

## Supporting Information

# Ru catalysts for levulinic acid hydrogenation with formic acid as a hydrogen source

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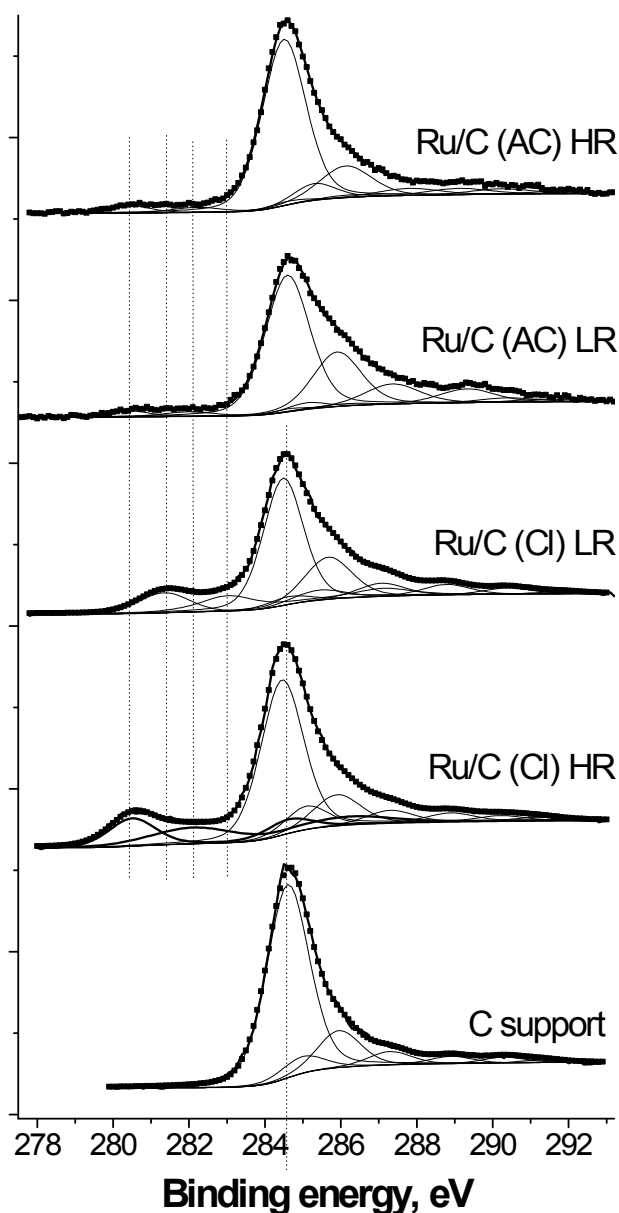
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**Supporting Information SI 1.** C 1s and Ru 3d XPS spectra of the Ru/C catalysts and of the bare carbon support material.



The carbon C 1s spectra of the carbon support displayed a usual pattern, with a major contribution at 284.6 eV corresponding to graphitic sp<sup>2</sup> carbon, a contribution at 285.1 eV due to aliphatic carbon resulting from the disordered structure of the high surface area activated carbon support, and contributions attributed with increasing binding energies to C-OH, C=O and COOH oxygenated surface groups, carbonate groups and surface plasmon peak/ $\pi \rightarrow \pi^*$  transition.

Due to a complex multi-contribution pattern, it is worth noting that the fit pattern of the C  $1s$  spectra tail is only used for allowing the low energy part of the spectra, *i.e.* corresponding to the Ru  $3d$  orbitals, to be fitted. The results were in agreement with those derived from the analysis of Ru  $3p$  spectra. They confirmed the presence of both Ru-based phases, *i.e.* metallic Ru<sup>0</sup> and Ru<sup>4+</sup>, and evidenced a shift towards higher binding energies for Ru  $3d$  orbitals in the case of the Ru/C (Cl) LR catalyst (*ca.* 1 eV).

### **Supporting Information SI 2 : catalytic activity**

In the LA hydrogenation, GVL was the only product observed. We did not observe any other components like the products of the GVL decomposition: 1,4-pentanediol and 2-Methyltetrahydrofuran (2-MTHF), or products of further reaction *e.g.* pentanoic acid (PA).

Additionally, in the control test performed only with bare active carbon, *i.e.* without any supported metal, 15% LA uptake was observed when 0.3 g of active carbon was used. When 0.6 g was used, around 20-25% uptake of LA was observed.

When the control test is performed in the presence of both GVL and LA components (in 1:1 molar ratio) with 0.6 g of active carbon, we observed the uptake of 15% of GVL and 5% of LA while no reaction products were detected by HPLC. Additionally when the same material was reused, no more uptake was observed. Therefore we conclude that this difference between LA conversion and GVL yield was only due to adsorption on the surface of active carbon.

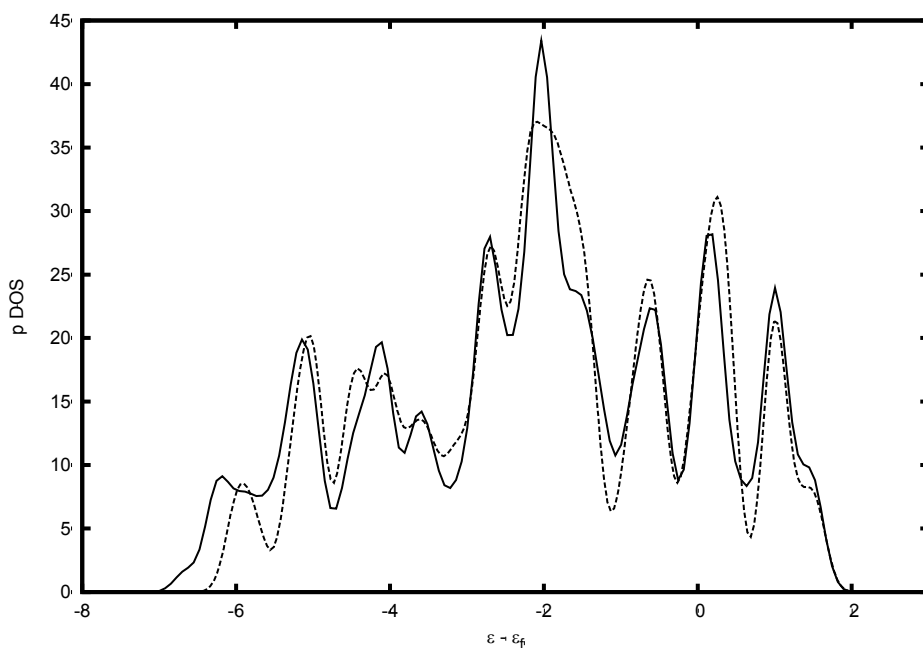
Below, Table 3A is a modification of Table 3 showing the molar ratio of products obtained in the gas phase. Based on that, the C balance is calculated. The reason for not closed carbon

balance is related probably to partial dissolution of CO<sub>2</sub> in the liquid phase or/and its remain on the catalysts as carbonates.

**Table 3A** Activity of selected metal catalysts in FA decomposition.

Catalyst	FA decomposition				Carbon balance	
	FA conversion [%]	Gaseous product amount [number of moles ×10 <sup>4</sup> ]				
		H <sub>2</sub>	CO	CH <sub>4</sub>	CO <sub>2</sub>	
Pd/C	23	0.41	0.10	0	0.26	0.86
Pt/C	31	0.45	0.08	0	0.26	0.71
Ru/C	48	0.24	0.08	0.08	0.22	0.90

### Supporting Information SI 3 : theoretical part



**Figure.** Projected density of states on the d orbitals of the top layer of Ru(0001) (dashed line) and of Ru(0001) covered by 1/4ML of chlorine (full line) in function of the energy relative to the Fermi level (eV).

## Coordinates of the structures obtained by DFT calculations in the VASP format

Acetone gas phase

C O H

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

C O H  
3 1 6

Direct

```
0.0756448317984794 0.1968148054082318 0.4871692912804564
0.0277317297787041 0.2530208797977044 0.5013598617288245
0.1162897051947694 0.1717010948019620 0.5452294861063364
0.0813824593140989 0.1726176289386174 0.4306310933526400
0.9987922531797154 0.2428008688439508 0.5470019860260754
0.9942533664280327 0.2615289656040903 0.4588022265273526
0.0568284043598859 0.2987944395766333 0.5112458764586471
0.1549108421851744 0.1365778654802526 0.5285360687614267
0.0825590608428567 0.1465168446763030 0.5808172875028770
0.1389386901921938 0.2138003184427030 0.5724679462995409
```

CO<sub>2</sub> gas phase

C O

```
1.0000000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
```

C O  
1 2

Direct

```
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0.5587745299031478 0.5000000000000000 0.5000000000000000
0.4412254700968523 0.5000000000000000 0.5000000000000000
```

dihydrogene molecule alone

```
1.0000000000000000
10.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.0000000000000000
```

H  
2

Direct

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0.0000000000000000 0.0000000000000000 0.0124555624429491
0.0000000000000000 0.0000000000000000 0.0875444375570524
```

HCOOH gas phase

C O H

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20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 20.0000000000000000
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C O H  
1 2 2

Direct

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0.4981543810404084 0.5000000000000000 0.5667175535972609
0.5545192583506022 0.5000000000000000 0.4679062965921272
0.5434034775764142 0.5000000000000000 0.5863355859412394
```

0.4519999735135204 0.5000000000000000 0.4773185892656350

iPrOH gas phase

C O H

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0.0000000000000000	20.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C O H  
3 1 8

Direct

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0.0980967067898509	0.0953198354347503	0.5006558874422232
0.2024659402261267	0.1226601304384184	0.4429995478392544
0.2015642257936879	0.1668090779564899	0.4638571510392795
0.1728986725563477	0.0279976311569525	0.4622626552717939
0.1885777371422962	0.0327101871573637	0.5864919996735338
0.2626647091297725	0.0580257773990129	0.5435844984585914
0.2089929121272935	0.1192276281270091	0.5805071752374780
0.0708632982538853	0.0992622727480559	0.4530793827731466
0.0731053103166049	0.0576599915030664	0.5320344651007771
0.0951338689993779	0.1437982303434190	0.5266824395431224

H on Cl-Ru

Ru H Cl

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0.0000000000000000	0.0000000000000000	7.3484692283495328

Ru H Cl  
64 1 4

Selective dynamics

Direct

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Hydrated Ru-Cl slab  
Ru O H Cl



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Ru O H Cl  
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Selective dynamics

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Ru-Cl Slab

Ru Cl

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4.0000000000000009	0.0000000000000000	0.0000000000000000
2.0000000000000004	3.4641016151377544	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.3484692283495328

Ru Cl

64 4

Selective dynamics

Direct

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F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1671453866770779	0.1671318154234060	0.2177238528618613	T	T
T	0.6671448406622769	0.1671361082418146	0.2177209858111320	T	T
T	0.1671439556363703	0.6671396767028972	0.2177243458314812	T	T

T	0.6671500398493604	0.6671363889718046	0.2177227710322448	T	T
T	0.4164727459901822	0.1669806878677260	0.2176779615668762	T	T
T	0.9164811234811445	0.1669767999780203	0.2176772127659530	T	T
T	0.4164796933078416	0.6669831479832012	0.2176802598794335	T	T
T	0.9164706618536341	0.6669858693763218	0.2176725876779607	T	T
T	0.1669871114232906	0.4164662229930239	0.2176777975045366	T	T
T	0.6669885598001190	0.4164665707145921	0.2176754825300297	T	T
T	0.1669932170220084	0.9164630805126301	0.2176807298959687	T	T
T	0.6669925700578270	0.9164625233917144	0.2176778039847959	T	T
T	0.4168623752442909	0.4168599582579007	0.2185593230513643	T	T
T	0.9168595525768249	0.4168634951627223	0.2185489171865264	T	T
T	0.4168577855672893	0.9168634322980972	0.2185506703473793	T	T
T	0.9168659960368248	0.9168535570099197	0.2185620855187030	T	T
T	0.0009803708505972	0.0009636552884077	0.3218407036372622	T	T
T	0.5009802430810633	0.0009677473523138	0.3218405382986925	T	T
T	0.0009839565226836	0.5009650127961545	0.3218412312368313	T	T
T	0.5009817743117861	0.5009670585385542	0.3218378890752907	T	T
T	0.2487912206991473	0.0011319958425370	0.3219081081551764	T	T
T	0.7487773580061778	0.0011521730338472	0.3218997797443510	T	T
T	0.2487815981978979	0.5011507532300510	0.3218986934731917	T	T
T	0.7487879704138295	0.5011436552955800	0.3218963192752338	T	T
T	0.2504762324475848	0.2504606869735083	0.3212855126664059	T	T
T	0.7504581637600797	0.2504856630950146	0.3212804493283138	T	T
T	0.2504772511635401	0.7504841553060903	0.3212829269359686	T	T
T	0.7504750445004980	0.7504810078662089	0.3212795070062837	T	T
T	0.5011548775466920	0.2487830179833223	0.3218977355318716	T	T
T	0.0011499649898326	0.2487748746564029	0.3219092369215826	T	T
T	0.5011608024491101	0.7487766711877664	0.3219118702435187	T	T
T	0.0011532865333433	0.7487846056003723	0.3219113068804285	T	T

	0.0833960718985771	0.0833855367464398	0.4197683432600128	T	T
T					
	0.5833933291271883	0.0833849199910714	0.4197657960025890	T	T
T					
	0.0833994572736454	0.5833813756504311	0.4197676741215328	T	T
T					
	0.5833967489910085	0.5833706166178483	0.4197671943801870	T	T
T					

Acetone Cl-Ru

Ru O H

2.7000000000000000		
4.0000000000000009	0.0000000000000000	0.0000000000000000
2.0000000000000004	3.4641016151377544	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.3484692283495328

Ru	C	O	H	Cl
64	3	2	8	4

Selective dynamics

Direct

	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					
	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					

F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.1675212890083841	0.1677924219832363	0.2211549030824500	F	F
F	0.6670573456327062	0.1677953087345827	0.2200431069047539	F	F
F	0.1680682302512650	0.6670185394974695	0.2201805504958756	F	F
F	0.6676729525762966	0.6677690948474151	0.2200798492508937	F	F
F	0.4147057634729663	0.1677834730540653	0.2211617072206238	F	F
F	0.9151592220210816	0.1677915559578338	0.2200567151811015	F	F
F	0.4145200658249450	0.6677748683501079	0.2201002616654151	F	F
F	0.9148871736269371	0.6670156527461231	0.2201873546340494	F	F
F	0.1679851838496589	0.4140496323006886	0.2216325535822889	F	F
F	0.6675630482801651	0.4148839034396659	0.2201274782181173	F	F
F	0.1680238218287329	0.9144073563425295	0.2200975400101441	F	F
F	0.6675506519557572	0.9143986960884902	0.2200961791825122	F	F
F	0.4163293711519529	0.4165062576960850	0.2217128424127495	F	F
F	0.9171762012789770	0.4164975974420528	0.2216992341364019	F	F
F	0.4162610604937456	0.9174528790125080	0.2221455856006429	F	F
F	0.9167632515982334	0.9164684968035388	0.2201070658035889	F	F
T	0.0029073107029013	0.0008706180543852	0.3219959664794714	T	T

T	0.5017129605851393	0.0018413976004413	0.3223571299871908	T	T
T	0.0022010383362807	0.5010667342571991	0.3226229404720573	T	T
T	0.4987622706191787	0.5042833297880568	0.3244910467177294	T	T
T	0.2456816757923030	0.0021842737218637	0.3224065639615131	T	T
T	0.7464597544216915	0.0021480664506791	0.3219218084234531	T	T
T	0.2459772089994818	0.5010937903302352	0.3226342084647594	T	T
T	0.7457793371013990	0.5056649379039525	0.3223746748081150	T	T
T	0.2501241702927423	0.2494745032100731	0.3225212892980163	T	T
T	0.7511847852823419	0.2491788159675408	0.3228839624775152	T	T
T	0.2484747424792720	0.7500741877937045	0.3220418543584974	T	T
T	0.7475058889999072	0.7480922508450297	0.3220383420748331	T	T
T	0.5003832511904026	0.2459342591957296	0.3224064987523172	T	T
T	0.0034599367211306	0.2450617995808000	0.3223166131842780	T	T
T	0.5052231956533036	0.7465109583831956	0.3224065689191052	T	T
T	0.0033217194323021	0.7462650921115199	0.3221755061951201	T	T
T	0.4229192739922417	0.5663657101298974	0.4831860058088092	T	T
T	0.3102147113262745	0.7169039302090809	0.4729087189373894	T	T
T	0.4506514931497136	0.5040511155037336	0.5517039384069466	T	T
T	0.4948028864224537	0.4901828552826827	0.4339909101575981	T	T
T	0.7515633323761034	0.2642694333196030	0.4322353632345005	T	T
T	0.4658127646020177	0.5742211010528255	0.5868635917092845	T	T
T	0.5422422892261111	0.3952472471049395	0.5532110310850784	T	T
T	0.3534724717823816	0.5039130407429516	0.5688076378430765	T	T
T	0.2483073163664950	0.7673268424700338	0.5185433949796486	T	T
T	0.2342504742716357	0.7211598335598591	0.4332862799620256	T	T
T	0.3595745214214934	0.7784909926975589	0.4544201992004367	T	T
T	0.7795101021024614	0.1774623893300855	0.4583936676622952	T	T
T	0.6524674909475977	0.3378740613654934	0.4453049397006476	T	T
T	0.0879357383122757	0.0791099552690878	0.4219154414006649	T	T



	0.5834909158599779	0.0790437519894011	0.4221462458450737	T	T
T					
	0.0789971410730896	0.5838132557267806	0.4223535072613499	T	T
T					
	0.6707862483276227	0.6671717092851415	0.4243788044849667	T	T
T					

CH3CH\_O\_CH3 on Ru-Cl

Ru C O H

2.7000000000000000		
4.0000000000000009	0.0000000000000000	0.0000000000000000
2.0000000000000004	3.4641016151377544	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.3484692283495328

Ru	C	O	H	Cl
64	3	2	9	4

Selective dynamics

Direct

	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					

F	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1676446482697974	0.1674437454224396	0.2177361912282883	T	T
T	0.6674073422919241	0.1672627919931434	0.2186342710561850	T	T
T	0.1669146345715755	0.6671726614153803	0.2184853252936097	T	T
T	0.6665578567475696	0.6665505683241032	0.2170598884044882	T	T
T	0.4158792917676500	0.1673067404858587	0.2177098590976695	T	T
T	0.9163889510632808	0.1662251803655138	0.2181141827424976	T	T
T	0.4165198147418899	0.6661667731682729	0.2189265184030698	T	T
T	0.9160988388694331	0.6681471738844037	0.2177973933099441	T	T
T	0.1674478901928106	0.4155550487781672	0.2176942147073717	T	T
T	0.6660770852012695	0.4161644492038156	0.2192350740844753	T	T
T	0.1666016240538832	0.9158494805182121	0.2179341825343677	T	T
T	0.6681476939585095	0.9163284477129021	0.2176871499160641	T	T
T	0.4170370184786110	0.4173550838131124	0.2193139330564773	T	T
T	0.9160948295007568	0.4159312089889651	0.2184250489798378	T	T
T	0.4170492524303320	0.9157507371244445	0.2181946938296710	T	T
T	0.9171816683985261	0.9172945201487359	0.2192071369275134	T	T

T	0.0036244196061118	0.0015918082739461	0.3208469583258408	T	T
T	0.5018934884809813	0.0012312199264869	0.3194971104965519	T	T
T	0.0015848480014422	0.5014328932695664	0.3194825237422031	T	T
T	0.4979178133694414	0.5025715460096268	0.3232369176803508	T	T
T	0.2465800615945770	0.0024507396353063	0.3195593633855395	T	T
T	0.7463664099847765	0.0018804739587330	0.3208303848829060	T	T
T	0.2452251137435830	0.5005964486373690	0.3202702661042747	T	T
T	0.7466051840195882	0.5058772284104375	0.3202519741805541	T	T
T	0.2498199520179363	0.2500080120255753	0.3189674174798349	T	T
T	0.7524813362815200	0.2486360757495019	0.3213143560339040	T	T
T	0.2488208007264062	0.7499629679048045	0.3206017490799176	T	T
T	0.7475251159857823	0.7481740634551528	0.3191592384902243	T	T
T	0.4991324691653548	0.2464867497164994	0.3201844721708511	T	T
T	0.0048792254232659	0.2445224933908671	0.3198450943784634	T	T
T	0.5057230179435167	0.7468615484696309	0.3204064330244496	T	T
T	0.0023972530296067	0.7461312733973887	0.3206556319265406	T	T
T	0.4044188081463144	0.5379197690356158	0.4768665943425346	T	T
T	0.3104678613010592	0.6988892020491148	0.4728034056786400	T	T
T	0.4806773530428416	0.4919145882120912	0.5445535890794521	T	T
T	0.5105726435412306	0.4861874056264188	0.4247794493477621	T	T
T	0.7475117816472403	0.2746227687784121	0.4274212262215795	T	T
T	0.5488559038771229	0.5395816862917815	0.5522443580688583	T	T
T	0.5473115632500148	0.3748811588201833	0.5469679666284339	T	T
T	0.4018417056172914	0.5267143890913512	0.5855736860171072	T	T
T	0.2313436153702215	0.7403253661944144	0.5137729124649610	T	T
T	0.2437775938212070	0.7307226979855698	0.4256710649772738	T	T
T	0.3740328195103984	0.7524926511892926	0.4737015083904051	T	T
T	0.7661391657296031	0.1930634844999034	0.4557180954944499	T	T
T	0.6421393159377660	0.3630706507387353	0.4357583313437662	T	T

T	0.3377225244359119	0.4876326060178522	0.4703668150076708	T	T
T	0.0909714542579505	0.0797683979801146	0.4193680939031456	T	T
T	0.5807746689997872	0.0796947900288629	0.4194831755974817	T	T
T	0.0757743743958564	0.5841599937245479	0.4191163521944836	T	T
T	0.6729781527233203	0.6694915408266736	0.4211859327886568	T	T

CH3C\_OH\_CH3 on Ru-Cl

Ru	C	O	H	Cl
1.0000000000000000				
10.799999999973024	0.0000000000000000	0.0000000000000000		
-5.399999999986512	9.3530743608696145	0.0000000000000000		
0.0000000000000000	0.0000000000000000	19.8408669165437317		

Ru	C	O	H	Cl
64	3	2	9	4

Selective dynamics

Direct

F	0.3333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.3333331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.5833332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.0833332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.0833331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.5833331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.5833339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.0833339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.3333339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F

F	0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
T	0.3341825871914888	0.1669673113475023	0.2178558214382082	T	T
T	0.8357562157417417	0.1685583136540297	0.2174699224306913	T	T
T	0.8325215271652724	0.6665671215064971	0.2176420568113308	T	T
T	0.3334536537685507	0.6673953844664965	0.2175917019358448	T	T
T	0.5842991485260015	0.1687335814307943	0.2177358620999513	T	T
T	0.0818837845056093	0.1666059776443748	0.2174720002271462	T	T
T	0.0839957542065757	0.6675894384184331	0.2178990144578968	T	T
T	0.5845468794529615	0.6670855924837499	0.2186157941609472	T	T
T	0.5832169161611430	0.4166341668025761	0.2191970556401347	T	T
T	0.0828121682135491	0.4153413452411105	0.2190338332840706	T	T
T	0.0825357048636180	0.9170656769784222	0.2181636225652042	T	T
T	0.5839752905030082	0.9159172933323750	0.2182304910709894	T	T
T	0.8331985655553527	0.4167318569680245	0.2180579334833784	T	T
T	0.3343685623170027	0.4177077717157348	0.2180905296827483	T	T
T	0.3314619394065270	0.9154384111419129	0.2178411244448027	T	T
T	0.8340939005417017	0.9159337098979222	0.2173761104795857	T	T

