

Appendix A. Supplementary Information

Understanding the reaction kinetics of heterogenous 1-hexene hydroformylation

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Supplementary methods

X-ray diffraction (XRD). The XRD patterns were measured using a Bruker D2 PHASER diffractometer from Bruker Corporation, Germany. Cu-K α radiation was utilized, with a tube power of 2.2 kW. The initial scan range was set from 5° to 90°, with a scan rate of 6°/min. A fine scan ranged from 30° to 50° with a rate of 1°/min was also applied to better reveal the crystal structure.

Transmission electron microscopy (TEM). TEM images are collected using a JEM-F200. The transmission electron microscope (TEM) has a point resolution of ≤ 0.23 nm at 200 kV. The line resolution is ≤ 0.10 nm at 200 kV and ≤ 0.14 nm at 80 kV. For scanning transmission electron microscopy (STEM) with high-angle annular dark field (HAADF) imaging, the resolution is ≤ 0.16 nm at 200 kV and ≤ 0.34 nm at 80 kV. The information resolution is 0.12 nm at 200 kV. The acceleration voltage ranges from 80 kV to 200 kV. The magnification in TEM mode is from 20x to 2.0 Mx, while in STEM mode it is from 200x to 1.5 Mx. The electron gun type is a high-brightness cold field emission gun. The condenser lens system consists of a four-stage condenser lens system, allowing for independent control of the convergence angle and brightness. The detector types include bright field (BF), dark field (DF), and backscattered electron imaging (BEI).

Supplementary note 1. Derivation of the three-variable model

For the purpose of simplifying calculations, we first focus on examining the hydroformylation activity of the catalyst without distinguishing the types of aldehydes. With reference to lumped kinetics, 1-heptanal, 2-methylhexanal and 2-ethylbutanal are collectively referred to as aldehydes. The reaction pathway is simplified into two main steps: direct hydroformylation of 1-hexene to aldehydes and hydroformylation of 2-hexene (formed from the isomerization of 1-hexene) to aldehydes. Wherein, the kinetic constant of 1-hexene isomerization to 2-hexene is defined as k_{iso} , and the kinetic constants of 1-hexene and 2-hexene hydroformylation to aldehydes are defined as k_{HF1} and k_{HF2} , respectively.

The three-variable model can be then constructed as follow:

$$\begin{cases} \frac{dY_\alpha}{dt} = -(k_{iso} + k_{HF1})Y_\alpha \\ \frac{dY_\beta}{dt} = k_{iso}Y_\alpha - k_{HF2}Y_\beta \\ \frac{dY_{ald}}{dt} = k_{HF1}Y_\alpha + k_{HF2}Y_\beta \end{cases} \quad (7)$$

By solving these differential equations, we can obtain:

$$\begin{cases} Y_\alpha = \exp [(-k_{iso} - k_{HF1})t] \\ Y_\beta = \frac{k_{iso}}{k_{HF2} - k_{iso} - k_{HF1}} \exp [(-k_{iso} - k_{HF1})t] - \frac{k_{iso}}{k_{HF2} - k_{iso} - k_{HF1}} \exp (-k_{HF2}t) \\ Y_{ald} = \frac{k_{HF1} - k_{HF2}}{k_{HF2} - k_{iso} - k_{HF1}} \{ \exp [(-k_{iso} - k_{HF1})t] - 1 \} + \frac{k_{iso}}{k_{HF2} - k_{iso} - k_{HF1}} [\exp (-k_{HF2}t) - 1] \end{cases} \quad (8)$$

Using these equations, we can fit the experimental data, which is shown in **Fig. S3**. Although the Arrhenius fitting shows good linearity, the three-variable model can only predict the catalytic activity but cannot distinguish the regioselectivity of aldehydes.

Supplementary note 2. Formula for l/b prediction model

$$\begin{cases} \ln K_1 = \frac{4507}{T} + 0.96 \times \ln P - 13.59 \\ \ln K_2 = \frac{6347}{T} + 0.96 \times \ln P - 19.39 \\ \ln S = \frac{6386}{T} + \ln P - 19.11 \end{cases} \quad (9)$$

As can be seen from equation (9), K_1 , K_2 and S are both functions of T and P . From equation (5), it can be inferred that l/b ratio is also a function of T and P . Therefore, by giving a set of (T , P), we can get the corresponding l/b ratio theoretically. According to this principle, by giving enough temperature and pressure, we get multiple sets of simulation results, and the predicted l/b ratio is supplemented in “Appendix B. Supplementary Data”. From this, the prediction chart is drawn.

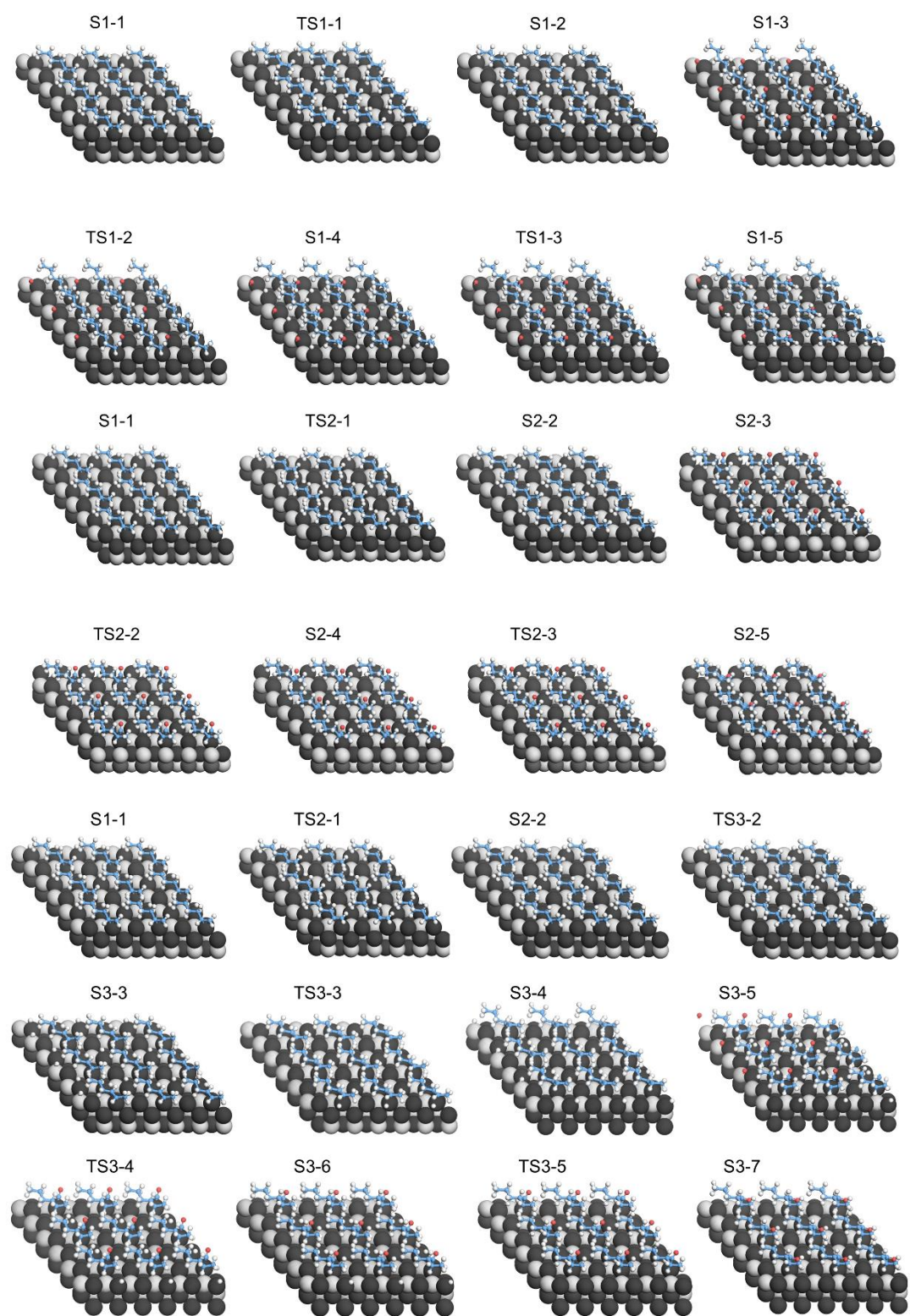


Figure S1. Cross view of steady states and transition states of 1-hexene hydroformylation.

Table S1. Energy profiles of 1-hexene hydroformylation on Rh₂P/SiO₂ catalysts.

Product		Reaction coordinate							
1-heptanal	ID	S1-1	TS1-1	S1-2	S1-3	TS1-2	S1-4	TS1-3	S1-5
	Gibbs free energy (eV)	-0.54	-0.26	-0.71	-0.99	-0.59	-1.58	-1.02	-1.36
	TDI/TDTS		TDTS $\delta E_1 = 1.33$ eV						
2-methylhexanal	ID	S1-1	TS2-1	S2-2	S2-3	TS2-2	S2-4	TS2-3	S2-5
	Gibbs free energy (eV)	-0.54	-0.30	-0.74	-1.11	-0.88	-1.57	-0.80	-1.32
	TDI/TDTS		TDTS $\delta E_2 = 1.29$ eV						
2-hexene	ID	S3-3	TS3-2	S2-2					
	Gibbs free energy (eV)	-0.48	0.12	-0.74					
	TDI/TDTS		TDTS $\delta E_{\text{iso}} = 1.71$ eV						
2-ethylbutanal	ID	S3-3	TS3-3	S3-4	S3-5	TS3-4	S3-6	TS3-5	S3-7
	Gibbs free energy (eV)	-0.48	0.01	-0.49	-0.77	-0.63	-1.59	-1.04	-1.38
	TDI/TDTS						TDI	TDTS $\delta E_3 = 0.55$ eV	

