

Electronic supplementary information

Essential role of CO coverage in CO₂ hydrogenation over Pt(111)

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Corrections to the transition state energies of CH_x-CO coupling

Abild-Pedersen et al. proposed a correction scheme of CO adsorption energies on metal surfaces based on the CO stretch vibrational frequency using RPBE calculations.¹ The energy correction is expressed as $E_{\text{corr}}=1.8 - 0.0008 \times \nu_{\text{CO}}$, where ν_{CO} is the vibrational frequency. Our calculations were performed using PBE-D3 and we take the frequency-dependant part of this equation. The adsorption energy of CO on Pt(111) at a 1/4 monolayer (ML) coverage was calculated to be -1.75 eV, which is stronger than the experimental value of -1.37 eV. The average vibrational frequency of CO was calculated to 1762.3 cm⁻¹. Then the original correction equation is slightly changed to be $E_{\text{corr}}=1.79 - 0.0008 \times \nu_{\text{CO}}$. For the CO adsorption at an minimum state in other cases (e.g. CO adsorption at a 6/16 ML), the vibrational frequency is essentially the same (around 1800 cm⁻¹) with those in a 1/4 ML coverage, we therefore take 0.38 eV as the energy correction. For those transition states of CH_x-CO coupling, the configuration of CO resembles a top configuration in a minimum state (the C-C bond distance is greater than 1.85 Å, much longer than that of 1.53 Å for typical C-C bond length) and vibrational frequency is significantly larger than that of CO adsorption in a 1/4 monolayer coverage. We therefore calculate the energy correction using $E_{\text{corr}}=1.79 - 0.0008 \times \nu_{\text{CO}}$. The vibrational frequency and the energy corrections are listed in Table S1. For the CO hydrogenation step, the bond distance of C-H in the TS (TS3 in Fig. 5b) is around 1.3 Å and it can be regarded that there is no separable CO molecule. Hence, we did not apply correction to the energy of TS3. Even if TS3 is stabilized by 0.38 eV as we used for CO adsorption, the energy of it is still 0.1 eV lower than that of TS4 and the reaction kinetics is essentially unchanged.

Table S1

Transition states	CO vibrational frequency(cm^{-1})	E_{corr}
CH-0CO	1924.434	0.25
CH-2CO	1927.227	0.25
CH-4CO	1933.693	0.24
CH-6CO	1944.115	0.23
CH-8CO	1942.326	0.24
CH ₂ -0CO	1932.498	0.24
CH ₂ -2CO	1941.240	0.24
CH ₂ -4CO	1944.060	0.23
CH ₂ -6CO	1967.499	0.22
CH ₂ -8CO	1976.035	0.21
CH ₃ -0CO	1918.305	0.26
CH ₃ -2CO	1876.692	0.29
CH ₃ -4CO	1881.605	0.28
CH ₃ -6CO	1893.628	0.27
CH ₃ -8CO	1905.286	0.27

Discussions on the error due to the inaccurate description of CO site preference

An important concern of our study is the $\text{CH}_x\text{-CO}$ coupling and the energy of CO in the transition state is corrected using the frequency-dependent correction scheme since the CO in the TS resembles that of a top site. Then CO is destabilized by a lesser extent (around 0.15 eV) than that of CO adsorption at a minimum state (see details in Table S1). After that, the energy difference between the TS and the optimized initial state (CO resides at hollow sites and bridge sites) should be well-described. Here, we also assume that the calculated energy of the initial state is correct since the experimental value is used to calibrate the CO adsorption energy at 1/4 ML coverage. In realistic cases, the reactive CO is expected to reside at either the top site or the bridge site. If CO resides at the top site in real case while it is located at hollow site in calculation, then its realistic energy should be 0.08 eV lower than the calculated value. Therefore, the barrier of $\text{CH}_x\text{-CO}$ coupling is underestimated by 0.08 eV. In the same vein, we can obtain that this error of activation energy is 0.04 eV for a top (real case)-bridge (calculated) or bridge (real case)-hollow (calculated) scenario. This is schematically shown in Fig. S1. By inspection of the values in Fig. 3a, we can obtain the trend that the barriers of $\text{CH}_x\text{-CO}$ ($x=1-3$) coupling decrease with the increase of CO coverage is unchanged if these errors are accounted for.

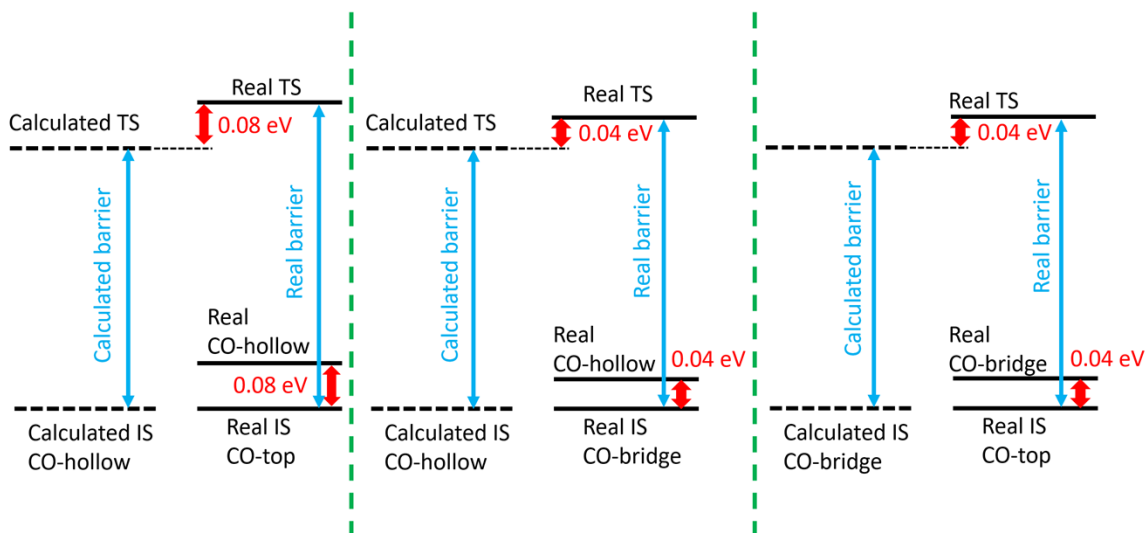


Fig. S1 Schematics of the error introduced by inaccurate description of CO site preference. IS=initial state, TS=transition state.

Discussions on the choice of reference state for CH-CO coupling

The most concerned case of CH-CO coupling is that for 8CO-CH. This is because Pt(111)-7CO-3H was determined to be the most stable structure from thermodynamic calculation and then used to examine the CO₂ hydrogenation mechanism under reaction conditions. Then one CO is generated first (Fig. 5a), which can desorb or undergoes further hydrogenation steps to form CH (Fig. 5b). The 7CO-CH species can be hydrogenated successively to form CH₄ (Fig. 5c) or accepts another CO from gas phase to undergo CH-CO coupling (Fig. 5d). Therefore, the CO-CH coupling in Fig. 5d is exactly the same with that of 8CO-CH in Fig. 3a. This process corresponds to $7\text{CO-CH}^*-\text{CO}^* \rightarrow \text{TS} \rightarrow 7\text{CO-CHCO}^*$. In this case, the initial/transition/final states are all in the same unit cell; the reactive CH* and CO* experience the lateral interactions from the same number of CO molecules in the transition state and the initial state, which is a reasonable way to account for the effect of lateral interactions on CH-CO coupling. This also help to directly compare the energetics of CH-CO coupling with CH* hydrogenation, that is $7\text{CO-CH}^*-\text{H}^* \rightarrow \text{TS} \rightarrow 7\text{CO-CH}_2^*$. If CH* and CO* are placed in different unit cells, then the coupling process would be $7\text{CO-CH}^*+7\text{CO-CO}^* \rightarrow \text{TS}+7\text{CO} \rightarrow 7\text{CO-CHCO}^*+7\text{CO}$. As such, CO* needs to desorb and then enters another unit cell containing CH* to allow the CH-CO coupling to occur. Also, in this way, CH* and CO* can experience the lateral interactions from different number of CO molecules in the transition state and the initial state. Still, we obtained the same trend that the barrier of CH-CO coupling decreases with the increase of CO coverage, which is provided in Fig. S2. We note that the way of placing CH* and CO* in different unit cells as initial state for the 2, 4, 6 and 8 CO cases allow us to draw a direct comparison of them with the 0CO case (CH* and CO* in different unit cells). But it does not directly reflect the barrier of the coupling step. By contrast, a merit of placing CH* and CO* in the same unit cell is that it is directly associated with the CH-CO coupling step for the 2, 4, 6 and 8 CO cases. Since the major concern of this study is the 8CO-CH case that reflects realistic reaction condition, our analysis is therefore mainly based on the results which place CH* and CO* in different unit cells. In summary, the different of choices of the initial state will not affect our conclusion that the barrier of CH-CO coupling will decrease with the increase of CO coverage.

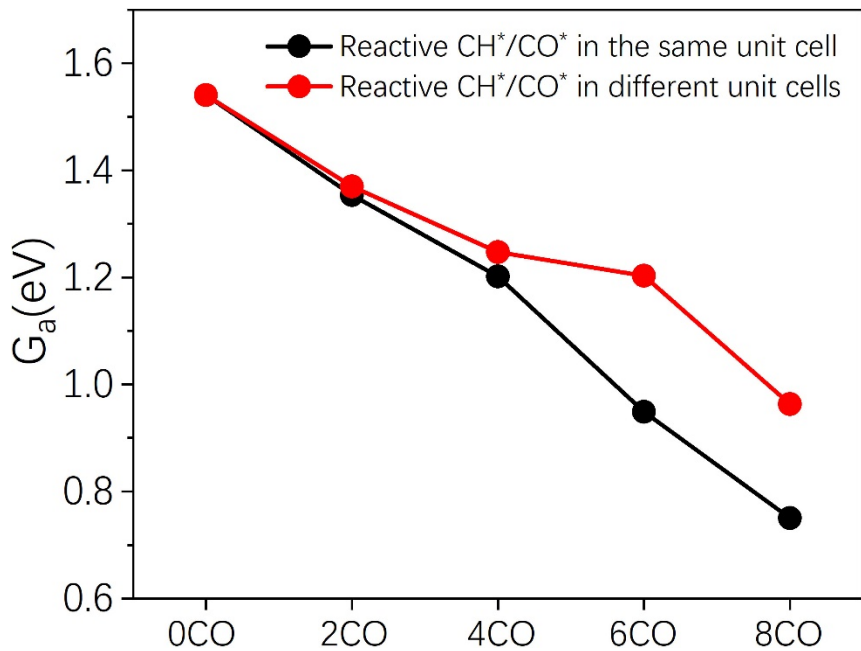


Fig. S2. Comparison of the free energy barriers for CH-CO coupling using different choice of initial states. The CH* are either placed in the same unit cell or different unit cells for the cases of 2, 4, 6 and 8 CO molecules.

Details of the microkinetic model

The forward (k_f) and backward (k_b) rate constants of each elementary reaction step are computed based on harmonic transition state theory. The rate constant of an adsorption step was calculated using an adsorption area per site of $4.58 \times 10^{-19} \text{ m}^2$. The desorption rate constant was obtained from the equilibrium constant, adsorption rate constant, and the relationship $K_{eq} = k_f/k_b$.

The Gibbs Free energies of each intermediate and transition state were calculated as $G = E_{DFT} + E_{ZPE} - k_B T \ln q_{vib}$ (1).

Here, E_{DFT} and $E_{ZPE} = \frac{1}{2} \sum_i h\nu_i$ are the DFT energy and zero-point energy (ZPE),

respectively. q_{vib} is the vibrational partition function. To reduce the error of small vibrational frequencies, we shifted all frequencies below 100 cm^{-1} to 100 cm^{-1} . It is found that when the frequencies below 50 cm^{-1} is shifted to 50 cm^{-1} , the effective barrier of **TS1** (the rate-determining step of CO formation) is changed from 1.23 eV using the 100 cm^{-1} threshold of frequency shift, to 1.22 eV, while that of **TS4** (the rate-determining step of CO consumption) is changed from 1.29 eV to 1.31 eV. Therefore, the reaction energy profile is marginally changed when using different thresholds to shift the low frequencies.

The Gibbs free energies of the gas molecules were calculated using

$$G_{\text{gas}} = E_{\text{DFT}} + E_{\text{ZPE}} + \Delta\mu(T, P^0) + k_B T \ln(P/P^0) \quad (2),$$

where $\Delta\mu$ was calculated from the rotational, translational, and vibrational partition functions of the gas molecules, while P and P^0 stands for the pressure/fugacity of the fluid molecule and 1 bar, respectively. The free energies of the gas molecules were used to calculate the free energy of adsorption. The calculated rate constants of all elementary steps are provided in Table S4.

Using the obtained rate constants of each elementary step, we developed a chemical Master equation of probability densities for the system to occupy each discrete state and solved for the steady-state solution. Here, the probability densities are also referred to as surface coverage θ . We solved the Master equation using Matlab. The reaction rate (turnover frequency) of each pathway was calculated using the obtained surface coverages. The apparent activation energy (E_{app}) was calculated using the expression (2). The temperature ranges for the calculation of E_{app} are specified in the main text.

$$E_{app} = RT^2 \left(\frac{\partial \ln r}{\partial T} \right)_{P, y_i} \quad (3)$$

where the total pressure (P) and the mole fraction of species i in the reaction mixtures (y_i) were

kept constant (i.e., the fluid species fugacities are kept constant).

To identify rate controlling steps in the microkinetic models, we also perform a Campbell's degree of rate control (DRC) ²⁻³ analysis.

$$\text{DRC}_i = \left(\frac{\partial \ln r}{\partial \ln k_i} \right)_{k_j, k_j \neq k_i} \quad (4).$$

Effect of the computational errors for gas phase reaction thermodynamics on the equilibrium partial pressures of CO and CH₃OH

There are still some errors for the calculations of gas phase reaction thermodynamics when the method by Calle-Vallejo et al. was applied (Ref. 41, ACS Catal. 2020, 10, 6900-6907). We mentioned in the Computational method section that the free energy change (ΔG , all gas phase species in 1 bar) of the reaction $\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ at 298K was calculated to be 0.26 eV, while the experimental value is 0.30 eV. Also, the reaction $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$ was calculated to be -0.14 eV, while the experimental value is 0.04 eV. The fact that these two reactions are calculated to be more exothermic than the experimental values makes the predicted equilibrium pressures higher than the expected values. If the DFT energy of CO and CH₃OH are destabilized by 0.04 and 0.18 eV to meet the experimental data, respectively, then the equilibrium pressures of CO and CH₃OH are 1.33 and 0.05 bar ($T=473\text{K}$, $P(\text{CO}_2)=10$ bar, $P(\text{H}_2)=30$ bar). If we neglect the contributions by CH₄ and C₂H₅OH, then the conversion of carbonaceous species is 12%. For the reaction $\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$ and $2\text{CO}_2 + 6\text{H}_2 \rightarrow \text{C}_2\text{H}_5\text{OH} + 3\text{H}_2\text{O}$, the experimental ΔG at 298K are -1.17 and -0.67 eV, respectively, and the computed values are -1.30 and -0.97 eV. Therefore, the equilibrium conversion of CH₄ and C₂H₅OH are much higher than that of CO and CH₃OH. Also, the choice of partial pressures of CH₄ and C₂H₅OH will essentially not affect the reaction rate. Therefore, we keep them to be constant value of 1 bar during microkinetic modelling. We note that if we adjust the energy of CO and CH₃OH to meet the experimental data (CO is destabilized by 0.04, $P(\text{CO})=1.33$ bar; CH₃OH is destabilized by 0.18 eV, $P(\text{CH}_3\text{OH})=0.05$ bar), then the overall reaction rate is 0.10/s, which is close to the original reaction rate of 0.13/s. Therefore, the ensuing analysis of the reaction kinetics are still based on the unadjusted energies of CO and CH₃OH.

Discussions on the formation rate of HCOOH, HCHO and CH₃CHO

We have added the pathway to the formation of HCOOH in Fig. 5a, whose transition state energy (**TS18**) is 1.27 eV and is significantly higher than that of **TS2** (0.72 eV) for CO formation. Also, the formation of gas phase HCOOH is endergonic by 1.02 eV (P(HCOOH)=1 bar, shown in dashed line in Fig. 5a). The formation rate of HCOOH equals to the consumption rate of it when the partial pressure of it is above 10⁻¹⁴ bar. When the partial pressure of HCOOH is above 10⁻¹⁴ bar, all the formed HCOOH will be converted to CO. Therefore, the formation rate of HCOOH is 0 when reaching equilibrium.

Similarly, the formation of gas phase HCHO is endergonic by 0.87 eV (P(HCHO)=1 bar, shown in Fig. 5b). The formation rate of HCHO equals to the consumption rate of it when the partial pressure of it is above 10⁻¹¹ bar. When the partial pressure of HCHO is above 10⁻¹¹ bar, all the formed HCHO will be converted to CH₃OH and other products. Therefore, the formation rate of HCHO is 0 when reaching equilibrium.

Regarding CH₃CHO, the equilibrium partial pressure of it is calculated to be 0.009 bar. When the partial pressure of it above 0.009 bar. The bare surface (Pt(111)-7CO-3H) through the desorption of CH₃CHO is above **TS16**. Therefore, all the formed CH₃CHO will be further hydrogenated. The formation rate of gas phase CH₃CHO is 0 when reaching equilibrium

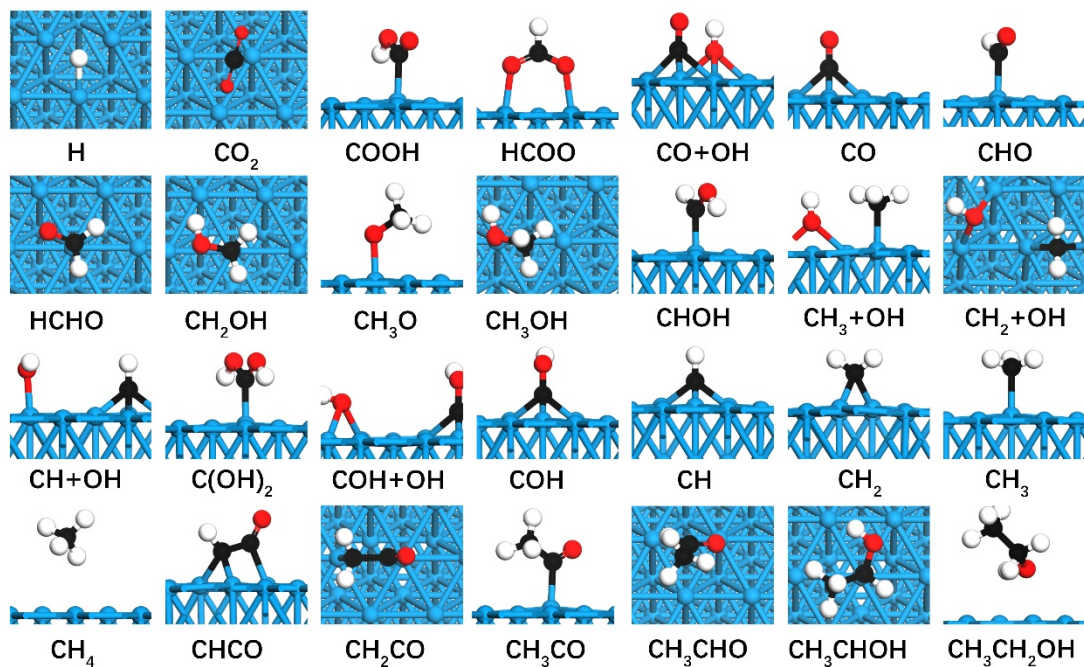


Fig. S3. Configurations of the intermediate states for CO₂ hydrogenation on Pt(111)

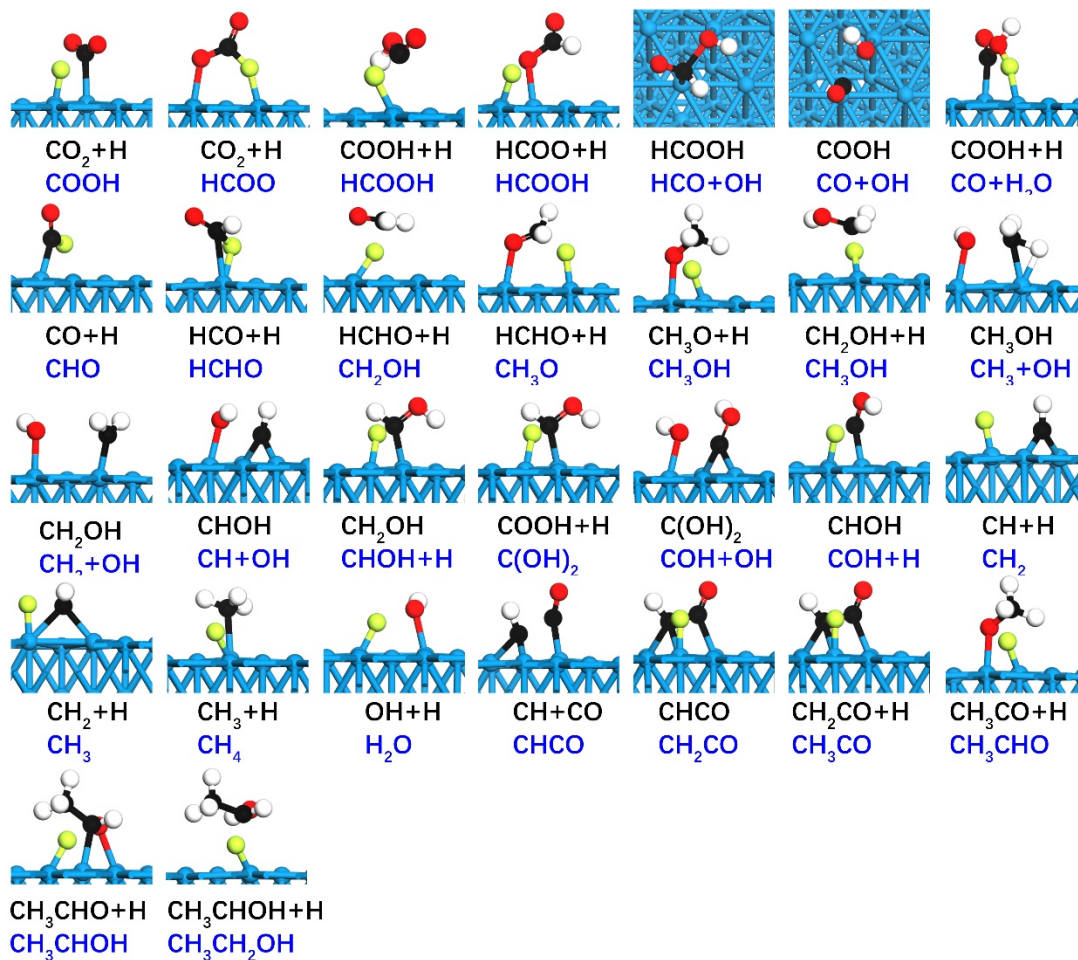


Fig. S4. Configurations of the transition states for CO₂ hydrogenation on Pt(111). The corresponding initial and final states are labelled in black and blue.