T	0.9921206393037124	0.9953398371445573	0.3206919919871447	T	T
T	0.5001805704807548	1.0005425397652743	0.3181762193573803	T	T
T	0.4989751915748344	0.5007267193265807	0.3223329353389299	T	T
T	-0.0000244168318356	0.5028711166125280	0.3205896678986864	T	T
T	0.2524244884663749	0.0034228134711247	0.3201809817872504	T	T
T	0.7559738874811398	0.0038262300857570	0.3210021449211059	T	T
T	0.7538756019239347	0.5035819762178221	0.3200731302930307	T	T
T	0.2516861096462786	0.5032282830172140	0.3194640700950118	T	T
T	0.4971703023159570	0.2465737821257337	0.3207019712514398	T	T
T	1.0060344573894437	0.2455123870405143	0.3252845637669822	T	T
T	0.9942350699443128	0.7477460981071002	0.3203601271072022	T	T
T	0.4950496971599367	0.7481055644906185	0.3201450433404939	T	T
T	0.7509433951073764	0.2468572242498251	0.3200133590533692	T	T
T	0.2477054522452300	0.2495788571135198	0.3189066188484956	T	T
T	0.2537627149996693	0.7483419429208831	0.3199915073994937	T	T
T	0.7566223216381034	0.7540619501064381	0.3197760922581745	T	T
T	0.0776619978806809	0.2552744585297970	0.4314804673057788	T	T
T	0.1190362388210919	0.3977000304258251	0.4634685916452684	T	T
T	0.9862810295468215	0.1341358740524413	0.4792248046313238	T	T
T	0.4834642808952981	0.4936320778983218	0.4321552080160928	T	T
T	0.2176686067321772	0.2560735310554272	0.4258676649710816	T	T
T	0.0487237398263034	0.1437089154262686	0.5250465213512135	T	T
T	0.3933173371092908	0.4069949212032413	0.4453336311686758	T	T
T	0.1637448171586269	0.4050390676585478	0.5144462413273914	T	T
T	0.2030901428470757	0.4893703533007015	0.4347018339880333	T	T
T	0.0264455521412638	0.4132831703530247	0.4672472672757879	T	T
T	0.5610943468817984	0.4945882444384852	0.4580124970192328	T	T
T	0.9474728422745313	0.0275954190161653	0.4568163549065699	T	T
T	0.8928418855356002	0.1411415343218941	0.4949740731343536	T	T

	0.2111641133995730	0.1713716631339633	0.4480292649520941	T	T
T					
	0.9123896711639926	0.5836954952447555	0.4200217873185431	T	T
T					
	0.3846673465582751	0.1021693165766538	0.4245670014403966	T	T
T					
	0.3806690382149098	0.7640917552454115	0.4247512538931152	T	T
T					
	0.6908193716042487	0.0995387780904140	0.4195357614113913	T	T
T					

iPrOH on Cl-Ru

Ru C O H Cl

2.7000000000000000			
4.0000000000000009	0.0000000000000000	0.0000000000000000	
2.0000000000000004	3.4641016151377544	0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.3484692283495328	

Ru	C	O	H	Cl
64	3	2	10	4

Selective dynamics

Direct

	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					

F	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1680155933787058	0.1676161801222859	0.2187982233912638	T	T
T	0.6677868721754183	0.1681412671651332	0.2179478601687492	T	T
T	0.1672033548602504	0.6657117593783060	0.2174341458611639	T	T
T	0.6665840126113479	0.6685084305476499	0.2183245717886070	T	T
T	0.4156656873016025	0.1670126267787263	0.2188913541327291	T	T
T	0.9147805785691215	0.1681344325718662	0.2177362317389172	T	T
T	0.4158632915944735	0.6683628688320036	0.2183616146464987	T	T
T	0.9150082750110521	0.6670473150349074	0.2177154473949543	T	T
T	0.1677408626688743	0.4158768981814723	0.2184627678396866	T	T
T	0.6679796223412080	0.4150473249818348	0.2177276726767615	T	T
T	0.1679369405885003	0.9163646913839604	0.2179940547688710	T	T
T	0.6662032171026235	0.9160380521387924	0.2181091324090912	T	T
T	0.4164244852473450	0.4159143875616986	0.2192341868697294	T	T
T	0.9176182729688318	0.4177159465710533	0.2186893498626486	T	T
T	0.4166880419524800	0.9175813477835235	0.2194320668307515	T	T
T	0.9164484813434555	0.9160618152035912	0.2187593426294445	T	T



T	0.0001816400383744	0.0036952224062394	0.3197231383960161	T	T
T	0.5025877053371063	0.0019044130895497	0.3215233685844689	T	T
T	0.9956529952994573	0.5077640004357059	0.3205600061035984	T	T
T	0.5043693285318084	0.5000440707176846	0.3201069173636980	T	T
T	0.2452139992642209	0.0030849025535284	0.3208255291365244	T	T
T	0.7470561465224627	0.0027390062618844	0.3203348378381257	T	T
T	0.2448965953436478	0.5057293993866937	0.3211260934739705	T	T
T	0.7480892007586483	0.5037726926697056	0.3210735255065320	T	T
T	0.2499363680398024	0.2510925834754056	0.3224196947028747	T	T
T	0.7501191347728762	0.2492132496980669	0.3198693552841311	T	T
T	0.2469029337109977	0.7488048977780934	0.3197063968465724	T	T
T	0.7556664014192060	0.7441252511499971	0.3201298589991852	T	T
T	0.5048561733563576	0.2453827612263486	0.3205260787205007	T	T
T	0.9997304239594967	0.2472089997059332	0.3201654970726215	T	T
T	0.5037877557898983	0.7465027285022433	0.3207219741049766	T	T
T	0.0039279719807478	0.7441928916666645	0.3208456849815576	T	T
T	0.9516413525854258	0.5476397693828946	0.5250423263431011	T	T
T	0.0756730645461706	0.5080171790026157	0.5724925709315020	T	T
T	0.8126361452910312	0.5905193083240821	0.5616620836660458	T	T
T	0.9905786077194345	0.4216272218376724	0.4831799555212933	T	T
T	0.2446197678486089	0.2713792743256808	0.4309960579464737	T	T
T	0.9183344017393180	0.4476631527153697	0.4474116611972475	T	T
T	0.0912157788855484	0.4197122268443105	0.6056689328397487	T	T
T	0.1751011457671067	0.4758053534390161	0.5445772364415590	T	T
T	0.0528001660072742	0.6006724525021815	0.6040529334206053	T	T
T	0.1453798393910406	0.3318097512103615	0.4517512695187080	T	T
T	0.2930850889337790	0.1820067654572733	0.4564890500974054	T	T
T	0.8249265836547023	0.5036264705490279	0.5949703695157327	T	T
T	0.7255059777795273	0.6156270182004425	0.5259089813164612	T	T

T	0.7819884293147389	0.6862759424294851	0.5924303723345438	T	T
T	0.9378865297624203	0.6347718065017274	0.4912132308732224	T	T
T	0.0813603697392334	0.0796442652912085	0.4192985155288199	T	T
T	0.5890420119751510	0.0795493894894126	0.4197417685934271	T	T
T	0.1688954453663129	0.6663803662025446	0.4216851475442183	T	T
T	0.5789614052195249	0.5866258775581243	0.4191964184821197	T	T

Acetone\_CH3CH\_O\_CH3 on Cl-Ru

Ru C O H Cl Ru C O H

2.7000000000000000								
4.0000000000000009	0.0000000000000000	0.0000000000000000	0.0000000000000000					
2.0000000000000004	3.4641016151377544	0.0000000000000000	0.0000000000000000					
0.0000000000000000	0.0000000000000000	7.3484692283495328						

Ru	C	O	H	Cl
64	3	2	9	4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208392	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.4166667055208394	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666661586767972	0.9166676826464056	0.0000000000000000	F	F
F	0.6666661586767975	0.9166676826464056	0.0000000000000000	F	F
F	0.4166660421142722	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166661586767973	0.9166676826464056	0.0000000000000000	F	F
F	0.9166661586767975	0.9166676826464056	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F

F	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.5000001165625252	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625251	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1681853840230233	0.1666878696695127	0.2181225120127738	T	T
T	0.6676704726528366	0.1675705014578385	0.2183631071414240	T	T
T	0.1669501150101622	0.6678456622801038	0.2177018620149190	T	T
T	0.6666194110386860	0.6669436816662720	0.2174185814329277	T	T
T	0.4156017151208838	0.1677938134207189	0.2175471097176151	T	T
T	0.9162778978215035	0.1666990998576525	0.2183098941153378	T	T
T	0.4162611808295797	0.6667936679786940	0.2182721068155145	T	T
T	0.9175622719631267	0.6673014600778872	0.2174170215591357	T	T
T	0.1672769144258178	0.4153428179637295	0.2175749934261796	T	T
T	0.6675363285653518	0.4157017835104215	0.2192426278617437	T	T
T	0.1669220578154096	0.9166889833687311	0.2179607723022135	T	T
T	0.6678377116804175	0.9158808248019171	0.2179228464842217	T	T
T	0.4170045741478821	0.4171929709917991	0.2181571636302319	T	T
T	0.9172772323197178	0.4161321572166772	0.2190958385295090	T	T
T	0.4163839361644258	0.9163140111050738	0.2181546460133051	T	T

T	0.9178356204792509	0.9171937339036156	0.2188980535460904	T	T
T	0.0047552749497802	0.0017167986898435	0.3205335511961666	T	T
T	0.5001640906370253	0.0033773747060652	0.3193796734999341	T	T
T	0.9995071404936680	0.5055961485833859	0.3210859621616868	T	T
T	0.4993656630126437	0.5006586905128896	0.3214669567652171	T	T
T	0.2472545506302121	0.0023705698134535	0.3203768068616392	T	T
T	0.7470717707525277	0.0018632964622839	0.3201827926972018	T	T
T	0.2507503878762987	0.4983368599664187	0.3201066543087882	T	T
T	0.7477918032228545	0.5066967324925634	0.3209003902722146	T	T
T	0.2511032300485542	0.2498784804894447	0.3193022375482166	T	T
T	0.7520038089179867	0.2485593415679949	0.3212872311195047	T	T
T	0.2497692516462809	0.7499560736283939	0.3199886318609789	T	T
T	0.7535016369844616	0.7452290246902322	0.3194830745766381	T	T
T	0.4996862204785652	0.2473087406980644	0.3196346098158352	T	T
T	0.0055655934148996	0.2445382474790809	0.3202334954317360	T	T
T	0.5043467564834954	0.7471774125914802	0.3199955454882679	T	T
T	0.0006885485456187	0.7459967555930932	0.3206051709334332	T	T
T	0.3815974699454348	0.5274737147153895	0.4645670621688042	T	T
T	0.2804506864847189	0.6844150766666341	0.4685449447373906	T	T
T	0.3790219642240549	0.4366418905965427	0.5206046971638262	T	T
T	0.4961021132039861	0.4794405517179167	0.4291947423330487	T	T
T	0.7514815966436774	0.2642347582450725	0.4300240722695633	T	T
T	0.4349244300162979	0.4512975122893226	0.5638479247084405	T	T
T	0.4358880235478224	0.3232726627371282	0.5066818257197659	T	T
T	0.2693704267840216	0.4705469983425882	0.5364541857026821	T	T
T	0.1689395210677600	0.7114746056437438	0.4741381004582027	T	T
T	0.2952595896169710	0.7423213637660689	0.4254949367181082	T	T
T	0.3103961411417656	0.7244379389117590	0.5133959279602754	T	T
T	0.7812896019765626	0.1778375848528869	0.4567877497824304	T	T

T	0.6507934743135696	0.3374062548078974	0.4426419423667332	T	T
T	0.2739554396516606	0.4840654983201051	0.4047653003206309	T	T
T	0.0902301473846180	0.0798688767702105	0.4200477436406062	T	T
T	0.5808748812908305	0.0778820091960343	0.4192377061975173	T	T
T	0.9585292881409679	0.6554711935658304	0.4244069483445870	T	T
T	0.6406073724282773	0.6608996232758285	0.4232611923896952	T	T

Acetone\_CH3CH\_O\_CH3 on Ru-Cl

Ru C O H Cl

1.0000000000000000		
10.799999999973024	0.0000000000000000	0.0000000000000000
-5.399999999986512	9.3530743608696145	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.8408669165437317

Ru	C	O	H	Cl
64	3	2	9	4

Selective dynamics

Direct

F	0.3333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.3333331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.5833332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.0833332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.0833331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.5833331779166286	0.6666663558332644	0.0000000000000000	F	F
F	0.5833339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.0833339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.3333339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F

F	0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.3333452182585575	0.1668403897356043	0.2190100198857436	F	F
F	0.8332657395010372	0.1671485762781728	0.2180966924904197	F	F
F	0.8341096670450909	0.6658735310134958	0.2186827551305015	F	F
F	0.3329428839174184	0.6669488555762300	0.2180442379847491	F	F
F	0.5850567797975259	0.1691288459513345	0.2182650546365181	F	F
F	0.0829030279833418	0.1657147011991356	0.2187578380800872	F	F
F	0.0839510213043084	0.6670614489542288	0.2186628204708612	F	F
F	0.5823803965470447	0.6649644068098723	0.2182666800664066	F	F
F	0.5839965986976097	0.4173452756263671	0.2191665974304939	F	F
F	0.0830830235491291	0.4170108746758672	0.2177450229176685	F	F
F	0.0827874305448546	0.9160461091115693	0.2192604098910849	F	F
F	0.5846881990549804	0.9154531899438183	0.2191011892260448	F	F
F	0.8331761857991182	0.4163088836717179	0.2185773878826325	F	F
F	0.3345042302157566	0.4171923270049902	0.2188861347513793	F	F
F	0.3309867135685636	0.9150731675009141	0.2182652178848130	F	F

F	0.8350128544990199	0.9175815934999036	0.2183255608083101	F	F
F	0.9909888963281261	0.9928995394876239	0.3226793340519762	F	F
F	0.5007675069033297	0.9995109673334994	0.3204160080348686	F	F
F	0.5074604075270415	0.5091675774001629	0.3226721513928510	F	F
F	0.0034905219569623	0.4964955305797432	0.3226801037026235	F	F
F	0.2571151109521495	0.0049408115492682	0.3224543025136555	F	F
F	0.7583664433479385	0.0073244597152211	0.3208448162634312	F	F
F	0.7510343624182667	0.5071625616144004	0.3223751326891460	F	F
F	0.2481071346675776	0.5072728975884644	0.3214595734495376	F	F
F	0.4952245466507819	0.2432994586676216	0.3224783129189888	F	F
F	0.9930097507424733	0.2519672516846114	0.3215840141746682	F	F
F	0.9928323243249793	0.7488804419167110	0.3223426769116742	F	F
F	0.4928351665962936	0.7415833421298359	0.3207989897065175	F	F
F	0.7546777754545246	0.2468073582881019	0.3214845094874548	F	F
F	0.2477419040569586	0.2516409299502769	0.3217304042575932	F	F
F	0.2536960677006235	0.7458253838378184	0.3214797477987830	F	F
F	0.7547221997207743	0.7446898603714729	0.3219233510490653	F	F
T	0.0720532662850530	0.2569380167398023	0.4302248843278704	T	T
T	0.1301416800817279	0.4038773013072046	0.4607100948669398	T	T
T	0.9728852406513084	0.1446432065795022	0.4803197628235196	T	T
T	0.4741995074725409	0.4856275264752696	0.4325903886584754	T	T
T	0.1928031234106911	0.2341702086987283	0.4224611533796008	T	T
T	0.0383108641509082	0.1472964180241831	0.5236934215212727	T	T
T	0.3875579187814111	0.3935537140289824	0.4431726167021282	T	T
T	0.1810859123629172	0.4099349855168697	0.5099672413668017	T	T
T	0.2165813019642258	0.4909522470394663	0.4303393231596502	T	T
T	0.0455594858939250	0.4305810588639361	0.4680773090586143	T	T
T	0.5518027259604352	0.4936366999237265	0.4611427893055833	T	T
T	0.9197132059816084	0.0360513102682489	0.4590982459485247	T	T

T	0.8912135780600607	0.1679571736452630	0.4988583828681854	T	T
T	0.1244746151328400	0.1002676981073520	0.3915004379433356	T	T
T	0.9122111458433935	0.5821262274896668	0.4215960808569008	T	T
T	0.3898588115928234	0.1098332451013349	0.4258300734870204	T	T
T	0.3818730302201203	0.7639976546510283	0.4258160566337139	T	T
T	0.6852805426836426	0.0933645164600634	0.4191076782758885	T	T

CH3CH\_O\_CH3\_iPrOH on Cl-Ru  
 Ru C O H Cl

1.0000000000000000		
10.799999999973024	0.0000000000000000	0.0000000000000000
-5.399999999986512	9.3530743608696003	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.8408669165437423

Ru	C	O	H	Cl
64	3	2	10	4

Selective dynamics

Direct

F	0.3333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333331779166289	0.6666663558332645	0.0000000000000000	F	F
F	0.3333331779166287	0.6666663558332645	0.0000000000000000	F	F
F	0.5833332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.0833332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.0833331779166286	0.6666663558332645	0.0000000000000000	F	F
F	0.5833331779166288	0.6666663558332645	0.0000000000000000	F	F
F	0.5833339578857277	0.4166679157714627	0.0000000000000000	F	F
F	0.0833339578857273	0.4166679157714627	0.0000000000000000	F	F
F	0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333339578857279	0.4166679157714627	0.0000000000000000	F	F
F	0.3333339578857278	0.4166679157714627	0.0000000000000000	F	F
F	0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333338413232027	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F



F	0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.3343204621124158	0.1667495698740069	0.2184708811960122	F	F
F	0.8357995920449498	0.1678792286950284	0.2176225296384757	F	F
F	0.8331021439368345	0.6656271093127232	0.2173675178720060	F	F
F	0.3352426771054625	0.6677476307006175	0.2177427249192974	F	F
F	0.5830804265597180	0.1669711505597178	0.2182490181069668	F	F
F	0.0829500630678695	0.1680218038045851	0.2181677711579511	F	F
F	0.0843853274616535	0.6677041733438713	0.2178641346289254	F	F
F	0.5831062447278015	0.6674012762102706	0.2177438171069853	F	F
F	0.5831167753876514	0.4166168747229266	0.2188385453791071	F	F
F	0.0827703298809439	0.4147868485040433	0.2181692587694926	F	F
F	0.0842734551875211	0.9166403916106064	0.2177017291694981	F	F
F	0.5822664077649337	0.9159537149513285	0.2176405919100830	F	F
F	0.8327452975965032	0.4164710665057427	0.2186286993647855	F	F
F	0.3346775094004215	0.4171776197858037	0.2192626125626660	F	F
F	0.3338156043111979	0.9174358155030973	0.2191279275943643	F	F

F	0.8330852273119405	0.9154880148805447	0.2179428153054914	F	F
F	0.0021939310514227	0.0012444101656399	0.3198081136224858	F	F
F	0.5047061537426458	0.0009969493698634	0.3205036865137956	F	F
F	0.5045349271384154	0.5057641880720425	0.3223646363903968	F	F
F	0.0028578517875886	0.5011232045712931	0.3197366571075904	F	F
F	0.2477264878982552	0.0018532162265643	0.3208113064910379	F	F
F	0.7467432379926322	0.9993758316732341	0.3196359206822947	F	F
F	0.7531986681129084	0.5071592759655346	0.3206144186670131	F	F
F	0.2471411086598536	0.5000505114039342	0.3224799608628218	F	F
F	0.5008181579539936	0.2497571632883293	0.3214061567929747	F	F
F	0.0005234867364763	0.2497108320199146	0.3198926909608986	F	F
F	0.9966131379445713	0.7470633294605449	0.3194486880820904	F	F
F	0.5050650377813923	0.7517463977157632	0.3198625251471868	F	F
F	0.7501818701289977	0.2444709873391276	0.3198587645629232	F	F
F	0.2450935216755639	0.2454030474737508	0.3214106854775807	F	F
F	0.2493142655689908	0.7459726144640300	0.3205922894621551	F	F
F	0.7481184364390643	0.7478721896632123	0.3196666545245678	F	F
T	0.4611103089433437	0.5716965282265202	0.4780535240667464	T	T
T	0.6133995527580094	0.6633467874266923	0.5021581539092697	T	T
T	0.3578523045088055	0.4888866303417514	0.5345715765406400	T	T
T	0.5165749206373551	0.2720513676473391	0.4294414697938955	T	T
T	0.4528355476325354	0.4693947936916553	0.4279722322887644	T	T
T	0.4273514395364429	0.6413705141047434	0.4527609629349998	T	T
T	0.4873660301734953	0.3460721518869427	0.4407348274165998	T	T
T	0.6174853299377994	0.7380071793697505	0.5409702842726246	T	T
T	0.6546028775819698	0.5972725193386357	0.5237522464145813	T	T
T	0.6834827548631317	0.7266960125870552	0.4603576348859751	T	T
T	0.4607738542546459	0.1868709077353039	0.4571115701745713	T	T
T	0.3916047130351907	0.4201732867043170	0.5601002831207270	T	T

T	0.3567643860894548	0.5637984804485435	0.5717834584783776	T	T
T	0.2488559546138549	0.4217308825049472	0.5151510760031039	T	T
T	0.3338581562358283	0.4221725290611218	0.3866675407395820	T	T
T	0.1698280834117249	0.5889706703638511	0.4192252774267166	T	T
T	0.6702244140442937	0.0806252628376722	0.4192941168633771	T	T
T	0.8740712084796399	0.6329636153863047	0.4240470754308521	T	T
T	0.1579513665683803	0.0740155318169654	0.4198191644518197	T	T

CH3C\_OH\_CH3\_iPrOH on Cl-Ru

Ru C O H Cl

1.0000000000000000

10.799999999973024 0.0000000000000000 0.0000000000000000

-5.399999999986512 9.3530743608695985 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.8408669165437423

Ru C O H Cl

64 3 2 10 4

Selective dynamics

Direct

F	0.3333332899999988	0.1666665899999984	0.0000000000000000	F	F
F	0.8333332899999988	0.1666665899999984	0.0000000000000000	F	F
F	0.8333331799999968	0.6666663600000007	0.0000000000000000	F	F
F	0.3333331799999968	0.6666663600000007	0.0000000000000000	F	F
F	0.5833332899999988	0.1666665899999984	0.0000000000000000	F	F
F	0.0833332899999988	0.1666665899999984	0.0000000000000000	F	F
F	0.0833331799999967	0.6666663600000007	0.0000000000000000	F	F
F	0.5833331799999968	0.6666663600000007	0.0000000000000000	F	F
F	0.5833339599999974	0.4166679200000019	0.0000000000000000	F	F
F	0.0833339599999974	0.4166679200000019	0.0000000000000000	F	F
F	0.0833338400000017	0.9166676800000033	0.0000000000000000	F	F
F	0.5833338400000017	0.9166676800000033	0.0000000000000000	F	F
F	0.8333339599999974	0.4166679200000019	0.0000000000000000	F	F
F	0.3333339599999974	0.4166679200000019	0.0000000000000000	F	F
F	0.3333338400000017	0.9166676800000033	0.0000000000000000	F	F
F	0.8333338400000017	0.9166676800000033	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111700000009	F	F