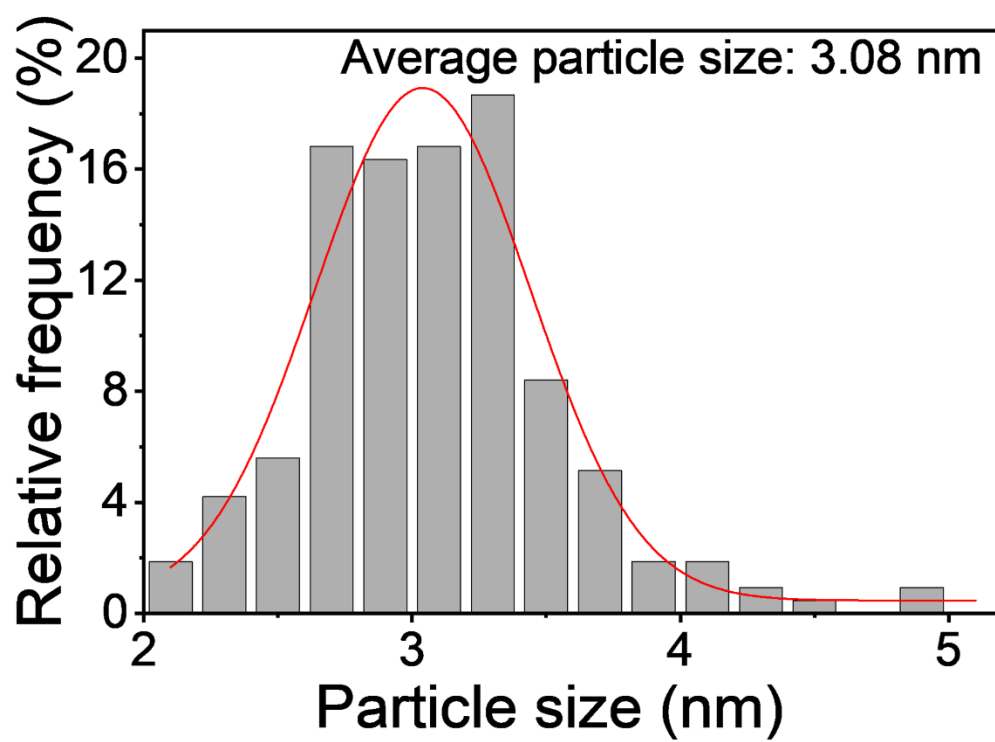


Figure S2. Particle size distribution diagram of Rh₂P/SiO₂

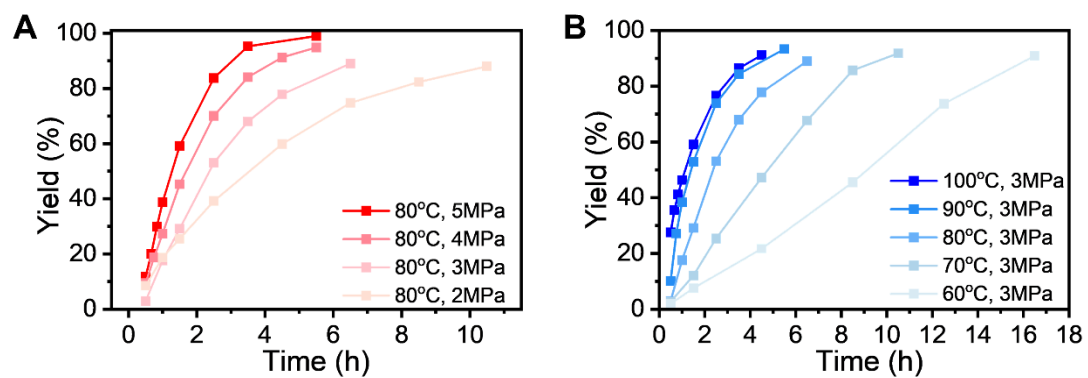


Figure S3. Aldehyde yields of 1-hexene hydroformylation on $\text{Rh}_2\text{P}/\text{SiO}_2$ under different conditions.

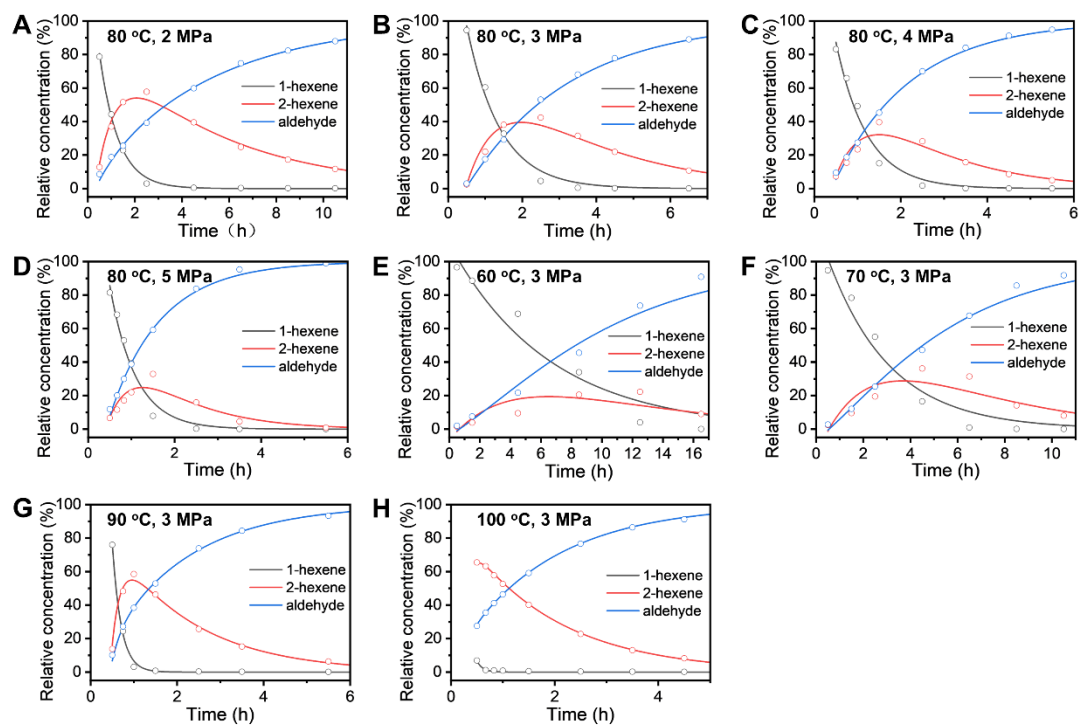


Figure S4. Fitting results of three-variable model under different reaction conditions.

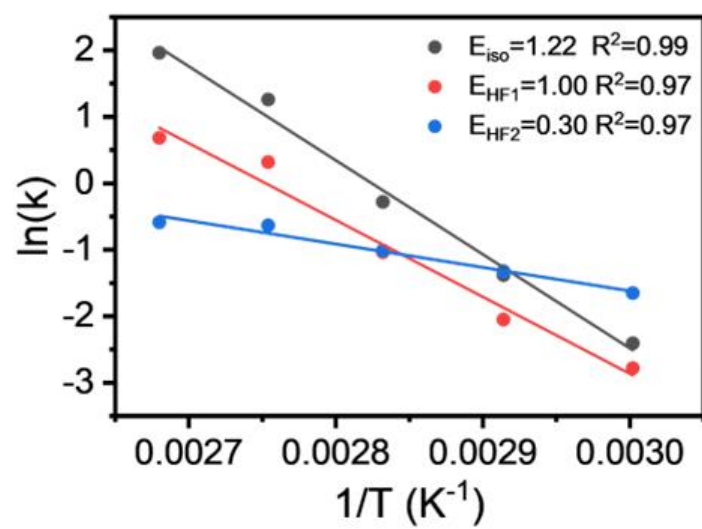


Figure S5. Arrhenius fitting of kinetic parameters in the three-variable model.

Table S2. The fitted apparent activation energies of kinetic parameters in the five-variable model.

E_1	E_2	E_3	E_{iso}	E_S
1.25 eV	1.04 eV	0.49 eV	1.65 eV	-0.55 eV

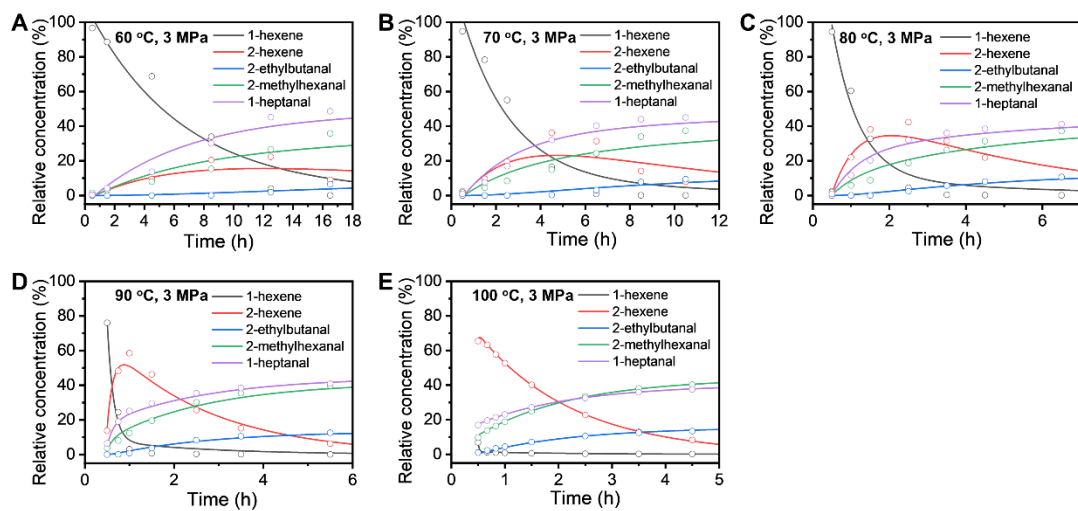


Figure S6. Fitting results of five-variable model under different reaction temperatures.

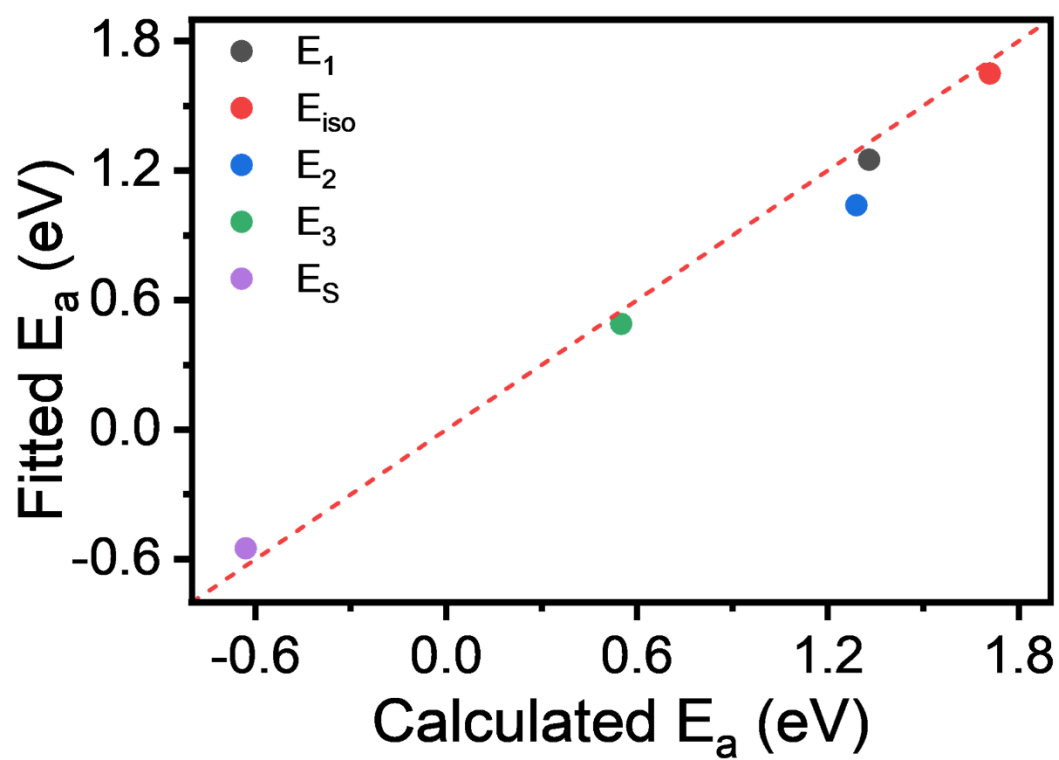


Figure S7. Comparison of activation energies obtained from DFT calculations and experimental evaluations.