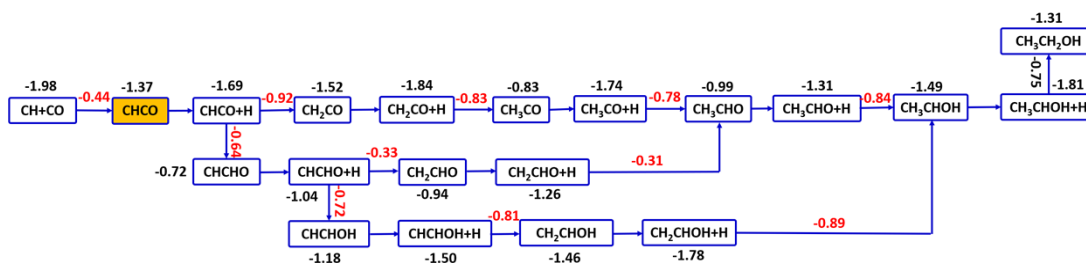


Fig. S5. Additional reaction pathways of CHCO hydrogenation to form ethanol

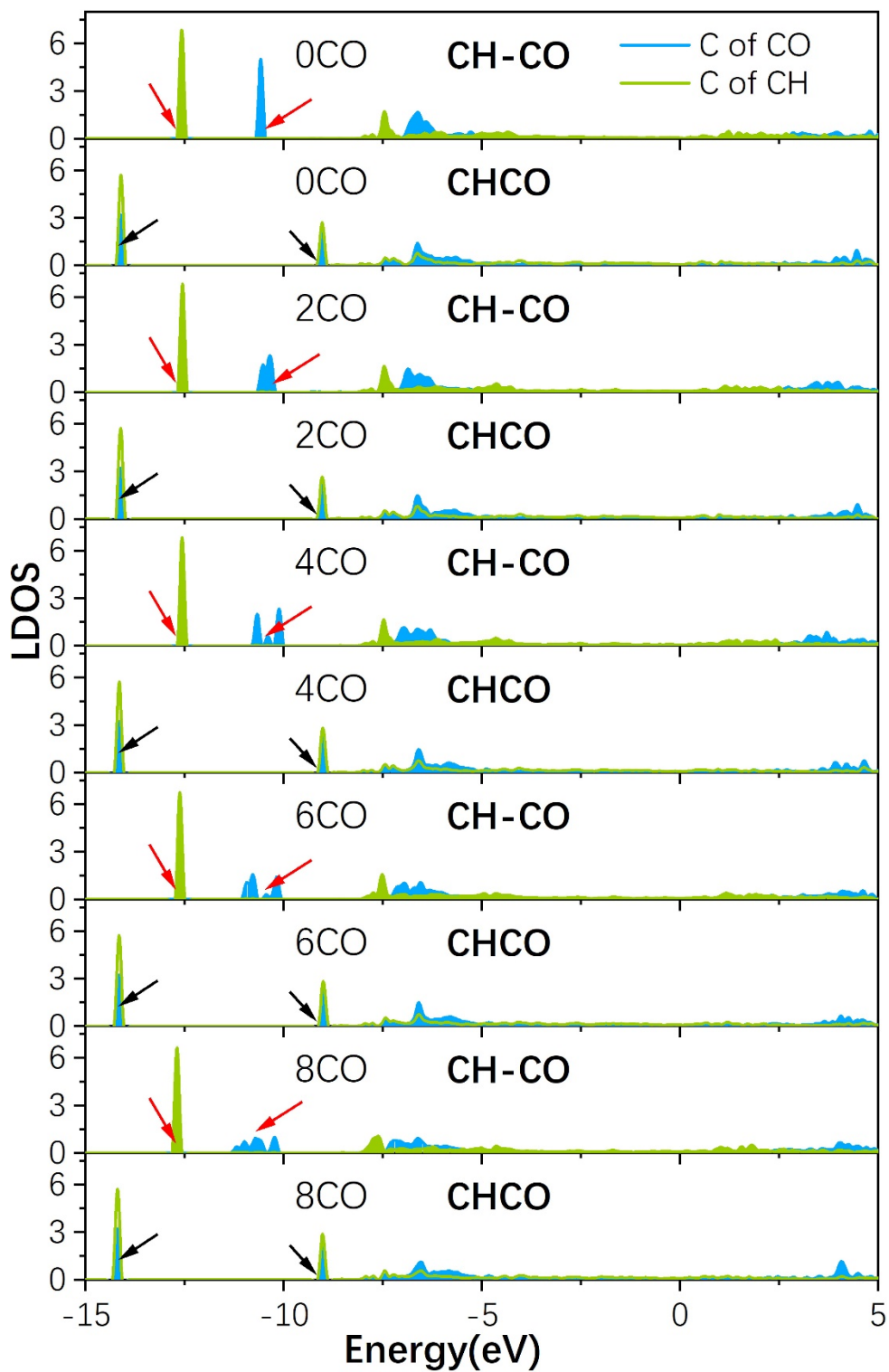


Fig. S6. Density of state for the carbon atoms involved in the C-C coupling before and after coupling.

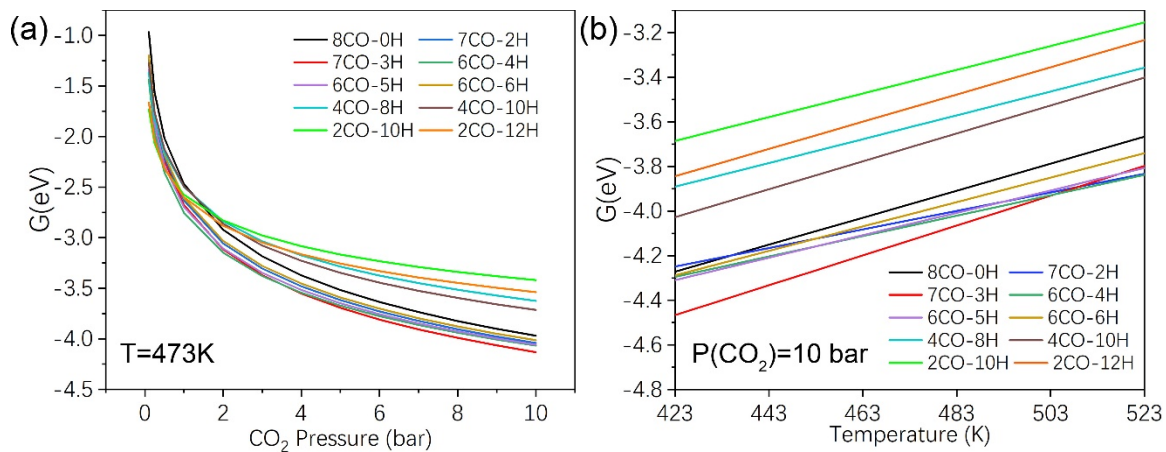


Fig. S7. Adsorption free energies of coadsorbed CO^* and H^* on Pt(111) at different (a) pressures and (b) temperatures. The H_2/CO ratio is 3. The adsorption free energy of CO^* is calculated with the free energy change the reaction $\text{CO}_2(\text{g})+\text{H}_2(\text{g})\rightarrow\text{CO}^*+\text{H}_2\text{O}(\text{g})$.

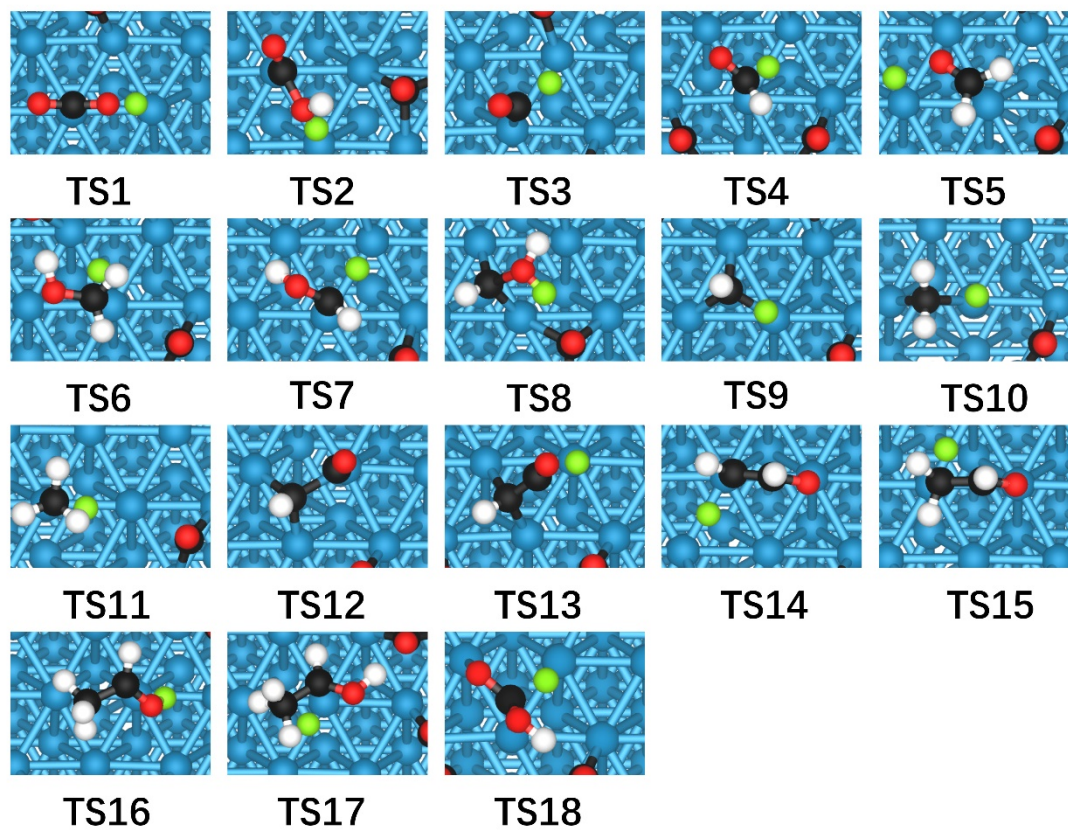


Fig. S8. Configurations of transition states on Pt(111)-7CO-3H.

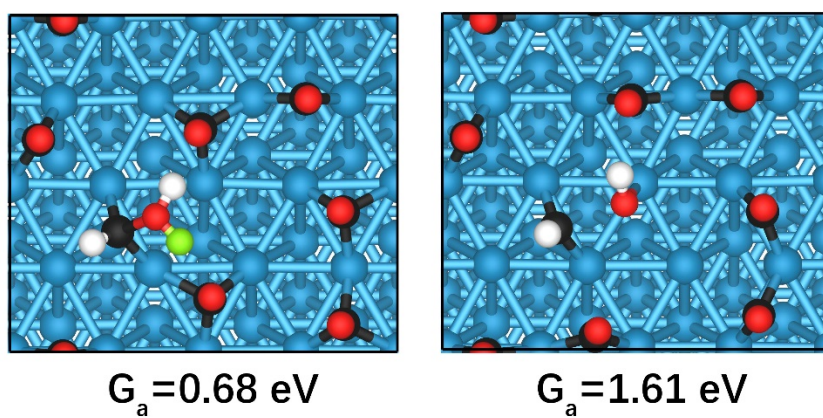


Fig. S9. Transition state configurations of CH-OH bond cleavage on Pt(111)-7CO

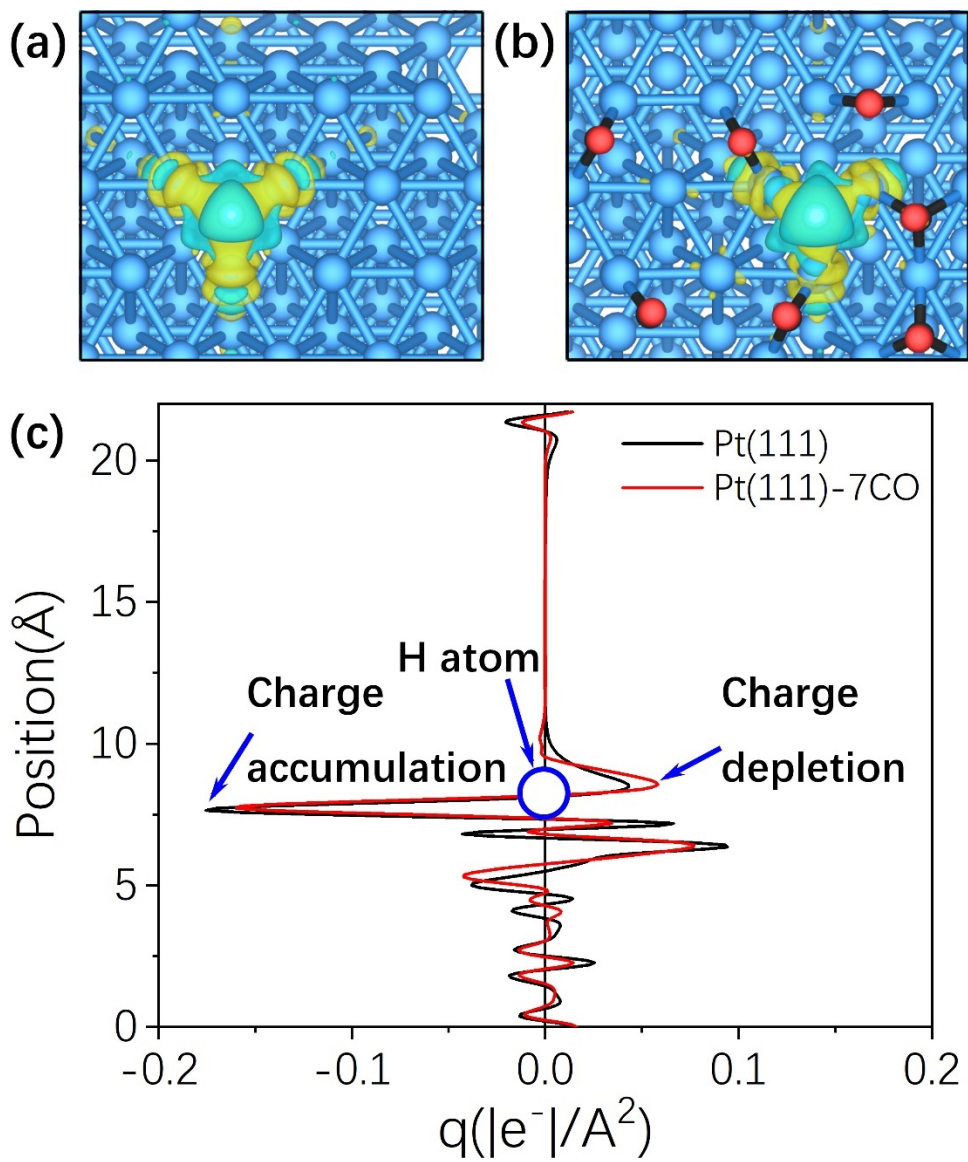


Fig. S10. Differential charge density of H adsorption on (a) Pt(111) and (b) Pt(111)-7CO. The isosurface is set to be $0.001 |e^-|/\text{\AA}^3$. Yellow denote charge accumulation and blue denotes charge depletion. (c) Plane-average charge differential charge density of H adsorption. The position of H-atom is marked.

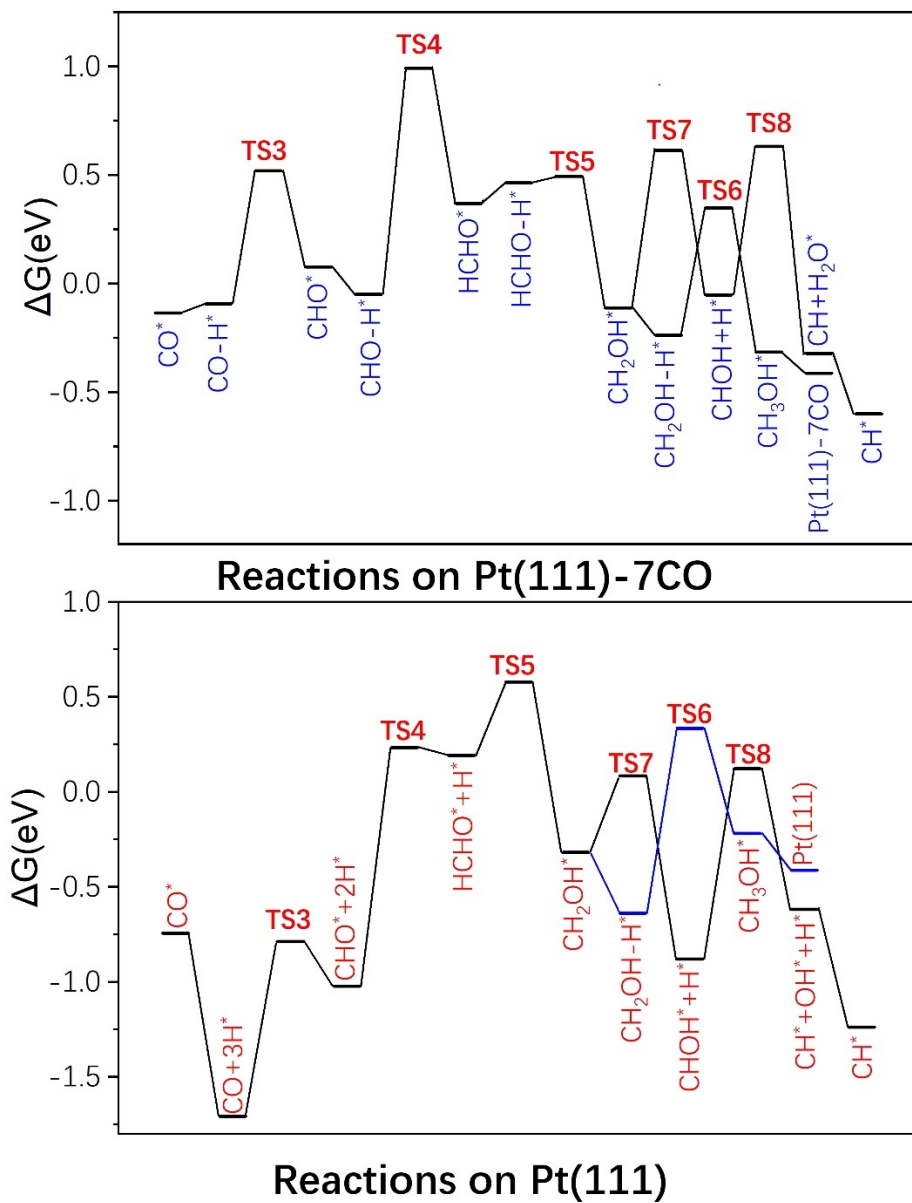


Fig. S11. Comparison of the free energy profiles for CO hydrogenation on Pt(111)-7CO and Pt(111). $T=473\text{K}$, the partial pressures of CO_2 and H_2 are set to be 10 bar and 30 bar, respectively, and those of all other molecules are set to be 1 bar. The same labeling of transition state is used for Pt(111) with that of Pt(111)-7CO. We added the energy of three H^* to correctly describe the effective barrier of CO hydrogenation. Including more H atoms to the system will not change the effective barrier.

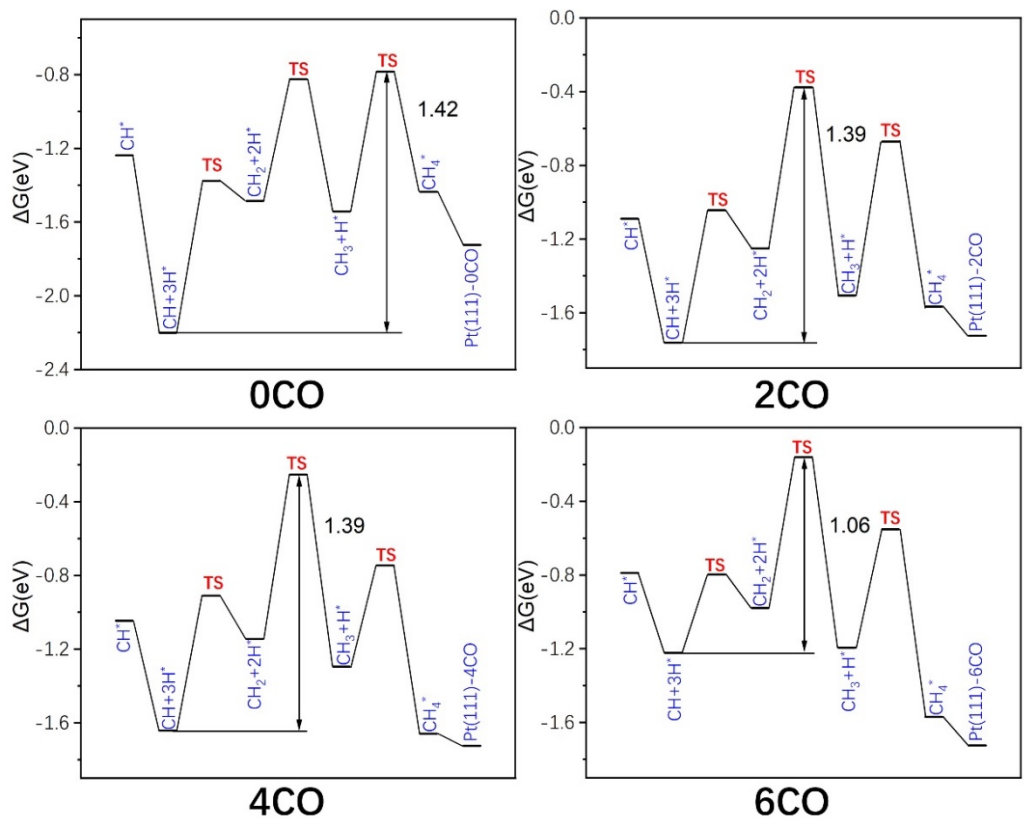


Fig. S12. Free energy profile of CH^* hydrogenation on Pt-nCO ($n=0, 2, 4, 6$). The partial pressure of H_2 is 30 bar.

