂	1.552	
C ₁ -O ₁	1.287	1.266
C ₁ -O ₂	1.289	1.264
C ₂ -O ₃	1.321	1.193
C ₂ -O ₄	1.226	1.193

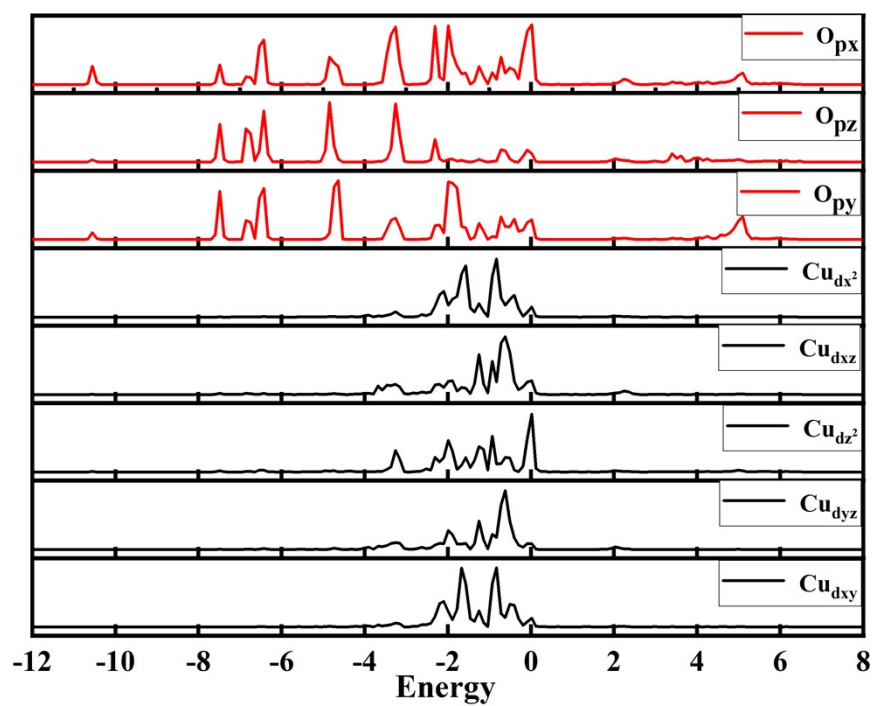
Table S4. Bader charges of free CO₂

	Bader charge transfer (e)
C	-2.10
O	1.05
O	1.04

Table S5. Bader charges of $^*\text{CO}_2+^*\text{CO}_2\rightarrow\text{TS1}\rightarrow^*\text{OOC}\text{COO}^*$

	atom	Bader charge transfer (e)
$^*\text{CO}_2+^*\text{CO}_2$	Cu ₁	-0.46
	Cu ₂	-0.25
	Cu ₃	-0.44
	Cu ₄	-0.25
	C ₁	-1.38
	O ₁	+1.08
	O ₂	+1.08
	C ₂	-1.61
	O ₃	+1.04
	O ₄	+1.06
TS1	Cu ₁	-0.47
	Cu ₂	-0.28
	Cu ₃	-0.39
	Cu ₄	-0.29
	C ₁	-1.47
	O ₁	+1.01
	O ₂	+1.11
	C ₂	-1.72
	O ₃	+1.07
	O ₄	+1.05
$^*\text{OOC}\text{COO}^*$	Cu ₁	-0.44
	Cu ₂	-0.30
	Cu ₃	-0.34
	Cu ₄	-0.31
	C ₁	-1.51
	O ₁	+1.12
	O ₂	+1.14
	C ₂	-1.60
	O ₃	+1.07
	O ₄	+1.11

Figure S1. pDOS of Cu₄/N₃GN adsorption-coupled CO₂



Coordinates for all structures

Adsorption CO₂

Structure01

top *CO₂

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999 12.8033199130999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O

4 9 63 2

Selective dynamics

Direct

0.3883999883824316 0.6109899878387068 0.1237199976883616 F F F

0.4263576239407567 0.5474738190662165 0.1985442450979715 T T T

0.2670471302641194 0.5538343853696647 0.2018633961853226 T T T

0.4321230452805908 0.7141980029482107 0.1981434693792862 T T T

0.3273999989159151 0.6724299788206594 0.0770300030666817 F F F

0.3273600042078257 0.4895400106801233 0.0762199982880674 F F F

0.5102499723826810 0.6724500060481091 0.0761599987757577 F F F

0.9996700287274507 0.0001800000324650 0.0573600009216477 F F F

0.0003299999634265 0.3344300090962307 0.0625099986649431 F F F

0.9996899962509573 0.6666100025562471 0.0586999989901287 F F F

0.3332400024166660 0.0001599999854633 0.0586900003380535 F F F

0.6654199958038518 0.9995099902101501 0.0625599995251847 F F F

0.6666899919723832 0.3331600129459886 0.0612300001087860 F F F

0.3321700096157301 0.3312500119332853 0.0634699985367249 F F F

0.6686199903697627 0.6676899790852886 0.0635500028781806 F F F

0.9991999865008054 0.1663299948336885 0.0593199990547291 F F F

0.0001500000141448 0.5002700090658863 0.0620899982600847 F F F

0.9999099969734431 0.8333100080615523 0.0571499988286135 F F F

0.3328500091896487 0.1653199940614059 0.0589599981996258 F F F

0.3319799900125986 0.8348799943726348 0.0628399997826108 F F F

0.6658499836809995 0.1663399934903538 0.0614599995434091 F F F

0.6657000184196491 0.4994199871907909 0.0623999982923920 F F F

0.6680499911019240 0.8350800275685089 0.0631899982792987 F F F

0.1665399968694743 0.9999399781380731 0.0571300014870246 F F F

0.1647700071264779 0.3318099975501880 0.0630899965588227 F F F

0.1649599969669993 0.6678699851318157 0.0628300011305356 F F F

0.4995799959066858 0.9996899962566772 0.0621200017787373 F F F

0.5004400015054742 0.3341600000654878 0.0623699985549493 F F F

0.8335300087518434 0.0006599999888621 0.0593699999149706 F F F

0.8335000276869380 0.3339900076717370 0.0614399984580416 F F F

0.8345299959310495 0.6670100092759697 0.0590099990224289 F F F

0.1655199974769772 0.1649699956211279 0.0588000007106046 F F F

0.1689099967855014 0.5010300278786701 0.0695900022914344 F F F

0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
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0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
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0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
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0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
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0.3825308647651620	0.5309151874415536	0.2778314712451781	T	T	T

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Structure02

bridge_1 *CO₂

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Cu	N	C	O
4	9	63	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4822203765113383	0.5975345127952001	0.1960390056950514	T	T	T
0.3011184077288275	0.5525686786157155	0.2008433497402076	T	T	T
0.4391346619897469	0.7326808206077019	0.1937054152811114	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
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0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
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0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.6341300207347729	0.7899104456327791	0.2322628232421513	T	T	T

0.6206813083023545	0.7002040860292090	0.2254721286069125	T	T	T
0.5802179545228394	0.8309327150276271	0.2214168883868043	T	T	T

Structure03

bridge_2 *CO₂

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-7.3920001983999999	12.8033199130999993	0.0000000000000000
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0.0000000000000000	0.0000000000000000	26.7110004425000014
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Cu	N	C	O
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4	9	63	2
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Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4364075533999533	0.5863636306467944	0.2041944210453363	T	T	T
0.2540604252755503	0.5583107747392347	0.1917155789935699	T	T	T
0.4047019336697154	0.7263775214784599	0.1937993020270143	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F

0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F

0.2098806839371564	0.6630792876389731	0.2046980423611053	T	T	T
0.1169978103616417	0.6366372208396635	0.2069188060611769	T	T	T
0.2922232051911843	0.7552416165351375	0.2083870903421970	T	T	T

Structure04

coupling 2*CO₂

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4219440486818910	0.5547522153667719	0.2038763826159971	T	T	T
0.2626138365440060	0.5584184169059828	0.1912656587350748	T	T	T
0.4293465988007806	0.7182224807812869	0.1984071614492052	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F

0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F

0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3557476400662427	0.6158820486624966	0.2803304365619118	T	T	T
0.2370335143260362	0.5620238295267281	0.2917485378645543	T	T	T
0.3964987989048830	0.5569850176505055	0.2767058069961230	T	T	T
0.4033613624782468	0.7146272850715478	0.2709550098945275	T	T	T
0.1809730989878906	0.5301498394310152	0.2502896859822238	T	T	T
0.2036424437726740	0.5524614299344457	0.3345754713435170	T	T	T

Structure05

isolating *CO₂

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4130632493383450	0.5404670479457077	0.1991811343395985	T	T	T
0.2537897738593287	0.5483782282608972	0.2120833744654479	T	T	T
0.4209896441899800	0.7074902778854264	0.1991783261762778	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F

0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F

0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3627751542427797	0.5994684373837431	0.2654256050762394	T	T	T
0.1083634201029452	0.4820485276278713	0.2359058856000218	T	T	T
0.3901710702524694	0.5338765571957554	0.2783010718968291	T	T	T
0.3997058658420994	0.6946057215195208	0.2778644595818222	T	T	T
0.1014817532874559	0.4770341815633291	0.1886418327368359	T	T	T
0.0586792694994209	0.4605463584714972	0.2740705975539928	T	T	T

CO₂ dimerization

Structure01

*CO₂+*CO₂

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4130632493383450	0.5404670479457077	0.1991811343395985	T	T	T
0.2537897738593287	0.5483782282608972	0.2120833744654479	T	T	T
0.4209896441899800	0.7074902778854264	0.1991783261762778	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F

0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F

0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3627751542427797	0.5994684373837431	0.2654256050762394	T	T	T
0.1083634201029452	0.4820485276278713	0.2359058856000218	T	T	T
0.3901710702524694	0.5338765571957554	0.2783010718968291	T	T	T
0.3997058658420994	0.6946057215195208	0.2778644595818222	T	T	T
0.1014817532874559	0.4770341815633291	0.1886418327368359	T	T	T
0.0586792694994209	0.4605463584714972	0.2740705975539928	T	T	T

Structure02

TS1

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387210	0.1237199976883616	F	F	F
0.4437601182100437	0.5579066858586401	0.1966699662415579	F	F	F
0.2898544608250617	0.5672253428407856	0.2056218852015377	F	F	F
0.4499852471488808	0.7248041598066877	0.1950994867346481	F	F	F
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801375	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.000329999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.000159999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101856	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141377	0.5002700090658863	0.0620899982600847	F	F	F

0.9999099969734573	0.8333100080615807	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726704	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871908052	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685231	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781381086	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066929	0.9996899962567127	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319563	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978258	0.8309299945801669	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178252	0.4998199939886305	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111918	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097657	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898967128	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116937123	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928238029	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610725	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F

0.5538799763018645	0.4459800124308231	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346234	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669572	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725294069	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777516	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137766	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620820	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147560309	0.0582900010185554	F	F	F
0.3797151105396921	0.6165647666226590	0.2683879413302606	T	T	T
0.2079003005197819	0.5376565749846804	0.2723896381117470	T	T	T
0.4152520047169119	0.5573292322294208	0.2807407331367386	T	T	T
0.4229849988294987	0.7154558331090541	0.2748137446142707	T	T	T
0.1414365836324620	0.5030840951580302	0.2364916953614937	T	T	T
0.1958760278762881	0.5372449102603768	0.3174449834473679	T	T	T