F	0.5000000000000000	0.0000000000000000	0.1111111700000009	F	F
F	0.4999998799999972	0.4999997700000023	0.1111111700000009	F	F
F	0.9999998799999971	0.4999997700000023	0.1111111700000009	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111700000009	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111700000009	F	F
F	0.7499998799999972	0.4999997700000023	0.1111111700000009	F	F
F	0.2499998799999972	0.4999997700000023	0.1111111700000009	F	F
F	0.4999999400000021	0.2499998799999972	0.1111111700000009	F	F
F	0.9999999400000021	0.2499998799999972	0.1111111700000009	F	F
F	0.0000005500000029	0.7500010899999978	0.1111111700000009	F	F
F	0.5000005500000029	0.7500010899999978	0.1111111700000009	F	F
F	0.2499999400000021	0.2499998799999972	0.1111111700000009	F	F
F	0.7499999400000020	0.2499998799999972	0.1111111700000009	F	F
F	0.7500005500000029	0.7500010899999978	0.1111111700000009	F	F
F	0.2500005500000027	0.7500010899999978	0.1111111700000009	F	F
F	0.3357500700000031	0.1676626499999969	0.2183969299999972	F	F
F	0.8354029699999971	0.1676744499999998	0.2177674499999966	F	F
F	0.8322539400000011	0.6653214999999975	0.2174506300000018	F	F
F	0.3358258199999966	0.6680430099999981	0.2175853199999977	F	F
F	0.5828218799999973	0.1672497100000001	0.2185602799999984	F	F
F	0.0828878800000012	0.1674122699999998	0.2175558100000003	F	F
F	0.0846271799999982	0.6670543500000008	0.2173222799999976	F	F
F	0.5839150099999983	0.6672869300000031	0.2191741700000023	F	F
F	0.5837412799999981	0.4157875499999975	0.2204120999999972	F	F
F	0.0827596700000013	0.4146651399999968	0.2175514699999965	F	F
F	0.0843871699999994	0.9166339800000004	0.2169939799999980	F	F
F	0.5824179399999992	0.9152227900000015	0.2178717899999967	F	F
F	0.8321348300000013	0.4165256100000008	0.2190596299999967	F	F
F	0.3348733999999993	0.4167279400000012	0.2191804099999999	F	F

F	0.3342116600000011	0.9170429699999970	0.2191753800000029	F	F
F	0.8323774999999998	0.9146800500000012	0.2178727699999996	F	F
F	0.0026986900000026	0.0007772100000025	0.3190160999999989	F	F
F	0.5053204900000026	0.0008280400000018	0.3203471400000026	F	F
F	0.5051117000000005	0.5048540599999995	0.3239255299999967	F	F
F	0.0044713799999982	0.5008440900000011	0.3191890399999977	F	F
F	0.2476693300000008	0.0019185900000025	0.3200638900000001	F	F
F	0.7474375700000027	0.9995999699999986	0.3197521399999985	F	F
F	0.7536601400000009	0.5070472700000010	0.3222666300000014	F	F
F	0.2475823700000035	0.5007949199999970	0.3200241600000027	F	F
F	0.4990006299999976	0.2473221600000031	0.3223425600000027	F	F
F	0.0014176099999972	0.2503912600000007	0.3191181299999996	F	F
F	0.9988228100000001	0.7483016600000028	0.3174940600000014	F	F
F	0.5029123500000026	0.7511441099999985	0.3200264399999995	F	F
F	0.7504994499999995	0.2450268899999983	0.3202124999999967	F	F
F	0.2462663599999999	0.2449132599999970	0.3200365900000008	F	F
F	0.2492424300000025	0.7449954200000022	0.3203605499999966	F	F
F	0.7502060899999989	0.7487754699999982	0.3212523600000026	F	F
F	0.5141560499999969	0.5356798299999994	0.4615896099999972	F	F
T	0.6262121719467754	0.5290118046041179	0.5032984760239800	T	T
T	0.4966013481661389	0.6608292920647644	0.4814612594032864	T	T
T	0.3875444645261812	0.4031058507853401	0.4677216108327545	T	T
T	0.4933829114743816	0.2377079068698176	0.4314840174245034	T	T
T	0.3054329616245334	0.4066280197083731	0.4486216324042552	T	T
T	0.5806587395787297	0.4979134432586634	0.5545390872349863	T	T
T	0.6547530789323055	0.4503780383965215	0.4860472936899198	T	T
T	0.7216629864210302	0.6345714746610520	0.5067198612568709	T	T
T	0.4372365583904967	0.2817457106931028	0.4487147432562764	T	T
T	0.4542215811091950	0.1436117911186557	0.4525870600084377	T	T

T	0.4543019450490389	0.6429346181098178	0.5334510829819086	T	T
T	0.4224508734887321	0.6749690192818260	0.4488790715922686	T	T
T	0.6005018687964643	0.7597664606987746	0.4804349590304208	T	T
T	0.5960523132459696	0.6541252167488950	0.3798182137658213	T	T
T	0.1675801807654691	0.5791932595377617	0.4188040668415399	T	T
T	0.6712457981876225	0.0796708717550482	0.4192991643034785	T	T
T	0.8981045008279698	0.6483560047033500	0.4225433737213773	T	T
T	0.1531142794950909	0.0734696829873714	0.4191022681139948	T	T

CO2 on Cl-Ru

Ru C O Cl

2.7000000000000000			
4.0000000000000009	0.0000000000000000	0.0000000000000000	
2.0000000000000004	3.4641016151377544	0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.3484692283495328	

Ru C O Cl  
64 1 2 4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F

F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1681098373910584	0.1663722984369264	0.2180775092279744	T	T
T	0.6677133559231913	0.1673329435864569	0.2180563563256697	T	T
T	0.1658659521090470	0.6663747328486249	0.2175730734901875	T	T
T	0.6675975769097140	0.6675664409573522	0.2182797869203028	T	T
T	0.4160598934329719	0.1663782764865417	0.2185921296088645	T	T
T	0.9153333167574197	0.1671534039387207	0.2178178588717583	T	T
T	0.4162120833582522	0.6679221566341061	0.2182275584276992	T	T
T	0.9145551227795944	0.6678227563970528	0.2169898008587347	T	T
T	0.1656611977763104	0.4166075364537625	0.2189650410312677	T	T
T	0.6675926788268679	0.4153676926697438	0.2178919167773065	T	T

T	0.1679970344224091	0.9160677290474070	0.2179029950638301	T	T
T	0.6663510122623926	0.9160729762070713	0.2179572587726430	T	T
T	0.4163477562165031	0.4162459112282125	0.2192411759617366	T	T
T	0.9173649635321681	0.4174115082781606	0.2186239354786946	T	T
T	0.4171826561435965	0.9168000034950102	0.2191515140974725	T	T
T	0.9161182591009770	0.9161217146809412	0.2183906485483406	T	T
T	0.0010336217974218	0.0018644295097874	0.3196199159056800	T	T
T	0.5046072634008100	0.9995269398037410	0.3210603252811927	T	T
T	0.0050319726219974	0.4968214575658788	0.3238142985096135	T	T
T	0.5038458495555540	0.5015119383337935	0.3202918102699038	T	T
T	0.2457322490124730	0.0018371338692268	0.3206033410646065	T	T
T	0.7460376624816931	0.0019446020266389	0.3200571633149095	T	T
T	0.2453663380431572	0.5054539493082927	0.3210929072216213	T	T
T	0.7469010965929540	0.5018084975779852	0.3202177543451190	T	T
T	0.2476571742422395	0.2531505118364980	0.3212599759375538	T	T
T	0.7489086545282388	0.2505739444564560	0.3194140214854279	T	T
T	0.2478181648137234	0.7481525682424884	0.3193347227191781	T	T
T	0.7502502165502785	0.7491488846130960	0.3202526012045084	T	T
T	0.0010220848797619	0.2467171758309341	0.3199103183929284	T	T
T	0.5042906983412678	0.2451723779117650	0.3206867255810833	T	T
T	0.0052812695990848	0.7457042974678486	0.3211973889633236	T	T
T	0.5049569549892190	0.7454355660085451	0.3208471349531825	T	T
F	0.0762869664512258	0.4190395544697447	0.4217512647299415	T	T
T	0.2038482497969318	0.3023045269540183	0.4225272912849484	T	T
T	0.0047531691163833	0.4790070762169643	0.4722128817189840	T	T
T	0.0825828448233954	0.0779972261449221	0.4186170367682026	T	T
T	0.5863017572073583	0.0807201033673278	0.4192863773025625	T	T
T	0.1663535964997484	0.6746781330711947	0.4209502140719570	T	T
T	0.5835612289901108	0.5852131351606938	0.4193198138227090	T	T



COOH on Cl-Ru

Ru	C	O	H	Cl	
2.7000000000000000					
4.0000000000000009				0.0000000000000000	0.0000000000000000
2.0000000000000004				3.4641016151377544	0.0000000000000000
0.0000000000000000				0.0000000000000000	7.3484692283495328

Ru	C	O	H	Cl	
64	1	2	1	4	

Selective dynamics

Direct

0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F				

F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1662991980310927	0.1679875369835333	0.2184745411494001	T	T
T	0.6689030224114794	0.1676097580250662	0.2171414586737872	T	T
T	0.1673598542367541	0.6680701598146835	0.2176354122830201	T	T
T	0.6683058865087697	0.6657072426215855	0.2180822652944540	T	T
T	0.4165660727839256	0.1671276139208533	0.2182149086532042	T	T
T	0.9158701903588762	0.1681360740580722	0.2180425939855391	T	T
T	0.4149599847325686	0.6674616114281695	0.2177079841929748	T	T
T	0.9166149316774135	0.6659790197138785	0.2178553022671973	T	T
T	0.1665109349056227	0.4159684594159708	0.2179462751359813	T	T
T	0.6677486302306299	0.4149173360231303	0.2181139126937767	T	T
T	0.1675092975577534	0.9151909295008135	0.2178708098943863	T	T
T	0.6664064617491984	0.9175224061624205	0.2173516126083582	T	T
T	0.4171933095366415	0.4162715251541216	0.2182497086697294	T	T
T	0.9170777987627636	0.4163077905876752	0.2191114723136824	T	T
T	0.416315728772957	0.9175119781560533	0.2190387362845058	T	T
T	0.9161204039375737	0.9178468440524330	0.2184793996897812	T	T
T	0.0019435508332058	0.0026860529725939	0.3201912008280718	T	T
T	0.5056089949324808	0.9991440704586826	0.3206666978094489	T	T
T	0.0025648317207349	0.5026016415139993	0.3204960334789043	T	T
T	0.5018591437371202	0.5018755355901294	0.3202894460206896	T	T
T	0.2454862443690801	0.0010007993375163	0.3203856154593189	T	T

T	0.7455434978691088	-0.0000315124535867	0.3210981216309420	T	T
T	0.2469225689756020	0.5035066400457069	0.3197128544044596	T	T
T	0.7457567431154160	0.5000161054441624	0.3205401940672913	T	T
T	0.2530705599075435	0.2494117072167429	0.3208838768035600	T	T
T	0.7483167045814900	0.2497467797532754	0.3201607511776484	T	T
T	0.2509255805566404	0.7507911778686259	0.3195632314449472	T	T
T	0.7486630877634504	0.7540036988541150	0.3191307534414833	T	T
T	0.4996819929689639	0.2477252436886691	0.3237611720951010	T	T
T	0.0004809294370594	0.2464487116386487	0.3209561455049462	T	T
T	0.5013271214863161	0.7452758840168990	0.3200263123384405	T	T
T	0.0023187249760050	0.7472865767012815	0.3196089629794899	T	T
T	0.4231972582658711	0.2523981875671565	0.4189936524122533	T	T
T	0.3078837423534793	0.2463034290674475	0.4238696097271450	T	T
T	0.4773918919979385	0.2588958827056677	0.4783930733403106	T	T
T	0.5659330407647946	0.2622951705992732	0.4726264937343061	T	T
T	0.0813126341866674	0.0839666619530858	0.4193975879159766	T	T
T	0.6736499264584725	0.9070032190690840	0.4211313412017351	T	T
T	0.0779373726958650	0.5890879847600956	0.4188569318871690	T	T
T	0.5862424696628847	0.5815911557209491	0.4193590510265631	T	T

HCOOH on Cl-Ru

Ru C O H Cl

2.7000000000000000				
4.0000000000000009	0.0000000000000000	0.0000000000000000	0.0000000000000000	
2.0000000000000004	3.4641016151377544	0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	0.0000000000000000	7.3484692283495328	

Ru C O H Cl  
64 1 2 2 4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F

F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1679781928968439	0.1679777063095453	0.2191587255935052	T	T
T	0.6678841218333419	0.1679563354438934	0.2178648230019996	T	T

T	0.1679574812875793	0.6678841253220473	0.2178651326172763	T	T
T	0.6674906100960345	0.6674903196908143	0.2181966113107035	T	T
T	0.4152337104379914	0.1676169774095193	0.2188861845257483	T	T
T	0.9153881243441245	0.1679933903437276	0.2181595615221385	T	T
T	0.4151640848761714	0.6677068316923893	0.2181083091502986	T	T
T	0.9157594085970258	0.6670931077894355	0.2178802043966313	T	T
T	0.1676172736989513	0.4152337576935881	0.2188856335054925	T	T
T	0.6677063840601569	0.4151653599878581	0.2181079419621014	T	T
T	0.1679949034558591	0.9153871451587986	0.2181593708761009	T	T
T	0.6670938925001924	0.9157587701286299	0.2178799021042634	T	T
T	0.4165001439306147	0.4164995796734982	0.2199469420852947	T	T
T	0.9172815115456495	0.4166894617303928	0.2193934857092421	T	T
T	0.4166900034549775	0.9172807890659112	0.2193935328441461	T	T
T	0.9170407174977157	0.9170386185034564	0.2179594302593967	T	T
T	0.0020149075951498	0.0020142630996389	0.3200817487730312	T	T
T	0.5046836153334184	0.0006795970221164	0.3206477766641689	T	T
T	0.0006808081520508	0.5046828259806195	0.3206474609323414	T	T
T	0.5021495850959077	0.5021492295817803	0.3212270840387248	T	T
T	0.2458243355080052	0.0009589087731095	0.3208686652217176	T	T
T	0.7473976726401135	0.0015892143438076	0.3196407421981619	T	T
T	0.2452867904707092	0.5050746335861818	0.3212892320090031	T	T
T	0.7455624911986402	0.5023799097159569	0.3208427827300039	T	T
T	0.2507771394717578	0.2507767245031207	0.3234421221778697	T	T
T	0.7496957957885407	0.2506121530345549	0.3198492442347688	T	T
T	0.2506089468448865	0.7496993472342750	0.3198495042901365	T	T
T	0.7500160565496248	0.7500169292684541	0.3192981961036263	T	T
T	0.5050753609949675	0.2452857319353779	0.3212897147624761	T	T
T	0.0009587608530970	0.2458248936329883	0.3208687892266732	T	T
T	0.5023804058251047	0.7455620475003313	0.3208428428745844	T	T

T	0.0015899620129750	0.7473961223260563	0.3196413650771601	T	T
T	0.2832526080886958	0.2832341108996319	0.4832909353027340	T	T
T	0.3535623877218931	0.3535655033664395	0.4844089936110814	T	T
T	0.2449315268481724	0.2449155047062136	0.4321278340042827	T	T
T	0.2593512030776669	0.2593087601548316	0.5338160002453711	T	T
T	0.3732460260311288	0.3732674836024025	0.4371186985373253	T	T
T	0.0792945714463424	0.0792935260578715	0.4192072499691243	T	T
T	0.5982677302807232	0.0689749824236049	0.4192789192988845	T	T
T	0.0689745296632673	0.5982653743867934	0.4192791322593462	T	T
T	0.5849203272341954	0.5849183015620901	0.4197783772152858	T	T

HCOO\_a Cl-Ru

Ru C O H Cl

2.7000000000000000				
4.0000000000000009	0.0000000000000000	0.0000000000000000	0.0000000000000000	
2.0000000000000004	3.4641016151377544	0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.3484692283495328		

Ru	C	O	H	Cl
64	1	2	1	4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F

F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1665409320259994	0.1680896306179051	0.2185901943122951	T	T
T	0.6674445291966802	0.1679718028889008	0.2187830383995468	T	T
T	0.1676387030148738	0.6676425410554996	0.2175781539911503	T	T
T	0.6682650497610856	0.6659329463969658	0.2180594652768841	T	T
T	0.4161244713858607	0.1677209475459100	0.2194198780355096	T	T
T	0.9154717305156872	0.1685166268796623	0.2180883878512985	T	T
T	0.4154147163191542	0.6675285517772389	0.2178262249237559	T	T
T	0.9166093019509660	0.6660698920232621	0.2178096361331821	T	T
T	0.1670801913860699	0.4158519178184140	0.2183634030560601	T	T
T	0.6677920673880423	0.4153877983409201	0.2182216073912258	T	T
T	0.1675708418382438	0.9154338961666797	0.2178226184629534	T	T

T	0.6665046450965630	0.9171979326318249	0.2172386186047089	T	T
T	0.4174527138665926	0.4159732181116318	0.2192306450176958	T	T
T	0.9173050688106277	0.4163489045855182	0.2191665939001836	T	T
T	0.4165868785839789	0.9177112422677948	0.2188276803039469	T	T
T	0.9161802394573504	0.9179577230455581	0.2183296902542862	T	T
T	0.0021851250805103	0.0027314428007422	0.3199805416750730	T	T
T	0.5064532166507714	0.9975627672487584	0.3204682276892393	T	T
T	0.0025539907041587	0.5027649921929987	0.3206450652616006	T	T
T	0.5013734578212832	0.5033037317104425	0.3202001717158838	T	T
T	0.2453656611609639	0.0012913737861854	0.3202678329861002	T	T
T	0.7471914851068570	0.9983905442976941	0.3205941784731354	T	T
T	0.2459007676833830	0.5052991277621957	0.3199320774950169	T	T
T	0.7461744327388253	0.5004733039164379	0.3207833830261588	T	T
T	0.2516637993548604	0.2499376752103447	0.3216510533814482	T	T
T	0.7510347456655376	0.2510512226695956	0.3202416671869194	T	T
T	0.2500234485998755	0.7506665652545400	0.3192665775524667	T	T
T	0.7485190564684113	0.7543645937854653	0.3192430831100667	T	T
T	0.5003067991797094	0.2490678604893339	0.3226010918117981	T	T
T	0.0005560043837516	0.2463541394634957	0.3212082670169830	T	T
T	0.5016198913487793	0.7465676507904146	0.3200499045945032	T	T
T	0.0018559135789723	0.7477830770508638	0.3196612845916133	T	T
T	0.3744716403974346	0.2515099124167677	0.4567573290322072	T	T
T	0.2748026798767045	0.2418577300564921	0.4272611347110146	T	T
T	0.4770445573279692	0.2574928236503591	0.4282839284030125	T	T
T	0.3715739758179971	0.2550298014113713	0.5122986058976422	T	T
T	0.0817326724341327	0.0816166858522212	0.4192749670347708	T	T
T	0.6714450955381212	0.9104736763801350	0.4210773184882168	T	T
T	0.0792057383614511	0.5892763591621391	0.4189676182591079	T	T
T	0.5845842890464550	0.5824150429903528	0.4193726690506104	T	T



HCOO\_b on Cl-Ru

Ru C O H Cl

2.7000000000000000				
4.0000000000000009	0.0000000000000000	0.0000000000000000	0.0000000000000000	
2.0000000000000004	3.4641016151377544	0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	0.0000000000000000	7.3484692283495328	

Ru	C	O	H	Cl
64	1	2	1	4

Selective dynamics

Direct

0.1666667049999973	0.1666665899999984	0.0000000000000000	F	F
F				
0.6666667049999973	0.1666665899999984	0.0000000000000000	F	F
F				
0.1666667049999973	0.6666665899999984	0.0000000000000000	F	F
F				
0.6666667049999973	0.6666665899999984	0.0000000000000000	F	F
F				
0.4166667049999973	0.1666665899999984	0.0000000000000000	F	F
F				
0.9166667049999973	0.1666665899999984	0.0000000000000000	F	F
F				
0.4166667049999973	0.6666665899999984	0.0000000000000000	F	F
F				
0.9166667049999973	0.6666665899999984	0.0000000000000000	F	F
F				
0.1666660400000026	0.4166679149999979	0.0000000000000000	F	F
F				
0.6666660400000026	0.4166679149999979	0.0000000000000000	F	F
F				
0.1666660400000026	0.9166679149999979	0.0000000000000000	F	F
F				
0.6666660400000026	0.9166679149999979	0.0000000000000000	F	F
F				
0.4166660400000026	0.4166679149999979	0.0000000000000000	F	F
F				
0.9166660400000026	0.4166679149999979	0.0000000000000000	F	F
F				
0.4166660400000026	0.9166679149999979	0.0000000000000000	F	F
F				
0.9166660400000026	0.9166679149999979	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111700000009	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111700000009	F	F
F				
0.0000000000000000	0.5000000000000000	0.1111111700000009	F	F
F				
0.5000000000000000	0.5000000000000000	0.1111111700000009	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111700000009	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111700000009	F	F
F				
0.2500000000000000	0.5000000000000000	0.1111111700000009	F	F
F				
0.7500000000000000	0.5000000000000000	0.1111111700000009	F	F
F				

F	0.2500000599999979	0.2499998850000011	0.1111111700000009	F	F
F	0.7500000599999979	0.2499998850000011	0.1111111700000009	F	F
F	0.2500000599999979	0.7499998850000011	0.1111111700000009	F	F
F	0.7500000599999979	0.7499998850000011	0.1111111700000009	F	F
F	0.0000000599999979	0.2499998850000011	0.1111111700000009	F	F
F	0.5000000599999979	0.2499998850000011	0.1111111700000009	F	F
F	0.0000000599999979	0.7499998850000011	0.1111111700000009	F	F
F	0.5000000599999979	0.7499998850000011	0.1111111700000009	F	F
T	0.1666971730175719	0.1658665253936119	0.2188847168975675	T	T
T	0.6669762302499722	0.1661899872962412	0.2192247038890749	T	T
T	0.1658436123833545	0.6680420652729342	0.2188104555611672	T	T
T	0.6665297637539080	0.6672187055315472	0.2190394087487658	T	T
T	0.4176811180750555	0.1660094592562738	0.2179866407574026	T	T
T	0.9171859747671202	0.1651063070051101	0.2184921098435122	T	T
T	0.4162415512655200	0.6670493537888040	0.2173095864021207	T	T
T	0.9173988047862626	0.6651944566254786	0.2180270838975616	T	T
T	0.1648431676023610	0.4177943207388931	0.2179097565483560	T	T
T	0.6661105866501703	0.4158793784704986	0.2180568244827062	T	T
T	0.1639149245016455	0.9180597717350247	0.2188550940564446	T	T
T	0.6655949069880011	0.9180431339964109	0.2187566014742116	T	T
T	0.4174831644044700	0.4161532610363855	0.2179237673499239	T	T
T	0.9178441966302292	0.4174946600428531	0.2179694289858579	T	T
T	0.4168497328752684	0.9166306331962565	0.2177886310311724	T	T
T	0.9163408137004923	0.9182733874929365	0.2184468072032643	T	T
T	0.9982606388773306	0.5017126306757682	0.3196929264059729	T	T
T	0.4974588902959148	0.5044189915274864	0.3194407633797146	T	T
T	0.9992207611303516	0.0003464921634025	0.3207621369638441	T	T
T	0.4947746986332056	0.9998658407204749	0.3204060786984018	T	T
T	0.2546679037964459	0.9973742569859118	0.3215832738024417	T	T