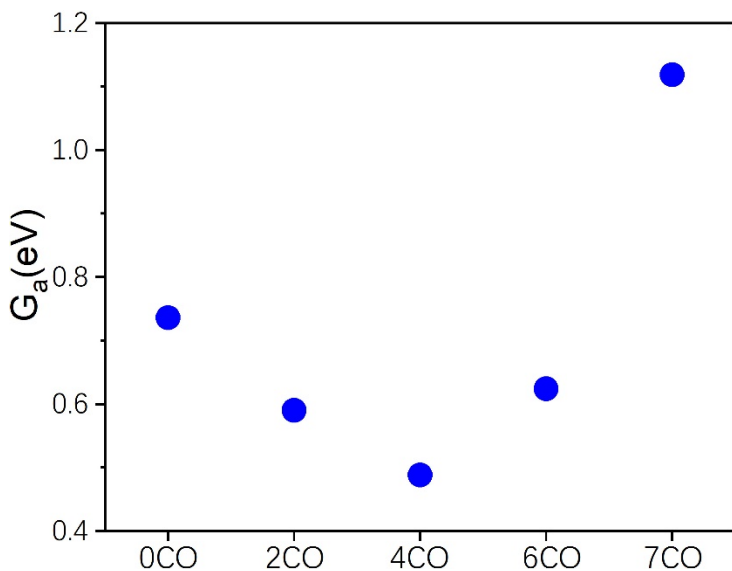


Fig. S13. Change of the free energy barrier (G_a) of CO_2 hydrogenation on Pt(111) at various CO coverage. Note that the initial state in each system is $\text{H}^* + \text{CO}_2^*$, therefore the barrier on Pt(111)-7CO is 1.12 eV, which differs with the value of 1.23 eV using Pt(111)-7CO-3H as the reference state.

Table S2 Intermediate and transition state energies of CO₂ hydrogenation on Pt(111). All the energies are referenced to gas phase CO₂ and H₂.

Intermediate state		Transition state		
Species	Energy(eV)	Initial state	Final state	Energy (eV)
H	-0.54	H-CO ₂	COOH	-0.36
CO ₂	-0.49	H-CO ₂	HCOO	0.09
COOH	-1.06	H-COOH	HCOOH	-0.48
CO-OH	-0.58	H-HCOO	HCOOH	0.02
CO	-1.15	COOH	CO-OH	-0.43
HCOO	-0.62	H-COOH	CO-H ₂ O	-0.85
H ₂ O	-0.46	CO-H	COH	-0.66
COH	-1.56	CO-H	CHO	-0.79
C(OH) ₂	-1.75	CHO-H	HCHO	-0.39
CHO	-1.09	HCHO-H	CH ₂ OH	-0.82
HCHO	-0.46	HCHO-H	CH ₃ O	-1.35
CH ₂ OH	-1.83	CH ₂ OH-H	CH ₃ OH	-1.35
CH ₃ O	-0.95	CH ₃ O-H	CH ₃ OH	-1.26
CH ₃ OH	-2.04	CH ₃ OH	CH ₃ -OH	-0.26
COH-OH	-0.83	CH ₂ OH	CH ₂ -OH	-0.36
CHOH	-1.44	CH ₂ OH	CHOH-H	-1.27
CH ₃ -OH	-1.56	CHOH	CH-OH	-0.36
CH ₂ -OH	-1.02	COOH-H	C(OH) ₂	-1.40
CH-OH	-1.44	C(OH) ₂	COH-OH	-2.46
CH	-1.90	COH-H	CHOH	0.19
CH ₂	-1.83	CH-H	CH ₂	-1.63
CH ₃	-2.50	CH ₂ -H	CH ₃	-1.74
CH ₄	-2.90	CH ₃ -H	CH ₄	-2.25
CHCO	-2.50	CH-CO	CHCO	-1.74
CH ₂ CO	-2.99	CHCO-H	CH ₂ CO	-2.29
CH ₃ CO	-3.53	CH ₂ CO-H	CH ₃ CO	-2.56
CH ₃ CHO	-3.05	CH ₃ CO-H	CH ₃ CHO	-2.78
CH ₃ CHOH	-4.05	CH ₃ CHO-H	CH ₃ CHOH	-3.29
CH ₃ CH ₂ OH	-4.20	CH ₃ CHOH-H	CH ₃ CH ₂ OH	-3.47

Table S3 Intermediate and transition state energies of CO₂ hydrogenation on Pt(111)-7CO-3H. All the energies are referenced to gas phase CO₂ and H₂.

Intermediate state		Transition state		
Species	Energy(eV)	Initial state	Final state	Energy (eV)
7CO-H	-0.38	H-CO ₂	COOH	0.14
7CO-3H	-1.02	H-COOH	CO-H ₂ O	-0.49
CO ₂ -H	-0.84	CO-H	CHO	-0.13
COOH	-0.59	CHO-H	HCHO	0.04
COOH+H	-0.87	HCHO-H	CH ₂ OH	-0.64
CO-H ₂ O	-1.53	CH ₂ OH	CHOH-H	-0.75
CO	-1.01	CH ₂ OH-H	CH ₃ OH	-1.42
CO-H	-1.43	CHOH-H	CH-H ₂ O	-0.88
CHO	-0.70	CH-H	CH ₂	-0.85
HCHO	-0.70	CH ₂ -H	CH ₃	-1.39
HCHO-H	-0.78	CH ₃ -H	CH ₄	-2.19
CH ₂ OH	-1.69	CH-CO	CHCO	-1.06
CHOH-H	-1.49	CHCO-H	CHCHO	-1.43
CH-H ₂ O	-1.72	CHCHO-H	CH ₂ CHO	-1.73
CH ₂ OH+H	-2.06	CH ₂ CHO-H	CH ₃ CHO	-2.40
CH ₃ OH	-2.20	CH ₃ CHO-H	CH ₃ CHOH	-2.87
CH	-1.26	CH ₃ CHOH-H	CH ₃ CH ₂ OH	-4.00
CH-H	-1.60			
CH ₂	-1.47			
CH ₂ -H	-1.80			
CH ₃	-2.37			
CH ₃ -H	-2.65			
CH ₄	-2.89			
CH-CO	-2.03			
CHCO	-1.88			
CHCO-H	-2.09			
CHCHO	-2.00			
CHCHO-H	-2.14			
CH ₂ CHO	-2.81			
CH ₂ CHO-H	-2.85			
CH ₃ CHO	-3.34			
CH ₃ CHO-H	-3.53			
CH ₃ CHOH	-4.00			
CH ₃ CHOH-H	-4.21			

Table S4. Forward (k_f) and backward (k_b) reaction rate constant, free energy of activation (ΔG^\ddagger) and reaction free energy (ΔG_{rxn}) of each elementary step the CO_2 hydrogenation on Pt(111)-7CO-3H. T=473K; P(CO_2)=10 bar, P(H_2)=30 bar; P(CO)=4.43 bar; P(CH_3OH)=4.88 bar, the partial pressures of all other molecules are set to be 1 bar.

Reaction label	Elementary Steps	$k_f(\text{s}^{-1})$	$k_b(\text{s}^{-1})$	$\Delta G^\ddagger(\text{eV})$	$\Delta G_{\text{rxn}}(\text{eV})$
R1	Pt(111)-7CO +0.5H ₂ (g)→H	1.177E+11	1.072E+09		-0.191
R2	H+CO ₂ (g)→H-CO ₂	8.364E+09	1.580E+13		0.307
R3	H-CO ₂ →COOH	2.264E+04	5.986E+07	0.811	0.321
R4	COOH+0.5H ₂ (g)→COOH-H	1.177E+11	2.880E+10		-0.057
R5	COOH-H→CO-H ₂ O	2.193E+09	5.293E+05	0.343	-0.340
R6	CO-H ₂ O→CO+H ₂ O(g)	3.034E+10	1.308E+09		-0.128
R7	CO→CO(g)+ Pt(111)-7CO	6.481E+08	4.928E+09		0.083
R8	CO+0.5H ₂ (g)→CO-H	1.177E+11	3.280E+11		0.042
R9	CO-H→CHO	9.441E+06	1.916E+08	0.565	0.123
R10	CHO+0.5H ₂ (g)→CHO-H	1.177E+11	5.294E+09		-0.126
R11	CHO-H→HCHO	4.639E+01	1.361E+06	1.063	0.419
R12	HCHO+0.5H ₂ (g)→HCHO-H	1.177E+11	1.177E+12		0.094
R13	HCHO-H→CH ₂ OH	4.721E+12	3.464E+06	0.030	-0.576
R14	CH ₂ OH+0.5H ₂ (g)→CH ₂ OH-H	1.177E+11	5.293E+09		-0.126
R15	CH ₂ OH-H→CH ₃ OH	5.542E+06	8.356E+05	0.587	-0.077
R16	CH ₃ OH→ Pt(111)-7CO +CH ₃ OH(g)	1.816E+10	7.846E+09		-0.034
R17	CH ₂ OH→CHOH-H	1.208E+05	5.228E+05	0.743	0.060
R18	CHOH-H→CH-H ₂ O	1.893E+05	2.568E+02	0.724	-0.269
R19	CH-H ₂ O→CH+H ₂ O(g)	1.219E+12	1.308E+09		-0.279
R20	CH+0.5H ₂ (g)→CH-H	1.177E+11	1.614E+10		-0.081
R21	CH-H→CH ₂	2.373E+05	8.217E+07	0.715	0.238
R22	CH ₂ +0.5H ₂ (g)→CH ₂ -H	1.177E+11	2.154E+10		-0.069
R23	CH ₂ -H→CH ₃	5.251E+08	2.536E+03	0.401	-0.499
R24	CH ₃ +0.5H ₂ (g)→CH ₃ -H	1.177E+11	2.026E+10		-0.072
R25	CH ₃ -H→CH ₄	2.101E+08	1.064E+05	0.438	-0.309
R26	CH ₄ →CH ₄ (g)+ Pt(111)-7CO	4.764E+12	1.387E+09		-0.332
R27	CH+CO(g)→CH-CO	4.928E+09	9.910E+10		0.122
R28	CH-CO→CHCO	1.000E+05	9.746E+01	0.750	-0.283
R29	CHCO+0.5H ₂ (g)→CHCO-H	1.177E+11	3.471E+11		0.044
R30	CHCO-H→CHCHO	2.307E+06	9.814E+08	0.622	0.247
R31	CHCHO+0.5H ₂ (g)→CHCHO-H	1.177E+11	1.525E+12		0.104
R32	CHCHO-H→CH ₂ CHO	5.641E+08	3.320E+02	0.398	-0.585
R33	CH ₂ CHO+0.5H ₂ (g)→CH ₂ CHO-H	1.177E+11	2.060E+13		0.211
R34	CH ₂ CHO-H→CH ₃ CHO	5.843E+08	4.613E+03	0.397	-0.479

R35	$\text{CH}_3\text{CHO}+0.5\text{H}_2(\text{g})\rightarrow\text{CH}_3\text{CHO-H}$	1.177E+11	3.566E+11		0.045
R36	$\text{CH}_3\text{CHO-H}\rightarrow\text{CH}_3\text{CHOH}$	1.042E+06	4.734E+03	0.655	-0.220
R37	$\text{CH}_3\text{CHOH}+0.5\text{H}_2(\text{g})\rightarrow\text{CH}_3\text{CHOH-H}$	1.177E+11	1.254E+11		0.003
R38	$\text{CH}_3\text{CHOH-H}\rightarrow\text{CH}_3\text{CH}_2\text{OH}$	1.190E+11	1.462E+10	0.180	-0.085
R39	$\text{CH}_3\text{CH}_2\text{OH}\rightarrow\text{CH}_3\text{CH}_2\text{OH}(\text{g})+\text{Pt}(\mathbf{11})\text{-7CO}$	9.515E+08	8.180E+08		-0.006
R40	$\text{H}+0.5\text{H}_2(\text{g})\rightarrow 3\text{H}$	1.177E+11	8.407E+09		-0.108

Table S5. Coverage of surface species for the reactions on Pt(111)-7CO-3H, the rate constants presented in Table S4 are used. For brevity, the “7CO” notation is omitted to describe each surface species.

Surface species	Coverage
1H	6.5144E-02
H-CO ₂	3.4478E-05
COOH	1.0845E-08
COOH-H	4.4318E-08
CO-H ₂ O	6.0342E-04
CO	1.4001E-02
CO-H	5.0237E-03
CHO	7.5237E-05
CHO-H	1.6726E-03
HCHO	1.4751E-11
HCHO-H	1.3633E-12
CH ₂ OH	1.8200E-06
CH ₂ OH-H	4.0468E-05
CH ₃ OH	2.6838E-04
CHOH-H	2.5587E-07
CH-H ₂ O	8.2682E-11
CH	7.6979E-08
CH-H	5.6134E-07
CH ₂	4.6217E-11
CH ₂ -H	2.4648E-10
CH ₃	1.2222E-10
CH ₃ -H	7.0371E-10
CH ₄	1.7283E-07
CH-CO	1.2597E-08
CHCO	3.7593E-08
CHCO-H	1.2747E-08

CHCHO	2.8692E-11
CHCHO-H	2.2128E-12
CH ₂ CHO	1.6513E-09
CH ₂ CHO-H	9.4317E-12
CH ₃ CHO	9.2406E-07
CH ₃ CHO-H	3.0493E-07
CH ₃ CHOH	6.6824E-05
CH ₃ CHOH-H	6.2708E-05
CH ₃ CH ₂ OH	5.1035E-04
Pt(111)-7CO	5.9367E-04
3H	9.1190E-01

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2. Stegelmann, C.; Andreasen, A.; Campbell, C. T., Degree of Rate Control: How Much the Energies of Intermediates and Transition States Control Rates. *Journal of the American Chemical Society* **2009**, *131* (23), 8077-8082.
3. Campbell, C. T., The Degree of Rate Control: A Powerful Tool for Catalysis Research. *ACS Catal.* **2017**, *7* (4), 2770-2779.

Pt(111)-7CO-3H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
7	3	7	64

Direct

0.878740013	0.068470001	0.378820002
0.875039995	0.409110010	0.383120000
0.754480004	0.740830004	0.383459985
0.199800000	0.137070000	0.385129988
0.552839994	0.128790006	0.386339992
0.457269996	0.646279991	0.387710005
0.081380002	0.630230010	0.388509989
0.372810006	0.915520012	0.360390007
0.364769995	0.402669996	0.354110003
0.626030028	0.413069993	0.359409988
0.876070023	0.059889998	0.433270007
0.866230011	0.409539998	0.437480003
0.756349981	0.739180028	0.437550008
0.207069993	0.145720005	0.439000010
0.546389997	0.134460002	0.440270007
0.465189993	0.650529981	0.441630006
0.088909999	0.630879998	0.442369998
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000

0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249320000	0.330769986	0.205329999
0.750180006	0.833029985	0.206100002
0.877030015	0.085400000	0.206809998
0.377739996	0.584999979	0.207359999
0.375180006	0.080210000	0.207379997
0.125650004	0.078620002	0.207440004
0.123590000	0.580500007	0.207310006
0.624819994	0.083769999	0.207849994
0.502070010	0.336450011	0.207920000
0.875299990	0.578960001	0.208370000
0.999830008	0.829490006	0.208389997
0.750129998	0.330570012	0.209189996
0.501839995	0.833850026	0.210199997
0.626559973	0.581709981	0.209470004
0.251549989	0.831560016	0.211190000
0.001120000	0.332850009	0.210740000
0.249909997	0.496549994	0.308389992
0.375310004	0.249239996	0.308270007
0.754499972	0.001140000	0.311190009
0.875270009	0.748170018	0.314020008
0.000420000	0.993359983	0.313879997
0.128069997	0.245069996	0.314990014
0.375239998	0.748690009	0.319310009
0.503289998	0.999480009	0.318179995

0.754849970	0.492689997	0.316379994
0.630530000	0.752219975	0.315640002
0.125970006	0.745289981	0.316109985
0.624300003	0.245409995	0.317860007
0.246429995	0.996370018	0.319680005
0.879970014	0.245120004	0.319279999
0.500970006	0.503470004	0.321509987
0.006190000	0.496740013	0.324019998

H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
7	1	7	64

Direct

0.879220009	0.069169998	0.378780007
0.751529992	0.739069998	0.383240014
0.873660028	0.409029990	0.382789999
0.206090003	0.130250007	0.384530008
0.549679995	0.122290000	0.385789990
0.435970008	0.628180027	0.386159986
0.077760004	0.632269979	0.388590008
0.619840026	0.414240003	0.358870000
0.876550019	0.060660001	0.433219999
0.753229976	0.737010002	0.437359989
0.865809977	0.409960002	0.437180012
0.212029994	0.137600005	0.438510001
0.545599997	0.126640007	0.439799994
0.435400009	0.626470029	0.440250009
0.082520001	0.632879972	0.442519993
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000

0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.248940006	0.330100000	0.205139995
0.750829995	0.833739996	0.206159994
0.377440006	0.583580017	0.206550002
0.877409995	0.085919999	0.207059994
0.375440001	0.078599997	0.207000002
0.122749999	0.581470013	0.207240000
0.125389993	0.079580002	0.207560003
0.625660002	0.084150001	0.207770005
0.502560019	0.335359991	0.207719997
0.875270009	0.579649985	0.208710000
0.999559999	0.830449998	0.208790004
0.627290010	0.582059979	0.209040001
0.750549972	0.331090003	0.209299996
0.502179980	0.833029985	0.209930003
0.250600010	0.830869973	0.210490003
0.001420000	0.333339989	0.210850000
0.251659989	0.494120002	0.307500005
0.375099987	0.250420004	0.307550013
0.754599988	0.001910000	0.311479986

0.002150000	0.993979990	0.314379990
0.874740005	0.748239994	0.314460009
0.628849983	0.752810001	0.315299988
0.131320000	0.244990006	0.316399992
0.500500023	0.996730030	0.317140013
0.128299996	0.746200025	0.316969991
0.753220022	0.492379993	0.316769987
0.375860006	0.749499977	0.317530006
0.251199991	0.993239999	0.318280011
0.621630013	0.244690001	0.318470001
0.497509986	0.501089990	0.318340003
0.880940020	0.245749995	0.319040000
0.007110000	0.496980011	0.323480010

CO2-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	1	9	64

Direct

0.879459977	0.070249997	0.378670007
0.873319983	0.409750015	0.382820010
0.752059996	0.739790022	0.383289993
0.564260006	0.112740003	0.386150002
0.194820002	0.122309998	0.384880006
0.444790006	0.637989998	0.385630012
0.075719997	0.634249985	0.388579994
0.319099993	0.380800009	0.488189995
0.618550003	0.413260013	0.359499991
0.876829982	0.061710000	0.433079988
0.865660012	0.410690010	0.437220007
0.753470004	0.737890005	0.437409997
0.570500016	0.107950002	0.440030009
0.193749994	0.124619998	0.439069986
0.448610008	0.641680002	0.439740002
0.078879997	0.636160016	0.442539990
0.394609988	0.335079998	0.456059992
0.243469998	0.426840007	0.519729972
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000

0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.248809993	0.330399990	0.205210000
0.750790000	0.834079981	0.206169993
0.377490014	0.583440006	0.206660002
0.502860010	0.335949987	0.207849994
0.122819997	0.581619978	0.207310006
0.877349973	0.086470000	0.206990004
0.375470012	0.078960001	0.207059994
0.625689983	0.084830001	0.207690001
0.125379995	0.080100000	0.207450002
0.875349998	0.579959989	0.208739996
0.750599980	0.331669986	0.209360003

0.627449989	0.582409978	0.209059998
0.999589980	0.830730021	0.208739996
0.502359986	0.833150029	0.209649995
0.001460000	0.333799988	0.210869998
0.250519991	0.830890000	0.210290000
0.252000004	0.494480014	0.307850003
0.375420004	0.251280010	0.307370007
0.754840016	0.002430000	0.311239988
0.001930000	0.994530022	0.314119995
0.752950013	0.492819995	0.316909999
0.874809980	0.748719990	0.314429998
0.628929973	0.753289998	0.315380007
0.131850004	0.245570004	0.316760004
0.621399999	0.245220006	0.318859994
0.497539997	0.502020001	0.318899989
0.128490001	0.746479988	0.316909999
0.500220001	0.998170018	0.316810012
0.881079972	0.246639997	0.319040000
0.251289994	0.994159997	0.317979991
0.375510007	0.750680029	0.316850007
0.007250000	0.497460008	0.323540002

COOH

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	1	9	64

Direct

0.885559976	0.076710001	0.381009996
0.858359993	0.412180007	0.381480008
0.757679999	0.748839974	0.385490000
0.605979979	0.093510002	0.376349986
0.176510006	0.112690002	0.383949995
0.483240008	0.659070015	0.378789991
0.064340003	0.638729990	0.387800008
0.359290004	0.335200012	0.404150009
0.471890002	0.211689994	0.444909990
0.888270020	0.072240002	0.435429990
0.851189971	0.416200012	0.435820013
0.762809992	0.746330023	0.439429998

0.596499979	0.101899996	0.431529999
0.169080004	0.114110000	0.437990010
0.481550008	0.652260005	0.433299989
0.064369999	0.640600026	0.441749990
0.412230015	0.286769986	0.453330010
0.288960010	0.436479986	0.409640014
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249180004	0.330309987	0.206970006
0.747160017	0.835240006	0.208179995
0.373490006	0.583989978	0.206740007

0.498530000	0.334329993	0.207499996
0.124580003	0.580529988	0.208770007
0.872780025	0.084739998	0.208140001
0.373750001	0.084610000	0.209380001
0.623899996	0.083039999	0.207249999
0.123269998	0.079839997	0.206770003
0.876550019	0.582090020	0.207580000
0.750729978	0.331620008	0.207130000
0.627210021	0.583859980	0.207210004
0.997940004	0.831260026	0.208619997
0.500530005	0.832849979	0.208700001
0.000730000	0.333539993	0.210109994
0.248760000	0.832729995	0.209670007
0.248030007	0.496019989	0.311769992
0.376349986	0.257149994	0.319130003
0.744350016	0.007170000	0.319720000
0.995469987	0.996070027	0.313380003
0.750230014	0.494709998	0.313059986
0.869759977	0.752149999	0.313239992
0.624239981	0.751550019	0.320490003
0.126670003	0.243110001	0.314249992
0.620490015	0.253210008	0.312709987
0.503250003	0.503130019	0.311749995
0.124940000	0.748489976	0.317050010
0.493409991	0.001540000	0.314420015
0.877560019	0.249190003	0.318639994
0.247060001	0.994650006	0.317279994
0.372000009	0.752479970	0.315439999
0.002130000	0.499639988	0.322299987

COOH-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	9	64

Direct

0.606109977	0.089659996	0.377420008
0.885280013	0.075309999	0.380879998
0.871479988	0.409869999	0.381989986
0.756730020	0.745389998	0.384939998

0.478430003	0.663550019	0.379999995
0.174410000	0.110820003	0.383800000
0.066299997	0.640839994	0.388159990
0.357439995	0.331779987	0.404309988
0.621540010	0.414270014	0.355809987
0.469110012	0.205980003	0.444660008
0.287959993	0.433420002	0.410360008
0.596319973	0.096490003	0.432559997
0.888570011	0.071999997	0.435310006
0.862119973	0.410869986	0.436320007
0.761380017	0.741720021	0.438930005
0.479600012	0.658379972	0.434460014
0.165840000	0.112130001	0.437790006
0.065940000	0.643410027	0.442090005
0.410659999	0.282040000	0.453260005
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003

