

Electronic Supplementary Information for

**Over 50 wt% loaded nanoparticulate Ru on hollow carbon spheres as efficient catalysts
for the conversion of levulinic acid to γ -valerolactone under ambient conditions**

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Fig. S1. Additional TEM images of (a) Ru/HC-1, (b) Ru/HC-2, and (c) Ru/HC-3.

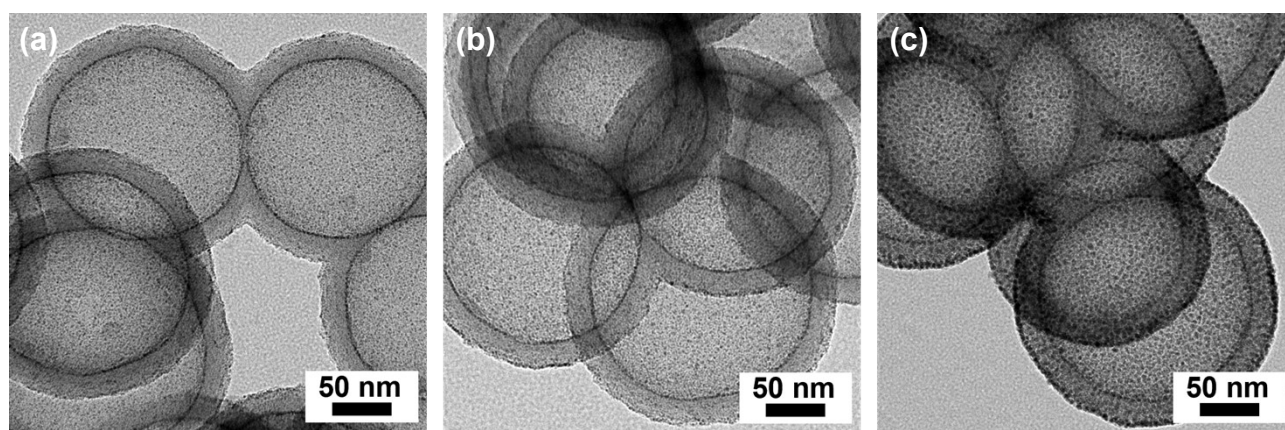


Fig. S2. (a-b) TEM images, (c) a size distribution diagram of Ru nanoparticles, (d) N₂ adsorption-desorption isotherm curves obtained at 77 K (Inset: a pore size distribution diagram based on the NL-DFT method), (e) an IR spectrum, (f) a PXRD pattern, and (g) a XPS Ru 3p orbital spectrum of control Ru/C (C-Ru) prepared by the same synthetic procedures as Ru/HC-3 using HMOP instead HMOP@TA.

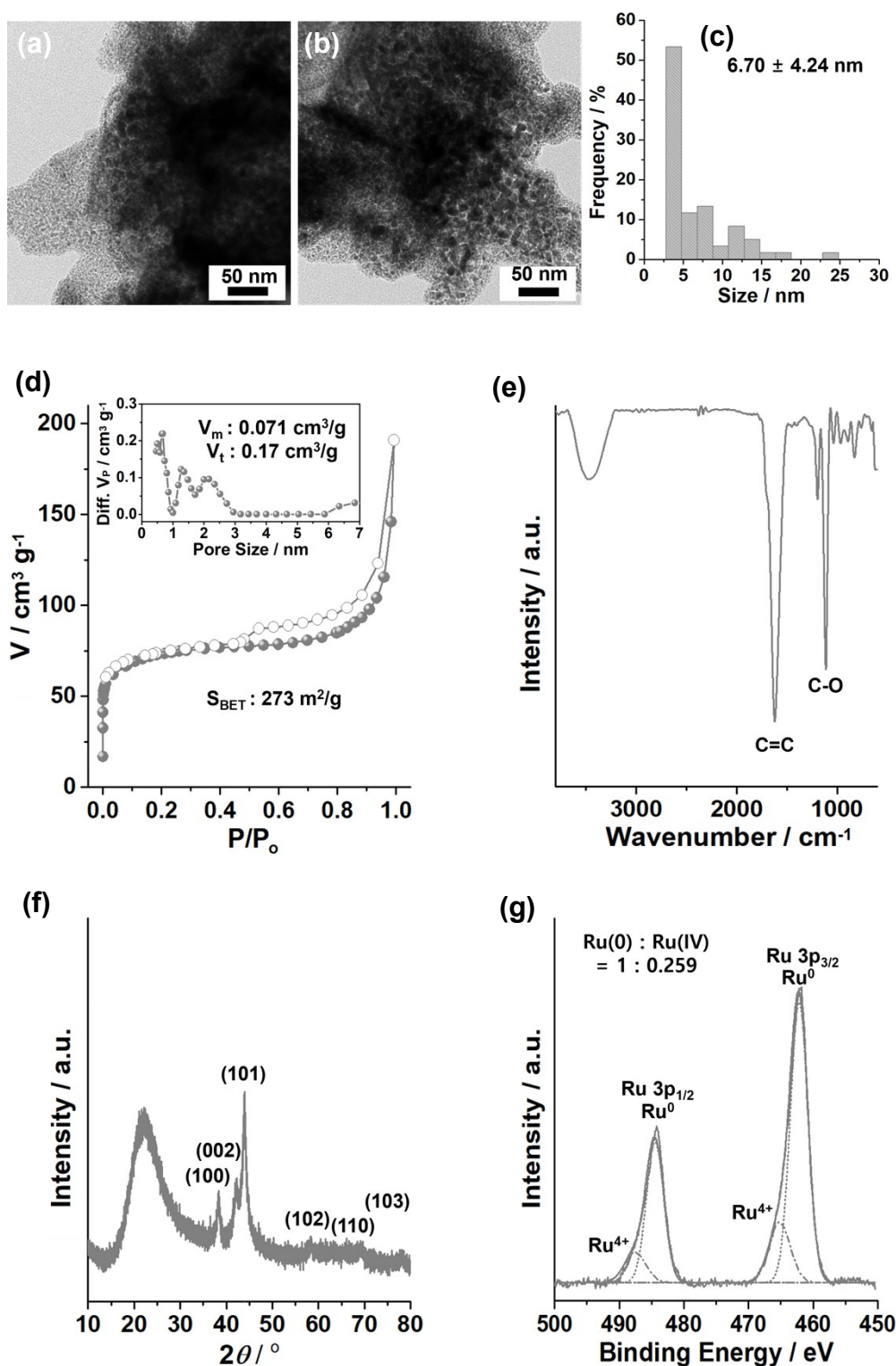
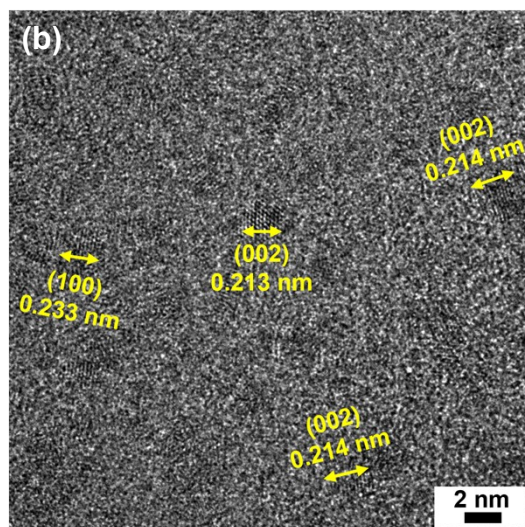
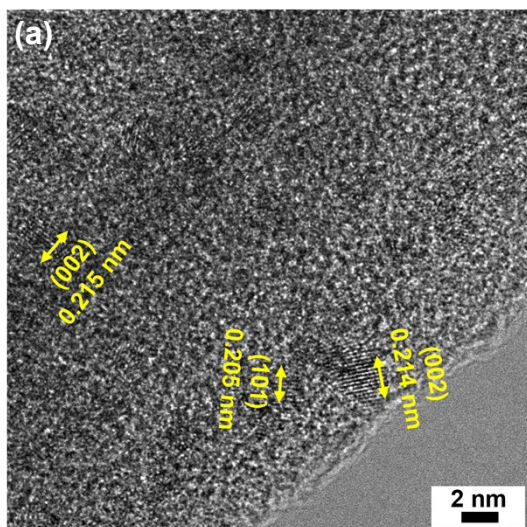
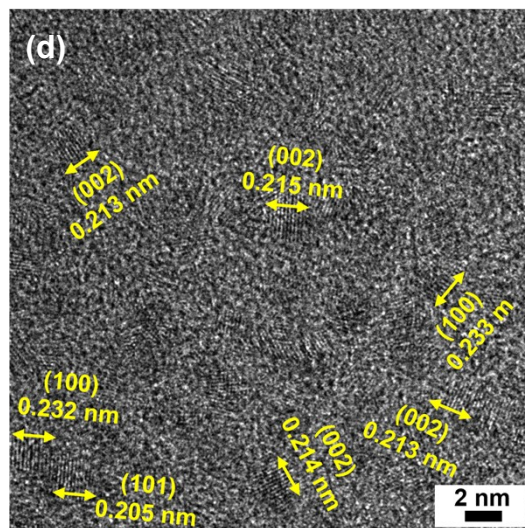
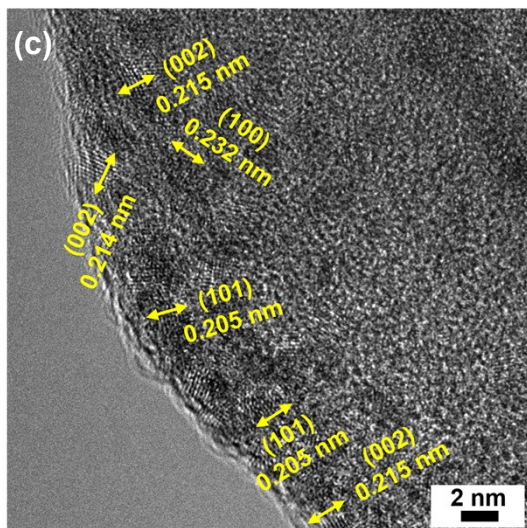


Fig. S3. HR-TEM images of (a-b) Ru/HC-1, (c-d) Ru/HC-2, and (e-f) Ru/HC-3.

Ru/HC-1



Ru/HC-2



Ru/HC-3

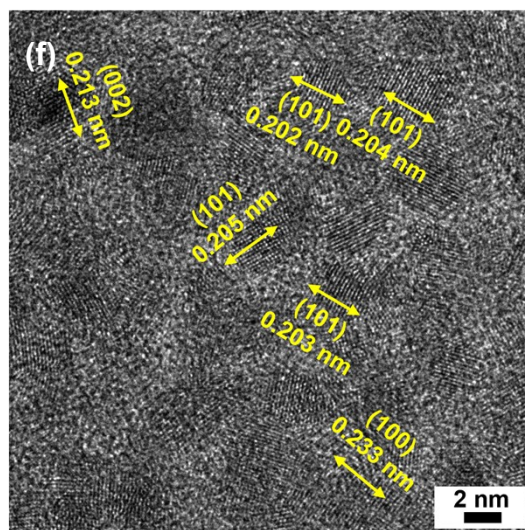
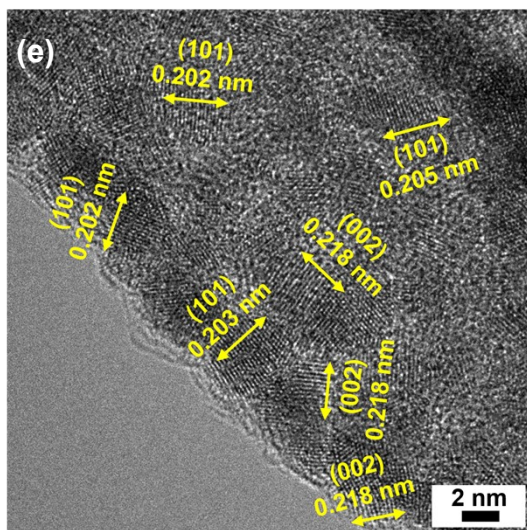


Fig. S4. EDS-based elemental mapping images of C, Ru, and O in Ru/HC-3.