T	0.7530087032926741	0.9962973898256507	0.3214473884299616	T	T
T	0.2506142276933139	0.4975597578743043	0.3199196010564091	T	T
T	0.7531498157806481	0.4955782311054556	0.3202014635194945	T	T
T	0.2505530438627954	0.2530462763590465	0.3193933220010865	T	T
T	0.7538168128977182	0.2504808461955086	0.3210268886392432	T	T
T	0.2543132560171046	0.7495444342634839	0.3210611341659629	T	T
T	0.7530578556465761	0.7510755130090712	0.3208064495881294	T	T
T	0.4949985504869122	0.2525892612834016	0.3204981432148373	T	T
T	0.9958698275638826	0.2525637057218028	0.3204734438922862	T	T
T	0.4953902875499532	0.7490017715722119	0.3199506101766493	T	T
T	0.9950877498810321	0.7527926803396299	0.3205068804025398	T	T
T	0.3579025090399821	0.0172351850942642	0.4753283352170007	T	T
T	0.2547538689116493	0.0267650642102526	0.5057184698985795	T	T
T	0.3732032163414305	0.0034204069106752	0.4087965609513503	T	T
T	0.4488381204084601	0.0186709732169744	0.5002876068435360	T	T
T	0.3349987482003550	0.3382051290535075	0.4192479441757945	T	T
T	0.8337901121938721	0.3316213033496082	0.4194677132949792	T	T
T	0.4153378953247316	0.6627261144574373	0.4211657599448864	T	T
T	0.8331423077729312	0.8338986978861811	0.4198026649564087	T	T

HCOO\_c on Cl-Ru

Ru	C	O	H	Cl	
	2.7000000000000000				
	4.0000000000000009		0.0000000000000000		0.0000000000000000
	2.0000000000000004		3.4641016151377544		0.0000000000000000
	0.0000000000000000		0.0000000000000000		7.3484692283495328

Ru	C	O	H	Cl
64	1	2	1	4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F

0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F				
0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F				
0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F				
0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F				
0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F				
0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F				

0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
F				
0.1675191477658100	0.1678947968630880	0.2189834555491086	T	T
T				
0.6672280778819205	0.1678305650789589	0.2181003858285108	T	T
T				
0.1680508108677447	0.6672313530059688	0.2181564176276287	T	T
T				
0.6675636750296379	0.6678403548249957	0.2183071941913370	T	T
T				
0.4153082024453448	0.1679116315107642	0.2189936935143167	T	T
T				
0.9156359992087169	0.1677265551017221	0.2179762048028422	T	T
T				
0.4153062071164478	0.6677881359942867	0.2182381091036990	T	T
T				
0.9154819296315928	0.6671935255211152	0.2180083270594486	T	T
T				
0.1676685608200146	0.4155683796959702	0.2189532661987799	T	T
T				
0.6675184827829370	0.4156501035750745	0.2181488953343782	T	T
T				
0.1677125999859921	0.9156179131959012	0.2180187940200529	T	T
T				
0.6671602153746239	0.9156461793956637	0.2179868235113524	T	T
T				
0.4167285204046046	0.4168326905682793	0.2195475022798920	T	T
T				
0.9172111514457830	0.4169229630196459	0.2194165879556981	T	T
T				
0.4164837505413383	0.9177559313264314	0.2198008552641386	T	T
T				
0.9168879224829906	0.9167513256620442	0.2178061549684488	T	T
T				
0.0013643811922019	0.0020198821894987	0.3196489930096983	T	T
T				
0.5049417736846556	0.0009540349406347	0.3211652883514899	T	T
T				
0.0008037899176994	0.5048063967307432	0.3208564842055059	T	T
T				
0.5024945505536338	0.5031705867527396	0.3208909331467327	T	T
T				
0.2449186669159724	0.0011414363696525	0.3211256835475755	T	T
T				
0.7476138518624341	0.0015388308123442	0.3197247145841738	T	T
T				
0.2455192293955161	0.5048761333831170	0.3210541509563982	T	T
T				
0.7455058921751452	0.5030314708372212	0.3208539565146554	T	T
T				
0.2505409412595518	0.2494506001908567	0.3225474038228575	T	T
T				
0.7499854161456574	0.2507117255366598	0.3194661935533835	T	T
T				
0.2507161872461751	0.7503233627948233	0.3197020163675627	T	T
T				
0.7498924185084268	0.7502158045695296	0.3196237025352651	T	T
T				

T	0.0004722093499032	0.2457011681782298	0.3207835687784201	T	T
T	0.5048852061284307	0.2455532678266592	0.3210437870182170	T	T
T	0.0015972765880334	0.7474441910939024	0.3198533654424928	T	T
T	0.5026135608824124	0.7458978950343110	0.3210540714363977	T	T
T	0.2898840265353082	0.1687149483616277	0.4731106598133517	T	T
T	0.2745834765938622	0.1987863388108270	0.5336562366725843	T	T
T	0.2421220692184678	0.2654921394857176	0.4252579161209438	T	T
T	0.3462687830084213	0.0553311446030585	0.4559000813550717	T	T
T	0.0711318229774149	0.0805614865324743	0.4194850997733535	T	T
T	0.5983356891227865	0.0795867828504968	0.4195235895433175	T	T
T	0.0777612273100022	0.5945379191492051	0.4188688892627688	T	T
T	0.5837708321139301	0.5831183926318873	0.4196682328958177	T	T

CO2 desorption on Cl-Ru

Ru	C	O	Cl		
	2.7000000000000000				
	4.0000000000000009	0.0000000000000000	0.0000000000000000		
	2.0000000000000004	3.4641016151377544	0.0000000000000000		
	0.0000000000000000	0.0000000000000000	7.3484692283495328		

Ru C O Cl  
64 1 2 4

Selective dynamics

Direct					
F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F

F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1658588782945145	0.1662489493327115	0.2191515317943953	T	T
T	0.6677620281288483	0.1671026656672510	0.2162000684804539	T	T
T	0.1660678220034626	0.6669596380468548	0.2190805005318808	T	T
T	0.6662490176737990	0.6654601476216868	0.2189337443980719	T	T
T	0.4165170867742845	0.1675228776165767	0.2182706483859747	T	T
T	0.9161704135267499	0.1675456918206422	0.2186446657366901	T	T
T	0.4170473320162458	0.6674063110355632	0.2190129785758543	T	T
T	0.9175775286684100	0.6643733296074359	0.2185514961153956	T	T
T	0.1646963870564520	0.4174538761923330	0.2186883659316692	T	T

T	0.6669880060738862	0.4166501165941057	0.2187657485355032	T	T
T	0.1674259610473641	0.9171467752222071	0.2188525980704981	T	T
T	0.6665614033101690	0.9177668309989073	0.2184741983254170	T	T
T	0.4169347398463756	0.4158128937824586	0.2180450995408805	T	T
T	0.9161150325992224	0.4166663820289926	0.2173732198236777	T	T
T	0.4160108676350731	0.9168900038117940	0.2177502380867367	T	T
T	0.9162820728948162	0.9169782754045670	0.2173425726888070	T	T
T	0.0026091293157293	0.0026603560916953	0.3207545352843724	T	T
T	0.5073121076641840	0.9991280953001578	0.3216972237157378	T	T
T	0.9974196634874986	0.5033008317924157	0.3221675071831882	T	T
T	0.4996597014716642	0.5045438006280349	0.3217334245486754	T	T
T	0.2471974607560341	0.9962208317886407	0.3223673619027423	T	T
T	0.7438607723015025	0.9985469093958486	0.3218099681352982	T	T
T	0.2461249271208956	0.5053813514242833	0.3214253209070392	T	T
T	0.7506589629119063	0.4930552771318943	0.3233789637541875	T	T
T	0.2524882580498868	0.2496811606002538	0.3208652658385844	T	T
T	0.7512313250077938	0.2529087869318332	0.3207446429578695	T	T
T	0.2517239771643744	0.7495562703467229	0.3206246180401848	T	T
T	0.7489826415774772	0.7554842832742921	0.3209030834835218	T	T
T	0.4978102449349677	0.2453047860121842	0.3241982507918024	T	T
T	0.9916708682898303	0.2501685303705941	0.3225833059665533	T	T
T	0.4974785013912992	0.7484233053368214	0.3227019989607669	T	T
T	0.0012827977433147	0.7469986940629170	0.3216419017747043	T	T
T	0.4213802442667429	0.2471663315821715	0.4214313909871379	T	T
T	0.4832493009553076	0.2521017892162334	0.4725823949491925	T	T
T	0.3005448410520444	0.2427258341503631	0.4215925621282111	T	T
T	0.0805901757067531	0.0814120534764626	0.3795803032547553	T	T
T	0.6686869432776064	0.9141130933994290	0.3823356389470050	T	T
T	0.0813018049267953	0.5872387952017348	0.3792788348860299	T	T



0.5834913393137313 0.5819353216415450 0.3785130355901662 T T  
T

HCOO\_a\_to\_b on Cl-Ru  
Ru C O H Cl

2.7000000000000000  
3.9999999999990008 0.0000000000000000 0.0000000000000000  
1.9999999999995004 3.4641016151368942 0.0000000000000000  
0.0000000000000000 0.0000000000000000 7.3484692283495301

Ru C O H Cl  
64 1 2 1 4

Selective dynamics

Direct

0.1666667055208393 0.1666665889583143 0.0000000000000000 F F  
F 0.6666667055208393 0.1666665889583143 0.0000000000000000 F F  
F 0.1666668220833714 0.6666663558332644 0.0000000000000000 F F  
F 0.6666668220833714 0.6666663558332644 0.0000000000000000 F F  
F 0.4166667055208393 0.1666665889583143 0.0000000000000000 F F  
F 0.9166667055208393 0.1666665889583143 0.0000000000000000 F F  
F 0.4166668220833714 0.6666663558332644 0.0000000000000000 F F  
F 0.9166668220833714 0.6666663558332644 0.0000000000000000 F F  
F 0.1666660421142723 0.4166679157714626 0.0000000000000000 F F  
F 0.6666660421142723 0.4166679157714626 0.0000000000000000 F F  
F 0.1666661586767972 0.9166676826464055 0.0000000000000000 F F  
F 0.6666661586767972 0.9166676826464055 0.0000000000000000 F F  
F 0.4166660421142723 0.4166679157714626 0.0000000000000000 F F  
F 0.9166660421142723 0.4166679157714626 0.0000000000000000 F F  
F 0.4166661586767972 0.9166676826464055 0.0000000000000000 F F  
F 0.9166661586767972 0.9166676826464055 0.0000000000000000 F F  
F 0.0000000000000000 0.0000000000000000 0.1111111681396224 F F  
F 0.5000000000000000 0.0000000000000000 0.1111111681396224 F F  
F 0.0000001165625250 0.4999997668749430 0.1111111681396224 F F  
F 0.5000001165625250 0.4999997668749430 0.1111111681396224 F F  
F 0.2500000000000000 0.0000000000000000 0.1111111681396224 F F  
F 0.7500000000000000 0.0000000000000000 0.1111111681396224 F F  
F 0.2500001165625250 0.4999997668749430 0.1111111681396224 F F  
F

F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1667248576446782	0.1667875369701975	0.2173151358572979	T	T
T	0.6662751608459667	0.1676741780794868	0.2180961892620170	T	T
T	0.1677036238233724	0.6659290369273285	0.2177931750053830	T	T
T	0.6676245262475881	0.6669798751112614	0.2176939162837795	T	T
T	0.4169051064768762	0.1678872694680041	0.2172229137750128	T	T
T	0.9150891926569568	0.1680714818772805	0.2189282064828005	T	T
T	0.4166839356437662	0.6659224862756702	0.2180035004730257	T	T
T	0.9154471066158830	0.6680983572183899	0.2176969460393189	T	T
T	0.1676256527734615	0.4156860985028547	0.2180704476345186	T	T
T	0.6668987871730361	0.4158842654293810	0.2181755505574730	T	T
T	0.1664786538617877	0.9171468181566257	0.2170165404191170	T	T
T	0.6674574503238796	0.9157746622573786	0.2175789109242728	T	T
T	0.4162914330883874	0.4154328617548239	0.2196291951816246	T	T
T	0.9170310787086655	0.4159150293350318	0.2187940927630508	T	T
T	0.4163262990895649	0.9180668135637381	0.2188631730490744	T	T
T	0.9164767639369421	0.9183775390556551	0.2182814575626996	T	T
T	0.0051515490046692	0.9992145073483939	0.3203817636291779	T	T
T	0.5045157845665799	0.9996792769421365	0.3204042476995215	T	T
T	0.0006739062068283	0.5040326788371414	0.3201077139626849	T	T
T	0.5033899679755266	0.5006395275504120	0.3208053429382741	T	T

T	0.2465097334383168	0.9991111662048043	0.3205103424147017	T	T
T	0.7452770816877087	0.0020714355455474	0.3196075668484762	T	T
T	0.2453652631317419	0.5017714458761747	0.3215334528649071	T	T
T	0.7460202968920282	0.5024727744867521	0.3199485912552852	T	T
T	0.2462213407779195	0.2538668974482558	0.3234434127993048	T	T
T	0.7477930011517265	0.2513100227749902	0.3198668280226963	T	T
T	0.2481293051184833	0.7554638378117072	0.3189246174621251	T	T
T	0.7478298558437125	0.7512768895811199	0.3189172494862082	T	T
T	0.4994373852298814	0.2465783300840743	0.3231078503161418	T	T
T	0.0028818518354935	0.2482589186861306	0.3222907208057384	T	T
T	0.5033339386788843	0.7459862564594161	0.3199907008256463	T	T
T	0.0011744490805203	0.7483077740826494	0.3194136877486133	T	T
T	0.1693812513131196	0.2548254074820396	0.4166421995092974	T	T
T	0.0534479881133835	0.2530281361687927	0.4278706936930522	T	T
T	0.2510244493196884	0.2610452102290701	0.4625183544444189	T	T
T	0.3233343868881910	0.2760547024985515	0.4061245377789875	T	T
T	0.1681894019930119	0.9091560543325651	0.4205948981391930	T	T
T	0.6001153084195758	0.0662520426263564	0.4201619068015315	T	T
T	0.0750018627831777	0.5974515914501969	0.4191459372640913	T	T
T	0.5847260213163600	0.5814434586225469	0.4191959156777914	T	T

HCOO\_b\_to\_C on Cl-Ru

Ru C O H Cl

2.700000000000000				
3.9999999999990008	0.0000000000000000	0.0000000000000000		
1.9999999999995004	3.4641016151368880	0.0000000000000000		
0.0000000000000000	0.0000000000000000	7.3484692283495328		

Ru C O H Cl  
64 1 2 2 4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208394	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F

F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.9166668220833716	0.6666663558332644	0.0000000000000000	F	F
F	0.1666660421142722	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166661586767973	0.9166676826464055	0.0000000000000000	F	F
F	0.9166661586767975	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.5000001165625252	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625251	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.1662769689776198	0.1677324694092945	0.2190418071668319	F	F

F	0.6656592283196333	0.1682180834976776	0.2196760255088392	F	F
F	0.1671917106944392	0.6683596589400267	0.2172410464550367	F	F
F	0.6688281641335792	0.6647437611119997	0.2179470654811695	F	F
F	0.4171951561041780	0.1668063787320690	0.2196218501600739	F	F
F	0.9150110296591123	0.1684133326000676	0.2182797930757587	F	F
F	0.4148659977921554	0.6670321230459848	0.2176941112864483	F	F
F	0.9172445688861970	0.6647661341086319	0.2176617278337644	F	F
F	0.1669299303244642	0.4146181815659062	0.2184052427767184	F	F
F	0.6673537887423251	0.4144886485629300	0.2184543107901433	F	F
F	0.1679375511142140	0.9150112997141804	0.2180579627011951	F	F
F	0.6663455334281849	0.9170607493048165	0.2175686686323814	F	F
F	0.4176895801444687	0.4156504656814661	0.2185119587418995	F	F
F	0.9174376086732039	0.4155170492518252	0.2191485191451719	F	F
F	0.4167431134464151	0.9176636629173133	0.2194069673449732	F	F
F	0.9156599759291240	0.9178336337875805	0.2188681529473157	F	F
F	0.0018983963635293	0.0020390453609878	0.3202260165728461	F	F
F	0.5065830824711597	0.9977737849689916	0.3217927145358175	F	F
F	0.0027383208134069	0.5016344891235889	0.3207232365795889	F	F
F	0.5007730963511322	0.5028666323155164	0.3207776400941427	F	F
F	0.2457263043277678	0.0015241873796299	0.3205360320521890	F	F
F	0.7463541895276293	0.9978805127009808	0.3220840000284609	F	F
F	0.2456252278911251	0.5058561976002167	0.3198010642874109	F	F
F	0.7462100951551350	0.4990674847842129	0.3207547498204093	F	F
F	0.2532466953593656	0.2480653573992555	0.3224076330214842	F	F
F	0.7489936991065350	0.2494441460412276	0.3211059602489001	F	F
F	0.2505020579712323	0.7493733186070912	0.3196580902523891	F	F
F	0.7494473598545142	0.7527084863465561	0.3189132544456186	F	F
F	0.5031228195796730	0.2432049307421664	0.3279932215732941	F	F
F	0.9998908311789592	0.2467269999909973	0.3210043772465809	F	F

F	0.5015495619430227	0.7448140558319309	0.3195643791858557	F	F
F	0.0024516958490253	0.7466026936622328	0.3192094724285681	F	F
T	0.3974178171037520	0.2483497181400086	0.4449613949398034	T	T
T	0.2936367347274825	0.2320633131913871	0.4284092538767323	T	T
T	0.4669957518222314	0.1900919833467122	0.5010640562218384	T	T
T	0.5380786758618061	0.2191671354330618	0.5113848701251560	T	T
T	0.4164889709625500	0.3330794639451375	0.4205556312607252	T	T
T	0.0809457006057149	0.0833521712813996	0.4194724800508370	T	T
T	0.6742684311592055	0.9004090242561783	0.4216672217541448	T	T
T	0.0794379966209762	0.5875015931026222	0.4189104903770440	T	T
T	0.5853900691784073	0.5816839511024882	0.4195708137892251	T	T

HCOOH\_to\_COOH on Cl-Ru

Ru C O H Cl

1.0000000000000000				
10.799999999973024	0.0000000000000000	0.0000000000000000	0.0000000000000000	
5.399999999986512	9.3530743608695985	0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.8408669165437388		

Ru	C	O	H	Cl
64	1	2	2	4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208394	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.9166668220833716	0.6666663558332644	0.0000000000000000	F	F
F	0.1666660421142722	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F

F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166661586767973	0.9166676826464055	0.0000000000000000	F	F
F	0.9166661586767975	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.5000001165625252	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625251	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.1668729082021088	0.1679686964486322	0.2189546196035010	F	F
F	0.6675044199233753	0.1680299316779497	0.2176740542979516	F	F
F	0.1675451740776950	0.6676260752906487	0.2175472156491693	F	F
F	0.6680988420185801	0.6669258606029729	0.2183006578238533	F	F
F	0.4155127196819279	0.1678758554488837	0.2186996080984684	F	F
F	0.9156916931509613	0.1676856851119766	0.2181969598174404	F	F
F	0.4148293982109053	0.6673760317797388	0.2178392304172120	F	F
F	0.9155047253928430	0.6666128397103606	0.2180581382967475	F	F
F	0.1661688418644830	0.4167068779443497	0.2187831266276206	F	F
F	0.6669813353385692	0.4161304859861730	0.2178920617486639	F	F

F	0.1668195885323982	0.9158325715134339	0.2179191364239798	F	F
F	0.6658483290969315	0.9178051150939837	0.2175629261699470	F	F
F	0.4162473890795937	0.4160465490182474	0.2186878607908156	F	F
F	0.9171373022069318	0.4163186546965463	0.2193420862999460	F	F
F	0.4153533314973572	0.9180069906222670	0.2190121809755538	F	F
F	0.9159160403757838	0.9180407332163939	0.2181536014029106	F	F
F	0.0023253331405400	0.0011398911430476	0.3199200614495936	F	F
F	0.5044191540484420	0.9991318280644776	0.3204425151370742	F	F
F	0.0007518349630686	0.5040725826739703	0.3208381272090292	F	F
F	0.5020861149078328	0.4987450089795971	0.3205067871741178	F	F
F	0.2439593587945836	0.0005509917686837	0.3205914527426543	F	F
F	0.7466432057969357	0.9995891799629389	0.3202060944648650	F	F
F	0.2512803511930741	0.4980865517701432	0.3224234528225338	F	F
F	0.7446070573030781	0.5018941469148857	0.3202740762496106	F	F
F	0.2503334163043789	0.2501012635484798	0.3231577295988473	F	F
F	0.7467105914472612	0.2528823773954443	0.3200670331912291	F	F
F	0.2505335857580917	0.7506484581814092	0.3198900383502945	F	F
F	0.7477710547321195	0.7554549441634606	0.3199379349634411	F	F
F	0.4963296861181803	0.2565917552402155	0.3213767692894932	F	F
F	0.0004015175869654	0.2445179504842372	0.3213798252203616	F	F
F	0.5009825552022137	0.7469178271856904	0.3201700320857341	F	F
F	0.0010878745854867	0.7479375908084762	0.3198401382340492	F	F
T	0.3104693872005017	0.2558492675104947	0.4774891334543709	T	T
T	0.4039353413675959	0.2933640196410011	0.4756940507270887	T	T
T	0.2453893229270082	0.2379429188496761	0.4277503989049861	T	T
T	0.2790047719523083	0.2357427326367087	0.5275633230846666	T	T
T	0.4407625319404093	0.2997398566818890	0.4066479356744758	T	T
T	0.0775593564047353	0.0776416388159168	0.4193803553535905	T	T
T	0.6637882673588442	0.9235588380565254	0.4207557850923614	T	T



	0.0745381821469840	0.5910288493987883	0.4193830991095884	T	T
T					
	0.5877055084681204	0.5822212576021721	0.4193375750254748	T	T
T					

HCOOH\_to\_HCOO on Cl-Ru

Ru	C	O	H		C
1.0000000000000000					
10.799999999973024	0.0000000000000000	0.0000000000000000			
5.399999999986512	9.3530743608695985	0.0000000000000000			
0.0000000000000000	0.0000000000000000	19.8408669165437388			
Ru	C	O	H	Cl	
64	1	2	1	4	

Selective dynamics

Direct

	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					
	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					
	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F					