Structure03

*OCCO*O*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4219440486818910	0.5547522153667719	0.2038763826159971	T	T	T
0.2626138365440060	0.5584184169059828	0.1912656587350748	T	T	T
0.4293465988007806	0.7182224807812869	0.1984071614492052	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F

0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F

0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3557476400662427	0.6158820486624966	0.2803304365619118	T	T	T
0.2370335143260362	0.5620238295267281	0.2917485378645543	T	T	T
0.3964987989048830	0.5569850176505055	0.2767058069961230	T	T	T
0.4033613624782468	0.7146272850715478	0.2709550098945275	T	T	T
0.1809730989878906	0.5301498394310152	0.2502896859822238	T	T	T
0.2036424437726740	0.5524614299344457	0.3345754713435170	T	T	T

Structure04

*COOH+*CO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4194435754205023	0.5699419560612911	0.2037902427895011	T	T	T
0.2491401905902602	0.5743747468857173	0.1971328957503611	T	T	T
0.4258965216696888	0.7303776783533019	0.1927621871198655	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F

0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F

0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2512913469874277	0.7083657963829614	0.2030720509774867	T	T	T
0.1682652591796102	0.4398806584497523	0.2176490469425374	T	T	T
0.1641422988813062	0.7163056247206658	0.2022188663724570	T	T	T
0.3369114664149034	0.7937841949308904	0.2087195677416377	T	T	T
0.1185112183437692	0.3546425180885628	0.2315548725629460	T	T	T
0.1864688670402007	0.7912625211492346	0.2059464258464727	T	T	T

Structure05

TS2

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O H

4 9 64 3 1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387077	0.1237199976883616	F	F	F
0.4518971469782195	0.5923770422226484	0.2007220966570020	T	T	T
0.2674350215855189	0.5407983721852475	0.1931805678975612	T	T	T
0.4023312067743161	0.7212075299707955	0.1943196812184122	T	T	T
0.3273999989159152	0.6724299788206597	0.0770300030666817	F	F	F

0.3273600042078258	0.4895400106801239	0.0762199982880674	F	F	F
0.5102499723826811	0.6724500060481094	0.0761599987757577	F	F	F
0.9996700286598070	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634263	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562472	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101511	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332855	0.0634699985367248	F	F	F
0.6686199903697628	0.6676899790852888	0.0635500028781806	F	F	F
0.9991999865008060	0.1663299948336886	0.0593199990547290	F	F	F
0.0001500000141445	0.5002700090658865	0.0620899982600846	F	F	F
0.9999099969734440	0.8333100080615534	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726359	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907915	0.0623999982923919	F	F	F
0.6680499911019241	0.8350800275685100	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380742	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501881	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066861	0.9996899962566783	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654880	0.0623699985549493	F	F	F
0.8335300088194800	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310500	0.6670100092759701	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211280	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786706	0.0695900022914344	F	F	F
0.1661600023717328	0.8336899876319361	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978191	0.8309299945801396	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178185	0.4998199939886169	0.0600900016626156	F	F	F
0.8348900079967697	0.8343399763111574	0.0588699989124350	F	F	F
0.0547900013529557	0.1105799972670668	0.0582499988478275	F	F	F
0.0574500001527696	0.4450300037547384	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364286	0.0577500015516321	F	F	F
0.3890799879994377	0.1110199987696633	0.0590200014557141	F	F	F
0.3847500086142550	0.4413599968097520	0.0698899999278808	F	F	F
0.3856300115637483	0.7774099707386032	0.0697999968969185	F	F	F
0.7216899990961426	0.1110199987696633	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195367	0.0617300011113215	F	F	F

0.0548500008969129	0.2779600024177144	0.0611100010467140	F	F	F
0.0548699982635698	0.6113299727824151	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966854	0.0569700002542319	F	F	F
0.3894000053534442	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536159	0.9449700116936779	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081721	0.0612899996210956	F	F	F
0.7228400111134907	0.6104599833518950	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237756	0.0611900016818296	F	F	F
0.2224700004002289	0.1112700029890165	0.0579399988155273	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610869	0.7781400084212831	0.0611599981631770	F	F	F
0.5554500222519395	0.1106600016727201	0.0609599985034350	F	F	F
0.5538799763018651	0.4459800124308094	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346168	0.1112200022076310	0.0597000010326383	F	F	F
0.8891900181671419	0.4444000124669506	0.0609400011618462	F	F	F
0.8885800242332567	0.7773900031831716	0.0579899996383304	F	F	F
0.2204699963058162	0.2759700119173589	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952091	0.0697799995553297	F	F	F
0.2220399975825631	0.9445899725293796	0.0577399991557783	F	F	F
0.5561599731237840	0.2784900069045197	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777312	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137421	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197190	0.6107800006620758	0.0590399987973029	F	F	F
0.8892800212255745	0.9450600147559964	0.0582900010185554	F	F	F
0.2120288951984161	0.6956400733089452	0.2246478788902254	T	T	T
0.1373183703388037	0.5186518937677744	0.2130369630257955	T	T	T
0.1494332207370978	0.7281810877394075	0.2431380499186550	T	T	T
0.3077881256752899	0.7666655336248981	0.2185892020863577	T	T	T
0.0472809218436042	0.4711466936633407	0.2209013741665392	T	T	T
0.1913717391142257	0.8054791742113288	0.2482744945118217	T	T	T

Structure06

*COCOOH

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999 12.8033199130999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O H

4 9 64 3 1

Selective dynamics

Direct

0.3883999883824316 0.6109899878387068 0.1237199976883616 F F F

0.4392763547480729	0.5871994149137666	0.2029226725689758	T	T	T
0.2549012784927376	0.5458141485975589	0.1921547915995275	T	T	T
0.3955564715646387	0.7199252836255121	0.1935084037277833	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F

0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2088287830413699	0.7003187949977605	0.2303902374282455	T	T	T
0.1537691786619513	0.5862454691995360	0.2089870368740852	T	T	T
0.1482721773847495	0.7251563785214857	0.2573880307082777	T	T	T
0.3045348490384225	0.7649918373858182	0.2258485648841843	T	T	T
0.0596701366558077	0.5453396633676229	0.2003968774719356	T	T	T
0.1924655303617271	0.7957854727406499	0.2709554667151666	T	T	T

Structure07

*CO+CO

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999 12.8033199130999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.3638925409506603	0.5125976375899015	0.1977741039769680	T	T	T
0.3151486538953924	0.6421226622622641	0.2007716926592291	T	T	T
0.4951503331375004	0.7024050506691387	0.1943721553173900	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F

0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2359551044404608	0.6804506305026675	0.2354967805960252	T	T	T
-0.0639337260118251	0.5544420656126509	0.2553012964990847	T	T	T
0.1883745436856193	0.7064626983966146	0.2602060994290081	T	T	T
-0.0587600414728097	0.4975928056005482	0.2825832978229738	T	T	T

Structure08

TS3

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O
4 9 64 2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4489117563020457	0.5817316770612990	0.1996420919717892	F	F	F
0.2705662548140850	0.5546454786882364	0.1973916292034801	F	F	F
0.4262892306244197	0.7279849648576970	0.1966085434091127	F	F	F
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700286598070	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300088194799	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F

0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2500824388295015	0.6358385212003128	0.2518488221540522	T	T	T
0.1068863693949993	0.6093613104221021	0.2633630969810881	T	T	T
0.3177573835008118	0.7303548347981490	0.2446344012485255	T	T	T
0.0356535336474408	0.5461245870179142	0.2914118030418267	T	T	T

Structure09

*OCCO

1.00000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4424428128097739	0.5754195930843953	0.1998533104227568	T	T	T
0.2704923047599229	0.5589630320675921	0.1990504019288104	T	T	T
0.4266642009364209	0.7279665069881117	0.1964385658164190	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F

0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.069889999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2502057181502524	0.6591067215280279	0.2365414843399728	T	T	T
0.1570903035946044	0.6174449004251451	0.2582169716147137	T	T	T
0.3334703260707893	0.7544864580509788	0.2365834810972113	T	T	T
0.0701122243907576	0.5669319946521808	0.2740837045240614	T	T	T

Structure10

*OCHO+CO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4801292302763676	0.6727473991699738	0.2007558694714578	T	T	T
0.3126228867497272	0.5216193722785052	0.2001477051711841	T	T	T
0.3290414438176519	0.6885182970674119	0.1897143673496114	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F

0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.1641662991338774	0.7357471035186246	0.1940053667639016	T	T	T
0.1896429024492453	0.7750210843058722	0.3271400540938331	T	T	T
0.1204728881041825	0.7832348679552322	0.1791653036793025	T	T	T
0.2639123852282966	0.7681246656118482	0.1884378894305946	T	T	T

0.2060611975331726	0.8581903551751553	0.3341615647505596	T	T	T
0.1183084097391353	0.6595383494428355	0.2140336378916995	T	T	T

Structure11

TS4

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
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-7.3920001983999999	12.8033199130999993	0.0000000000000000
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0.0000000000000000	0.0000000000000000	26.7110004425000014
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Cu	N	C	O	H
4	9	64	3	1

Selective dynamics

Direct

0.3883999883824319	0.6109899878387083	0.1237199976883616	F	F	F
0.4673142199894835	0.6198586308743931	0.2017965136632612	T	T	T
0.2826011107511517	0.5289011567062322	0.1958920871254385	T	T	T
0.3769073237911778	0.7150634162597528	0.1954033274950313	T	T	T
0.3273999989159152	0.6724299788206597	0.0770300030666817	F	F	F
0.3273600042078260	0.4895400106801243	0.0762199982880674	F	F	F
0.5102499723826811	0.6724500060481094	0.0761599987757577	F	F	F
0.9996700286598081	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634262	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509580	0.6666100025562472	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038519	0.9995099902101519	0.0625599995251847	F	F	F
0.6666899919723834	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157302	0.3312500119332855	0.0634699985367248	F	F	F
0.6686199903697627	0.6676899790852888	0.0635500028781806	F	F	F
0.9991999865008062	0.1663299948336886	0.0593199990547290	F	F	F
0.0001500000141444	0.5002700090658865	0.0620899982600846	F	F	F
0.9999099969734443	0.8333100080615541	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125990	0.8348799943726366	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196500	0.4994199871907919	0.0623999982923919	F	F	F
0.6680499911019246	0.8350800275685106	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380749	0.0571300014870246	F	F	F
0.1647700071264776	0.3318099975501881	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066861	0.9996899962566790	0.0621200017787373	F	F	F
0.5004400015054744	0.3341600000654880	0.0623699985549493	F	F	F
0.8335300088194799	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869382	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310497	0.6670100092759701	0.0590099990224289	F	F	F

