Reaction of CO, H_2O, H_2 and CO_2 on the clean as well as O, OH and H pre-covered Fe(100) and Fe(111) Surfaces

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	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
$CO+H_2O$	-2.39	-2.49	2.003; 2.020; 2.150; 2.241	2.153; 2.180; 2.249		1.318	0.978; 0.983
TS1	-2.23	-2.12	1.951; 1.955; 2.171; 2.206	2.121; 2.132; 2.003	1.901; 1.965	1.316	0.981
CO+OH+H-t1	-3.42	-3.33	1.948; 1.986; 2.149; 2.200	2.126; 2.130; 1.970; 2.006	1.755; 1.802; 1.960; 2.171; 2.451	1.317	0.976
TS2	-2.67	-2.36	1.966; 2.007; 2.115; 2.186	2.125; 2.133; 1.841; 1.929	1.775; 1.900; 2.136; 2.151; 1.917; 1.925	1.317	
CO+O+2H	-3.84	-3.62	1.987; 2.018; 2.095; 2.137	1.950; 1.983; 2.181; 2.212; 2.151; 2.157	1.916; 1.863; 1.846; 1.868	1.309	
TS3	-2.01	-1.75	1.985; 2.087; 2.231; 2.386	1.844; 1.948; 2.062	1.745; 1.915; 1.976; 2.222; 2.273; 1.778; 1.844; 1.902	1.284	
CO_2+2H-t1	-2.83	-2.63	1.960; 2.243	2.037; 2.060; 1.989	1.781; 1.836; 1.911; 1.750; 1.877; 1.957	1.296; 1.359	
TS4	-2.80	-2.49	1.922; 1.941; 1.991; 2.033	1.943; 1.990; 2.191; 2.215; 1.886; 1.905	1.752; 1.880; 1.932; 1.730; 1.980; 2.075		
C+2O+2H	-4.78	-4.52	1.919; 1.933; 1.950; 1.954	1.964; 1.992; 2.132; 2.193; 1.959; 1.998	1.836; 1.911; 1.872; 1.890		
TS5	-1.65	-1.55	1.927; 2.025	2.052; 2.145; 2.022		1.305	0.979
COOH+H	-2.04	-2.03	1.939; 2.433; 2.458	2.015; 2.162	1.747; 1.930; 1.947	1.329; 1.372	0.984
TS6	-1.30	-1.08	1.928; 2.351; 2.448	2.037; 2.271	1.746; 1.920; 1.988; 1.825	1.306; 1.326	
CO_2+2H-t2	-2.77	-2.57	1.969; 2.239	2.039; 2.043; 2.000	1.788; 1.860; 1.934; 2.190; 1.766; 1.989; 1.966; 2.060	1.295; 1.361	
TS7	-0.91	-0.82	1.934; 1.954	1.855; 1.859	1.741; 1.946; 1.952	1.372	0.980
COH+O+H	-2.83	-2.76	1.988; 1.990; 2.072; 2.074	1.962; 2.007; 2.118; 2.145	1.747; 1.822; 1.963	1.413	0.981
TS8	-2.38	-2.11	2.001; 2.008; 2.288	2.078; 2.090; 1.965; 1.980	1.743; 1.929; 1.994; 2.217; 2.254; 1.979; 2.000	1.347	
HCO+O+H	-3.08	-2.99	2.018; 2.022	1.990; 1.992; 1.941; 1.972; 2.169; 2.196	1.747; 1.815; 1.971	1.369	
CO+OH+H-t2	-3.37	-3.32	1.948; 1.971; 2.158; 2.188	2.118; 2.150; 1.971; 2.003	1.750; 1.908; 1.963; 2.179	1.314	0.976
TS9	-2.28	-2.24	1.959; 2.000; 2.150	1.998; 2.293; 1.938; 2.037	1.586; 2.269	1.339	0.975
HCO+OH	-2.58	-2.65	1.964; 2.039	1.986; 2.003; 1.970; 2.010		1.384	0.977
TS10	-1.90	-1.92	1.940; 1.987; 2.228; 2.298	1.871; 1.882; 1.968; 2.019			0.976
CH+O+OH	-3.92	-3.92	1.980; 2.022; 2.063; 2.079	1.983; 2.003; 2.158; 2.168; 1.980; 2.004			0.976
TS11	-1.41	-1.51	1.961; 2.448	2.066; 2.066		1.345	0.979
HCOOH	-1.56	-1.72	2.050	2.006; 2.078		1.391; 1.486	0.983
CO+OH+H-t3	-3.44	-3.36	1.949; 1.993; 2.216; 2.178	2.134; 2.162; 1.971; 1.999	1.811; 1.814	1.313	0.976
TS12	-1.58	-1.46	1.958; 1.979; 2.105; 2.166	1.973; 1.999	1.882; 1.979	1.365	0.976
COH+OH	-2.64	-2.36	2.010; 2.027; 2.030; 2.364	1.969; 2.009		1.422	0.976; 0.981

Table S2. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of $CO+H_2O$ on the Fe(100) surface, and the bond distances (Å) of the transition states on the Fe(100) surface

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
$CO+H_2O$→TS1→CO+OH+H-t1	0.16	0.37	-1.03	-0.84	1.303
CO+OH+H-t1→TS2→CO+O+2H	0.75	0.97	-0.42	-0.29	1.419
CO+O+2H→TS3→CO_2+2H-t1	1.83	1.87	1.01	0.99	1.867
CO+O+2H→TS4→C+2O+2H	1.04	1.13	-0.94	-0.90	1.901
CO+OH+H-t1→TS5→COOH+H	1.77	1.78	1.38	1.30	1.811
COOH+H→TS6→CO_2+2H-t2	0.74	0.95	-0.73	-0.54	1.416
COOH+H→TS7→COH+O+H	1.13	1.21	-0.79	-0.73	2.017
CO+OH+H-t1→TS8→HCO+O+H	1.04	1.22	0.34	0.34	1.369/1.464
CO+OH+H-t2→TS9→HCO+OH	1.09	1.08	0.79	0.67	1.402
HCO+OH→TS10→HC+O+OH	0.68	0.73	-1.34	-1.27	1.895
HCO+OH→TS11→HCOOH	1.17	1.14	1.02	0.93	1.884
CO+OH+H-t3→TS12→COH+OH	1.86	1.90	0.80	1.00	1.300

Table S3. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of $CO+H_2O$ on the Fe(111) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
$CO+H_2O$	-2.61	-2.75	1.778; 2.261; 2.243	2.085		1.227	0.977; 0.999
TS1’	-2.05	-2.01	1.768	1.917	1.770	1.205	0.981
CO+OH+H-t1	-3.11	-3.09	1.769	2.061; 2.153; 2.188	1.624; 1.888	1.198	
TS2’	-2.38	-2.17	1.770; 1.948; 2.006; 2.068	1.637; 1.902; 1.681		1.197	
CO+O+2H	-3.12	-2.99	1.770; 1.978; 2.016; 2.018	1.647; 1.673; 1.643; 1.803		1.197	
TS3’	-1.48	-1.32	1.869; 2.225	1.758	1.643; 1.813; 1.679; 1.695	1.207	
CO_2+2H	-3.16	-3.04	1.976	1.956; 1.957	1.645; 1.790; 1.647; 1.787	1.295; 1.295	
TS4’	-2.21	-1.97	1.876; 1.953; 2.239	1.885; 1.982; 2.005; 2.068; 1.928; 2.028; 2.117	1.644; 1.802; 1.656; 1.674		
C+2O+2H	-3.30	-3.09	1.878; 1.890; 1.903; 1.979	1.878; 1.972; 1.997; 2.082; 1.866; 1.954; 1.974	1.661; 1.667; 1.644; 1.817		
TS5’	-2.12	-2.09	1.844; 2.281	1.953; 2.147	1.645; 1.816	1.237	0.979
COOH+H	-2.30	-2.33	1.899	2.015; 2.165	1.650; 1.808	1.280; 1.435	0.987
TS6’	-1.35	-1.20	1.936	1.965; 2.030	1.646; 1.815; 1.687		
TS7’	-2.22	-2.21	1.882; 1.982	2.138; 1.986; 2.023	1.602	1.251	0.974
HCO+OH	-2.31	-2.35	1.868; 2.189	1.996; 1.932; 2.044		1.289	0.976
CO+OH+H-t2	-3.15	-3.15	1.769	2.080; 2.099; 2.244	1.644; 1.820	1.198	
TS8’	-1.60	-1.47	1.817; 1.988; 2.207	2.098; 2.148; 2.183	2.013	1.287	0.978
COH+OH	-1.78	-1.87	1.861; 1.976; 2.028; 2.044	2.099; 2.159; 2.162		1.379	0.978; 0.990

Table S4. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of $CO+H_2O$ on the Fe(111) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
$CO+H_2O$→TS1′→CO+OH+H-t1	0.56	0.74	-0.50	-0.34	1.411
CO+OH+H-t1→TS2′→CO+O+2H	0.73	0.92	-0.01	0.10	1.383
CO+O+2H→TS3′→CO_2+2H	1.64	1.67	-0.04	-0.05	1.862
CO+O+2H→TS4′→C+2O+2H	0.91	1.02	-0.18	-0.10	1.872
CO+OH+H-t1→TS5′→COOH+H	0.99	1.00	0.81	0.76	1.843
COOH+H→TS6′→CO_2+2H	0.95	1.13	-0.86	-0.71	1.323
CO+OH+H-t1→TS7′→HCO+OH	0.89	0.88	0.80	0.74	1.406
CO+OH+H-t2→TS8′→COH+OH	1.55	1.68	1.37	1.28	1.363

Table S5. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of $CO+H_2O$ on the 3O (0.25 ML) pre-covered Fe(100) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
3O+CO+H_2O	-2.44	-2.57	1.937;1.963; 2.188; 2.226	2.103; 2.131; 2.191; 2.008; 2.078; 2.108; 2.281		1.324	0.972; 0.985
TS13	-0.04	-0.16	1.9004; 2.176; 2.243; 2.297	0.259; 2.238; 1.735; 2.169		1.293	0.980; 0.985
2O+CO_2+H_2O	-1.31	-1.50	1.941; 2.230	2.026; 2.112; 2.085; 2.096		1.312; 1.350	0.982; 0.995
TS14	-2.37	-2.38	1.940; 1.964; 2.176; 2.227	2.104; 2.128; 1.976; 1.900; 1.920		1.323	0.973
2O+CO+2OH-t1	-2.93	-3.08	1.943; 1.967; 2.162; 2.263	2.102; 2.119; 1.958; 1.979; 2.010; 2.037		1.323	0.976; 0.992
TS15	-1.96	-1.89	1.949; 1.987; 2.190; 2.216	2.084; 2.133; 1.960; 1.982; 1.892; 1.894	1.765; 1.854	1.322	0.987
3O+CO+OH+H-t1	-2.85	-2.81	1.979; 2.012; 2.096; 2.171	2.118; 2.131; 1.970; 2.003; 1.945; 2.011; 2.171	1.868; 1.905	1.316	0.976
TS16	-1.11	-1.02	2.055; 2.060; 2.125; 2.167	2.146; 2.153; 1.881; 1.916; 1.974; 2.002	1.728; 1.972; 1.995	1.303	0.976
2O+CO_2+OH+H	-1.89	-1.88	1.983; 2.254	2.051; 2.062; 1.989; 1.979; 2.004	1.751; 1.913; 2.005	1.347	0.976
3O+CO+OH+H-t2	-2.99	-2.95	1.991; 1.999; 2.089; 2.192	2.115; 2.133; 1.931; 2.052; 2.071	1.753; 1.828; 1.837	1.316	
TS17	-1.89	-1.85	1.904; 2.039; 2.227; 2.285	2.056; 2.119; 1.972; 2.001	1.593	1.332	0.976
3O+HCO+OH	-2.04	-2.14	1.987; 2.038	1.988; 2.008; 1.974; 2.004		1.364	0.976
TS18	-1.89	-1.82	1.883; 1.919; 2.054; 2.146	1.972; 2.010; 1.862; 1.898	1.782; 1.856		0.976
3O+C+O+OH+H	-3.68	-3.64	1.897; 1.944; 1.945; 2.039	1.937; 2.041; 2.135; 2.217; 1.977; 2.012	1.764; 1.830		0.976
2O+CO+2OH-t2	-2.65	-2.77	1.959; 1.966; 2.143; 2.214	2.103; 2.117; 1.917; 2.004	1.751; 1.913; 2.005	1.347	0.976
TS19	-0.26	-0.34	1.876; 2.014	2.081;2.205; 1.971; 2.004		1.295	0.976; 0.986
2O+COOH+OH	-1.25	-1.44	1.938	1.999; 2.253; 1.972; 2.010		1.321; 1.374	0.976; 0.981

Table S6. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of CO+H_2O on the 3O (0.25 ML) pre-covered Fe(100) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
3O+CO+H_2O→TS13→2O+CO_2+H_2O	2.40	2.41	1.13	1.07	1.938
3O+CO+H_2O→TS14→2O+CO+2OH-t1	0.07	0.19	-0.49	-0.51	1.207/1.221
2O+CO+2OH-t1→TS15→3O+CO+OH+H-t1	0.97	1.19	0.08	0.27	1.422
3O+CO+OH+H-t1→TS16→2O+CO_2+OH+H	1.74	1.79	0.96	0.93	1.933
3O+CO+OH+H-t2→TS17→3O+HCO+OH	1.10	1.10	0.95	0.81	1.453
3O+CO+OH+H-t2→TS18→3O+C+O+OH+H	1.10	1.13	-0.69	-0.69	1.999
2O+CO+2OH-t2→TS19→2O+COOH+OH	2.39	2.43	1.40	1.33	1.826

Table S7. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of CO+H_2O on the 3O (0.33 ML) pre-covered Fe(111) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
3O+CO+H_2O	-2.72	-2.87	1.773, 2	2.081		1.199	0.976, 1.019
TS9′	-0.90	-0.95	1.889; 1.933; 1.952	1.942; 2.037; 2.167			
3O+C+O+H_2O	-2.51	-2.57	1.875; 1.896; 1.901; 1.975	1.881; 1.943; 1.961			
TS10′	-2.72	-2.76	1.773	1.949		1.198	0.974
2O+CO+2OH-t1	-2.75	-2.90	1.772	1.881; 1.922; 1.991		1.197	0.974; 1.011
2O+CO+2OH-t2	-2.77	-2.93	1.772	1.949; 2.050; 1.940; 2.023		1.201	0.977; 0.981
TS11′	-2.13	-2.06	1.774	1.941; 2.033; 2.078; 2.023; 2.102	1.930; 1.990	1.198	0.997
3O+CO+OH+ H	-3.16	-3.17	1.775	1.826; 1.962; 1.972; 1.939; 2.022	1.640; 1.808	1.196	0.980
TS12′	-1.56	-1.50	1.916; 2.202; 2.196	1.876; 2.038; 2.028; 2.089	1.634; 1.869	1.224	0.992
2O+CO_2+OH+H	-2.78	-2.84	1.977	1.948; 1.955; 1.940; 2.025	1.661; 1.781	1.295; 1.297	0.981
TS13′	-1.91	-1.88	1.853; 2.159; 2.274	1.816; 1.917; 2.042; 2.025; 2.170	1.576	1.224	0.996
3O+HCO+OH	-2.30	-2.38	1.920; 2.177	1.974; 1.813; 1.912; 2.043; 1.938; 2.023		1.317	0.980
TS14′	-1.67	-1.77	1.861; 2.271	1.958; 2.033; 2.039; 2.106		1.242	0.980; 0.994
2O+COOH+OH	-1.85	-2.05	1.906	2.016; 2.142; 1.935; 2.035		1.279; 1.444	0.981; 0.987