F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1671226332944329	0.1683211108638005	0.2192965272063745	T	T
T	0.6687525932860225	0.1676739758706844	0.2182329729981234	T	T
T	0.1674662561709113	0.6681058948119443	0.2186358779574320	T	T
T	0.6669066485003370	0.6669051979253311	0.2189419575652920	T	T
T	0.4142944770952255	0.1678500771746272	0.2177452244536084	T	T
T	0.9157736415548428	0.1676739914160805	0.2193302809887214	T	T
T	0.4155447451821743	0.6676494194854996	0.2196701742827329	T	T
T	0.9150636939056653	0.6681339552586039	0.2190016039672287	T	T
T	0.1673344834854547	0.4150231129613218	0.2185461505720738	T	T
T	0.6667683869182284	0.4163183872660454	0.2192555026164058	T	T
T	0.1671058648877022	0.9157504259071416	0.2190368673012699	T	T
T	0.6664528455967584	0.9186618070207828	0.2183254320667345	T	T
T	0.4169796746454253	0.4164606069261936	0.2201512743273142	T	T
T	0.9158623338394420	0.4166637546879883	0.2198307298114131	T	T
T	0.4158590284765324	0.9175448254615617	0.2198853727202206	T	T
T	0.9163446678603719	0.9183907263911664	0.2198452788669130	T	T
T	0.0031026291671381	0.0024112110787797	0.3224197698266593	T	T
T	0.5048201277777196	0.0005451226048763	0.3220620502442699	T	T
T	0.0023347806898002	0.5019404256127515	0.3213163479647037	T	T

T	0.4986121622040258	0.4999035887189009	0.3225774876580445	T	T
T	0.2455147835062945	0.0023245035590804	0.3219464393643676	T	T
T	0.7450622908313136	0.0030615028679151	0.3221712342031111	T	T
T	0.2442385488624055	0.5033862774717619	0.3208726910495159	T	T
T	0.7459839671392743	0.5046681051690669	0.3222044920012763	T	T
T	0.2500936704789751	0.2523218774934719	0.3211028572798043	T	T
T	0.7491573435172256	0.2502156930750417	0.3216392152330982	T	T
T	0.2481917671716971	0.7516807829086147	0.3213690245614060	T	T
T	0.7444989299414857	0.7551151671886913	0.3208791800487347	T	T
T	0.4984783452233117	0.2534200724766222	0.3252830416263919	T	T
T	0.0028654138187250	0.2452052014837989	0.3217336134578161	T	T
T	0.5049640176809120	0.7481936311733932	0.3224835697818023	T	T
T	0.0030510247781095	0.7470863398468737	0.3211605190217028	T	T
T	0.5066163841432143	0.3329060147614769	0.4340049986304706	T	T
T	0.5481774122998928	0.2583672380095621	0.4846731073849426	T	T
T	0.4916619116099454	0.4594171367635269	0.4253351235113243	T	T
T	0.4044073823367782	0.3176961185998337	0.4001416222525194	T	T
T	0.0840583373029204	0.0850502344713462	0.4211546426261421	T	T
T	0.6586967949529381	0.9451884069968983	0.4229371029386044	T	T
T	0.0756818188518125	0.5887999184453392	0.4203979087379111	T	T
T	0.6461642391523554	0.6337772321463220	0.4243207273876796	T	T

COOH\_to\_CO2 on Cl-Ru  
Ru C O H Cl  
1.0000000000000000  
10.799999999973024 0.0000000000000000 0.0000000000000000  
5.399999999986512 9.3530743608696003 0.0000000000000000  
0.0000000000000000 0.0000000000000000 19.8408669165437388

Ru C O H Cl  
64 1 2 1 4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F

0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
F				

T	0.1669116726299970	0.1682716313072973	0.2187619162181283	T	T
T	0.6671738674162833	0.1669098598526939	0.2183677264705293	T	T
T	0.1681721096043715	0.6675991940060462	0.2179571738345818	T	T
T	0.6681240382733716	0.6655094319102828	0.2180491888033649	T	T
T	0.4152474470745665	0.1675885681250369	0.2187915671243520	T	T
T	0.9157714278899340	0.1681979571863714	0.2191588144500091	T	T
T	0.4154610405076917	0.6678288136450568	0.2178934598424959	T	T
T	0.9171481472855161	0.6654274872351605	0.2180131828109310	T	T
T	0.1677183326001413	0.4152131259946916	0.2184007134892962	T	T
T	0.6678153814390261	0.4158773369474551	0.2180880962738159	T	T
T	0.1677642425820128	0.9155721757183706	0.2182127694998007	T	T
T	0.6665211522907074	0.9171090211882462	0.2173110834522828	T	T
T	0.4169258474897445	0.4162391187742754	0.2185341529398841	T	T
T	0.9174722883818176	0.4161271034502491	0.2192662719274852	T	T
T	0.4165673523341091	0.9179844501260722	0.2188961435575981	T	T
T	0.9169212038705357	0.9175546619746635	0.2189298539931880	T	T
T	0.0035662077177036	0.0019119938482866	0.3207620431922676	T	T
T	0.5064946129914425	-0.0012308417963671	0.3211139916830075	T	T
T	0.0050311057471927	0.5000135528932317	0.3209175091628064	T	T
T	0.5005876641275729	0.5035019412509021	0.3196346333160572	T	T
T	0.2461464735690308	0.0026690053502521	0.3207020410247318	T	T
T	0.7470399475647004	-0.0016225497647648	0.3201920055811493	T	T
T	0.2469578691443315	0.5030763981952411	0.3202605453094084	T	T
T	0.7458629641198017	0.5014477909073192	0.3205704256823216	T	T
T	0.2504878164080125	0.2504617397754139	0.3208739622626122	T	T
T	0.7482249329709209	0.2495359895008566	0.3205703518780200	T	T
T	0.2497506815934545	0.7512629154436760	0.3196125882800359	T	T
T	0.7485131096638865	0.7541857644691660	0.3190125185214653	T	T
T	0.5051852104874516	0.2483083830012112	0.3210156666310857	T	T

T	0.0039277552101739	0.2467179779172522	0.3217630928160759	T	T
T	0.5013146111548520	0.7473476454972299	0.3201381014402254	T	T
T	0.0033913323996403	0.7461750236790448	0.3202102453282541	T	T
T	0.5220962101911155	0.2465667560351962	0.4738707341624521	T	T
T	0.4185669118767592	0.2280170799748181	0.4784428846875651	T	T
T	0.5770520412347961	0.2603662541773857	0.4171136666527748	T	T
T	0.5796694742772139	0.2531785358400759	0.5187699643587309	T	T
T	0.0838452112460987	0.0831670863786847	0.4199447554709288	T	T
T	0.6730850686236652	0.9050912364632535	0.4209794613339513	T	T
T	0.0846518029362014	0.5819407499282498	0.4192868685616062	T	T
T	0.5853409805601342	0.5849069690704348	0.4191308235646466	T	T

HCOO\_to\_CO2 on Cl-Ru

Ru C O H Cl

2.700000000000000				
3.999999999999008	0.000000000000000	0.000000000000000		
1.999999999995004	3.4641016151368880	0.000000000000000		
0.000000000000000	0.000000000000000	7.3484692283495328		

Ru	C	O	H	Cl
64	1	2	1	4

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.000000000000000	F	F
F	0.9166668220833714	0.6666663558332644	0.000000000000000	F	F
F	0.1666660421142723	0.4166679157714626	0.000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.000000000000000	F	F
F	0.1666661586767972	0.9166676826464055	0.000000000000000	F	F
F	0.6666661586767972	0.9166676826464055	0.000000000000000	F	F

F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1666124099144357	0.1673149169683290	0.2188869185630650	T	T
T	0.6659901721720540	0.1686105598097438	0.2180609091652118	T	T
T	0.1678872077326019	0.6672233393504702	0.2177175366221191	T	T
T	0.6681974529765711	0.6661068691446076	0.2185621540651395	T	T
T	0.4154202588767983	0.1673532303767307	0.2189068191844938	T	T
T	0.9151620593133437	0.1682617872608592	0.2182487892226402	T	T
T	0.4149660725810279	0.6669841805768060	0.2178909514895402	T	T
T	0.9158823180668285	0.6661057085207567	0.2179950799743031	T	T
T	0.1671480305663444	0.4153036735521142	0.2186316902758760	T	T

T	0.6674859503605534	0.4154446383201814	0.2183619634166040	T	T
T	0.1676636263322526	0.9147710553463122	0.2178059835082805	T	T
T	0.6656538060130586	0.9173206691283361	0.2175412869130200	T	T
T	0.4169910040024832	0.4149836333231893	0.2187969521462202	T	T
T	0.9171202286829541	0.4159779948687058	0.2195849918770359	T	T
T	0.4157486692338292	0.9177877904169931	0.2193189379583988	T	T
T	0.9153014499921135	0.9178067237871486	0.2182463754395059	T	T
T	0.0018884687367894	0.0005691088834232	0.3196915740970940	T	T
T	0.5047504384356016	0.9994121218233091	0.3212547142947407	T	T
T	0.0018525843798286	0.5034524316063307	0.3208326734665014	T	T
T	0.5028887128840634	0.4992243796262157	0.3210148422509338	T	T
T	0.2442298531485635	0.0001798557668542	0.3205435714051043	T	T
T	0.7443390583948509	0.0011155203298687	0.3206844802709979	T	T
T	0.2463120385464146	0.5036983331830197	0.3204406524581520	T	T
T	0.7452703561133646	0.5002976035387097	0.3207667297174250	T	T
T	0.2489373653389622	0.2501430245231203	0.3218611660568701	T	T
T	0.7441671169445696	0.2513397615847091	0.3202577709268729	T	T
T	0.2493414888480904	0.7508353495834696	0.3197394086868345	T	T
T	0.7481903552457538	0.7548862810448888	0.3196976638801651	T	T
T	0.5046688547059581	0.2480734874773514	0.3212129426929762	T	T
T	0.0003827658147942	0.2450547827486436	0.3214420741726318	T	T
T	0.5000858259629050	0.7457944863385866	0.3203543310450366	T	T
T	0.0023322978390874	0.7474295093177861	0.3194912476866782	T	T
T	0.2853220772407965	0.2586116539282810	0.4775559970713923	T	T
T	0.2386957267455183	0.2624103065633128	0.5347290528028026	T	T
T	0.2209356263647865	0.2513707298860701	0.4229812062318538	T	T
T	0.3858768412169094	0.2613397304832100	0.4692172587405796	T	T
T	0.0778349051588239	0.0736186539161213	0.4190897154602400	T	T
T	0.6648014391613198	0.9183518641959896	0.4213942726876097	T	T



	0.0794347845727351	0.5932802995847902	0.4190420768276870	T	T
T					
	0.5856314593957469	0.5814822758665383	0.4192999308523622	T	T
T					

H2O on Ru

Ru	O	H		
	2.7000000000000000			
	4.0000000000000009	0.0000000000000000	0.0000000000000000	
	2.0000000000000004	3.4641016151377544	0.0000000000000000	
	0.0000000000000000	0.0000000000000000	7.3484692283495328	

	Ru	O	H		
	64	1	2		
	Selective dynamics				
	Direct				
	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F					
	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F					
	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F					
	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					
	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F					
	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F					

F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1667193598976526	0.1666415559123174	0.2180877308107509	T	T
T	0.6650839200774407	0.1650151206017844	0.2168175776314669	T	T
T	0.1665186664941124	0.6658295337668060	0.2186603610855134	T	T
T	0.6671284488135850	0.6664231776738490	0.2178642108069179	T	T
T	0.4165786180259877	0.1668214009534002	0.2180646342735266	T	T
T	0.9195750790507969	0.1652711430087433	0.2167050909551161	T	T
T	0.4169183127990669	0.6665212519948366	0.2177000353141917	T	T
T	0.9171987320152133	0.6658680831507241	0.2191906958377053	T	T
T	0.1657575143229541	0.4172583242033662	0.2189701291856320	T	T
T	0.6653789950767586	0.4193461021832645	0.2168537612992595	T	T
T	0.1666012167928119	0.9167715559809086	0.2176090522314615	T	T
T	0.6668025673772351	0.9161931556610144	0.2178777788208640	T	T
T	0.4169484811432116	0.4169457811112723	0.2183179665883106	T	T
T	0.9177961347971332	0.4172483133637537	0.2178580571305323	T	T
T	0.4170073833841578	0.9167780072785874	0.2182798760001276	T	T
T	0.9173662066173186	0.9164195683739031	0.2179840592207661	T	T
T	0.0095643041084329	0.9930247744035491	0.3208985995203872	T	T
T	0.5059013686897894	0.0024909428336989	0.3215823343751165	T	T
T	0.9975276147879493	0.4923797919707444	0.3224067916363971	T	T

T	0.4929950821386759	0.5110445290360738	0.3209874815778204	T	T
T	0.2426931982187751	0.0061939919217746	0.3209671396966869	T	T
T	0.7480783585500191	0.9934780838285521	0.3202520253462428	T	T
T	0.2569450118237424	0.5007607933445474	0.3217128678642772	T	T
T	0.7496423785607839	0.5067298873078435	0.3204766592051308	T	T
T	0.2486660856756797	0.2468834757670317	0.3220210733018824	T	T
T	0.7514792478574883	0.2495656273923008	0.3135891416463900	T	T
T	0.2472131782457855	0.7450898814832363	0.3222432712812120	T	T
T	0.7431521312920736	0.7530867894124164	0.3221697545921100	T	T
T	0.4958965521834129	0.2466363620460611	0.3205215482320488	T	T
T	0.0073887599803982	0.2485263509760677	0.3209294261838310	T	T
T	0.5073947559369513	0.7423493198979341	0.3211429387975392	T	T
T	0.0010464985588983	0.7577260428107827	0.3216371340201213	T	T
F	0.7546725287305591	0.2487140567774873	0.4135360000000006	F	F
T	0.7633338739228246	0.1707099997036217	0.4420742748728758	T	T
T	0.7199112477439366	0.3340504445413105	0.4418570317393404	T	T

H on Ru

Ru H

2.7000000000000000			
3.0000000000000004	0.0000000000000000	0.0000000000000000	0.0000000000000000
-1.5000000000000002	2.5980762113533160		0.0000000000000000
0.0000000000000000	0.0000000000000000		7.3484692283495336

Ru H

36 1

Selective dynamics

Direct

F	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F
F	0.3333333333333357	0.0000000000000000	0.0000000000000000	F	F
F	0.6666666666666643	0.0000000000000000	0.0000000000000000	F	F
F	0.3333333333333357	0.3333333333333357	0.0000000000000000	F	F
F	0.6666666666666643	0.3333333333333357	0.0000000000000000	F	F
F	0.0000000000000000	0.3333333333333357	0.0000000000000000	F	F
F	0.3333333333333357	0.6666666666666643	0.0000000000000000	F	F
F	0.6666666666666643	0.6666666666666643	0.0000000000000000	F	F

0.0000000000000000	0.6666666666666643	0.0000000000000000	F	F
F				
0.1111111111111143	0.222222222222214	0.1111111111111072	F	F
F				
0.4444444444444429	0.222222222222214	0.1111111111111072	F	F
F				
0.7777777777777786	0.222222222222214	0.1111111111111072	F	F
F				
0.4444444444444429	0.5555555555555571	0.1111111111111072	F	F
F				
0.7777777777777786	0.5555555555555571	0.1111111111111072	F	F
F				
0.1111111111111143	0.5555555555555571	0.1111111111111072	F	F
F				
0.4444444444444429	0.8888888888888857	0.1111111111111072	F	F
F				
0.7777777777777786	0.8888888888888857	0.1111111111111072	F	F
F				
0.1111111111111143	0.8888888888888857	0.1111111111111072	F	F
F				
0.0001151198297791	0.0000575599148931	0.2170765754395845	T	T
T				
0.3333979489538592	0.0000305329108414	0.2172311972014427	T	T
T				
0.6666063059198493	0.0000812867274647	0.2169583123526522	T	T
T				
0.3333979489538592	0.3333674160430249	0.2172311972014427	T	T
T				
0.6673210403990169	0.3336605201995084	0.2172123735956291	T	T
T				
0.9994028623846773	0.3337542556083264	0.2171231091580808	T	T
T				
0.3332242110584644	0.6666121055292251	0.2170020651311830	T	T
T				
0.6666063059198493	0.6665250191923846	0.2169583123526522	T	T
T				
0.9994028623846773	0.6656486067763581	0.2171231091580808	T	T
T				
0.1098891533318778	0.2234452794003161	0.3228552976051731	T	T
T				
0.4463625394656248	0.2231812697328053	0.3229982427221074	T	T
T				
0.7771555322632722	0.2207134600553644	0.3218257996558833	T	T
T				
0.4450869042773462	0.5569677207854653	0.3218510564035100	T	T
T				
0.7771555322632722	0.5564420722079078	0.3218257996558833	T	T
T				
0.1120846265697821	0.5560423132848840	0.3217191034620726	T	T
T				
0.4450869042773462	0.8881191834918809	0.3218510564035100	T	T
T				
0.7766385248025074	0.8883192624012537	0.3218029455582752	T	T
T				
0.1098891533318778	0.8864438739315545	0.3228552976051731	T	T
T				
0.2220000000000013	0.1109999999999971	0.3766680849817732	F	F
T				

```

Ru_slab
Ru
  2.7000000000000000
  4.0000000000000009  0.0000000000000000  0.0000000000000000
  2.0000000000000004  3.4641016151377544  0.0000000000000000
  0.0000000000000000  0.0000000000000000  7.3484692283495328

```

```

Ru
  64
Selective dynamics

```

```

Direct
  0.1666667055208393  0.1666665889583143  0.0000000000000000  F  F
F
  0.6666667055208393  0.1666665889583143  0.0000000000000000  F  F
F
  0.1666667055208393  0.6666665889583143  0.0000000000000000  F  F
F
  0.6666667055208393  0.6666665889583143  0.0000000000000000  F  F
F
  0.4166667055208393  0.1666665889583143  0.0000000000000000  F  F
F
  0.9166667055208393  0.1666665889583143  0.0000000000000000  F  F
F
  0.4166667055208393  0.6666665889583143  0.0000000000000000  F  F
F
  0.9166667055208393  0.6666665889583143  0.0000000000000000  F  F
F
  0.1666660421142652  0.4166679157714626  0.0000000000000000  F  F
F
  0.6666660421142723  0.4166679157714626  0.0000000000000000  F  F
F
  0.1666660421142652  0.9166679157714626  0.0000000000000000  F  F
F
  0.6666660421142723  0.9166679157714626  0.0000000000000000  F  F
F
  0.4166660421142723  0.4166679157714626  0.0000000000000000  F  F
F
  0.9166660421142723  0.4166679157714626  0.0000000000000000  F  F
F
  0.4166660421142723  0.9166679157714626  0.0000000000000000  F  F
F
  0.9166660421142723  0.9166679157714626  0.0000000000000000  F  F
F
  0.0000000000000000  0.0000000000000000  0.1111111681396224  F  F
F
  0.5000000000000000  0.0000000000000000  0.1111111681396224  F  F
F
  0.0000000000000000  0.5000000000000000  0.1111111681396224  F  F
F
  0.5000000000000000  0.5000000000000000  0.1111111681396224  F  F
F
  0.2500000000000000  0.0000000000000000  0.1111111681396224  F  F
F
  0.7500000000000000  0.0000000000000000  0.1111111681396224  F  F
F
  0.2500000000000000  0.5000000000000000  0.1111111681396224  F  F
F
  0.7500000000000000  0.5000000000000000  0.1111111681396224  F  F
F

```

F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1665706197906643	0.1667455905410820	0.2178753749539497	T	T
T	0.6665722443197146	0.1667597630726421	0.2178889668173094	T	T
T	0.1665662871178226	0.6667446802317303	0.2178929258911869	T	T
T	0.6665913740923299	0.6667247515767815	0.2178909883787618	T	T
T	0.4165399276247104	0.1668199545909671	0.2177507580642391	T	T
T	0.9165384014470356	0.1668171444168685	0.2177628300026247	T	T
T	0.4165515528505763	0.6668016409663141	0.2177500963615543	T	T
T	0.9165391221273860	0.6668361411325304	0.2177547459675353	T	T
T	0.1667021871921321	0.4166838659053307	0.2177706712324521	T	T
T	0.6667066112619517	0.4166747101494485	0.2177684007616042	T	T
T	0.1666949768750356	0.9166663134990248	0.2177423701878882	T	T
T	0.6666701844993937	0.9166975541720055	0.2177631026468013	T	T
T	0.4165309395859785	0.4166796875921044	0.2177635455739411	T	T
T	0.9165253760038173	0.4166969655423231	0.2177589009163177	T	T
T	0.4165600889738826	0.9166897208105254	0.2177704888166855	T	T
T	0.9165204210727294	0.9167085478141390	0.2177514561222677	T	T
T	-0.0000734616569923	0.0000568178898742	0.3218279382809195	T	T
T	0.4999280080499708	0.0000904354194396	0.3218314453957680	T	T
T	-0.0000800488237815	0.5000568295317596	0.3218529495401728	T	T
T	0.4999216319669107	0.5000505193450083	0.3218443975082252	T	T
T	0.2499343816639646	0.0000407661745392	0.3220921269286962	T	T

T	0.7499427197165548	0.0000578127452645	0.3221102143941437	T	T
T	0.2499309002510059	0.5000682779991059	0.3221143140411725	T	T
T	0.7499724773155585	0.5000300943973154	0.3221256106626188	T	T
T	0.2499339282680926	0.2500856392540476	0.3221047408836280	T	T
T	0.7499538197410608	0.2500847595451495	0.3221149215702150	T	T
T	0.2499600873609787	0.7500700699734094	0.3221080603828390	T	T
T	0.7499623467111264	0.7500668293013745	0.3221110089514490	T	T
T	0.4998361117742343	0.2500944573917867	0.3220982346142376	T	T
T	0.9998432428427303	0.2501026275842849	0.3221061182477729	T	T
T	0.4998182427209478	0.7501078639911308	0.3221042436309025	T	T
T	0.9998242133256459	0.7501269342860650	0.3221044771045282	T	T

Acetone on Ru

Ru	C	O	H	C
2.7000000000000000				
4.0000000000000009	0.0000000000000000			0.0000000000000000
2.0000000000000004	3.4641016151377544			0.0000000000000000
0.0000000000000000	0.0000000000000000			7.3484692283495328

Ru C O H  
64 3 2 8

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F

F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.1675212890083841	0.1677924219832363	0.2211549030824500	F	F
F	0.6670573456327062	0.1677953087345827	0.2200431069047539	F	F
F	0.1680682302512650	0.6670185394974695	0.2201805504958756	F	F
F	0.6676729525762966	0.6677690948474151	0.2200798492508937	F	F
F	0.4147057634729663	0.1677834730540653	0.2211617072206238	F	F
F	0.9151592220210816	0.1677915559578338	0.2200567151811015	F	F
F	0.4145200658249450	0.6677748683501079	0.2201002616654151	F	F
F	0.9148871736269371	0.6670156527461231	0.2201873546340494	F	F
F	0.1679851838496589	0.4140496323006886	0.2216325535822889	F	F