0.1655199974769772	0.1649699956211280	0.0588000007106046	F	F	F
0.1689099967855015	0.5010300278786706	0.0695900022914344	F	F	F
0.1661600023717328	0.8336899876319368	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978192	0.8309299945801403	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178190	0.4998199939886173	0.0600900016626156	F	F	F
0.8348900079967702	0.8343399763111581	0.0588699989124350	F	F	F
0.0547900013529557	0.1105799972670669	0.0582499988478275	F	F	F
0.0574500001527695	0.4450300037547388	0.0647099986659398	F	F	F
0.0552599988734522	0.7778099775364286	0.0577500015516321	F	F	F
0.3890799879994379	0.1110199987696634	0.0590200014557141	F	F	F
0.3847500086142551	0.4413599968097524	0.0698899999278808	F	F	F
0.3856300115637482	0.7774099707386032	0.0697999968969185	F	F	F
0.7216899990961428	0.1110199987696634	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781851	0.7793800235195367	0.0617300011113215	F	F	F
0.0548500008969130	0.2779600024177144	0.0611100010467140	F	F	F
0.0548699982635697	0.6113299727824156	0.0609100013869721	F	F	F
0.0557399988174792	0.9441199898966861	0.0569700002542319	F	F	F
0.3894000053534443	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536159	0.9449700116936787	0.0609200000764787	F	F	F
0.7219600081768296	0.2778800130081721	0.0612899996210956	F	F	F
0.7228400111134917	0.6104599833518950	0.0612800009690204	F	F	F
0.7218999862732436	0.9449999928237762	0.0611900016818296	F	F	F
0.2224700004002289	0.1112700029890166	0.0579399988155273	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610868	0.7781400084212837	0.0611599981631770	F	F	F
0.5554500222519398	0.1106600016727202	0.0609599985034350	F	F	F
0.5538799763018648	0.4459800124308098	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346173	0.1112200022076311	0.0597000010326383	F	F	F
0.8891900181671427	0.4444000124669510	0.0609400011618462	F	F	F
0.8885800242332579	0.7773900031831716	0.0579899996383304	F	F	F
0.2204699963058162	0.2759700119173589	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952091	0.0697799995553297	F	F	F
0.2220399975825630	0.9445899725293803	0.0577399991557783	F	F	F
0.5561599731237837	0.2784900069045198	0.0609700009367202	F	F	F
0.5584899783382445	0.6151199936777317	0.0699099972694697	F	F	F
0.5548200011515053	0.9423800111137428	0.0647599995261743	F	F	F
0.8888199925564068	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197194	0.6107800006620764	0.0590399987973029	F	F	F
0.8892800212255747	0.9450600147559971	0.0582900010185554	F	F	F

0.1849855348392153	0.7031063000584467	0.2167702792629285	T	T	T
0.2220597702647501	0.7697231602052578	0.2680554506305453	T	T	T
0.1197784749956156	0.7105075152600379	0.1902281213725944	T	T	T
0.3026235479062593	0.7835619589735356	0.2124670856195736	T	T	T
0.2414085715374152	0.8378451132126570	0.2957790004621877	T	T	T
0.1761244139296485	0.6236592279113035	0.2239259324226130	T	T	T

Structure12

*OCOCHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4484384266647232	0.5858773804468611	0.2008905794273000	T	T	T
0.2706367918087608	0.5452029298293490	0.1941422901103948	T	T	T
0.4059417710759569	0.7214819242549124	0.1963902397400545	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F

0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F

0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.1920234004016005	0.6861713845792677	0.2190348645460142	T	T	T
0.2791764400576177	0.7864742698689012	0.2440163029151038	T	T	T
0.1236460289363406	0.6806745038432190	0.1920532461285731	T	T	T
0.3735379275672392	0.8134449210074440	0.2295009383318054	T	T	T
0.2527195269597287	0.8313467761420120	0.2742353443830129	T	T	T
0.1977498643598479	0.6111423255433798	0.2275473327118529	T	T	T

Structure13

TS5

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387214	0.1237199976883616	F	F	F
0.4581397746374792	0.5603408990063095	0.1906225778131222	T	T	T
0.2856181612898299	0.5260941954779479	0.2057416463605923	T	T	T
0.4272675537958449	0.7054042705927115	0.1998820519943147	T	T	T
0.3273999989159152	0.6724299788206597	0.0770300030666817	F	F	F
0.3273600042078263	0.4895400106801452	0.0762199982880674	F	F	F
0.5102499723826811	0.6724500060481094	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634263	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562472	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101866	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332855	0.0634699985367248	F	F	F
0.6686199903697628	0.6676899790852888	0.0635500028781806	F	F	F
0.9991999865008060	0.1663299948336886	0.0593199990547290	F	F	F
0.0001500000141334	0.5002700090658865	0.0620899982600846	F	F	F
0.9999099969734652	0.8333100080615888	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726715	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196504	0.4994199871908128	0.0623999982923919	F	F	F
0.6680499911019240	0.8350800275685243	0.0631899982792987	F	F	F

0.1665399968694744	0.9999399781381098	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501881	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066893	0.9996899962567138	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654880	0.0623699985549493	F	F	F
0.8335300087518440	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310500	0.6670100092759701	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211280	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786706	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319591	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978204	0.8309299945801666	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178293	0.4998199939886382	0.0600900016626156	F	F	F
0.8348900079967698	0.8343399763111928	0.0588699989124350	F	F	F
0.0547900013529561	0.1105799972670686	0.0582499988478275	F	F	F
0.0574500001527694	0.4450300037547393	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364286	0.0577500015516321	F	F	F
0.3890799879994401	0.1110199987696651	0.0590200014557141	F	F	F
0.3847500086142550	0.4413599968097733	0.0698899999278808	F	F	F
0.3856300115637483	0.7774099707386032	0.0697999968969185	F	F	F
0.7216899990961438	0.1110199987696651	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195367	0.0617300011113215	F	F	F
0.0548500008969129	0.2779600024177144	0.0611100010467140	F	F	F
0.0548699982635698	0.6113299727824170	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898967209	0.0569700002542319	F	F	F
0.3894000053534442	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536164	0.9449700116937133	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081721	0.0612899996210956	F	F	F
0.7228400111134907	0.6104599833518950	0.0612800009690204	F	F	F
0.7218999862732441	0.9449999928238111	0.0611900016818296	F	F	F
0.2224700004002299	0.1112700029890182	0.0579399988155273	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610742	0.7781400084212852	0.0611599981631770	F	F	F
0.5554500222519416	0.1106600016727218	0.0609599985034350	F	F	F
0.5538799763018654	0.4459800124308307	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346283	0.1112200022076328	0.0597000010326383	F	F	F
0.8891900181671419	0.4444000124669573	0.0609400011618462	F	F	F
0.8885800242332567	0.7773900031831716	0.0579899996383304	F	F	F
0.2204699963058162	0.2759700119173589	0.0616400018241308	F	F	F

0.2224200070404621	0.6142200231952091	0.0697799995553297	F	F	F
0.2220399975825631	0.9445899725294151	0.0577399991557783	F	F	F
0.5561599731237840	0.2784900069045198	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777521	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137777	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197190	0.6107800006620824	0.0590399987973029	F	F	F
0.8892800212255745	0.9450600147560320	0.0582900010185554	F	F	F
0.3062054898363181	0.7030361767420877	0.2682240953917274	T	T	T
0.2561395663395236	0.6363601544545424	0.2194827067313799	T	T	T
0.2522091740869952	0.6903404436430746	0.3057426919552981	T	T	T
0.4044853701729892	0.7685384393311556	0.2612904619621569	T	T	T
0.2424294477953431	0.3991967814923780	0.2242392278865521	T	T	T
0.1867141525050759	0.6421449414135512	0.1971157947276627	T	T	T

Structure14

*O₃+*CO₂*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O
4 9 64 4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4312258063663581	0.5449092408217646	0.1972897752262702	T	T	T
0.2615849237317285	0.5440090536885697	0.2011994219733609	T	T	T
0.4226888265521631	0.7086030148445142	0.2000004834173896	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F

0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F

0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2728756054005387	0.7356598060840628	0.2437348330254357	T	T	T
0.2151021237643997	0.6430533361053821	0.2035664547537805	T	T	T
0.2186688667939253	0.7500420900270921	0.2737204236291947	T	T	T
0.3734274570476822	0.7859060072629069	0.2381391663396365	T	T	T
0.2980515281770629	0.4444791386902827	0.2059899239174974	T	T	T
0.1506450888077651	0.6441787372038281	0.1754795260371914	T	T	T

Structure15

*O₂+*COCOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O
4 9 64 4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.3865129165322657	0.5056742038813115	0.1945195358867301	T	T	T
0.2632350212094252	0.5834357145345279	0.1973237877890122	T	T	T
0.4590127600777317	0.6919769112837684	0.2043504199379414	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F

0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F

0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.94238001111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2728503678423365	0.3942813413870608	0.2304382966602358	T	T	T
0.1670685360430287	0.3657006025170011	0.2011912592016913	T	T	T
0.2718468927000408	0.3590270892422520	0.2712753139988570	T	T	T
0.3556065173844535	0.7217427069880971	0.1991467667283167	T	T	T
0.1531800089325983	0.4439900177943749	0.1932058966149539	T	T	T
0.1118098066859614	0.2740864783757456	0.1884560781635788	T	T	T

Structure16

*O₄+*COCOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000	
-7.3920001983999999	12.8033199130999993	0.0000000000000000	
0.0000000000000000	0.0000000000000000	26.7110004425000014	
Cu	N	C	O
4	9	64	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.5052683435153659	0.6529751588608614	0.2207541814528568	T	T	T
0.3205785551253504	0.5775996235236369	0.2181803039154686	T	T	T
0.4007423593829499	0.7470998527927413	0.1771352364416578	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F

0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F

0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.4513645489139435	0.7693414382566065	0.2595263419464637	T	T	T
0.3406590650953982	0.6721536586174632	0.2726025806558124	T	T	T
0.5339910969164949	0.7639174910679084	0.2685583643000584	T	T	T
0.4478358928858323	0.8433286427586468	0.2361236229244619	T	T	T
0.2928713882491008	0.6650779949115996	0.3107268935974568	T	T	T
0.4119170789406781	0.5448143066493412	0.1799878814886793	T	T	T

Structure17

*O₁+*COCOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O
4 9 64 4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4255349698356273	0.5234668917697988	0.1966439159803162	T	T	T
0.2715629082360690	0.5477226671641934	0.1935580706425726	T	T	T
0.4433499715848465	0.6894773806607613	0.2051921777557635	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F

0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F

0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.4197405106566217	0.5771280711957104	0.2642402472677715	T	T	T
0.3024118232024054	0.5072515296351555	0.2886697714780911	T	T	T
0.4406067674506771	0.4275614935587548	0.1694874648613622	T	T	T
0.4958963076659514	0.6335299141939407	0.2894508277360004	T	T	T
0.2272743353379022	0.4960545555977966	0.2600360259860531	T	T	T
0.3008370964315632	0.4751781221879634	0.3309085579706980	T	T	T

Formation of ethane

Structure01

*OH+*COCOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	4	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.3714566102558433	0.5270735896249249	0.2004776891079399	T	T	T

0.2218673323105973	0.5345025627548590	0.2357200479872127	T	T	T
0.3791990746686262	0.6915308211467057	0.1986018289717798	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.000159999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F