Table S8. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of $CO+H_2O$ on the 3O (0.33 ML) pre-covered Fe(111) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
3O+CO+H_2O→TS9'→3O+C+O+H_2O	1.82	1.92	0.21	0.30	1.766
3O+CO+H_2O→TS10'→2O+CO+2OH-t1	0.00	0.11	-0.03	-0.03	1.266
2O+CO+2OH-t2→TS11'→3O+CO+OH+H	0.64	0.87	-0.39	-0.24	1.363
3O+CO+OH+H→TS12'→2O+CO_2+OH+H	1.60	1.67	0.38	0.33	1.769
3O+CO+OH+H→TS13'→3O+HCO+OH	1.25	1.29	0.86	0.79	1.667
2O+CO+2OH-t2→TS14'→2O+COOH+OH	1.10	1.16	0.92	0.88	1.826

Table S9. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of $CO+H_2O$ on the 3OH (0.25 ML) pre-covered Fe(100) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
3OH+CO+H_2O	-2.52	-2.64	1.910; 2.072; 2.267; 2.328	2.044; 2.209		1.316	0.976; 0.992
TS20	-2.19	-2.07	1.917; 2.114; 2.151; 2.329	2.020; 2.068; 2.289		1.305	0.983
3OH+CO+OH+H-t1	-3.36	-3.29	1.913; 2.052; 2.251; 2.331	2.019; 1.970; 2.015	1.752; 1.813; 1.982	1.300	0.987
TS21	-2.73	-2.44	1.923; 2.115; 2.115	2.061; 2.251; 1.889; 1.897	1.727; 1.860; 2.036; 1.839; 1.866	1.308	
3OH+CO+O+2H	-3.82	-3.56	1.948; 2.023; 2.189; 2.209	2.145; 2.159; 2.000; 2.039; 2.057; 2.231	1.754; 1.851; 1.948; 1.726; 1.855; 2.082	1.309	
TS22	-1.42	-1.16	1.945; 2.188; 2.232; 2.309	2.067; 2.203; 1.775; 2.299	1.711; 2.024; 2.041	1.294	
3OH+CO_2+2H	-2.63	-2.44	1.991; 2.317	2.021; 2.069; 1.987	1.698; 1.877; 2.002	1.297; 1.358	
TS23	-2.47	-2.38	1.882; 2.105; 2.129	2.071; 2.254; 1.984; 2.002	1.626	1.319	0.978
3OH+HCO+ OH	-2.53	-2.60	1.925; 2.138	1.974; 2.096; 1.981; 2.008		1.371	0.981
TS24	-2.93	-2.68	1.903; 2.097; 2.127	2.062; 2.253; 1.977; 2.040; 2.068; 2.096	1.763; 1.863; 1.920	1.319	
3OH+HCO+O+H	-3.05	-2.93	1.943; 2.057	2.002; 2.018; 1.995; 2.053; 2.054; 2.112	1.747; 1.890; 1.987		
3OH+CO+OH+H-t2	-3.41	-3.35	1.896; 2.113; 2.181	1.976; 2.007; 2.014	1.810	1.302	0.978
TS25	-1.74	-1.66	1.881; 2.231	2.048; 2.238; 1.989	1.738; 1.837	1.298	0.981
3OH+COOH+H	-2.05	-2.05	1.947	2.019; 2.174	1.732; 1.891; 1.900	1.341; 1.371	0.986
TS26	-2.66	-2.35	1.887; 1.936; 2.058; 2.060	1.881; 1.902; 1.967; 2.044; 2.049; 2.122	1.748; 1.833; 1.723		
3OH+C+2O+2H	-4.36	-4.07	1.878; 1.952; 1.960; 2.002	2.026; 2.053; 2.066; 2.092	1.741; 1.821; 1.723		

Table S10. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of CO+H_2O on the 3OH (0.25 ML) pre-covered Fe(100) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
3OH+CO+H_2O→TS20→3OH+CO+OH+H-t1	0.33	0.57	-0.84	-0.65	1.332
3OH+CO+OH+H-t1→TS21→3OH+CO+O+2H	0.63	0.85	-0.46	-0.27	1.416
3OH+CO+O+2H→TS22→3OH+CO_2+2H	2.40	2.40	1.19	1.12	1.894
3OH+CO+OH+H-t1→TS23→3OH+HCO+OH	0.89	0.91	0.83	0.69	1.576
3OH+CO+O+2H→TS24→3OH+HCO+O+H	0.89	0.88	0.77	0.63	1.522
3OH+CO+OH+H-t2→TS25→3OH+COOH+H	1.67	1.69	1.36	1.30	1.830
3OH+CO+O+2H→TS26→3OH+C+2O+2H	1.16	1.21	-0.54	-0.51	1.941

Table S11. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of $CO+H_2O$ on the 3OH (0.33 ML) pre-covered Fe(111) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
3OH+CO+H_2O	-2.81	-2.92	1.899; 2.216	2.104; 2.065		1.288	0.975; 1.104
TS15′	-1.26	-1.36	1.836; 2.291	1.957; 2.134; 2.128		1.249	1.978; 0.985
2OH+COOH+ H_2O	-1.51	-1.68	1.891	2.112; 2.051		1.301; 1.427	0.977; 1.000
TS16′	-2.18	-2.11	1.881; 1.921; 2.151	1.910; 2.118	1.770; 1.866	1.259	0.984
3OH+CO+OH+H	-3.16	-3.12	1.854; 2.004; 2.137	2.106; 2.046; 2.063	1.710; 1.818	1.244	0.977
TS17′	-2.48	-2.27	1.869; 2.149	2.089; 1.924; 2.004; 2.113	1.705; 1.846; 1.887; 1.696		
3OH+CO+O+2H-t1	-3.55	-3.39	1.778	1.894; 1.940; 1.949; 2.150	1.733; 1.798; 1.810; 1.706; 1.825; 1.910	1.198	
TS18′	-2.43	-2.24	1.997; 2.119	2.024; 2.021; 2.025; 2.180; 2.267	1.666; 1.682; 1.707; 1.825; 1.901	1.266	
3OH+CO_2+2H	-3.02	-2.87	1.995; 2.325	1.940; 1.977	1.657; 1.797; 1.712; 1.813; 1.884	1.248; 1.287	
TS19′	-2.50	-2.24	1.891; 1.939; 1.959; 2.042	1.949; 1.972; 2.221			
3OH+C+2O+2H	-3.26	-3.07	1.815; 1.898; 1.913; 1.986	1.796; 1.799			
3OH+CO+O+2H-t2	-3.70	-3.53	1.775	1.850; 1.938; 1.961; 2.296	1.643; 1.809	1.198	
TS20′	-2.58	-2.40	1.918; 2.015	1.857; 1.936; 1.948; 2.244	1.609	1.219	
3OH+HCO+O+H	-2.57	-2.50	1.899; 2.279	1.839; 1.927; 1.991; 2.202		1.298	
TS21′	-1.60	-1.55	1.893; 2.146	2.098; 1.924	1.708; 1.799	1.236	0.976
3OH+COOH+H	-2.18	-2.20	1.913; 2.320	1.991; 2.209	1.707; 1.809; 1.911	1.285; 1.414	0.987

Table S12. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of CO+H_2O on the 3OH (0.33 ML) pre-covered Fe(111) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
3OH+CO+H_2O→TS15'→2OH+COOH+H_2O	1.55	1.56	1.30	1.24	1.828
3OH+CO+H_2O→TS16'→3OH+CO+OH+H	0.63	0.81	-0.35	-0.20	1.399
3OH+CO+OH+H→TS17'→3OH+CO+O+2H-t1	0.68	0.85	-0.39	-0.27	1.359
3OH+CO+O+2H-t1→TS18'→3OH+CO_2+2H	1.12	1.15	0.53	0.52	1.681
3OH+CO+O+2H-t1→TS19'→3OH+C+O+O+2H	1.05	1.15	0.29	0.32	1.833
3OH+CO+O+2H-t2→TS20'→3OH+HCO+O+H	1.12	1.13	1.13	1.03	1.465
3OH+CO+OH+H→TS21'→3OH+COOH+H	1.56	1.57	0.98	0.92	1.826

Table S13. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of CO+H_2O on the 3H (0.25 ML) pre-covered Fe(100) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
3H+CO+H_2O	-2.41	-2.45	1.950; 1.976; 2.144; 2.197	2.129; 2.157; 2.220		1.316	0.978; 0.984
TS27	-1.45	-1.56	1.854; 2.024; 2.242	2.077; 2.124; 2.126	1.633	1.332	0.978; 0.994
2H+HCO+H_2O	-1.45	-1.68	1.938; 2.061	1.994; 1.999; 2.212		1.380	0.993; 0.994
TS28	-2.20	-2.04	1.953; 1.954; 2.135; 2.209	2.132; 2.143; 1.993	1.946; 1.993	1.313	0.981
3H+CO+OH+H	-3.36	-3.25	1.955; 1.985; 2.113; 2.227	2.131; 2.141; 1.979; 2.005	1.767; 1.895; 1.907	1.315	0.976
TS29	-2.63	-2.29	1.977; 2.000; 2.084; 2.187	2.135; 2.140; 1.852; 1.926	1.761; 1.958; 2.067	1.314	
3H+CO+O+2H	-3.82	-3.59	1.994; 2.020; 2.070; 2.144	2.160; 2.171; 1.956; 1.964; 2.155; 2.220	1.794; 1.805; 1.856	1.307	
TS30	-1.93	-1.67	2.058; 2.088; 2.117; 2.205	2.158; 2.240; 1.886; 1.913	1.786; 1.781; 1.835; 1.842	1.292	
3H+CO_2+2H	-2.75	-2.59	1.964; 2.244	2.022; 2.081; 1.989.1.811; 1.860; 1.776; 1.836	1.358		
TS31	-2.66	-2.34	1.922; 1.954; 1.958; 2.036	1.884; 1.913	1.775; 1.816; 1.746		
3H+C+2O+2H	-4.68	-4.45	1.932; 1.941; 1.951; 1.958	1.948; 1.999; 2.111; 2.247	1.789; 1.792; 1.780; 1.829; 1.847		
TS32	-2.47	-2.40	1.856; 2.032; 2.249	2.075; 2.127; 1.975; 2.005	1.631	1.331	0.977
3H+HCO+OH	-2.49	-2.55	1.959; 2.041	1.989; 2.004; 1.974; 2.010		1.380	0.977
TS33	-1.56	-1.47	1.938; 1.994	2.074; 2.127; 2.020	1.794; 1.847	1.303	0.978
3H+COOH+H	-2.00	-2.02	1.942	2.015; 2.186	1.786; 1.862	1.327; 1.371	0.981

Table S14. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of CO+H_2O on the 3H (0.25 ML) pre-covered Fe(100) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
3H+CO+H_2O→TS27→2H+HCO+H_2O	0.96	0.89	0.96	0.77	1.352
3H+CO+H_2O→TS28→3H+CO+OH+H	0.21	0.41	-0.95	-0.80	1.341
3H+CO+OH+H→TS29→3H+CO+O+2H	0.73	0.96	-0.46	-0.34	1.403
3H+CO+O+2H→TS30→3H+CO_2+2H	1.89	1.92	1.07	1.00	1.915
3H+CO+O+2H→TS31→3H+C+2O+2H	1.16	1.25	-0.86	-0.86	1.893
3H+CO+OH+H→TS32→3H+HCO+OH	0.89	0.85	0.87	0.70	1.365
3H+CO+OH+H→TS33→3H+COOH+H	1.80	1.78	1.36	1.23	1.840

Table S15. Computed adsorption energies (E_{ads}, eV), and the relevant bond distances (d, Å) of the IS, TS and FS in the reaction of $CO+H_2O$ on the 3H (0.33 ML) pre-covered Fe(111) surface

	$E_{ads\text{-}ZPE}$	E_{ads}	$d_{Fe\text{-}C}$	$d_{Fe\text{-}O}$	$d_{Fe\text{-}H}$	$d_{C\text{-}O}$	$d_{O\text{-}H}$
3H+CO+H_2O	-2.68	-2.81	1.777; 2.257; 2.259	2.085		1.227	0.977; 0.999
TS22’	-1.92	-2.05	1.858; 1.912; 2.331	2.084; 2.072	1.571	1.288	0.975; 1.011
2H+HCO+H_2O	-1.96	-2.18	1.893; 1.997	2.022; 2.070	1.840	1.322	0.975; 1.015
TS23’	-2.16	-2.08	1.775; 2.268	1.916	1.785	1.209	0.982
3H+CO+OH+H	-3.19	-3.15	1.786	2.069; 2.108; 2.252	1.635; 1.912; 2.164	1.197	0.977
TS24’	-2.30	-2.11	1.773; 2.325	1.900; 1.985; 2.241	1.627; 1.857; 1.678	1.198	
3H+CO+O+2H	-3.22	-3.07	1.771	1.862; 1.981; 2.025; 2.027	1.636; 1.807	1.197	
TS25’	-2.23	-2.00	1.926; 2.118; 2.226	2.084; 1.983; 2.067; 2.173; 2.234	1.668; 1.677; 1.629	1.250	
3H+CO_2+2H	-3.09	-2.99	1.975	1.954; 1.965	1.643; 1.787; 1.639; 1.780	1.292; 1.295	
TS26’	-2.52	-2.29	1.848; 1.922; 2.011; 2.124	1.999; 2.038; 2.042			
3H+C+2O+2H	-3.13	-2.95	1.877; 1.911; 1.917; 1.976; 2.094	1.888; 1.918; 1.947			
TS27’	-1.83	-1.80	1.877; 2.174	2.125; 1.910	1.641; 1.795	1.233	0.975
3H+COOH+H	-2.30	-2.34	1.903	2.018; 2.161	1.646; 1.785	1.278; 1.433	0.987

Table S16. Barriers E_a (eV) and reaction energies E_r (eV) of the reaction of CO+H_2O on the 3H (0.33 ML) pre-covered Fe(111) surface, and the bond distances (Å) of the transition states

	$E_{a\text{-}ZPE}$	E_a	$E_{r\text{-}ZPE}$	E_r	d
3H+CO+H_2O→TS22'→2H+HCO+H_2O	0.76	0.76	0.72	0.63	1.589
3H+CO+H_2O→TS23'→3H+CO+OH+H	0.52	0.73	-0.51	-0.34	1.399
3H+CO+OH+H→TS24'→3H+CO+O+2H	0.89	1.04	-0.03	0.08	1.376
3H+CO+O+2H→TS25'→3H+CO_2+2H	0.99	1.07	0.13	0.08	1.742
3H+CO+O+2H→TS26'→3H+C+2O+2H	0.70	0.78	0.09	0.12	1.901
3H+CO+OH+H→TS27'→3H+COOH+H	1.36	1.35	0.89	0.81	1.818

Figure S1. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O for route P1 on the Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