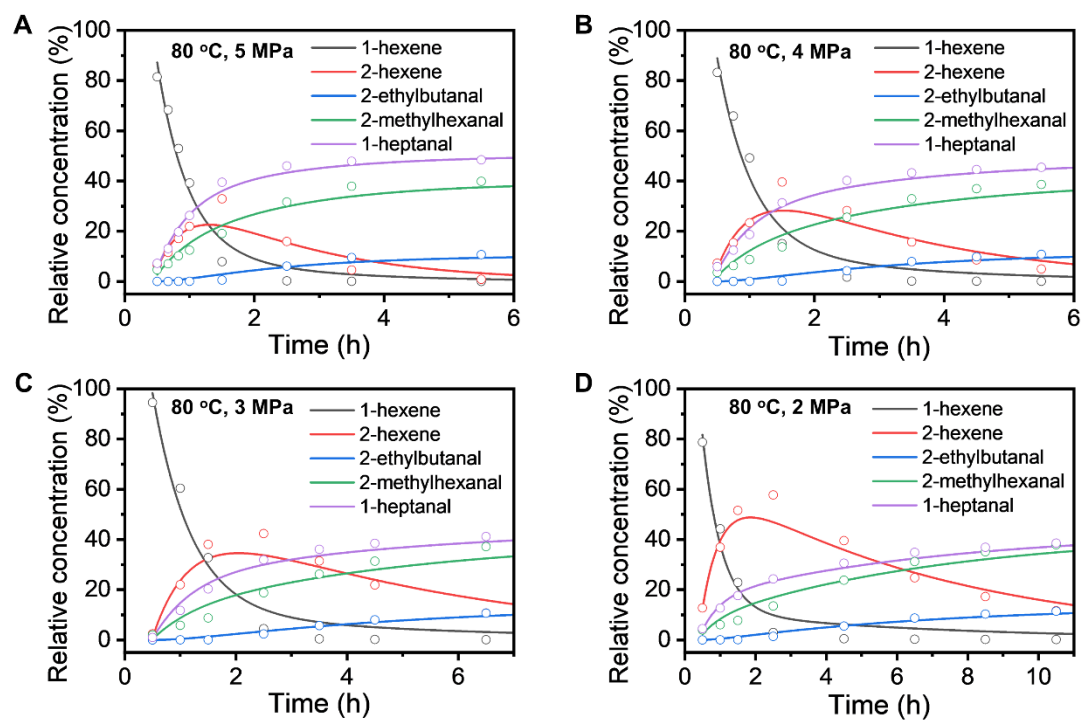


Figure S8. Fitting results of five-variable model under different reaction pressures.

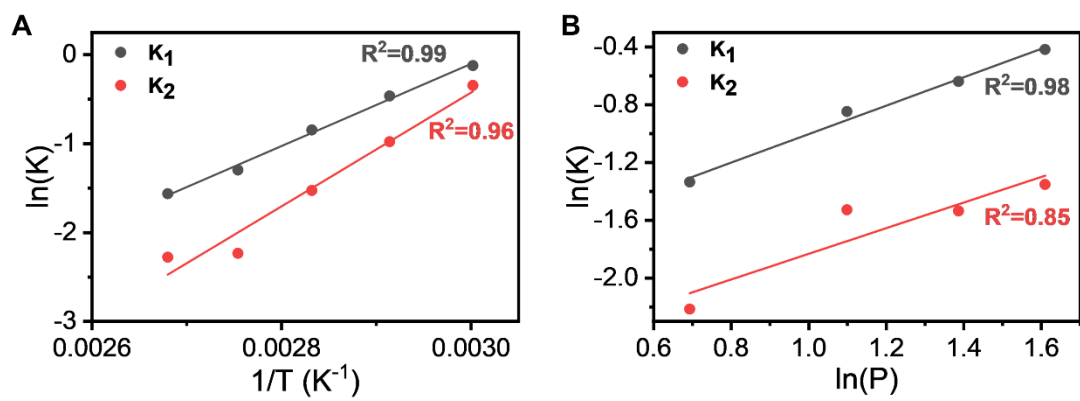


Figure S9. Arrhenius fitting (A) and pressure fitting (B) of K_1 and K_2 .

Path1

S1-1

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7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
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0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
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0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
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TS1-1

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-3.8620861857000000 6.6897080140999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
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S1-2

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P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

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S1-3

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7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
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0.5893741716585160	0.3890913422904374	0.2582282731496422	T	T	T
0.5872474670972727	0.8865929230662367	0.2552320917413652	T	T	T
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9169042380645731	0.0644731978755742	0.2164511290122110	T	T	T
0.9179682862764603	0.5509710631309412	0.2149551442709699	T	T	T
0.4259131133350377	0.5533034978794485	0.2139432762284546	T	T	T
0.4385118363482848	0.0644363010891416	0.2173068513809075	T	T	T
0.2576481238138787	0.7200303754546040	0.2902191662909288	T	T	T
0.2544772294676859	0.2221476225195939	0.2936105138414086	T	T	T
0.7641510111082955	0.2586400037763470	0.3179238575770714	T	T	T
0.7646450621291858	0.7378494230095771	0.2937919402284227	T	T	T
0.4553443609271590	0.1573600078943549	0.4346772057383952	T	T	T
0.5870346394235588	0.0842839957369218	0.4033694173232846	T	T	T
0.5580155747669929	0.3742589885959307	0.4580398266208484	T	T	T
0.4173651711765333	0.4386316974955012	0.4882304358511696	T	T	T
0.5309367674038922	0.6493588386440056	0.5181274194091592	T	T	T
0.3931176086138001	0.7223107581853158	0.5451594997728106	T	T	T
0.9193168406965438	0.4357921869435994	0.3856399282783133	T	T	T
0.4948664631272600	0.9307068084692587	0.3838180156458904	T	T	T
0.6905959767672941	0.0803009433132034	0.4409452377093648	T	T	T
0.6344020358855491	0.4730581616881636	0.4143293527077060	T	T	T
0.6761042958678573	0.4010433297771545	0.4951287169286550	T	T	T
0.3233505525696280	0.3320286699618885	0.5279622912137424	T	T	T
0.3143276007090261	0.4324922242509204	0.4481232468107538	T	T	T
0.6311536096855944	0.7536364693072506	0.4789045868896448	T	T	T
0.6289378085744387	0.6507283204189013	0.5591837842364191	T	T	T
0.2830435965033899	0.6131599382136531	0.5809415131043169	T	T	T
0.3095942261577486	0.7414411409140202	0.5035697812592562	T	T	T
0.4774540505767141	0.8662866643353868	0.5717469652284958	T	T	T
0.3770936344122460	0.0600705147427111	0.4786861513766842	T	T	T
0.3344327849486812	0.1313519770279198	0.3977927963190936	T	T	T
0.8353810741020998	0.8875778579147147	0.3559570450371844	T	T	T
0.0167660127799550	0.5448536201962964	0.4284602718953367	T	T	T

TS1-2

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0949107484061614	0.8925405684386962	0.2554873230171017	T	T	T
0.0944355541238487	0.3934505958510297	0.2542488990456091	T	T	T
0.5891631986885877	0.3891710862644662	0.2565877836524834	T	T	T
0.5913777053157190	0.8929850295017585	0.2569347655813826	T	T	T
0.2546800080000250	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000213	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000092	0.3899199960000033	0.1350599969999990	F	F	F
0.9198259800177095	0.0631557668408601	0.2161090235247086	T	T	T
0.9204582019900345	0.5554164853975405	0.2144144540273993	T	T	T
0.4269474498347405	0.5565214871951615	0.2137880273385172	T	T	T
0.4340419309175539	0.0621884092060621	0.2162304439531794	T	T	T
0.2620632192344274	0.7249948783801730	0.2912955697014610	T	T	T
0.2573180878366355	0.2248585168569507	0.2931347122656299	T	T	T
0.7745136143345800	0.2565585583420367	0.3096033851452366	T	T	T
0.7629488174124572	0.7353564959171124	0.2940968266491706	T	T	T
0.5168213791720490	0.1951419348598831	0.4439454325129035	T	T	T
0.6702163636139166	0.1419160704163751	0.4191245161076388	T	T	T
0.5991141283068109	0.4125401436593406	0.4653483014423270	T	T	T
0.4405685642637087	0.4570380359777845	0.4923754287205246	T	T	T
0.5329251452772925	0.6689009666147213	0.5211263538590553	T	T	T
0.3773470512677887	0.7257197632073235	0.5419477013383600	T	T	T
0.9139830823776000	0.4136879220137580	0.3821152898585530	T	T	T
0.6087183783088339	0.9867245447586197	0.4021090757512999	T	T	T
0.7854793118886122	0.1712999281507790	0.4572926335774445	T	T	T
0.6723454213604683	0.5128742716169401	0.4215983120578844	T	T	T
0.7174613224090912	0.4537083769421188	0.5038151706062003	T	T	T

0.3509976403655702	0.3479544710139809	0.5321738992767795	T	T	T
0.3357736292805837	0.4374511805889853	0.4509243189374145	T	T	T
0.6348728395735439	0.7758861414228584	0.4828990399917541	T	T	T
0.6272320208018090	0.6815472556326783	0.5650569995999976	T	T	T
0.2662954307050483	0.6134433198076056	0.5767718471561313	T	T	T
0.2958664000842381	0.7333898525098732	0.4974685095918655	T	T	T
0.4464919797759276	0.8717100272500863	0.5677068400149353	T	T	T
0.4385308417144949	0.0973273274102572	0.4877646307272834	T	T	T
0.4017744411746667	0.1562503245348716	0.4040817671349050	T	T	T
0.8406248991151863	0.8755767120161007	0.3587283405298609	T	T	T
0.0249384997954589	0.5321739999879912	0.4211567092442265	T	T	T

S1-4

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0851599327630949	0.8856111789789521	0.2570340044755862	T	T	T
0.0912682907588576	0.3888631653259289	0.2528465502864147	T	T	T
0.5891156433790877	0.3909516220314335	0.2564620997920279	T	T	T
0.5840775969075975	0.8854702512963973	0.2557975520025457	T	T	T
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9173084478682680	0.0501793472051925	0.2149604180542055	T	T	T
0.9218726408040876	0.5604760601054597	0.2143729215096117	T	T	T
0.4226630719048617	0.5581397053659162	0.2138864273090103	T	T	T
0.4203485829856609	0.0519942738108531	0.2163335315569579	T	T	T
0.2512893776023092	0.7195759719154520	0.2974327787066269	T	T	T
0.2546901844820621	0.2261693907636981	0.2916121815517514	T	T	T
0.7673628611716371	0.2360430799267275	0.2942266046000760	T	T	T