0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.123649999	0.079379998	0.206660002
0.747259974	0.835659981	0.208010003
0.750729978	0.332450002	0.207550004
0.249449998	0.330110013	0.206790000
0.374280006	0.583199978	0.207090005
0.624239981	0.084330000	0.207460001
0.627089977	0.583809972	0.207479998
0.875750005	0.581359982	0.208059996
0.872979999	0.084830001	0.208100006
0.997839987	0.830640018	0.208489999
0.124360003	0.580200016	0.208629996
0.498899996	0.334890008	0.207890004
0.500720024	0.833090007	0.208560005
0.000890000	0.333550006	0.209910005
0.374080002	0.084430002	0.209360003
0.249100000	0.832059979	0.209600002
0.248249993	0.495330006	0.311549991
0.996100008	0.995270014	0.313160002
0.620450020	0.249589995	0.313059986
0.870230019	0.752170026	0.313160002
0.753759980	0.495539993	0.315079987
0.127030000	0.242540002	0.314040005
0.501250029	0.505400002	0.313459992
0.624319971	0.753229976	0.319700003
0.493710011	0.001010000	0.314359993
0.125229999	0.748319983	0.316799998
0.371459991	0.752849996	0.315329999
0.879299998	0.247820005	0.317860007
0.247370005	0.994340003	0.317279994
0.745230019	0.006520000	0.320030004
0.003800000	0.499520004	0.322800010
0.374749988	0.255439997	0.318940014

CO-H2O

1.0

11.1216001511	0.0000000000	0.0000000000
---------------	--------------	--------------

	0.0000000000	9.6316003799	0.0000000000
	0.0000000000	0.0000000000	21.7964000702
C	H	O	Pt
8	2	9	64
Direct			
0.554979980	0.132290006	0.383830011	
0.877139986	0.069890000	0.378259987	
0.869889975	0.411920011	0.380730003	
0.764400005	0.742550015	0.387580007	
0.482910007	0.758390009	0.389770001	
0.193240002	0.127039999	0.384409994	
0.076080002	0.634019971	0.387989998	
0.369870007	0.419910014	0.375860006	
0.545539975	0.433910012	0.469529986	
0.685530007	0.441139996	0.466549993	
0.365480006	0.415459991	0.430669993	
0.553309977	0.134719998	0.438019991	
0.875249982	0.062880002	0.432770014	
0.863189995	0.412869990	0.435440004	
0.776369989	0.742359996	0.441190004	
0.476310015	0.763999999	0.443520010	
0.193299994	0.131119996	0.438529998	
0.078699999	0.635240018	0.441949993	
0.612280011	0.483880013	0.450780004	
0.000000000	0.000000000	0.000000000	
0.000000000	0.500000000	0.000000000	
0.125000000	0.250000000	0.000000000	
0.125000000	0.750000000	0.000000000	
0.250000000	0.000000000	0.000000000	
0.250000000	0.500000000	0.000000000	
0.375000000	0.250000000	0.000000000	
0.375000000	0.750000000	0.000000000	
0.500000000	0.000000000	0.000000000	
0.500000000	0.500000000	0.000000000	
0.625000000	0.250000000	0.000000000	
0.625000000	0.750000000	0.000000000	
0.750000000	0.000000000	0.000000000	
0.750000000	0.500000000	0.000000000	
0.875000000	0.250000000	0.000000000	
0.875000000	0.750000000	0.000000000	
0.000000000	0.166669995	0.103940003	

0.00000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.124519996	0.079729997	0.207120001
0.747539997	0.830479980	0.207690001
0.749970019	0.330680013	0.208169997
0.249489993	0.331299990	0.206300005
0.376509994	0.585609972	0.207320005
0.625779986	0.081840001	0.207059994
0.625129998	0.582790017	0.209959999
0.875739992	0.579859972	0.207640007
0.876330018	0.084770001	0.206660002
0.999050021	0.829429984	0.208519995
0.125170007	0.580139995	0.208260000
0.500819981	0.333629996	0.206660002
0.502399981	0.834100008	0.209610000
0.001390000	0.333290011	0.210500002
0.374779999	0.082120001	0.207969993
0.250400007	0.832220018	0.210439995
0.253060013	0.500020027	0.311969995
0.999719977	0.993539989	0.313789994
0.626030028	0.247920007	0.315629989
0.871249974	0.747619987	0.313279986
0.750469983	0.491780013	0.314110011
0.127200007	0.244939998	0.315079987
0.504040003	0.496549994	0.315970004
0.623929977	0.749400020	0.326599985
0.501209974	0.003540000	0.316040009
0.128179997	0.747330010	0.316359997

0.376610011	0.755490005	0.316210002
0.878690004	0.246669993	0.318459988
0.248579994	0.996640027	0.317730010
0.753329992	0.000720000	0.311329991
0.005700000	0.498490006	0.322629988
0.375270009	0.251249999	0.312390000

CO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	O	Pt
8	8	64

Direct

0.552730024	0.132499993	0.384200007
0.875209987	0.069810003	0.378360003
0.330269992	0.390700012	0.382679999
0.862259984	0.411379993	0.381839991
0.762539983	0.745739996	0.385899991
0.488680005	0.667100012	0.379979998
0.180910006	0.112319998	0.384710014
0.073940001	0.632430017	0.388260007
0.552429974	0.135649994	0.438320011
0.874069989	0.060720000	0.432770014
0.854189992	0.414940000	0.436170012
0.769360006	0.743560016	0.439749986
0.483980000	0.659879982	0.434430003
0.334609985	0.391550004	0.436720014
0.175150007	0.114110000	0.438710004
0.076329999	0.635060012	0.442209989
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000

0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.124750003	0.079329997	0.207020000
0.748279989	0.831640005	0.207169995
0.249239996	0.330440015	0.206650004
0.749849975	0.330199987	0.207949996
0.626619995	0.583270013	0.208269998
0.375120014	0.584450006	0.207130000
0.875720024	0.084720001	0.206799999
0.877009988	0.579379976	0.207519993
0.624409974	0.082939997	0.207230002
0.125790000	0.579010010	0.209059998
0.999610007	0.829060018	0.208350003
0.500029981	0.335139990	0.207450002
0.501760006	0.834529996	0.209680006
0.001170000	0.332700014	0.210800007
0.374850005	0.083750002	0.209030002
0.250310004	0.832130015	0.209779993
0.251489997	0.496569991	0.313849986
0.998679996	0.993160009	0.313360006
0.873210013	0.747780025	0.313169986
0.126000002	0.240490004	0.315160006

0.623290002	0.249430001	0.315479994
0.627229989	0.752810001	0.322010010
0.751590014	0.491780013	0.313129991
0.499480009	0.001730000	0.317299992
0.505389988	0.503250003	0.314639986
0.127660006	0.745559990	0.316610008
0.375699997	0.754069984	0.315439999
0.877080023	0.246240005	0.319189996
0.248989999	0.993229985	0.317620009
0.751600027	0.001190000	0.311329991
0.375270009	0.253410012	0.314799994
0.004390000	0.496829987	0.323300004

CO-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	1	8	64

Direct

0.556360006	0.124339998	0.384889990
0.878350019	0.068190001	0.378410012
0.370160013	0.417490005	0.376569986
0.874840021	0.409220010	0.382620007
0.765209973	0.739809990	0.386649996
0.483660012	0.745620012	0.388720006
0.193030000	0.125019997	0.384510010
0.079000004	0.633669972	0.388520002
0.626049995	0.415850013	0.356929988
0.555360019	0.125340000	0.438950002
0.876689970	0.059769999	0.432830006
0.865530014	0.409310013	0.436940014
0.775170028	0.737380028	0.440420002
0.478709996	0.741880000	0.442640007
0.369899988	0.412519991	0.431149989
0.192729995	0.128539994	0.438620001
0.082419999	0.635519981	0.442449987
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000

0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.124860004	0.079369999	0.207020000
0.747910023	0.830690026	0.207509995
0.249420002	0.331200004	0.206239998
0.750519991	0.330650002	0.208719999
0.625930011	0.582120001	0.209900007
0.376980007	0.584609985	0.207320005
0.876959980	0.084930003	0.206630006
0.875419974	0.578760028	0.208079994
0.626399994	0.082769997	0.207259998
0.125220001	0.579670012	0.208320007
0.999260008	0.828809977	0.208269998
0.501240015	0.332949996	0.206499994
0.502860010	0.834129989	0.209360003

0.001630000	0.333139986	0.210759997
0.374909997	0.081900001	0.207870007
0.250809997	0.831459999	0.210199997
0.252730012	0.499139994	0.312489986
0.000790000	0.992670000	0.313549995
0.872990012	0.747730017	0.312940001
0.127780005	0.243929997	0.315239996
0.626299977	0.243750006	0.316520005
0.624719977	0.751540005	0.325430006
0.754549980	0.493180007	0.315800011
0.500880003	0.002150000	0.315600008
0.501619995	0.498279989	0.315250009
0.128539994	0.746609986	0.316339999
0.376230001	0.755209982	0.315840006
0.880599976	0.245299995	0.318910003
0.248999998	0.995720029	0.317550004
0.754740000	0.999759972	0.311109990
0.374639988	0.250569999	0.311789989
0.007220000	0.497579992	0.323599994

CHO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	1	8	64

Direct

0.575339973	0.113289997	0.383419991
0.867100000	0.076320000	0.380360007
0.346789986	0.284790009	0.413370013
0.861739993	0.413309991	0.381500006
0.752479970	0.742789984	0.383450001
0.451889992	0.634289980	0.384240001
0.140880004	0.082120001	0.378549993
0.074989997	0.631290019	0.387639999
0.383080006	0.197750002	0.441379994
0.583239973	0.110579997	0.437640011
0.860090017	0.071920000	0.434670001
0.854969978	0.416850001	0.435889989
0.753040016	0.740819991	0.437530011
0.456349999	0.637269974	0.438320011

0.296979994	0.383830011	0.435259998
0.144830003	0.088289998	0.433219999
0.079539999	0.632740021	0.441549987
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.125459999	0.079650000	0.207169995
0.750890017	0.833999991	0.206320003
0.251210004	0.328330010	0.206729993
0.748839974	0.330790013	0.207990006
0.626209974	0.581820011	0.208030000
0.376260012	0.582870007	0.206420004

0.878040016	0.086029999	0.207589999
0.875509977	0.581740022	0.208210006
0.624769986	0.083540000	0.207259998
0.122309998	0.581099987	0.206909999
0.999629974	0.833169997	0.209820002
0.498800009	0.333370000	0.209810004
0.501800001	0.833310008	0.209370002
0.999939978	0.334179997	0.209790006
0.376080006	0.082439996	0.209340006
0.250499994	0.829670012	0.209150001
0.250349998	0.494700015	0.307440013
0.003360000	0.997089982	0.320490003
0.874570012	0.750599980	0.314579993
0.128450006	0.245619997	0.313120008
0.620220006	0.249699995	0.316370010
0.628989995	0.751959980	0.315299988
0.748700023	0.493580014	0.313879997
0.500159979	0.998459995	0.317209989
0.500490010	0.500919998	0.316509992
0.127979994	0.745000005	0.316049993
0.376349986	0.749409974	0.316769987
0.876749992	0.249190003	0.318569988
0.253619999	0.993439972	0.314700007
0.754000008	0.003200000	0.310950011
0.372070014	0.254869998	0.323309988
0.003830000	0.498180002	0.322400004

CHO-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	8	64

Direct

0.866869986	0.075669996	0.380219996
0.872340024	0.411190003	0.382019997
0.573889971	0.107660003	0.384730011
0.446969986	0.638840020	0.385369986
0.752030015	0.740930021	0.382840008
0.140110001	0.080849998	0.378479987
0.077179998	0.632350028	0.387930006

0.345889986	0.281260014	0.413320005
0.619099975	0.414869994	0.358350009
0.378270000	0.191000000	0.440580010
0.859799981	0.071649998	0.434549987
0.300339997	0.381960005	0.436080009
0.863699973	0.412010014	0.436390013
0.581309974	0.104199998	0.438890010
0.144280002	0.087229997	0.433160007
0.452730000	0.642979980	0.439350009
0.752430022	0.738979995	0.436969995
0.081960000	0.634249985	0.441810012
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003

0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.377260000	0.582140028	0.206619993
0.750909984	0.834559977	0.206080005
0.122040004	0.580799997	0.206760004
0.878220022	0.086319998	0.207369998
0.125550002	0.079429999	0.207029998
0.624880016	0.084990002	0.207519993
0.251480013	0.328040004	0.206569999
0.748799980	0.331580013	0.208580002
0.626529992	0.581629992	0.208299994
0.874989986	0.581139982	0.208519995
0.999539971	0.832889974	0.209680006
0.501999974	0.833670020	0.209230006
0.499300003	0.333660007	0.210130006
0.250710011	0.829180002	0.208979994
0.376249999	0.082439996	0.209340006
0.000050000	0.334100008	0.209680006
0.249929994	0.494329989	0.307000011
0.754599988	0.002900000	0.310640007
0.752049983	0.494670004	0.315800011
0.003520000	0.996349990	0.320470005
0.874979973	0.750609994	0.314269990
0.619960010	0.245869994	0.317730010
0.629100025	0.753430009	0.314570010
0.128389999	0.245269999	0.313039988
0.375310004	0.749979973	0.316410005
0.497680008	0.503319979	0.317880005
0.128000006	0.745119989	0.315869987
0.499760002	0.997489989	0.317119986
0.253259987	0.993510008	0.314449996
0.878189981	0.247999996	0.317999989
0.005290000	0.498129994	0.322880000
0.370510012	0.253580004	0.323029995

HCHO

1.0

11.1216001511	0.0000000000	0.0000000000	
0.0000000000	9.6316003799	0.0000000000	
0.0000000000	0.0000000000	21.7964000702	
C	H	O	Pt
8	2	8	64

Direct

0.878319979	0.072049998	0.378540009
0.858839989	0.410730004	0.381449997
0.546959996	0.134880006	0.383749992
0.487430006	0.656849980	0.379159987
0.757790029	0.751250029	0.386260003
0.208399996	0.134690002	0.383419991
0.047359999	0.653079987	0.385800004
0.321669996	0.426189989	0.453229994
0.401069999	0.369569987	0.435730010
0.306479990	0.430629998	0.503329992
0.876969993	0.063570000	0.433050007
0.249439999	0.484030008	0.419010013
0.853269994	0.415950000	0.435869992
0.540459991	0.142619997	0.437909991
0.217570007	0.145630002	0.437460005
0.484670013	0.649100006	0.434029996
0.763790011	0.751540005	0.440189987
0.037500001	0.662159979	0.439500004
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003

0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.374379992	0.584190011	0.207259998
0.748549998	0.832379997	0.207450002
0.124399997	0.581430018	0.208680004
0.876240015	0.085359998	0.207289994
0.124990001	0.080760002	0.207230002
0.625140011	0.082549997	0.207409993
0.248620003	0.332500011	0.206139997
0.750199974	0.330440015	0.208020002
0.626739979	0.583920002	0.208289996
0.876169980	0.581130028	0.207619995
0.998839974	0.831560016	0.208389997
0.501860023	0.832949996	0.210099995
0.501720011	0.335480005	0.206359997
0.249569997	0.831809998	0.210219994
0.375239998	0.078890003	0.206819996
0.001130000	0.333939999	0.210779995
0.252649993	0.495860010	0.312940001
0.752149999	0.002500000	0.312079996
0.749779999	0.492179990	0.313149989
0.000580000	0.996609986	0.313879997
0.871840000	0.749840021	0.314190000
0.621860027	0.249699995	0.316159993
0.625599980	0.751160026	0.321669996
0.129549995	0.246500000	0.315869987
0.374949992	0.752990007	0.316659987
0.501399994	0.498890013	0.314280003
0.128429994	0.749000013	0.316379994
0.500140011	0.000560000	0.317530006
0.250349998	0.995739996	0.318010002
0.878470004	0.247860000	0.319200009
0.003430000	0.499460012	0.321700007

0.376670003	0.252649993	0.307289988
HCHO-H		
1.0		
11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	8	64

Direct

0.861869991	0.070660003	0.382950008
0.804030001	0.389829993	0.387690008
0.446969986	0.631070018	0.384770006
0.534630001	0.137889996	0.383329988
0.140320003	0.004880000	0.388170004
0.749490023	0.741509974	0.384530008
0.050310001	0.645070016	0.385839999
0.308539987	0.344669998	0.475970000
0.077030003	0.367890000	0.364600003
0.400550008	0.387780011	0.481979996
0.282940000	0.254330009	0.505029976
0.851320028	0.065669999	0.437200010
0.801999986	0.394259989	0.441689998
0.238179997	0.393610001	0.438760012
0.450980008	0.631609976	0.439020008
0.525070012	0.148690000	0.437299997
0.145439997	0.009980000	0.442180008
0.750500023	0.738150001	0.438630015
0.045660000	0.650829971	0.439850003
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000

0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.248919994	0.330839992	0.204439998
0.751370013	0.834039986	0.206790000
0.377099991	0.584190011	0.206119999
0.501190007	0.335579991	0.207269996
0.373549998	0.077569999	0.207450002
0.878589988	0.085809998	0.209600002
0.625349998	0.082520001	0.207249999
0.123640001	0.081019998	0.207910001
0.122939996	0.582989991	0.206290007
0.627219975	0.583559990	0.209020004
0.749000013	0.330339998	0.208489999
0.875389993	0.582249999	0.209010005
0.998830020	0.834529996	0.209999993
0.501860023	0.833260000	0.210069999
0.249650002	0.829639971	0.209779993
0.996630013	0.335280001	0.210030004
0.370840013	0.250220001	0.308440000
0.252929986	0.496769994	0.307099998
0.752780020	0.002290000	0.311879992
0.744769990	0.494010001	0.314790010
0.003000000	0.004230000	0.324239999
0.496890008	0.499469995	0.317220002

0.872990012	0.749809980	0.315869987
0.126900002	0.252119988	0.310840011
0.627170026	0.753679991	0.316460013
0.616649985	0.248439997	0.315820009
0.497920007	0.998329997	0.317710012
0.375640005	0.749909997	0.317790002
0.250790000	0.998910010	0.316300005
0.127509996	0.746879995	0.315719992
0.870800018	0.251610011	0.323249996
0.003400000	0.501060009	0.320659995

CH2OH-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	4	8	64

Direct

0.871460021	0.413729995	0.381540000
0.870289981	0.079650000	0.381339997
0.751519978	0.742139995	0.383210003
0.102030002	0.607060015	0.383789986
0.571129978	0.108779997	0.385470003
0.431479990	0.625909984	0.385320008
0.139909998	0.971210003	0.386469990
0.333640009	0.258789986	0.418110013
0.616500020	0.413960010	0.359090000
0.351680011	0.152079999	0.432779998
0.399749994	0.334589988	0.434839994
0.205300003	0.391490012	0.437590003
0.216260001	0.290840000	0.433050007
0.860870004	0.076410003	0.435609996
0.866289973	0.416009992	0.436089993
0.123130001	0.594319999	0.436980009
0.751529992	0.740419984	0.437390000
0.578390002	0.105870001	0.439599991
0.425399989	0.621209979	0.439480007
0.143150002	0.963829994	0.440490007
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000

0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.252640009	0.329459995	0.205369994
0.378380001	0.582279980	0.206389993
0.121629998	0.581889987	0.206349999
0.750689983	0.834969997	0.206410006
0.125400007	0.078809999	0.207059994
0.624490023	0.084299996	0.207660004
0.997860014	0.334349990	0.208049998
0.873749971	0.581489980	0.208619997
0.878740013	0.084490001	0.208230004
0.626640022	0.581459999	0.208739996
0.748269975	0.330659986	0.208959997
0.250990003	0.828719974	0.208949998

0.502099991	0.833280027	0.209450006
0.499469995	0.332470000	0.209989995
0.999300003	0.832300007	0.209930003
0.374449998	0.080159999	0.210020006
0.249410003	0.495759994	0.306360006
0.127560005	0.250349998	0.307469994
0.754790008	0.003530000	0.311690003
0.873820007	0.750850022	0.314689994
0.749629974	0.494060010	0.316190004
0.252389997	0.996580005	0.315930009
0.126570001	0.744449973	0.315970004
0.628170013	0.753769994	0.315210015
0.495629996	0.500609994	0.317919999
0.617349982	0.245379999	0.318199992
0.376839995	0.749539971	0.316740006
0.499170005	0.997510016	0.317409992
0.878390014	0.248260006	0.318280011
0.001980000	0.499139994	0.320510000
0.004800000	0.999620020	0.322120011
0.365550011	0.250640005	0.321790010

CH3OH

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	4	8	64

Direct

0.863330007	0.412950009	0.380129993
0.867919981	0.077509999	0.381119996
0.753809988	0.741379976	0.384050012
0.092000000	0.609619975	0.384820014
0.545729995	0.133520007	0.384059995
0.439300001	0.620809972	0.384909987
0.138429999	0.956080019	0.385520011
0.236939996	0.277929991	0.455020010
0.283140004	0.374929994	0.442690015
0.294149995	0.188569993	0.444339991
0.214440003	0.277359992	0.504109979
0.068559997	0.330269992	0.433099985
0.127140000	0.260430008	0.419900000

0.859040022	0.075250000	0.435499996
0.866789997	0.415529996	0.434980005
0.105460003	0.597639978	0.438450009
0.756129980	0.739350021	0.438190013
0.539349973	0.141320005	0.438160002
0.435409993	0.617810011	0.439119995
0.141259998	0.945540011	0.439579993
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249210000	0.330379993	0.205090001
0.377939999	0.583589971	0.206119999

0.122740000	0.582729995	0.206919998
0.751169980	0.834259987	0.206589997
0.125489995	0.080820002	0.208629996
0.625270009	0.082340002	0.207310006
0.999450028	0.333689988	0.209230006
0.874750018	0.581889987	0.207920000
0.879490018	0.083760001	0.208480000
0.627399981	0.582629979	0.209000006
0.749809980	0.329869986	0.208379999
0.250490010	0.828679979	0.209470004
0.502569973	0.832589984	0.210189998
0.501659989	0.334479988	0.207249999
0.000250000	0.832889974	0.209849998
0.373970002	0.076760001	0.207870007
0.253149986	0.494340003	0.307429999
0.130840003	0.250039995	0.312929988
0.754209995	0.002670000	0.311870009
0.873899996	0.749960005	0.314390004
0.747789979	0.492269993	0.315239996
0.254770011	0.995769978	0.317319989
0.128769994	0.743309975	0.317039996
0.628970027	0.751709998	0.316929996
0.499790013	0.496780008	0.317169994
0.620360017	0.248809993	0.316399992
0.379629999	0.747399986	0.317570001
0.500810027	0.997590005	0.317939997
0.877489984	0.247620001	0.318179995
0.002530000	0.499330014	0.318540007
0.004520000	0.998809993	0.321839988
0.373349994	0.248190001	0.308739990