F	0.6675630482801651	0.4148839034396659	0.2201274782181173	F	F
F	0.1680238218287329	0.9144073563425295	0.2200975400101441	F	F
F	0.6675506519557572	0.9143986960884902	0.2200961791825122	F	F
F	0.4163293711519529	0.4165062576960850	0.2217128424127495	F	F
F	0.9171762012789770	0.4164975974420528	0.2216992341364019	F	F
F	0.4162610604937456	0.9174528790125080	0.2221455856006429	F	F
F	0.9167632515982334	0.9164684968035388	0.2201070658035889	F	F
T	0.0071821684459634	0.9921955994289697	0.3226570750409726	T	T
T	0.5087925524877633	0.9980873833422139	0.3242453303452800	T	T
T	0.0009302114453980	0.4919160845591889	0.3241939354452636	T	T
T	0.4944444881678477	0.5067198498221366	0.3258563835572534	T	T
T	0.2485435441282077	0.9996547484563916	0.3229735856386868	T	T
T	0.7441513964213299	0.9969756585705488	0.3229118270805590	T	T
T	0.2444715400455403	0.5077984387411909	0.3235206133383821	T	T
T	0.7578510917512101	0.4979338350124589	0.3232666502325582	T	T
T	0.2476083890755572	0.2486619548978072	0.3242332799036405	T	T
T	0.7542748176034089	0.2482647630359094	0.3242303506081995	T	T
T	0.2411934930486685	0.7488069090564863	0.3242796003868125	T	T
T	0.7414782619568099	0.7538099670176545	0.3240780735828123	T	T
T	0.5005434759072191	0.2405063542805769	0.3234589691542833	T	T
T	0.9983748110899406	0.2578319113235599	0.3240027543123101	T	T
T	0.5012349298773001	0.7533620053675441	0.3231642895121543	T	T
T	0.0053368590177871	0.7529952761403518	0.3235785880866051	T	T
T	0.4457450399953683	0.5633476545523604	0.4872757684009266	T	T
T	0.3282426661019849	0.7122464754550337	0.4809532248494096	T	T
T	0.4914849542640274	0.4984769367314234	0.5549383702032125	T	T
T	0.5075109797452003	0.4896930106247527	0.4355552222270517	T	T
T	0.7531947333577261	0.2493686359348863	0.4335125406030123	T	T
T	0.5204030295773827	0.5655123593282635	0.5854157126283959	T	T

	0.5804117939352917	0.3882405132698946	0.5530917169886953	T	T
T					
	0.3986590923983733	0.5025070666366637	0.5802565004010517	T	T
T					
	0.2825035099989545	0.7621630511625788	0.5295751319600467	T	T
T					
	0.2428571554745500	0.7137737147224789	0.4488034653438037	T	T
T					
	0.3675697314225376	0.7756308697530719	0.4540006379942272	T	T
T					
	0.7614886331937143	0.1647288243579237	0.4558711362320573	T	T
T					
	0.6576860535333815	0.3332093168553942	0.4451864418727793	T	T
T					

CH3CH\_O\_CH3 on Ru

Ru	C	O	H		
	2.7000000000000000				
	4.0000000000000009	0.0000000000000000	0.0000000000000000		
	-2.0000000000000004	3.4641016151377544	0.0000000000000000		
	0.0000000000000000	0.0000000000000000	7.3484692283495328		

Ru	C	O	H	
64	3	2	9	

Selective dynamics

Direct

	0.3333332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.8333332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.8333331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.3333331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.5833332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.0833332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.0833331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.5833331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.5833339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.0833339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.8333339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.3333339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.8333338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					

F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
T	0.3333452182585545	0.1668403897356016	0.2190100198857460	T	T
T	0.8332657395010377	0.1671485762781725	0.2180966924904205	T	T
T	0.8341096670450935	0.6658735310134941	0.2186827551305005	T	T
T	0.3329428839174182	0.6669488555762314	0.2180442379847481	T	T
T	0.5850567797975286	0.1691288459513348	0.2182650546365216	T	T
T	0.0829030279833400	0.1657147011991331	0.2187578380800883	T	T
T	0.0839510213043049	0.6670614489542263	0.2186628204708597	T	T
T	0.5823803965470437	0.6649644068098720	0.2182666800664061	T	T
T	0.5839965986976077	0.4173452756263684	0.2191665974304942	T	T
T	0.0830830235491319	0.4170108746758664	0.2177450229176714	T	T
T	0.0827874305448531	0.9160461091115703	0.2192604098910817	T	T
T	0.5846881990549783	0.9154531899438201	0.2191011892260415	T	T
T	0.8331761857991168	0.4163088836717156	0.2185773878826290	T	T
T	0.3345042302157592	0.4171923270049913	0.2188861347513797	T	T

T	0.3309867135685609	0.9150731675009118	0.2182652178848161	T	T
T	0.8350128544990193	0.9175815934999019	0.2183255608083066	T	T
T	-0.0090111036718743	0.9928995394876230	0.3226793340519745	T	T
T	0.5007675069033310	-0.0004890326665001	0.3204160080348687	T	T
T	0.5074604075270425	0.5091675774001632	0.3226721513928479	T	T
T	0.0034905219569634	0.4964955305797419	0.3226801037026266	T	T
T	0.2571151109521494	0.0049408115492653	0.3224543025136584	T	T
T	0.7583664433479405	0.0073244597152203	0.3208448162634315	T	T
T	0.7510343624182672	0.5071625616144008	0.3223751326891454	T	T
T	0.2481071346675791	0.5072728975884618	0.3214595734495345	T	T
T	0.4952245466507810	0.2432994586676185	0.3224783129189899	T	T
T	0.9930097507424717	0.2519672516846108	0.3215840141746714	T	T
T	0.9928323243249823	0.7488804419167117	0.3223426769116722	T	T
T	0.4928351665962951	0.7415833421298365	0.3207989897065173	T	T
T	0.7546777754545232	0.2468073582881017	0.3214845094874537	T	T
T	0.2477419040569601	0.2516409299502761	0.3217304042575936	T	T
T	0.2536960677006258	0.7458253838378169	0.3214797477987812	T	T
T	0.7547221997207773	0.7446898603714728	0.3219233510490667	T	T
T	0.4449468038103164	0.0559530146632751	0.4548856409532453	T	T
T	0.3283583018609320	0.9373958229786981	0.4964047499851457	T	T
T	0.5643456155452163	0.1727443059493936	0.4959612833149760	T	T
T	0.3832605517935209	0.1175171391009431	0.4114210441580672	T	T
T	0.2394409044946743	0.2421123565614761	0.4303771627058979	T	T
T	0.3731782278249402	0.8853741984990938	0.5276525500860133	T	T
T	0.2775807775237038	0.3321799661750103	0.4552156329846528	T	T
T	0.3010452722120858	0.1980733811925914	0.4399410843190893	T	T
T	0.5203528073757206	0.2228545488168837	0.5291837408003492	T	T
T	0.2454408774473281	0.8563969880385213	0.4633826456287691	T	T
T	0.2787658969110983	-0.0177920961725119	0.5294677356852641	T	T

	0.6167565806887900	0.1280303850704677	0.5269985972730102	T	T
T					
	0.6448914550265945	0.2552275069078286	0.4625982918826119	T	T
T					
	0.4957781555153244	0.0043436324389445	0.4229423667229589	T	T
T					

CH3C\_OH\_CH3 on Ru

0.00000000E+00 0.00000000E+00 0.00000000E+00

Ru C O H

2.7000000000000000

3.999999999999008 0.0000000000000000 0.0000000000000000

-1.999999999995004 3.4641016151368942 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3484692283495301

Ru C O H

64 3 2 9

Selective dynamics

Direct

	0.3333332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.8333332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.8333331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.3333331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.5833332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.0833332944791607	0.1666665889583143	0.0000000000000000	F	F
F					
	0.0833331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.5833331779166286	0.6666663558332644	0.0000000000000000	F	F
F					
	0.5833339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.0833339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.8333339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.3333339578857277	0.4166679157714626	0.0000000000000000	F	F
F					
	0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.8333338413232028	0.9166676826464055	0.0000000000000000	F	F
F					
	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F					
	0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F					
	0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F					

F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
T	0.3318767757072834	0.1662841399096868	0.2182723967491034	T	T
T	0.8329126650947042	0.1656843016438092	0.2178771203809725	T	T
T	0.8335003252704749	0.6668902627994250	0.2184004918341325	T	T
T	0.3342097529725784	0.6672814266983342	0.2195387949678527	T	T
T	0.5825139882947217	0.1648033986577596	0.2179793587660034	T	T
T	0.0826926410451887	0.1657913087712713	0.2184199593177114	T	T
T	0.0820189376386565	0.6655924876141933	0.2182067659033674	T	T
T	0.5826701814908536	0.6661730773211247	0.2191122149124027	T	T
T	0.5830271905235825	0.4180127250032971	0.2180495211086169	T	T
T	0.0821054181521633	0.4164051141365390	0.2182391235573009	T	T
T	0.0826959656263848	0.9166986097316969	0.2185757116460713	T	T
T	0.5829014347615241	0.9167934055200799	0.2188522735082127	T	T
T	0.8328330608622139	0.4165054352570148	0.2181253458096127	T	T
T	0.3348374639394645	0.4171531857490139	0.2191497407983334	T	T
T	0.3352405088525963	0.9181614071543140	0.2185436377275137	T	T
T	0.8343773448086802	0.9172947048064402	0.2176986411800429	T	T
T	0.9913895064311968	0.9981516951227831	0.3228986571761275	T	T

T	0.5020280190123765	0.0103635904002702	0.3222586485101427	T	T
T	0.5058577590575077	0.4945763098631505	0.3223943368312913	T	T
T	0.0083467729099674	0.5043517897936967	0.3248531508705344	T	T
T	0.2587567799438231	0.0080745043348317	0.3215044457380707	T	T
T	0.7574116063329630	0.0062036510898400	0.3217202097048251	T	T
T	0.7502849378775532	0.5078715183646570	0.3214374782316892	T	T
T	0.2459050319258747	0.4982555408239910	0.3215598723657438	T	T
T	0.4912180236462001	0.2457510411829003	0.3215189675710567	T	T
T	0.9919663786676082	0.2442999984195605	0.3206733319518025	T	T
T	0.9919423101471019	0.7451472305389839	0.3212044006855378	T	T
T	0.5026901116983211	0.7516268603166740	0.3227557739539840	T	T
T	0.7492749990520048	0.2426238701429926	0.3207111280905897	T	T
T	0.2547960966070693	0.2481262529790186	0.3215072889282986	T	T
T	0.2481354972311878	0.7514306905558675	0.3210170700572198	T	T
T	0.7570859393069755	0.7498571347615667	0.3219011681277916	T	T
T	0.0840995633702132	0.5321186205134442	0.4287095880962485	T	T
T	0.1475167004010469	0.6842147721262787	0.4537926358101731	T	T
T	0.9714221982489772	0.4274320997499370	0.4768573892923824	T	T
T	0.4857211731517581	0.7433820158688988	0.4325174083876885	T	T
T	0.2092446216885604	0.5065961379109791	0.4291263537322438	T	T
T	0.0155689836020239	0.4426142972618439	0.5284273775735367	T	T
T	0.3987192476832815	0.6553648558417828	0.4470204246217567	T	T
T	0.1956983635601973	0.6962198293172259	0.5042741786110050	T	T
T	0.2410805466054619	0.7680761103501554	0.4235987208303930	T	T
T	0.0663385036906133	0.7169178958648704	0.4562529418807308	T	T
T	0.5662887665545286	0.7508889553519569	0.4584990863521850	T	T
T	0.9306932360557156	0.3158805681703432	0.4614096347418292	T	T
T	0.8803984472323716	0.4461446656164110	0.4778796359236455	T	T
T	0.1849716504251719	0.4178936523798140	0.4533323907040688	T	T

iPrOH on Ru  
 Ru C O H C  
 2.7000000000000000  
 4.0000000000000009 0.0000000000000000 0.0000000000000000  
 2.0000000000000004 3.4641016151377544 0.0000000000000000  
 0.0000000000000000 0.0000000000000000 7.3484692283495328

Ru C O H  
 64 3 2 10

Selective dynamics

Direct

0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				



F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1678831261269867	0.1659870543014175	0.2196286031448237	T	T
T	0.6664760070145272	0.1668505130348273	0.2191503109172820	T	T
T	0.1666563782283743	0.6652231674648111	0.2188127462189703	T	T
T	0.6647981124901958	0.6677445371429087	0.2177963002448388	T	T
T	0.4156188688783268	0.1676983629399489	0.2191711831686435	T	T
T	0.9159861689893238	0.1672153798080160	0.2186625631842843	T	T
T	0.4176725437783557	0.6664190365935342	0.2178829950165063	T	T
T	0.9156825245564508	0.6674229602756570	0.2189355360009462	T	T
T	0.1677241873189206	0.4161740339066068	0.2198236389767272	T	T
T	0.6650492659807782	0.4172511189755851	0.2179492221284390	T	T
T	0.1668742719275585	0.9178204714378375	0.2183036598495981	T	T
T	0.6664598613151955	0.9163250679613917	0.2186159383474327	T	T
T	0.4171582115957590	0.4174055793564557	0.2187536240816235	T	T
T	0.9170866071141397	0.4168658334205830	0.2182833628019847	T	T
T	0.4167171064335417	0.9157461031129699	0.2179889565640367	T	T
T	0.9180459157781025	0.9161579658934559	0.2185790658762559	T	T
T	0.0095500062624823	0.9941091988151334	0.3215408790976110	T	T
T	0.5084598162779843	0.0012763106573472	0.3223145303068815	T	T
T	0.9901504535661905	0.5016324548691413	0.3216666021604084	T	T
T	0.4980729404574285	0.5035485825627927	0.3222424625472678	T	T
T	0.2520669069483449	0.9914872583140513	0.3220710587799592	T	T

T	0.7422646486296799	0.0007560646346892	0.3210726582700601	T	T
T	0.2502413606218106	0.5088673045943604	0.3223561798873660	T	T
T	0.7590078227161082	0.4925381970107327	0.3223572786675651	T	T
T	0.2527600562022050	0.2473904620086442	0.3240523312507441	T	T
T	0.7473346938141090	0.2580616461764008	0.3214957530053091	T	T
T	0.2414731846816031	0.7529515597839298	0.3228773349124235	T	T
T	0.7444242251133765	0.7497347077540134	0.3215254390721967	T	T
T	0.5083838925996386	0.2396158716907544	0.3224309558177129	T	T
T	0.9897619361602320	0.2580362779007510	0.3217362922257932	T	T
T	0.4973109536095605	0.7515969315599164	0.3223778008729746	T	T
T	0.0083010451871713	0.7487810941814458	0.3221160365758803	T	T
T	0.9600259764353348	0.5550919646007837	0.5140986220184726	T	T
T	0.0710747615781582	0.5287400022191655	0.5672073391725677	T	T
T	0.8092832526089863	0.6211135013052584	0.5417231711259294	T	T
T	0.0009195249101391	0.4157553632212176	0.4841869033752066	T	T
T	0.2529261795793772	0.2609346326132950	0.4320432393572575	T	T
T	0.9311399140672070	0.4296059078172884	0.4485263168461777	T	T
T	0.0706592630007633	0.4572566551439894	0.6066321622467714	T	T
T	0.1786002974095741	0.4802667691597454	0.5450310044675191	T	T
T	0.0466026411215271	0.6306001809387065	0.5907526883433939	T	T
T	0.1541039355372111	0.3223537659664751	0.4535458057460882	T	T
T	0.3028079623967352	0.1707959130773927	0.4569493272593613	T	T
T	0.8034077377771194	0.5518390123448033	0.5807227569956249	T	T
T	0.7327767500045383	0.6368845348742491	0.5013648505756251	T	T
T	0.7772980457253511	0.7260087681085673	0.5641243517246567	T	T
T	0.9637652701335991	0.6239218190546247	0.4737595845551258	T	T

Acetone\_to\_CH3CH\_O\_CH3 on Ru  
Ru C O H  
1.0000000000000000  
10.799999999973024 0.0000000000000000 0.0000000000000000  
-5.399999999986512 9.3530743608695985 0.0000000000000000  
0.0000000000000000 0.0000000000000000 19.8408669165437423

	Ru	C	O	H			
	64	3	2	9			
Selective dynamics							
Direct							
	0.3333332944791607	0.1666665889583143	0.0000000000000000		F	F	
F	0.8333332944791607	0.1666665889583143	0.0000000000000000		F	F	
F	0.8333331779166286	0.6666663558332644	0.0000000000000000		F	F	
F	0.3333331779166286	0.6666663558332644	0.0000000000000000		F	F	
F	0.5833332944791607	0.1666665889583143	0.0000000000000000		F	F	
F	0.0833332944791607	0.1666665889583143	0.0000000000000000		F	F	
F	0.0833331779166286	0.6666663558332644	0.0000000000000000		F	F	
F	0.5833331779166286	0.6666663558332644	0.0000000000000000		F	F	
F	0.5833339578857277	0.4166679157714626	0.0000000000000000		F	F	
F	0.0833339578857277	0.4166679157714626	0.0000000000000000		F	F	
F	0.0833338413232028	0.9166676826464055	0.0000000000000000		F	F	
F	0.5833338413232028	0.9166676826464055	0.0000000000000000		F	F	
F	0.8333339578857277	0.4166679157714626	0.0000000000000000		F	F	
F	0.3333339578857277	0.4166679157714626	0.0000000000000000		F	F	
F	0.3333338413232028	0.9166676826464055	0.0000000000000000		F	F	
F	0.8333338413232028	0.9166676826464055	0.0000000000000000		F	F	
F	0.0000000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.5000000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.4999998834374750	0.4999997668749430	0.1111111681396224		F	F	
F	0.9999998834374750	0.4999997668749430	0.1111111681396224		F	F	
F	0.2500000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.7500000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.7499998834374750	0.4999997668749430	0.1111111681396224		F	F	
F	0.2499998834374750	0.4999997668749430	0.1111111681396224		F	F	
F	0.4999999417187340	0.2499998834374750	0.1111111681396224		F	F	
F	0.9999999417187340	0.2499998834374750	0.1111111681396224		F	F	
F	0.0000005468440492	0.7500010936880912	0.1111111681396224		F	F	

F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
T	0.3322535689736650	0.1677227463754042	0.2179196968467848	T	T
T	0.8325954961381156	0.1670915474250553	0.2187834984935005	T	T
T	0.8341980873536615	0.6660276247172349	0.2179849799198690	T	T
T	0.3329486396525617	0.6673052791530809	0.2188806651785385	T	T
T	0.5839788680424929	0.1681616905077266	0.2177675421516681	T	T
T	0.0822648611920701	0.1660161919020067	0.2191540961128710	T	T
T	0.0831919837321305	0.6676922077175970	0.2178284440198483	T	T
T	0.5822530715919124	0.6649891081509993	0.2184551280576946	T	T
T	0.5845556636230431	0.4184087607640221	0.2188286699059313	T	T
T	0.0838930930344673	0.4161750924350000	0.2179781266790249	T	T
T	0.0816055811664717	0.9155163547414200	0.2186812893741749	T	T
T	0.5841233275324685	0.9157602912460474	0.2177041211771017	T	T
T	0.8321643754561743	0.4166424492817868	0.2178370123870582	T	T
T	0.3340183714486266	0.4178241766027261	0.2191228051442303	T	T
T	0.3317813027364993	0.9160400513604297	0.2177034789508202	T	T
T	0.8351592639157307	0.9178629149829332	0.2184463330997068	T	T
T	0.9922964450429066	0.9921516835844344	0.3215373669933475	T	T
T	0.4978954372140131	0.0016198553755756	0.3221859719497639	T	T
T	0.5078314727674758	0.5076990914584807	0.3215617514679549	T	T
T	0.0038948042092984	0.4955107618705667	0.3223567816326939	T	T
T	0.2585561853341510	0.0074879659426198	0.3215291096958373	T	T
T	0.7513467060072404	0.9912368003533333	0.3218387749858800	T	T
T	0.7536739575060462	0.5043456538095915	0.3217634357465260	T	T
T	0.2410262136596454	0.5020838607512763	0.3218042323358769	T	T

T	0.4925047550936191	0.2412492492404215	0.3216302181147360	T	T
T	0.9976210608936475	0.2588920774940527	0.3217232803512196	T	T
T	0.9956213209906405	0.7466843258949825	0.3217995350942697	T	T
T	0.5091401857905055	0.7488907205336255	0.3218594099183485	T	T
T	0.7562885871891878	0.2583404549060480	0.3211018686587795	T	T
T	0.2503121641068523	0.2505583698636059	0.3225699830641649	T	T
T	0.2416448207354809	0.7438603478510313	0.3211279991216954	T	T
T	0.7465349769979530	0.7543988240362528	0.3225535546603078	T	T
T	0.4598618657211143	0.0374426393619034	0.4352586405402533	T	T
T	0.3556527480745498	0.9059293161658076	0.4744346570223148	T	T
T	0.5894159731712646	0.1402388098153366	0.4759710047582794	T	T
T	0.3893045826386049	0.1089179973748841	0.4101854308048765	T	T
T	0.2602660759822097	0.2565015028962745	0.4320492760562495	T	T
T	0.4073531872784945	0.8474311188676544	0.4932862105657758	T	T
T	0.1704768576396124	0.2238242003531609	0.4565132343952220	T	T
T	0.3009663305793427	0.1957996286734269	0.4459141621107097	T	T
T	0.5535122895724159	0.1798522553319684	0.5186545981821624	T	T
T	0.2630820672423353	0.8327849046625466	0.4430021104145883	T	T
T	0.3146949173238431	0.9395493228166473	0.5174530700357008	T	T
T	0.6465233258350850	0.0875830031570393	0.4954448449083970	T	T
T	0.6643187019595671	0.2334432246517705	0.4454447947347637	T	T
T	0.5378456648579257	0.9628776691156399	0.3976374164441580	T	T

Acetone\_to\_CH3C\_OH\_CH3 on Ru

Ru	C	O	H
1.0000000000000000			
10.799999999973024	0.0000000000000000	0.0000000000000000	
-5.399999999986512	9.3530743608696145	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.8408669165437317	

Ru C O H  
64 3 2 9

Selective dynamics

Direct

F	0.3333332944791607	0.1666665889583143	0.0000000000000000	F	F
F	0.8333332944791607	0.1666665889583143	0.0000000000000000	F	F

0.8333331779166286	0.6666663558332644	0.0000000000000000	F	F
F				
0.3333331779166286	0.6666663558332644	0.0000000000000000	F	F
F				
0.5833332944791607	0.1666665889583143	0.0000000000000000	F	F
F				
0.0833332944791607	0.1666665889583143	0.0000000000000000	F	F
F				
0.0833331779166286	0.6666663558332644	0.0000000000000000	F	F
F				
0.5833331779166286	0.6666663558332644	0.0000000000000000	F	F
F				
0.5833339578857277	0.4166679157714626	0.0000000000000000	F	F
F				
0.0833339578857277	0.4166679157714626	0.0000000000000000	F	F
F				
0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.8333339578857277	0.4166679157714626	0.0000000000000000	F	F
F				
0.3333339578857277	0.4166679157714626	0.0000000000000000	F	F
F				
0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.8333338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F				
0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F				
0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F				