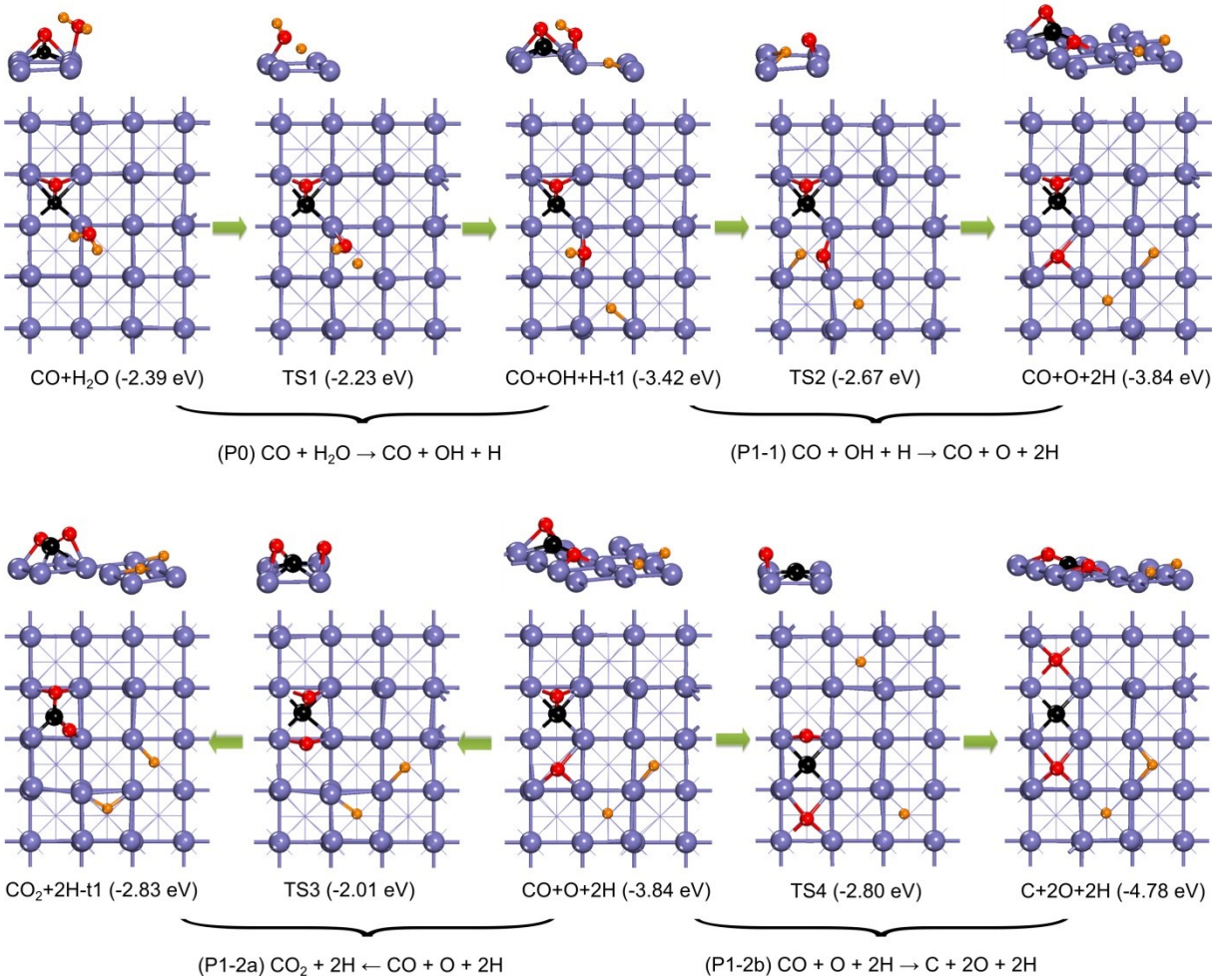


Figure S2. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O for route P2 on the Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

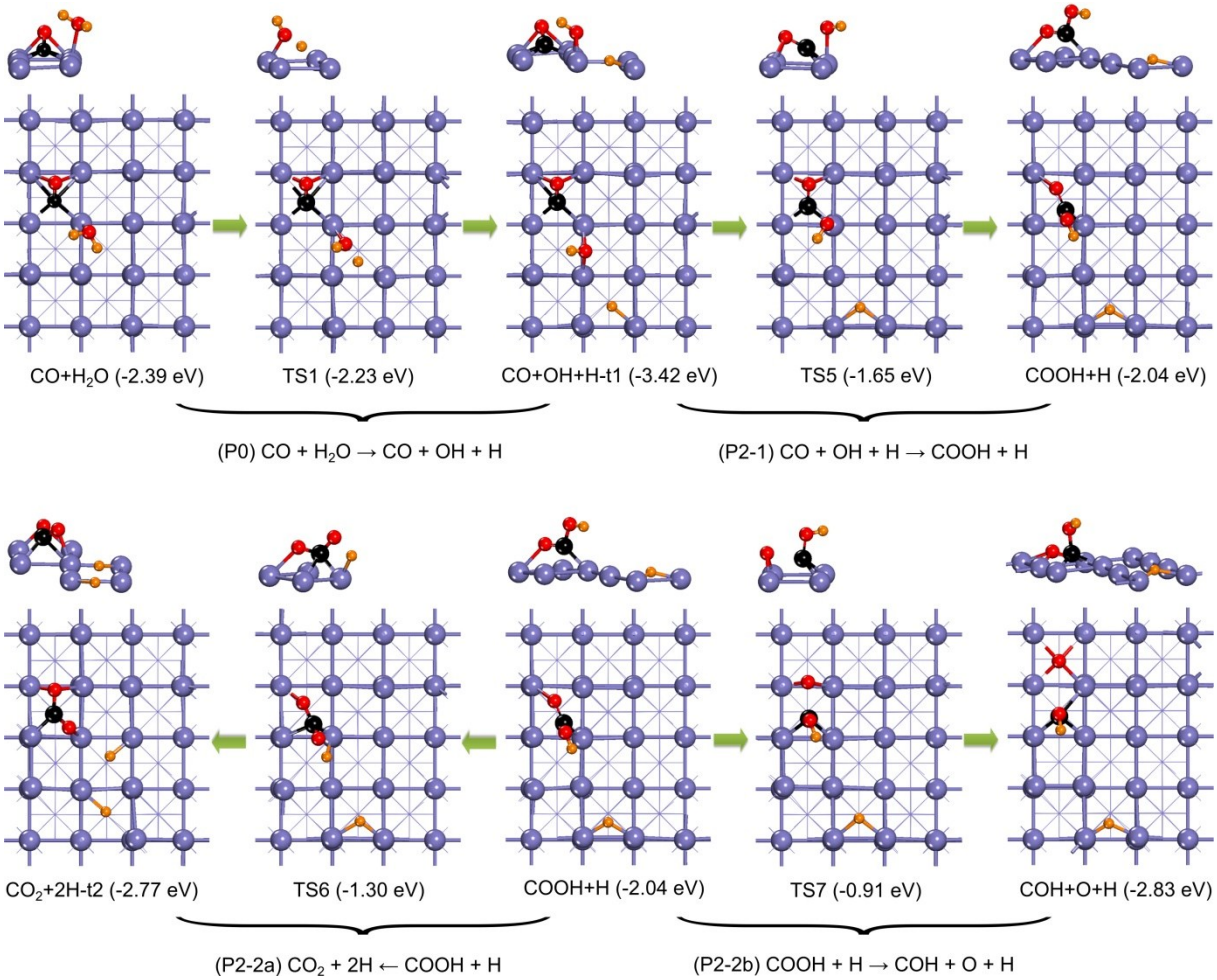


Figure S3. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O for route P3 on the Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

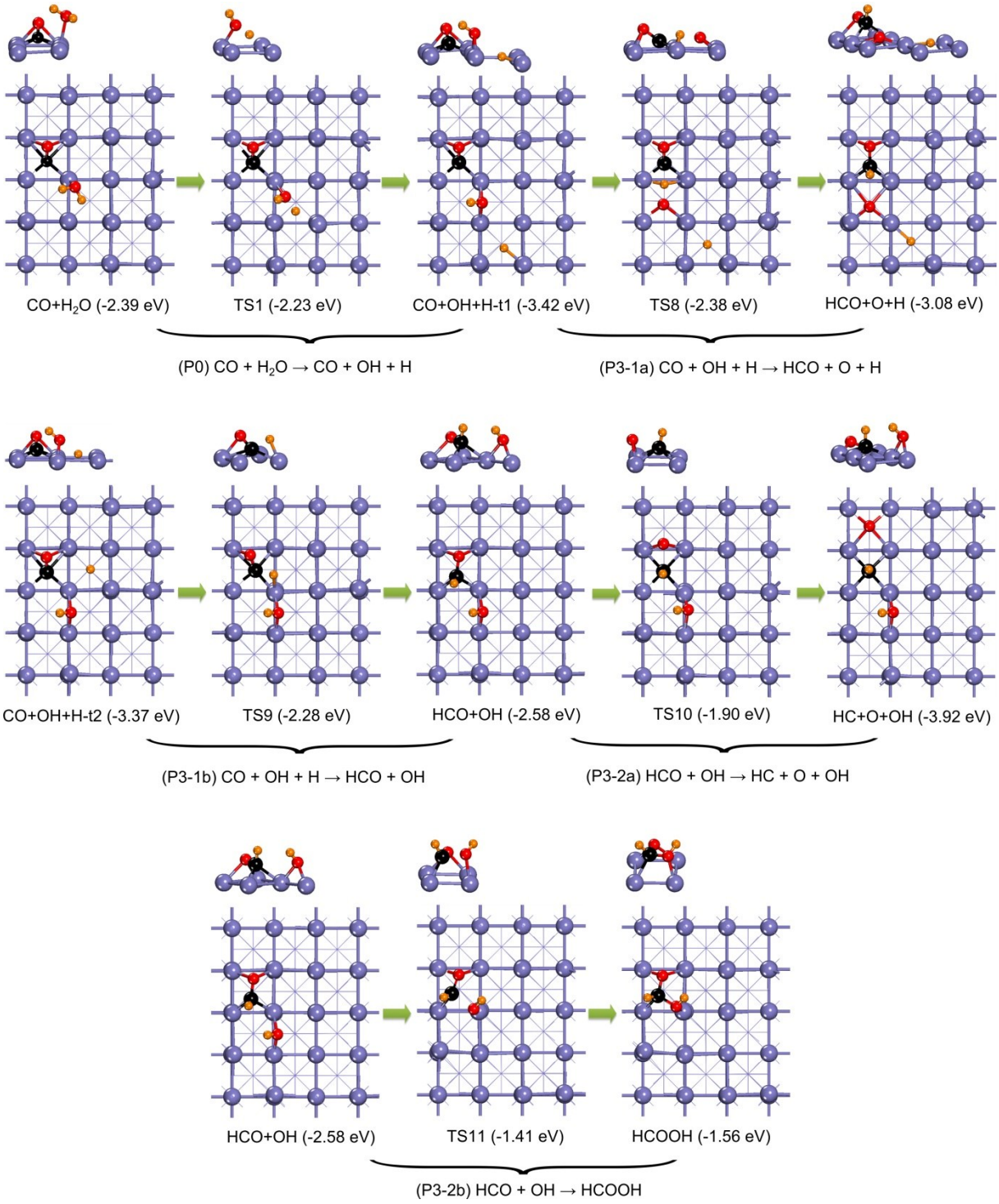


Figure S4. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O for route P4 on the Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

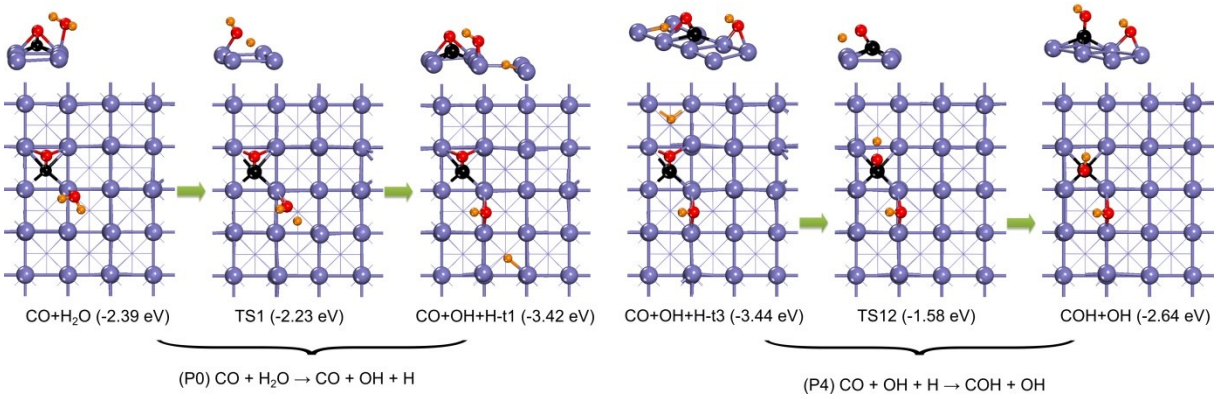


Figure S5. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the Fe(111) surface (Fe/blue; C/black; O/red; H/yellow)

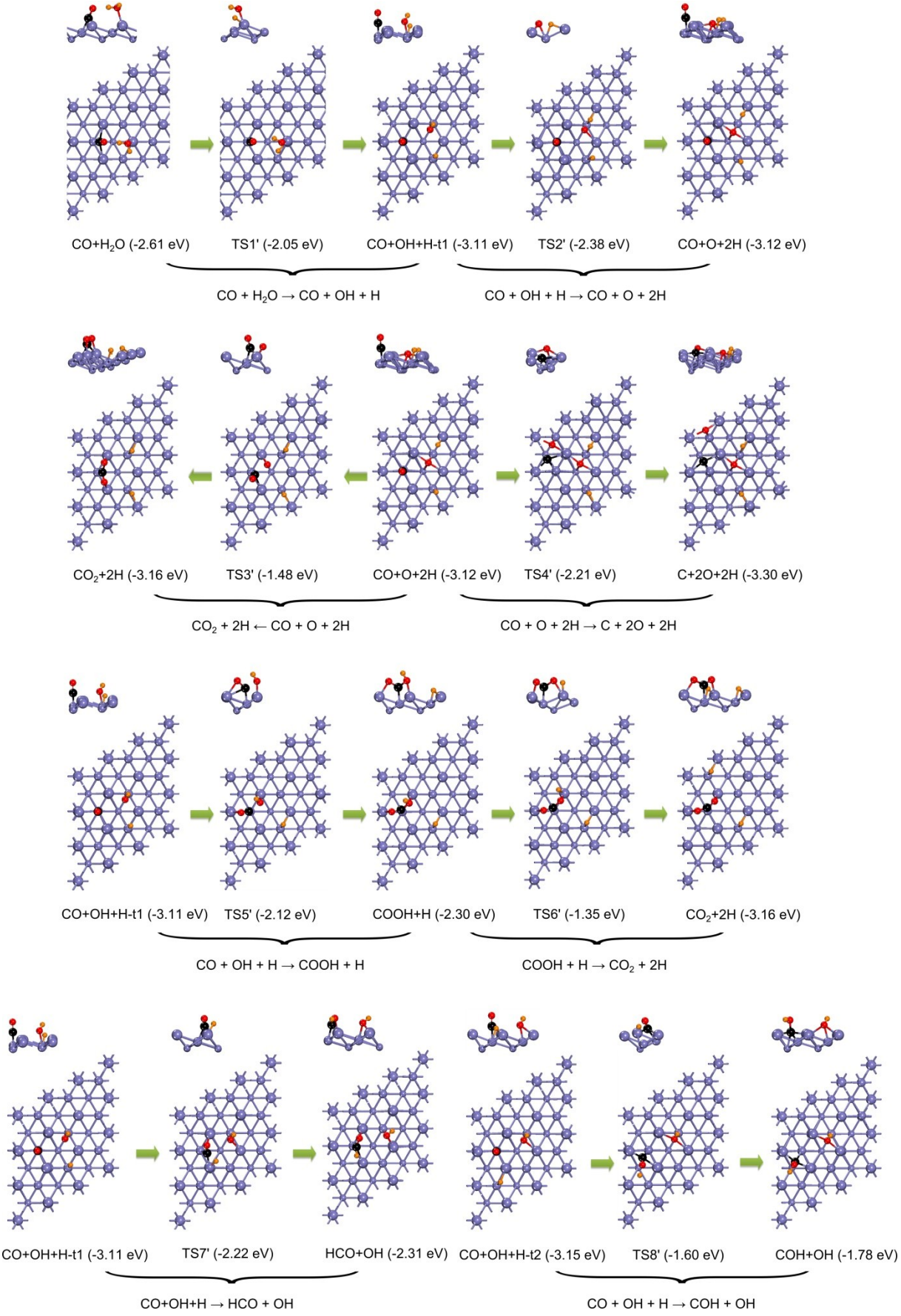


Figure S6. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the 3O (0.25 ML) precovered Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