CHOH-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	8	64

Direct

0.871779978	0.078860000	0.381359994
0.871060014	0.412490010	0.382090002
0.437359989	0.632979989	0.385690004

0.578299999	0.103370003	0.384790003
0.141609997	0.981890023	0.386480004
0.751860023	0.741540015	0.383240014
0.086719997	0.622089982	0.386370003
0.339709997	0.251470000	0.409179986
0.257059991	0.423079997	0.415190011
0.618460000	0.414790004	0.359219998
0.369439989	0.164590001	0.438329995
0.862469971	0.075680003	0.435649991
0.864610016	0.413709998	0.436610013
0.285589993	0.344969988	0.441830009
0.434720010	0.633369982	0.439949989
0.584819973	0.099639997	0.439029992
0.145549998	0.980310023	0.440649986
0.751709998	0.739939988	0.437400013
0.099789999	0.619390011	0.440200001
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003

0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.253089994	0.330000013	0.205720007
0.750769973	0.834590018	0.206340000
0.378259987	0.582120001	0.206640005
0.498499990	0.331490010	0.211359993
0.375019997	0.080920003	0.210099995
0.878830016	0.084940001	0.208179995
0.625109971	0.083980002	0.207660004
0.125389993	0.078740001	0.206709996
0.121459998	0.581990004	0.206310004
0.626060009	0.580460012	0.208759993
0.747770011	0.330890000	0.208759993
0.873600006	0.581709981	0.208739996
0.999170005	0.832599998	0.209840000
0.502290010	0.832939982	0.209150001
0.251190007	0.829119980	0.208849996
0.997380018	0.335330009	0.208090007
0.368490010	0.251679987	0.322829992
0.248879999	0.496950001	0.306760013
0.755930007	0.002720000	0.311800003
0.750649989	0.493900001	0.316300005
0.005880000	0.000000000	0.322169989
0.496619999	0.501760006	0.319110006
0.874059975	0.750699997	0.314639986
0.126650006	0.251399994	0.306089997
0.628740013	0.752669990	0.315039992
0.620310009	0.244560003	0.318430007
0.500970006	0.996200025	0.317030013
0.376580000	0.749620020	0.316190004
0.252880007	0.996230006	0.315230012
0.126980007	0.744840026	0.315409988
0.878939986	0.248300001	0.318370014
0.003060000	0.499300003	0.322279990

CH-H2O

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	8	64

Direct

0.865320027	0.077339999	0.381909996
0.855660021	0.412869990	0.382120013
0.446920007	0.628359973	0.384499997
0.547379971	0.131679997	0.384389997
0.140200004	0.974889994	0.387100011
0.752229989	0.744319975	0.383870006
0.069660001	0.629270017	0.387360007
0.250120014	0.331110001	0.367610008
0.388520002	0.437090009	0.496419996
0.415259987	0.279390007	0.494879991
0.257699996	0.334170014	0.418599993
0.854669988	0.073100001	0.436129987
0.850920022	0.418419987	0.436529994
0.349559993	0.346469998	0.494120002
0.446570009	0.627179980	0.438919991
0.543550014	0.137600005	0.438710004
0.144010007	0.969190001	0.441109985
0.753989995	0.741829991	0.437970012
0.074239999	0.631030023	0.441339999
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000

0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249760002	0.330769986	0.205280006
0.750450015	0.833980024	0.206420004
0.375499994	0.582449973	0.207200006
0.499839991	0.333389997	0.208539993
0.373869985	0.079219997	0.208649993
0.879260004	0.084799998	0.208729997
0.625060022	0.082580000	0.207220003
0.124499999	0.081110001	0.208320007
0.123389997	0.581210017	0.207790002
0.626049995	0.582040012	0.208210006
0.749210000	0.329930007	0.208389997
0.874989986	0.581990004	0.207690001
0.999650002	0.832989991	0.209739998
0.501359999	0.832719982	0.209840000
0.250000000	0.829159975	0.209390000
0.998719990	0.334479988	0.210069999
0.374359995	0.247020006	0.314249992
0.251419991	0.496230006	0.312189996
0.754199982	0.003110000	0.311459988
0.747430027	0.493180007	0.313639998
0.004100000	0.000050000	0.323089987
0.501489997	0.499879986	0.317000002
0.872539997	0.751420021	0.314190000
0.125799999	0.249860004	0.313789994
0.628189981	0.752690017	0.316329986

0.620660007	0.248870000	0.316599995
0.500980020	0.998019993	0.317669988
0.378300011	0.748730004	0.317350000
0.252530009	0.993449986	0.316109985
0.126829997	0.743659973	0.316080004
0.876200020	0.248950005	0.320069999
0.999010026	0.501259983	0.321449995

CH

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	1	7	64

Direct

0.866110027	0.077030003	0.381810009
0.855459988	0.411949992	0.382110000
0.752610028	0.744430006	0.383859992
0.552540004	0.128340006	0.384710014
0.447490007	0.627979994	0.384700000
0.140770003	0.974940002	0.387080014
0.070060000	0.628859997	0.387169987
0.250039995	0.331019998	0.368189991
0.248590007	0.333860010	0.418660015
0.855620027	0.072839998	0.436030000
0.851580024	0.417490005	0.436509997
0.754490018	0.742340028	0.437929988
0.552540004	0.132190004	0.438859999
0.447270006	0.626990020	0.438910007
0.074689999	0.630100012	0.441170007
0.144309998	0.969879985	0.441119999
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000

0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.250220001	0.330790013	0.205459997
0.123860002	0.581110001	0.207870007
0.750699997	0.833729982	0.206389993
0.375479996	0.582379997	0.207259998
0.124779999	0.081150003	0.208309993
0.625230014	0.082410000	0.207130000
0.999040008	0.334289998	0.210040003
0.879530013	0.084670000	0.208639994
0.749400020	0.329829991	0.208279997
0.875280023	0.581759989	0.207640007
0.626179993	0.581839979	0.208179995
0.250200003	0.829320014	0.209380001
0.501510024	0.832589984	0.209739998
0.999899983	0.832889974	0.209690005
0.374049991	0.079590000	0.208869994
0.499749988	0.333090007	0.208719999
0.126519993	0.249709994	0.313529998
0.251839995	0.495999992	0.312599987
0.754859984	0.002740000	0.311309993

0.872979999	0.751039982	0.314130008
0.628589988	0.752399981	0.316260010
0.253320009	0.993359983	0.316240013
0.127149999	0.743740022	0.316049993
0.747879982	0.492859989	0.313670009
0.378670007	0.748480022	0.317209989
0.501529992	0.997829974	0.317380011
0.621169984	0.248559996	0.316320002
0.876829982	0.248610005	0.319940001
0.501890004	0.499669999	0.316769987
0.004780000	0.999800026	0.322990000
0.999480009	0.501049995	0.321179986
0.375000000	0.246900007	0.315490007

CH-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	7	64

Direct

0.865890026	0.076920003	0.381689996
0.868709981	0.411330014	0.382209986
0.751860023	0.743239999	0.383289993
0.551029980	0.120180003	0.385939986
0.442009985	0.633239985	0.385670006
0.141430005	0.979130030	0.387320012
0.072430000	0.631579995	0.387419999
0.249990001	0.330500007	0.367839992
0.618200004	0.413500011	0.358880013
0.248779997	0.332839996	0.418309987
0.854719996	0.073330000	0.435889989
0.861869991	0.413659990	0.436670005
0.753019989	0.740930021	0.437409997
0.549749970	0.123539999	0.440039992
0.442690015	0.633019984	0.439830005
0.077220000	0.633729994	0.441399992
0.145620003	0.975719988	0.441370010
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000

0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.250279993	0.330720007	0.205200002
0.123439997	0.580619991	0.207810000
0.750790000	0.834330022	0.206149995
0.376260012	0.581520021	0.207509995
0.124609999	0.081009999	0.208140001
0.625280023	0.083920002	0.207420006
0.998889983	0.334349990	0.209849998
0.879599988	0.084840000	0.208340004
0.749140024	0.330440015	0.208949998
0.874520004	0.581130028	0.208100006
0.626359999	0.581510007	0.208350003
0.250299990	0.828920007	0.209150001

0.501649976	0.832809985	0.209460005
0.999740005	0.832589984	0.209519997
0.374009997	0.079449996	0.208660007
0.500310004	0.333169997	0.209000006
0.126320004	0.249579996	0.313089997
0.251109987	0.495730013	0.312420011
0.755339980	0.002750000	0.310900003
0.873449981	0.751349986	0.314040005
0.628790021	0.753880024	0.315299988
0.252629995	0.993929982	0.315890014
0.126980007	0.744210005	0.315510005
0.750810027	0.493990004	0.315549999
0.377180010	0.749360025	0.316680014
0.500790000	0.996569991	0.316830009
0.620509982	0.244739994	0.318269998
0.878080010	0.247390002	0.319110006
0.499280006	0.502860010	0.317930013
0.004900000	0.999080002	0.323390007
0.000580000	0.501389980	0.321980000
0.373589993	0.245989993	0.314529985

CH2

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	7	64

Direct

0.864090025	0.078019999	0.381150007
0.859480023	0.412889987	0.381240010
0.762889981	0.748499990	0.386570007
0.549170017	0.134240001	0.384350002
0.489259988	0.658070028	0.378989995
0.138349995	0.984879971	0.387620002
0.076590002	0.624310017	0.387149990
0.306419998	0.369370013	0.389030010
0.376089990	0.412770003	0.419090003
0.231199995	0.324000001	0.414950013
0.854960024	0.074139997	0.435440004
0.853039980	0.417439997	0.435649991
0.769370019	0.747160017	0.440470010

0.549430013	0.137689993	0.438540012
0.483550012	0.646160007	0.433440000
0.080159999	0.627430022	0.441159993
0.140090004	0.983669996	0.441689998
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.251190007	0.331669986	0.206070006
0.125359997	0.578930020	0.208550006
0.748749971	0.832539976	0.207509995
0.374790013	0.583220005	0.207580000
0.124600001	0.077370003	0.206579998

0.624530017	0.082149997	0.207220003
0.997080028	0.334699988	0.208279997
0.878250003	0.083059996	0.208179995
0.748560011	0.329510003	0.207980007
0.875760019	0.581860006	0.207739994
0.626900017	0.583649993	0.207460001
0.250459999	0.829249978	0.209230006
0.501879990	0.833959997	0.209849998
0.999660015	0.830749989	0.209869996
0.373450011	0.081529997	0.209649995
0.498939991	0.332359999	0.207959995
0.124210000	0.246050000	0.305660009
0.252680004	0.491679996	0.317059994
0.752740026	0.001870000	0.311349988
0.872969985	0.749870002	0.313749999
0.627059996	0.752789974	0.322869986
0.250910014	0.996200025	0.316870004
0.128910005	0.740130007	0.315450013
0.749509990	0.492359996	0.312759995
0.376879990	0.751529992	0.315860003
0.498400003	0.002010000	0.317409992
0.620029986	0.249799997	0.315519989
0.876590014	0.247339994	0.319050014
0.503600001	0.501320004	0.311749995
0.003510000	0.997879982	0.322329998
0.002120000	0.497060001	0.321709991
0.368360013	0.250070006	0.318260014

CH2-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	7	64

Direct

0.487170011	0.666249990	0.379729986
0.871599972	0.411330014	0.381579995
0.864400029	0.077959999	0.381049991
0.548959970	0.126650006	0.385650009
0.762660027	0.747009993	0.386220008
0.079329997	0.626139998	0.387320012

0.138990000	0.986320019	0.387569994
0.306329995	0.367680013	0.388709992
0.620450020	0.413269997	0.356099993
0.230800003	0.323009998	0.414590001
0.376230001	0.410239995	0.418859988
0.482760012	0.654959977	0.434179991
0.863499999	0.413340002	0.435999990
0.855030000	0.074610002	0.435350001
0.548139989	0.130119994	0.439770013
0.768830001	0.744840026	0.440160006
0.082960002	0.629710019	0.441309988
0.141190007	0.986100018	0.441630006
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003

0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.251179993	0.331750005	0.205890000
0.124490000	0.077119999	0.206410006
0.624629974	0.083889998	0.207530007
0.627110004	0.583800018	0.207609996
0.375490010	0.582530022	0.207790002
0.748560011	0.833249986	0.207389995
0.874979973	0.581439972	0.208169997
0.748449981	0.330509990	0.208590001
0.499309987	0.332940012	0.208320007
0.997060001	0.334939986	0.208120003
0.878310025	0.083379999	0.207900003
0.125149995	0.578610003	0.208470002
0.250640005	0.828710020	0.208890006
0.373530000	0.081529997	0.209450006
0.502149999	0.834460020	0.209670007
0.999379992	0.830489993	0.209769994
0.124320000	0.245810002	0.305339992
0.753719985	0.002040000	0.311049998
0.502009988	0.504610002	0.312640011
0.753180027	0.493880004	0.314700007
0.873290002	0.750370026	0.313620001
0.619780004	0.245959997	0.317039996
0.375739992	0.752009988	0.315400004
0.128989995	0.740769982	0.315120012
0.252739996	0.491569996	0.317110002
0.250629991	0.996330023	0.316430002
0.497700006	0.001300000	0.317110002
0.367080003	0.249329999	0.317389995
0.878549993	0.246399999	0.318370014
0.003980000	0.497669995	0.321969986
0.626839995	0.755299985	0.322530001
0.003840000	0.997219980	0.322510004

CH3

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C H O Pt

Direct

0.434170008	0.618619978	0.384730011
0.817460001	0.389690012	0.386949986
0.869530022	0.068790004	0.381350011
0.546509981	0.130579993	0.384240001
0.752160013	0.738919973	0.383650005
0.059420001	0.614459991	0.386409998
0.138589993	0.923950016	0.381839991
0.147200003	0.261240005	0.415749997
0.223800004	0.196579993	0.429300010
0.063369997	0.220719993	0.435240000
0.161599994	0.369280010	0.429529995
0.428330004	0.615390003	0.438800007
0.819850028	0.396780014	0.440899998
0.861840010	0.062530003	0.435719997
0.542190015	0.137700006	0.438279986
0.754830003	0.736620009	0.437739998
0.057390001	0.609730005	0.440439999
0.142480001	0.927839994	0.436379999
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003

0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.247510001	0.330529988	0.205699995
0.124380000	0.082149997	0.209240004
0.625670016	0.082340002	0.207100004
0.627219975	0.582159996	0.209240004
0.377629995	0.583320022	0.206060007
0.751139998	0.834150016	0.206420004
0.874740005	0.581749976	0.207709998
0.750090003	0.329879999	0.208370000
0.501190007	0.334080011	0.207279995
0.999520004	0.333719999	0.210749999
0.879209995	0.085969999	0.208829999
0.124030001	0.585389972	0.206819996
0.249919996	0.829200029	0.209549993
0.373750001	0.077739999	0.206990004
0.502219975	0.832539976	0.209869996
0.000040000	0.833500028	0.209700003
0.131410003	0.252359986	0.320569992
0.754329979	0.002560000	0.311690003
0.498519987	0.496549994	0.317099988
0.747590005	0.491450012	0.315299988
0.872720003	0.748369992	0.313840002
0.618789971	0.247020006	0.315690011
0.379240006	0.747349977	0.316810012
0.128289998	0.746810019	0.321660012
0.252669990	0.495000005	0.307099998
0.253549993	0.997820020	0.315180004
0.499949992	0.997290015	0.317389995
0.371879995	0.248150006	0.308140010
0.877950013	0.250779986	0.322329998
0.006060000	0.499359995	0.314770013

0.628189981	0.751689970	0.316289991
0.003510000	0.001750000	0.319799989

CH3-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	4	7	64

Direct

0.487729996	0.664430022	0.380800009
0.870500028	0.069559999	0.380980015
0.139970005	0.922909975	0.381599993
0.818870008	0.390850008	0.386629999
0.549269974	0.133330002	0.383819997
0.764989972	0.743390024	0.386530012
0.063419998	0.613139987	0.386400014
0.144970000	0.258150011	0.415540010
0.373890013	0.411289990	0.353720009
0.153280005	0.366549999	0.429910004
0.225020006	0.198919997	0.428750008
0.063740000	0.210879996	0.434799999
0.479330003	0.660589993	0.435250014
0.863520026	0.062749997	0.435400009
0.143370003	0.927550018	0.436140001
0.820439994	0.398270011	0.440569997
0.545549989	0.139799997	0.437889993
0.772880018	0.740170002	0.440369993
0.061469998	0.607640028	0.440420002
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000

0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.378380001	0.583750010	0.206479996
0.248229995	0.331099987	0.206269994
0.501259983	0.334380001	0.207130000
0.626259983	0.082369998	0.207000002
0.749379992	0.832189977	0.207289994
0.374069989	0.079690002	0.207269996
0.875320017	0.581449986	0.207399994
0.125550002	0.584670007	0.207149997
0.750509977	0.329759985	0.207900003
0.879159987	0.085170001	0.208629996
0.627009988	0.582729995	0.209900007
0.250099987	0.829750001	0.208939999
0.124499999	0.082240000	0.208849996
0.000170000	0.832710028	0.209370002
0.503780007	0.833670020	0.209500000
0.000040000	0.333460003	0.210649997
0.253089994	0.498589993	0.308470011
0.373070002	0.247030005	0.309560001
0.755089998	0.001720000	0.311450005
0.873300016	0.748929977	0.312909991
0.751010001	0.491279989	0.314150006

0.253250003	0.999080002	0.314660013
0.379720002	0.752479970	0.313870013
0.503589988	0.499249995	0.317680001
0.622619987	0.246849999	0.314790010
0.501209974	0.000060000	0.317090005
0.129700005	0.747020006	0.321669996
0.879360020	0.250420004	0.322380006
0.006780000	0.499969989	0.314680010
0.004040000	0.001050000	0.319200009
0.628409982	0.751929998	0.323599994
0.130500004	0.251700014	0.320219994

CH4

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	4	7	64

Direct

0.437689990	0.621070027	0.385149986
0.864929974	0.078019999	0.381909996
0.139349997	0.976610005	0.387349993
0.858169973	0.412759990	0.382180005
0.542010009	0.134480000	0.384160012
0.751659989	0.742039979	0.384020001
0.073459998	0.627330005	0.387320012
0.194830000	0.309139997	0.468629986
0.256190002	0.318489999	0.429199994
0.195510000	0.406960011	0.494329989
0.225130007	0.223250002	0.497790009
0.103030004	0.288060009	0.452529997
0.435110003	0.618309975	0.439280003
0.855589986	0.073689997	0.436190009
0.142059997	0.968529999	0.441280007
0.853619993	0.417549998	0.436610013
0.535529971	0.142309994	0.438149989
0.753459990	0.739799976	0.438109994
0.078180000	0.630469978	0.441269994
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000

0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.376940012	0.583150029	0.206440002
0.249980003	0.330419987	0.204229996
0.500980020	0.334140003	0.207589999
0.624949992	0.082269996	0.207450002
0.750620008	0.834299982	0.206650004
0.373640001	0.076870002	0.207959995
0.874210000	0.582170010	0.208320007
0.121730000	0.581250012	0.206949994
0.748979986	0.329769999	0.208759993
0.878880024	0.084420003	0.208719999
0.626470029	0.582530022	0.208790004
0.249860004	0.828019977	0.209639996

0.124650002	0.078680001	0.207409993
0.999080002	0.832759976	0.209979996
0.501720011	0.832629979	0.210140005
0.997229993	0.334980011	0.209279999
0.250860006	0.492559999	0.307810009
0.370920002	0.248280004	0.309500009
0.753790021	0.003000000	0.311949998
0.873000026	0.750069976	0.314700007
0.746749997	0.492130011	0.314649999
0.252680004	0.996110022	0.316989988
0.377220005	0.747030020	0.317640007
0.498270005	0.497060001	0.317140013
0.619050026	0.248689994	0.316439986
0.499509990	0.997399986	0.317880005
0.127470002	0.741999984	0.315719992
0.877780020	0.248349994	0.319959998
0.002380000	0.497480005	0.322140008
0.004780000	0.000370000	0.322789997
0.627740026	0.751770020	0.316419989
0.129250005	0.249829993	0.308640003

CH-CO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	1	8	64

Direct

0.369159997	0.408950001	0.368550003
0.133939996	0.100790001	0.381080002
0.077090003	0.633050025	0.387010008
0.510469973	0.658439994	0.384429991
0.770560026	0.751770020	0.386830002
0.862990022	0.077059999	0.380129993
0.567780018	0.144759998	0.386830002
0.862370014	0.416350007	0.380970001
0.366549999	0.920009971	0.383910000
0.365040004	0.406709999	0.418969989
0.135790005	0.108719997	0.435449988
0.081589997	0.636460006	0.440959990
0.505760014	0.654380023	0.438919991

0.777220011	0.751659989	0.440660000
0.854749978	0.073500000	0.434460014
0.568300009	0.153410003	0.440710008
0.853640020	0.419050008	0.435299993
0.363359988	0.920080006	0.438349992
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.125349998	0.580269992	0.207900003
0.876060009	0.582000017	0.207139999
0.501519978	0.834540009	0.211300001
0.000080000	0.832719982	0.209429994

0.251789987	0.831759989	0.209729999
0.747439981	0.831369996	0.207289994
0.999610007	0.333990008	0.209790006
0.125929996	0.079080001	0.207959995
0.877950013	0.084220000	0.207059994
0.623660028	0.583029985	0.209759995
0.376289994	0.586989999	0.208560005
0.623139977	0.081009999	0.207670003
0.375559986	0.082829997	0.208509997
0.749040008	0.330240011	0.207379997
0.249170005	0.332219988	0.206110001
0.500230014	0.335979998	0.207190007
0.251590014	0.499639988	0.313389987
0.503650010	0.003740000	0.323520005
0.752240002	0.494520009	0.311390013
0.002820000	0.998570025	0.321680009
0.127379999	0.745790005	0.314269990
0.876190007	0.752290010	0.313080013
0.004500000	0.499170005	0.322589993
0.250059992	0.998310030	0.317449987
0.126599997	0.247559994	0.312700003
0.379999995	0.752160013	0.321200013
0.754740000	0.002440000	0.309720010
0.876730025	0.249329999	0.318439990
0.631760001	0.751290023	0.323480010
0.503769994	0.498109996	0.320210010
0.625490010	0.249139994	0.313549995
0.373589993	0.249720007	0.311729997

CHCO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	1	8	64

Direct

0.862420022	0.070830002	0.380600005
0.137610003	0.095449999	0.381060004
0.860279977	0.410279989	0.381749988
0.372999996	0.892279983	0.382770002
0.747910023	0.738770008	0.383899987