F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.3355280163328301	0.1667659241211913	0.2183773673051221	F	F
F	0.8333697260889701	0.1679928225464417	0.2183572120592569	F	F
F	0.8321092197147374	0.6681318443164953	0.2181302750329354	F	F
F	0.3336142700310347	0.6682978841100505	0.2191027437810454	F	F
F	0.5836477775281446	0.1684174822786833	0.2179727940221961	F	F
F	0.0807344898566531	0.1655349601099507	0.2179245700429302	F	F
F	0.0842353298126066	0.6666361595452487	0.2179529363874438	F	F
F	0.5841276195251267	0.6677770559768732	0.2193536294544072	F	F
F	0.5830047349411323	0.4166993547216369	0.2189187372282119	F	F
F	0.0823050793549351	0.4160143130175640	0.2187002511625709	F	F
F	0.0842581472747227	0.9181361230128295	0.2179121697914507	F	F
F	0.5827989224526950	0.9159715879001591	0.2184766676887305	F	F
F	0.8348318877307180	0.4172339652682480	0.2186065970275175	F	F
F	0.3354954801036933	0.4186278770725637	0.2185628687926156	F	F
F	0.3335003620990793	0.9159485930766622	0.2179304314756150	F	F
F	0.8334339262811651	0.9153627463872406	0.2173881224968454	F	F
F	1.0096943748222376	0.9971864012033098	0.3223369210152178	F	F
F	0.5092483112718396	1.0010818799163683	0.3219090565800776	F	F
F	0.4994676931145537	0.4986552888355187	0.3232955072532224	F	F
F	-0.0039936511660356	0.5062671124832742	0.3212352376428170	F	F
F	0.2489160237029638	0.0002623084161405	0.3216102829394443	F	F
F	0.7427344553037273	-0.0006617124822495	0.3213471297700313	F	F
F	0.7610306120285326	0.5075677936450156	0.3215966865511823	F	F
F	0.2496719219046452	0.4983844682930104	0.3215938719169781	F	F
F	0.5032487846238758	0.2465737972822472	0.3212408423340519	F	F
F	1.0085017304690644	0.2504992551335091	0.3237989963669041	F	F
F	0.9902822348144024	0.7442892659676498	0.3221444578171425	F	F
F	0.4984345706742094	0.7585832406641113	0.3214307411867759	F	F

F	0.7421379904285824	0.2482658992888585	0.3219114634200492	F	F
F	0.2462796152483308	0.2510257937872777	0.3195345900869893	F	F
F	0.2535620042240504	0.7552525964763966	0.3217818849362279	F	F
F	0.7589697734938099	0.7505162423690642	0.3229610467972110	F	F
T	0.0812181200415048	0.2553612167606306	0.4270754705696572	T	T
T	0.1388188780822577	0.4026766660641405	0.4573228544734970	T	T
T	0.9646643342092550	0.1404688207065196	0.4706193738008741	T	T
T	0.4732818167183927	0.4732471136740580	0.4325901685360173	T	T
T	0.2012700315024213	0.2292145687325054	0.4238468626612508	T	T
T	0.0072202332439982	0.1428758946834224	0.5216054549771866	T	T
T	0.3862413001413432	0.3808262181584431	0.4431651658623368	T	T
T	0.1902101907004718	0.4098955534069478	0.5065174526171378	T	T
T	0.2273583783147302	0.4919541843853040	0.4272737693120084	T	T
T	0.0540291793126060	0.4293564062942473	0.4641414051322359	T	T
T	0.5526091123266073	0.4785350174422902	0.4588471689640046	T	T
T	0.9265666802935111	0.0328299948577376	0.4495232258269233	T	T
T	0.8728399110461638	0.1574385880955706	0.4750293372320170	T	T
T	0.1514394756086075	0.0978489070274169	0.3950258143544450	T	T

CH3CH\_O\_CH3\_to\_iPrOH on Ru

Ru C O H

1.000000000000000			
10.799999999973024	0.000000000000000	0.000000000000000	
-5.399999999986512	9.3530743608696003	0.000000000000000	
0.000000000000000	0.000000000000000	19.8408669165437423	

Ru	C	O	H
64	3	2	10

Selective dynamics

Direct

F	0.3333332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.8333332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.8333331779166289	0.6666663558332645	0.000000000000000	F	F
F	0.3333331779166287	0.6666663558332645	0.000000000000000	F	F
F	0.5833332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.0833332944791607	0.1666665889583143	0.000000000000000	F	F



0.0833331779166286	0.6666663558332645	0.0000000000000000	F	F
F				
0.5833331779166288	0.6666663558332645	0.0000000000000000	F	F
F				
0.5833339578857277	0.4166679157714627	0.0000000000000000	F	F
F				
0.0833339578857273	0.4166679157714627	0.0000000000000000	F	F
F				
0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.8333339578857279	0.4166679157714627	0.0000000000000000	F	F
F				
0.3333339578857278	0.4166679157714627	0.0000000000000000	F	F
F				
0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F				
0.8333338413232027	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F				
0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F				
0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F				
0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F				
0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F				
0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
F				
0.3326368006787130	0.1661229459557623	0.2196966769845009	T	T
T				
0.8318364709011321	0.1661914611387480	0.2184765323474769	T	T
T				
0.8337327797497511	0.6660806355729701	0.2182056160907741	T	T
T				

T	0.3325924782636812	0.6659767856897888	0.2176376588073597	T	T
T	0.5832533527832547	0.1665677852362077	0.2189151115426859	T	T
T	0.0847441034810323	0.1676249995421217	0.2185497515014606	T	T
T	0.0832334335166310	0.6660298603107265	0.2180381148690510	T	T
T	0.5837431948973661	0.6675304684551454	0.2187093800819592	T	T
T	0.5837737146470779	0.4168708569450483	0.2199045427527643	T	T
T	0.0837045840665775	0.4181674763197002	0.2176274766241184	T	T
T	0.0838414541003493	0.9171890878934663	0.2181547306818689	T	T
T	0.5832087751264549	0.9167827385899044	0.2184637320891041	T	T
T	0.8325467989411883	0.4159732687778007	0.2183789526115828	T	T
T	0.3326081837619883	0.4162205773606439	0.2193940414166109	T	T
T	0.3316531430342700	0.9152160331715591	0.2180188817714938	T	T
T	0.8331377447662687	0.9165871415636322	0.2183656382737881	T	T
T	0.9972870085724714	0.9945205017923481	0.3213077949373615	T	T
T	0.4920865767888023	0.9912469741091416	0.3214480635593712	T	T
T	0.5001023094415444	0.5031091312163192	0.3224702027193143	T	T
T	0.9946672314333658	0.4910313358840392	0.3224734373656044	T	T
T	0.2488173850819314	0.9899585321231861	0.3218697263960563	T	T
T	0.7487329705975094	0.0014090133316337	0.3207300424081206	T	T
T	0.7580153634264296	0.5086815293474218	0.3214920764748801	T	T
T	0.2433992423796051	0.4916913097255406	0.3231115244114964	T	T
T	0.4983833389255912	0.2450075592625110	0.3229978263139558	T	T
T	0.9997262961610098	0.2569756672071391	0.3218365453653179	T	T
T	0.9963731697009843	0.7546143966954056	0.3222271122997420	T	T
T	0.4965815349337904	0.7537856757504471	0.3212553274925396	T	T
T	0.7556938559055145	0.2480649094438423	0.3218200783825113	T	T
T	0.2425139256088774	0.2524036571617382	0.3223805420720703	T	T
T	0.2571538652205591	0.7562591297939839	0.3226356812426245	T	T
T	0.7583903394695107	0.7489537641057737	0.3215791275837067	T	T

T	0.4906081833617179	0.5838023737824739	0.4769687395515407	T	T
T	0.6466818179389923	0.6468375934260367	0.4954901251486994	T	T
T	0.3911997564225017	0.5201608753435104	0.5369237478631032	T	T
T	0.5059087032818710	0.2635653976766474	0.4310442812418526	T	T
T	0.4516222244668985	0.4708694228712038	0.4272576509202818	T	T
T	0.4738436017706136	0.6671111797944812	0.4528708457892540	T	T
T	0.4798102908594307	0.3399556871525644	0.4409887372208082	T	T
T	0.6783900624547905	0.7346620253710474	0.5317169501039301	T	T
T	0.6663053069834983	0.5652506641307260	0.5181632252868059	T	T
T	0.7158354864921617	0.6903350877731176	0.4505436414644312	T	T
T	0.4426348404504697	0.1776857506434974	0.4570219042262005	T	T
T	0.4056046473847812	0.4357040281666144	0.5601658789061940	T	T
T	0.4159393444920862	0.6036252020270952	0.5748364383238056	T	T
T	0.2790219949017417	0.4743413554302707	0.5214767563397699	T	T
T	0.3220765927013896	0.4309910381734579	0.3959008703192922	T	T

CH3C\_OH\_CH3\_to\_iPrOH on Ru

Ru C O H

2.700000000000000			
3.999999999999008	0.000000000000000	0.000000000000000	
-1.999999999995004	3.4641016151368880	0.000000000000000	
0.000000000000000	0.000000000000000	7.3484692283495336	

Ru C O H  
64 3 2 10

Selective dynamics

Direct

F	0.3333332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.8333332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.8333331779166286	0.6666663558332644	0.000000000000000	F	F
F	0.3333331779166286	0.6666663558332644	0.000000000000000	F	F
F	0.5833332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.0833332944791607	0.1666665889583143	0.000000000000000	F	F
F	0.0833331779166286	0.6666663558332644	0.000000000000000	F	F
F	0.5833331779166286	0.6666663558332644	0.000000000000000	F	F
F	0.5833339578857277	0.4166679157714626	0.000000000000000	F	F

F	0.0833339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.0833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.5833338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.3333339578857277	0.4166679157714626	0.0000000000000000	F	F
F	0.3333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.8333338413232028	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.4999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.9999998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.2499998834374750	0.4999997668749430	0.1111111681396224	F	F
F	0.4999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.9999999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.0000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.5000005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7499999417187340	0.2499998834374750	0.1111111681396224	F	F
F	0.7500005468440492	0.7500010936880912	0.1111111681396224	F	F
F	0.2500005468440492	0.7500010936880912	0.1111111681396224	F	F
T	0.3337934581252373	0.1670544476486897	0.2192982131008855	T	T
T	0.8328752727792086	0.1673752763614949	0.2183122698533422	T	T
T	0.8321090699522832	0.6670304099483437	0.2183092525022232	T	T
T	0.3313690702020203	0.6660138673304078	0.2175507668149156	T	T
T	0.5830710566150198	0.1668212997393363	0.2191318021631056	T	T
T	0.0827942700233585	0.1655548419008189	0.2189833033644704	T	T

T	0.0837471953662591	0.6664839808895603	0.2178041905725330	T	T
T	0.5828850582248659	0.6644964193545018	0.2193801648160442	T	T
T	0.5827452062327263	0.4159462477243918	0.2204832251527908	T	T
T	0.0843479875914839	0.4171484648560687	0.2183176854608245	T	T
T	0.0839262407434223	0.9164763116545480	0.2179659496946882	T	T
T	0.5832964186770412	0.9174348350382875	0.2181738817404755	T	T
T	0.8339381204212111	0.4159468898150390	0.2182276044270482	T	T
T	0.3340761817312929	0.4165009147634060	0.2190625443344510	T	T
T	0.3328628191006404	0.9156830613417748	0.2173378562725733	T	T
T	0.8333015730800173	0.9155972440924018	0.2181108077498770	T	T
T	0.0051738071518542	0.9944504371853816	0.3215033851546312	T	T
T	0.4992566372913296	0.9913637414952872	0.3209891171559428	T	T
T	0.4985887626678742	0.5054259342748778	0.3276220748079068	T	T
T	0.9935212258245466	0.4913244436039740	0.3218843297294557	T	T
T	0.2431316677636111	0.9957396302996482	0.3214524661102588	T	T
T	0.7464142723430146	0.0017070611296451	0.3204889343500848	T	T
T	0.7613174357402167	0.5053142334039268	0.3216787485492863	T	T
T	0.2504454402649813	0.5047254834007908	0.3215398100698368	T	T
T	0.4986345527674408	0.2448781066749415	0.3233695361027549	T	T
T	0.0004530562386751	0.2550976492215436	0.3209164552839826	T	T
T	0.9951523159472534	0.7524800222946046	0.3222004363429325	T	T
T	0.4927881641859320	0.7521817175793024	0.3211396371221611	T	T
T	0.7575590909807863	0.2519191305539133	0.3218801048664914	T	T
T	0.2419405025260506	0.2431856086189525	0.3219658630937257	T	T
T	0.2581519277055043	0.7543724157890943	0.3221362467763138	T	T
T	0.7574587968695169	0.7510279782039430	0.3225664657252623	T	T
T	0.5168554498429485	0.5363475645585122	0.4565175355097640	T	T
T	0.6477280396022368	0.5489705993268148	0.4906365753972758	T	T
T	0.4818304653314304	0.6491878503995206	0.4778742227292645	T	T

T	0.4024582932817017	0.3972769260653744	0.4689192455044894	T	T
T	0.4929344749800859	0.2260481419421228	0.4317694750031085	T	T
T	0.3092501258915021	0.3908748301778723	0.4629769485262144	T	T
T	0.6235873822813587	0.5260689375877506	0.5447382462594760	T	T
T	0.6774467428390059	0.4728768795167879	0.4700893522280319	T	T
T	0.7388639671150217	0.6575028349647111	0.4848218516267192	T	T
T	0.4426967779987978	0.2749687488270902	0.4512507369797705	T	T
T	0.4507087073678988	0.1305257745979268	0.4516686301501030	T	T
T	0.4690964645749719	0.6445144561576609	0.5332101360964365	T	T
T	0.3820546846349345	0.6332392320074691	0.4549767069068354	T	T
T	0.5690130305634464	0.7563437432559472	0.4643315565652907	T	T
T	0.6184194008829833	0.6130432703662985	0.3886815157157989	T	T

CO2 on Ru

Ru	C	O			
	2.7000000000000000				
	4.0000000000000009	0.0000000000000000	0.0000000000000000		
	2.0000000000000004	3.4641016151377544	0.0000000000000000		
	0.0000000000000000	0.0000000000000000	7.3484692283495328		

Ru C O  
64 1 2

Selective dynamics

Direct					
F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F

F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1676267749535990	0.1658424429043035	0.2192326479637328	T	T
T	0.6658548039851130	0.1669453635207052	0.2190631634052150	T	T
T	0.1664898196188268	0.6666983232027289	0.2189653122865818	T	T
T	0.6667833411658538	0.6667973929979848	0.2184240593818890	T	T
T	0.4172324492733243	0.1662375306919486	0.2191019763260279	T	T
T	0.9163768580221341	0.1659588331757576	0.2189758432860381	T	T
T	0.4173384307763287	0.6659473717440647	0.2188202214685070	T	T
T	0.9157446522951375	0.6673502874856410	0.2170381400132379	T	T
T	0.1653731192565553	0.4173313244141309	0.2194651535241232	T	T

T	0.6657579516364716	0.4171032833888612	0.2187148602834486	T	T
T	0.1674744336863677	0.9167637102533051	0.2183220205244408	T	T
T	0.6667244846220024	0.9160247894941230	0.2181470969533907	T	T
T	0.4172992017334166	0.4160475409501780	0.2193814206336289	T	T
T	0.9167887167377058	0.4175650461660169	0.2186630035996654	T	T
T	0.4166569769090727	0.9157171910349186	0.2182547674624028	T	T
T	0.9171459396322267	0.9171163276943147	0.2187669506825997	T	T
T	0.0064129608382497	0.9964262367600918	0.3212001916048741	T	T
T	0.5081202066891859	0.9906408255426491	0.3217436474230269	T	T
T	0.0053724025121751	0.4964058021285783	0.3248782615154099	T	T
T	0.5043569052097872	0.4946069862282386	0.3221786080962515	T	T
T	0.2542714674522977	0.9917948708285688	0.3216205691073266	T	T
T	0.7434934176032425	0.9987750483055846	0.3208236540328692	T	T
T	0.2438890977047616	0.5081772698720365	0.3217659758423813	T	T
T	0.7506442400475910	0.4922615421476024	0.3220977550927646	T	T
T	0.2495191128706517	0.2509190190134442	0.3217844907701360	T	T
T	0.7460027978555372	0.2591682700816537	0.3220589414478088	T	T
T	0.2418632703762234	0.7538310017546059	0.3222417505891797	T	T
T	0.7442909856503209	0.7550657982016346	0.3218649417632092	T	T
T	0.9917969166777841	0.2526666531139656	0.3216917264323186	T	T
T	0.5081189057072931	0.2451333552001674	0.3225674836098702	T	T
T	0.0079217499017638	0.7480791458684378	0.3221827230131618	T	T
T	0.5011310686342633	0.7561990704118283	0.3225174378549429	T	T
T	0.0815717460973267	0.4210665759795080	0.4221158677993578	T	T
T	0.2057658449184576	0.2995542857301178	0.4228675052932908	T	T
T	0.0150173595771795	0.4857580087869158	0.4729036682689220	T	T

COOH on Ru

Ru C O H

2.7000000000000000			
4.0000000000000009	0.0000000000000000	0.0000000000000000	0.0000000000000000
2.0000000000000004	3.4641016151377544	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.3484692283495328	



	Ru	C	O	H			
	64	1	2	1			
Selective dynamics							
Direct							
F	0.1666667055208393	0.1666665889583143	0.0000000000000000		F	F	
F	0.6666667055208393	0.1666665889583143	0.0000000000000000		F	F	
F	0.1666667055208393	0.6666665889583143	0.0000000000000000		F	F	
F	0.6666667055208393	0.6666665889583143	0.0000000000000000		F	F	
F	0.4166667055208393	0.1666665889583143	0.0000000000000000		F	F	
F	0.9166667055208393	0.1666665889583143	0.0000000000000000		F	F	
F	0.4166667055208393	0.6666665889583143	0.0000000000000000		F	F	
F	0.9166667055208393	0.6666665889583143	0.0000000000000000		F	F	
F	0.1666660421142652	0.4166679157714626	0.0000000000000000		F	F	
F	0.6666660421142723	0.4166679157714626	0.0000000000000000		F	F	
F	0.1666660421142652	0.9166679157714626	0.0000000000000000		F	F	
F	0.6666660421142723	0.9166679157714626	0.0000000000000000		F	F	
F	0.4166660421142723	0.4166679157714626	0.0000000000000000		F	F	
F	0.9166660421142723	0.4166679157714626	0.0000000000000000		F	F	
F	0.4166660421142723	0.9166679157714626	0.0000000000000000		F	F	
F	0.9166660421142723	0.9166679157714626	0.0000000000000000		F	F	
F	0.0000000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.5000000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.0000000000000000	0.5000000000000000	0.1111111681396224		F	F	
F	0.5000000000000000	0.5000000000000000	0.1111111681396224		F	F	
F	0.2500000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.7500000000000000	0.0000000000000000	0.1111111681396224		F	F	
F	0.2500000000000000	0.5000000000000000	0.1111111681396224		F	F	
F	0.7500000000000000	0.5000000000000000	0.1111111681396224		F	F	
F	0.2500000582812589	0.2499998834374750	0.1111111681396224		F	F	
F	0.7500000582812589	0.2499998834374750	0.1111111681396224		F	F	
F	0.2500000582812589	0.7499998834374679	0.1111111681396224		F	F	

F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1673423960913977	0.1662731547069571	0.2191548153488436	T	T
T	0.6665553381786147	0.1663896745561540	0.2183627470233718	T	T
T	0.1676474771922582	0.6662853239011957	0.2187198492733545	T	T
T	0.6679953417422919	0.6645964595365434	0.2184421996117620	T	T
T	0.4178672328139815	0.1658363893619317	0.2174930467418635	T	T
T	0.9165418359390303	0.1657421007954952	0.2189863172192499	T	T
T	0.4171114020043046	0.6654766324490473	0.2186284100181893	T	T
T	0.9161652110952699	0.6672380313233949	0.2187405932784572	T	T
T	0.1672879845006468	0.4164216520110438	0.2181241417624906	T	T
T	0.6658944647387453	0.4172268499970719	0.2181848342578032	T	T
T	0.1656201379213243	0.9170130337373718	0.2190020890406623	T	T
T	0.6672725012365389	0.9156566873016583	0.2187967090196499	T	T
T	0.4169585203451786	0.4161955304906997	0.2179563991203949	T	T
T	0.9160184000657334	0.4160157498418308	0.2192204866817305	T	T
T	0.4172124268633693	0.9165088929195009	0.2184276409109251	T	T
T	0.9176820484949811	0.9173077735331646	0.2186394422655590	T	T
T	0.9967037212148159	0.9955231933247866	0.3226119472150484	T	T
T	0.4976328602610962	0.9935359761803049	0.3220342653224763	T	T
T	0.0021412021773672	0.5075760397342093	0.3216101151206504	T	T
T	0.5073256708506700	0.4904128621297231	0.3226368578659394	T	T
T	0.2598271296951205	0.9938944638644308	0.3215164565265140	T	T
T	0.7494728548516186	0.0064638556239897	0.3209286374572869	T	T
T	0.2430106187801967	0.5062259624451042	0.3219859849217026	T	T
T	0.7430237971226726	0.5014008033644585	0.3219612677709400	T	T

T	0.2482053712070000	0.2473763621425337	0.3250987192509612	T	T
T	0.7408085338312032	0.2516892281234815	0.3220068094863547	T	T
T	0.2442116492313444	0.7522986116494729	0.3218464611568936	T	T
T	0.7483122619894694	0.7461652737869571	0.3212289004452837	T	T
T	0.5058961355503067	0.2496877420997556	0.3216581844697949	T	T
T	0.9994874013508394	0.2498653365101413	0.3222284864767798	T	T
T	0.5036856150274608	0.7546612589983538	0.3220573633233335	T	T
T	0.0102277162533600	0.7438000120036702	0.3220962175469718	T	T
T	0.1727977585927199	0.2492786979592953	0.4202095938119144	T	T
T	0.0540535588696938	0.2493587544567416	0.4249972385950482	T	T
T	0.2297437233455326	0.2504314643353889	0.4795074709536434	T	T
T	0.3202434489849033	0.2501483976292554	0.4738870746264249	T	T

HCOOH on Ru

Ru	C	O	H
2.7000000000000000			
4.0000000000000009	0.0000000000000000	0.0000000000000000	0.0000000000000000
2.0000000000000004	3.4641016151377544	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	7.3484692283495328	

Ru	C	O	H		
64	1	2	2		
Selective dynamics					
Direct					
F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F

F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1670292227063936	0.1669492349396424	0.2196391629450910	T	T
T	0.6674801379886715	0.1654558231440646	0.2183940721112634	T	T
T	0.1653121367738734	0.6678093148076059	0.2181795791572191	T	T
T	0.6658483380399322	0.6656602695344026	0.2188352824931585	T	T
T	0.4169453114337209	0.1661474008299852	0.2190903353461041	T	T
T	0.9155009503188630	0.1678106942706940	0.2188689068103495	T	T
T	0.4158806005731777	0.6680539813862220	0.2186262729257090	T	T
T	0.9178501400366466	0.6653961035401045	0.2180802438465214	T	T
T	0.1658741157255522	0.4170743607247407	0.2190047368977412	T	T

T	0.6677748942500337	0.4161772266352076	0.2186926932841825	T	T
T	0.1676487291192852	0.9157274818096207	0.2188639331748021	T	T
T	0.6653828932589129	0.9178646622080567	0.2181631859619177	T	T
T	0.4169325341455223	0.4169395705670944	0.2181263964347357	T	T
T	0.9169655059387462	0.4177072751825872	0.2188889042633694	T	T
T	0.4176934749292407	0.9169372019354816	0.2190101864257808	T	T
T	0.9160867505376139	0.9162671530700086	0.2179334894864235	T	T
T	0.0038802258905356	0.0059099829710761	0.3219600558158532	T	T
T	0.5101448975292681	0.9923320980312582	0.3222191805467685	T	T
T	0.9927099740139946	0.5100533545522213	0.3222355593195133	T	T
T	0.4943815567659446	0.4967988700688338	0.3221725524311477	T	T
T	0.2419598759746030	0.9978444906014714	0.3218988812758908	T	T
T	0.7508520408371222	0.9979032073049721	0.3215950136961164	T	T
T	0.2603617338172547	0.4957697607691596	0.3215777810856322	T	T
T	0.7526278238648209	0.5069450492753629	0.3226319069643004	T	T
T	0.2521742543972464	0.2529598772802826	0.3240850527623152	T	T
T	0.7518276552801698	0.2439413496759298	0.3218992133836249	T	T
T	0.2444507312320807	0.7508652740540565	0.3218572663371463	T	T
T	0.7456176720999823	0.7460243505774319	0.3227322965289856	T	T
T	0.4951063119983825	0.2609074342288932	0.3215550084013556	T	T
T	0.9975273706152566	0.2420987216294583	0.3219669409029314	T	T
T	0.5073818877886858	0.7519468141434392	0.3225527184120286	T	T
T	0.9981114377113673	0.7504499352173427	0.3214977737850350	T	T
T	0.2775799474988387	0.2761331067277412	0.4818915407864418	T	T
T	0.3475768580131287	0.3460678747837390	0.4815791254423872	T	T
T	0.2372328050508579	0.2369500535375364	0.4313663566378309	T	T
T	0.2548053853114417	0.2522227822396599	0.5326485646860877	T	T
T	0.3661597435681655	0.3657646957004276	0.4332925082518979	T	T