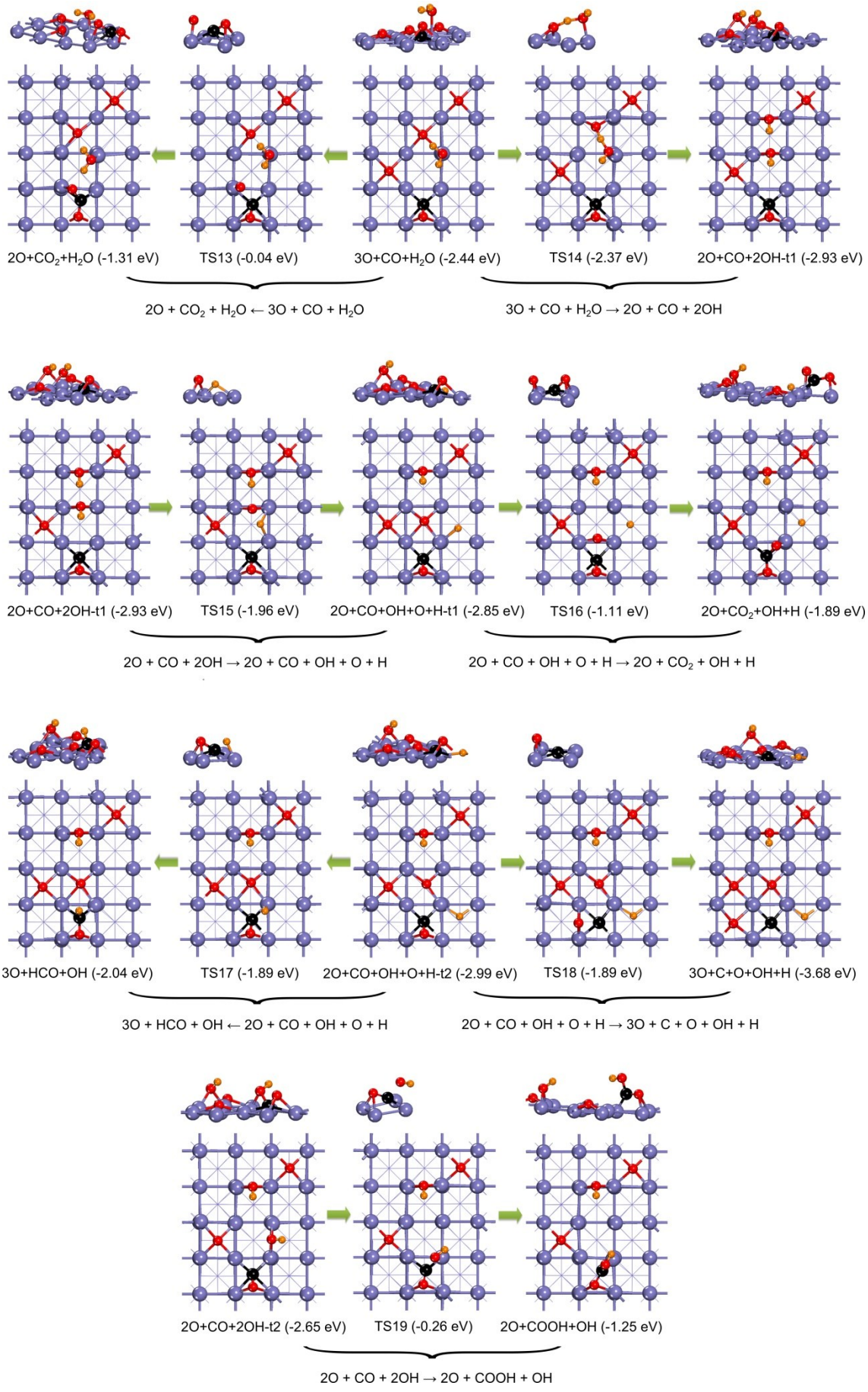


Figure S7. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the 3O (0.33 ML) precovered Fe(111) surface (Fe/blue; C/black; O/red; H/yellow)

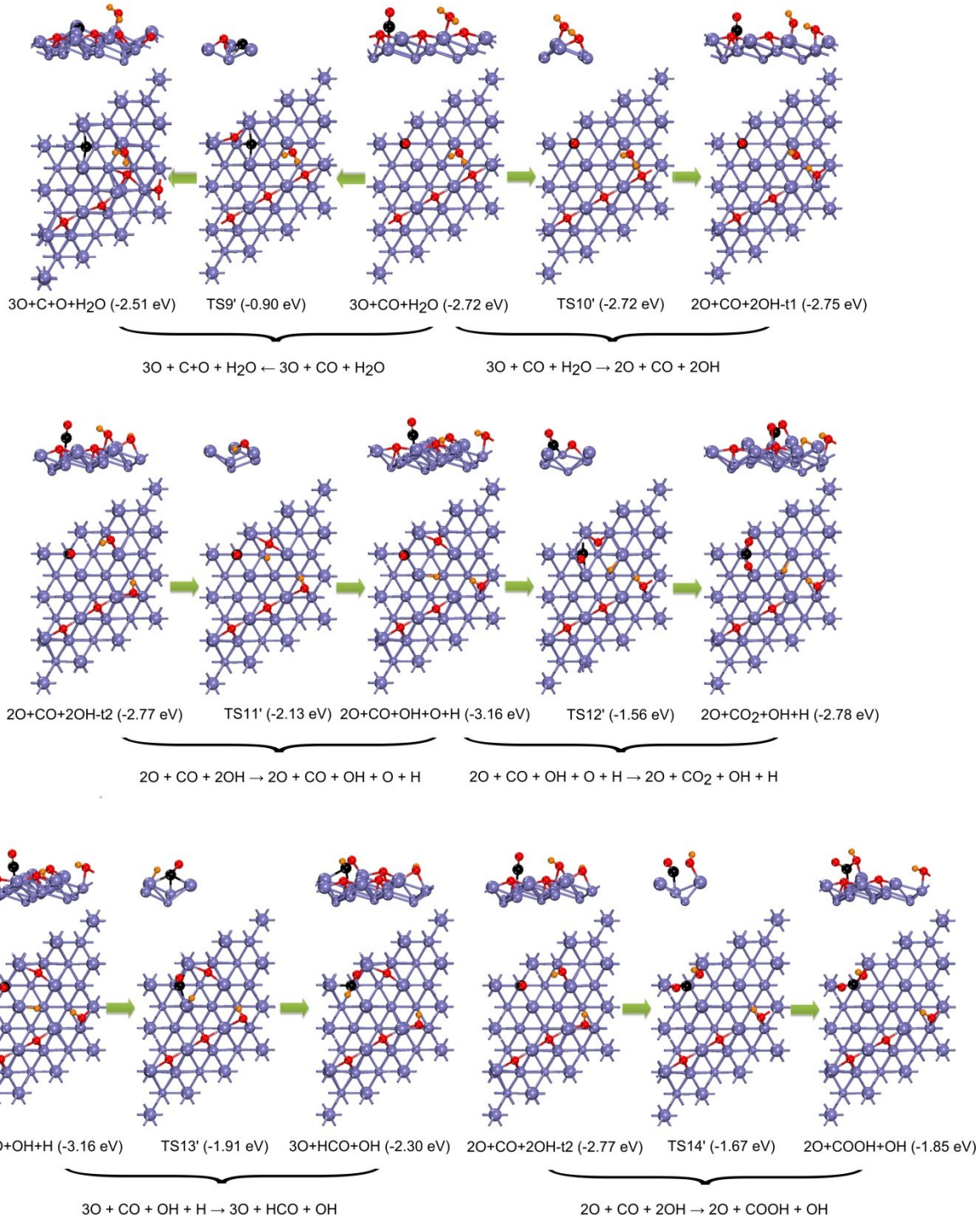


Figure S8. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the 3OH (0.25 ML) dispersed precovered Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

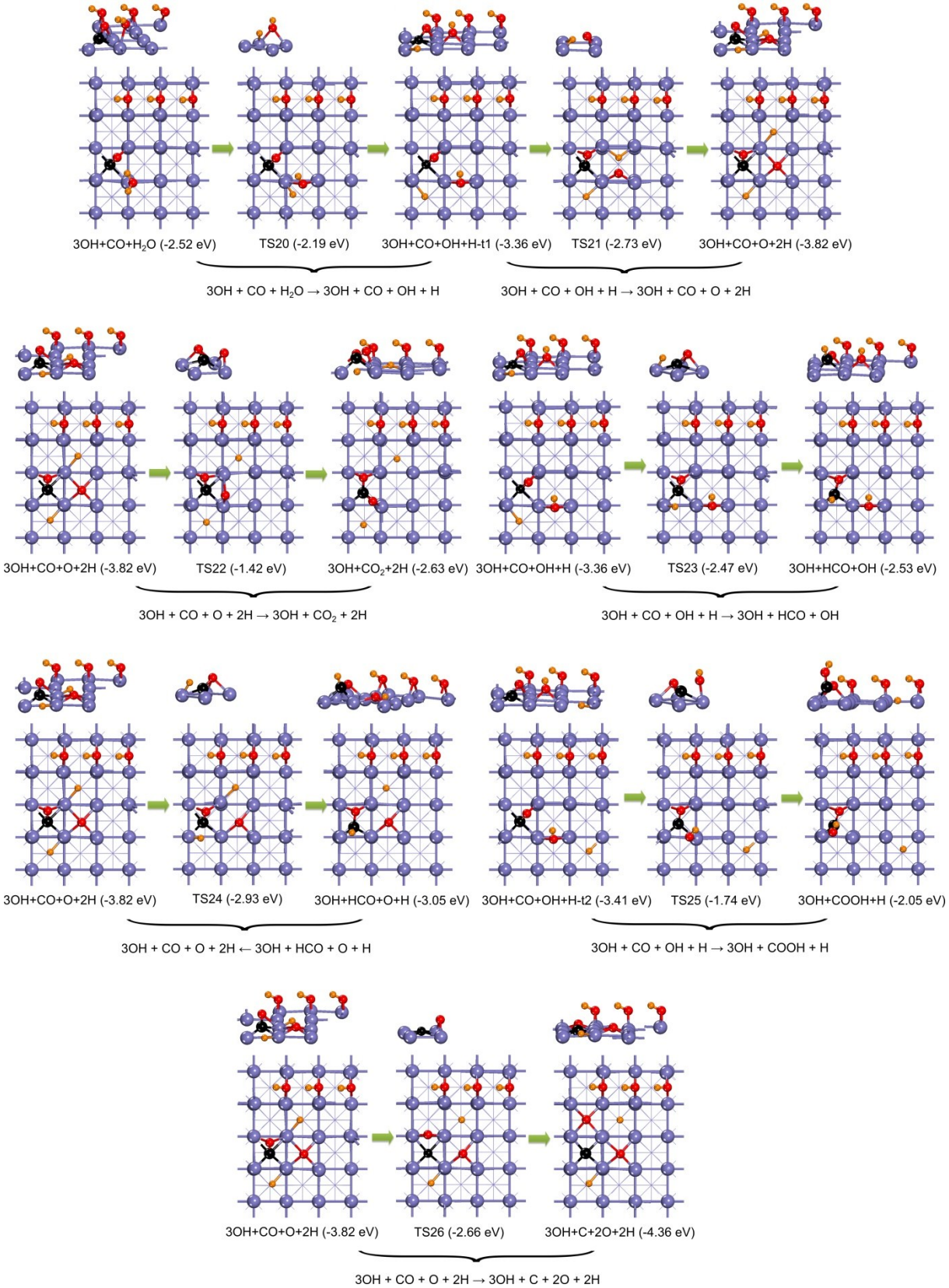
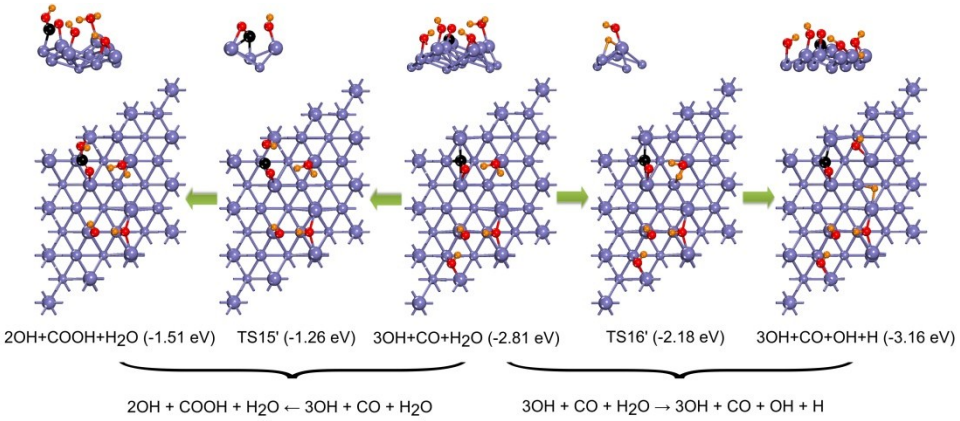
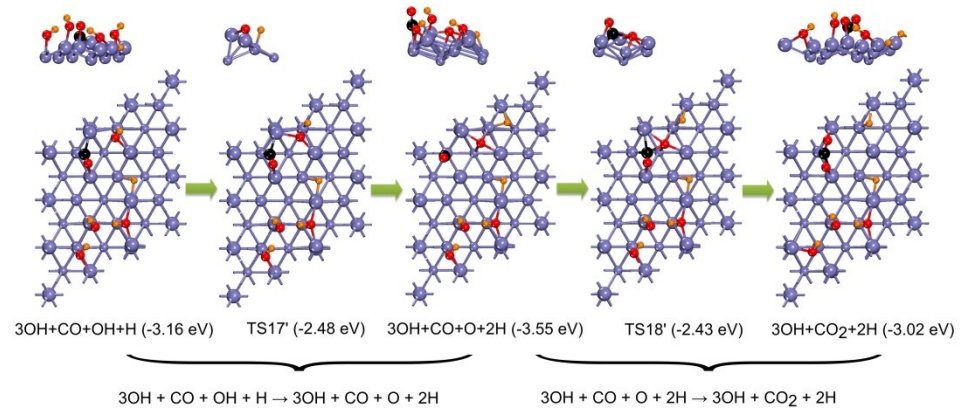
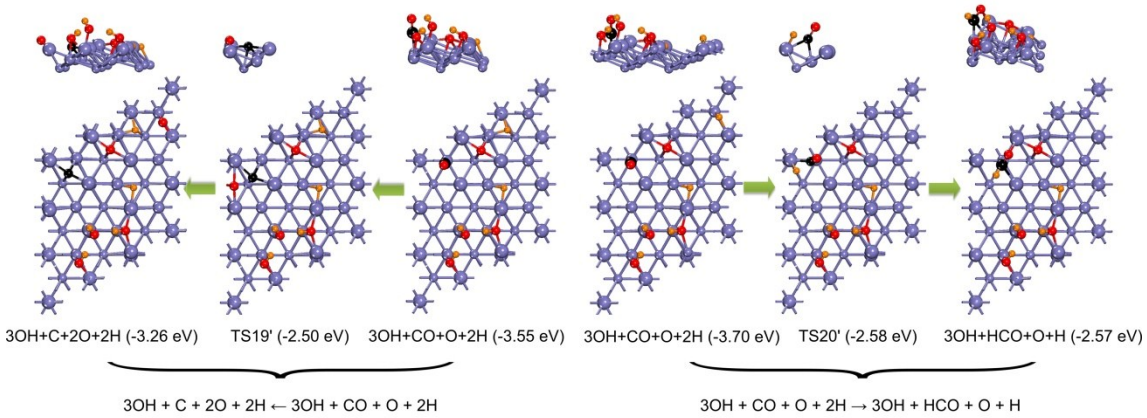