0.7490399372632829	0.7216976617745053	0.2951851336926822	T	T	T
0.5968733068435712	0.2876058499086304	0.4515993018679674	T	T	T
0.7864602364024373	0.2738706983062029	0.4403050358418726	T	T	T
0.6413655433456876	0.5017293098303932	0.4610289465856218	T	T	T
0.4609807679677742	0.5150800649366388	0.4849879393930119	T	T	T
0.5132502640991490	0.7271249091702208	0.5044052352633071	T	T	T
0.3338584818195475	0.7399427242046102	0.5302965364506965	T	T	T
0.8974866172684903	0.3850507633734915	0.3770070318552909	T	T	T
0.7463164808214447	0.1161764917225611	0.4354211615655120	T	T	T
0.8898562666057128	0.3402341966920800	0.4835991237732498	T	T	T
0.6964434869959925	0.5849584307886104	0.4121788923382096	T	T	T
0.7664638636712686	0.5796489242961888	0.4971189250737401	T	T	T
0.3918817207368330	0.4144513957003315	0.5288608272019910	T	T	T
0.3464133721870662	0.4589809545810190	0.4444917110014934	T	T	T
0.5778739928580883	0.8235608392941256	0.4594780448569781	T	T	T
0.6321461254963067	0.7840106519294693	0.5432366024003203	T	T	T
0.2642886683261758	0.6383873100720325	0.5737469997823021	T	T	T
0.2199738168057442	0.6967914006383403	0.4903895519189195	T	T	T
0.3775263006578874	0.8921823322713117	0.5472624998039626	T	T	T
0.5207765041144737	0.1988138271122639	0.4970167324132586	T	T	T
0.4933691980214994	0.2176272604786899	0.4085466166067294	T	T	T
0.2326926980717639	0.3064130492718847	0.3624987030225427	T	T	T
0.0532229021510129	0.5528972668105047	0.3825715644806546	T	T	T

TS1-3

1.000000000000000					
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-3.8620861857000000		6.6897080140999998		0.0000000000000000	
0.0000000000000000		0.0000000000000000		19.7301998137999988	
P	Rh	C	H	O	
8	16	7	14	1	

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0900147900563384	0.8892327497662469	0.2580883557762648	T	T	T
0.0941204806342450	0.3919079334409888	0.2508899674838174	T	T	T
0.5874496451856297	0.3909116732386085	0.2577087569288381	T	T	T
0.5830178257622179	0.8817717361948707	0.2556540806161897	T	T	T
0.2546800080000174	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F

0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000135	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000053	0.3899199960000033	0.1350599969999990	F	F	F
0.9189794575370887	0.0513252422056214	0.2142182822045643	T	T	T
0.9191618413547185	0.5570968934085537	0.2162572521424222	T	T	T
0.4231387531241769	0.5564010639781578	0.2136515196321768	T	T	T
0.4294079089123625	0.0570175697244411	0.2169091235991560	T	T	T
0.2548579976120819	0.7194405551633059	0.2979327213657721	T	T	T
0.2542869248147273	0.2234062583122018	0.2923161135036286	T	T	T
0.7673668430038734	0.2213688947568092	0.3002930045951193	T	T	T
0.7501447867934012	0.7232445583172116	0.2954085560752039	T	T	T
0.6157727292875784	0.2883957112688860	0.4612613709891435	T	T	T
0.8064047082010184	0.2760223559244317	0.4525561137510270	T	T	T
0.6628273504782577	0.5022028544730537	0.4730359793995035	T	T	T
0.4781478755351780	0.5150556320694269	0.4911982294976756	T	T	T
0.5295393067853812	0.7240910921961541	0.5138628177879746	T	T	T
0.3451022780737031	0.7375193124165245	0.5327721828114429	T	T	T
0.9108653801116691	0.3741638143523582	0.3870338015649977	T	T	T
0.7694996110393097	0.1190077068072952	0.4512327342617382	T	T	T
0.9104459772424407	0.3525327768418332	0.4949104946004032	T	T	T
0.7354004842814498	0.5942805489752930	0.4272681598303140	T	T	T
0.7746707241439290	0.5685799100344667	0.5141274838820229	T	T	T
0.3964568834582594	0.4074434867042548	0.5323388041449546	T	T	T
0.3761067395832930	0.4686996601185983	0.4471300442377785	T	T	T
0.6120227786574820	0.8292914445253778	0.4723919063124837	T	T	T
0.6336917713063148	0.7688664072390097	0.5572622154750312	T	T	T
0.2597531803671464	0.6286856394997949	0.5729830791203423	T	T	T
0.2462345406014322	0.7034060357881233	0.4886269681814850	T	T	T
0.3852009568589477	0.8871848981448583	0.5516043235921784	T	T	T
0.5310929100362021	0.1940567645822334	0.5046676977466131	T	T	T
0.5197733461099572	0.2250804963732794	0.4159545494735060	T	T	T
-0.0706751767273186	0.2022478045010301	0.3493178822873380	T	T	T
0.0629719987058116	0.5439286817108833	0.3877010376208219	T	T	T

S1-5

1.000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0888952767774198	0.8895315605260723	0.2576066170089713	T	T	T
0.0915197425286154	0.3905563216135539	0.2539413881189883	T	T	T
0.5897701297194444	0.3900539512850929	0.2559834161962408	T	T	T
0.5862752719693803	0.8893312884801823	0.2564445405273226	T	T	T
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9221654448275212	0.0549872968516015	0.2140834336858964	T	T	T
0.9245741726023702	0.5591694037348121	0.2150555607474944	T	T	T
0.4211267917244725	0.5585018400025472	0.2141620438033620	T	T	T
0.4195601397111374	0.0525557941597068	0.2149070327020884	T	T	T
0.2581229269162573	0.7256853086081949	0.2991179536731365	T	T	T
0.2570895621969983	0.2247346718256868	0.2927380638710702	T	T	T
0.7587570955978986	0.2218905795426321	0.2934840182441557	T	T	T
0.7512502648311838	0.7238681624773041	0.2939025993107985	T	T	T
0.6289284850225904	0.2966151818439120	0.4537287080895342	T	T	T
0.8156792786765125	0.2753777012972561	0.4533241206484232	T	T	T
0.6687364659753359	0.5068352264474325	0.4689703968160057	T	T	T
0.4794664469039371	0.5121402307751270	0.4870900775105939	T	T	T
0.5261834794158906	0.7197756775451873	0.5100474871024758	T	T	T
0.3421822989496250	0.7330706519317942	0.5298520218284390	T	T	T
0.9753930597716685	0.3912525673288743	0.4019430919592294	T	T	T
0.7739668495615893	0.1175460784894989	0.4470930889863939	T	T	T
0.8911157288540260	0.3225086370432486	0.5033642533070956	T	T	T
0.7420614052131931	0.6051142536562417	0.4247473147422803	T	T	T
0.7773623030362489	0.5719140598132479	0.5110694999641923	T	T	T
0.3985844383989807	0.4024209758726184	0.5278647896712610	T	T	T
0.3784192196129021	0.4643460788358676	0.4426634125940810	T	T	T
0.6068386112676001	0.8259910185215429	0.4686366705879320	T	T	T
0.6312498757267763	0.7653795029445846	0.5531703813090660	T	T	T
0.2571122469657230	0.6242993326178398	0.5700859149159563	T	T	T
0.2422532619459358	0.7022029957394962	0.4862129929535703	T	T	T
0.3839102698044502	0.8829208510347811	0.5490828730546848	T	T	T
0.5257748068217596	0.1918161342388120	0.4920860003653838	T	T	T

0.5508322366192301	0.2453945292131519	0.4045550903920498	T	T	T
0.0672327659400330	0.3224569442330574	0.3879665319441255	T	T	T
0.0397305511883932	0.5725689884953289	0.3871221035871741	T	T	T

Path2

S1-1(same as above)

TS2-1

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0896705596564888	0.8849064316217551	0.2532058339376113	T	T	T
0.0867707495210608	0.3835348020092152	0.2551590205120476	T	T	T
0.5805234298177555	0.3869520642216953	0.2567588064727948	T	T	T
0.5877848971311671	0.8887140234230374	0.2557579200404925	T	T	T
0.2546800080000323	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000283	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000128	0.3899199960000033	0.1350599969999990	F	F	F
0.9210399453395808	0.0568873378829067	0.2108921578827067	T	T	T
0.9046306622222896	0.5370740114029280	0.2196046774818153	T	T	T
0.4242373027119884	0.5532286343795075	0.2166132487209743	T	T	T
0.4360251027324142	0.0675522126096206	0.2172323712010786	T	T	T
0.2561086371615166	0.7281576267048780	0.2901164661765915	T	T	T
0.2401258292231416	0.2112565181673010	0.2949274989652827	T	T	T
0.7841633998020791	0.1916685348240309	0.3109329540696881	T	T	T
0.7730507632758886	0.7515892617754254	0.2972506513461441	T	T	T
0.6380472601277964	0.2267241264449928	0.4095228502469550	T	T	T
0.7786816095902378	0.1698457663046700	0.4234654773512430	T	T	T

0.6658631191547209	0.4288478185680149	0.4263357948794171	T	T	T
0.4669251690805502	0.4169373200563365	0.4411115914211691	T	T	T
0.4862235542973884	0.6197108862635787	0.4535760713617619	T	T	T
0.2864371144493927	0.6079112932080107	0.4668686404335149	T	T	T
0.7331624844888395	0.0131089901433014	0.4314100177484940	T	T	T
0.9255970916007675	0.2790739651989912	0.4432679752397509	T	T	T
0.7413669751549252	0.5388414058423878	0.3841498264250347	T	T	T
0.7680526080465379	0.4940619273602679	0.4699181531818915	T	T	T
0.3919298851557009	0.3147834785079195	0.4840748386656629	T	T	T
0.3653238170264670	0.3448189813446777	0.3964708190000446	T	T	T
0.5566509563722940	0.7130341295977836	0.4080256994852871	T	T	T
0.5905636045801740	0.6938355225474334	0.4961052292011755	T	T	T
0.2063972070837185	0.5048581376555856	0.5090741798814569	T	T	T
0.1918931897518507	0.5536702636054234	0.4210977657961962	T	T	T
0.3054618499913684	0.7552707082313440	0.4793530859779920	T	T	T
0.4833503983472730	0.1080076328852950	0.4012386629213808	T	T	T
0.2908522005915022	0.8496038114064339	0.3575220864388933	T	T	T
0.8725230682918754	0.9443282605016852	0.3473620725061789	T	T	T

S2-2

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0859641146706534	0.8911075318673625	0.2562830636416593	T	T	T
0.0884470546961600	0.3879964830385240	0.2549830471872565	T	T	T
0.5861900386582873	0.3938444147016028	0.2555530659932401	T	T	T
0.5878002686064308	0.8916766812542271	0.2571691157414978	T	T	T
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F