0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2462780865779847	0.7423413606072835	0.2481434568304300	T	T	T
0.1754692297092953	0.6299769708222100	0.2228884911719542	T	T	T
0.2053103749249202	0.7755906121668406	0.2769135519973289	T	T	T
0.3417845143576998	0.7830653405473434	0.2330586206833405	T	T	T
0.2604245928409378	0.4299007441001556	0.2454170873525329	T	T	T
0.1053600400863437	0.6143067943158190	0.1941131176869226	T	T	T
0.2804075159314572	0.4224771167421625	0.2792600622342633	T	T	T

Structure02

*O+*COHCOO*

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999 12.8033199130999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O H

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4292643375304163	0.5614405418000726	0.2012633584870474	T	T	T
0.2465836420423261	0.5451195135895908	0.2068910158474755	T	T	T
0.4142640749574460	0.7156575538309156	0.1968908974222325	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F

0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2555785862986244	0.7526446229234259	0.2196294146145316	T	T	T
0.1904025070377952	0.6313111725727818	0.2119749395937614	T	T	T
0.1987308116729467	0.7932347413817423	0.2245724714953405	T	T	T
0.3552650713670634	0.7993960379171750	0.2196250255697241	T	T	T
0.2980048068482301	0.4590197047090880	0.2115912537271659	T	T	T
0.0929005506723124	0.6071592939649597	0.2113521272374785	T	T	T
0.1020139451745427	0.6827537977124361	0.2175667574226754	T	T	T

Structure03

*O+*COCOHO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	4	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4255267361371969	0.5415605846833658	0.1967699970402015	T	T	T
0.2532799917805850	0.5386279555802610	0.2031073453959872	T	T	T
0.4214084647470115	0.7029413204526451	0.2011404993047044	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.000159999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F

0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.069889999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2664438831933977	0.7251764035901523	0.2441085671795784	T	T	T
0.2023283716520420	0.6330663717095328	0.2074249930842372	T	T	T
0.2110389807302811	0.7474444676981015	0.2761141471328670	T	T	T
0.3640274973099358	0.7729180907457915	0.2455350620510486	T	T	T
0.2929509802928963	0.4417161738148161	0.2069263139812764	T	T	T

0.1305318655746122	0.6347803938156686	0.1846109890087974	T	T	T
0.2596412823714759	0.8026849501845299	0.2989127851594443	T	T	T

Structure04

*O+*COCOO*H

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000		
-7.3920001983999999	12.8033199130999993	0.0000000000000000		
0.0000000000000000	0.0000000000000000	26.7110004425000014		
Cu	N	C	O	H
4	9	64	4	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4150602001668953	0.5355584838289628	0.1975483387405438	T	T	T
0.2494243634890037	0.5452552157959992	0.2045747502793446	T	T	T
0.4214789876631598	0.7018617769138300	0.2008971018376761	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F

0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F

0.2570455295574100	0.7315352087970968	0.2474075273010531	T	T	T
0.2030901010923983	0.6435401323186570	0.2074223926504169	T	T	T
0.2177210404703336	0.7539894922208076	0.2812194936968699	T	T	T
0.3675160060192329	0.7826379395863604	0.2427793955435083	T	T	T
0.2808801450357156	0.4424208208861491	0.2089378214285442	T	T	T
0.1333126210473032	0.6453452085852105	0.1827880298757486	T	T	T
0.3981343348050791	0.8312854882649211	0.2709781170499010	T	T	T

Structure05

H₂O+*CO₂O*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	4	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4029891197574968	0.5515904807421702	0.2037213529820064	T	T	T
0.2551231649439090	0.5836550828197735	0.1888494869619322	T	T	T
0.4278820185028208	0.7232511342480794	0.1956772066382537	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F

0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F

0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2891806880887716	0.7680229736162495	0.2446055557731249	T	T	T
0.2112145448801344	0.6831918846769983	0.2054103447888077	T	T	T
0.2518628728910036	0.7879568005812000	0.2810492878634420	T	T	T
0.3872223431990577	0.8072994271507136	0.2325448151204587	T	T	T
0.4098000172348972	0.4600732338561034	0.2595487974129741	T	T	T
0.1488986840046229	0.6978047189711518	0.1821028903616505	T	T	T
0.3738978953573376	0.4620084622695895	0.2897960452478970	T	T	T
0.3826914873861658	0.3864898088105544	0.2519147454035002	T	T	T

Structure06

*OH+*COHCOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	4	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.3601365527586912	0.5480908065740444	0.2066817769952869	T	T	T
0.2351739346962962	0.5729030563291452	0.2638945980739705	T	T	T
0.3503723595906915	0.6963555694716778	0.1892786190575972	T	T	T
0.327399989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F

0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F

0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2147342179308109	0.7555941700337186	0.2270465478450666	T	T	T
0.1713827089748150	0.6516202127872168	0.2572236460402670	T	T	T
0.1535560760484673	0.7919089224581932	0.2269901476802675	T	T	T
0.3025969502818148	0.7925655534436001	0.2047401734361715	T	T	T
0.2943749658232392	0.4859291238773017	0.2707122222426989	T	T	T
0.0775962233054554	0.6268825711748679	0.2713367400886015	T	T	T
0.0737423968677643	0.6921893817210865	0.2572390865463273	T	T	T
0.3418627358593778	0.5024963934203127	0.2988633268111212	T	T	T

Structure07

*OH+*COCOHO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	4	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.3491402456532064	0.5181851970131287	0.1995173431759683	T	T	T
0.2041997530193716	0.5238204329011008	0.2439730878501593	T	T	T
0.3653131592555764	0.6832372571867946	0.1984853668063657	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F

0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F

0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2350812760573652	0.7307031950963534	0.2509772692670386	T	T	T
0.1570348092405540	0.6188344866868898	0.2336960751118864	T	T	T
0.1986060014243289	0.7772278099822137	0.2812287487636634	T	T	T
0.3296467544009953	0.7749407138502522	0.2392620122640766	T	T	T
0.2475368363175162	0.4214505456315076	0.2475980211128612	T	T	T
0.0803333210467089	0.6064947447048440	0.2092604320221075	T	T	T
0.2767782979325688	0.4185393075950032	0.2798116678693891	T	T	T
0.2575394205225174	0.8454708696413644	0.2910982473069549	T	T	T

Structure08

*OH+*COCOO*H

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	4	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.3457723918583348	0.5195599439098252	0.2005635609097721	T	T	T
0.2022005384552982	0.5310752156823808	0.2430872965550784	T	T	T
0.3657072310709852	0.6854321731994477	0.1976026595973593	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F

0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F

0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2251040722829709	0.7358173140657215	0.2554523712898639	T	T	T
0.1574150098459592	0.6274568709159160	0.2309982293367944	T	T	T
0.2035097920982849	0.7771405361773478	0.2887542348953171	T	T	T
0.3286346338053759	0.7828187300786131	0.2365447448862285	T	T	T
0.2415070909368721	0.4258008085862168	0.2482623135459354	T	T	T
0.0847047860555301	0.6158109576213924	0.2036910615180158	T	T	T
0.2683736346138429	0.4214371305210587	0.2808947544634058	T	T	T
0.3731437242005118	0.8453859137977791	0.2565010647450537	T	T	T

Structure09

COCOO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O
4 9 64 3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4236768266358624	0.5645346432278657	0.2020598536475759	F	F	F

0.2639509989035602	0.5801479599939583	0.1935216703132738	F	F	F
0.4340973036528339	0.7283825546935816	0.1963555277731004	F	F	F
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.000159999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F

0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2907546463969766	0.7711606188764364	0.2404475979300429	T	T	T
0.2157360134614024	0.6790097944889339	0.2037949122865967	T	T	T
0.2519863227255215	0.7943196024726262	0.2750620291922985	T	T	T
0.3893280555106315	0.8132782287471301	0.2284748761498960	T	T	T
0.1506503247452358	0.6858822291068593	0.1782023433406097	T	T	T

Structure10

CHOCOO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4333828095814956	0.5762234667229466	0.2023366127165808	T	T	T
0.2707930774006564	0.5760697913715350	0.1936935855474118	T	T	T
0.4298718240502113	0.7350902309472035	0.1929590627153832	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F

0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2990035404637406	0.7855635279190334	0.2420136555383855	T	T	T
0.2161660012239930	0.6837161522606909	0.2165943322584861	T	T	T
0.2646371901586270	0.8213208434152196	0.2734804926089576	T	T	T
0.3959003018966486	0.8249465948140762	0.2279624531193454	T	T	T
0.1563189036457325	0.6789896244037669	0.1833529420568641	T	T	T
0.1965116207394271	0.6068625707080392	0.2391027884736013	T	T	T

Structure11

COHCOO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014
 Cu N C O H
 4 9 64 3 1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4204736966994110	0.5679530334351377	0.2031313131018552	T	T	T
0.2636345458552100	0.5829557931111325	0.1922217715003129	T	T	T
0.4315400607218217	0.7331313909294259	0.1945862278575122	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F

0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2816380039418779	0.7815363502306251	0.2251629753663784	T	T	T
0.2065539088655358	0.6630256223464523	0.2155029501412639	T	T	T
0.2354565328556875	0.8293529011565257	0.2387776523933187	T	T	T
0.3808146869931752	0.8216524372790116	0.2186552762685050	T	T	T
0.1115669718157311	0.6441349374831299	0.2235740199999607	T	T	T
0.1261524862456659	0.7187217733602632	0.2340913502465348	T	T	T

Structure12

*COCOHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4126199972623939	0.5592125754825639	0.2026376551529347	T	T	T
0.2597880995553786	0.5848804217130356	0.1910270942122813	T	T	T
0.4332180547806771	0.7280627165179313	0.1945831683595277	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F

0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2861438311606033	0.7714062168968034	0.2370498220146014	T	T	T
0.2027733765453200	0.6723670393544449	0.2086052453029074	T	T	T
0.2486578073116314	0.8110067267272791	0.2707239459616942	T	T	T
0.3829732275606950	0.8092601807723976	0.2324677009573241	T	T	T

0.1224676888295708	0.6711209135208834	0.1953776876255221	T	T	T
0.3083313457472615	0.8679201958963533	0.2883853149035581	T	T	T

Structure13

*COCOOH

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
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-7.3920001983999999	12.8033199130999993	0.0000000000000000
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0.0000000000000000	0.0000000000000000	26.7110004425000014
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Cu	N	C	O	H
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4	9	64	3	1
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Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4162393589662553	0.5632326013668113	0.2030612534740958	T	T	T
0.2650059794534455	0.5903936838896142	0.1927366627570806	T	T	T
0.4393128249826702	0.7321992286947659	0.1925677683725277	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F

0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F

0.2808773090631205	0.7737227908911352	0.2425494168816579	T	T	T
0.2091840677270808	0.6800043613491740	0.2075332571658837	T	T	T
0.2566053590651750	0.8032859014481250	0.2795801013490002	T	T	T
0.3895189878346493	0.8197014573023867	0.2297658488278936	T	T	T
0.1337200984988373	0.6813480847201360	0.1891545130440186	T	T	T
0.4284238860377658	0.8731379594045968	0.2553146163163129	T	T	T

Structure14

CHOHCOO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4313832636682087	0.5791029104276514	0.2036382473701648	T	T	T
0.2672399390815201	0.5845367941147057	0.1947846264576560	T	T	T
0.4328578503446432	0.7379282379673767	0.1931359868788291	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F