Figure S9. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the 3OH (0.33 ML) dispersed pre-covered Fe(111) surface (Fe/blue; C/black; O/red; H/yellow)







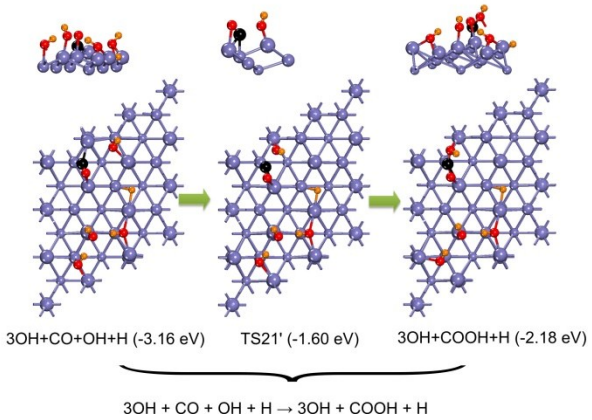


Figure S10. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the 3H (0.25 ML) pre-covered Fe(100) surface (Fe/blue; C/black; O/red; H/yellow)

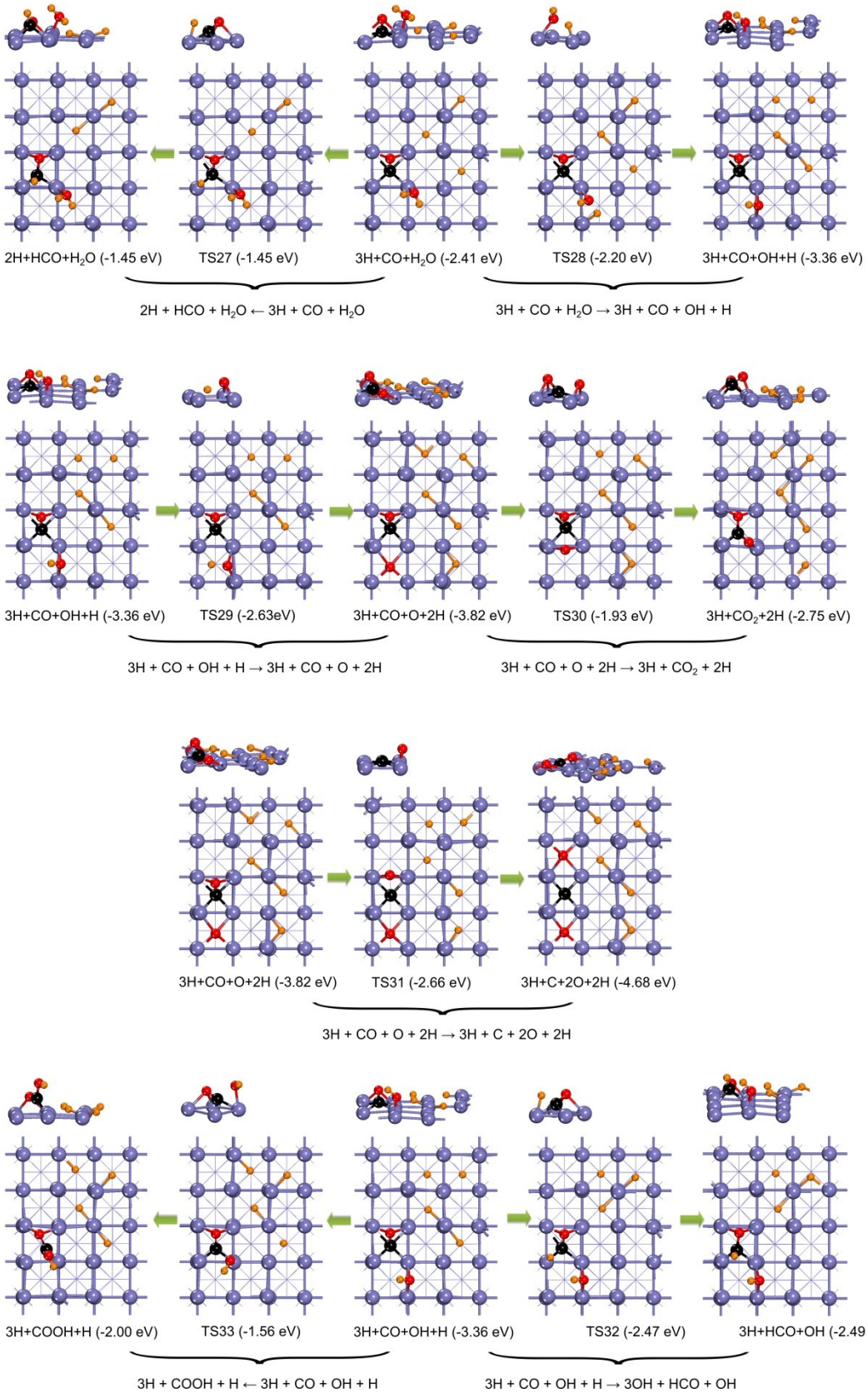
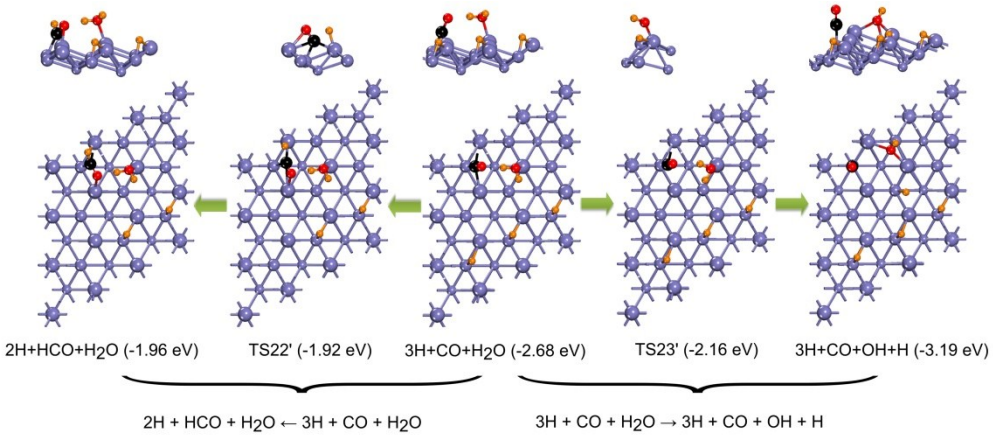
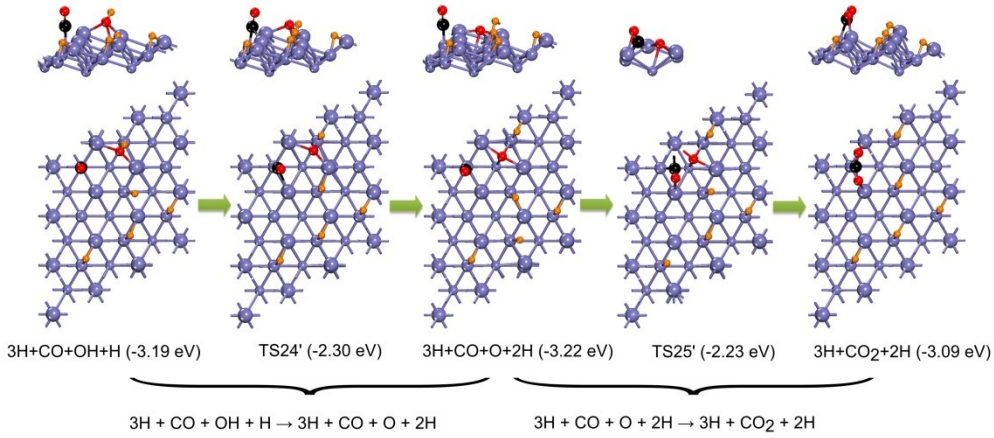


Figure S11. Top (below) and side (above) views of the optimized geometries and adsorption energies for the stationary points in the reaction of CO+H_2O on the 3H (0.33 ML) precovered Fe(111) surface (Fe/blue; C/black; O/red; H/yellow)





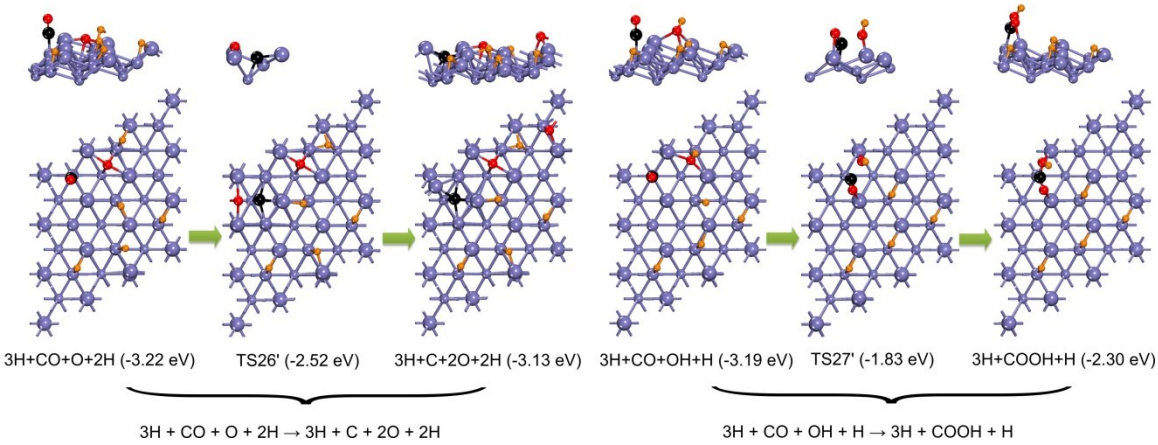


Table SX1. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the Fe(100) surface

	CO+H_2O (-407.036777; ZPE= 0.801722184)					**TS1 (-406.661686; ZPE= 0.582293)**			
H	0.2856664338507069	0.2006051046597274	0.3664958720095521	T	H	0.3591462529018198	0.1464315206721470	0.3565911521888163	T
H	0.4357892660265434	0.1364299175677873	0.3371748877055232	T	H	0.4974534671028555	0.0767747326451381	0.2863348697183014	T
C	0.1601906413487690	0.3651428437482078	0.2592117976122157	T	C	0.1617425160889168	0.3643883846172113	0.2607580708677485	T
O	0.3834320440541728	0.2134765692881852	0.3408658548379422	T	O	0.4145425999952471	0.1621973115383892	0.3129038875351270	T
O	0.1653231043544607	0.4521865658462159	0.3045478204951655	T	O	0.1612009905687143	0.4540746892923339	0.3041568146341497	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0005605212580785	-0.0000780121111494	0.2239082376957076	F	F	0.9997760709089690	0.0027078401050081	0.2242142293437061	T
e	0.0043105052972124	0.2561673659888236	0.2236674969440499	F	e	0.0037400226537431	0.2567367604207270	0.2237184956387973	T
F	0.9885164179789072	0.4989562971178168	0.2293758884734439	F	F	0.9896869520833806	0.4994938012684231	0.2288020206969411	T
e	0.0002985179500857	0.7432838860247888	0.2245254264746008	F	e	-0.0001236916439624	0.7493309207652856	0.2236026843325808	T
F	0.3336250877135843	0.9910061194150447	0.2232974079786583	F	F	0.3491074998730078	0.0011393322913213	0.2274255955859249	T
e	0.3297747605910899	0.2555476914081403	0.2308630563355629	F	e	0.3234710925647478	0.2515516503535747	0.2326819791686763	T
F	0.3343303946501651	0.4991642804651993	0.2287793062613823	F	F	0.3335897065019631	0.4939981075738057	0.2273138869775879	T
e	0.3346025044546531	0.7447413728834599	0.2245374583086531	F	e	0.3300917396411232	0.7533990024688166	0.2237505874104748	T
F	0.6593469236719477	0.0060276981210221	0.2246891326726461	F	F	0.6576441299119035	-0.0000921363747770	0.2283717020840240	T
e	0.6755891340095199	0.2475502770654938	0.2239171472898630	F	e	0.6755405405000410	0.2407522216440547	0.2247817662280229	T
F	0.6661674507550831	0.5024654356805577	0.2250363185505156	F	F	0.6648891077827598	0.5004948042033267	0.2240213465596539	T
e	0.6694080808411298	0.7568036887126199	0.2246380477245941	F	e	0.6665865315735860	0.7577793280166661	0.2241056599991693	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1677860679888154	0.1244041888849565	0.1517716704746348	F	F	0.1680055494526163	0.1239913621094812	0.1512491745360089	T
e	0.1681385240765037	0.3761127833082735	0.1494878983637494	F	e	0.1672297568601337	0.3761306773572311	0.1489911978350752	T
F	0.1663577726395023	0.6244772909718290	0.1505154088885207	F	F	0.1667665730951033	0.6252461997509979	0.1507849758455057	T
e	0.1654957565297286	0.8741142660221257	0.1512028035340729	F	e	0.1668434580300233	0.8770375703493288	0.1514214332943827	T
F	0.4970819613312796	0.1267228727861436	0.1518508423488207	F	F	0.5004417699167196	0.1262448059297012	0.1493543215895205	T
e	0.5003493319008139	0.3745781425343914	0.1516679806072216	F	e	0.5004495462742806	0.3726052054640209	0.1518643461317231	T
F	0.5003230885733320	0.6248257576717459	0.1514539076683885	F	F	0.4987781346247382	0.6248875165833800	0.1518628228987321	T
e	0.5008577175583682	0.8742329784250408	0.1508719398060327	F	e	0.5001411555137186	0.8747446073454028	0.1504175249029918	T
F	0.8347823697864685	0.1246144472619948	0.1511036077876899	F	F	0.8349431832101456	0.1237191283679474	0.1509295989900003	T
e	0.8318154954193717	0.3757693098626774	0.1506081505068232	F	e	0.8309124707247203	0.3752661858941813	0.1509857705581024	T
F	0.8324132280005130	0.6251254953369748	0.1511260081545830	F	F	0.8323757094367977	0.6254633092794163	0.1515103428642102	T
e	0.8336344533430559	0.8755387442654160	0.1513784481390157	F	e	0.8332359411410591	0.8761539733223204	0.1510775274895879	T
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	CO+OH+H-t1 (-407.877285; ZPE= 0.614579236)					**TS2 (-406.906537; ZPE = 0.39530933)**			
H	0.2546450895961650	0.1267065652914553	0.3399889798256619	T	H	0.1292218972924425	0.1199441591210142	0.2567964698781873	T
H	0.5184191693828810	0.8558229415290640	0.2435352241978459	T	H	0.5052182969174073	0.8762353117861198	0.2437654017012513	T
C	0.1611971231120915	0.3652651513289624	0.2604667363193821	T	C	0.1644294277230246	0.3670312751025525	0.2579320672127426	T
O	0.3447845955012704	0.1248968481410367	0.3086257944607123	T	O	0.2743608702643175	0.1117292420379463	0.2928468815731273	T
O	0.1603380888672599	0.4535938965325955	0.3048378369081426	T	O	0.1620306874444493	0.4526680982715492	0.3040876075571635	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0000875471304057	0.9927154442910386	0.2235028981164633	T	F	0.9831895625199799	0.0027785502042551	0.2252646689356492	T
e	0.0043375289263160	0.2572275987681859	0.2232620890867559	T	e	0.0099447840146756	0.2523816517557509	0.2231402056313446	T