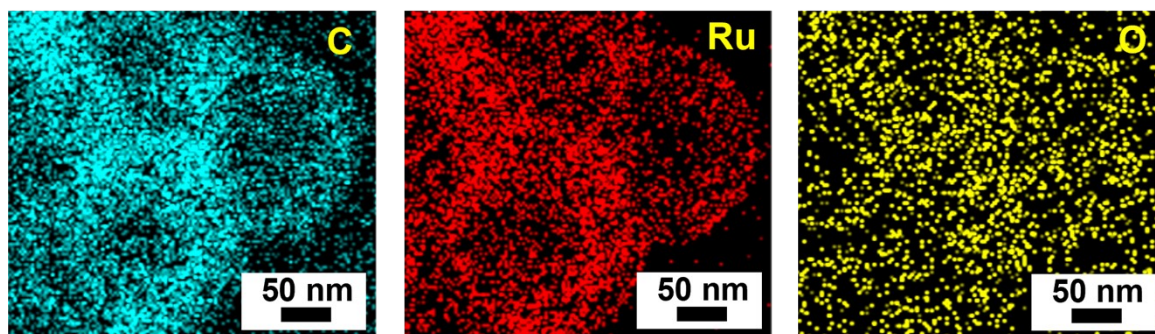


Fig. S5. Pore size distribution diagrams based on the NL-DFT method of Ru/HC-1~3.

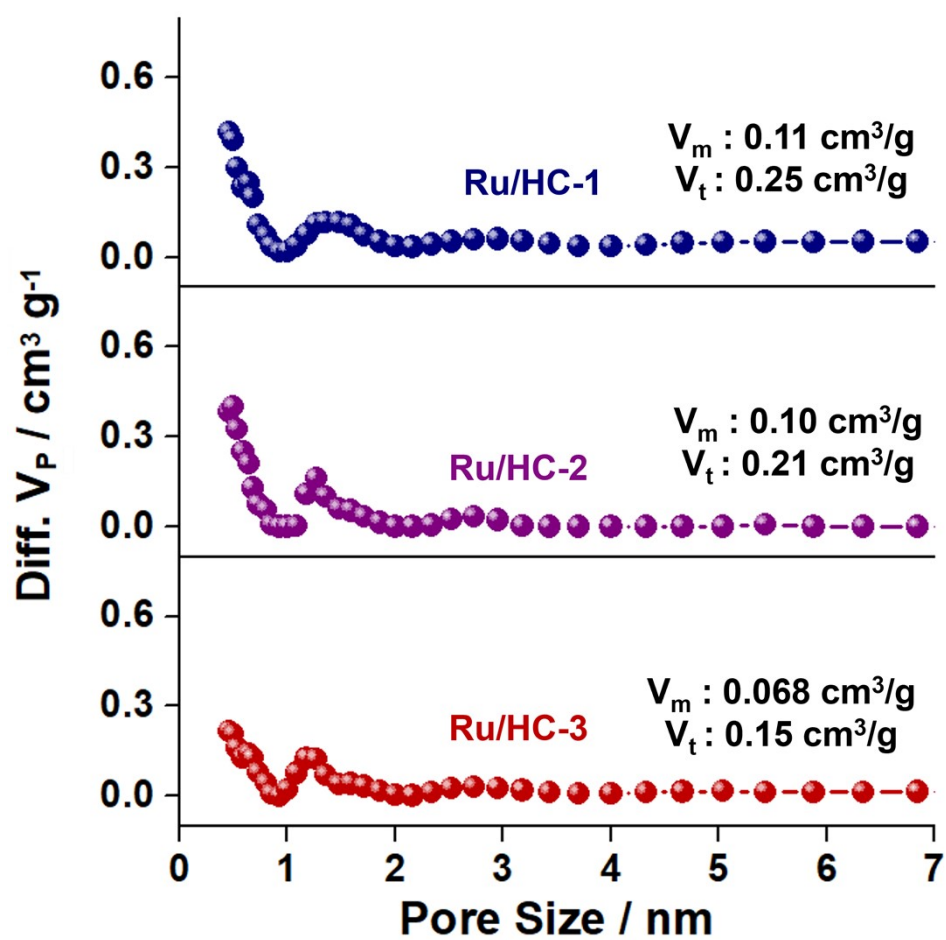
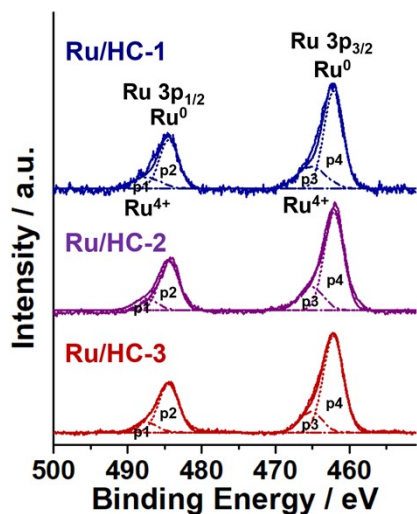


Fig. S6. Analysis of XPS (a) Ru 3p and (b) O 1s orbital peaks of Ru/HC-1~3.

(a)



Ru /HC-1	Peak	p1	p2	p3	p4
	Position (eV)	487.53	484.45	465.20	462.18
	FWHM	4.65	3.06	4.65	3.06
	Area (%)	8.69	24.6	17.2	49.5
	r ²	0.9804			

$$\text{Ru(0) : Ru(IV)} = 1 : 0.349$$

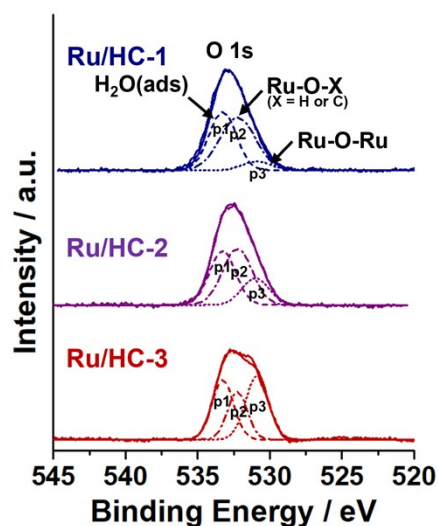
Ru /HC-2	Peak	p1	p2	p3	p4
	Position (eV)	487.55	484.42	465.20	462.12
	FWHM	3.82	3.14	3.81	3.12
	Area (%)	7.66	25.7	15.4	51.2
	r ²	0.9808			

$$\text{Ru(0) : Ru(IV)} = 1 : 0.300$$

Ru /HC-3	Peak	p1	p2	p3	p4
	Position (eV)	487.55	484.48	465.20	462.19
	FWHM	3.46	3.23	3.46	3.23
	Area (%)	6.26	27.1	12.5	54.2
	r ²	0.9933			

$$\text{Ru(0) : Ru(IV)} = 1 : 0.231$$

(b)



Ru /HC-1	Peak	p1	p2	p3
	Position (eV)	533.27	532.23	530.91
	FWHM	2.24	2.90	2.34
	Area (%)	42.83	50.32	6.85
	r ²	0.9949		

$$\text{Ru-O-Ru : Ru-O-X} = 1 : 7.346$$

Ru /HC-2	Peak	p1	p2	p3
	Position (eV)	533.27	532.25	530.99
	FWHM	2.14	2.43	2.22
	Area (%)	37.20	43.87	18.93
	r ²	0.9980		

$$\text{Ru-O-Ru : Ru-O-X} = 1 : 2.317$$

Ru /HC-3	Peak	p1	p2	p3
	Position (eV)	533.26	532.25	530.90
	FWHM	1.78	1.61	1.89
	Area (%)	34.94	25.59	39.47
	r ²	0.9964		

$$\text{Ru-O-Ru : Ru-O-X} = 1 : 0.648$$

Fig. S7. ^1H NMR spectra of the reaction mixtures obtained by Ru/HC-1~3 and control Ru/C.

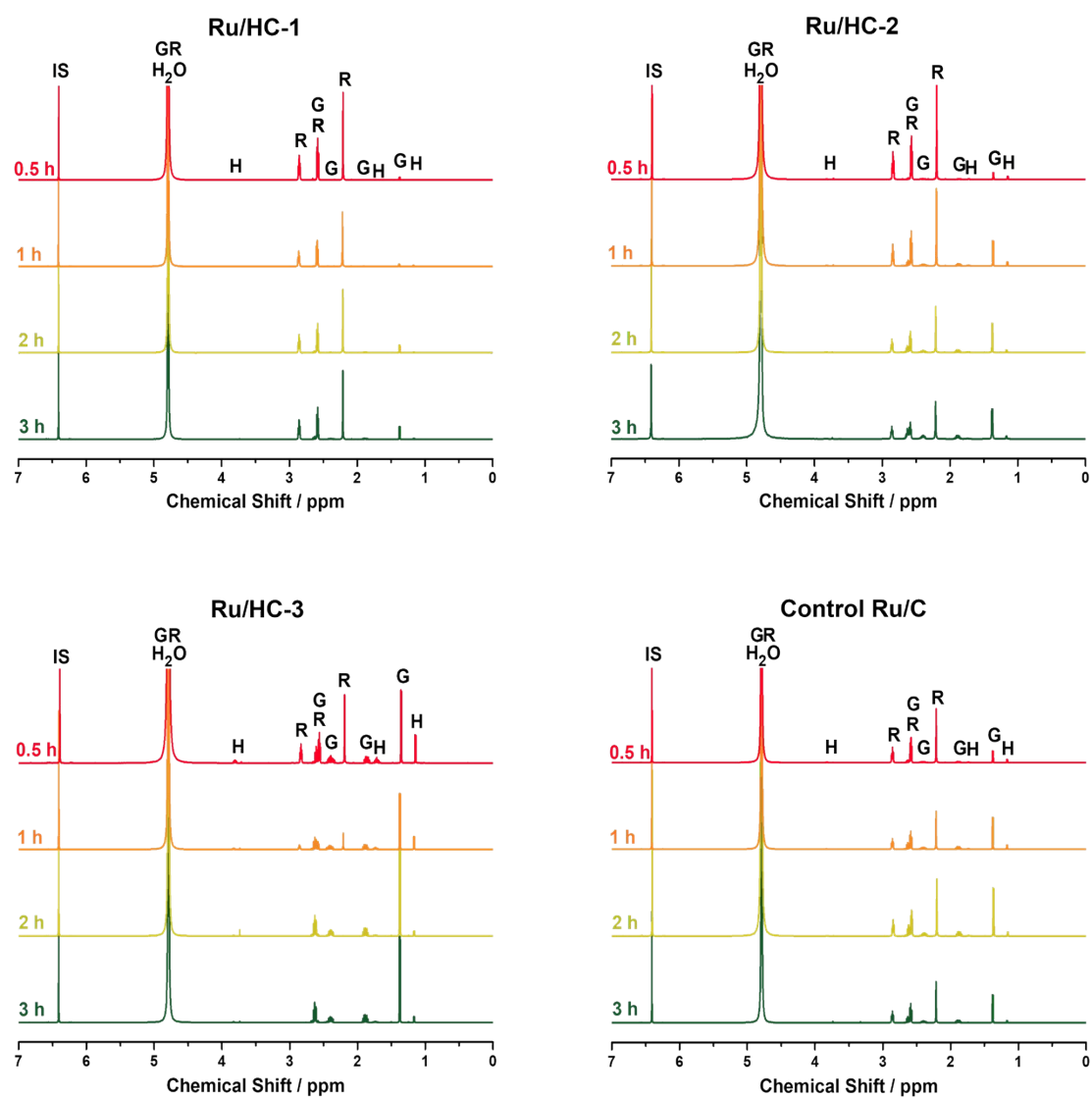


Fig. S8. ^1H and ^{13}C NMR spectra of the isolated GVL.