0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F

0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2768505516032303	0.7807878065012037	0.1977267331098790	T	T	T
0.2137981923788400	0.6740084112870429	0.2217852423116719	T	T	T
0.2264574542819070	0.8171979771181866	0.1763449602033709	T	T	T
0.3794673573708650	0.8300325798138194	0.1997692630322097	T	T	T
0.1062354688802463	0.6384432099107685	0.2182658495487599	T	T	T
0.1065134228168126	0.6948405179252728	0.1977889799235633	T	T	T
0.2369512836210806	0.6738726843466452	0.2611634724987489	T	T	T

Structure15

CH₂*OCOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4229387523293178	0.5854622498906062	0.2070219355255214	T	T	T
0.2622827022516943	0.5812572770131941	0.1917852600632311	T	T	T
0.4184444093353271	0.7413860593608687	0.1894184855933912	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F

0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F

0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2817712143122613	0.8232086155241342	0.1899023912309786	T	T	T
0.2007778277004517	0.7257946561192820	0.2199912111353869	T	T	T
0.2533331268779675	0.8808912093611577	0.1698352981809542	T	T	T
0.3792704623837135	0.8435805285489693	0.1871382001554255	T	T	T
0.1685205397904952	0.6274629949933876	0.1974640257871457	T	T	T
0.2342555293941580	0.7319081921048173	0.2579086525520871	T	T	T
0.1313496189531879	0.7348393889612784	0.2238672976006353	T	T	T

Structure16

*CHOCOHO

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999 12.8033199130999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O H
4 9 64 3 2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4142669909469692	0.5483810163269539	0.1998490608382886	T	T	T
0.2582507775555905	0.5673642517501406	0.1890662960072681	T	T	T
0.4273802807462409	0.7124251534716194	0.2029302347526487	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F

0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F

0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2766295136799671	0.7553019251839465	0.2165166698477859	T	T	T
0.1886662071209995	0.6469637715851007	0.2209759752860022	T	T	T
0.2532081883901072	0.8226345360805601	0.1935818823266768	T	T	T
0.3696675534956944	0.7916848712551487	0.2338514658911367	T	T	T
0.0974660032520102	0.6160099435240513	0.2039011705417267	T	T	T
0.2023143093574021	0.6062463345783832	0.2537347889166430	T	T	T
0.3179937493175705	0.8902921599670165	0.1942765653232307	T	T	T

Structure17

*CHOCOO*H

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4126669330281595	0.5462210011363531	0.2000585413137448	T	T	T
0.2599431199112150	0.5745906107738804	0.1887545628272491	T	T	T
0.4323925588048507	0.7128407583705986	0.2015167961381840	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F

0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F

0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2822310633704032	0.7696587846191887	0.2081522244393385	T	T	T
0.1970169494861521	0.6607136843199676	0.2179227594689356	T	T	T
0.2831324774320775	0.8380336845476147	0.1823897900367110	T	T	T
0.3794648546938080	0.7977027088722770	0.2367889286244683	T	T	T
0.1067454154645341	0.6260370676679821	0.1982729893104787	T	T	T
0.2069684895994849	0.6304736035294093	0.2550435390878540	T	T	T
0.4209795245994469	0.8736385633113567	0.2325638641088852	T	T	T

Structure18

CHOHCOHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4137677100225282	0.5661661045993702	0.2038323992550017	T	T	T
0.2577143729899863	0.5810786585845761	0.1896044663601419	T	T	T
0.4278665495079121	0.7315228458891687	0.1948169456502791	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F

0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F

0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2647121627167290	0.7647978547389555	0.2110494554969266	T	T	T
0.1985643107203300	0.6559808673014276	0.2272650511992926	T	T	T
0.2148351212569158	0.8126158282835910	0.1927233335892930	T	T	T
0.3636577799567897	0.8159452918136735	0.2112599364531790	T	T	T
0.0887302993796062	0.6249240278415347	0.2232767874303730	T	T	T
0.1396701376261943	0.7599500571504558	0.1968867363062591	T	T	T
0.2199406997424165	0.6440361053301112	0.2651907023330748	T	T	T
0.0612068831952987	0.6221878305403843	0.2567407173309100	T	T	T

Structure19

*CHOHCOHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
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0.4071006227209017	0.5561790754850325	0.2029264582939007	T	T	T
0.2593851713475057	0.5852532344198533	0.1898602879289139	T	T	T
0.4348392342261472	0.7271548017190013	0.1968490416645048	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F

0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2772412588894713	0.7678104109341566	0.2145535170253430	T	T	T
0.2059416381224889	0.6630871031055755	0.2313653939086286	T	T	T
0.2306087159323841	0.8189088947157610	0.1941652870721233	T	T	T
0.3772160262201486	0.8164984860899666	0.2156423699636213	T	T	T
0.0980666321951096	0.6304561318794615	0.2330599023910870	T	T	T
0.0860946991905356	0.6746505369308269	0.2101175820759809	T	T	T
0.2303356155890679	0.6452147210455447	0.2671125896100873	T	T	T
0.2870525305007631	0.8851511108720413	0.1811694567082164	T	T	T

Structure20

HOCH₂COO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014
 Cu N C O H
 4 9 64 3 3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4715063535606444	0.6279750236771574	0.2020462934634048	T	T	T
0.2867382936459545	0.5309389943392452	0.1967112860251337	T	T	T
0.3755516172726853	0.7163422823619192	0.1924958856442612	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F

0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2504210888781649	0.8104945131265926	0.2000438697923958	T	T	T
0.1666313381389699	0.7100561719728218	0.2254070877318236	T	T	T
0.2246013613637422	0.8746002939501075	0.1859999382214882	T	T	T
0.3437914482878136	0.8233009181964195	0.1948061589297154	T	T	T
0.0694758984890998	0.7069746282353594	0.2260257633127617	T	T	T
0.0875314293638778	0.7752265555674378	0.2111751600445579	T	T	T
0.1930738063619811	0.7070393671866915	0.2637916240149855	T	T	T
0.1605830268244610	0.6419319315325979	0.2049032301168459	T	T	T

Structure21

*CHOHCOHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4126077352208609	0.5653239271131899	0.2038751997754915	T	T	T
0.2586281140677277	0.5825117821708886	0.1890289509851615	T	T	T
0.4280463969735188	0.7312677353460800	0.1942083787532942	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F

0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2636002583902679	0.7637924399232233	0.2110309204460184	T	T	T
0.1978223760731063	0.6555529865743995	0.2271274858966024	T	T	T

0.2146480777541513	0.8123517092796664	0.1923775595300646	T	T	T
0.3631033365486986	0.8160296720341358	0.2115693896367877	T	T	T
0.0884574590553676	0.6229242575054447	0.2233598647724273	T	T	T
0.1389618537567721	0.7621038521519414	0.1966330931067366	T	T	T
0.2199237533256605	0.6426673157758584	0.2646765625495209	T	T	T
0.0622782960248592	0.6241863883289649	0.2567493089304795	T	T	T

Structure22

*OCHCHOHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4441495740063037	0.5761256500833661	0.1989578513160357	T	T	T
0.2759479386565185	0.5640557724887877	0.1970247351990492	T	T	T
0.4290854362740009	0.7300187170012036	0.1967899119074001	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F

0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F

0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2845393901339313	0.7818685805609882	0.2356629221759757	T	T	T
0.2277085574008972	0.6806522096810924	0.2660941632428289	T	T	T
0.2366245467870048	0.7699002675569495	0.1878424530795755	T	T	T
0.3885632671523415	0.8105081023492763	0.2349111678434690	T	T	T
0.2040174691981390	0.5915448522424742	0.2508895500717461	T	T	T
0.2507980092895608	0.7213782110080585	0.1688570678955630	T	T	T
0.2109859001959498	0.6876861665312267	0.3059299998217750	T	T	T
0.2732949146807028	0.8420772748574330	0.2547623135914960	T	T	T

Structure23

CH₂OHCOHO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4711524657654217	0.6248629274786374	0.2021768639024163	T	T	T
0.2778781715024806	0.5279156239178041	0.1949030725276964	T	T	T
0.3779694237804416	0.7136871799478038	0.1926886985867140	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F

0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F

0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2476925295040627	0.8037883316398658	0.2093907300221377	T	T	T
0.1593048066640053	0.7029830934517467	0.2299170774781802	T	T	T
0.2257987921727974	0.8790115568000855	0.1994697957951242	T	T	T
0.3365978729921634	0.8182473292636611	0.2013855240663857	T	T	T
0.0662746942088946	0.7100433491144170	0.2278366703425413	T	T	T
0.1510670748429322	0.8500743154043262	0.2078734187698840	T	T	T
0.1796593151478309	0.6930843635880195	0.2684908299721841	T	T	T
0.1541900574487102	0.6374363880824947	0.2074047406565155	T	T	T
0.0144289289895423	0.6608167673244191	0.2510291589259181	T	T	T

Structure24

HOCH₂CO*OH

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4771578068964031	0.6234391113586617	0.2004272335182445	T	T	T
0.2824937380325295	0.5264255682423826	0.1959918928061018	T	T	T
0.3835377549378599	0.7114400783657649	0.1941258250461820	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.000329999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F

0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F

0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2479931956048037	0.8157874171044524	0.2057224119093103	T	T	T
0.1647166973041319	0.7120378626438947	0.2254152847918096	T	T	T
0.2346247518171990	0.8862991075901155	0.1916927080960098	T	T	T
0.3471471455620938	0.8261700161744010	0.2049266911063777	T	T	T
0.0654825491933628	0.7034876213666738	0.2234272890137342	T	T	T
0.0756893993124413	0.7705461860833497	0.2114741201611257	T	T	T
0.1857362859504574	0.7036232407806591	0.2642292233634257	T	T	T
0.1666904147604439	0.6490371493477126	0.2035847039417632	T	T	T
0.3951014682543810	0.8952005876879200	0.1907104363327685	T	T	T

Structure25

HOCH₂CHOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4439989793630489	0.6064180590942303	0.2059261571578168	T	T	T
0.2701969719268145	0.5753908308211158	0.1940032564681583	T	T	T
0.4095148807132905	0.7449670686211255	0.1885268695657492	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F

0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F

0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2678461346140633	0.8235413371131401	0.2001102386970959	T	T	T
0.1905572723623730	0.7159259531705870	0.2265524981686125	T	T	T
0.2200932540700571	0.8287593597171333	0.1577528439834982	T	T	T
0.3700907506272788	0.8423819716286459	0.1955356559335718	T	T	T
0.0890872416918576	0.6942451332062318	0.2178056932429767	T	T	T
0.1027121948377671	0.7377493871747126	0.1864191333338881	T	T	T
0.2054189594541827	0.7128115415342395	0.2666966273015338	T	T	T
0.2072204277359728	0.6551932700133619	0.2065295221394857	T	T	T
0.2722875029405160	0.8830253820340156	0.2280187282856667	T	T	T