0.9201373078609791	0.0594505903551995	0.2141565433726106	T	T	T
0.9204167520204519	0.5561196563245594	0.2141794759507583	T	T	T
0.4199754762918998	0.5575022340340278	0.2140810664942282	T	T	T
0.4221104349349728	0.0598601756388074	0.2156960596137439	T	T	T
0.2530920427150212	0.7260041818649107	0.2923428346236330	T	T	T
0.2500349260396826	0.2237754656947853	0.2935055715118703	T	T	T
0.7519601681472645	0.2290750095814119	0.2951649654820218	T	T	T
0.7548792759029990	0.7274763384777952	0.2925411050780328	T	T	T
0.6568906483293836	0.1976608197421285	0.3966942145065537	T	T	T
0.8035742156533033	0.1435960305562467	0.4276575481399719	T	T	T
0.6690306215032172	0.3849635058229217	0.4274835242748872	T	T	T
0.4707367690171335	0.3804203795495988	0.4370533948327761	T	T	T
0.4996839169669236	0.5850468131867528	0.4556368187468853	T	T	T
0.3066700017164783	0.5884174546430828	0.4676187097667632	T	T	T
0.7827180109589507	0.1284949411145710	0.4834693463915086	T	T	T
0.9596458804274771	0.2618138787340947	0.4188526044662076	T	T	T
0.7715309163619242	0.5189603520838347	0.3975599168798923	T	T	T
0.7411372300149716	0.4106964419676871	0.4778357383158672	T	T	T
0.3771591456938949	0.2665998423653417	0.4749423326789994	T	T	T
0.3810237187884188	0.3301121478433457	0.3884805489040800	T	T	T
0.5838591279618728	0.6891536211691386	0.4137755232877434	T	T	T
0.5969966347063396	0.6418437049678567	0.5007343069182919	T	T	T
0.2126605256305527	0.4789928395596014	0.5064021495492063	T	T	T
0.2190095470561441	0.5539816465802267	0.4203334613701015	T	T	T
0.3374879786554446	0.7373559793256897	0.4841119319395136	T	T	T
0.5027138877908646	0.0700551235219471	0.3969427395393471	T	T	T
0.2771247972122595	0.8398998288651893	0.3613529203730900	T	T	T
0.7841623430388633	0.0024737011959410	0.4073563339785790	T	T	T

S2-3

1.0000000000000000

7.7241001129000004 0.0000000000000000 0.0000000000000000

-3.8620861857000000 6.6897080140999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.7301998137999988

P Rh C H O

8 16 7 14 1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0937473521309230	0.8937962000330832	0.2557869715899507	T	T	T
0.0848058629570093	0.3890864205719280	0.2563551094091590	T	T	T

0.5875835164718107	0.3886595089840038	0.2568930952817922	T	T	T
0.5882033472560078	0.8936662525355795	0.2543347337421902	T	T	T
0.2546800080000153	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000111	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000040	0.3899199960000033	0.1350599969999990	F	F	F
0.9192961385647734	0.0619188673694367	0.2173412504557585	T	T	T
0.9204661633173917	0.5541318863964344	0.2163584458066752	T	T	T
0.4166699899082448	0.5533240542918009	0.2128030106730511	T	T	T
0.4312393714985193	0.0619131143584646	0.2165047226445695	T	T	T
0.2582754885368034	0.7227473912438954	0.2929334184453976	T	T	T
0.2559889322031385	0.2259483192353459	0.2946767044220724	T	T	T
0.7516787949968756	0.2495711434780273	0.3197319248203976	T	T	T
0.7376169272616807	0.7174435199308736	0.2921530433032914	T	T	T
0.6089629441938111	0.0577924682517696	0.4093776539774132	T	T	T
0.7535903176838075	-0.0006587901892423	0.4395003642532353	T	T	T
0.5319687375322363	0.1385050547986258	0.4656952927961516	T	T	T
0.3898408229555409	0.2167721174950430	0.4471095119792986	T	T	T
0.4573498464000231	0.4288407318650251	0.4715424037016892	T	T	T
0.3002294853379482	0.4893207299317733	0.4590635234902271	T	T	T
0.8724984581632381	0.4367316940232373	0.3875391534752837	T	T	T
0.6800644849032512	0.8892165210948402	0.4808262120396307	T	T	T
0.8857982323894298	0.1304042691754181	0.4610550687055864	T	T	T
0.6607206642654333	0.2550288702554572	0.4940804579045103	T	T	T
0.4535877294192893	0.0132024961459061	0.5018591724403026	T	T	T
0.2373297675535783	0.1145440590886655	0.4654813320816611	T	T	T
0.3770710175349088	0.2161655377964892	0.3902927446242520	T	T	T
0.5980606714819672	0.5342678760205620	0.4458099936108523	T	T	T
0.4932324196309655	0.4402173815717967	0.5261685589600543	T	T	T
0.1654806817880501	0.3991138884113210	0.4897867417153630	T	T	T
0.2538221674866369	0.4656910392897535	0.4052132560050541	T	T	T
0.3553664687302716	0.6477733747674546	0.4707167992356221	T	T	T
0.4795615384251556	0.9259758463148665	0.3859172966126632	T	T	T
0.5817111011303469	0.6308156211662367	0.3523175093687735	T	T	T
0.8064370410635309	0.9307469111227776	0.4017972394391231	T	T	T
0.9416413594721630	0.5511510692917645	0.4320396833607481	T	T	T

TS2-2

1.000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999957	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0933298008566745	0.8935853835377271	0.2564491638272377	T	T	T
0.0850518751768466	0.3887066411850074	0.2559316416076454	T	T	T
0.5861816362978416	0.3885507432901041	0.2552553799339409	T	T	T
0.5882735371723147	0.8944819048471209	0.2543908791945465	T	T	T
0.2546800080000166	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000120	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000046	0.3899199960000033	0.1350599969999990	F	F	F
0.9204232789196086	0.0579854429726477	0.2169866451961706	T	T	T
0.9211982703303619	0.5583831776293109	0.2158944801465103	T	T	T
0.4167922990516063	0.5540240890488418	0.2124733746241933	T	T	T
0.4262761547694346	0.0588442039027304	0.2154861968339439	T	T	T
0.2589152135154216	0.7218507596275043	0.2932189585285536	T	T	T
0.2574808132902091	0.2279524972169031	0.2947027247391435	T	T	T
0.7594131566583147	0.2456392647166435	0.3077687768391891	T	T	T
0.7340139495941571	0.7154428063044462	0.2934266688028105	T	T	T
0.6287530227516008	0.0838755211501618	0.4172793024627535	T	T	T
0.7609483678938261	0.0071824652579449	0.4441439305886957	T	T	T
0.5352467322974470	0.1478424238488104	0.4727460787041644	T	T	T
0.3931400274522702	0.2232360315067047	0.4505934050522579	T	T	T
0.4569843946117488	0.4358578171450119	0.4734588285723129	T	T	T
0.2974918091931278	0.4926691154365363	0.4600732644125657	T	T	T
0.8381443277559895	0.3829199638116415	0.3885150637066444	T	T	T
0.6796979992304681	0.8908881746077042	0.4829463032877395	T	T	T
0.8970909502195282	0.1273508741765072	0.4679523901491992	T	T	T
0.6537756772094986	0.2600713534013561	0.5055860874394027	T	T	T
0.4514153349824535	0.0129902976754611	0.5046232949452244	T	T	T
0.2400692349219696	0.1203187821594687	0.4684822087114480	T	T	T
0.3824938390355395	0.2184961602591750	0.3937416270204984	T	T	T

0.5974527693683913	0.5414250186004352	0.4475509382738276	T	T	T
0.4925486315799098	0.4497576424325653	0.5281332974427133	T	T	T
0.1634161548887415	0.4031660614596414	0.4911811182495576	T	T	T
0.2499985759397620	0.4663832011292945	0.4063837239949408	T	T	T
0.3509378407357857	0.6514095482843346	0.4709325352707440	T	T	T
0.5081298753344996	0.9732119479296178	0.3846965998340992	T	T	T
0.5717863949401257	0.6281299303598379	0.3520023402613686	T	T	T
0.8062837957156012	0.9397462255135854	0.4036106201341014	T	T	T
0.9088732783894332	0.5016463361084311	0.4323361791236487	T	T	T

S2-4

1.0000000000000000

7.7241001129000004 0.0000000000000000 0.0000000000000000

-3.8620861857000000 6.6897080140999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0936540728820132	0.8931054431705429	0.2577826085607263	T	T	T
0.0924843252783624	0.3923519723233703	0.2547824981310715	T	T	T
0.5869196189519325	0.3908255600068776	0.2550937805801660	T	T	T
0.5867608686638375	0.8891039692592223	0.2538871808657407	T	T	T
0.2546800080000224	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000182	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000040	0.3899199960000033	0.1350599969999990	F	F	F
0.9262459167850232	0.0522254596835901	0.2160475095959334	T	T	T
0.9250091630880921	0.5670786752006276	0.2161030455312531	T	T	T
0.4191078466009876	0.5550214882925628	0.2128870709625949	T	T	T
0.4176953598886725	0.0554203778521115	0.2147871006416572	T	T	T
0.2607273868674299	0.7228036625958758	0.2947416487207878	T	T	T
0.2593587575715951	0.2295368833429628	0.2956273673714253	T	T	T
0.7588970287284926	0.2269254552813338	0.2887836534359287	T	T	T
0.7324329803223618	0.7148424105162940	0.2964955666872727	T	T	T
0.6319623368180637	0.0964058980168369	0.4277270181671639	T	T	T

0.7607162373465350	0.0104129630600861	0.4531272234982110	T	T	T
0.5357247250344648	0.1545860592738914	0.4846886270389614	T	T	T
0.3958720633770985	0.2300428738282683	0.4593850984452582	T	T	T
0.4605626869177767	0.4451238673595538	0.4795367831659684	T	T	T
0.2993433218602036	0.4986238727134820	0.4647025153181939	T	T	T
0.7685194059597312	0.2841330992338624	0.3855175974375414	T	T	T
0.6732021872227041	0.8846796370247353	0.4876851255479280	T	T	T
0.8935755610897599	0.1252189939428788	0.4799867942030910	T	T	T
0.6562807086745917	0.2704544527731581	0.5159054921209053	T	T	T
0.4528350679621810	0.0215430648159272	0.5169921376144977	T	T	T
0.2418169200396759	0.1295205083481977	0.4770630813964979	T	T	T
0.3862184479459895	0.2206965690813860	0.4026995821746202	T	T	T
0.5998351357120593	0.5471626182316569	0.4523954840597690	T	T	T
0.4975889010817263	0.4647047852638569	0.5340513688282488	T	T	T
0.1638629231678568	0.4064942730250491	0.4950047966709269	T	T	T
0.2541518755587740	0.4723477672708486	0.4107672313907290	T	T	T
0.3493011144653070	0.6565562597767767	0.4757988983033374	T	T	T
0.5135500801141377	-0.0141152068765021	0.3943419842909197	T	T	T
0.5636977462655257	0.6262233894984400	0.3533244972656393	T	T	T
0.8105739786251515	0.9544091690882438	0.4102226280765298	T	T	T
0.8774788554900812	0.4476526169666888	0.4104441011390544	T	T	T