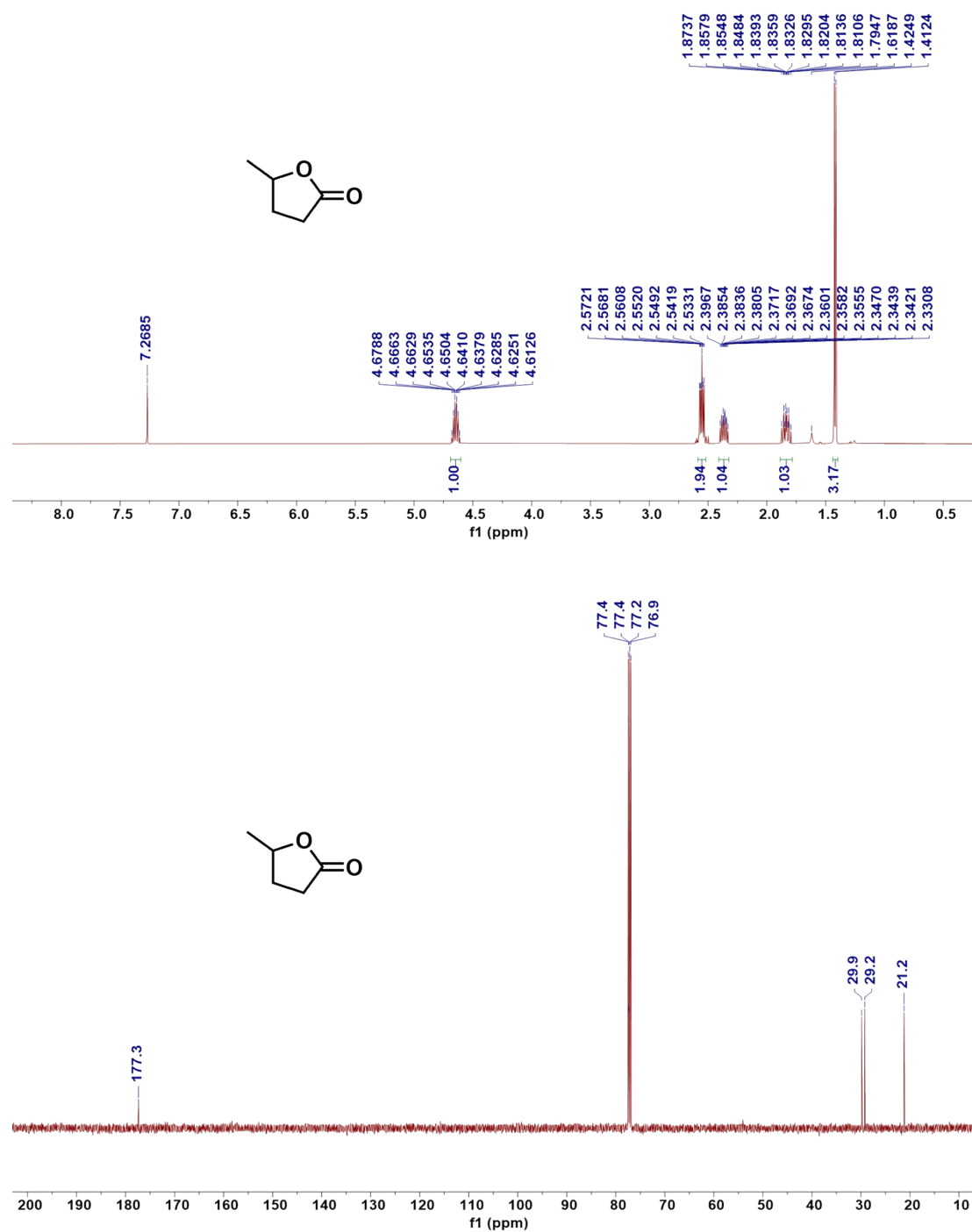


Fig. S9. DFT-optimized structures of reaction intermediates involved in the conversion of LA to GVL on the Ru(002) surface.

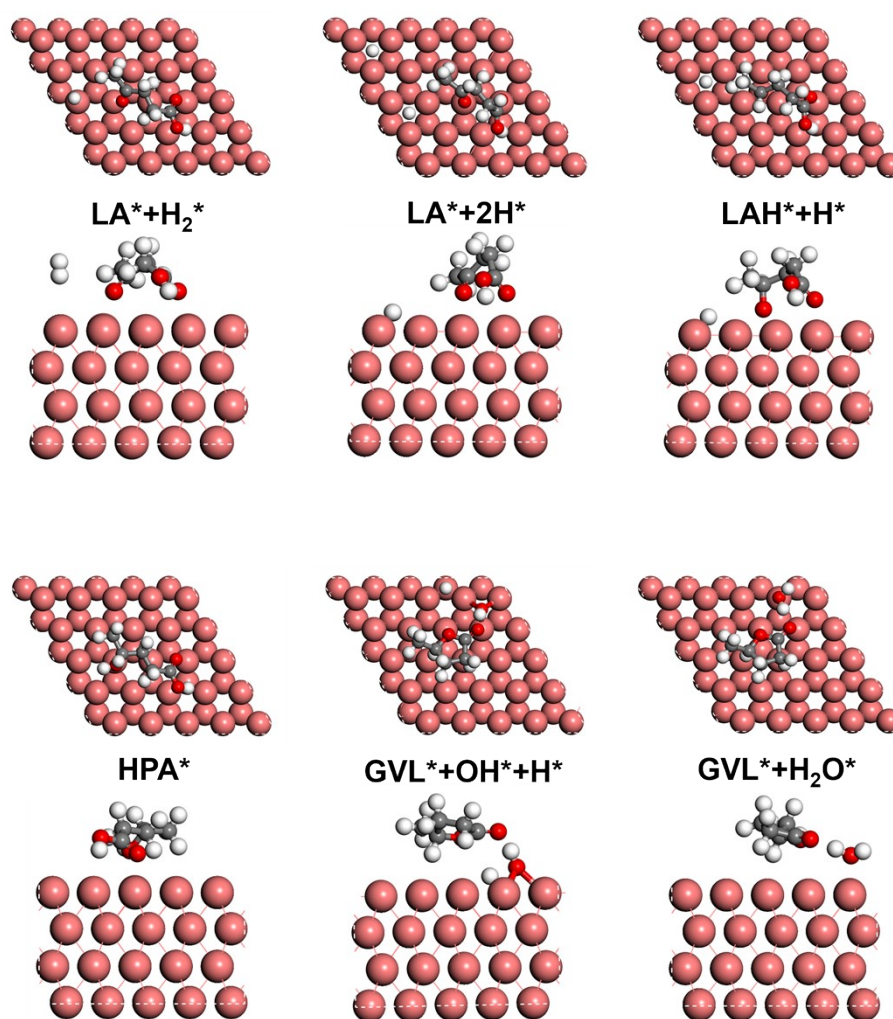


Fig. S10. Cartesian coordinates of all optimized intermediate structures involved in the catalytic conversion of LA to GVL on the Ru(002) surface.

Ru (002)										LA*+H ₂ *									
1.000000000000000										1.000000000000000									
11.7252320000000001 -6.7695660000000002 0.0000000000000000										11.7252320000000001 -6.7695660000000002 0.0000000000000000									
0.0000000000000000 13.5391320000000004 0.0000000000000000										0.0000000000000000 13.5391320000000004 0.0000000000000000									
0.0000000000000000 0.0000000000000000 21.4021529999999984										0.0000000000000000 0.0000000000000000 21.4021529999999984									
Ru										H C O Ru									
100										10 5 3 100									
Selective dynamics										Selective dynamics									
Direct										Direct									
0.0666670000000025	0.1333330000000004	0.0033859999999990	F	F	F					0.6401449774721015	0.2865627590046398	0.4006268901420416	T	T	T				
0.0666670000000025	0.1333330000000004	0.1995300000000029	T	T	T					0.5210960801311968	0.3813877404732706	0.5196005999137807	T	T	T				
0.1333330000000004	0.0666670000000025	0.0996060000000014	F	F	F					0.4440976536162180	0.3516205248362606	0.4493058657673579	T	T	T				
0.1333330000000004	0.0666670000000025	0.2957499999999982	T	T	T					0.5554889687234617	0.5719593542001646	0.5178947380676124	T	T	T				
0.2666669999999982	0.1333330000000004	0.0033859999999990	F	F	F					0.6119180527568068	0.5895111480239821	0.4417842312251313	T	T	T				
0.2666669999999982	0.1333330000000004	0.1995300000000029	T	T	T					0.4461008334414334	0.6632827625669006	0.5071982517933532	T	T	T				
0.3333330000000032	0.0666670000000025	0.0996060000000014	F	F	F					0.4898570675295886	0.7130787252362260	0.4296461463170722	T	T	T				
0.3333330000000032	0.0666670000000025	0.2957499999999982	T	T	T					0.3419986505814764	0.6251208050272711	0.4453097993112825	T	T	T				
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0.6666669999999968	0.1333330000000004	0.0033859999999990	F	F	F					0.5373116621516796	0.5325571283242171	0.4714495919061724	T	T	T				
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						0.1333006137263816	0.8667614144725307	0.2958076531612358	T	T	T
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						0.3337063339430396	0.8669780639783135	0.2958003890750833	T	T	T
						0.4666670000000011	0.9333329999999975	0.0033859999999990	F	F	F
						0.4666202537992002	0.9334549354716162	0.1993100572933223	T	T	T
						0.5333329999999989	0.8666669999999996	0.0996060000000014	F	F	F
						0.5335661493827626	0.8671626265555321	0.2958320401853714	T	T	T
						0.6666669999999968	0.9333329999999975	0.0033859999999990	F	F	F
						0.6666525884204556	0.9337141487252841	0.1993835368739551	T	T	T
						0.7333330000000018	0.8666669999999996	0.0996060000000014	F	F	F
						0.7336190565566636	0.8674221753986383	0.2958299148609940	T	T	T
						0.8666669999999996	0.9333329999999975	0.0033859999999990	F	F	F
						0.8672497981145956	0.9338217529458543	0.1994425272631462	T	T	T
						0.9333329999999975	0.8666669999999996	0.0996060000000014	F	F	F
						0.9336598500332409	0.8671435466326105	0.2958858906810023	T	T	T