Structure26

CH₃OH+*OCO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	4

Selective dynamics

Direct

0.3881900012654427	0.6059700250918354	0.1243999973027243	F	F	F
0.4714620304639258	0.6018762380710464	0.2004878574503819	T	T	T
0.2796638135907770	0.5380300372684276	0.1975422656617482	T	T	T
0.4066631051358789	0.7174421023872454	0.1940331744621729	T	T	T
0.3271900117312896	0.6674100160737950	0.0777100026436059	F	F	F
0.3271499871871910	0.4845199882612334	0.0768999979024301	F	F	F
0.5100399851915896	0.6674299836292192	0.0768399983526749	F	F	F
0.9994599819312597	0.9951599836198284	0.0580400004985719	F	F	F
0.0001200000273016	0.3294099867554436	0.0631899982792987	F	F	F
0.9994800090598659	0.6615899801373502	0.0593799986044843	F	F	F
0.3330299853944041	0.9951400160644042	0.0593699999149706	F	F	F
0.6652100086192263	0.9944900274632786	0.0632399991021018	F	F	F
0.6664800048203432	0.3281399906052016	0.0619099996857031	F	F	F
0.3319599926627319	0.3262299895143883	0.0641499981136491	F	F	F
0.6684100031460858	0.6626700162603143	0.0642300024551048	F	F	F
0.9989899993077103	0.1613100021727050	0.0599999986690847	F	F	F
0.9999399781436722	0.4952499866469964	0.0627700015807804	F	F	F
0.9997000098499953	0.8282899856426624	0.0578299984429691	F	F	F
0.3326399922060688	0.1603000014785252	0.0596400015203216	F	F	F
0.3317700028605586	0.8298599720318478	0.0635199993969664	F	F	F
0.6656399965269628	0.1613200009074731	0.0621399991203262	F	F	F
0.6654899716065188	0.4943999946079103	0.0630799979067476	F	F	F
0.6678400040175276	0.8300600052277218	0.0638699978562229	F	F	F
0.1663299947648440	0.9949200153131059	0.0578100010639488	F	F	F
0.1645600050914879	0.3267900049673074	0.0637700036232900	F	F	F
0.1647499948623761	0.6628500223068414	0.0635100007074527	F	F	F
0.4993700087155943	0.9946699738377873	0.0627999976118829	F	F	F
0.5002300143514304	0.3291400074826143	0.0630500018756450	F	F	F
0.8333200216341652	0.9956399798271960	0.0600499994918877	F	F	F
0.8332899809043965	0.3289699852528472	0.0621200017787373	F	F	F
0.8343200087790095	0.6619899869351826	0.0596899986367845	F	F	F
0.1653099954419872	0.1599500030382472	0.0594800002875289	F	F	F
0.1686999946458201	0.4960100054597802	0.0702700019057900	F	F	F
0.1659500003061538	0.8286700248850636	0.0590000003703537	F	F	F
0.4998199939779653	0.1615899950202078	0.0607700012769783	F	F	F
0.4980500042549494	0.4965800047294593	0.0701600015332318	F	F	F
0.4986000061067273	0.8259099721612486	0.0703099965889677	F	F	F
0.8330299854427636	0.1615899950202078	0.0616899989405937	F	F	F
0.8330299854637815	0.4948000014057357	0.0607700012769783	F	F	F
0.8346800207730922	0.8293200134861820	0.0595499984893522	F	F	F
0.0545799993282259	0.1055599972642369	0.0589299984247518	F	F	F
0.0572400018380179	0.4400100111718572	0.0653899982428570	F	F	F
0.0550500005567045	0.7727900147114539	0.0584300011285492	F	F	F
0.3888700008556611	0.1059999987668334	0.0597000010326383	F	F	F

0.3845399916306746	0.4363400042268708	0.0705699995048050	F	F	F
0.3854199946172159	0.7723900079917314	0.0704799965112741	F	F	F
0.7214800119523659	0.1059999987668334	0.0623099990051941	F	F	F
0.7211499809978719	0.4386700093507301	0.0616599992031510	F	F	F
0.7236899733956434	0.7743600011006464	0.0624100007256772	F	F	F
0.0546399987942863	0.2729400098348336	0.0617900006610697	F	F	F
0.0546599998791706	0.6063100099574470	0.0615900010013277	F	F	F
0.0555300005007311	0.9391000270717100	0.0576499998685875	F	F	F
0.3891899883698571	0.2720000148115318	0.0619000010336279	F	F	F
0.3883099854396690	0.9399499893528898	0.0615999996534029	F	F	F
0.7217500209857377	0.2728599905892821	0.0619699992354583	F	F	F
0.7226300239574499	0.6054400205269204	0.0619600005459446	F	F	F
0.7216899991212031	0.9399799704829874	0.0618700012587539	F	F	F
0.2222599983078553	0.1062500029861866	0.0586199983924445	F	F	F
0.2236900031708942	0.4370599984988672	0.0705600008527298	F	F	F
0.2214999944280933	0.7731199860804949	0.0618400014838727	F	F	F
0.5552399754776616	0.1056400015917802	0.0616400018241308	F	F	F
0.5536699891107730	0.4409599900119190	0.0655300021340608	F	F	F
0.5575500131050575	0.7709000110901840	0.0706000029860192	F	F	F
0.8884199857517885	0.1062000021266982	0.0603800006095554	F	F	F
0.8889799714236517	0.4393799901261630	0.0616200007387633	F	F	F
0.8883699774897735	0.7723699808423845	0.0586699992526860	F	F	F
0.2202599942728227	0.2709499895765717	0.0623200014384864	F	F	F
0.2222100049007807	0.6092000007763190	0.0704599991322468	F	F	F
0.2218299955455691	0.9395700097044042	0.0584199987327025	F	F	F
0.5559499859697397	0.2734700143216386	0.0616500005136444	F	F	F
0.5582799911471525	0.6100999712588333	0.0705899968838253	F	F	F
0.5546100139604135	0.9373599886948512	0.0654399991030985	F	F	F
0.8886100054023700	0.2731299996200178	0.0622799992677585	F	F	F
0.8886200189676785	0.6057599783212879	0.0597199983742271	F	F	F
0.8890699744430322	0.9400399923371054	0.0589700005954796	F	F	F
0.3578712369424437	0.8949363358920945	0.2005700130872554	T	T	T
0.1125408297528828	0.6702334528230031	0.2496949193032740	T	T	T
0.3078764505038887	0.9344608404574340	0.1920261341198788	T	T	T
0.4081557270895421	0.8547636278507716	0.2095260554390026	T	T	T
0.0173215255278341	0.6654323944240351	0.2350530242364929	T	T	T
0.0330814561009221	0.7180420639780881	0.2095125483491372	T	T	T
0.0924388343855540	0.6105022253219869	0.2786730515551208	T	T	T
0.1504230806055113	0.6524491999830916	0.2184829313533601	T	T	T
0.1687303377898463	0.7468498681432297	0.2660374439874085	T	T	T

Structure27

CH₃COO*+H₂O

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	5

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4764118495982494	0.6380618695953797	0.2016253740275553	T	T	T
0.2925172462166464	0.5263812781366372	0.1975289337914915	T	T	T
0.3659273307517042	0.7107401020793481	0.1924139859537418	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F

0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.069889999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2390303808514098	0.8033807220689431	0.2101901809791510	T	T	T
0.1824413486368251	0.7257566465965596	0.2523382213096020	T	T	T
0.2026402565250490	0.8564613981521810	0.1921936310327256	T	T	T
0.3265696503894305	0.8120396692480850	0.1941704821271331	T	T	T
-0.0082356235569018	0.7646978159242845	0.1779987507969880	T	T	T
0.0676648639153330	0.8018828134179992	0.1863067023909757	T	T	T

0.2378846570997827	0.7335372783383819	0.2817122735893008	T	T	T
0.1471363097875476	0.6457316588159933	0.2374937422154533	T	T	T
-0.0414278566529305	0.7780799550195663	0.2061036940991791	T	T	T
0.1204607294010010	0.7369248174967316	0.2683688786266443	T	T	T

Structure28

*CH₂COHO+H₂O

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	5

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4798503564294138	0.6886879195531482	0.1989174548712853	T	T	T
0.3359810033960908	0.5187202735887192	0.2005003854406673	T	T	T
0.3065345397761070	0.6639590947067125	0.1946152216479018	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F

0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F

0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2710881254411933	0.8369601861178950	0.2025850278947823	T	T	T
0.2166683119385849	0.7203965070311650	0.2117691878815941	T	T	T
0.2195518378482971	0.8880105090417555	0.2170311520409834	T	T	T
0.3570696484702505	0.8884195025334175	0.1829376190564443	T	T	T
0.0151117206089740	0.7424407786333483	0.2483815375227542	T	T	T
0.1491378175853811	0.8376182064991889	0.2298680838966357	T	T	T
0.1900032486543680	0.7038236821583099	0.2511017899180853	T	T	T
0.1457914924541859	0.6821971624796993	0.1880386142173114	T	T	T
0.0222103911386755	0.6803814310326162	0.2491559828265125	T	T	T
0.0079343066244253	0.7480860326193995	0.2817422770749434	T	T	T

Structure29

HOCH₂CHOHO

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	5

Selective dynamics

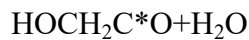
Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4690661371543391	0.6299105168735926	0.2027984680377659	T	T	T
0.2850792884563159	0.5289444195369907	0.1959282276305792	T	T	T
0.3676158678135732	0.7131776915532815	0.1931860642568256	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F

0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F

0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2532988350037718	0.8175537677957692	0.2208559195622413	T	T	T
0.1609634777575922	0.7065496889278755	0.2293327163471637	T	T	T
0.2234384081951891	0.8670369992061974	0.1821905439277418	T	T	T
0.3425368321145649	0.8194609963966331	0.2066194831313250	T	T	T
0.0674141658980650	0.7120661150827857	0.2375688997681067	T	T	T
0.1558544205160948	0.8573727193230158	0.1928076280223718	T	T	T
0.1781449305148434	0.6711970865857748	0.2616318933762659	T	T	T
0.1530865520020676	0.6604098049912549	0.1952893015264216	T	T	T
0.0231457516365806	0.6584657310779118	0.2613319183032465	T	T	T
0.2665522964448495	0.8634623474488291	0.2559600973342469	T	T	T

Structure30



1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	3	5

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4782253680274717	0.6609416038733837	0.2010213000923506	T	T	T
0.3060409230921195	0.5205377202999684	0.1987438491332285	T	T	T
0.3326313364379811	0.6937594935715402	0.1916044712043393	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F

0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F

0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2613393745943962	0.7702646359552237	0.2046530675911113	T	T	T
0.1555607829129260	0.7091781298781106	0.2304891595738969	T	T	T
0.1849283546359360	0.9703552441098989	0.1799946414414887	T	T	T
0.2963972845836955	0.8622629013414232	0.1919890134843712	T	T	T
0.1039707098110404	0.7677528475495266	0.2394210497583136	T	T	T
0.1229176727906637	0.9232046040476495	0.1990316243459028	T	T	T
0.1700473248003182	0.6788701504193227	0.2656932025098054	T	T	T
0.1083681692346188	0.6402028235240693	0.2063131756442660	T	T	T
0.0439929180739392	0.7260721994749995	0.2607872881361403	T	T	T
0.2295166450827061	0.9393095311147064	0.1862469373301348	T	T	T