TS2-3

1.000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0877315007341134	0.8945803718526570	0.2567694933060192	T	T	T
0.0914976856399085	0.3936631440635041	0.2562275377377525	T	T	T
0.5762103458677108	0.3915597319274552	0.2526506745375805	T	T	T
0.5858688469893147	0.8887117651993336	0.2559742091197967	T	T	T
0.2546800080000374	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F

0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000332	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000081	0.3899199960000033	0.1350599969999990	F	F	F
0.9146032928169557	0.0593379234855705	0.2173672888481322	T	T	T
0.9232651965715095	0.5605196840556400	0.2142679512341228	T	T	T
0.4186737987209080	0.5599763456374998	0.2134240590089016	T	T	T
0.4256683997711223	0.0585914603363287	0.2160962396670843	T	T	T
0.2550921079265718	0.7252923716131512	0.2939407685364607	T	T	T
0.2540826510410762	0.2273748118859749	0.2937072515475666	T	T	T
0.7637497166128793	0.2474688370308245	0.3006587792124369	T	T	T
0.7491889950623407	0.7174356555836668	0.2932132108584781	T	T	T
0.6347390390023055	0.1070801253767129	0.4346158375068984	T	T	T
0.7523624795958196	0.0067956295669985	0.4583452799596597	T	T	T
0.5269653399786174	0.1502857998837946	0.4920389265645861	T	T	T
0.3877119718468815	0.2285943237756591	0.4687525115026686	T	T	T
0.4640251302849902	0.4500271196893194	0.4830645781477556	T	T	T
0.3103435960618766	0.5094060337088375	0.4628842531299054	T	T	T
0.7915252628170991	0.3043519355364928	0.4005112046171742	T	T	T
0.6562763426829611	0.8744088849658287	0.4890791463012223	T	T	T
0.8826099268770677	0.1113090006861746	0.4887497311841431	T	T	T
0.6399345628911070	0.2568150288376128	0.5277311570570070	T	T	T
0.4394933278307428	0.0076383840045432	0.5193143229630872	T	T	T
0.2404189112535521	0.1404755270821946	0.4932959428112564	T	T	T
0.3573250359153562	0.2015369226880808	0.4134173345516778	T	T	T
0.6068231661957935	0.5434565428482135	0.4563722263889115	T	T	T
0.4969666806356480	0.4775595698850861	0.5377940365815509	T	T	T
0.1677152577474343	0.4174629635954848	0.4893924369791302	T	T	T
0.2787008596594878	0.4880577628475732	0.4079147242094860	T	T	T
0.3587424532715119	0.6665381503523267	0.4745305018369335	T	T	T
0.5212780049225970	0.0095491391664824	0.3972702622953952	T	T	T
0.7362867630030580	0.4296111441021322	0.3320092833850996	T	T	T
0.8059794226033671	0.9591402492149346	0.4141457604911603	T	T	T
0.9063063852165637	0.4517179348222587	0.4322680942489212	T	T	T

S2-5

1.000000000000000

7.7241001129000004 0.0000000000000000 0.0000000000000000

-3.8620861857000000 6.6897080140999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.7301998137999998

P Rh C H O

8 16 7 14 1

Selective dynamics

Direct

0.4213500019999969 0.5565900209999981 0.0951000009999987 F F F

0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0906309176411705	0.8921381533128966	0.2571288726073581	T	T	T
0.0914506737101776	0.3910318601055228	0.2550125817743547	T	T	T
0.5892697977336903	0.3909801137496464	0.2567001751431902	T	T	T
0.5895068811385783	0.8910650482244541	0.2551834776605265	T	T	T
0.2546800080000224	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000182	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000040	0.3899199960000033	0.1350599969999990	F	F	F
0.9255654321174580	0.0602693770760253	0.2146911444483061	T	T	T
0.9228367097504274	0.5566807013294949	0.2153101730938820	T	T	T
0.4213034986827104	0.5560791614497316	0.2136291087802730	T	T	T
0.4226847515286083	0.0579748632422725	0.2142775597335510	T	T	T
0.2596168409118376	0.7251187632142897	0.2940238031431645	T	T	T
0.2596818815905893	0.2276323894407960	0.2948181104491080	T	T	T
0.7466855159724435	0.2184281170900273	0.2972594787628837	T	T	T
0.7539698156527368	0.7254869431052842	0.2926776568791907	T	T	T
0.6099206671886660	0.0917532384196564	0.4446205233015499	T	T	T
0.7422457677397062	0.0058650552211713	0.4648711645744167	T	T	T
0.5068914634257000	0.1350046599046298	0.5040226483084335	T	T	T
0.3690777284980156	0.2147700576165728	0.4799154766580551	T	T	T
0.4487193714205301	0.4365396865387595	0.4944273485415215	T	T	T
0.3121368245350696	0.5079328063535496	0.4657372648700381	T	T	T
0.7277275354639889	0.2834032621838207	0.4034359256269536	T	T	T
0.6608106833916139	0.8739564208633305	0.4973533698251181	T	T	T
0.8767593380856226	0.1174370034231054	0.4918240010352676	T	T	T
0.6212743517369037	0.2432164384973287	0.5391974051426709	T	T	T
0.4210709511810203	0.9947477671417477	0.5326797298511410	T	T	T
0.2195339467678284	0.1274119638425278	0.5027830338545216	T	T	T
0.3435675558947893	0.1893624783828095	0.4244006457960672	T	T	T
0.6006083829893795	0.5269583115709331	0.4731348399494426	T	T	T
0.4657204421344848	0.4604508272815934	0.5497760565140141	T	T	T
0.1579692491601874	0.4157609568280369	0.4842668466873520	T	T	T
0.3042589403944809	0.4955533335673870	0.4099531794039221	T	T	T
0.3628354558146278	0.6646960581630105	0.4787944069449139	T	T	T
0.4872245979605724	0.9821139626310906	0.4121144967972373	T	T	T
0.6652584703172377	0.3848145924938345	0.4010363636518764	T	T	T
0.7928012323978485	0.9608584007123194	0.4192360792902554	T	T	T

0.9161840204417585	0.3597231131637430	0.3912719721719738	T	T	T
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Path3

S1-1(same as above)

TS2-1(same as above)

S2-2(same as above)

TS3-2

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0865032315414468	0.8894625412598879	0.2561514585037887	T	T	T
0.0867420427355406	0.3845701164428068	0.2550307072736798	T	T	T
0.5845366251221362	0.3876663089527031	0.2549917929716160	T	T	T
0.5887033395906301	0.8906366230306295	0.2571861644815772	T	T	T
0.2546800080000168	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000128	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000050	0.3899199960000033	0.1350599969999990	F	F	F
0.9158738378101250	0.0536591534863185	0.2145107661596041	T	T	T
0.9207968167388494	0.5546994133868266	0.2142338939743330	T	T	T
0.4212529640624525	0.5564536724787479	0.2144834190147449	T	T	T
0.4234367718878083	0.0584049119083626	0.2150443898343907	T	T	T
0.2556489754851066	0.7254273737872095	0.2923744976678535	T	T	T
0.2487136212609973	0.2203977330343513	0.2929286432859402	T	T	T
0.7553627998274925	0.2232665745000274	0.2958441263861207	T	T	T
0.7568521458392300	0.7149947764987753	0.2953438215108923	T	T	T
0.6683326341106705	0.1910759516135318	0.4034634413224025	T	T	T

0.8177137079734040	0.1375999982659691	0.4323292564299133	T	T	T
0.6796632973478836	0.3750499942787957	0.4200032536752266	T	T	T
0.4908328501832476	0.3781853814410960	0.4334058601107114	T	T	T
0.5188957229936649	0.5802079418137844	0.4540963059938523	T	T	T
0.3227945233936794	0.5774800757671812	0.4654885596652257	T	T	T
0.7898261318928468	0.1057296707352867	0.4872034499480635	T	T	T
0.9724124174395934	0.2604598707009244	0.4262141013766457	T	T	T
0.7466653445661287	0.5494736215462580	0.3552160933976993	T	T	T
0.8169289846495368	0.4894785223470760	0.4447088716817731	T	T	T
0.3999237697113751	0.2627336103778546	0.4713570949940088	T	T	T
0.3942451604760711	0.3250605903664565	0.3858077414402635	T	T	T
0.6044526373076264	0.6886253908020075	0.4134063576524085	T	T	T
0.6134350110153726	0.6330726783612182	0.4999158900087627	T	T	T
0.2282126313190743	0.4628769979474914	0.5029172351643825	T	T	T
0.2385344226780327	0.5444433539316639	0.4174644188216697	T	T	T
0.3479648940415945	0.7232561224588736	0.4834084359959026	T	T	T
0.5151612800885752	0.0639340691304092	0.3991644025356029	T	T	T
0.2686092110523962	0.8365885899035493	0.3612264236092825	T	T	T
0.8051466464713912	1.0039026760680259	0.4078271762877004	T	T	T

S3-3

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0865246318374203	0.8913689933187706	0.2547627010652525	T	T	T
0.0843961976947633	0.3854444944460237	0.2556404619456777	T	T	T
0.5871111391772580	0.3867536059120936	0.2566962316319554	T	T	T
0.5877534297583981	0.8943376683438248	0.2578850414918525	T	T	T
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F

0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9158656365141199	0.0568943481523325	0.2138920692018950	T	T	T
0.9208407179607346	0.5502696968089107	0.2139568488165972	T	T	T
0.4189877615600539	0.5567766499634265	0.2147474134818063	T	T	T
0.4257233841670843	0.0607697813166646	0.2143858226214663	T	T	T
0.2560836039170185	0.7327072864639604	0.2922808183987967	T	T	T
0.2485167496370226	0.2200687442721867	0.2926236381215182	T	T	T
0.7575618377941196	0.2253755792428573	0.3004292493683912	T	T	T
0.7588571946134125	0.7184656756222735	0.2898249051265364	T	T	T
0.6935130858373081	0.0957276389750898	0.4048082700709468	T	T	T
0.8623600780967482	0.0666338265828440	0.4282759050968434	T	T	T
0.6937632754113803	0.2764754477830816	0.4103731586633173	T	T	T
0.5091430543520797	0.2877502084479493	0.4273814054130954	T	T	T
0.5539676515837064	0.4937098214793660	0.4507296027784242	T	T	T
0.3676212349931803	0.5096811630100744	0.4621685048622457	T	T	T
0.8432585696666433	0.0298860496862101	0.4829748336311538	T	T	T
0.0089665947169020	0.2017296383111911	0.4208893463226934	T	T	T
0.8738749717094698	0.6919093532928462	0.3513238320543750	T	T	T
0.8362639647227388	0.4112514903851093	0.4224225739626360	T	T	T
0.4215566837654290	0.1751147749066337	0.4664340438686988	T	T	T
0.4038008106399021	0.2423193234064649	0.3828504722391750	T	T	T
0.6480358081229272	0.6045929271758885	0.4118513628677718	T	T	T
0.6460828797607732	0.5353523186806501	0.4971320819450903	T	T	T
0.2663249327706519	0.3990136449084471	0.4994432697979530	T	T	T
0.2848112502630519	0.4830427694123277	0.4139780900616415	T	T	T
0.4054678014712432	0.6593928553659743	0.4803853145482326	T	T	T
0.5466644207540485	0.9591543372934247	0.4036673496851351	T	T	T
0.2867641546819034	0.8699794157075388	0.3560456243588656	T	T	T
0.8628906595382685	0.9420271453905406	0.4011651684393508	T	T	T