LA*+2H*						LAH*													
1.0000000000000000						1.0000000000000000													
11.7252320000000001		-6.7695660000000002		0.0000000000000000		11.7252320000000001		-6.7695660000000002		0.0000000000000000									
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0.0000000000000000		0.0000000000000000		21.4021529999999984		0.0000000000000000		0.0000000000000000		21.4021529999999984									
H C O Ru						H C O Ru													
10 5 3 100						9 5 3 100													
Selective dynamics						Selective dynamics													
Direct						Direct													
0.6452647976553406	0.2813108372825796	0.3899827619274673	T	T	T	0.6284443638334571	0.3025368931162623	0.4001576194942070	T	T	T								
0.7373657439494040	0.4802277936596087	0.5313809930092270	T	T	T	0.6914180138013581	0.5374847762792333	0.5193223405651453	T	T	T								
0.5900125521273885	0.3807469136969980	0.5236584191365746	T	T	T	0.5479916435743190	0.4253106431891715	0.5151736409157748	T	T	T								
0.6149671042397695	0.5736199773376885	0.5395202638920920	T	T	T	0.5892370586795505	0.6334833680757441	0.5060667216250638	T	T	T								
0.7197202010667119	0.6324626833996631	0.4806739670944302	T	T	T	0.6477573428964483	0.6413468865286546	0.4315873977896137	T	T	T								
0.5158246602807913	0.6598936888382502	0.4885727755446206	T	T	T	0.3949673248160616	0.5970963143153554	0.5062156757702577	T	T	T								
0.5599206659879751	0.6879127772269769	0.4085330702024332	T	T	T	0.4605581242990721	0.6906300317861185	0.4412111098078088	T	T	T								
0.4209473774456159	0.5745508223597854	0.4262337998073132	T	T	T	0.3236179437401234	0.5659205984952338	0.4325143191657025	T	T	T								
0.2004186507790654	0.8003526324045926	0.3458615860118400	T	T	T	0.4100600735437228	0.4425338006969312	0.4495970483654035	T	T	T								
0.1995206210696132	0.3994671119035136	0.3464097514039929	T	T	T	0.6522214196030569	0.4418342174925355	0.4368248840540948	T	T	T								
0.6846976545374441	0.4151205086478212	0.4396352532967531	T	T	T	0.6170794874514293	0.4938945483404277	0.4879684141579035	T	T	T								
0.6623607205905749	0.4542476131459591	0.5012357539236462	T	T	T	0.5840995576656525	0.5816357507617255	0.4652827141019674	T	T	T								
0.6401706075252441	0.5539440203197624	0.4944340486234946	T	T	T	0.4644693127322170	0.5330623512244063	0.4364481964341424	T	T	T								
0.5565381505056605	0.5406848919034787	0.4440094845887281	T	T	T	0.4073972639350979	0.6006825415900218	0.4552865818117194	T	T	T								
0.5093638838180445	0.6187484231526047	0.4434194140749633	T	T	T	0.7214817149439136	0.5030706868642307	0.3957705886537919	T	T	T								
0.7463483388755993	0.4849597025480069	0.3988562872035827	T	T	T	0.6046816569711984	0.3294298789186415	0.4385636704706437	T	T									

0.6666146117826681	0.1332351314289666	0.1994473619744671	T	T	T	0.7333330000000018	0.0666670000000025	0.0996060000000014	F	F	F
0.7333330000000018	0.0666670000000025	0.0996060000000014	F	F	F	0.7332647159472557	0.0672607449706582	0.2958187469238364	T	T	T
0.7334048907089721	0.0667350150918712	0.2955007876133654	T	T	T	0.8666669999999996	0.1333330000000004	0.0033859999999990	F	F	F
0.8666669999999996	0.1333330000000004	0.0033859999999990	F	F	F	0.8666470902414702	0.1333730778749416	0.1995522600808604	T	T	T
0.8668014729344532	0.1331368872393588	0.1993738274260894	T	T	T	0.9333329999999997	0.0666670000000025	0.0996060000000014	F	F	F
0.9333329999999997	0.0666670000000025	0.0996060000000014	F	F	F	0.9336906711525172	0.0668884100017571	0.2956818499489416	T	T	T
0.9330185519260218	0.0668521274629322	0.2956010505416704	T	T	T	0.0666670000000025	0.3333330000000032	0.0033859999999990	F	F	F
0.0666670000000025	0.3333330000000032	0.0033859999999990	F	F	F	0.0663768191829321	0.3331745200797062	0.1994347671281154	T	T	T
0.0665937015467492	0.3333845636021859	0.1995892047791263	T	T	T	0.1333330000000004	0.2666669999999982	0.0996060000000014	F	F	F
0.1333330000000004	0.2666669999999982	0.0996060000000014	F	F	F	0.1329370137794853	0.2665833766806352	0.2958741468191587	T	T	T
0.1323881407953700	0.2649459779089593	0.2963720044196583	T	T	T	0.2666669999999982	0.3333330000000032	0.0033859999999990	F	F	F
0.2666669999999982	0.3333330000000032	0.0033859999999990	F	F	F	0.2660317013319295	0.3337163840657303	0.1998414108092139	T	T	T
0.2668380045596335	0.3333621186901884	0.1992407637447404	T	T	T	0.3333330000000032	0.2666669999999982	0.0996060000000014	F	F	F
0.3333330000000032	0.2666669999999982	0.0996060000000014	F	F	F	0.3312126230308890	0.2627201245802687	0.2951174040564045	T	T	T
0.3319593507890368	0.26411930982250092	0.2952153366399697	T	T	T	0.4666670000000011	0.3333330000000032	0.0996060000000014	F	F	F
0.4666670000000011	0.3333330000000032	0.0033859999999990	F	F	F	0.4671854115464231	0.3333905558900695	0.1990759193763571	T	T	T
0.4667871451611081	0.3338782787471216	0.1992791523869740	T	T	T	0.5333329999999989	0.2666669999999982	0.0996060000000014	F	F	F
0.5333329999999989	0.2666669999999982	0.0996060000000014	F	F	F	0.5310979757997899	0.2638965184477327	0.2950544997293341	T	T	T
0.5310698343261703	0.2629221433214984	0.2948106611117970	T	T	T	0.6666669999999968	0.3333330000000032	0.0033859999999990	F	F	F
0.6666669999999968	0.3333330000000032	0.0033859999999990	F	F	F	0.6668805667438213	0.3331449358100761	0.1998858859193731	T	T	T
0.6666056491738603	0.3333438233451790	0.1997789328604254	T	T	T	0.7333330000000018	0.2666669999999982	0.0996060000000014	F	F	F
0.7333330000000018	0.2666669999999982	0.0996060000000014	F	F	F	0.7333915608261204	0.2651781892971117	0.2959502059176331	T	T	T
0.7338532601516333	0.2642185882189460	0.2950041248222002	T	T	T	0.8666669999999996	0.3333330000000032	0.0033859999999990	F	F	F
0.8666669999999996	0.3333330000000032	0.0033859999999990	F	F	F	0.8667338093710504	0.3335257332763614	0.1992158486919133	T	T	T
0.8671682593714782	0.3339637906499761	0.1987770440712282	T	T	T	0.9333329999999997	0.2666669999999982	0.0996060000000014	F	F	F
0.9333329999999997	0.2666669999999982	0.0996060000000014	F	F	F	0.9328203964221783	0.2664608931541333	0.2959740080477359	T	T	T
0.9320544882446596	0.2660229564606666	0.2955367296490238	T	T	T	0.0666670000000025	0.5333329999999989	0.0996060000000014	F	F	F
0.0666670000000025	0.5333329999999989	0.0033859999999990	F	F	F	0.0665246615213509	0.5331650558834186	0.1997085960260663	T	T	T
0.0660146307079308	0.5330304033946135	0.1989982252881060	T	T	T	0.1333330000000004	0.4666670000000011	0.0996060000000014	F	F	F
0.1333330000000004	0.4666670000000011	0.0996060000000014	F	F	F	0.1326637209884806	0.4665309175383842	0.2958391371225934	T	T	T
0.1328667283999500	0.4673856638780235	0.2963569833119388	T	T	T	0.2666669999999982	0.5333329999999989	0.0033859999999990	F	F	F
0.2666669999999982	0.5333329999999989	0.0033859999999990	F	F	F	0.2662710505793769	0.5327276725421514	0.1999853875802602	T	T	T
0.2665831473497028	0.53291297361559305	0.1995280662393308	T	T	T	0.3333330000000032	0.4666670000000011	0.0996060000000014	F	F	F
0.3333330000000032	0.4666670000000011	0.0996060000000014	F	F	F	0.3337988706100699	0.4668321199076354	0.2968191244767983	T	T	T
0.3317796407357481	0.4667161160351062	0.2956034591527805	T	T	T	0.4666670000000011	0.5333329999999989	0.0033859999999990	F	F	F
0.4666670000000011	0.5333329999999989	0.0033859999999990	F	F	F	0.4665303052475053	0.5333491020762275	0.1979069706204004	T	T	T
0.4671823852984875	0.5334025700914745	0.19963894779702422	T	T	T	0.5333329999999989	0.4666670000000011	0.0996060000000014	F	F	F
0.5333329999999989	0.4666670000000011	0.0996060000000014	F	F	F	0.5309420945401450	0.4666664023922702	0.2947841056002583	T	T	T
0.5301057157320689	0.4667282653253357	0.2985721393393292	T	T	T	0.6666669999999968	0.5333329999999989	0.0033859999999990	F	F	F
0.6666669999999968	0.5333329999999989	0.0033859999999990	F	F	F	0.6665811553549549	0.5324826895860775	0.1997814741843130	T	T	T
0.6660182518773737	0.5325153079385172	0.2005759809510156	T	T	T	0.7333330000000018	0.4666670000000011	0.0996060000000014	F	F	F
0.7333330000000018	0.4666670000000011	0.0996060000000014	F	F	F	0.7334337354394600	0.4667605824094030	0.2976770193260563	T	T	T
0.7359810325294994	0.4662638641275190	0.2978308448152765	T	T	T	0.8666669999999996	0.5333329999999989	0.0033859999999990	F	F	F
0.8666669999999996	0.5333329999999989	0.0033859999999990	F	F	F	0.8668195933197171	0.5331122750935606	0.1996702536530775	T	T	T
0.866826031920763	0.5329911440846765	0.1996088196049136	T	T	T	0.9333329999999997	0.4666670000000011	0.0996060000000014	F	F	F
0.9333329999999997	0.4666670000000011	0.0996060000000014	F	F	F	0.9348003885966779	0.4669398005073411	0.2956356461535407	T	T	T
0.9346020253740926	0.4661194617660778	0.2952514219411613	T	T	T	0.0666670000000025	0.7333330000000018	0.0033859999999990	F	F	F
0.0666670000000025	0.7333330000000018	0.0033859999999990	F	F	F	0.066489522658648	0.7334877147051576	0.2954008215931714	T	T	T
0.0667325171555987	0.7334978456611050	0.1998330517352609	T	T	T	0.1333330000000004	0.6666669999999968	0.0996060000000014	F	F	F
0.1333330000000004	0.6666669999999968	0.0996060000000014	F	F	F	0.1335713313593227	0.6666589342410605	0.2958931015667342	T	T	T
0.133310837888902	0.6665706173576611	0.2963264583683830	T	T	T	0.2666669999999982	0.7333330000000018	0.0033859999999990	F	F	F
0.2666669999999982	0.7333330000000018	0.0033859999999990	F	F	F	0.2668073413136182	0.7337039585261280	0.1995223505050732	T	T	T
0.266691923551115	0.7335498342556441	0.1994403224674296	T	T	T	0.3333330000000032	0.6666669999999968	0.0996060000000014	F	F	F
0.3333330000000032	0.6666669999999968	0.0996060000000014	F	F	F	0.3312784029556290	0.6687552240169816	0.2954008215931714	T	T	T
0.3338400785323419	0.6674651839285008	0.2951921638139278	T	T	T	0.4666670000000011	0.7333330000000018	0.0033859999999990	F	F	F
0.4666670000000011	0.7333330000000018	0.0033859999999990	F	F	F	0.4674456088368806	0.7338919942101662	0.1999676455350487	T	T	T
0.466910494248060	0.7339664304106149	0.1993824172254699	T	T	T	0.5333329999999989	0.6666669999999982	0.0996060000000014	F	F	F
0.5333329999999989	0.6666669999999968	0.0996060000000014	F	F	F	0.5333641817657687	0.6668738964113177	0.2967568937081875	T	T	T
0.5334667043937387	0.6669730756470392	0.2950924215425493	T	T	T	0.6666669999999968	0.7333330000000018	0.0033859999999990	F	F	F
0.6666669999999968	0.7333330000000018	0.0033859999999990	F	F	F	0.666579239047918	0.7340114172073526	0.2002230836177529	T	T	T
0.6667799534028558	0.7329701658818332	0.1994939240192032	T	T	T	0.7333330000000018	0.6666669999999968	0.0996060000000014	F	F	F
0.7333330000000018	0.6666669999999968	0.0996060000000014	F	F	F	0.7369515328636966	0.6703209818633357	0.2946039639069132	T	T	T
0.7353061704215620	0.6702499773628015	0.2947868826335813	T	T	T	0.8666669999999996	0.7333330000000018	0.0033859999999990	F	F	F
0.8666669999999996	0.7333330000000018	0.0033859999999990	F	F	F	0.8670654851902379	0.7334526236345821	0.1991964568668562	T	T	T
0.8663451160456732	0.7332980582208865	0.1992705015183587	T	T	T	0.9333329999999975	0.6666669999999968	0.0996060000000014	F	F	F
0.9333329999999975	0.6666669999999968	0.0996060000000014	F	F	F	0.9358850759918987	0.6685110257221922	0.2952045751554635	T	T	T
0.9348210329784552	0.6684733925399062	0.2949535843982611	T	T	T	0.0666670000000025	0.9333329999999975	0.0033859999999990	F	F	F
0.0666670000000025	0.9333329999999975	0.0033859999999990	F	F	F	0.0667242554274332	0.9335962013576227	0.1993832118158367	T	T	T
0.0667158403973094	0.9338946303328034	0.1991695778601340	T	T	T	0.1333330000000004	0.8666669999999996	0.0996060000000014	F	F	F
0.1333330000000004	0.8666669999999996	0.0996060000000014	F	F	F	0.1332281991121058	0.8668334224413503	0.2955279142080055	T	T	T
0.1325585455617889	0.8674220070388714	0.2964201578612060	T	T	T	0.2666669999999982	0.9333329999999975	0.0033859999999990	F	F	F
0.2666669999999982	0.9333329999999975	0.0033859999999990	F								