F	-0.0111621451358430	0.4998352473650828	0.2292580484388293	T	F	0.9892895982927740	0.4990070607399448	0.2285209788576658	T
e	0.0004705898939642	0.7478891323409760	0.2243680827610069	T	e	0.0035828494370589	0.7517737703635036	0.2262079659561739	T
F	0.3238844421565483	0.0137055301357382	0.2305239475815575	T	F	0.3581160444467961	0.0011413799775791	0.2333852184468437	T
e	0.3254401467001910	0.2487510240941366	0.2347287367886066	T	e	0.3278766236484438	0.2452541725092711	0.2354923739048047	T
F	0.3329160558231443	0.4930032588051923	0.2281394811479106	T	F	0.3331731927206285	0.4937794047386220	0.2273871786962422	T
e	0.3342822037147986	0.7576779318340333	0.2234744410007790	T	e	0.3213105311063972	0.7527853715898938	0.2233917954289979	T
F	0.6756240667898659	0.0024060299525738	0.2225896004517962	T	F	0.6637369174152321	-0.0036819726579247	0.2264369588399252	T
e	0.6683675074989233	0.2502630561575686	0.2235991896823380	T	e	0.6651028713697014	0.2474883280943528	0.2243243944750479	T
F	0.6661072714808477	0.5025421434767788	0.2260854095021559	T	F	0.6623603604554915	0.5034157320310263	0.2245633369100167	T
e	0.6663287706015745	0.7355048722700425	0.2243522251442421	T	e	0.6887904020852862	0.7501537258577409	0.2238875073208328	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1653578177945751	0.1248959564046520	0.1500946937664763	T	F	0.1655360858454476	0.1219714028111828	0.1509727617496096	T
e	0.1683974185857817	0.3761533112252768	0.1494977842790391	T	e	0.1681499499199936	0.3764389414750975	0.1490925671405396	T
F	0.1678244857136603	0.6254622001168024	0.1512820593078521	T	F	0.1668268549555358	0.6252821308368754	0.1506817296775532	T
e	0.1671038910733579	0.8757250903692810	0.1507338626977402	T	e	0.1661366038389151	0.8787717631189469	0.1514740046628336	T
F	0.4990638224608455	0.1258414323569061	0.1505075860743148	T	F	0.4994028279877440	0.1256524946848282	0.1501293506332710	T
e	0.4994961139397645	0.3736206219646933	0.1516133844155798	T	e	0.4997206302294768	0.3734021347021249	0.1517779969140547	T
F	0.4960155155063051	0.6229287099008690	0.1510244942742648	T	F	0.4988254967167645	0.6251172965110225	0.1517858962120589	T
e	0.5004626566440249	0.8773980920932813	0.1536280777326144	T	e	0.5016689723849732	0.8715017727965074	0.1516157976574967	T
F	0.8348251317194856	0.1253592898167591	0.1512803038282269	T	F	0.8312741224091120	0.1256163382431778	0.1509214722749939	T
e	0.8325166347357920	0.3757989219154793	0.1506692236790054	T	e	0.8322503257858233	0.3746101747334807	0.1512970484457088	T
F	0.8338688886060129	0.6245718779128568	0.1507745050063836	T	F	0.8345768762310135	0.6243932043690575	0.1508603389260318	T
e	0.8326685924235643	0.8734973467468748	0.1508315592254616	T	e	0.8361181054919316	0.8756481490729981	0.1495203137456823	T
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	CO+O+2H (-408.17082; ZPE= 0.482326967)					**TS3 (-406.293882; ZPE= 0.438953)**			
H	0.7928313364888435	0.1255632302071167	0.2439800378609757	T	H	0.8134804585241866	0.1195906926887111	0.2437560603766524	T
H	0.4954513047708561	0.8949879036299105	0.2449949486170971	T	H	0.5017695901687408	0.8940077577081693	0.2445096636877782	T
C	0.1704030258181738	0.3758505766246324	0.2600213301991492	T	C	0.1488999945275943	0.3851633175847924	0.2600141363689248	T
O	0.1724105108609922	0.1071339262547610	0.2586437341813863	T	O	0.1737358531036996	0.2343333369077819	0.2973391940815613	T
O	0.1672979460810996	0.4604380656558963	0.3062556716866857	T	O	0.1913599701866763	0.4594079373281331	0.3067053465711055	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0076695984471643	0.9967821146780732	0.2256437061867540	T	F	0.0033748860289879	0.9894312414377380	0.2235683850357595	T
e	0.0181391787587252	0.2549737651410664	0.2274540548511927	T	e	0.0057265914107109	0.2568118421671762	0.2298495239389162	T
F	0.9919245565164524	0.4973842364052615	0.2287410811797289	T	F	0.9776743210838965	0.5034820775968661	0.2257207756110257	T
e	0.9954498842907662	0.7534849456964116	0.2258745043135060	T	e	0.9987008099015396	0.7487447416010496	0.2278511215168114	T
F	0.3364342269886271	-0.0018052271994749	0.2288169778215172	T	F	0.3427718825631583	0.0069050228273581	0.2244567083593267	T
e	0.3283071735370722	0.2525047789757811	0.2310346436452810	T	e	0.3299995132539730	0.2322497072316216	0.2309445308459526	T
F	0.3415948570022331	0.4968050264378217	0.2277504823453191	T	F	0.3418567146656954	0.5064241552985475	0.2274630999023425	T
e	0.3205808197348141	0.7508059927094717	0.2233628170315309	T	e	0.3201212642664127	0.7481742938973240	0.2229015698486856	T
F	0.6476482844284095	0.0085647824639308	0.2259384146882102	T	F	0.6523939728392318	0.0060820928832114	0.2249008420627087	T
e	0.6546785652163404	0.2492292234869395	0.2244550825575619	T	e	0.6652328726228778	0.2493562850383892	0.2238053387052678	T
F	0.6652623253884342	0.5017101594875882	0.2259049020446233	T	F	0.6623854940182151	0.5030647066417050	0.2261275798022521	T
e	0.6846124244415618	0.7429071274295281	0.2240612582580415	T	e	0.6870590055383531	0.7479984861407049	0.2248486215012509	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F

F	0.1675593159835290	0.1246405854855083	0.1475021965278921	T	F	0.1651395879784630	0.1232644610612869	0.1492582841493474	T
e	0.1676125832717212	0.3776588422104341	0.1495906266512899	T	e	0.1706111218088420	0.3761896671964514	0.1537804284140092	T
F	0.1663823694318891	0.6250651986760113	0.1503850012204092	T	F	0.1656449365493390	0.6243025497840452	0.1501052190132465	T
e	0.1658087110290418	0.8753249945469140	0.1499322590713575	T	e	0.1662522306739772	0.8750350874078694	0.1501679382088556	T
F	0.4947493116771240	0.1265009543507377	0.1497845319422134	T	F	0.5004801674233692	0.1268272405143525	0.1484604493882557	T
e	0.5005465618038183	0.3744369757810884	0.1510212889999998	T	e	0.4998376795910174	0.3742055006518525	0.1516281918299182	T
F	0.4993122778326624	0.6251355820481211	0.1513547385396362	T	F	0.5010307003957472	0.6267793035878003	0.1511030022142068	T
e	0.5018292695601057	0.8723202222883031	0.1532697297828216	T	e	0.5010657209536126	0.8721001359126848	0.1530833239569199	T
F	0.8336639856678006	0.1246785654457373	0.1538690785335629	T	F	0.8362491750528490	0.1245667451868184	0.1537090639409751	T
e	0.8337042844516571	0.3741304130526661	0.1518041623366045	T	e	0.8326750747823721	0.3749204308392718	0.1507223350868898	T
F	0.8355371910162634	0.6233211729716608	0.1505503501636144	T	F	0.8329628136980910	0.6255062373851533	0.1492811288856566	T
e	0.8334358838252861	0.8760221191422800	0.1511553376717724	T	e	0.8334527935287324	0.8750344627614441	0.1500338907852486	T
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	CO_2+2H-t1 (-407.173176; ZPE= 0.497221148)					**TS4 (-407.034954; ZPE= 0.393853)**			
H	0.8056836308726285	0.1174638387432455	0.2431803139492352	T	H	0.5198411620156087	0.8750873515249997	0.2431741696605850	T

H	0.5021328722626450	0.8913311632329649	0.2444928483179845	T	H	0.8029452737953742	0.1314804470002459	0.2432019555728225	T
C	0.1559825247876694	0.3388502936053294	0.2932931151745009	T	C	0.1691510992424755	0.3716741693198233	0.2466178177691968	T
O	0.2539767191563622	0.2738257226159116	0.3278349733560030	T	O	0.1641686226384453	0.5134237764133608	0.2993232999668116	T
O	0.1635690820472903	0.4573787117707115	0.3031401385390045	T	O	0.1673701213072603	0.1065484072213083	0.2592538795067946	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0022244967918964	0.9982181171512106	0.2227482779034335	T	F	0.0023712526470986	0.9945230371483095	0.2273645575650056	T
e	0.0139209902484979	0.2644013517440867	0.2261966060141244	T	e	0.0120224644849343	0.2540549914013681	0.2280394571179873	T
F	-0.0008539496257821	0.5088508143934494	0.2324665843750909	T	F	0.0042877895330379	0.4990884940536166	0.2319513023533800	T
e	0.9937906402316000	0.7465179366162157	0.2264282119470607	T	e	0.9992441688745471	0.7511744571589192	0.2244752609291078	T
F	0.3420230199684714	0.0051087870494619	0.2254496246804568	T	F	0.3304909181749635	0.0011865048843213	0.2254966685962821	T
e	0.3335150080750444	0.2334114772543916	0.2336205742393128	T	e	0.3259274247031856	0.2505073217484404	0.2299577165738306	T
F	0.3284572358489848	0.5016625988992123	0.2292420129807436	T	F	0.3261316556568880	0.4993813824987902	0.2315193986038481	T
e	0.3196075315375378	0.7473890234097021	0.2224077257258049	T	e	0.3378658759337601	0.7529757724936561	0.2230170510073412	T
F	0.6500010810173749	0.0044495214970697	0.2247302561368900	T	F	0.6763917775441978	-0.0001917333911717	0.2233388776937772	T
e	0.6645961845318191	0.2497178201064195	0.2237736315061149	T	e	0.6489584604725210	0.2523820462418451	0.2239818789603319	T
F	0.6662415318429784	0.4981336293035052	0.2242250460516776	T	F	0.6658148808554094	0.4981027718208400	0.2259654524942559	T
e	0.6841595154425907	0.7498027340658832	0.2242374134487242	T	e	0.6731361969659894	0.7365175108082948	0.2240009321017493	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1665625879105477	0.1247299431480460	0.1507446405135912	T	F	0.1667643805237899	0.1256693564588747	0.1477893804708034	T
e	0.1703512634266455	0.3747472828962658	0.1493433972822565	T	e	0.1665857835418862	0.3762605091634032	0.1458685598969504	T
F	0.1657538367392139	0.6240274748303862	0.1500352837194325	T	F	0.1672671715123380	0.6256832392473366	0.1502192445518778	T
e	0.1648851838073382	0.8756645092888229	0.1506927717712663	T	e	0.1663664724813954	0.8747464415274150	0.1505791970597072	T
F	0.4991439987912249	0.1270651124554264	0.1488803919964570	T	F	0.4978234256877201	0.1248895825189361	0.1511017005315670	T
e	0.4982389383751337	0.3745827947463000	0.1519738350840882	T	e	0.4972372786848721	0.3758671463488882	0.1515690753549204	T
F	0.4990151354653162	0.6249654026415111	0.1517286570405942	T	F	0.4983092788955397	0.6225003711005077	0.1513585346022942	T
e	0.5001927609661374	0.8718818763886707	0.1527276109321909	T	e	0.5028321716523787	0.8759275364865948	0.1536551124719778	T
F	0.8351053238807181	0.1255991866999712	0.1533257370266589	T	F	0.8337854589138451	0.1262353608040323	0.1533049878575732	T
e	0.8350941388726032	0.3761796934779562	0.1514864274841776	T	e	0.8341768142690492	0.3749096602797196	0.1522796227350443	T
F	0.8332728268410210	0.6238987632581173	0.1504071610272386	T	F	0.8349255870546787	0.6226736479065327	0.1514108160794095	T
e	0.8345698745379391	0.8759066757111017	0.1504983547542841	T	e	0.8340483709616328	0.8731611312282904	0.1509694276507575	T
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	C+2O+2H (-409.065722; ZPE= 0.442128599)					**TS5 (-406.0916649; ZPE= 0.598227)**			
H	0.7928313364888435	0.1255632302071167	0.2439800378609757	T	H	0.2259024157735551	0.1865999763300457	0.3481900203293502	T
H	0.4954513047708561	0.8949879036299105	0.2449949486170971	T	H	0.5032574936372491	0.8521716200892598	0.2433834636818235	T
C	0.1704030258181738	0.3758505766246324	0.2600213301991492	T	C	0.1635971878398668	0.3431766523794967	0.2807140962187648	T
O	0.1724105108609922	0.1071339262547610	0.2586437341813863	T	O	0.2886954046454702	0.2564766204369610	0.3371590733653255	T
O	0.1672979460810996	0.4604380656558963	0.3062556716866857	T	O	0.1712190795045845	0.4494799075593457	0.3064160377371942	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0076695984471643	0.9967821146780732	0.2256437061867540	T	F	0.9937189722978356	0.0008460293400972	0.2236903518387524	T
e	0.0181391787587252	0.2549737651410664	0.2274540548511927	T	e	0.0118371679689129	0.2581527505680855	0.2258447384039896	T
F	0.9919245565164524	0.4973842364052615	0.2287410811797289	T	F	0.9961179444316655	0.4975390688022370	0.2314282290214947	T
e	0.9954498842907662	0.7534849456964116	0.2258745043135060	T	e	0.9961005961654067	0.7490334770993751	0.2239683558045971	T
F	0.3364342269886271	-0.0018052271994749	0.2288169778215172	T	F	0.3305212691724326	0.0064593536088600	0.2222473517957666	T
e	0.3283071735370722	0.2525047789757811	0.2310346436452810	T	e	0.3357011178009504	0.2482633236101026	0.2343142956452875	T