TS3-3

1.000000000000000		
7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H
8	16	6	14

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0909870887121192	0.8933864905031969	0.2544394983757768	T	T	T

0.0865688877746129	0.3887290664234955	0.2583072339921660	T	T	T
0.5866332485585708	0.3876958322887338	0.2565987354307146	T	T	T
0.5844906619700958	0.8864166849841622	0.2534801953307163	T	T	T
0.2546800080000288	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000245	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000144	0.3899199960000033	0.1350599969999990	F	F	F
0.9157804292420897	0.0618959282837731	0.2159600113510909	T	T	T
0.9186927323579916	0.5447292590201299	0.2163526421376938	T	T	T
0.4205204896983368	0.5561612346194238	0.2145674514744188	T	T	T
0.4255490411353555	0.0589937227315789	0.2135096519587702	T	T	T
0.2574039622638020	0.7279070000354586	0.2927358859068162	T	T	T
0.2539892218781926	0.2214711490426412	0.2925885304766500	T	T	T
0.7363372104960306	0.2113728591520392	0.3070812638941740	T	T	T
0.7643546610977314	0.7218684327692489	0.2915173611155080	T	T	T
0.7320712766234722	0.1514256251138693	0.4208161472319163	T	T	T
0.9098871613445927	0.1252105941470387	0.4331269806267012	T	T	T
0.7321253868570635	0.3319415356916106	0.4153484227084847	T	T	T
0.5472926012388155	0.3439368340005823	0.4320767283895672	T	T	T
0.5881700124980502	0.5526868190742185	0.4505179962006142	T	T	T
0.3981820021031887	0.5634953727549056	0.4598000328997551	T	T	T
0.9234358667791899	0.1046487346175219	0.4879986502156069	T	T	T
0.0490315635259105	0.2543913587652527	0.4150503964717696	T	T	T
0.8975469449795458	0.6973440738212809	0.3476324858664882	T	T	T
0.8756619678398821	0.4718505803938070	0.4148965135926722	T	T	T
0.4638904142242835	0.2383463302202761	0.4734623134961202	T	T	T
0.4405586729190659	0.2895593161939801	0.3880397199661472	T	T	T
0.6779091329657574	0.6561347829880736	0.4089309863346952	T	T	T
0.6835649615758109	0.6065888628694437	0.4961009887925916	T	T	T
0.2941208884643743	0.4490766520142699	0.4955460773277516	T	T	T
0.3203849291641140	0.5383645988686546	0.4105810633518299	T	T	T
0.4308346560107629	0.7108266784399968	0.4787870543729336	T	T	T
0.5899744780303995	0.0235236470096475	0.4376140217796448	T	T	T
0.5674858485218779	0.0070533793025900	0.3408935566173140	T	T	T
0.8921449229677405	0.9913953402805055	0.4067655047671639	T	T	T

S3-4

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-3.8620861857000000	6.6897080140999998	0.0000000000000000

0.0000000000000000				0.0000000000000000				19.7301998137999988			
P	Rh	C	H								
8	16	6	14								
Selective dynamics											
Direct											
0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F						
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F						
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F						
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F						
0.0901543493806691	0.8940351196781188	0.2542642987006008	T	T	T						
0.0888315182323121	0.3917730219960210	0.2566265526900422	T	T	T						
0.5844350388485035	0.3889924021459811	0.2551163895893204	T	T	T						
0.5852473738917033	0.8903981561746849	0.2560884561633808	T	T	T						
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F						
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F						
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F						
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F						
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F						
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F						
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F						
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F						
0.9160529958773392	0.0589334290704013	0.2147918843800452	T	T	T						
0.9218707883154335	0.5532779128267691	0.2147411719440444	T	T	T						
0.4233084482244310	0.5619208318805069	0.2152739016365336	T	T	T						
0.4227793987016636	0.0576913954902147	0.2143478759974018	T	T	T						
0.2535799538978281	0.7279259527882512	0.2939320577564620	T	T	T						
0.2493525553838543	0.2226152272217065	0.2915769129830882	T	T	T						
0.7485068372875709	0.2252652084754727	0.2977268408049111	T	T	T						
0.7647984440029586	0.7229039963181310	0.2930372220967803	T	T	T						
0.6863545689568881	0.0905226814092504	0.4371731476171928	T	T	T						
0.8826844972751355	0.0861940238991217	0.4372754706579975	T	T	T						
0.6941082009757503	0.2692749700534663	0.4014093613199237	T	T	T						
0.5191041316823514	0.2988516906716729	0.4204532413903145	T	T	T						
0.5728304370009883	0.5105713025994136	0.4399438119522924	T	T	T						
0.3898378050213772	0.5303838392641661	0.4536384345791160	T	T	T						
0.9048536443855639	0.0282947172111846	0.4854692128366462	T	T	T						
0.0098477807130687	0.2378195714227843	0.4297406497503991	T	T	T						
0.9176123374649712	0.7345758666118994	0.3497467905026433	T	T	T						
0.8372269184521512	0.4067826653725065	0.4125079873553297	T	T	T						
0.4326173249590030	0.1961347335217788	0.4622517831578633	T	T	T						
0.4061552597431818	0.2498209990744130	0.3782325641034980	T	T	T						
0.6601955900341644	0.6137698750963111	0.3975309588320620	T	T	T						
0.6764192536141358	0.5621044062257821	0.4834846265587788	T	T	T						
0.2899018400158657	0.4192353723299133	0.4909865670725135	T	T	T						

0.3040883770396465	0.5045755321516844	0.4060958153996467	T	T	T
0.4304738817365485	0.6799503242774853	0.4724656013540824	T	T	T
0.6427995268000176	0.0956621813068621	0.4904338125163886	T	T	T
0.5623681056850341	0.9506769270996704	0.4160444391105723	T	T	T
0.8887552057258516	0.9929829473386684	0.3961138238625180	T	T	T

S3-5

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0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0952011015899206	0.8953708940945017	0.2542877961286095	T	T	T
0.0944487873930469	0.3937854707418719	0.2555371290575498	T	T	T
0.5920684846657176	0.3900318828747594	0.2605227499979041	T	T	T
0.5853776031255175	0.8926152394528069	0.2551007097524303	T	T	T
0.2546800080000082	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000040	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9155043244361107	0.0691227876357885	0.2164478848489866	T	T	T
0.9199300347379087	0.5438766933668568	0.2159916516668780	T	T	T
0.4220652291785946	0.5554430560143346	0.2135201681108454	T	T	T
0.4349957610564859	0.0661417640860019	0.2167177446043294	T	T	T
0.2591858250646759	0.7265440072441502	0.2918402250943652	T	T	T
0.2541362252446066	0.2243332669309097	0.2929593239572306	T	T	T
0.7517243473577724	0.2368897847540465	0.3208000229003333	T	T	T
0.7622611770064412	0.7287067472569877	0.2864043246751582	T	T	T
0.5876870612223367	0.9158000248914889	0.4375946730997185	T	T	T
0.7858665195350106	0.9244376641042804	0.4522496421825228	T	T	T
0.6130986533622544	0.1207687588339823	0.4229384035205550	T	T	T
0.4311849929037496	0.1454792026385980	0.4332888661242046	T	T	T
0.4826805163680566	0.3565181213346988	0.4543022771195956	T	T	T

0.2969679334217401	0.3715083611740043	0.4689209735971411	T	T	T
0.9089934009743086	0.4265149581312648	0.3835090616697833	T	T	T
0.7638032211120326	0.7783879969094301	0.4682673157484832	T	T	T
0.8675841165519635	0.0336224988658948	0.4928282791736172	T	T	T
0.7957376428923209	0.6739316757256214	0.3588804599172412	T	T	T
0.7229890041552526	0.2192619855318408	0.4609798236105500	T	T	T
0.3356915363478825	0.0393090213608369	0.4733411135425880	T	T	T
0.3356953269440099	0.1004281927967006	0.3870743490656954	T	T	T
0.5709638762290274	0.4633997173631663	0.4139246457590853	T	T	T
0.5797664229602737	0.4011368658189107	0.4996032136029742	T	T	T
0.2074357294753980	0.2683156350395158	0.5099363489131639	T	T	T
0.2005138664180517	0.3300135523808340	0.4235006519626939	T	T	T
0.3341968837204760	0.5236843689542539	0.4835455928624942	T	T	T
0.4912308108013944	0.8580821194714241	0.4832214483079947	T	T	T
0.5062946737444839	0.8069533706013168	0.3967529374900364	T	T	T
0.8829637713270440	0.9721301091126707	0.4071517281692071	T	T	T
0.0040463282330760	0.5464818959418092	0.4244172345592823	T	T	T

TS3-4

1.0000000000000000

7.7241001129000004 0.0000000000000000 0.0000000000000000

-3.8620861857000000 6.6897080140999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 19.7301998137999988

P Rh C H O

8 16 7 14 1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0930900605669540	0.8944439198751130	0.2552314779596984	T	T	T
0.0882051382223004	0.3906532938190951	0.2563330217918738	T	T	T
0.5892135786278445	0.3895393121186499	0.2584510000076610	T	T	T
0.5847220957281468	0.8938952310775642	0.2556055337919430	T	T	T
0.2546800080000172	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000129	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000015	0.3899199960000033	0.1350599969999990	F	F	F
0.9170847242071816	0.0635536747677797	0.2155745957471443	T	T	T