Structure31

CH₃COO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	3

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4763614185375661	0.6454855535850536	0.2017677434202137	T	T	T
0.2934678813593881	0.5305946533110054	0.1983064149499415	T	T	T
0.3619332547310436	0.7133143614120774	0.1901759425136809	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F

0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F

0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2370529598450425	0.8112268859927030	0.2056220681471617	T	T	T
0.1813555867842432	0.7370550595821098	0.2491886858372931	T	T	T
0.2041750748608059	0.8667966450727175	0.1880548935872817	T	T	T
0.3215303788335679	0.8129978291535208	0.1882122831221635	T	T	T
0.2367064651661980	0.7506721369282672	0.2796379793382353	T	T	T
0.1499671185452704	0.6557714312993823	0.2368031607842542	T	T	T
0.1173892524383771	0.7473215992506060	0.2631893795131346	T	T	T

Structure32

CH₃COHO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4677066243814490	0.6305110768187754	0.2034736155767387	T	T	T
0.2751451163440408	0.5305390290429318	0.1947462526836431	T	T	T
0.3719877250748259	0.7158025906612733	0.1899224042481085	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F

0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2500258019276656	0.8106391287189022	0.2185583302655617	T	T	T
0.1810529008490704	0.7232728129026640	0.2529535256694494	T	T	T
0.2263103490215417	0.8856562633811057	0.2078228832430179	T	T	T
0.3293070428229826	0.8187779834933511	0.1983121119712365	T	T	T
0.2218149658144918	0.7335231948927784	0.2887949114815606	T	T	T
0.1694731598100850	0.6493992758216084	0.2366233954364084	T	T	T
0.1054489920161334	0.7180550068493925	0.2601295420630861	T	T	T
0.1625363882198224	0.8717611540234418	0.2251958273207881	T	T	T

Structure33

CH₃COO*H

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999	12.8033199130999993	0.0000000000000000		
0.0000000000000000	0.0000000000000000	26.7110004425000014		
Cu	N	C	O	H
4	9	64	2	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4749039612393310	0.6289392249394167	0.2015534089338769	T	T	T
0.2813610511480797	0.5256406801472054	0.1957445958469515	T	T	T
0.3754012709996615	0.7107705975956521	0.1920042462079355	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F

0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2442137217065798	0.8171581412775363	0.2166394730448001	T	T	T
0.1869148011723605	0.7276360433169595	0.2517528627796637	T	T	T
0.2210959431644694	0.8806647704437957	0.2024664595152149	T	T	T
0.3373448580441887	0.8234876774875378	0.1991422122243126	T	T	T
0.2353174601562631	0.7381418793284531	0.2848848606331422	T	T	T
0.1721988498554659	0.6542999285706171	0.2337127052051023	T	T	T
0.1135727722413001	0.7229636373489805	0.2629628248452106	T	T	T

0.3682170133915197 0.8812148459701903 0.1749086242466414 T T T

Structure34

CH₄+COO*

1.0000000000000000

14.7840003966999998 0.0000000000000000 0.0000000000000000

-7.3920001983999999 12.8033199130999993 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.7110004425000014

Cu N C O H

4 9 64 2 4

Selective dynamics

Direct

0.3883999883824316 0.6109899878387068 0.1237199976883616 F F F

0.4755845446011821 0.6131452131860792 0.1996177698310020 T T T

0.2818818106643254 0.5369972509558243 0.1968308635725388 T T T

0.3998819168986962 0.7190776927129693 0.1936957453326602 T T T

0.3273999989159151 0.6724299788206594 0.0770300030666817 F F F

0.3273600042078257 0.4895400106801233 0.0762199982880674 F F F

0.5102499723826810 0.6724500060481091 0.0761599987757577 F F F

0.9996700287274507 0.0001800000324650 0.0573600009216477 F F F

0.0003299999634265 0.3344300090962307 0.0625099986649431 F F F

0.9996899962509573 0.6666100025562471 0.0586999989901287 F F F

0.3332400024166660 0.0001599999854633 0.0586900003380535 F F F

0.6654199958038518 0.9995099902101501 0.0625599995251847 F F F

0.6666899919723832 0.3331600129459886 0.0612300001087860 F F F

0.3321700096157301 0.3312500119332853 0.0634699985367249 F F F

0.6686199903697627 0.6676899790852886 0.0635500028781806 F F F

0.9991999865008054 0.1663299948336885 0.0593199990547291 F F F

0.0001500000141448 0.5002700090658863 0.0620899982600847 F F F

0.9999099969734431 0.8333100080615523 0.0571499988286135 F F F

0.3328500091896487 0.1653199940614059 0.0589599981996258 F F F

0.3319799900125986 0.8348799943726348 0.0628399997826108 F F F

0.6658499836809995 0.1663399934903538 0.0614599995434091 F F F

0.6657000184196491 0.4994199871907909 0.0623999982923920 F F F

0.6680499911019240 0.8350800275685089 0.0631899982792987 F F F

0.1665399968694743 0.9999399781380731 0.0571300014870246 F F F

0.1647700071264779 0.3318099975501880 0.0630899965588227 F F F

0.1649599969669993 0.6678699851318157 0.0628300011305356 F F F

0.4995799959066858 0.9996899962566772 0.0621200017787373 F F F

0.5004400015054742 0.3341600000654878 0.0623699985549493 F F F

0.8335300087518434 0.0006599999888621 0.0593699999149706 F F F

0.8335000276869380 0.3339900076717370 0.0614399984580416 F F F

0.8345299959310495 0.6670100092759697 0.0590099990224289 F F F

0.1655199974769772 0.1649699956211279 0.0588000007106046 F F F

0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3332343291090298	0.8839900460371114	0.1993952762991621	T	T	T

0.1346663236560453	0.6594597365955891	0.2810811315652428	T	T	T
0.2802308130614445	0.9197115751095249	0.1900061774491749	T	T	T
0.3872727223551249	0.8483712819757883	0.2091499456245928	T	T	T
0.1874197192417089	0.6942739713063292	0.3130485769349098	T	T	T
0.0608881929108320	0.5930790082003563	0.2939623133658509	T	T	T
0.1188194485602852	0.7175329665209967	0.2639004198748358	T	T	T
0.1705637038285290	0.6319342173853291	0.2534531301520043	T	T	T

Structure35

CH₃CHOO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4657770734261124	0.6292376695229401	0.2042030487356850	T	T	T
0.2826204837703634	0.5497373828805636	0.1975190354980762	T	T	T
0.3841854768167346	0.7315597036592816	0.1896410360965249	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F

0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F

0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2565523662163358	0.8299703265137628	0.1969735704925791	T	T	T
0.1879573042821823	0.7403971154049869	0.2339287671390730	T	T	T
0.2066010620741253	0.8246864800161217	0.1541155996735737	T	T	T
0.3557365675533778	0.8361957927914712	0.1905392676542281	T	T	T
0.2279493328008693	0.7515363679834480	0.2700269509852779	T	T	T
0.1739061211216176	0.6664174152138965	0.2168134083194414	T	T	T
0.1125779958429031	0.7367054240273126	0.2399690261991368	T	T	T
0.2770888365448410	0.9048974145960597	0.2172255688921859	T	T	T

Structure36



1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	5

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4748743839168369	0.6597642423759066	0.2016431646035037	T	T	T
0.3001769112517537	0.5271223287210509	0.1984556401943546	T	T	T
0.3374761603011390	0.7040001982210840	0.1942467581169666	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F

0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F

0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.94238001111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2835211655402245	0.7923849769878659	0.2205245435470498	T	T	T
0.1925207897872332	0.7365998830162817	0.2570482197994516	T	T	T
0.2537092110801060	0.8327724758575807	0.1794656160642959	T	T	T
0.3671780449158802	0.8848510841689295	0.2448391507664679	T	T	T
0.1664152336173921	0.7910891358423465	0.2700816878959826	T	T	T
0.2146822733774343	0.7073728574114123	0.2900440907413296	T	T	T
0.1266215616344708	0.6696514622767752	0.2386232122705924	T	T	T
0.2354783507730484	0.8833009393495075	0.1933312687911859	T	T	T
0.3831859882596407	0.8625659117245666	0.2763031938889041	T	T	T

Structure37

CH₃CHOHO*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	5

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4663149183782191	0.6268292640410343	0.2031002750488433	T	T	T
0.2823076165771550	0.5316445750754593	0.1952464712415719	T	T	T
0.3710257807130588	0.7162186416058270	0.1926989958574349	T	T	T
0.327399989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F

0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F

0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2705184772190041	0.8316718155604936	0.2242398748385989	T	T	T
0.1944927745581485	0.7324612558424938	0.2528075700276897	T	T	T
0.2124516938287034	0.8536297165994943	0.1860859117764112	T	T	T
0.3495482823622154	0.8262976062534556	0.2006596581926452	T	T	T
0.2365281714911024	0.7152613576399605	0.2817825382444551	T	T	T
0.1591200907122040	0.6669593859092170	0.2261915618096031	T	T	T
0.1317989600954118	0.7400915228735993	0.2709804233158504	T	T	T
0.1760125284894678	0.8840453464246909	0.2034399176887006	T	T	T
0.3040151692044495	0.8994959771159272	0.2505327860750022	T	T	T

Structure38

CH₃CO*+H₂O

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	5

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4695639373291928	0.6212493781956795	0.2012968231717038	T	T	T
0.2840768384622285	0.5386424158839971	0.1977063044074894	T	T	T
0.3825282169153792	0.7213878518958597	0.1922396772014727	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F

0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F

0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2629269864335645	0.8218078768726514	0.2156172100867216	T	T	T
0.1829074991766449	0.7216905164438501	0.2395539426010219	T	T	T
0.2115156074313790	0.9737898531208996	0.1784567138104126	T	T	T
0.3444810725673454	0.8265444265511163	0.1986252160635638	T	T	T
0.1808828992085895	0.7358814531267746	0.2799815017306643	T	T	T
0.2022528231030510	0.6582923024301295	0.2336916864831195	T	T	T
0.1045622689221475	0.6982498200874712	0.2250845379829883	T	T	T
0.2103016316358783	0.0164382065646028	0.2058423494332938	T	T	T
0.2325496744676952	0.9252906425500894	0.1950580723230790	T	T	T

Structure39



1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O H
4 9 64 2 6

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4648606246473940	0.6048034029906986	0.2010908136597050	T	T	T
0.2748731560394414	0.5310358616224727	0.1936197345951261	T	T	T
0.3921689600731948	0.7143449565069115	0.1964524909122460	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F

0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3150111624452654	0.8334831016882869	0.2466624865518805	T	T	T
0.2310833872199345	0.7404237864680248	0.2724881139586914	T	T	T
0.1684636217824755	0.8996959510867953	0.1911523180454489	T	T	T
0.3819408339438923	0.8310456545605323	0.2186526621043217	T	T	T
0.2589603400583127	0.7314875506903465	0.3094861880641430	T	T	T
0.2111392940926350	0.6690985827542822	0.2507448191638864	T	T	T
0.1620480527758859	0.7487022645394763	0.2784107226001339	T	T	T
0.1220275781618468	0.9277192922564416	0.1960741653672690	T	T	T
0.3193131372286991	0.9096350347662920	0.2513893706711380	T	T	T
0.1737840445991609	0.8963827755722105	0.1548730635682532	T	T	T