0.332830012	0.387930006	0.385109991
0.563830018	0.138029993	0.386660010
0.070280001	0.630630016	0.387690008
0.442009985	0.463330001	0.401369989
0.275500000	0.350479990	0.422769994
0.854330003	0.067890003	0.434920013
0.137740001	0.106720001	0.435400009
0.852349997	0.413190007	0.436080009
0.369630009	0.886650026	0.437169999
0.749960005	0.737540007	0.437940001
0.565909982	0.145449996	0.440589994
0.074340001	0.634540021	0.441650003
0.490240008	0.498250008	0.448089987
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003

0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.750270009	0.832189977	0.206430003
0.249449998	0.331070006	0.206689999
0.499680012	0.332760006	0.207139999
0.877219975	0.083860002	0.207340002
0.626089990	0.581669986	0.207589999
0.876060009	0.580630004	0.207670003
0.375030011	0.585560024	0.207810000
0.622399986	0.079599999	0.207890004
0.124969997	0.077909999	0.207870007
0.748480022	0.328689992	0.207920000
0.247700006	0.831690013	0.208800003
0.124739997	0.577929974	0.208890006
0.500670016	0.834280014	0.209460005
0.998700023	0.332879990	0.209900007
0.374179989	0.082750000	0.209989995
0.998769999	0.831300020	0.210020006
0.752139986	0.999379992	0.310479999
0.124729998	0.243100002	0.311749995
0.748549998	0.492110014	0.313279986
0.621429980	0.246590003	0.314090014
0.504159987	0.502529979	0.314249992
0.376269996	0.746940017	0.314429998
0.251139998	0.494879991	0.314590007
0.371149987	0.251399994	0.314619988
0.123939998	0.741819978	0.315319985
0.872070014	0.748319983	0.315259993
0.626070023	0.747250021	0.315640002
0.874180019	0.246140003	0.318720013
0.249349996	0.993409991	0.319200009
0.000560000	0.995209992	0.321489990
0.001490000	0.495209992	0.323060006
0.500949979	0.998030007	0.323320001

CHCO-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C H O Pt
9 2 8 64

Direct

0.862540007	0.070230000	0.380369991
0.136580005	0.093970001	0.380699992
0.873319983	0.407389998	0.382279992
0.372480005	0.891520023	0.382930011
0.748260021	0.737999976	0.383439988
0.326790005	0.385039985	0.385159999
0.563359976	0.133829996	0.388390005
0.073559999	0.632870018	0.387739986
0.429890007	0.467750013	0.403499991
0.628820002	0.413919985	0.354930013
0.267839998	0.345750004	0.421779990
0.853590012	0.067560002	0.434650004
0.137720004	0.107009999	0.435000002
0.863449991	0.407779992	0.436569989
0.368050009	0.885259986	0.437290013
0.750339985	0.736079991	0.437519997
0.564920008	0.142220005	0.442270011
0.078019999	0.636789978	0.441670001
0.472240001	0.508499980	0.450729996
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003

0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.750100017	0.832769990	0.206190005
0.249799997	0.331059992	0.206359997
0.500039995	0.333270013	0.207719997
0.877579987	0.084020004	0.207169995
0.625810027	0.581439972	0.208389997
0.875440001	0.580250025	0.207890004
0.376419991	0.585030019	0.208230004
0.622430027	0.081529997	0.208210006
0.125259995	0.077459998	0.207619995
0.748459995	0.329439998	0.208360001
0.248180002	0.831269979	0.208519995
0.124679998	0.577970028	0.208550006
0.501230001	0.835139990	0.209360003
0.998730004	0.333059996	0.209629998
0.374570012	0.082879998	0.210120007
0.998640001	0.831049979	0.209800005
0.752950013	0.999610007	0.309850007
0.125049993	0.242320001	0.310990006
0.754050016	0.493939996	0.314700007
0.621580005	0.244169995	0.315690011
0.501829982	0.505630016	0.317140013
0.376069993	0.748030007	0.313950002
0.250380009	0.494509995	0.313699991
0.370499998	0.251410007	0.314449996
0.124530002	0.742609978	0.314790010
0.872770011	0.749080002	0.314870000
0.626429975	0.750060022	0.315310001
0.876309991	0.244839996	0.318069994

0.249899998	0.993830025	0.318940014
0.001480000	0.994329989	0.321929991
0.004040000	0.495669991	0.323379993
0.500760019	0.997979999	0.324119985

CHCHO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	2	8	64

Direct

0.859899998	0.073239997	0.380730003
0.133070007	0.090360001	0.380230010
0.861150026	0.410299987	0.381240010
0.374579996	0.891709983	0.382360011
0.747929990	0.739359975	0.383879989
0.313560009	0.375640005	0.389849991
0.559499979	0.143940002	0.385989994
0.071510002	0.630169988	0.387870014
0.405360013	0.436289996	0.427639991
0.396739990	0.430669993	0.478040010
0.241300002	0.328729987	0.416979998
0.851520002	0.070610002	0.435059994
0.134849995	0.104840003	0.434560001
0.852060020	0.413430005	0.435579985
0.370790005	0.885200024	0.436820000
0.748449981	0.736630023	0.437979996
0.559669971	0.153779998	0.439999998
0.075319998	0.633520007	0.441920012
0.498540014	0.497119993	0.407909989
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000

0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.750999987	0.832769990	0.206210002
0.249699995	0.331010014	0.206880003
0.499069989	0.332740009	0.207039997
0.877370000	0.083530001	0.207369998
0.626079977	0.582120001	0.207509995
0.877210021	0.581560016	0.207190007
0.374900013	0.584969997	0.208049998
0.622380018	0.079790004	0.207640007
0.125139996	0.076949999	0.207289994
0.748700023	0.328929991	0.207540005
0.247810006	0.831239998	0.208509997
0.125619993	0.577939987	0.209140003
0.500909984	0.834599972	0.209279999
0.998560011	0.333149999	0.209470004
0.374260008	0.082889996	0.210260004
0.999130011	0.831229985	0.210449994
0.751919985	0.000100000	0.310589999
0.124179997	0.240750000	0.309729993
0.752550006	0.492980003	0.312249988

0.621829987	0.248170003	0.313459992
0.507849991	0.505010009	0.311390013
0.377149999	0.746739984	0.313890010
0.252840012	0.493950009	0.315950006
0.371019989	0.252339989	0.315880001
0.125070006	0.741280019	0.315699995
0.873049974	0.748870015	0.315820009
0.627900004	0.750880003	0.315019995
0.874689996	0.245649993	0.318250000
0.249870002	0.992820024	0.319160014
0.000530000	0.994220018	0.322109997
0.003450000	0.494599998	0.323159993
0.500649989	0.999830008	0.323549986

CHCHO-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	3	8	64

Direct

0.858020008	0.065159999	0.381819993
0.132359996	0.088780001	0.381909996
0.801819980	0.386359990	0.385729998
0.371419996	0.892579973	0.382090002
0.734860003	0.740490019	0.386510015
0.553059995	0.144140005	0.385569990
0.313950002	0.381900012	0.390179992
0.014920000	0.662670016	0.380970001
0.407090008	0.440420002	0.427630007
0.069250003	0.372260004	0.363620013
0.241889998	0.335779995	0.417679995
0.399589986	0.434280008	0.478060007
0.849659979	0.061620001	0.436150014
0.133919999	0.099579997	0.436329991
0.799170017	0.391999990	0.439689994
0.368759990	0.886250019	0.436560005
0.731339991	0.737609982	0.440459996
0.553149998	0.155169994	0.439550012
0.500440001	0.500010014	0.407359987
0.020439999	0.661719978	0.435530007

0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.626800001	0.582830012	0.207440004
0.498149991	0.333270013	0.206939995
0.753019989	0.831700027	0.207269996
0.375380009	0.586489975	0.207409993
0.248879999	0.332179993	0.207629994
0.876760006	0.084710002	0.208320007
0.622879982	0.079429999	0.207389995
0.124349996	0.080700003	0.208189994
0.748030007	0.328960001	0.207220003

0.877260029	0.581990004	0.207880005
0.247749999	0.834450006	0.207690001
0.127030000	0.581070006	0.207959995
0.501280010	0.835409999	0.209220007
0.373510003	0.084380001	0.210429996
0.997929990	0.332810014	0.209050000
0.998009980	0.833549976	0.210199997
0.504170001	0.507510006	0.310680002
0.750620008	0.998520017	0.310829997
0.118730001	0.243809998	0.312629998
0.747969985	0.493470013	0.312279999
0.616989970	0.246989995	0.312649995
0.367680013	0.254949987	0.316500008
0.626479983	0.752219975	0.314209998
0.374049991	0.749880016	0.313239992
0.124339998	0.746110022	0.313950002
0.873090029	0.745890021	0.322059989
0.254020005	0.500249982	0.316029996
0.866689980	0.248129994	0.321350008
0.246969998	0.996800005	0.319079995
0.498059988	0.999989986	0.322849989
0.997370005	0.997659981	0.322259992
0.002630000	0.497640014	0.317039996

CH2CHO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	3	8	64

Direct

0.875750005	0.066100001	0.379519999
0.191210002	0.142089993	0.386539996
0.811410010	0.387160003	0.386709988
0.373789996	0.889680028	0.382640004
0.735339999	0.740339994	0.386680007
0.552259982	0.144649997	0.385540009
0.271470010	0.500029981	0.412820011
0.011640000	0.661379993	0.379110008
0.392540008	0.492709994	0.439539999
0.217590004	0.414950013	0.432920009

0.230179995	0.595730007	0.431510001
0.397810012	0.487729996	0.490319997
0.874840021	0.055300001	0.433979988
0.196170002	0.152219996	0.440589994
0.809239984	0.395049989	0.440660000
0.373210013	0.878430009	0.437110007
0.733539999	0.738470018	0.440690011
0.547070026	0.158140004	0.439350009
0.490920007	0.492900014	0.412429988
0.016430000	0.657830000	0.433910012
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003

0.875000000	0.916670024	0.103940003
0.626739979	0.581979990	0.208790004
0.500970006	0.333920002	0.205679998
0.752439976	0.831499994	0.207690001
0.374909997	0.586070001	0.207859993
0.248009995	0.335409999	0.206650004
0.875559986	0.085589997	0.207570001
0.623920023	0.078649998	0.207870007
0.125719994	0.081890002	0.208130002
0.749450028	0.329010010	0.207969993
0.875559986	0.581019998	0.207499996
0.247280002	0.835020006	0.209020004
0.126159996	0.582989991	0.208010003
0.502070010	0.833410025	0.209490001
0.374460012	0.078610003	0.207379997
0.000310000	0.332159996	0.210179999
0.997690022	0.832300007	0.208529994
0.499879986	0.501450002	0.312269986
0.752250016	0.999130011	0.312599987
0.126939997	0.250829995	0.315919995
0.748359978	0.490990013	0.313870013
0.620209992	0.245550007	0.313290000
0.373600006	0.252530009	0.305920005
0.625360012	0.748889983	0.315219998
0.373629987	0.749270022	0.313030005
0.123640001	0.749769986	0.314289987
0.872099996	0.745540023	0.321099997
0.253829986	0.499570012	0.318390012
0.876169980	0.249809995	0.322910011
0.246669993	0.998920023	0.323150009
0.499870002	0.997829974	0.323179990
0.998319983	0.999339998	0.313329995
0.005530000	0.497999996	0.314929992

CH2CHO-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	4	8	64

Direct

0.008750000	0.657040000	0.379700005
0.143289998	0.102380000	0.381139994
0.377889991	0.901889980	0.382039994
0.864669979	0.068030000	0.381779999
0.553990006	0.149649993	0.385399997
0.735939980	0.741389990	0.387320012
0.811829984	0.389369994	0.386409998
0.275070012	0.460060000	0.415569991
0.395729989	0.483449996	0.441280007
0.252299994	0.667800009	0.352079988
0.251280010	0.351590008	0.427630007
0.209380001	0.524219990	0.440930009
0.402410001	0.487190008	0.492069989
0.492399991	0.496329993	0.413249999
0.015939999	0.651300013	0.434410006
0.143619999	0.109810002	0.435710013
0.857749999	0.061700001	0.436179996
0.371109992	0.893790007	0.436479986
0.547469974	0.164199993	0.439119995
0.733349979	0.739470005	0.441320002
0.809369981	0.397430003	0.440349996
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003

0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.501559973	0.334699988	0.205420002
0.248140007	0.335220009	0.206499994
0.374890000	0.077650003	0.206919998
0.624450028	0.078100003	0.207680002
0.876030028	0.582570016	0.207399994
0.753340006	0.831700027	0.207790002
0.749480009	0.328999996	0.207609996
0.125139996	0.080610000	0.207810000
0.247690007	0.831780016	0.208440006
0.877579987	0.085029997	0.208370000
0.374350011	0.584940016	0.208749995
0.626749992	0.582570016	0.208649993
0.126289994	0.582149982	0.208600000
0.998929977	0.332910001	0.209350005
0.502319992	0.832639992	0.209549993
0.998539984	0.833609998	0.210099995
0.375039995	0.250050008	0.305280000
0.754630029	0.999360025	0.311749995
0.127839997	0.249349996	0.313199997
0.502080023	0.500590026	0.312519997
0.621890008	0.246730000	0.312599987
0.749379992	0.492379993	0.313190013
0.378760010	0.751240015	0.314429998
0.627359986	0.748989999	0.315360010
0.122079998	0.749939978	0.315360010
0.004380000	0.496859998	0.314709991
0.250840008	0.999409974	0.317860007
0.254619986	0.489850014	0.321599990
0.001600000	0.002480000	0.320749998

0.873310030	0.746930003	0.322079986
0.503480017	0.999689996	0.323439986
0.875349998	0.250690013	0.322880000

CH3CHO

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	4	8	64

Direct

0.058600001	0.627170026	0.384559989
0.197870001	0.145219997	0.386570007
0.375490010	0.888509989	0.383569986
0.875450015	0.063129999	0.379770011
0.545799971	0.148790002	0.385190010
0.745700002	0.733219981	0.383610010
0.815140009	0.386940002	0.386539996
0.332670003	0.477589995	0.462449998
0.464219987	0.493090004	0.461050004
0.294620007	0.468450010	0.415840000
0.308550000	0.385529995	0.489899993
0.293099999	0.568260014	0.485949993
0.512040019	0.498730004	0.505670011
0.529709995	0.501330018	0.415179998
0.058470000	0.625689983	0.438870013
0.206080005	0.156279996	0.440479994
0.873109996	0.053339999	0.434280008
0.374749988	0.878669977	0.438129991
0.537450016	0.165380001	0.438870013
0.747060001	0.729369998	0.437790006
0.812990010	0.395420015	0.440519989
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000

0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.500549972	0.333799988	0.206330001
0.248679996	0.331099987	0.205390006
0.374130011	0.077790000	0.207749993
0.622940004	0.079539999	0.208039999
0.875230014	0.580349982	0.207430005
0.750320017	0.833270013	0.206459999
0.749239981	0.328669995	0.208120003
0.125279993	0.079920001	0.208480000
0.247119993	0.833909988	0.210010007
0.875609994	0.085620001	0.207870007
0.377559990	0.586650014	0.207130000
0.627139986	0.582069993	0.208849996
0.123779997	0.583369970	0.205929995
0.000280000	0.331600010	0.210759997
0.501269996	0.833949983	0.210189998
0.997789979	0.831950009	0.209130004
0.374060005	0.251839995	0.307859987
0.751370013	0.999650002	0.312550008

0.127480000	0.248410001	0.316089988
0.498010010	0.500079989	0.314179987
0.620869994	0.245849997	0.313749999
0.750169992	0.490590006	0.313760012
0.374000013	0.746010005	0.315070003
0.625450015	0.747910023	0.315279990
0.123750001	0.746370018	0.316619992
0.006770000	0.497200012	0.316240013
0.246600002	0.996280015	0.323700011
0.253199995	0.497269988	0.308169991
0.998570025	0.996169984	0.314469993
0.871240020	0.746869981	0.315620005
0.499749988	0.996819973	0.323909998
0.876850009	0.248219997	0.322930008

CH3CHO-H

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	5	8	64

Direct

0.876020014	0.064659998	0.379759997
0.747399986	0.738259971	0.384110004
0.375519991	0.890829980	0.383850008
0.058189999	0.627770007	0.384600013
0.546549976	0.150729999	0.385109991
0.817179978	0.389319986	0.386619985
0.198609993	0.148939997	0.386440009
0.478500009	0.512239993	0.469440013
0.345800012	0.519529998	0.472640008
0.366950005	0.408879995	0.350270003
0.305290014	0.543259978	0.427929997
0.318370014	0.597199976	0.506929994
0.311960012	0.418199986	0.489019990
0.527989984	0.508610010	0.513750017
0.541289985	0.508260012	0.422719985
0.873880029	0.054740001	0.434260011
0.749300003	0.736129999	0.438279986
0.375730008	0.881179988	0.438410014
0.057510000	0.626659989	0.438899994

0.538999975	0.166329995	0.438859999
0.816479981	0.398000002	0.440569997
0.207379997	0.162259996	0.440219998
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249449998	0.331209987	0.205899999
0.125119999	0.582570016	0.206129998
0.500289977	0.333719999	0.206770003
0.750530005	0.832669973	0.206520006
0.377480000	0.587249994	0.207509995
0.875490010	0.580160022	0.207369998

0.374190003	0.079360001	0.207859993
0.875569999	0.085359998	0.207739994
0.623179972	0.079350002	0.208140001
0.749180019	0.328700006	0.208000004
0.125249997	0.079700001	0.208389997
0.998220026	0.831239998	0.208969995
0.626760006	0.581879973	0.208949998
0.247449994	0.834640026	0.210060000
0.501489997	0.834399998	0.210079998
0.000270000	0.331499994	0.210649997
0.374280006	0.247600004	0.309630007
0.251179993	0.500039995	0.309219986
0.751890004	0.999920011	0.312570006
0.998549998	0.996100008	0.314289987
0.622709990	0.246360004	0.313600004
0.502390027	0.503960013	0.315329999
0.750819981	0.491510004	0.313760012
0.374909997	0.748799980	0.315070003
0.626439989	0.749310017	0.315829992
0.871720016	0.747319996	0.315640002
0.123709999	0.746749997	0.316489995
0.006010000	0.497689992	0.316199988
0.125599995	0.247240007	0.315239996
0.876730025	0.248579994	0.323009998
0.500840008	0.997389972	0.323920012
0.245989993	0.996179998	0.324470013

CH3CHOH

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	5	8	64

Direct

0.876290023	0.063759997	0.379000008
0.747789979	0.726769984	0.382149994
0.372579992	0.892620027	0.382030010
0.064240001	0.626969993	0.384539992
0.564400017	0.133169994	0.386790007
0.833019972	0.392659992	0.385729998
0.190490007	0.141749993	0.386590004

0.481290013	0.520030022	0.425969988
0.372049987	0.444209993	0.448670000
0.647119999	0.538699985	0.452769995
0.381209999	0.331369996	0.443760008
0.289869994	0.479319990	0.425359994
0.362089992	0.467290014	0.498050004
0.474720001	0.633840024	0.428429991
0.582849979	0.468719989	0.452760011
0.873470008	0.054159999	0.433459997
0.746819973	0.717090011	0.436650008
0.373780012	0.883159995	0.436589986
0.065669999	0.625440001	0.438749999
0.565590024	0.136920005	0.440849990
0.839619994	0.403699994	0.439630002
0.193770006	0.148819998	0.440629989
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003

0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249129996	0.331640005	0.205280006
0.124490000	0.583039999	0.206090003
0.501709998	0.335700005	0.207420006
0.750069976	0.832849979	0.206389993
0.378960013	0.585929990	0.207300007
0.874539971	0.580349982	0.207870007
0.374779999	0.079099998	0.207870007
0.876010001	0.086209998	0.207399994
0.623440027	0.081479996	0.208069995
0.749220014	0.330110013	0.208700001
0.125650004	0.080130003	0.208289996
0.998139977	0.831489980	0.208910003
0.626190007	0.580690026	0.210240006
0.247940004	0.833809972	0.209570006
0.502129972	0.833599985	0.209490001
0.000550000	0.332650006	0.210519999
0.376419991	0.254999995	0.307370007
0.256419986	0.498879999	0.307880014
0.751999974	0.000130000	0.311549991
0.999270022	0.996249974	0.313800007
0.620150030	0.247879997	0.315890014
0.497599989	0.500069976	0.326040000
0.748369992	0.490630001	0.315800011
0.375930011	0.746720016	0.313930005
0.624949992	0.745559990	0.315380007
0.872080028	0.747479975	0.315380007
0.125489995	0.746930003	0.315950006
0.008000000	0.498389989	0.316219985
0.129030004	0.249689996	0.315450013
0.877799988	0.248249993	0.321660012
0.501179993	0.997430027	0.321969986
0.247850001	0.998250008	0.322649986

CH3CHOH-H

1.0

11.1216001511	0.0000000000	0.0000000000
---------------	--------------	--------------

	0.0000000000	9.6316003799	0.0000000000
	0.0000000000	0.0000000000	21.7964000702
C	H	O	Pt
9	6	8	64
Direct			
0.878369987	0.064680003	0.378930002	
0.373829991	0.893429995	0.382380009	
0.749589980	0.730849981	0.382519990	
0.062479999	0.628589988	0.384469986	
0.831399977	0.392879993	0.385720015	
0.198109999	0.148379996	0.386020005	
0.570630014	0.131150007	0.386460006	
0.493519992	0.545729995	0.434940010	
0.371399999	0.512499988	0.460429996	
0.412220001	0.370209992	0.365159988	
0.299989998	0.566070020	0.435169995	
0.515540004	0.656809986	0.433369994	
0.353839993	0.400279999	0.460900009	
0.659290016	0.509190023	0.458240002	
0.369399995	0.549589992	0.508310020	
0.874620020	0.054380000	0.433360010	
0.375090003	0.884360015	0.436969995	
0.749189973	0.723569989	0.436989993	
0.062660001	0.628040016	0.438710004	
0.835380018	0.403470010	0.439870000	
0.574469984	0.135399997	0.440459996	
0.205320001	0.158940002	0.439880013	
0.579670012	0.465990007	0.461739987	
0.000000000	0.000000000	0.000000000	
0.000000000	0.500000000	0.000000000	
0.125000000	0.250000000	0.000000000	
0.125000000	0.750000000	0.000000000	
0.250000000	0.000000000	0.000000000	
0.250000000	0.500000000	0.000000000	
0.375000000	0.250000000	0.000000000	
0.375000000	0.750000000	0.000000000	
0.500000000	0.000000000	0.000000000	
0.500000000	0.500000000	0.000000000	
0.625000000	0.250000000	0.000000000	
0.625000000	0.750000000	0.000000000	
0.750000000	0.000000000	0.000000000	