0.9207733501600585	0.5494473224636601	0.2156096209614045	T	T	T
0.4197318659567286	0.5563193365097536	0.2134833448712234	T	T	T
0.4294698574843396	0.0625312088039603	0.2159352190299316	T	T	T
0.2573046268672849	0.7244528748137586	0.2928869948132896	T	T	T
0.2538538998983255	0.2257828114915001	0.2929195739737537	T	T	T
0.7606554389807859	0.2373085683864145	0.3110652454411932	T	T	T
0.7572760528836926	0.7257884798543621	0.2878636257980113	T	T	T
0.5964547106789231	0.9263726203608895	0.4402642050250116	T	T	T
0.7922253751314559	0.9300475777871526	0.4546160514889999	T	T	T
0.6236291909032633	0.1333961975189623	0.4318882902316930	T	T	T
0.4399295844416761	0.1553715349438594	0.4359270160612476	T	T	T
0.4863082800499131	0.3645766259923597	0.4569442689339495	T	T	T
0.2990092011250499	0.3760007625386189	0.4720233704209049	T	T	T
0.8758875718161898	0.3897221712765512	0.3871310650809786	T	T	T
0.7661835985318287	0.7848404885716380	0.4733113170763892	T	T	T
0.8787335015848966	0.0441894791716449	0.4932741411216844	T	T	T
0.7981657639563151	0.6703457732158060	0.3594664063999556	T	T	T
0.7235974228868203	0.2229400699508250	0.4733511098707858	T	T	T
0.3389700312378575	0.0461635234781212	0.4742629371821387	T	T	T
0.3525086881904730	0.1101800082471526	0.3879249855492101	T	T	T
0.5728638327121031	0.4718078118416628	0.4164056898453535	T	T	T
0.5841623270169845	0.4103660948878602	0.5020640316066189	T	T	T
0.2110733528079840	0.2718053398096492	0.5129916997380459	T	T	T
0.2021210143534314	0.3353239537854633	0.4268195510575992	T	T	T
0.3352056223532659	0.5273758216649398	0.4873336201061962	T	T	T
0.4968760969968831	0.8624980924255119	0.4849638512649913	T	T	T
0.5156114222189191	0.8252449329820085	0.3975994669995315	T	T	T
0.8852499326800056	0.9677337876863558	0.4086804595939951	T	T	T
0.9797418344916577	0.5192374843263847	0.4247867096528569	T	T	T

S3-6

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0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0908913148871950	0.8930907490666754	0.2561496798602212	T	T	T

0.0926144812928483	0.3921244400611696	0.2553336021268901	T	T	T
0.5876592526641952	0.3914394088112423	0.2571981627509187	T	T	T
0.5832751254933358	0.8887425672979521	0.2547577792865937	T	T	T
0.2546800080000082	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099980000040	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9214609228090928	0.0575801091989423	0.2148427179639100	T	T	T
0.9244120771154171	0.5557556937905473	0.2154433143136665	T	T	T
0.4223370121648194	0.5593115055612260	0.2143279241226168	T	T	T
0.4210949348240156	0.0588475266213564	0.2143441461485641	T	T	T
0.2584752142516226	0.7279737219872925	0.2947485508406048	T	T	T
0.2564602213912300	0.2254748221900598	0.2933183499246150	T	T	T
0.7528936489360638	0.2192456275872376	0.2948725408438751	T	T	T
0.7599338394895316	0.7220066907830793	0.2919129122900019	T	T	T
0.6034700368874367	0.9395151499636104	0.4453908443825179	T	T	T
0.7930293454409848	0.9268284194285387	0.4527581506918182	T	T	T
0.6444428754821829	0.1541713120153846	0.4463541779147631	T	T	T
0.4524337430685220	0.1657334833185697	0.4446109640168047	T	T	T
0.4870394371927674	0.3756504499209239	0.4562962049488642	T	T	T
0.2922681833489710	0.3795105946715511	0.4596740664223737	T	T	T
0.7955321866914877	0.2932435520677442	0.3921557650446063	T	T	T
0.7606391523655380	0.7712798458794052	0.4542055477889170	T	T	T
0.8741324516036364	0.0017710099105940	0.4995059589214529	T	T	T
0.8443719345623319	0.6637448415744629	0.3552242387025695	T	T	T
0.7233576763167323	0.2241352792767361	0.4942199300517083	T	T	T
0.3508068301677513	0.0624235279815876	0.4836955410665104	T	T	T
0.3763848332011431	0.1067068520221245	0.3953307611370379	T	T	T
0.5813482055946784	0.4738743684434629	0.4148756373830855	T	T	T
0.5735199686852901	0.4365873712546202	0.5035753326581517	T	T	T
0.1945376004482847	0.2802933961388218	0.5000599926578254	T	T	T
0.2082317411118702	0.3267168295636138	0.4114754634768931	T	T	T
0.3165807461923882	0.5306378847914743	0.4686708014442672	T	T	T
0.4985548849123794	0.8606510269046850	0.4873242292403081	T	T	T
0.5240340913632260	0.8652066730598142	0.3981838451141965	T	T	T
0.8946958431120260	0.0005937984935109	0.4096972083396600	T	T	T
0.9425896475982900	0.4504434052313643	0.4080306978602679	T	T	T

TS3-5

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0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999951	0.0565899979999997	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0856258303257237	0.8905153507007144	0.2568917147649457	T	T	T
0.0875426226908264	0.3897552390511415	0.2563795597016294	T	T	T
0.5700727826035956	0.3852781190173206	0.2517636154155973	T	T	T
0.5844902455424569	0.8868138250973380	0.2575194180663904	T	T	T
0.2546800080000770	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999996	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000809	0.8899199960000027	0.1350599969999990	F	F	F
0.0880099980000320	0.3899199960000033	0.1350599969999990	F	F	F
0.9097291405481117	0.0529886696221228	0.2187736999826820	T	T	T
0.9252037376808476	0.5594292284944518	0.2137229881645361	T	T	T
0.4182053047604398	0.5605590757570484	0.2141285667049070	T	T	T
0.4229860155222204	0.0541017256613619	0.2156634701318205	T	T	T
0.2540420064007002	0.7238711706452918	0.2954791608052330	T	T	T
0.2512919512089735	0.2238732632921962	0.2931299639578706	T	T	T
0.7545796394011977	0.2479403303446591	0.3010893672678296	T	T	T
0.7474680593416201	0.7025399827929920	0.2954742982704810	T	T	T
0.6135342599675808	0.9693199548525314	0.4466903092482813	T	T	T
0.7996829247698709	0.9491478333317078	0.4497404877218037	T	T	T
0.6606111959979097	0.1864810740655987	0.4507347681777377	T	T	T
0.4692264703828452	0.1993790013202622	0.4490289976791647	T	T	T
0.4995354266769225	0.4051471279179615	0.4654588406793773	T	T	T
0.3014588860064943	0.3997801469172138	0.4744940898484874	T	T	T
0.8239998253830682	0.3242101186188691	0.3996080866806370	T	T	T
0.7614612770622671	0.7932081475293746	0.4570253581471733	T	T	T
0.8971935521523217	0.0381796690192699	0.4919019652283828	T	T	T
0.7522308976143344	0.4586689032657602	0.3315994398505826	T	T	T
0.7353069405332963	0.2491057183607169	0.4997221268043203	T	T	T
0.3660238124040719	0.0896201677512545	0.4863987056727100	T	T	T
0.3940811885837807	0.1484249591852517	0.3991285636252380	T	T	T

0.5840612246828845	0.5083408184081389	0.4235475646597699	T	T	T
0.5924190287268021	0.4638417697479527	0.5115088653386313	T	T	T
0.2158588071483029	0.3028423206157416	0.5173401227714742	T	T	T
0.2092582000162944	0.3394468594648432	0.4285345723891877	T	T	T
0.3202047448575329	0.5486906661247543	0.4833549490886670	T	T	T
0.5127115444048371	0.8902106531289118	0.4894464490604815	T	T	T
0.5270232518889828	0.8995068347668272	0.4000326388177771	T	T	T
0.8880422238534711	1.0044568519059638	0.4026616759068473	T	T	T
0.9816564424390463	0.4651664792752666	0.4181663322653217	T	T	T

S3-7

1.0000000000000000

7.7241001129000004	0.0000000000000000	0.0000000000000000
-3.8620861857000000	6.6897080140999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	19.7301998137999988

P	Rh	C	H	O
8	16	7	14	1

Selective dynamics

Direct

0.4213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.4213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.0565899979999998	0.0951000009999987	F	F	F
0.9213500019999969	0.5565900209999981	0.0951000009999987	F	F	F
0.0891116877692408	0.8901845232915404	0.2568703989535735	T	T	T
0.0933807062439473	0.3917279914158360	0.2538937246085279	T	T	T
0.5894207373853558	0.3912714459767238	0.2566241970450401	T	T	T
0.5896327847037695	0.8894158979431666	0.2560950154355634	T	T	T
0.2546800080000011	0.7232699990000029	0.0551499990000011	F	F	F
0.2546800080000011	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.2232699990000029	0.0551499990000011	F	F	F
0.7546799779999986	0.7232699990000029	0.0551499990000011	F	F	F
0.5880100130000017	0.3899199960000033	0.1350599969999990	F	F	F
0.5880100130000017	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.8899199960000033	0.1350599969999990	F	F	F
0.0880099979999969	0.3899199960000033	0.1350599969999990	F	F	F
0.9228877246727968	0.0596563400246895	0.2154028573980285	T	T	T
0.9218182606608673	0.5543878077150821	0.2155906969545551	T	T	T
0.4230711671925261	0.5570801478832513	0.2139223758584466	T	T	T
0.4252912995095535	0.0584159330717130	0.2139119237820986	T	T	T
0.2596091001706423	0.7267431218062749	0.2934419231681066	T	T	T
0.2609542868339689	0.2240343403695192	0.2937939855298511	T	T	T
0.7403382460439044	0.2167071116923077	0.2990462237360322	T	T	T
0.7544143105449641	0.7227619578177276	0.2938927728769013	T	T	T
0.6076370737669402	0.9632062200373042	0.4523063259745674	T	T	T

0.7895747370159149	0.9346430129617820	0.4577245288125802	T	T	T
0.6518494490735038	0.1798383139748107	0.4558763114901757	T	T	T
0.4609570513953876	0.1937488384719590	0.4575801411608131	T	T	T
0.4996806815171316	0.4046221316265814	0.4712983522366499	T	T	T
0.3095489904902022	0.4106058170047035	0.4860084025539283	T	T	T
0.7991450299271838	0.3224405844684020	0.4045409055582672	T	T	T
0.7472173804681441	0.7859861589899969	0.4777224161940666	T	T	T
0.9046673872885839	0.0471619705410062	0.4913662255675516	T	T	T
0.8147142940035794	0.4733120979961032	0.4028103250628683	T	T	T
0.7302720233169981	0.2425551509883239	0.5048246945309658	T	T	T
0.3609972119673134	0.0907468479479261	0.4970083451267062	T	T	T
0.3812204848826264	0.1384479113654536	0.4085560705514282	T	T	T
0.5743613096930847	0.5007076242083319	0.4269138154420122	T	T	T
0.6058021608506181	0.4690603246282368	0.5140611526808211	T	T	T
0.2272607679383469	0.3115800700273803	0.5287853083626769	T	T	T
0.2106524749192169	0.3607414612617475	0.4415168980867852	T	T	T
0.3426490197778820	0.5628439934795635	0.4987612974952284	T	T	T
0.5023373526784141	0.8833013916968838	0.4939691228082661	T	T	T
0.5248024632303631	0.8945317397635151	0.4048641454915808	T	T	T
0.8619509898449997	0.9521094816517541	0.4079430911273554	T	T	T
-0.0495872487441390	0.3086776758500459	0.3836246010316726	T	T	T