F	0.3415948570022331	0.4968050264378217	0.2277504823453191	T
e	0.3205808197348141	0.7508059927094717	0.2233628170315309	T
F	0.6476482844284095	0.0085647824639308	0.2259384146882102	T
e	0.6546785652163404	0.2492292234869395	0.2244550825575619	T
F	0.6652623253884342	0.5017101594875882	0.2259049020446233	T
e	0.6846124244415618	0.7429071274295281	0.2240612582580415	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1675593159835290	0.1246405854855083	0.1475021965278921	T
e	0.1676125832717212	0.3776588422104341	0.1495906266512899	T
F	0.1663823694318891	0.6250651986760113	0.1503850012204092	T
e	0.1658087110290418	0.8753249945469140	0.1499322590713575	T
F	0.4947493116771240	0.1265009543507377	0.1497845319422134	T
e	0.5005465618038183	0.3744369757810884	0.1510212889999998	T
F	0.4993122778326624	0.6251355820481211	0.1513547385396362	T
e	0.5018292695601057	0.8723202222883031	0.1532697297828216	T
F	0.8336639856678006	0.1246785654457373	0.1538690785335629	T
e	0.8337042844516571	0.3741304130526661	0.1518041623366045	T
F	0.8355371910162634	0.6233211729716608	0.1505503501636144	T
e	0.8334358838252861	0.8760221191422800	0.1511553376717724	T
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F	0.3264534435474988	0.4930528531512989	0.2289519969922351	T
e	0.3328038991131681	0.7451407421312811	0.2222572607408415	T
F	0.6694567593290963	0.0101446851212343	0.2230464946048811	T
e	0.6682459240768398	0.2528699558647087	0.2251036021157043	T
F	0.6692904731188091	0.4992719759477553	0.2254153159829719	T
e	0.6678070393016430	0.7368112246642837	0.2236607242191460	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1661938808145858	0.1255765558058923	0.1510687647847526	T
e	0.1681274786403843	0.3750696682226616	0.1483078674831954	T
F	0.1662294428217386	0.6241136231467355	0.1511876356627200	T
e	0.1655453507207416	0.8751034172045185	0.1514493611628919	T
F	0.4989853004037828	0.1277482643197186	0.1505733290957173	T
e	0.4992113023763207	0.3745739525245493	0.1511691748529719	T
F	0.4977972628589016	0.6211945975221926	0.1510012358024298	T
e	0.5012509060201205	0.8751677354088195	0.1539358923746070	T
F	0.8341978219639345	0.1271012631195443	0.1510957775261549	T
e	0.8345127578687203	0.3750952800689547	0.1510195479351383	T
F	0.8348449574649944	0.6236058227386372	0.1509856145834652	T
e	0.8319969421556351	0.8746723073269598	0.1513393977909742	T
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	COOH+H (-406.580624; ZPE= 0.691456269)					**TS6 (-405.6229867; ZPE= 0.479603)**			
H	0.4991432398303677	0.8517089620172489	0.2437631732526714	T	H	0.5129569982217718	0.8569419532589598	0.2442059044046517	T
H	0.2632760765882375	0.2103672708786971	0.3651151084535049	T	H	0.2961577202234202	0.1699334637499178	0.3054349654299707	T
C	0.2111440801945107	0.3355350506290228	0.3033073939093795	T	C	0.2100828748155433	0.3283670007536100	0.2990122543092086	T
O	0.1500228051925796	0.4433242954462196	0.3056568220893829	T	O	0.1432662359815911	0.4326844939175639	0.3090140140917736	T
O	0.2199368831402290	0.2902041648643902	0.3692780404150086	T	O	0.2420630087205227	0.2588166947618833	0.3512308368022131	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0020790191153254	0.0003819759953338	0.2242437520734024	T	F	0.0003587289056362	0.9991826927427367	0.2244002858025117	T
e	0.0172505185966132	0.2431837115845503	0.2279730412636035	T	e	0.0185756728927606	0.2442028492121420	0.2262510729299320	T
F	0.0094214868430740	0.5008636004788967	0.2285676480905099	T	F	0.0092430249785020	0.4996582213824696	0.2306734407477345	T
e	-0.0045147453221476	0.7526147809597400	0.2231681500314247	T	e	0.9970654664168837	0.7500231635810851	0.2236968939170246	T
F	0.3347149037315734	0.0119185951362226	0.2238325800321469	T	F	0.3288399648441541	0.0281457498367116	0.2307672800925006	T
e	0.3208668554470639	0.2593716400601747	0.2272945097117726	T	e	0.3255012733602549	0.2527772525510785	0.2252168026618945	T
F	0.3317622464114856	0.4915978934521794	0.2325108324365283	T	F	0.3280962179136074	0.4866620964338342	0.2300821105796085	T
e	0.3334931075039125	0.7406324636749224	0.2234485796375571	T	e	0.3324688850596504	0.7512905937825517	0.2235311883720943	T
F	0.6671604091138718	0.0108801208248353	0.2235552656718006	T	F	0.6658658289305820	0.0054724923583637	0.2233242998986356	T
e	0.6633641701212101	0.2531282461168280	0.2249108047651270	T	e	0.6641153924180041	0.2529363061103815	0.2240830349626358	T
F	0.6656539922347298	0.4984862525744195	0.2252699833055426	T	F	0.6662111895768644	0.5001214173104407	0.2246778290254741	T
e	0.6652814960431522	0.7389102559090815	0.2232539635787902	T	e	0.6670913497281588	0.7386902826443371	0.2228404681738838	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1675842343202544	0.1243691362304384	0.1501171575736098	T	F	0.1664318236848890	0.1242126659944131	0.1487725666440692	T
e	0.1650811616106820	0.3754988150976569	0.1472701681831913	T	e	0.1648289339787418	0.3750661113674483	0.1470654477392605	T
F	0.1675208125926766	0.6240290604550545	0.1509897269943072	T	F	0.1681269811243358	0.6243232800983735	0.1518492013612187	T
e	0.1673556707455198	0.8751319876420369	0.1516200526126684	T	e	0.1680774465475713	0.8768349217546932	0.1520421827811123	T

F	0.4990607082836048	0.1285109173269823	0.1505869754313035	T	F	0.5003700175870547	0.1267981995949076	0.1501567606769823	T
e	0.4990322145197909	0.3753689212683793	0.1510269883728072	T	e	0.4996300646772841	0.3753562762241203	0.1506727649177291	T
F	0.4976449093234943	0.6205648973895643	0.1509749598508125	T	F	0.4958671245873464	0.6220355357950482	0.1514019268834896	T
e	0.4998769771374314	0.8755372481247832	0.1541391660453114	T	e	0.4987480758436221	0.8774907977970611	0.1545573490713036	T
F	0.8347592158990333	0.1272297925432973	0.1517711122169373	T	F	0.8344015708128576	0.1264065721590033	0.1518019828521919	T
e	0.8366482307916521	0.3747222390015159	0.1521341207071383	T	e	0.8361459487518544	0.3749846495393013	0.1521718724251655	T
F	0.8346946521661862	0.6234750540175382	0.1514828245976625	T	F	0.8352777542709019	0.6231321366997818	0.1515744778821349	T
e	0.8316415720167540	0.8753306318485605	0.1514079409411873	T	e	0.8326795513090405	0.8753331071926150	0.1514755262458883	T
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	CO_2+2H-t2 (-407.116012; ZPE= 0.498647057)					**TS7 (-405.362689;ZPE= 0.612187)**			
H	0.4807190124503054	0.8845651428897259	0.2441309971434295	T	H	0.5008988705004066	0.8531623215713755	0.2436613083602378	T
H	0.1599369654029510	0.0852725400200414	0.2421852976576652	T	H	0.2211960763784491	0.2484642980582763	0.3675644858700780	T
C	0.1538260028954280	0.3436766808451802	0.2904021322665479	T	C	0.1766968982811887	0.3372298269751585	0.2858656681110052	T
O	0.2531714660687766	0.2774627882414292	0.3231437625960283	T	O	0.1700033876583545	0.5143320013202340	0.2952242074596935	T
O	0.1598634279423433	0.4616027516713038	0.3025536173841963	T	O	0.1820605306066071	0.3276404400077904	0.3568559811586367	T

F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0082124994261566	0.9913626664074751	0.2236175664024102	T	F	0.9956511719817926	0.0019825730855443	0.2241627812063418	T
e	0.0038394036223255	0.2659113601289331	0.2266757932779100	T	e	0.0146966891968905	0.2625747181410300	0.2289123636973471	T
F	0.9941578047033550	0.5123466975387067	0.2321925974005071	T	F	0.0062594802316722	0.4935022915540410	0.2324150939427672	T
e	-0.0070951851804406	0.7482756760566570	0.2252781691530867	T	e	0.9993648473499711	0.7523418492575591	0.2230672929869826	T
F	0.3216248942914774	-0.0093861182078294	0.2237145526913349	T	F	0.3338211837545657	0.0090284140909488	0.2232150550057848	T
e	0.3462453058531511	0.2423927208567932	0.2303109109052158	T	e	0.3284563737052583	0.2606884356366340	0.2261572071252842	T
F	0.3228328139518270	0.5101537947313445	0.2298943693189226	T	F	0.3325074783481777	0.4906402135100215	0.2325010612295060	T
e	0.3467598047615452	0.7513673750862883	0.2239066084877542	T	e	0.3299792406889747	0.7443225643160033	0.2220166370679082	T
F	0.6711872264391057	0.0133969656575794	0.2237637000898985	T	F	0.6718632032353725	0.0115161647997905	0.2234898173618644	T
e	0.6674282795142725	0.2512216280642260	0.2250542063912023	T	e	0.6657458941373733	0.2508073884039783	0.2253281926870154	T
F	0.6665125776469724	0.4939747967167644	0.2256599230321784	T	F	0.6666360625747982	0.4988824877149110	0.2252209509801721	T
e	0.6682168981778152	0.7331614796161406	0.2245881355078533	T	e	0.6661859721543315	0.7400499010766558	0.2225613671823983	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1661424206769865	0.1255682106059645	0.1529881564379811	T	F	0.1663881183025503	0.1260344052212714	0.1513900879591137	T
e	0.1696387918510187	0.3755874020264570	0.1507697222222265	T	e	0.1669581530045006	0.3769065861028604	0.1472617268630531	T
F	0.1656752359665681	0.6258736470674521	0.1505244569656588	T	F	0.1660869402145293	0.6243300200141024	0.1498815835833106	T
e	0.1640486551515533	0.8714687425191552	0.1501333399926677	T	e	0.1666556020861178	0.8761476087229285	0.1513338355024954	T
F	0.5010338470325693	0.1248632959214621	0.1501348204102528	T	F	0.4994559495189221	0.1277311898268420	0.1507915227197726	T
e	0.4979253551661178	0.3758770102669917	0.1513247309164082	T	e	0.5012134699284229	0.3752304368921685	0.1502442617345702	T
F	0.4990432630538596	0.6222533735531887	0.1502514360924815	T	F	0.4981830630406463	0.6211624559185540	0.1509007401950490	T
e	0.5050701420548154	0.8762256153611711	0.1529745813559176	T	e	0.5007198695001892	0.8754259223501437	0.1542032535200704	T
F	0.8356032679617201	0.1271618200325362	0.1508364218838144	T	F	0.8363496456710618	0.1285291958937735	0.1517466295259320	T
e	0.8350839776171107	0.3765072482805866	0.1508509631952113	T	e	0.8346442100817840	0.3748032062502692	0.1513238956871237	T
F	0.8326912689955852	0.6240712580234669	0.1498269115878492	T	F	0.8350671462464023	0.6229738456341131	0.1517007388551216	T
e	0.8301392564303801	0.8744006204612379	0.1512327498071366	T	e	0.8322801575416195	0.8753010237824840	0.1513840331861642	T
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	COH+O+H (-407.309454; ZPE= 0.632062886)					**TS8 (-406.656539; ZPE= 0.433083)**			
H	0.4877304306028529	0.8449206193960508	0.2436605614071569	T	H	0.1666469689736207	0.2206368143642555	0.2807620157556799	T
H	0.1760961706958842	0.2983224074995889	0.3658791088285556	T	H	0.5075515224512338	0.8645387285284113	0.2439126120036963	T
C	0.1670539844913642	0.3656373810221572	0.2714246164127286	T	C	0.1678299719608503	0.3444164160014321	0.2591077775279530	T
O	0.1665133325213805	0.3766822254160532	0.3447517406561932	T	O	0.1600006966442508	0.1012413373093288	0.2707183943561642	T
O	0.1645091730671646	0.6334056383465509	0.2589919898054506	T	O	0.1618073454142452	0.4396443587766775	0.3008397422714280	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9976780940603635	-0.0010140447086752	0.2247245879856599	T	F	0.9968125496041277	0.9990660054916897	0.2287467767271470	T
e	0.0102659135933352	0.2597040335360881	0.2267587901178895	T	e	0.9790971536319231	0.2570221141942672	0.2238640419368045	T
F	0.0149771437803690	0.4915420533334042	0.2315530584791325	T	F	0.9947306084008697	0.4992349461943372	0.2303609210362005	T
e	-0.0004116291193524	0.7478133395684803	0.2271349852787169	T	e	0.9963674676926959	0.7511199481101819	0.2237893613781140	T
F	0.3339126848256170	0.0059344004317478	0.2232864468463900	T	F	0.3245435853330588	0.0053122653790007	0.2266379397442638	T
e	0.3230429385833726	0.2601356895867454	0.2261141301621706	T	e	0.3578184157982304	0.2583891438021933	0.2245575490182076	T
F	0.3192979661188707	0.4913888008486872	0.2318385307015197	T	F	0.3240447897356222	0.4995258513260885	0.2273658713539637	T
e	0.3283613579660772	0.7417515463894202	0.2261870634256085	T	e	0.3446293581232576	0.7512843364949862	0.2237547439343300	T
F	0.6777883170452480	0.0126234477634255	0.2226331979019566	T	F	0.6781276293553371	0.0086215284620252	0.2243713341342621	T
e	0.6650346763791259	0.2508799119867962	0.2255137622643373	T	e	0.6655451465494616	0.2470943418953975	0.2265331055116011	T