HCOO on Ru  
Ru C O H

```

2.7000000000000000
4.0000000000000009 0.0000000000000000 0.0000000000000000
2.0000000000000004 3.4641016151377544 0.0000000000000000
0.0000000000000000 0.0000000000000000 7.3484692283495328

```

```

Ru    C    O    H
64    1    2    1

```

Selective dynamics

Direct

0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F				
0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F				
0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F				

F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
T	0.1664081191571911	0.1669543107050112	0.2189667846364948	T	T
T	0.6661331716119520	0.1666841172811375	0.2193533921869242	T	T
T	0.1658443408062223	0.6674985414879562	0.2180808293913818	T	T
T	0.6670742428271542	0.6649709006903883	0.2185356833302229	T	T
T	0.4162276271330281	0.1672114649239611	0.2204165981060915	T	T
T	0.9155607346394573	0.1678144702005343	0.2186499827740840	T	T
T	0.4165819436056948	0.6657899228947743	0.2186570453221906	T	T
T	0.9178750290074065	0.6647600309357039	0.2181367768082055	T	T
T	0.1655852976561396	0.4169725478702974	0.2189075007979863	T	T
T	0.6663077877356717	0.4170140771647660	0.2188635162385545	T	T
T	0.1677371816661359	0.9167891343210627	0.2183627456293045	T	T
T	0.6663548119617668	0.9171928483540902	0.2181974320483437	T	T
T	0.4181689497044080	0.4166011675061375	0.2189006137515206	T	T
T	0.9174225395328740	0.4175102650239272	0.2183377357972530	T	T
T	0.4174451409230963	0.9168394158435949	0.2189842374300058	T	T
T	0.9161631910307576	0.9159723748897385	0.2184089916260817	T	T
T	0.0003095831075041	0.0078175576663440	0.3214270693755193	T	T
T	0.5100761082695023	0.9891682851625345	0.3215125069441818	T	T
T	0.9953458904931104	0.5059637313124752	0.3226076994096130	T	T
T	0.4896292545324757	0.5083505491945765	0.3227411870258298	T	T
T	0.2434092844049072	0.0018525258325957	0.3214633448736924	T	T
T	0.7515735242985683	0.9966934657290338	0.3215350776037819	T	T

T	0.2509274809531911	0.5084653097559662	0.3213472569734707	T	T
T	0.7537697575629552	0.5038340049870408	0.3226627155249423	T	T
T	0.2488657077690674	0.2525671646173548	0.3228514246444015	T	T
T	0.7592369263320413	0.2433476161124912	0.3218485248249435	T	T
T	0.2467175199718468	0.7464111559925664	0.3212454858302097	T	T
T	0.7424805285744361	0.7487658461725886	0.3222730268578004	T	T
T	0.4957613625926976	0.2536848528329928	0.3233915045592398	T	T
T	0.9964633151271234	0.2435906047278780	0.3220059695600092	T	T
T	0.5084939120363280	0.7474667723803868	0.3218297140770053	T	T
T	0.0033936068182911	0.7465519376323816	0.3210107811330358	T	T
T	0.3713940456144530	0.2528714214133977	0.4576453180096053	T	T
T	0.2680908925953503	0.2493989451187485	0.4283799594849870	T	T
T	0.4768241171184365	0.2530211736847216	0.4288607151074517	T	T
T	0.3697451687590799	0.2552829460082038	0.5131735966400464	T	T

CO2 desorption on Ru

Ru C O H Cl

1.0000000000000000			
10.8000000000000025	0.0000000000000000	0.0000000000000000	
5.4000000000000012	9.3530743608719380	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.8408669165437388	

Ru C O  
64 1 2

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.1666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.6666667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.6666665889583143	0.0000000000000000	F	F
F	0.1666660421142652	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F



F	0.1666660421142652	0.9166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.9166679157714626	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.5000000000000000	0.1111111681396224	F	F
F	0.2500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.2500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.7500000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812589	0.2499998834374750	0.1111111681396224	F	F
F	0.0000000582812660	0.7499998834374679	0.1111111681396224	F	F
F	0.5000000582812589	0.7499998834374679	0.1111111681396224	F	F
F	0.1671414680067471	0.1668727705014135	0.2192470453930895	F	F
F	0.6661377227496956	0.1656195507763840	0.2183212211937331	F	F
F	0.1683063949668977	0.6666837374458652	0.2187351656700471	F	F
F	0.6674489651262405	0.6664769267552302	0.2192056336665047	F	F
F	0.4157945387033664	0.1674999833188764	0.2180530786276265	F	F
F	0.9169379055232412	0.1654030552621819	0.2189295811689220	F	F
F	0.4156708790854040	0.6670030452153171	0.2188611940890155	F	F

F	0.9163988668200389	0.6657578084566964	0.2184568123563579	F	F
F	0.1658284132048138	0.4165037720219900	0.2192051161312349	F	F
F	0.6653212342757087	0.4176873152024783	0.2183869894079535	F	F
F	0.1654502467348706	0.9164757371421999	0.2184437305772562	F	F
F	0.6679592824576517	0.9159407268349113	0.2182705870471935	F	F
F	0.4167148214252521	0.4154419445385997	0.2183531018649276	F	F
F	0.9160074863902494	0.4166264499784660	0.2195972229411325	F	F
F	0.4170418323173024	0.9156777708836543	0.2188879866554529	F	F
F	0.9166198369421394	0.9176204107807706	0.2180387880168126	F	F
F	0.9975496912388664	0.9940133705974077	0.3221736284057499	F	F
F	0.4927380915305761	0.9975063479884412	0.3224549637729481	F	F
F	0.0030430634497023	0.5071254847310769	0.3216897739128726	F	F
F	0.5072750386438329	0.4907505924859521	0.3224203277005984	F	F
F	0.2597399378295648	0.9990334698925309	0.3216447015001904	F	F
F	0.7521312707898602	0.9992751967944855	0.3213975081798779	F	F
F	0.2424435018911595	0.5084360187315369	0.3224069904617579	F	F
F	0.7441698967645536	0.4951168832777384	0.3219272738922214	F	F
F	0.2537034031846801	0.2423385766773620	0.3225538589064385	F	F
F	0.7414585604411599	0.2589772982941057	0.32182034111119021	F	F
F	0.2418893221512448	0.7515342878888802	0.3228807374709177	F	F
F	0.7503525884807303	0.7543837923042602	0.3217496950617402	F	F
F	0.5052524610921836	0.2483432271925707	0.3215436969215091	F	F
F	0.9975213550144986	0.2483315013249054	0.3227585183737176	F	F
F	0.5017888126609193	0.7549926588923910	0.3220153532088332	F	F
F	0.0081489179434868	0.7427855997093218	0.3227043126188605	F	F
T	0.1279191762759950	0.2488822197251892	0.4509139013656522	T	T
T	0.2161530579959106	0.2517312709303638	0.4849865997068505	T	T
T	0.0197620996128265	0.2475137814368935	0.4355968187399270	T	T

COOH\_CO2 on Ru

Ru C O H Ru C O H - Geom 4/ 9

2.7000000000000000			
3.9999999999990008	0.0000000000000000	0.0000000000000000	
1.9999999999995004	3.4641016151368942	0.0000000000000000	
0.0000000000000000	0.0000000000000000	7.3484692283495301	

Ru	C	O	H
64	1	2	1

Selective dynamics

Direct

0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.6666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.9166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.1666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.9166661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.5000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.7500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F				

F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1656943841495102	0.1673588033548355	0.2189931806738824	T	T
T	0.6663810622308881	0.1675139099767350	0.2189657256502519	T	T
T	0.1662946234944092	0.6669126467241953	0.2189254098457916	T	T
T	0.6659648851669144	0.6673781801797073	0.2182715114977555	T	T
T	0.4186270884344973	0.1690416938645527	0.2163808134440127	T	T
T	0.9155756375283485	0.1685409124775060	0.2201276167239233	T	T
T	0.4170360610238593	0.6667985357454969	0.2178215550035501	T	T
T	0.9159325850196094	0.6679146117460059	0.2192559046353041	T	T
T	0.1657191810032399	0.4172164004832652	0.2186281561368437	T	T
T	0.6654408403466757	0.4171896490028502	0.2183436975474841	T	T
T	0.1665165188271099	0.9172635045759232	0.2187184301621348	T	T
T	0.6682086941834741	0.9158704286900317	0.2184722561794635	T	T
T	0.4170929170665185	0.4159404064561411	0.2179381297282079	T	T
T	0.9167003111302541	0.4161467238734252	0.2193076887318310	T	T
T	0.4149867199011073	0.9167506510626359	0.2188581456382903	T	T
T	0.9165876281676085	0.9168854064489980	0.2197517554464321	T	T
T	0.0071445697301181	-0.0075492529047361	0.3218831428192079	T	T
T	0.5031185165254828	0.0030667273786301	0.3209557155638391	T	T
T	0.0001663074385139	0.5056180970765661	0.3217904143810962	T	T
T	0.5052720266339055	0.5015001391180879	0.3218237663500936	T	T
T	0.2505050297260594	-0.0037512845956879	0.3218616076402409	T	T
T	0.7434081524229186	0.0030358527483511	0.3214352425015549	T	T

T	0.2441545210312291	0.5031397502981838	0.3222112849022423	T	T
T	0.7410940072912782	0.5029764763648222	0.3218682560565380	T	T
T	0.2524913579719310	0.2540236984746642	0.3253807558618415	T	T
T	0.7430065095075162	0.2579686546524105	0.3213761102661713	T	T
T	0.2439912850373975	0.7557001993817078	0.3213455788728175	T	T
T	0.7442454846886528	0.7508725182128309	0.3207255590796455	T	T
T	0.4949346842686798	0.2431006541649193	0.3245059155135731	T	T
T	-0.0007790624823421	0.2520617537435619	0.3240927344250269	T	T
T	0.5054748993337411	0.7428615734084866	0.3217166186290276	T	T
T	0.0094896926109827	0.7502547590362316	0.3227148696070645	T	T
T	0.1762670776927583	0.2521811395680443	0.4186280648127012	T	T
T	0.0588914747611281	0.2516497023798506	0.4287156350786518	T	T
F	0.2616906301135131	0.2494043045905272	0.4646439579667572	F	F
F	0.3491892800787681	0.2498918810826396	0.4086640457818120	F	F

HCOOH\_COOH on Ru

Ru C O H Ru C O H - Geom 5/ 9

1.0000000000000000			
10.799999999973024	0.0000000000000000	0.0000000000000000	
5.399999999986512	9.3530743608695985	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.8408669165437388	

Ru C O H  
64 1 2 2

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208394	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.9166668220833716	0.6666663558332644	0.0000000000000000	F	F
F	0.1666660421142722	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F

0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166661586767973	0.9166676826464055	0.0000000000000000	F	F
F				
0.9166661586767975	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.5000001165625252	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.7500001165625251	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F				
0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
F				
0.1665830680698264	0.1659513801620278	0.2192002683394776	F	F
F				
0.6658375327441989	0.1664120664110982	0.2192639180288864	F	F
F				
0.1657583197165096	0.6672526351092358	0.2181946933266729	F	F
F				
0.6670546785789213	0.6659057608750700	0.2187357382757184	F	F
F				
0.4175372560672130	0.1664807958236239	0.2195486002787490	F	F
F				
0.9164910792993907	0.1663765747397008	0.2185681944613052	F	F
F				
0.4174699591880326	0.6659349923075553	0.2185269480887584	F	F
F				

F	0.9177614710326125	0.6650816175564316	0.2183579427868665	F	F
F	0.1659742153666244	0.4161591198990280	0.2193236374198051	F	F
F	0.6663889635374645	0.4160522164835498	0.2181411343695174	F	F
F	0.1678873742345814	0.9173768188446871	0.2182591695558216	F	F
F	0.6676320220505758	0.9157248388370647	0.2182989735229199	F	F
F	0.4168178698131655	0.4170065480213907	0.2184091587298695	F	F
F	0.9160933345576012	0.4176539132346022	0.2183370869816485	F	F
F	0.4153443238994328	0.9173847733649508	0.2187144396988216	F	F
F	0.9172629192240009	0.9165347748127247	0.2182739384620191	F	F
F	0.0010102244818739	0.0009654578565588	0.3209241066780279	F	F
F	0.5113649579095778	0.9935808060522930	0.3216064187272422	F	F
F	0.9952646132068352	0.4960827674172137	0.3222178654757712	F	F
F	0.4928817644916849	0.5094477772878321	0.3222533777520482	F	F
F	0.2496180357038469	0.9935094905508564	0.3221887921331187	F	F
F	0.7455195660471361	0.9952328558583119	0.3225356730892485	F	F
F	0.2468963391623618	0.5118911801263053	0.3212296756387829	F	F
F	0.7566965842834890	0.4904881151024796	0.3226473786460530	F	F
F	0.2482220735533289	0.2505682591053855	0.3229096236522651	F	F
F	0.7567072015784504	0.2483763800710506	0.3217771763177808	F	F
F	0.2590311392175552	0.7454139710151182	0.3228914132376062	F	F
F	0.7529306019791306	0.7546723020667088	0.3216960426090907	F	F
F	0.5059553675442459	0.2411277884152057	0.3250429463448299	F	F
F	0.9914649685341743	0.2592540417889779	0.3219280676314469	F	F
F	0.4915007996760039	0.7525935026620516	0.3218597639178994	F	F
F	0.9998915135693025	0.7510467157156597	0.3210229366662957	F	F
T	0.4104560912895336	0.2376719322898291	0.4400218353713268	T	T
T	0.2997563921759540	0.2297185967536612	0.4282560304597346	T	T
T	0.4861218515625553	0.1763371434159330	0.4942632345503467	T	T
T	0.5629874192247137	0.1990679953716385	0.5012724998507471	T	T

0.4272197852906597 0.3256233479272119 0.4151769023515693 T T  
T

HCOOH\_HCOO

Ru C O H

2.7000000000000000

3.9999999999990008 0.0000000000000000 0.0000000000000000

1.9999999999995004 3.4641016151368880 0.0000000000000000

0.0000000000000000 0.0000000000000000 7.3484692283495328

Ru C O H

64 1 2 2

Selective dynamics

Direct

0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.6666667055208394	0.1666665889583143	0.0000000000000000	F	F
F				
0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F				
0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F
F				
0.9166668220833716	0.6666663558332644	0.0000000000000000	F	F
F				
0.1666660421142722	0.4166679157714626	0.0000000000000000	F	F
F				
0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F				
0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F				
0.4166661586767973	0.9166676826464055	0.0000000000000000	F	F
F				
0.9166661586767975	0.9166676826464055	0.0000000000000000	F	F
F				
0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F				
0.5000001165625252	0.4999997668749430	0.1111111681396224	F	F
F				
0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F				
0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F				



F	0.7500001165625251	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1674432633706992	0.1667397637041693	0.2192194598090424	T	T
T	0.6677829721480379	0.1659743002382132	0.2183550019613061	T	T
T	0.1666977893018086	0.6676332337414583	0.2178452538551019	T	T
T	0.6665612672934824	0.6652642618402795	0.2180280601539355	T	T
T	0.4173532361842426	0.1654175874696768	0.2198570149100512	T	T
T	0.9155540115821104	0.1676964211196817	0.2186594175197461	T	T
T	0.4160236033827671	0.6680663104772475	0.2181913593318139	T	T
T	0.9175992968979702	0.6649812897843372	0.2183744270427035	T	T
T	0.1652423521036434	0.4174963724739161	0.2195320978464016	T	T
T	0.6678709348366112	0.4164697729113892	0.2179467485455885	T	T
T	0.1670927595583051	0.9159194000652283	0.2193086235382827	T	T
T	0.6651739595576567	0.9175740822854657	0.2187391576640539	T	T
T	0.4156437764760644	0.4149000075186238	0.2186946352897871	T	T
T	0.9158023856011078	0.4173800616122610	0.2179832200542628	T	T
T	0.4171860579492176	0.9154815312901856	0.2188559826689948	T	T
T	0.9157765988682087	0.9153222360533260	0.2185432675739439	T	T
T	0.9981156486073237	0.0080159226512285	0.3207426321259900	T	T
T	0.5085304994749775	0.9907008309230504	0.3220311035152178	T	T
T	0.9921563419817410	0.5059132019201030	0.3219649395266615	T	T
T	0.4923547688380966	0.5007205372082046	0.3217218907061967	T	T

T	0.2392055538476015	0.0013988571189898	0.3221246893821109	T	T
T	0.7512794451119419	0.9907051248650178	0.3219674934846514	T	T
T	0.2605345108277590	0.4971395810767371	0.3229887547355140	T	T
T	0.7504641903316569	0.5014375494622764	0.3221533268158766	T	T
T	0.2476291768618735	0.2494123158582423	0.3236688957665815	T	T
T	0.7513502828756635	0.2540766233967581	0.3215714655074297	T	T
T	0.2587192064354554	0.7435634094879989	0.3217288920370332	T	T
T	0.7528998993384292	0.7551142923151921	0.3229164383794986	T	T
T	0.4967164268476394	0.2593053187947464	0.3225396843828284	T	T
T	0.0001023362227834	0.2403629573977324	0.3219299032500205	T	T
T	0.5039811754104548	0.7467459992384866	0.3219268374343257	T	T
T	0.9926743966885140	0.7477446440017947	0.3215239683752631	T	T
T	0.2935932916866215	0.2695043193643987	0.4754208887414053	T	T
T	0.3598953829589115	0.3377428271121342	0.4692379349769627	T	T
T	0.2409875678558257	0.2288122093062198	0.4282095315673182	T	T
T	0.2783264708391707	0.2405089510067774	0.5269050553387130	T	T
T	0.3684527927338693	0.3679560805368749	0.3993987273036447	T	T

HCOO\_to\_CO2 on Ru

Ru C O H

1.0000000000000000			
10.799999999973024	0.0000000000000000	0.0000000000000000	
5.399999999986512	9.3530743608695985	0.0000000000000000	
0.0000000000000000	0.0000000000000000	19.8408669165437388	

Ru C O H

64 1 2 1

Selective dynamics

Direct

F	0.1666667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.6666667055208394	0.1666665889583143	0.0000000000000000	F	F
F	0.1666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.6666668220833714	0.6666663558332644	0.0000000000000000	F	F
F	0.4166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.9166667055208393	0.1666665889583143	0.0000000000000000	F	F
F	0.4166668220833714	0.6666663558332644	0.0000000000000000	F	F

F	0.9166668220833716	0.6666663558332644	0.0000000000000000	F	F
F	0.1666660421142722	0.4166679157714626	0.0000000000000000	F	F
F	0.6666660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.1666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.6666661586767972	0.9166676826464055	0.0000000000000000	F	F
F	0.4166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.9166660421142723	0.4166679157714626	0.0000000000000000	F	F
F	0.4166661586767973	0.9166676826464055	0.0000000000000000	F	F
F	0.9166661586767975	0.9166676826464055	0.0000000000000000	F	F
F	0.0000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.5000000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.0000001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.5000001165625252	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.7500000000000000	0.0000000000000000	0.1111111681396224	F	F
F	0.2500001165625250	0.4999997668749430	0.1111111681396224	F	F
F	0.7500001165625251	0.4999997668749430	0.1111111681396224	F	F
F	0.2500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.7500000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.2499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.7499994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.0000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.5000000582812660	0.2499998834374750	0.1111111681396224	F	F
F	0.9999994531559508	0.7500010936880912	0.1111111681396224	F	F
F	0.4999994531559508	0.7500010936880912	0.1111111681396224	F	F
T	0.1659118108168612	0.1668207303636278	0.2179624783537221	T	T
T	0.6676988416584149	0.1665063147681759	0.2186766069727760	T	T
T	0.1666856823511588	0.6671517561499732	0.2193770690657090	T	T
T	0.6648821674159284	0.6683076305295589	0.2186254759344338	T	T

T	0.4172397915390031	0.1643632883022638	0.2182712812601673	T	T
T	0.9155354879320702	0.1673045686389709	0.2181132125200907	T	T
T	0.4177422816611954	0.6651145349086595	0.2184443522857406	T	T
T	0.9168007938468715	0.6657449065811114	0.2194066891960152	T	T
T	0.1667202419260400	0.4166598235037774	0.2196299063946610	T	T
T	0.6645665336231401	0.4172138070574127	0.2177907173478719	T	T
T	0.1671323276524547	0.9168962550234578	0.2186761632242253	T	T
T	0.6663687275769625	0.9170629629785384	0.2189220317274628	T	T
T	0.4169845644969628	0.4177471651126623	0.2185592109148538	T	T
T	0.9174780513101746	0.4165021519491031	0.2179089088078089	T	T
T	0.4165418278480115	0.9171178962718873	0.2189201542663480	T	T
T	0.9161834412472524	0.9164224911674463	0.2188976805620469	T	T
T	0.0091640159285678	0.9917482731639667	0.3218166393349574	T	T
T	0.5043140854636516	0.0059190174126602	0.3230014011898057	T	T
T	0.9902907271250720	0.4991032360352538	0.3213307747578174	T	T
T	0.5076227166020306	0.4988692288829238	0.3222932221884169	T	T
T	0.2419056667211759	0.0008831051136778	0.3219280442721406	T	T
T	0.7465192698931461	0.0049597907305286	0.3213571307215908	T	T
T	0.2537246307580908	0.4961158614084860	0.3218577651360752	T	T
T	0.7477434707738648	0.5086480545650686	0.3224800613172669	T	T
T	0.2560336151786037	0.2505249644070003	0.3246748594600629	T	T
T	0.7482093789448465	0.2516732461078637	0.3206584209501446	T	T
T	0.2438870984647564	0.7608401446236761	0.3218945145030996	T	T
T	0.7479353989608939	0.7433209426662214	0.3219445922962032	T	T
T	0.5021153054357030	0.2436063638818367	0.3214493203087289	T	T
T	0.9956104155727916	0.2512474779355326	0.3212495549927201	T	T
T	0.5050639633977637	0.7410948756251730	0.3225161187488089	T	T
T	0.0005819869773356	0.7574390081869068	0.3217928243343186	T	T
T	0.2564202645296545	0.3336990696237846	0.4347479520565340	T	T

0.2931269076111263	0.2578852330927764	0.4850766601952414	T	T
T				
0.2611436714044543	0.4509473259043891	0.4246211648681860	T	T
T				
0.1538402193955875	0.3319429264100677	0.3998885643183661	T	T
T				