LAH*+H*										HPA*									
1.000000000000000										1.000000000000000									
11.7252320000000001										11.7252320000000001									
0.0000000000000000										0.0000000000000000									
0.0000000000000000										0.0000000000000000									
0.0000000000000000										0.0000000000000000									
H C O Ru										H C O Ru									
10 5 3 100										10 5 3 100									
Selective dynamics										Selective dynamics									
Direct										Direct									
0.6283284920478872	0.3024837728939648	0.4001632787973430	T	T	T					0.6518698176310380	0.2934229877569905	0.4092790056900810	T	T	T				
0.6913342077997763	0.5373901542849183	0.5193777742217593	T	T	T					0.5068535285879605	0.3843059003728087	0.5140749014256372	T	T	T				
0.5479274160834712	0.4252273503749547	0.5150821042790584	T	T	T					0.4328983321848909	0.3376006630342800	0.4427512278799028	T	T	T				
0.5893142511776095	0.6334387653303255	0.5061784617111855	T	T	T					0.5715712997671432	0.5850868348818707	0.4889581435043908	T	T	T				
0.6476587469790948	0.6414130260638505	0.4316466998099049	T	T	T					0.5487937622672661	0.5565540474646353	0.408533400060875	T	T	T				
0.3951451089813215	0.5972161194971964	0.5062975886666805	T	T	T					0.4510444349124541	0.6778296522503950	0.5013262915465617	T	T	T				
0.4605838288480136	0.6906678523290301	0.4412355101947832	T	T	T					0.4517691141655078	0.6780955048466026	0.4178853413361949	T	T	T				
0.3237635019790687	0.5659950804087955	0.4326260562421254	T	T	T					0.3201254980130557	0.6203621879677286	0.4591338169194756	T	T	T				
0.4100184569722891	0.4425847411319888	0.4496971735777586	T	T	T					0.3523827540767357	0.4651037667964530	0.5024419784237466	T	T	T				
0.1992703228139836	0.6007405805333579	0.3464174798280862	T	T	T					0.2476755971552933	0.4193152207990778	0.4140598686361514	T	T	T				
0.6522438897342498	0.4418743463247983	0.4368079917716661	T	T	T					0.6064473701301836	0.4007187577248246	0.4331391595937433	T	T	T				
0.6171127551973482	0.4938925082465355	0.4879709094425972	T	T	T					0.5106125956053376	0.4077304894610236	0.4644831826256635	T	T	T				
0.5841585978201929	0.5816537798733090	0.4653693466495723	T	T	T					0.5133459642210525	0.5209888608296041	0.4552467067128632	T	T	T				
0.4645299761336178	0.5331122713782421	0.4365383348877798	T	T	T					0.3971799867476236	0.5128098649563029	0.4598836817920997	T	T	T				
0.4074872450918910	0.6007631103570787	0.4553703528707154	T	T	T					0.4052457663596059	0.6287151111246061	0.4596108230708396	T	T	T				
0.7214949453895251	0.5030999356627456	0.3957253514652695	T	T	T					0.6792762998961734	0.4779828761540443	0.3994336244164742	T	T	T				
0.6046866312666306	0.3294573240768628	0.4385925882185749	T	T	T					0.6001868157913890	0.3000292648052522	0.4403637343750901	T	T	T				
0.4696356990611767	0.5325484222315743	0.3682536829439889	T	T	T					0.3277980041196287	0.4418622342475018	0.4072200298376387	T	T	T				
0.0666670000000025	0.1333330000000004	0.0033859999999990	F	F	F					0.0666670000000025	0.1333330000000004	0.0033859999999990	F	F	F				
0.0668154415369050	0.1337062389654763	0.1996071087514516	T	T	T					0.0667106716124053	0.1334912487586237	0.1994517137483456	T	T	T				
0.1333330000000004	0.0666670000000025	0.0996060000000014	F	F	F					0.1333330000000004	0.0666670000000025	0.0996060000000014	F	F	F				
0.1334171861715264	0.1334467521276955	0.2957886825777496	T	T	T					0.1333002517227584	0.0666013724459518	0.2957342666800074	T	T	T				
0.2666669999999982	0.1333330000000004	0.0033859999999990	F	F	F					0.2666669999999982	0.1333330000000004	0.0033859999999990	F	F	F				
0.2662124683781757	0.1328964994909746	0.1993895359023869	T	T	T					0.2666647842054104	0.1335438582213158	0.1996748811064393	T	T	T				
0.3333330000000032	0.0666670000000025	0.0996060000000014	F	F	F					0.3333330000000032	0.0666670000000025	0.0996060000000014	F	F	F				
0.3336184101333369	0.0670482748289219	0.2956386472550033	T	T	T					0.3332334932076293	0.0664869173136466	0.2956986385639766	T	T	T				
0.4666670000000011	0.1333330000000004	0.0033859999999990	F	F	F					0.4666670000000011	0.1333330000000004	0.0033859999999990	F	F	F				
0.4667114157767344	0.1334467521276955	0.1994424243015231	T	T	T					0.4665499427228781	0.1330605610195761	0.1993625213767771	T	T	T				
0.5333329999999989	0.0666670000000025	0.0996060000000014	F	F	F					0.5333329999999989	0.0666670000000025	0.0996060000000014	F	F	F				
0.5332133601455689	0.0666658268607014	0.2957422722829798	T	T	T					0.5334500881736872	0.0664090555294408	0.2957615881139688	T	T	T				
0.6666669999999968	0.1333330000000004	0.0033859999999990	F	F	F					0.6666669999999968	0.1333330000000004	0.0033859999999990	F	F	F				
0.6669227530126510	0.1336405365396631	0.1995631427319055	T	T	T					0.6668313729429727	0.1335449032960412	0.1994254355518876	T	T	T				
0.7333330000000018	0.0666670000000025	0.0996060000000014	F	F	F					0.7333330000000018	0.0666670000000025	0.0996060000000014	F	F	F				
0.7331232595250770	0.06671208558554218	0.2958218474645319	T	T	T					0.7332637190143509	0.0670213894261877	0.2957100611184913	T	T	T				
0.8666669999999996	0.1333330000000004	0.0033859999999990	F	F	F					0.8666669999999996	0.1333330000000004	0.0033859999999990	F	F	F				
0.8667632683243378	0.1335728629055248	0.1996057951820072	T	T	T					0.8666664176247068	0.1333095367420825	0.1995265086713474	T	T	T				
0.9333329999999975	0.0666670000000025	0.0996060000000014	F	F	F					0.9333329999999975	0.0666670000000025	0.0996060000000014	F	F	F				
0.9337631629057298	0.0669114170885989	0.2956148377683873	T	T	T					0.93352922298594027	0.0669798350225577	0.2957167001891889	T	T	T				
0.0666670000000025	0.3333330000000032	0.0033859999999990	F	F	F					0.0666670000000025	0.3333330000000032	0.0033859999999990	F	F	F				
0.0660421387555137	0.3333330000000032	0.1992095979954993	T	T	T					0.0669615823767344	0.3334521453754604	0.1993329252322332	T	T	T				
0.1333330000000004	0.2666669999999982	0.0996060000000014	F	F	F					0.1333330000000004	0.2666669999999982	0.0996060000000014	F	F	F				
0.1330467575516104	0.2665009958724917	0.2958629046310139	T	T	T					0.1315327639684938	0.2651455395652249	0.2955551495887860	T	T	T				
0.2666669999999982	0.3333330000000032	0.0033859999999990	F	F	F					0.2666669999999982	0.3333330000000032	0.0033859999999990	F	F	F				
0.2658734016698237	0.3335157362862644	0.1996842558037902	T	T	T					0.2665752664059298	0.3335275282034260	0.1999008872192363	T	T	T				
0.3333330000000032	0.2666669999999982	0.0996060000000014	F	F	F					0.3333330000000032	0.2666669999999982	0.0996060000000014	F	F	F				
0.3311018083544254	0.2627212365867172	0.2950202357407163	T	T	T					0.3327496205185199	0.2646259229199472	0.2954222334168293	T	T	T				
0.4666670000000011	0.3333330000000032	0.0033859999999990	F	F	F					0.4666670000000011	0.3333330000000032	0.0033859999999990	F	F	F				
0.4671699249401281	0.3332583169438440	0.1990318601739792	T	T	T					0.4664641406893111	0.3334221513547746	0.1988646499392388	T	T	T				
0.5333329999999989	0.2666669999999982	0.0996060000000014	F	F	F					0.5333329999999989	0.2666669999999982	0.0996060000000014	F	F	F				
0.5311304750559840	0.2638945482842829	0.2950201210144744	T	T	T					0.5310297763159468	0.2632546461259793	0.2946602802548526	T	T	T				
0.6666669999999968	0.3333330000000032	0.003385999999																	