Structure40

CH₃CHOHO*H

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	2	6

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4772723941839648	0.6299365847910584	0.2007291099232602	T	T	T
0.2868232584173071	0.5348218876448382	0.1977597637765525	T	T	T
0.3840912320429274	0.7197349509441580	0.1906350036791457	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F

0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2765195325757848	0.8424895305477071	0.2150366771134804	T	T	T
0.2656322430064844	0.8084227607392624	0.2690009391171762	T	T	T
0.1891468667854466	0.7688378715908489	0.1886140115181157	T	T	T
0.3737959176528142	0.8488615008661988	0.1960567039346766	T	T	T

0.3331287752877500	0.8642262095004566	0.2910742805096120	T	T	T
0.2593424934091613	0.7310343121098466	0.2706961535445971	T	T	T
0.1942073068495147	0.8019550990262669	0.2848320168148238	T	T	T
0.1884919613462047	0.7942667132469955	0.1549194716950464	T	T	T
0.2885703755260926	0.9220197314152568	0.2106932966501604	T	T	T
0.3914988375223561	0.8844878204788080	0.1635891320531192	T	T	T

Structure41



1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	1	4

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4596043953092761	0.6046801921152019	0.2025707438562477	T	T	T
0.2705346642843558	0.5365114117445404	0.1927103556021999	T	T	T
0.3929704661126489	0.7187567568592818	0.1943406005077922	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F

0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F

0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3169853944998203	0.8368916815209246	0.2447859496066516	T	T	T
0.2474213684083037	0.7460302299371021	0.2764490869378008	T	T	T
0.3793170577244047	0.8347257042980065	0.2131314109379504	T	T	T
0.2937189929333158	0.7287811555059380	0.3032118436995728	T	T	T
0.2066391573509804	0.6752707488928772	0.2524256709958465	T	T	T
0.1907283710797811	0.7586152473966554	0.2973218901908217	T	T	T
0.3140957436773210	0.9098954830716061	0.2474905604593713	T	T	T

Structure42



1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu N C O H
4 9 64 1 6

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4767606302833553	0.6224468775089463	0.2000064597543145	T	T	T
0.2844670184113550	0.5350426964698241	0.1970176943154922	T	T	T
0.3919186497416836	0.7202929323357500	0.1919784810063168	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F

0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F

0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.3317045268346591	0.8610240993497179	0.2483708463857186	T	T	T
0.2358180023810314	0.7632355472887478	0.2668965020640841	T	T	T
0.3727544188514800	0.8437729056009979	0.2015253983454232	T	T	T
0.2524129915455309	0.6987756050404293	0.2706296019977566	T	T	T
0.1691823050412700	0.7378106395481537	0.2413265766850067	T	T	T
0.2126442353874427	0.7777941422398564	0.3037949380007956	T	T	T
0.3162655177073744	0.9255783290627082	0.2419097144990589	T	T	T
0.3968529185577816	0.8877623588340980	0.2749216342050113	T	T	T
0.3335614355267980	0.8481076716106128	0.1731223470237350	T	T	T

Structure43



1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	64	1	7

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4634080160917425	0.6000102909223368	0.2003098206193247	T	T	T
0.2926285877648873	0.5744336770838464	0.1995092424778430	T	T	T
0.4382611989665887	0.7463391139893893	0.1910820152421392	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F
0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F

0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F
0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F

0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.2981969298630693	0.8573441374017721	0.3140561130484694	T	T	T
0.2098296874667740	0.7529913305327995	0.2947863017081379	T	T	T
0.4821430597767001	0.8842956174204857	0.1934119706550159	T	T	T
0.2112957292863225	0.6868718405913868	0.3128197316734219	T	T	T
0.2162463560039617	0.7454351743546298	0.2541338558647399	T	T	T
0.1328947632172105	0.7446391035983306	0.3023120368023366	T	T	T
0.2966260563752672	0.9235963989617524	0.2962574205798876	T	T	T
0.2930108284238272	0.8651498209662680	0.3547563319843859	T	T	T
0.4744161317646729	0.9076931222328002	0.2263602664294350	T	T	T
0.3750148379889189	0.8655326528404683	0.3062470913414597	T	T	T

Structure44

O*H

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	62	1	1

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4634099900707298	0.6000099778136345	0.2003100067523818	T	T	T
0.2926299869793780	0.5744299888558544	0.1995099932131623	T	T	T
0.4382599890270527	0.7463399768073415	0.1910800039851424	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F

0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F

0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.4821400046111322	0.8842999935052518	0.1934099942501604	T	T	T
0.4744200110684034	0.9076899886028187	0.2263599932176135	T	T	T

Structure45

H₂O*

1.0000000000000000

14.7840003966999998	0.0000000000000000	0.0000000000000000
-7.3920001983999999	12.8033199130999993	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.7110004425000014

Cu	N	C	O	H
4	9	62	1	2

Selective dynamics

Direct

0.3883999883824316	0.6109899878387068	0.1237199976883616	F	F	F
0.4651500862699671	0.5955047876313943	0.1997110794663279	T	T	T
0.2851814716709609	0.5669628361035106	0.1983531718066067	T	T	T
0.4335287845398628	0.7361989446016884	0.1913878594651489	T	T	T
0.3273999989159151	0.6724299788206594	0.0770300030666817	F	F	F
0.3273600042078257	0.4895400106801233	0.0762199982880674	F	F	F
0.5102499723826810	0.6724500060481091	0.0761599987757577	F	F	F

0.9996700287274507	0.0001800000324650	0.0573600009216477	F	F	F
0.0003299999634265	0.3344300090962307	0.0625099986649431	F	F	F
0.9996899962509573	0.6666100025562471	0.0586999989901287	F	F	F
0.3332400024166660	0.0001599999854633	0.0586900003380535	F	F	F
0.6654199958038518	0.9995099902101501	0.0625599995251847	F	F	F
0.6666899919723832	0.3331600129459886	0.0612300001087860	F	F	F
0.3321700096157301	0.3312500119332853	0.0634699985367249	F	F	F
0.6686199903697627	0.6676899790852886	0.0635500028781806	F	F	F
0.9991999865008054	0.1663299948336885	0.0593199990547291	F	F	F
0.0001500000141448	0.5002700090658863	0.0620899982600847	F	F	F
0.9999099969734431	0.8333100080615523	0.0571499988286135	F	F	F
0.3328500091896487	0.1653199940614059	0.0589599981996258	F	F	F
0.3319799900125986	0.8348799943726348	0.0628399997826108	F	F	F
0.6658499836809995	0.1663399934903538	0.0614599995434091	F	F	F
0.6657000184196491	0.4994199871907909	0.0623999982923920	F	F	F
0.6680499911019240	0.8350800275685089	0.0631899982792987	F	F	F
0.1665399968694743	0.9999399781380731	0.0571300014870246	F	F	F
0.1647700071264779	0.3318099975501880	0.0630899965588227	F	F	F
0.1649599969669993	0.6678699851318157	0.0628300011305356	F	F	F
0.4995799959066858	0.9996899962566772	0.0621200017787373	F	F	F
0.5004400015054742	0.3341600000654878	0.0623699985549493	F	F	F
0.8335300087518434	0.0006599999888621	0.0593699999149706	F	F	F
0.8335000276869380	0.3339900076717370	0.0614399984580416	F	F	F
0.8345299959310495	0.6670100092759697	0.0590099990224289	F	F	F
0.1655199974769772	0.1649699956211279	0.0588000007106046	F	F	F
0.1689099967855014	0.5010300278786701	0.0695900022914344	F	F	F
0.1661600023717327	0.8336899876319350	0.0583200007559981	F	F	F
0.5000299811505329	0.1666100025210966	0.0600900016626156	F	F	F
0.4982599914069894	0.5016000270702463	0.0694800019188762	F	F	F
0.4988099932978187	0.8309299945801385	0.0696299970120435	F	F	F
0.8332399726153312	0.1666100025210966	0.0610099993636766	F	F	F
0.8332399726178181	0.4998199939886163	0.0600900016626156	F	F	F
0.8348900079967692	0.8343399763111563	0.0588699989124351	F	F	F
0.0547900013529556	0.1105799972670667	0.0582499988478276	F	F	F
0.0574500001527696	0.4450300037547379	0.0647099986659398	F	F	F
0.0552599988734528	0.7778099775364282	0.0577500015516321	F	F	F
0.3890799879994375	0.1110199987696632	0.0590200014557141	F	F	F
0.3847500086142546	0.4413599968097515	0.0698899999278808	F	F	F
0.3856300115637481	0.7774099707386029	0.0697999968969185	F	F	F
0.7216899990961423	0.1110199987696632	0.0616299994282770	F	F	F
0.7213600277433585	0.4436900019336107	0.0609799995887954	F	F	F
0.7239000201781849	0.7793800235195363	0.0617300011113215	F	F	F
0.0548500008969128	0.2779600024177142	0.0611100010467140	F	F	F
0.0548699982635696	0.6113299727824142	0.0609100013869721	F	F	F

0.0557399988174794	0.9441199898966843	0.0569700002542319	F	F	F
0.3894000053534441	0.2770200073944125	0.0612200014192723	F	F	F
0.3885200023536157	0.9449700116936768	0.0609200000764787	F	F	F
0.7219600081768291	0.2778800130081720	0.0612899996210956	F	F	F
0.7228400111134903	0.6104599833518947	0.0612800009690204	F	F	F
0.7218999862732431	0.9449999928237744	0.0611900016818296	F	F	F
0.2224700004002287	0.1112700029890163	0.0579399988155274	F	F	F
0.2239000052058842	0.4420799910817479	0.0698800012383671	F	F	F
0.2217099964610867	0.7781400084212819	0.0611599981631770	F	F	F
0.5554500222519394	0.1106600016727199	0.0609599985034350	F	F	F
0.5538799763018645	0.4459800124308089	0.0648500025197052	F	F	F
0.5577600002220393	0.7759199738370555	0.0699200034090950	F	F	F
0.8886299729346163	0.1112200022076308	0.0597000010326383	F	F	F
0.8891900181671417	0.4444000124669500	0.0609400011618462	F	F	F
0.8885800242332564	0.7773900031831715	0.0579899996383304	F	F	F
0.2204699963058161	0.2759700119173587	0.0616400018241308	F	F	F
0.2224200070404621	0.6142200231952089	0.0697799995553297	F	F	F
0.2220399975825629	0.9445899725293785	0.0577399991557783	F	F	F
0.5561599731237834	0.2784900069045193	0.0609700009367202	F	F	F
0.5584899783382440	0.6151199936777303	0.0699099972694697	F	F	F
0.5548200011515050	0.9423800111137410	0.0647599995261743	F	F	F
0.8888199925564066	0.2781499922028985	0.0615999996534029	F	F	F
0.8888300061197185	0.6107800006620749	0.0590399987973029	F	F	F
0.8892800212255736	0.9450600147559953	0.0582900010185554	F	F	F
0.4895549086583598	0.8893367196557923	0.2041081545219007	T	T	T
0.4581602893087315	0.9113594943521099	0.2299144594836041	T	T	T
0.5649756423139066	0.9319331591363834	0.2077688129785838	T	T	T