0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249939993	0.332060009	0.205369994
0.125039995	0.583010018	0.206110001
0.750000000	0.832310021	0.206379995
0.380030006	0.586359978	0.207680002
0.876739979	0.086470000	0.207190007
0.374769986	0.080729999	0.208430007
0.501850009	0.336510003	0.207760006
0.623660028	0.081670001	0.207800001
0.874339998	0.580200016	0.207839996
0.126049995	0.080169998	0.208330005
0.749530017	0.330480009	0.208560005
0.998459995	0.831219971	0.208859995
0.502300024	0.834200025	0.209460005
0.248610005	0.834249973	0.209549993
0.000850000	0.332980007	0.210529998
0.625400007	0.580150008	0.210979998
0.377350003	0.254480004	0.308360010
0.255950004	0.501879990	0.307159990
0.753840029	0.000530000	0.310880005
0.000570000	0.996730030	0.313789994
0.376549989	0.748369992	0.314000010
0.129030004	0.250530005	0.314990014

0.126049995	0.747829974	0.316009998
0.872759998	0.748260021	0.315210015
0.007940000	0.499240011	0.316359997
0.625899971	0.745800018	0.315450013
0.748899996	0.491589993	0.316009998
0.622959971	0.246840000	0.314830005
0.502849996	0.997380018	0.322210014
0.878809988	0.249109998	0.321929991
0.248620003	0.998820007	0.323069990
0.499749988	0.505460024	0.334989995

CH3CH2OH

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	6	8	64

Direct

0.875249982	0.062799998	0.379629999
0.374300003	0.893930018	0.382809997
0.746890008	0.727999985	0.382880002
0.062070001	0.625249982	0.384959996
0.817650020	0.386700004	0.386370003
0.183170006	0.134580001	0.387180001
0.556280017	0.142030001	0.385919988
0.426420003	0.532400012	0.463999987
0.326409996	0.427740008	0.462610006
0.394970000	0.637700021	0.452960014
0.256720006	0.455619991	0.496109992
0.471049994	0.534550011	0.509130001
0.282539994	0.426600009	0.416970015
0.591440022	0.546649992	0.428020000
0.359140009	0.322629988	0.472510010
0.872929990	0.053119998	0.434100002
0.374020010	0.887019992	0.437500000
0.744949996	0.717999995	0.437229991
0.062639996	0.623539984	0.439190000
0.815230012	0.395729989	0.440400004
0.553430021	0.152999997	0.439830005
0.181569993	0.138150007	0.441289991
0.519469976	0.491120011	0.419800013

0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.248500004	0.331490010	0.205410004
0.124119997	0.583060026	0.206159994
0.750509977	0.833029985	0.206489995
0.377490014	0.586489975	0.207249999
0.875869989	0.085610002	0.207770005
0.374260008	0.077569999	0.207609996
0.501089990	0.333810002	0.206180006
0.623350024	0.079630002	0.207890004
0.875400007	0.580349982	0.207619995

0.125340000	0.079719998	0.208279997
0.749549985	0.329050004	0.208100006
0.998030007	0.831409991	0.209209993
0.501359999	0.833620012	0.210069999
0.247459993	0.833350003	0.209979996
0.000380000	0.331779987	0.210749999
0.627260029	0.582009971	0.208820000
0.374630004	0.252180010	0.307000011
0.254500002	0.496969998	0.308919996
0.751789987	0.999149978	0.312290013
0.998549998	0.995469987	0.314229995
0.374890000	0.746349990	0.315589994
0.128250003	0.247779995	0.316069990
0.124559999	0.745500028	0.316729993
0.871819973	0.746840000	0.315899998
0.007540000	0.496859998	0.316469997
0.625339985	0.747269988	0.315439999
0.750050008	0.490599990	0.314130008
0.621029973	0.245940000	0.313840002
0.500609994	0.997470021	0.322930008
0.877340019	0.248060003	0.322719991
0.247030005	0.996590018	0.322829992
0.498829991	0.499890000	0.314260006

TS1

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C H O Pt
8 1 9 64

Direct

0.875199974	0.087140001	0.385190010
0.860490024	0.414370000	0.382110000
0.755699992	0.724799991	0.382220000
0.604330003	0.993690014	0.387140006
0.138510004	0.977469981	0.386940002
0.443450004	0.632839978	0.384039998
0.079389997	0.624480009	0.386839986
0.375259995	0.273380011	0.420240015
0.565980017	0.277249992	0.384059995
0.873849988	0.088409998	0.439570010

0.855899990	0.419919997	0.436450005
0.753679991	0.718159974	0.436250001
0.604520023	0.987550020	0.440979987
0.140939996	0.968850017	0.440780014
0.446040004	0.632700026	0.438149989
0.087320000	0.623700023	0.440640002
0.480599999	0.276919991	0.438400000
0.272060007	0.278629988	0.437240005
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.251130015	0.330139995	0.205119997

0.750159979	0.837670028	0.207300007
0.375519991	0.583339989	0.206009999
0.498979986	0.334699988	0.207699999
0.121660002	0.582700014	0.206630006
0.874859989	0.084100001	0.211170003
0.374949992	0.078520000	0.209419996
0.625379980	0.084909998	0.207920000
0.123580001	0.080150001	0.206949994
0.874719977	0.583840013	0.207900003
0.750630021	0.332520008	0.207870007
0.626619995	0.582910001	0.207890004
0.998149991	0.834670007	0.210030004
0.501850009	0.832069993	0.208509997
0.997739971	0.334850013	0.208790004
0.249400005	0.830009997	0.209250003
0.249290004	0.495429993	0.307509989
0.371069998	0.251080006	0.316709995
0.744379997	0.011650000	0.321429998
0.001610000	0.003330000	0.322499990
0.747669995	0.495240003	0.314720005
0.872919977	0.754760027	0.313679993
0.627950013	0.749629974	0.314639986
0.129050002	0.252149999	0.308349997
0.615379989	0.257990003	0.313300014
0.496309996	0.502300024	0.315640002
0.125909999	0.745509982	0.315660000
0.495680004	0.003110000	0.315640002
0.876510024	0.251340002	0.319559991
0.251120001	0.999350011	0.316300005
0.374260008	0.749849975	0.316119999
0.002330000	0.499879986	0.321269989

TS2

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	9	64

Direct

0.621140003	0.434489995	0.378989995
0.875209987	0.085759997	0.376060009

0.560930014	0.114940003	0.386330009
0.170359999	0.127619997	0.387479991
0.731459975	0.749580026	0.387989998
0.012540000	0.744899988	0.388669997
0.338990003	0.871490002	0.387360007
0.269230008	0.499150008	0.412380010
0.367370009	0.307520002	0.385729998
0.381900012	0.389189988	0.469209999
0.616479993	0.439590007	0.433809996
0.875190020	0.080270000	0.430729985
0.558719993	0.112470001	0.440450013
0.159649998	0.127859995	0.441300005
0.725220025	0.752110004	0.441879988
0.017519999	0.749979973	0.442519993
0.349330008	0.874310017	0.441100001
0.244320005	0.581979990	0.451189995
0.329540014	0.371039987	0.433519989
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003

0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.501030028	0.334109992	0.206770003
0.625670016	0.584490001	0.207039997
0.250149995	0.334630013	0.207300007
0.876519978	0.082610004	0.205720007
0.374210000	0.079879999	0.207949996
0.625689983	0.084700003	0.207320005
0.752799988	0.832149982	0.208059996
0.998489976	0.829289973	0.207920000
0.127859995	0.080320001	0.208560005
0.002300000	0.329490006	0.207159996
0.749119997	0.331539989	0.208480000
0.873430014	0.581480026	0.208690003
0.501439989	0.834249973	0.209160000
0.374960005	0.585179985	0.209910005
0.248119995	0.832920015	0.209830001
0.127719998	0.582140028	0.208710000
0.374949992	0.255369991	0.309210002
0.752629995	0.492790014	0.315710008
0.753610015	0.002440000	0.311589986
0.998600006	0.999530017	0.311509997
0.501200020	0.505370021	0.313499987
0.127629995	0.250310004	0.316700011
0.626559973	0.753660023	0.314350009
0.503269970	0.002970000	0.315050006
0.000560000	0.491739988	0.309760004
0.120329998	0.746209979	0.315510005
0.375169992	0.750649989	0.315750003
0.878849983	0.251150012	0.315380007
0.624029994	0.249500006	0.320859998
0.250990003	0.501730025	0.321960002
0.873570025	0.743529975	0.325470001
0.248830006	0.998250008	0.324149996

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	1	8	64

Direct

0.577210009	0.113150001	0.382820010
0.877309978	0.069739997	0.378659993
0.385259986	0.330940008	0.400319993
0.861320019	0.409289986	0.382140011
0.754440010	0.741779983	0.384499997
0.457329988	0.669139981	0.384600013
0.171969995	0.108250000	0.384719998
0.076700002	0.628970027	0.387989998
0.480690002	0.409429997	0.392080009
0.586080015	0.114399999	0.436850011
0.874719977	0.061620001	0.433050007
0.855000019	0.411579996	0.436549991
0.757309973	0.739480019	0.438540012
0.462819993	0.668640018	0.438730001
0.337449998	0.334630013	0.448659986
0.162680000	0.105010003	0.438620001
0.082819998	0.629700005	0.441920012
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003

0.00000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.125070006	0.080380000	0.207369998
0.749109983	0.832170010	0.206550002
0.249850005	0.329459995	0.206839994
0.749880016	0.331110001	0.207719997
0.625230014	0.581409991	0.209979996
0.377339989	0.583440006	0.207059994
0.876580000	0.085670002	0.206829995
0.875010014	0.580560029	0.208000004
0.624440014	0.082670003	0.206760004
0.122299999	0.581849992	0.206430003
0.999000013	0.831110001	0.208660007
0.499700010	0.334729999	0.208120003
0.501510024	0.833940029	0.209150001
0.000920000	0.333829999	0.210490003
0.374639988	0.083169997	0.209529996
0.250270009	0.832009971	0.209749997
0.248930007	0.498310000	0.306899995
0.999830008	0.993650019	0.314060003
0.872979999	0.747650027	0.314229995
0.128069997	0.244519994	0.316529989
0.624469995	0.246439993	0.313439995
0.627650023	0.751439989	0.317889988
0.751450002	0.491549999	0.314379990
0.500299990	0.999620020	0.316830009
0.503030002	0.502200007	0.321940005
0.126149997	0.745980024	0.316610008

0.373320013	0.753629982	0.314669997
0.878759980	0.246490002	0.318760008
0.249029994	0.994769990	0.317990005
0.753400028	0.000810000	0.311219990
0.372729987	0.253839999	0.316579998
0.004490000	0.496939987	0.323060006

TS4

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	8	64

Direct

0.879029989	0.071780004	0.378919989
0.861949980	0.411159992	0.381749988
0.578459978	0.113410003	0.382459998
0.456959993	0.648930013	0.384200007
0.753859997	0.743439972	0.383839995
0.176090002	0.110930003	0.384180009
0.071439996	0.633970022	0.388280004
0.366569996	0.317970008	0.426200002
0.434340000	0.364349991	0.377330005
0.411940008	0.235159993	0.452719986
0.876389980	0.064390004	0.433349997
0.290699989	0.396450013	0.443549991
0.854709983	0.414119989	0.436150014
0.585600019	0.114399999	0.436830014
0.168870002	0.109099999	0.438369989
0.463250011	0.651170015	0.438369989
0.755670011	0.741620004	0.437909991
0.072999999	0.636820018	0.442240000
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000

0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.376410007	0.584460020	0.206550002
0.749970019	0.833060026	0.206369996
0.122010000	0.582970023	0.206469998
0.877189994	0.085890003	0.206980005
0.125640005	0.080590002	0.207379997
0.624909997	0.082989998	0.207010001
0.249950007	0.330330014	0.206410006
0.750299990	0.331169993	0.207729995
0.625769973	0.581939995	0.208930001
0.875549972	0.581149995	0.207980007
0.999620020	0.831889987	0.208810002
0.501489997	0.834219992	0.209330007
0.500370026	0.335480005	0.208330005
0.250809997	0.832690001	0.210099995
0.375310004	0.084009998	0.209889993
0.001240000	0.334179997	0.210419998
0.249390006	0.497709990	0.306320012
0.754379988	0.001970000	0.311650008

0.751230001	0.492579997	0.313970000
0.001070000	0.994799972	0.314550012
0.874090016	0.748769999	0.314249992
0.624549985	0.247630000	0.314359993
0.628889978	0.751590014	0.316260010
0.129549995	0.245230004	0.316020012
0.375479996	0.751810014	0.316179991
0.502449989	0.502099991	0.319169998
0.127710000	0.746460021	0.316870004
0.501119971	0.998170018	0.317570001
0.250779986	0.994109988	0.318069994
0.879450023	0.247659996	0.318740010
0.005210000	0.497689992	0.323009998
0.375200003	0.254009992	0.316219985

TS5

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	8	64

Direct

0.863709986	0.072549999	0.382620007
0.817740023	0.395420015	0.387080014
0.444409996	0.629010022	0.384950012
0.546440005	0.131459996	0.384119987
0.140809998	0.995800018	0.387919992
0.751100004	0.742089987	0.384160012
0.057640001	0.639339983	0.385919988
0.315890014	0.324070007	0.466230005
0.100380003	0.339230001	0.373210013
0.408340007	0.367029995	0.471219987
0.300190002	0.217010006	0.483610004
0.852859974	0.067829996	0.436780006
0.820029974	0.402359992	0.441089988
0.235430002	0.392309994	0.442799985
0.446570009	0.628859997	0.439209998
0.542330027	0.138009995	0.438369989
0.145490006	0.996519983	0.442039996
0.752579987	0.739400029	0.438290000
0.054609999	0.644410014	0.439949989

0.00000000	0.00000000	0.00000000
0.00000000	0.50000000	0.00000000
0.12500000	0.25000000	0.00000000
0.12500000	0.75000000	0.00000000
0.25000000	0.00000000	0.00000000
0.25000000	0.50000000	0.00000000
0.37500000	0.25000000	0.00000000
0.37500000	0.75000000	0.00000000
0.50000000	0.00000000	0.00000000
0.50000000	0.50000000	0.00000000
0.62500000	0.25000000	0.00000000
0.62500000	0.75000000	0.00000000
0.75000000	0.00000000	0.00000000
0.75000000	0.50000000	0.00000000
0.87500000	0.25000000	0.00000000
0.87500000	0.75000000	0.00000000
0.00000000	0.166669995	0.103940003
0.00000000	0.666670024	0.103940003
0.12500000	0.416669995	0.103940003
0.12500000	0.916670024	0.103940003
0.25000000	0.166669995	0.103940003
0.25000000	0.666670024	0.103940003
0.37500000	0.416669995	0.103940003
0.37500000	0.916670024	0.103940003
0.50000000	0.166669995	0.103940003
0.50000000	0.666670024	0.103940003
0.62500000	0.416669995	0.103940003
0.62500000	0.916670024	0.103940003
0.75000000	0.166669995	0.103940003
0.75000000	0.666670024	0.103940003
0.87500000	0.416669995	0.103940003
0.87500000	0.916670024	0.103940003
0.248989999	0.330980003	0.204539999
0.751230001	0.834619999	0.206650004
0.377370000	0.584150016	0.206100002
0.501330018	0.335399985	0.207379997
0.373800009	0.077830002	0.207609996
0.878929973	0.086340003	0.209409997
0.625469983	0.082860000	0.207120001
0.124100000	0.082139999	0.208260000
0.123109996	0.583480000	0.206220001

0.627250016	0.583299994	0.209199995
0.749000013	0.330819994	0.208499998
0.874939978	0.582989991	0.208489999
0.999329984	0.835120022	0.209759995
0.502030015	0.833220005	0.209979996
0.249990001	0.830009997	0.209570006
0.996609986	0.336160004	0.209680006
0.371080011	0.250690013	0.308539987
0.253010005	0.497180015	0.307110012
0.753939986	0.002930000	0.311670005
0.745890021	0.493970007	0.315149993
0.004100000	0.004280000	0.323839992
0.497590005	0.499100000	0.317440003
0.873499990	0.750530005	0.315100014
0.126080006	0.255070001	0.311289996
0.627839983	0.753489971	0.316410005
0.617470026	0.248730004	0.316020012
0.498849988	0.998950005	0.317609996
0.377020001	0.749949992	0.317629993
0.251929998	0.999559999	0.316350013
0.128389999	0.747179985	0.315629989
0.873170018	0.252220005	0.322490007
0.004220000	0.503009975	0.319649994

TS6

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	4	8	64

Direct

0.869099975	0.416819990	0.380789995
0.868669987	0.078840002	0.381520003
0.754960001	0.742169976	0.384550005
0.131430000	0.581260026	0.378190011
0.563369989	0.122740000	0.384460002
0.453280002	0.635420024	0.383459985
0.139239997	0.965879977	0.386669993
0.315369993	0.273710012	0.437480003
0.331849992	0.364850014	0.371490002
0.340640008	0.164430007	0.437150002

0.381770015	0.349000007	0.454430014
0.179089993	0.393629998	0.453969985
0.199839994	0.293460011	0.449479997
0.859080017	0.075280003	0.435829997
0.867129982	0.421429992	0.435400009
0.139139995	0.571630001	0.433360010
0.754790008	0.740249991	0.438679993
0.566219985	0.123089999	0.438859999
0.453119993	0.632539988	0.437860012
0.142959997	0.958679974	0.440780014
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003

0.875000000	0.916670024	0.103940003
0.251069993	0.333090007	0.205850005
0.376379997	0.583480000	0.207240000
0.123190001	0.582069993	0.206980005
0.750859976	0.833559990	0.206780002
0.125200003	0.077699997	0.206640005
0.625060022	0.083200000	0.207289994
0.997009993	0.332920015	0.207169995
0.874800026	0.581600010	0.208079994
0.878470004	0.082730003	0.208289996
0.626760006	0.582650006	0.208260000
0.748399973	0.329979986	0.208489999
0.252299994	0.830359995	0.209010005
0.502430022	0.834270000	0.209450006
0.499630004	0.333970010	0.209360003
0.000049949	0.831179976	0.210160002
0.374330014	0.083540000	0.210370004
0.248009995	0.497810006	0.312189996
0.125110000	0.246570006	0.305770010
0.754239976	0.001710000	0.311969995
0.874800026	0.748730004	0.315420002
0.748260021	0.492320001	0.314859986
0.251850009	0.995959997	0.316570014
0.125729993	0.743809998	0.316419989
0.629429996	0.752200007	0.317070007
0.501039982	0.500670016	0.316249996
0.620239973	0.249369994	0.316890001
0.379200011	0.751789987	0.316599995
0.500840008	0.999170005	0.317770004
0.876100004	0.247040004	0.318820000
0.999710023	0.496969998	0.317869991
0.003620000	0.997500002	0.322539985
0.367670000	0.249039993	0.317660004

TS7

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	8	64

Direct

0.875050008	0.078249998	0.381889999
0.858889997	0.411399990	0.382220000
0.454070002	0.661040008	0.385320008
0.588689983	0.101319999	0.381320000
0.142780006	0.979740024	0.387400001
0.754670024	0.743130028	0.384590000
0.077959999	0.625660002	0.387059987
0.374500006	0.294180006	0.408239990
0.224739999	0.392509997	0.411920011
0.456389993	0.403079987	0.390520006
0.433690012	0.234750003	0.438899994
0.866050005	0.074620001	0.436150014
0.853900015	0.413839996	0.436710000
0.281899989	0.344399989	0.439740002
0.457260013	0.667089999	0.439489990
0.598720014	0.099200003	0.435539991
0.144600004	0.974759996	0.441410005
0.756219983	0.741490006	0.438679993
0.087269999	0.625699997	0.441020012
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003

0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.251890004	0.329580009	0.205210000
0.749639988	0.832769990	0.206929997
0.378829986	0.581529975	0.206809998
0.499819994	0.332610011	0.209390000
0.374289989	0.080880001	0.209889993
0.878820002	0.083899997	0.208430007
0.625419974	0.082110003	0.206809998
0.125039995	0.078829996	0.206919998
0.120810002	0.582350016	0.205860004
0.624639988	0.579429984	0.210639998
0.749249995	0.330069989	0.208069995
0.873510003	0.582120001	0.208279997
0.998809993	0.832819998	0.209849998
0.502250016	0.832199991	0.208749995
0.250559986	0.829089999	0.209000006
0.997319996	0.335319996	0.208529994
0.368680000	0.247319996	0.318720013
0.248919994	0.496540010	0.304949999
0.756219983	0.001250000	0.312420011
0.748790026	0.490920007	0.314740002
0.006630000	0.998790026	0.322259992
0.499639988	0.496289998	0.325650007
0.873210013	0.749080002	0.314599991
0.127529994	0.250779986	0.307159990
0.628130019	0.749000013	0.317609996
0.622139990	0.245590001	0.314319998
0.501290023	0.996680021	0.315800011
0.375589997	0.749189973	0.314029992
0.253100008	0.997150004	0.316359997
0.126819998	0.742879987	0.315459996
0.879289985	0.247299999	0.319050014

0.002250000	0.497619987	0.322930008
TS8		
1.0		
11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	8	64

Direct

0.861479998	0.082050003	0.381320000
0.860059977	0.415430009	0.380899996
0.492720008	0.662230015	0.377319992
0.516059995	0.156800002	0.378809988
0.136989996	0.987450004	0.387109995
0.763480008	0.751950026	0.386799991
0.074150003	0.629559994	0.387290001
0.278690010	0.357329994	0.383379996
0.419559985	0.491659999	0.449510008
0.438609987	0.327410012	0.455969989
0.213119999	0.323900014	0.417860001
0.853439987	0.078929998	0.435689986
0.852670014	0.419319987	0.435350001
0.377039999	0.401549995	0.455249995
0.485170007	0.650059998	0.432529986
0.521319985	0.162560001	0.434029996
0.140489995	0.987550020	0.441219985
0.769819975	0.750790000	0.440710008
0.077950001	0.632749975	0.441329986
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000

0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.252249986	0.332309991	0.206540003
0.748780012	0.833180010	0.207699999
0.374100000	0.583769977	0.207859993
0.498199999	0.333270013	0.208110005
0.373780012	0.083169997	0.209830001
0.878099978	0.083559997	0.208320007
0.624970019	0.082599998	0.207029998
0.124679998	0.078960001	0.206540003
0.126069993	0.579930007	0.209160000
0.626619995	0.584119976	0.207359999
0.749230027	0.330749989	0.207220003
0.876349986	0.583109975	0.207550004
0.999520004	0.831979990	0.209749997
0.501820028	0.833890021	0.209330007
0.250169992	0.830600023	0.209000006
0.997749984	0.335519999	0.208210006
0.370240003	0.247170001	0.323060006
0.252750009	0.495299995	0.318450004
0.751730025	0.004680000	0.311989993
0.750050008	0.494870007	0.312150002
0.002530000	0.001180000	0.322369993
0.503139973	0.503629982	0.312139988