0.0666670000000025	0.7333330000000018	0.0033859999999990	F	F	F	0.0666670000000025	0.7333330000000018	0.0033859999999990	F	F	F
0.0661359495798680	0.7337711586835959	0.1992367378787786	T	T	T	0.0663432536698991	0.7333303171671304	0.1995736162014623	T	T	T
0.1333330000000004	0.6666669999999968	0.0996060000000014	F	F	F	0.1333330000000004	0.6666669999999968	0.0996060000000014	F	F	F
0.1329561074716646	0.6675176719226001	0.2964326764077510	T	T	T	0.1333857250713777	0.6666351147110490	0.2958362923056583	T	T	T
0.2666669999999982	0.7333330000000018	0.0033859999999990	F	F	F	0.2666669999999982	0.7333330000000018	0.0033859999999990	F	F	F
0.2667612513221027	0.7335054335607468	0.1996151663412717	T	T	T	0.2669366663396602	0.7333476651012631	0.1996678416594762	T	T	T
0.3333330000000032	0.6666669999999968	0.0996060000000014	F	F	F	0.3333330000000032	0.6666669999999968	0.0996060000000014	F	F	F
0.3325525421768296	0.6694820645594550	0.2958309044587716	T	T	T	0.3329829800583894	0.6681732134425005	0.2956042794455698	T	T	T
0.4666670000000011	0.7333330000000018	0.0033859999999990	F	F	F	0.4666670000000011	0.7333330000000018	0.0033859999999990	F	F	F
0.4679707464738588	0.7342652489924383	0.1997151080337513	T	T	T	0.4666527971569963	0.7333131011451570	0.1991910699425716	T	T	T
0.5333329999999989	0.6666669999999968	0.0996060000000014	F	F	F	0.5333329999999989	0.6666669999999968	0.0996060000000014	F	F	F
0.5331268366147338	0.6663926921946416	0.2965908370534472	T	T	T	0.5352016227672749	0.6691765675273658	0.2949988390486666	T	T	T
0.6666669999999968	0.7333330000000018	0.0033859999999990	F	F	F	0.6666669999999968	0.7333330000000018	0.0033859999999990	F	F	F
0.6666213638274117	0.7340413796140381	0.2002328086467098	T	T	T	0.6668422032322781	0.7334868957478236	0.1995355194693502	T	T	T
0.7333330000000018	0.6666669999999968	0.0996060000000014	F	F	F	0.7333330000000018	0.6666669999999968	0.0996060000000014	F	F	F
0.7369558382450977	0.6703367291621468	0.2945920845154963	T	T	T	0.7340375168692219	0.6692405219326076	0.2949487811744902	T	T	T
0.8666669999999996	0.7333330000000018	0.0033859999999990	F	F	F	0.8666669999999996	0.7333330000000018	0.0033859999999990	F	F	F
0.8672065959321354	0.7334057219564144	0.1992314484270156	T	T	T	0.8667532561499556	0.7333542364386929	0.1992627012852211	T	T	T
0.9333329999999975	0.6666669999999968	0.0996060000000014	F	F	F	0.9333329999999975	0.6666669999999968	0.0996060000000014	F	F	F
0.9355746385298673	0.6683137894167027	0.2951745114956696	T	T	T	0.9348993881558556	0.6680313899016497	0.2955642780352790	T	T	T
0.0666670000000025	0.9333299999999975	0.0033859999999990	F	F	F	0.0666670000000025	0.9333299999999975	0.0033859999999990	F	F	F
0.0668077179646100	0.9335048914197155	0.1994463571779951	T	T	T	0.0667467261466825	0.9332687783826046	0.1994220090093464	T	T	T
0.1333330000000004	0.8666669999999996	0.0996060000000014	F	F	F	0.1333330000000004	0.8666669999999996	0.0996060000000014	F	F	F
0.1334702373036498	0.8671156983685908	0.2955134286286007	T	T	T	0.1330452544634184	0.8664604112084717	0.2957264832131174	T	T	T
0.2666669999999982	0.9333329999999975	0.0033859999999990	F	F	F	0.2666669999999982	0.9333329999999975	0.0033859999999990	F	F	F
0.2666086487077036	0.9330629173020959	0.1992530436584216	T	T	T	0.2663855645121558	0.9328555665192297	0.1993149573678039	T	T	T
0.3333330000000032	0.8666669999999996	0.0996060000000014	F	F	F	0.3333330000000032	0.8666669999999996	0.0996060000000014	F	F	F
0.3340492036174649	0.8679623021054758	0.2956769271519509	T	T	T	0.3334760512645332	0.8666623250886900	0.2956982408119160	T	T	T
0.4666670000000011	0.9333329999999975	0.0033859999999990	F	F	F	0.4666670000000011	0.9333329999999975	0.0033859999999990	F	F	F
0.4665672220002676	0.9328946903222025	0.1995109995029948	T	T	T	0.4665150225446766	0.9331873769887906	0.1992945942988982	T	T	T
0.5333299999999989	0.8666669999999996	0.0996060000000014	F	F	F	0.5333299999999989	0.8666669999999996	0.0996060000000014	F	F	F
0.5335706004361833	0.8675326882917243	0.2959907051092278	T	T	T	0.5334446721259312	0.8669965891873943	0.2957450241879371	T	T	T
0.6666669999999968	0.9333299999999975	0.0033859999999990	F	F	F	0.6666669999999968	0.9333299999999975	0.0033859999999990	F	F	F
0.6663366585379514	0.9333894554816228	0.1994572823836671	T	T	T	0.6664782628760051	0.9334093258684462	0.1993499298696335	T	T	T
0.7333330000000018	0.8666669999999996	0.0996060000000014	F	F	F	0.7333330000000018	0.8666669999999996	0.0996060000000014	F	F	F
0.7338368968285851	0.8677687890687362	0.2958916715978815	T	T	T	0.7332997828110024	0.8670128495217995	0.295729507523374	T	T	T
0.8666669999999996	0.9333329999999975	0.0033859999999990	F	F	F	0.8666669999999996	0.9333329999999975	0.0033859999999990	F	F	F
0.8667274261065305	0.9334958112022830	0.1995712429820457	T	T	T	0.8669586809836218	0.9335175546354932	0.1994015080986173	T	T	T
0.9333329999999975	0.8666669999999996	0.0996060000000014	F	F	F	0.9333329999999975	0.8666669999999996	0.0996060000000014	F	F	F
0.9334943685141461	0.8671634535528703	0.2957472859725896	T	T	T	0.9335211800409908	0.8669749169040486	0.2958101236473638	T	T	T

GVL*+OH*+H*						GVL*+H₂O*					
1.000000000000000						1.000000000000000					
11.7252320000000001	-6.7695660000000002	0.0000000000000000				11.7252320000000001	-6.7695660000000002	0.0000000000000000			
0.0000000000000000	13.5391320000000004	0.0000000000000000				0.0000000000000000	13.5391320000000004	0.0000000000000000			
0.0000000000000000	0.0000000000000000	21.4021529999999984				0.0000000000000000	0.0000000000000000	21.4021529999999984			
H	C	O	Ru			H	C	O	Ru		
10	5	3	100			10	5	3	100		
Selective dynamics						Selective dynamics					
Direct						Direct					
0.3881009512094064	0.5058406580073876	0.4063619301138428	T	T	T	0.3674268663108139	0.4935959878100949	0.4046779438896581	T	T	T
0.4126345485834780	0.4637021920914572	0.5445624403504569	T	T	T	0.4164251952278019	0.4475937867458556	0.5379776054995018	T	T	T
0.3581877785141922	0.3638203942527178	0.4817928056843247	T	T	T	0.3617524063985599	0.3521317130834221	0.4731906023166441	T	T	T
0.5880112126987047	0.4586630527003008	0.5204821995175519	T	T	T	0.5978304930049454	0.4653258444372551	0.5024916186804177	T	T	T
0.5493178430550758	0.4292219667458879	0.4403900629186541	T	T	T	0.5489015277653168	0.4353270573036757	0.4240592726806214	T	T	T
0.3443487723166164	0.6508482353710051	0.4463794354339600	T	T	T	0.3121820526141337	0.6223996699140310	0.4549707134631351	T	T	T
0.2523032674589667	0.5163427722525695	0.4814264676837726	T	T	T	0.2349524259147502	0.4841875126901466	0.4887659429077334	T	T	T
0.3692207280670128	0.6240682067444708	0.5251687416876862	T	T	T	0.3520546622857130	0.5961979711547025	0.5303778151424817	T	T	T
0.6670173844297363	0.9325624661960824	0.3447019204270172	T	T	T	0.7216357782902908	0.7973557251935971	0.4190166006329300	T	T	T
0.7715461431781210	0.7624887697491259	0.4101507113545945	T	T	T	0.8144211361136335	0.9302052544562623	0.4124656488563963	T	T	T
0.6078910761376205	0.6002012988120222	0.4644082608921480	T	T	T	0.5948937248746817	0.6017037058361763	0.4519017062951494	T	T	T
0.4146266025215006	0.5394450648827303	0.4546817119064092	T	T	T	0.3983772693075573	0.5250655065110528	0.4529755600814753	T	T	T
0.4237696104435593	0.4507542323554121	0.4948343539416138	T	T	T	0.4228156276503709	0.4401576929407992	0.4870898196552402	T	T	T
0.5452413258668894	0.4758316242424										

0.0666670000000025	0.3333330000000032	0.0033859999999990	F	F	F	0.0666670000000025	0.3333330000000032	0.0033859999999990	F	F	F
0.066716546058136	0.3334795661022892	0.1994709145875437	T	T	T	0.0667585970985219	0.3335007352273859	0.1994880407412460	T	T	T
0.1333330000000004	0.2666669999999982	0.0996060000000014	F	F	F	0.1333330000000004	0.2666669999999982	0.0996060000000014	F	F	F
0.1336237262583602	0.2670925787968229	0.2957392678643088	T	T	T	0.1333742829187754	0.2667132916580352	0.2957764317491668	T	T	T
0.2666669999999982	0.3333330000000032	0.0033859999999990	F	F	F	0.2666669999999982	0.3333330000000032	0.0033859999999990	F	F	F
0.266722440944657	0.3333155404744647	0.1994613288996849	T	T	T	0.266670925408734	0.3332138310627181	0.1993511574837025	T	T	T
0.3333330000000032	0.2666669999999982	0.0996060000000014	F	F	F	0.3333330000000032	0.2666669999999982	0.0996060000000014	F	F	F
0.3336734979332153	0.2668259529563259	0.2958891383517067	T	T	T	0.3334137375597174	0.2665800826188529	0.2956995241390247	T	T	T
0.4666670000000011	0.3333330000000032	0.0033859999999990	F	F	F	0.4666670000000011	0.3333330000000032	0.0033859999999990	F	F	F
0.4663661005487673	0.3332425954634411	0.1994862413692389	T	T	T	0.4665167875550062	0.3331059027751562	0.1992595129708887	T	T	T
0.5333329999999989	0.2666669999999982	0.0996060000000014	F	F	F	0.5333329999999989	0.2666669999999982	0.0996060000000014	F	F	F
0.5332922589411738	0.2669082361132418	0.2957407784073590	T	T	T	0.5333023241091693	0.2667228193787375	0.2957626292277825	T	T	T
0.6666669999999968	0.3333330000000032	0.0033859999999990	F	F	F	0.6666669999999968	0.3333330000000032	0.0033859999999990	F	F	F
0.6669784868306505	0.2667375325168397	0.1995264943838574	T	T	T	0.6665788455387539	0.3333006482391260	0.1994225875856714	T	T	T
0.7333330000000018	0.3336669999999982	0.0996060000000014	F	F	F	0.7333330000000018	0.2666669999999982	0.0996060000000014	F	F	F
0.7333293125899093	0.26666329713176728	0.2956861461810100	T	T	T	0.7334556297416992	0.2668387891497235	0.2957784742184311	T	T	T
0.8666669999999996	0.3333330000000032	0.0033859999999990	F	F	F	0.8666669999999996	0.3333330000000032	0.0033859999999990	F	F	F
0.8666123605657721	0.3333126877143562	0.1994026052346305	T	T	T	0.8667758043828852	0.3335256880267947	0.19957595888385794	T	T	T
0.9333329999999975	0.2666669999999982	0.0996060000000014	F	F	F	0.9333329999999975	0.2666669999999982	0.0996060000000014	F	F	F
0.9331523328556138	0.2665323246162100	0.2956307142710593	T	T	T	0.9335349429757090	0.2667540613727346	0.2959055431623667	T	T	T
0.0666670000000025	0.5333329999999989	0.0033859999999990	F	F	F	0.3333330000000025	0.5333329999999989	0.0033859999999990	F	F	F
0.0667386355432171	0.5332476320502494	0.1994477595283805	T	T	T	0.0666636801013553	0.5333203936475448	0.1995110648222642	T	T	T
0.1333330000000004	0.4666670000000011	0.0996060000000014	F	F	F	0.1333330000000004	0.4666670000000011	0.0996060000000014	F	F	F
0.1334243759648644	0.4666720848908141	0.2956757402449089	T	T	T	0.1332946847577588	0.4667576362544876	0.2957595888385794	T	T	T
0.2666669999999982	0.5333329999999989	0.0033859999999990	F	F	F	0.2666669999999982	0.5333329999999989	0.0033859999999990	F	F	F
0.2665351304686333	0.5333621067714557	0.1993653727006755	T	T	T	0.2664930372565273	0.5333712549991894	0.1994115687782966	T	T	T
0.3333330000000032	0.4666670000000011	0.0996060000000014	F	F	F	0.3333330000000032	0.4666670000000011	0.0996060000000014	F	F	F
0.3330071200910900	0.4663624999749001	0.2956252573738680	T	T	T	0.3331943988176421	0.4664732844700717	0.2956573486089960	T	T	T
0.4666670000000011	0.5333329999999989	0.0033859999999990	F	F	F	0.4666670000000011	0.5333329999999989	0.0033859999999990	F	F	F
0.4670317250103395	0.5334200365823270	0.1996101138346305	T	T	T	0.4667913837699860	0.5336513216580741	0.1994781216482638	T	T	T
0.5333329999999989	0.4666670000000011	0.0996060000000014	F	F	F	0.5333329999999989	0.4666670000000011	0.0996060000000014	F	F	F
0.5335416262240307	0.4660085459881356	0.2953224202715901	T	T	T	0.5330687432120206	0.4654228923214275	0.2952317665734618	T	T	T
0.6666669999999968	0.5333329999999989	0.0033859999999990	F	F	F	0.6666669999999968	0.5333329999999989	0.0033859999999990	F	F	F
0.6663025185434713	0.5325189852170442	0.1992684888904611	T	T	T	0.6669520164568268	0.5335218219636390	0.1995941967364955	T	T	T
0.7333330000000018	0.4666670000000011	0.0996060000000014	F	F	F	0.7333330000000018	0.4666670000000011	0.0996060000000014	F	F	F
0.7331079676038944	0.466670451368475633	0.2956424804752216	T	T	T	0.7334663226659343	0.4666182005323104	0.2957324276594006	T	T	T
0.8666669999999996	0.5333329999999989	0.0033859999999990	F	F	F	0.8666669999999996	0.5333329999999989	0.0033859999999990	F	F	F
0.8664323552552728	0.5332858352247074	0.1995661869703912	T	T	T	0.8668577853474354	0.5333994888047475	0.1995039477299225	T	T	T
0.9333329999999975	0.4666670000000011	0.0996060000000014	F	F	F	0.9333329999999975	0.4666670000000011	0.0996060000000014	F	F	F
0.9333935525767132	0.4663876709032851	0.2956605490241774	T	T	T	0.9335103301786598	0.4667298005356956	0.2958014096057801	T	T	T
0.0666670000000025	0.7333330000000018	0.0033859999999990	F	F	F	0.0666670000000025	0.7333330000000018	0.0033859999999990	F	F	F
0.0668200353031019	0.733333000470634604	0.1996174089701697	T	T	T	0.0666549647671374	0.7332589705024031	0.199589137332642	T	T	T
0.1333330000000004	0.6666669999999968	0.0996060000000014	F	F	F	0.1333330000000004	0.6666669999999968	0.0996060000000014	F	F	F
0.1337968481402855	0.6667010176354059	0.2956746059407276	T	T	T	0.1333128112226247	0.6664982330937096	0.2958116952332357	T	T	T
0.2666669999999982	0.7333330000000018	0.0033859999999990	F	F	F	0.2666669999999982	0.7333330000000018	0.0033859999999990	F	F	F
0.2667709449812292	0.7333822623440391	0.1993749813701398	T	T	T	0.2665293755899313	0.7332716839098803	0.1995026222939499	T	T	T
0.3333330000000032	0.6666669999999968	0.0996060000000014	F	F	F	0.3333330000000032	0.6666669999999968	0.0996060000000014	F	F	F
0.333382005097587	0.66670451368475633	0.2954686854221857	T	T	T	0.3329897950814613	0.6668262926325262	0.2956736018901474	T	T	T
0.4666670000000011	0.7333330000000018	0.0033859999999990	F	F	F	0.4666670000000011	0.7333330000000018	0.0033859999999990	F	F	F
0.4668969893111716	0.73333954714368404	0.1994101262621362	T	T	T	0.4667932795649696	0.7334145499146780	0.1992131826097797	T	T	T
0.5333329999999989	0.6666669999999968	0.0996060000000014	F	F	F	0.5333329999999989	0.6666669999999968	0.0996060000000014	F	F	F
0.5298601235328692	0.6643601419699665	0.2955718236923697	T	T	T	0.5315257303807827	0.6651314624410153	0.2953329271135802	T	T	T
0.6666669999999968	0.7333330000000018	0.0033859999999990	F	F	F	0.6666669999999968	0.7333330000000018	0.0033859999999990	F	F	F
0.6661845863909945	0.7331398218185865	0.1989077507831124	T	T	T	0.6666481890373785	0.7333522163133870	0.1999322225403805	T	T	T
0.7333330000000018	0.6666669999999968	0.0996060000000014	F	F	F	0.7333330000000018	0.6666669999999968	0.0996060000000014	F	F	F
0.7346088248984122	0.6690243597267921	0.2955432705311641	T	T	T	0.7331515997333026	0.6646279813864622	0.2956950305861447	T	T	T
0.8666669999999996	0.7333330000000018	0.0033859999999990	F	F	F	0.8666669999999996	0.7333330000000018	0.0033859999999990	F	F	F
0.8670172615164108	0.7331024027327662	0.1988625146369559	T	T	T	0.8664685247817997	0.7333122169908778	0.1993358839145090	T	T	T
0.9333329999999975	0.6666669999999968	0.0996060000000014	F	F	F	0.9333329999999975	0.6666669999999968	0.0996060000000014	F	F	F
0.9350985639080484	0.6649234429570369	0.2954163938548832	T	T	T	0.9334986808186562	0.6667000865513409	0.2958665571784083	T	T	T
0.0666670000000025	0.9333329999999975	0.0033859999999990	F	F	F	0.0666670000000025	0.9333329999999975	0.0033859999999990	F	F	F
0.0672246460116155	0.9336362934454877	0.1999747530831022	T	T	T	0.0664639850020344	0.9330901663352830	0.1996788164942292	T	T	T
0.1333330000000004	0.8666669999999996	0.0996060000000014	F	F	F	0.1333330000000004	0.8666669999999996	0.0996060000000014	F	F	F
0.1339972642180771	0.8667204870775937	0.2958011656668484	T	T	T	0.1333167948166054	0.8666046714811513	0.2957874830857372	T	T	T
0.2666669999999982	0.9333329999999975	0.0033859999999990	F	F	F	0.2666669999999982	0.9333329999999975	0.0033859999999990	F	F	F
0.2665460725900654	0.9330731021578056	0.1995800183648593	T	T	T	0.2667794667813916	0.9335995449526013	0.1994094829404460	T	T	T
0.3333330000000032	0.8666669999999996	0.0996060000000014	F	F	F	0.3333330000000032	0.8666669999999996	0.0996060000000014	F	F	F
0.3335082948341846	0.8666008033487029	0.2957139042369716	T	T	T	0.3332524083266573	0.8665654756595009	0.2957868861877577	T	T	T
0.4666670000000011	0.9333329999999975	0.0033859999999990	F	F	F	0.4666670000000011	0.9333329999999975	0.0033859999999990	F	F	F
0.4664928290304970	0.9332349080404899	0.1994951462828016	T	T	T	0.4666807085600137	0.9331205604772504	0.1997018297086314	T	T	T
0.5333329999999989	0.8666669999999996	0.0996060000000014	F	F	F	0.5333329999999989	0.8666669999999996	0.0996060000000014	F	F	F
0.5305975320480623	0.8656907408620665	0.2967579212662622									

Fig. S11. ^1H NMR spectra of the reaction mixtures of each reaction in the recyclability tests (IS: maleic acid internal standard, R: levulinic acid reactant, GVL: γ -valerolactone, HPA: 4-hydroxypentanoic acid).

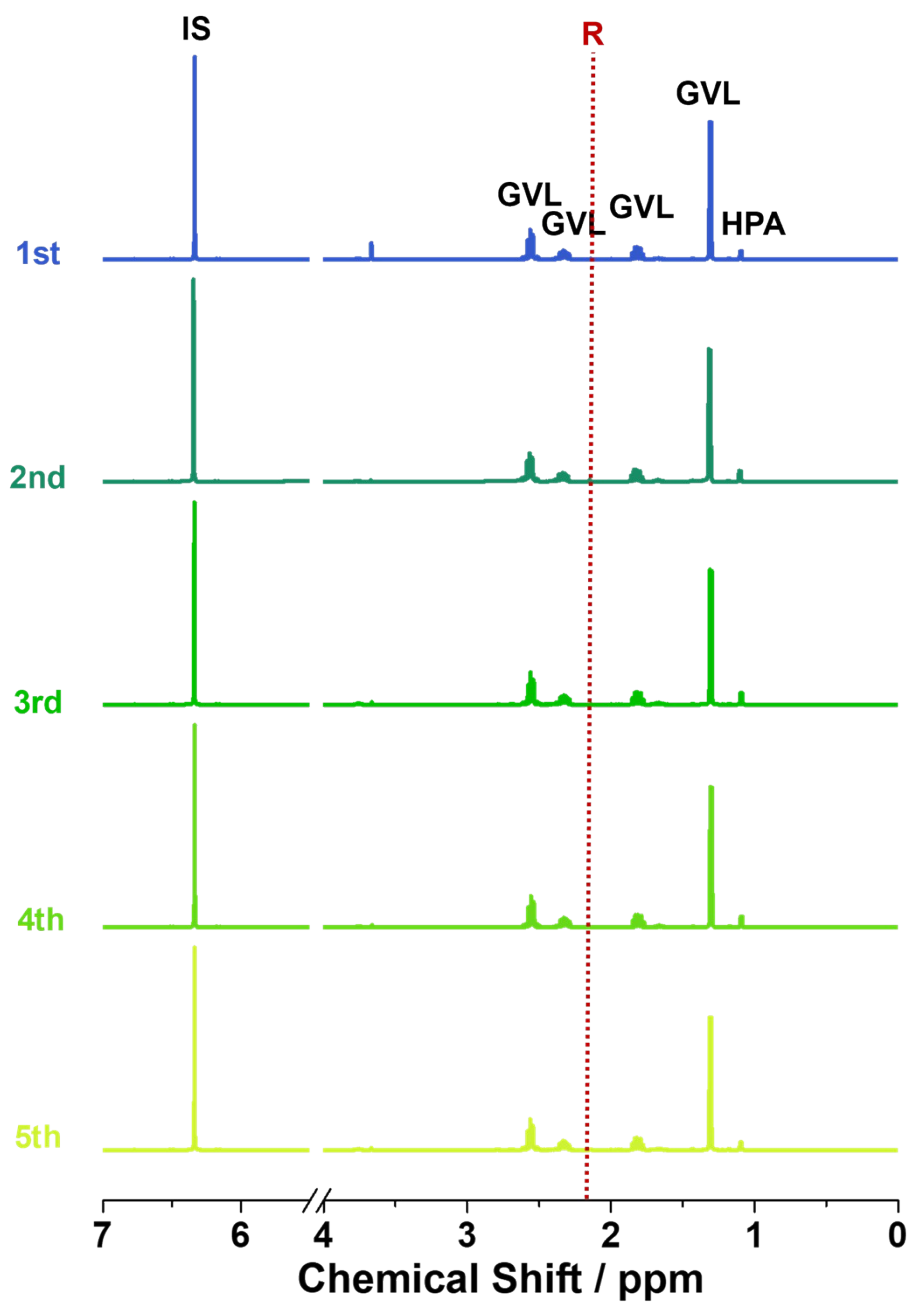


Fig. S12. IR spectra of Ru/HC-3 before and after five successive reactions.