0.872780025	0.752550006	0.313899994
0.124090001	0.249149993	0.305770010
0.627520025	0.754960001	0.322890013
0.620999992	0.252779990	0.313270003
0.499669999	0.000940000	0.316000015
0.376459986	0.752789974	0.315809995
0.250000000	0.996550024	0.316190004
0.127700001	0.744329989	0.315670013
0.875829995	0.249929994	0.318520010
0.001590000	0.500720024	0.321929991

TS9

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	2	7	64

Direct

0.870150030	0.079630002	0.382050008
0.856589973	0.414180011	0.381859988
0.763180017	0.751309991	0.386610001
0.570129991	0.120010003	0.384640008
0.486299992	0.654919982	0.380039990
0.143649995	0.982129991	0.387109995
0.071690001	0.633329988	0.386629999
0.244829997	0.341019988	0.370770007
0.353689998	0.268689990	0.389750004
0.223700002	0.356530011	0.419640005
0.860430002	0.075960003	0.436329991
0.852750003	0.420639992	0.436239988
0.769640028	0.751259983	0.440519989
0.573090017	0.121480003	0.438800007
0.480479985	0.648479998	0.434549987
0.075999998	0.634419978	0.440660000
0.147670001	0.979130030	0.441170007
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000

0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.250340015	0.332659990	0.205219999
0.124569997	0.583109975	0.207560003
0.749689996	0.833000004	0.207450002
0.375959992	0.584089994	0.206980005
0.125049993	0.083039999	0.208130002
0.626609981	0.082390003	0.207220003
0.999400020	0.335299999	0.209749997
0.879410028	0.084880002	0.208759993
0.749870002	0.330269992	0.207530007
0.876299977	0.582769990	0.207460001
0.627099991	0.583299994	0.208000004
0.250589997	0.831900001	0.208550006
0.503069997	0.833890021	0.209399998
0.000030000	0.834469974	0.209629998
0.375600010	0.081969999	0.209570006

0.499949992	0.332470000	0.208729997
0.127880007	0.253609985	0.312629998
0.254299998	0.501510024	0.312290013
0.757080019	0.003110000	0.311940014
0.873459995	0.752499998	0.313630015
0.628549993	0.751489997	0.322840005
0.254750013	0.996410012	0.315719992
0.128889993	0.747340024	0.315439999
0.750249982	0.493129998	0.312620014
0.379550010	0.752370000	0.315149993
0.504700005	0.999689996	0.317389995
0.624800026	0.248720005	0.316489995
0.878989995	0.250519991	0.319940001
0.504180014	0.500670016	0.314139992
0.006850000	0.002170000	0.322990000
0.001460000	0.504469991	0.320879996
0.376819998	0.249829993	0.315409988

TS10

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	3	7	64

Direct

0.442310005	0.625970006	0.385369986
0.850780010	0.409610003	0.382979989
0.876269996	0.077280000	0.381209999
0.575879991	0.110880002	0.384959996
0.753880024	0.744799972	0.383679986
0.086659998	0.604409993	0.388209999
0.139300004	0.924809992	0.380589992
0.234239995	0.257750005	0.390879989
0.383819997	0.272130013	0.394300014
0.230660006	0.166160002	0.420610011
0.226150006	0.354449987	0.417199999
0.438120008	0.625779986	0.439539999
0.850950003	0.416209996	0.437310010
0.868520021	0.071840003	0.435510010
0.583419979	0.109849997	0.439049989
0.754480004	0.744340003	0.437790006

0.101450004	0.592469990	0.441529989
0.146009997	0.934329987	0.435070008
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.250999987	0.331140012	0.206129998
0.125320002	0.081820004	0.207959995
0.625549972	0.083049998	0.207359999
0.626789987	0.580680013	0.208600000
0.378760010	0.584029973	0.205770001
0.751119971	0.834050000	0.206300005
0.875050008	0.581160009	0.208130002

0.749350011	0.329919994	0.207980007
0.498079985	0.331959993	0.211140007
0.000950000	0.334149987	0.210170001
0.878960013	0.085649997	0.208269998
0.121600002	0.585789979	0.206939995
0.250759989	0.829259992	0.207910001
0.375800014	0.082510002	0.209340006
0.502610028	0.833440006	0.209450006
0.000000000	0.832880020	0.209910005
0.128959998	0.252750009	0.314249992
0.755819976	0.003700000	0.312079996
0.500850022	0.500259995	0.318040013
0.748000026	0.492430001	0.314539999
0.873399973	0.750119984	0.313899994
0.620959997	0.247590005	0.317389995
0.380890012	0.748870015	0.316810012
0.127480000	0.747250021	0.322360009
0.250979990	0.503549993	0.304149985
0.255230010	0.992219985	0.311820000
0.502990007	0.997380018	0.317640007
0.372079998	0.255010009	0.321630001
0.879270017	0.250290006	0.319909990
0.003200000	0.500819981	0.320060015
0.629630029	0.751649976	0.315759987
0.004420000	0.001120000	0.319040000

TS11

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
8	4	7	64

Direct

0.439929992	0.622959971	0.385149986
0.869509995	0.071560003	0.381080002
0.137439996	0.926039994	0.380989999
0.818059981	0.392980009	0.386869997
0.539830029	0.136910006	0.383540004
0.752539992	0.741310000	0.383899987
0.064240001	0.615069985	0.386680007
0.150780007	0.263419986	0.420960009

0.242070004	0.241500005	0.371170014
0.160710007	0.372189999	0.434119999
0.217620000	0.198129997	0.444519997
0.061620001	0.221630007	0.431400001
0.436839998	0.621370018	0.439319998
0.863510013	0.065399997	0.435579985
0.141990006	0.932359993	0.435579985
0.821250021	0.400530010	0.440829992
0.533829987	0.145860001	0.437570006
0.755550027	0.739229977	0.437979996
0.065770000	0.608780026	0.440750003
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003

0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.378490001	0.584779978	0.205809996
0.249259993	0.331470013	0.205740005
0.500880003	0.334760010	0.207440004
0.625750005	0.083240002	0.207090005
0.751010001	0.834949970	0.206340000
0.374159992	0.079449996	0.207300007
0.875060022	0.581809998	0.207589999
0.123930000	0.585959971	0.206589997
0.750680029	0.330749989	0.208010003
0.879239976	0.086209998	0.208820000
0.627489984	0.582920015	0.209250003
0.250330001	0.829819977	0.209120005
0.125080004	0.082450002	0.208859995
0.000090000	0.833609998	0.209509999
0.502520025	0.833469987	0.209940001
0.001550000	0.332949996	0.212129995
0.253199995	0.500069976	0.305949986
0.373019993	0.249809995	0.310600013
0.753539979	0.004120000	0.311969995
0.872210026	0.750129998	0.313620001
0.747539997	0.493389994	0.315070003
0.254249990	0.995649993	0.314260006
0.380369991	0.748849988	0.317299992
0.498890013	0.498479992	0.317290008
0.618879974	0.249320000	0.315219998
0.500819981	0.998560011	0.317369998
0.128389999	0.748600006	0.321559995
0.875769973	0.252139986	0.322259992
0.004620000	0.503679991	0.315439999
0.002470000	0.001890000	0.318989992
0.628480017	0.753260016	0.316619992
0.127719998	0.255510002	0.319099993

TS12

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C H O Pt
9 1 8 64

Direct

0.360080004	0.407860011	0.373030007
0.143450007	0.100079998	0.382160008
0.074740000	0.635789990	0.388020009
0.489630014	0.503139973	0.405660003
0.752780020	0.744390011	0.384240001
0.865970016	0.074850000	0.380510002
0.563639998	0.145820007	0.385960013
0.867100000	0.413239986	0.382250011
0.377220005	0.895240009	0.382099986
0.328150004	0.381469995	0.419440001
0.143179998	0.106840000	0.436610013
0.079530001	0.640320003	0.441969991
0.511240005	0.527999997	0.456970006
0.753099978	0.741590023	0.438340008
0.856850028	0.071640000	0.434810013
0.561619997	0.157000005	0.439850003
0.857190013	0.415199995	0.436580002
0.373039991	0.887139976	0.436459988
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003

0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.125850007	0.580200016	0.208210006
0.877730012	0.582080007	0.207499996
0.502799988	0.835619986	0.208890006
0.999989986	0.833180010	0.209859997
0.248699993	0.833440006	0.208100006
0.752099991	0.832949996	0.206290007
0.000980020	0.334580004	0.210229993
0.126269996	0.080459997	0.208379999
0.879109979	0.085680000	0.207179993
0.626020014	0.582109988	0.210189998
0.377719998	0.586000025	0.208059996
0.624010026	0.081019998	0.207479998
0.375759989	0.083839998	0.209199995
0.750220001	0.330540001	0.207770005
0.250209987	0.332139999	0.206320003
0.500930011	0.335559994	0.207230002
0.252270013	0.500760019	0.312240005
0.504199982	0.001150012	0.323559999
0.757380009	0.495119989	0.313360006
0.004090000	0.998499990	0.321689993
0.126350001	0.746029973	0.314949989
0.876389980	0.751900017	0.315800011
0.006360000	0.498169988	0.324140012
0.251720011	0.996550024	0.318910003
0.129179999	0.247070000	0.314040005
0.378639996	0.752569973	0.312429994
0.756550014	0.002610000	0.310050011
0.879140019	0.248809993	0.318679988
0.631519973	0.755050004	0.315809995
0.513639987	0.507439971	0.319260001
0.627099991	0.247659996	0.312779993

0.375999987	0.251260012	0.312240005
TS13		
1.0		
11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	2	8	64

Direct

0.860960007	0.073579997	0.380679995
0.133910000	0.092340000	0.380109996
0.861549973	0.410250008	0.381390005
0.372429997	0.893060029	0.382710010
0.749260008	0.739929974	0.384099990
0.315109998	0.377059996	0.388130009
0.561039984	0.140279993	0.386519998
0.070060000	0.631330013	0.387639999
0.399619997	0.448020011	0.424919993
0.514549971	0.496069998	0.384889990
0.246439993	0.330100000	0.418119997
0.852930009	0.070900001	0.435000002
0.135450006	0.107699998	0.434379995
0.853299975	0.412910014	0.435770005
0.369289994	0.887489974	0.437189996
0.750549972	0.737389982	0.438210011
0.561720014	0.149389997	0.440499991
0.074290000	0.634400010	0.441650003
0.427210003	0.488660008	0.473930001
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000

0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.750320017	0.832830012	0.206410006
0.249640003	0.331609994	0.206660002
0.499300003	0.332309991	0.206890002
0.877189994	0.083679996	0.207330003
0.626339972	0.582669973	0.207359999
0.876569986	0.581480026	0.207499996
0.374720007	0.585810006	0.207920000
0.622550011	0.079949997	0.207810000
0.125220001	0.077590004	0.207310006
0.748440027	0.329250008	0.207729995
0.248190001	0.831870019	0.208859995
0.125499994	0.578599989	0.209150001
0.500490010	0.834739983	0.209670007
0.998369992	0.333460003	0.209350005
0.374280006	0.083300002	0.210370004
0.999019980	0.831579983	0.210130006
0.751999974	0.999949992	0.310710013
0.124119997	0.241960004	0.309720010
0.750699997	0.492680013	0.312999994
0.621699989	0.247180000	0.314310014
0.506009996	0.503069997	0.311230004
0.377020001	0.746280015	0.315070003

0.251239985	0.495409995	0.315290004
0.371549994	0.253349990	0.315780014
0.124169998	0.742609978	0.315600008
0.872590005	0.749249995	0.315369993
0.627240002	0.749239981	0.316020012
0.874379992	0.246040002	0.318150014
0.250099987	0.993640006	0.319160014
0.000710000	0.994939983	0.321920007
0.002000000	0.495590001	0.322950006
0.500970006	0.998769999	0.323419988

TS14

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	3	8	64

Direct

0.874050021	0.064980000	0.379720002
0.177330002	0.115610003	0.390619993
0.810130000	0.385890007	0.387279987
0.379929990	0.889090002	0.383240014
0.734200001	0.740629971	0.386920005
0.558099985	0.141709998	0.386059999
0.274190009	0.510209978	0.407559991
0.009150000	0.661650002	0.378560007
0.386480004	0.498930007	0.434269994
0.202930003	0.374839991	0.373039991
0.198599994	0.541239977	0.436390013
0.394069999	0.506980002	0.484560013
0.872669995	0.053029999	0.434100002
0.173360005	0.112159997	0.444629997
0.807749987	0.393260002	0.441190004
0.377169997	0.880240023	0.437610000
0.733309984	0.739289999	0.440880001
0.556500018	0.153410003	0.439859986
0.489360005	0.479620010	0.407150000
0.014070000	0.656430006	0.433279991
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000

0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.625810027	0.581539989	0.209409997
0.501110017	0.333880007	0.205610007
0.751879990	0.831160009	0.207509995
0.374709994	0.586049974	0.207780004
0.246739998	0.334639996	0.207059994
0.875919998	0.085830003	0.207450002
0.623780012	0.078259997	0.207499996
0.125770003	0.083789997	0.208930001
0.749740005	0.328920007	0.207939997
0.874629974	0.580980003	0.207130000
0.246979997	0.835030019	0.208989993
0.125009999	0.583469987	0.207049996

0.501619995	0.832809985	0.209549993
0.374029994	0.077260002	0.207020000
0.000980000	0.331010014	0.211019993
0.997560024	0.833469987	0.208370000
0.501850009	0.498710006	0.313089997
0.752770007	0.998420000	0.311989993
0.129250005	0.251740009	0.324180007
0.748470008	0.490130007	0.314249992
0.621110022	0.243340001	0.312700003
0.375070006	0.249139994	0.304080009
0.625010014	0.747959971	0.315279990
0.373919994	0.749140024	0.313520014
0.122010000	0.750349998	0.313959986
0.870970011	0.745869994	0.320850015
0.253760010	0.502260029	0.315070003
0.876219988	0.249259993	0.323460013
0.246610001	0.997789979	0.322279990
0.500249982	0.997210026	0.323430002
0.998650014	0.000849962	0.313360006
0.002220000	0.498789996	0.313360006

TS15

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	4	8	64

Direct

0.011900000	0.658760011	0.378630012
0.191949993	0.140919998	0.386220008
0.375539988	0.891889989	0.383630008
0.875779986	0.063380003	0.379759997
0.553049982	0.144319996	0.385829985
0.734820008	0.737529993	0.386949986
0.813750029	0.385089993	0.386999995
0.279069990	0.504260004	0.419030011
0.401580006	0.506550014	0.444409996
0.295899987	0.612200022	0.370970011
0.247600004	0.395310014	0.420069993
0.214680001	0.564719975	0.446429998
0.410030007	0.517409980	0.494850010

0.496399999	0.494929999	0.414900005
0.018800000	0.654760003	0.433450013
0.197870001	0.153300002	0.440250009
0.874589980	0.052400000	0.434210002
0.373210013	0.881179988	0.438160002
0.547649980	0.158950001	0.439579993
0.732900023	0.735170007	0.440970004
0.811890006	0.393519998	0.440939993
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.501030028	0.333260000	0.205550000

0.248270005	0.335970014	0.207159996
0.374579996	0.077569999	0.207200006
0.623730004	0.077459998	0.207749993
0.875069976	0.580690026	0.207440004
0.751999974	0.830739975	0.207709998
0.749379992	0.328130007	0.207929999
0.125860006	0.081340000	0.207870007
0.247580007	0.834439993	0.209330007
0.875440001	0.085000001	0.207629994
0.375180006	0.586260021	0.207530007
0.626869977	0.581260026	0.208680004
0.125300005	0.582799971	0.207629994
0.000060000	0.331470013	0.209910005
0.501550019	0.832509995	0.209900007
0.997250021	0.832069993	0.208110005
0.375400007	0.248420000	0.306129992
0.752219975	0.996850014	0.312610000
0.126259997	0.247840002	0.315459996
0.503430009	0.496879995	0.311729997
0.621179998	0.242730007	0.313030005
0.749490023	0.488770008	0.314300001
0.373950005	0.748269975	0.314709991
0.625440001	0.746379972	0.315270007
0.121239997	0.750159979	0.313490003
0.003720000	0.495880008	0.314619988
0.246910006	0.997690022	0.323220015
0.253340006	0.494540006	0.316100001
0.998120010	0.997529984	0.313479990
0.871619999	0.743690014	0.321460009
0.500810027	0.995329976	0.324119985
0.876240015	0.247089997	0.323060006

TS16

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	5	8	64

Direct

0.876860023	0.064000003	0.379159987
0.749830008	0.734570026	0.383729994

0.372009993	0.890630007	0.383430004
0.063780002	0.627690017	0.384900004
0.559710026	0.135900006	0.385969996
0.832939982	0.389840007	0.387039989
0.193810001	0.142739996	0.386810005
0.468230009	0.534020007	0.457069993
0.351709992	0.470860004	0.468989998
0.587180018	0.486719996	0.384820014
0.345789999	0.377590001	0.440580010
0.281639993	0.546790004	0.457580000
0.339280009	0.436690003	0.516820014
0.481350005	0.646059990	0.463209987
0.547020018	0.459850013	0.431849986
0.874029994	0.054540001	0.433739990
0.750240028	0.732290030	0.438340008
0.373609990	0.882640004	0.437929988
0.064750001	0.626190007	0.439009994
0.558640003	0.143209994	0.440129995
0.838469982	0.397509992	0.441080004
0.197799996	0.153129995	0.440990001
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000
0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003

0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249329999	0.331440002	0.205349997
0.124200001	0.583700001	0.206200004
0.501389980	0.329499990	0.204019994
0.751800001	0.833750010	0.206839994
0.375389993	0.588630021	0.205300003
0.876169980	0.580259979	0.208770007
0.374740005	0.077390000	0.207929999
0.876730025	0.086280003	0.207670003
0.624220014	0.079599999	0.208000004
0.750680029	0.329789996	0.208539993
0.126110002	0.080210000	0.208409995
0.999090016	0.831789970	0.209020004
0.631340027	0.583649993	0.206469998
0.248280004	0.835030019	0.210460007
0.502210021	0.833320022	0.210280001
0.001340000	0.332520008	0.210679993
0.375510007	0.252759993	0.307440013
0.257070005	0.497590005	0.308010012
0.752919972	0.999729991	0.312050015
0.000110030	0.996039987	0.313980013
0.620790005	0.244179994	0.314020008
0.502799988	0.496749997	0.304930001
0.748839974	0.489879996	0.317759991
0.377270013	0.742500007	0.316439986
0.626850009	0.745720029	0.316300005
0.873350024	0.746640027	0.316040009
0.126289994	0.746429980	0.316439986
0.007780000	0.498070002	0.317059994
0.129759997	0.249090001	0.315580010
0.879119992	0.247920007	0.321880013

0.501420021	0.994870007	0.322510004
0.248730004	0.996590018	0.324160010

TS17

1.0

11.1216001511	0.0000000000	0.0000000000
0.0000000000	9.6316003799	0.0000000000
0.0000000000	0.0000000000	21.7964000702

C	H	O	Pt
9	6	8	64

Direct

0.876919985	0.060649998	0.379500002
0.371190012	0.890630007	0.382959992
0.748420000	0.715319991	0.381220013
0.069190003	0.619979978	0.384799987
0.823700011	0.384759992	0.386990011
0.207069993	0.153840005	0.385670006
0.557420015	0.138640001	0.385910004
0.483119994	0.562640011	0.459490001
0.376320004	0.486099988	0.479589999
0.451350003	0.417860001	0.374179989
0.302819997	0.495900005	0.446249992
0.475309998	0.660300016	0.433950007
0.396030009	0.377009988	0.490189999
0.653150022	0.592100024	0.465530008
0.345079988	0.537880003	0.522159994
0.873790026	0.051309999	0.434049994
0.373439997	0.880219996	0.437759995
0.747009993	0.703459978	0.436470002
0.074390002	0.615409970	0.439060003
0.824800014	0.392639995	0.441159993
0.554059982	0.152349994	0.439850003
0.219040006	0.168310001	0.439319998
0.586790025	0.526130021	0.479649991
0.000000000	0.000000000	0.000000000
0.000000000	0.500000000	0.000000000
0.125000000	0.250000000	0.000000000
0.125000000	0.750000000	0.000000000
0.250000000	0.000000000	0.000000000
0.250000000	0.500000000	0.000000000
0.375000000	0.250000000	0.000000000
0.375000000	0.750000000	0.000000000

0.500000000	0.000000000	0.000000000
0.500000000	0.500000000	0.000000000
0.625000000	0.250000000	0.000000000
0.625000000	0.750000000	0.000000000
0.750000000	0.000000000	0.000000000
0.750000000	0.500000000	0.000000000
0.875000000	0.250000000	0.000000000
0.875000000	0.750000000	0.000000000
0.000000000	0.166669995	0.103940003
0.000000000	0.666670024	0.103940003
0.125000000	0.416669995	0.103940003
0.125000000	0.916670024	0.103940003
0.250000000	0.166669995	0.103940003
0.250000000	0.666670024	0.103940003
0.375000000	0.416669995	0.103940003
0.375000000	0.916670024	0.103940003
0.500000000	0.166669995	0.103940003
0.500000000	0.666670024	0.103940003
0.625000000	0.416669995	0.103940003
0.625000000	0.916670024	0.103940003
0.750000000	0.166669995	0.103940003
0.750000000	0.666670024	0.103940003
0.875000000	0.416669995	0.103940003
0.875000000	0.916670024	0.103940003
0.249139994	0.331339985	0.205430001
0.123829998	0.583180010	0.206129998
0.749989986	0.831619978	0.206609994
0.377139986	0.587109983	0.206520006
0.876330018	0.085029997	0.207570001
0.374630004	0.078709997	0.208210006
0.500630021	0.332029998	0.206239998
0.624029994	0.079140000	0.207859993
0.874379992	0.579729974	0.208039999
0.125740007	0.079429999	0.208580002
0.749610007	0.329299986	0.208480000
0.997990012	0.830730021	0.209260002
0.501680017	0.833530009	0.210079998
0.247909993	0.834280014	0.210170001
0.000410000	0.331609994	0.210590005
0.625970006	0.579879999	0.209840000
0.374370009	0.250539988	0.308970004

0.253980011	0.498600006	0.307790011
0.752579987	0.998000026	0.312130004
0.999979973	0.994979978	0.314280003
0.375640005	0.745209992	0.315169990
0.127470002	0.248380005	0.315439999
0.124820001	0.745959997	0.316960007
0.872669995	0.746439993	0.316289991
0.007160000	0.497029990	0.316359997
0.625150025	0.744669974	0.316089988
0.749350011	0.489329994	0.316749990
0.621980011	0.243530005	0.313690007
0.501839995	0.994549990	0.323500007
0.877960026	0.246610001	0.322380006
0.247889996	0.996339977	0.324339986
0.499220014	0.497429997	0.315169990