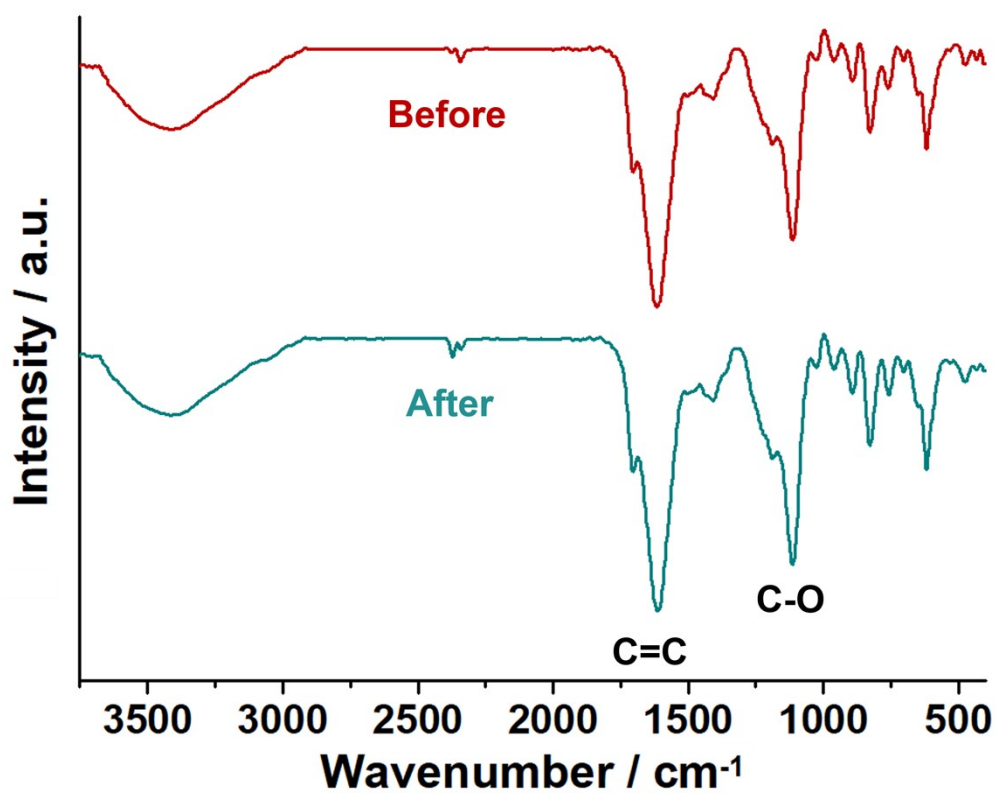


Fig. S13. Analysis of the XPS (a) Ru 3p and (b) O 1s orbital peaks of Ru/HC-3 before and after five successive reactions.

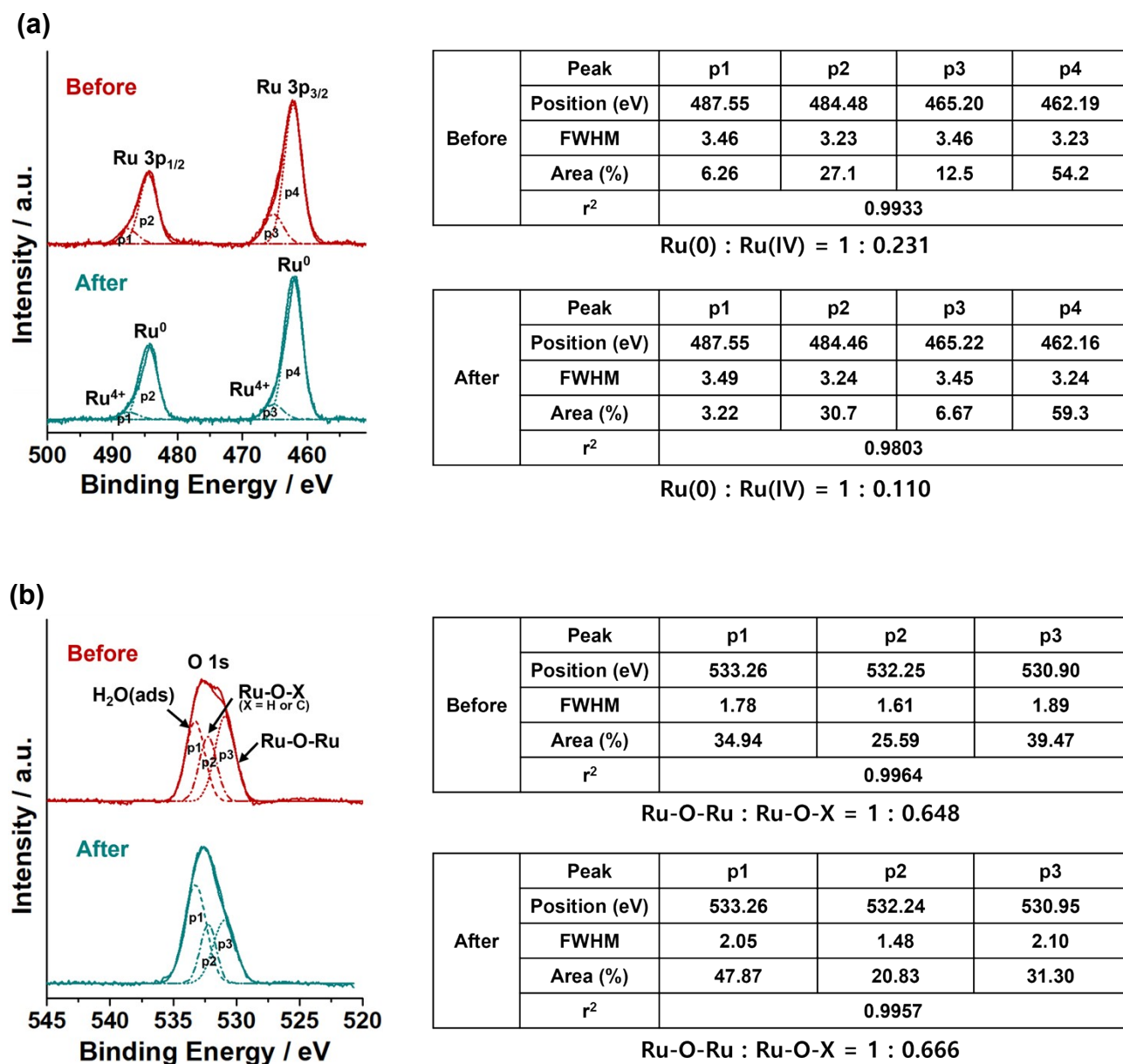


Table S1. Comparison of the catalytic performance of recent Ru-based heterogeneous catalysts for the conversion of LA to GVL reported in the literature.

Entry	Catalyst (Ru loading wt%)	Amount (mol%)	Temp. (°C)	H ₂ (bar)	Time (h)	Conv. ^a (%)	GVL Yield (%)	TON	TOF (h ⁻¹)	Year	Ref
1	Ru/TiO ₂ (0.6)	0.4	150	35	5	100	93	232.5	46.6	2011	S1
2	5 % Ru-NOMC (5)	0.29	120	13	4	100	100	344.8	114.9	2016	S2
3	Ru/C (5)	0.23	90	45	6	98	83	360.9	60.2	2016	S3
4	Ru ⁴⁰ @Meso-TiO ₂ (0.37)	0.5	150	10	5	98	99	198	39.6	2018	S4
5	Ru ⁴⁰ @Meso-SiO ₂ (0.39)	0.5	150	10	5	100	100	200	40	2018	S4
6	Ru/ZrO ₂ , Ru/TiO ₂ (1)	0.25	150	50	- ^b	>90	>90	—	—	2020	S5
7	Ru/HCSs-m (-)	0.17	180	40	4	98.45	92.74	545.5	136.4	2021	S6
8	Ru ⁵ /Al ₂ O ₃ (4.8)	1.84	190	50	4	>99.9	88.9	48.3	12.1	2023	S7
9	Ru-PC (5.6)	1.8	140	IPA	4	100	93.8	52.1	13	2024	S8
10	5Ru@FC-30% (8.6)	2.8	120	IPA	3	100	92.4	33	11	2025	S9
11	MO-Ru (1)	1	150	FA	1.5	100	99	99	66	2025	S10
12	Ru/HC-3 (51.6)	0.25	100	5	2	100	94	376	188	This Work	

^a Conversion yields of LA. ^b Continuous flow system.

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Table S2. Physical parameters of HMOP, HMOP@TA, Ru/HC-1~3, and control Ru/C.

Materials	$S_{\text{BET}}^{\text{a}}$ (m^2/g)	$V_{\text{mic}}^{\text{b}}$ (cm^3/g)	V_{t}^{c} (cm^3/g)
HMOP	544	0.13	0.27
HMOP@TA	415	0.10	0.28
Ru/HC-1	407	0.11	0.25
Ru/HC-2	351	0.10	0.21
Ru/HC-3	243	0.068	0.15
Control Ru/C	273	0.071	0.17

^a Surface area obtained by a BET plot. ^b Micropore volume obtained by a t-plot. ^c Total pore volume.

Table S3. DFT-calculated energies of the intermediates involved in the conversion of LA to GVL on the Ru (002) surface. LA, HPA, and GVL represent levulinic acid, 4-hydroxypentanoic acid, γ -valerolactone, respectively.

Systems	Relative Energy (eV)
LA(g)+H ₂ (g)	0
HPA(g)	-0.73
GVL(g)+H ₂ O(g)	-0.53
LA*+H ₂ *	-1.40
LA*+2H*	-2.91
LAH*+H*	-3.03
HPA*	-2.24
GVL*+OH*+H*	-2.75
GVL*+H ₂ O*	-2.60

Table S4. Comparison of the first and second TPR temperatures of Ru-based heterogeneous catalysts reported in the literature.

Entry	Catalyst	The first TPR Temp. ^a (°C)	The second TPR Temp. ^b (°C)	Year	Ref
1	Ru/TiO ₂	126-160		2014	S1
2	Ru/C	100-175	250-400	2017	S2
3	Ru/ZrO ₂	175-250		2017	S3
4	Ru/CeO ₂	144-164	225-279	2018	S4
5	Ru/TiO ₂	131-200		2020	S5
6	Ru/BaCeO ₃	181-209		2021	S6
7	Ru-MnAl ₂ O ₃	100-105	175-217	2023	S7
8	Ru/Ti-S-A and Ru/Ti	95-105	128-131	2024	S8
9	Ru/HC-3	80	163	This Work	

^a Corresponding to the reduction temperature of surface RuO_x species. ^b Corresponding to the reduction temperature of RuO_x species at the interface of solid supports.

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