F	0.6669356994845935	0.4968813225805448	0.2259037542410418	T
e	0.6672003752246396	0.7418333701712497	0.2231710576787977	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1662196783044843	0.1251837929450952	0.1516142672338565	T
e	0.1663261620286026	0.3757636422818203	0.1468218020588397	T
F	0.1660041440821078	0.6239161593429997	0.1475210693779442	T
e	0.1662741754462905	0.8748821680619971	0.1516408289942644	T
F	0.4987455751128900	0.1275794140350513	0.1512526379812859	T
e	0.4993592108408743	0.3758106868292331	0.1517829973391100	T
F	0.4984331945530767	0.6211638660251699	0.1517992387067841	T
e	0.5002199318465594	0.8747327523798639	0.1548208242334206	T
F	0.8369426710870227	0.1284956229917368	0.1510176594419049	T
e	0.8344517897496394	0.3756294855042704	0.1519681608416391	T
F	0.8347698289248692	0.6229371203321420	0.1519809054271703	T
e	0.8335896252973455	0.8741390035692831	0.1520493640677944	T
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F	0.6729129603198554	0.5000801464733164	0.2265635333174680	T
e	0.6627297491540740	0.7367621606028650	0.2247463875263654	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1667160930952834	0.1258251712497981	0.1496518979844023	T
e	0.1658569112899440	0.3718289523076830	0.1510100226636470	T
F	0.1663088642835826	0.6253783108153875	0.1513253591002099	T
e	0.1654669306212865	0.8746934584222725	0.1512836696143777	T
F	0.5015198376468107	0.1241559124928828	0.1500272936707139	T
e	0.5026302252416661	0.3779207816355946	0.1498821422406437	T
F	0.4982724518243008	0.6214089852265560	0.1510158318210437	T
e	0.5018212252009553	0.8774055243739137	0.1537459963404157	T
F	0.8333552860423656	0.1245714000893449	0.1492600267988162	T
e	0.8313073750480744	0.3768050064663401	0.1495228886767231	T
F	0.8337957432792598	0.6243951738788328	0.1513724088222149	T
e	0.8329447001806718	0.8748649224119457	0.1514497478861587	T
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	HCO+O+H (-407.5337; ZPE= 0.607976861)					**CO+OH+H-t2 (-407.870365; ZPE= 0.660577699)**			
H	0.4906522619221008	0.9054671873385961	0.2432115231656471	T	H	0.2639053415693094	0.1223227249371766	0.3409447603672404	T
H	0.1678790288024956	0.2998714485861239	0.3441572477458756	T	H	0.5176616872681625	0.3903031347736026	0.2437674000453842	T
C	0.1670437373409249	0.3466845287078863	0.2930422300394512	T	C	0.1595122411661747	0.3645708602122266	0.2608743734254117	T
O	0.1642386880918868	0.1101230445126301	0.2592670299134384	T	O	0.3516510036534412	0.1250993109170878	0.3083216482089559	T
O	0.1662833756986197	0.4664183484376252	0.3021290737890537	T	O	0.1578946129193603	0.4525976339922995	0.3052829988338766	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0006619436292405	0.0011916973041764	0.2265331670912214	T	F	0.9996226348644360	0.9977600924877857	0.2230942327824456	T
e	0.0153304038144516	0.2581429860341317	0.2316498042263408	T	e	0.0028596299640944	0.2569901910203120	0.2229863168088118	T
F	0.0045453698773908	0.4982359489737139	0.2298649454066136	T	F	0.9893231642695011	0.4987314312504324	0.2290077380217443	T
e	0.9915612457359996	0.7551158785326458	0.2239121085133945	T	e	0.0029531852731502	0.7479799314503696	0.2236031752145326	T
F	0.3297594996984543	0.0065756319155363	0.2262073164495037	T	F	0.3415887234694099	0.0102325096550707	0.2316493107006903	T
e	0.3196105840941761	0.2576647905362056	0.2319239773266159	T	e	0.3196244384050612	0.2471451801129050	0.2344488225721479	T
F	0.3310319934818778	0.4927933393538366	0.2302411299485853	T	F	0.3336500838487260	0.4914074794080337	0.2283408288965723	T
e	0.3339298138463566	0.7472010137131861	0.2218166213473458	T	e	0.3317507234445732	0.7560002979125066	0.2250131601919314	T
F	0.6670965122813041	0.0131754924676902	0.2236468542431170	T	F	0.6680907010240233	0.9927517612154434	0.2242347036493041	T
e	0.6669686052013777	0.2517253875045183	0.2258611442873214	T	e	0.6746359435475759	0.2426967152047951	0.2227052873036946	T
F	0.6661315546019220	0.4928630817073564	0.2251647753754011	T	F	0.6672053620905604	0.5111250110592229	0.2239249541112368	T
e	0.6738770901493174	0.7355413644055935	0.2225857196362307	T	e	0.6585849700990363	0.7491531238607008	0.2248393303240206	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1668360940574049	0.1262065671493262	0.1476387809485040	T	F	0.1672494531609938	0.1238770908613056	0.1507442489866591	T
e	0.1665672866685177	0.3751976286512225	0.1473792151706124	T	e	0.1674753023382579	0.3762106232880491	0.1492018917377481	T
F	0.1663776492947778	0.6247133200573070	0.1510066939738849	T	F	0.1679441257377621	0.6249258593092754	0.1511847854062028	T
e	0.1659236319282751	0.8752126564400092	0.1511780964079673	T	e	0.1683348922621270	0.8768096075281491	0.1515482114074863	T
F	0.4981730238006606	0.1285224345522918	0.1509918916476033	T	F	0.5001651440821706	0.1248904533158426	0.1499825099718804	T
e	0.4985023463327192	0.3735463474664306	0.1513136154416921	T	e	0.5012679415369705	0.3722122046347436	0.1537887740199528	T
F	0.4987084751276543	0.6216721674903630	0.1511899446317291	T	F	0.4955971123712457	0.6253944774464181	0.1511380034651060	T
e	0.5019010539056022	0.8755150727068434	0.1543420890333128	T	e	0.4983958561764459	0.8759821593993011	0.1509491759409382	T

F	0.8349045539901178	0.1269288142949859	0.1511332872201568	T	F	0.8345088680924889	0.1238211394381136	0.1509060728646273	T
e	0.8362694181928036	0.3740406617726497	0.1517710750877142	T	e	0.8317606447620677	0.3758310725483831	0.1505637966733954	T
F	0.8358115710390863	0.6217887055308313	0.1509195921429771	T	F	0.8335062430112380	0.6258533128526269	0.1510058056631005	T
e	0.8312638088632130	0.8763226075627139	0.1517587110287321	T	e	0.8338300583656880	0.8736530764056916	0.1510732061248264	T
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e					e				
	TS9 (-406.783006; ZPE= 0.662912)					**HCO+OH (-407.194638; ZPE= 0.775319877)**			
H	0.2758199432780573	0.1079590582740814	0.3455454386446160	T	H	0.2813227964430114	0.1202875321987520	0.3463704522958261	T
H	0.3205435847253521	0.3335877178750235	0.2950174562831360	T	H	0.1306418916980983	0.2933318187015626	0.3464753632014552	T
C	0.1769206751425531	0.3593201008667361	0.2626208686608726	T	C	0.1493336837643569	0.3338401515183210	0.2941883278369574	T
O	0.3571085817366178	0.1075430860221449	0.3098298823026865	T	O	0.3580331065281005	0.1245647817717482	0.3086964580899732	T
O	0.1346269247926827	0.4504168269301477	0.3027639140644234	T	O	0.1694482351376729	0.4542462048893747	0.3016179353847772	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F

F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0025467684956781	0.9962984872138203	0.2229764814697021	T	F	-0.0022285738226392	0.0012164965325471	0.2221419309705631	T
e	0.0081360147500088	0.2562367681766671	0.2232590632549854	T	e	0.0117115686771792	0.2599181205554695	0.2247807420701298	T
F	0.9901893454230297	0.5134265298462285	0.2298198445347297	T	F	0.0044775519355409	0.4956557964280871	0.2314673653515028	T
e	0.0002609573254209	0.7480439792229709	0.2237467363550652	T	e	0.0028792551623442	0.7456180832900438	0.2232174608380910	T
F	0.3333056886360772	0.0021922343410654	0.2312928002794891	T	F	0.3374806154026876	0.0121254444725729	0.2312163610760526	T
e	0.3256075346490611	0.2350085366256293	0.2366166743633422	T	e	0.3166628751318517	0.2494663008551397	0.2368796438660586	T
F	0.3318651798201908	0.4955808446328200	0.2260188169804537	T	F	0.3262482159696921	0.4947196912767740	0.2289602085464858	T
e	0.3322792198495405	0.7571134575658766	0.2247129063167880	T	e	0.3335040023257043	0.7568169873614377	0.2236384060198850	T
F	0.6687275869387932	0.0010987286148718	0.2229237270595535	T	F	0.6680176901641027	-0.0003655819844683	0.2230110198745980	T
e	0.6710641330056695	0.2502373023782059	0.2233226103230460	T	e	0.6671382947155482	0.2498985370634594	0.2236577215573917	T
F	0.6673868683569866	0.5006370682017216	0.2239976320699610	T	F	0.6659282592624546	0.4971792127455145	0.2237874497443153	T
e	0.6557513797917657	0.7488816391928581	0.2238966489465754	T	e	0.6644440182566081	0.7474333141835243	0.2224524981066671	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1678041911437950	0.1241923387872400	0.1504929177612802	T	F	0.1665525612022912	0.1250080916249143	0.1503622590730791	T
e	0.1687757417517754	0.3752044218928738	0.1512735124157671	T	e	0.1693343299915817	0.3748486071125007	0.1471311154772027	T
F	0.1678286125518474	0.6247670952126276	0.1506129939829578	T	F	0.1678103863545388	0.6241717771316889	0.1509711034727189	T
e	0.1673484541590879	0.8755329846721319	0.1505889189330143	T	e	0.1676907753000584	0.8769174587793609	0.1516008634604331	T
F	0.5001510479328679	0.1245502814499372	0.1501030549946894	T	F	0.4987734227145582	0.1265113818732768	0.1500187747051552	T
e	0.4991829925900262	0.3726778019837236	0.1520513926919665	T	e	0.4968268772179210	0.3731456693127108	0.1522460519870339	T
F	0.4958450496243859	0.6237450294528919	0.1517644490777346	T	F	0.4978593808840692	0.6237193692352838	0.1518222221053671	T
e	0.4995783949931977	0.8755120813814431	0.1507600424408180	T	e	0.4990790216856955	0.8765447215425183	0.1514723230000384	T
F	0.8363246736689882	0.1260502336415305	0.1516575059272979	T	F	0.8335032732994128	0.1260460838154678	0.1509786279075075	T
e	0.8346297252549102	0.3762440708971093	0.1510861278161910	T	e	0.8337683580121512	0.3751185011342800	0.1511213166220757	T
F	0.8303031807754628	0.6272946569559001	0.1504054318099140	T	F	0.8350301767516389	0.6232936603780134	0.1518896823696501	T
e	0.8323415959940870	0.8747753159393218	0.1511260036370962	T	e	0.8338035376746279	0.8741554704288623	0.1514803634570409	T
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	TS10 (-406.4653361; ZPE= 0.724496)					**CH+O+OH (-408.4647133; ZPE= 0.700566812)**			
H	0.2737241645978033	0.1192724624569486	0.3436662905934096	T	H	0.2679702558994307	0.1211442146654571	0.3415574383448040	T
H	0.1575929043277077	0.3340122995921193	0.3325119768279476	T	H	0.1632449276265956	0.3785237977019436	0.3167622937638454	T
C	0.1626433410205874	0.3491825339270290	0.2756669688697762	T	C	0.1623825453889749	0.3695293852238289	0.2590182845042122	T
O	0.3566181127887060	0.1219529015744176	0.3086182017944376	T	O	0.3550667565213243	0.1247599653758817	0.3085853612965439	T
O	0.1625211949810298	0.5122106075796757	0.2972692874638214	T	O	0.1675869551754707	0.6373835547106041	0.2590808132729245	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9971840883831247	-0.0000096802929602	0.2221385301845752	T	F	0.9939181809105503	-0.0005328025557575	0.2229966770547378	T
e	0.0067146034701254	0.2600067023619267	0.2241814055073419	T	e	0.0018277463015305	0.2584379195384084	0.2235195745651147	T
F	0.9992301468238696	0.4934344599365271	0.2330930107248161	T	F	0.0050443868252313	0.5003789704914521	0.2292510272109971	T
e	0.0080530340431949	0.7477932253054960	0.2233343835981625	T	e	0.0044976774156300	0.7493933557591557	0.2264100190471308	T
F	0.3384780386494483	0.0094115679020673	0.2312475658234573	T	F	0.3440118570706572	0.0089449023753881	0.2317903479880451	T
e	0.3280978886160574	0.2466968442517967	0.2348312331933348	T	e	0.3263015838674326	0.2472168277193778	0.2345986681434171	T
F	0.3252205064408057	0.4851556597945053	0.2329885434253830	T	F	0.3229012187947282	0.4953291125909579	0.2279893677323801	T
e	0.3309198290699730	0.7551556982897311	0.2245470997523857	T	e	0.3319310541953531	0.7521705608698420	0.2276958547219972	T
F	0.6672480819777450	0.9981076349716770	0.2227144934144662	T	F	0.6681270418146977	0.9912058389487201	0.2235914016980351	T
e	0.6699070538517584	0.2517999546628861	0.2232604649948063	T	e	0.6664919177019453	0.2488038014017990	0.2233066276741136	T
F	0.6650893703099312	0.5020921112559463	0.2242229575720402	T	F	0.6690099673568576	0.5007066612102681	0.2242657844848849	T
e	0.6615898844734223	0.7474392426575264	0.2222562062210212	T	e	0.6613087660951770	0.7490672700008565	0.2243429320352633	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F

F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1670576525325799	0.1250774796653603	0.1506018203445486	T
e	0.1686484660669705	0.3754619578535713	0.1494064390951379	T
F	0.1683836479989976	0.6244117765146084	0.1504460691978962	T
e	0.1682243813797254	0.8772075816496474	0.1512538942386996	T
F	0.4997786706051865	0.1262313832451558	0.1499116027067104	T
e	0.4988885151671914	0.3735409151745253	0.1517057970413030	T
F	0.4954548716068861	0.6226674282168250	0.1522284093971313	T
e	0.4986031559915431	0.8758312201800121	0.1511614390270257	T
F	0.8341579434923203	0.1261164909384344	0.1511171200432190	T
e	0.8322656349589648	0.3760781337347031	0.1506965921062165	T
F	0.8350355404385796	0.6240459130315289	0.1518740670805016	T
e	0.8336977990887884	0.8736160605850142	0.1512615814934443	T
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F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1671167497403787	0.1240541599053454	0.1512337406068057	T
e	0.1684688764983236	0.3743777183604863	0.1495404858935206	T
F	0.1675028877014742	0.6251222895341234	0.1473069287944323	T
e	0.1686417889880634	0.8768988085268646	0.1520281355034616	T
F	0.5003707211004396	0.1256514849002869	0.1500823943893907	T
e	0.4985794814127851	0.3746075135108587	0.1526870339231799	T
F	0.4981398046386723	0.6240110898553557	0.1516421236009901	T
e	0.4974912720413722	0.8751537742862616	0.1514607628110404	T
F	0.8333776542292934	0.1256134368033091	0.1513769122777947	T
e	0.8325496183376403	0.3761790627875903	0.1513986080161092	T
F	0.8340374296601355	0.6250625936143979	0.1514586593352314	T
e	0.8344935310545929	0.8731698270131737	0.1512177385221843	T
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	TS11 (-406.05452; ZPE= 0.800905)					**HCOOH (-406.267163; ZPE= 0.862184526)**			
H	0.3439749468117263	0.3010312242487317	0.3637301555776078	T	H	0.0361734063856544	0.3263368287228410	0.3582745244628475	T
H	0.0447861811169725	0.3196339758187182	0.3573548705437216	T	H	0.3270822284791140	0.3254947561112038	0.3632029269906161	T
C	0.1067083100700733	0.3419342227999864	0.3084659629045252	T	C	0.1184104344229544	0.3385372485890595	0.3140745208094399	T
O	0.2816316172671028	0.2494610103934179	0.3336995082961091	T	O	0.1545514364811685	0.4573938537035275	0.3062337263574041	T
O	0.1625273207552425	0.4529048364674328	0.3073700346981820	T	O	0.2642576550660827	0.2738865508190415	0.3329678868079657	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9991321893202988	0.0092410549415666	0.2242190786664267	T	F	-0.0009336675264787	0.0095872265286132	0.2244593162367175	T
e	0.0119099055870942	0.2642993329791113	0.2276391148235946	T	e	0.0120120049429995	0.2650912101613989	0.2288805602913540	T
F	0.0020857577408564	0.4932180661506450	0.2304074760452405	T	F	0.0026247866535787	0.5003768343083536	0.2306965923549051	T
e	0.9982524546793572	0.7484807245809704	0.2233012027029751	T	e	-0.0028968599185167	0.7483722926637617	0.2231811376067115	T
F	0.3331960798118447	0.0029046574770560	0.2232687080817945	T	F	0.3328005917574388	0.0010593063202534	0.2233791064052728	T
e	0.3296232783126172	0.2420740194009957	0.2348820660609622	T	e	0.3313682442389954	0.2402343073650871	0.2307485010308824	T
F	0.3208240353186324	0.4932233182287412	0.2295301068589709	T	F	0.3186265586085355	0.4977234965687491	0.2298890858131888	T
e	0.3339056962490020	0.7502766850691688	0.2228259124434825	T	e	0.3359093944973027	0.7507358944018546	0.2227301115174480	T
F	0.6748537920297626	0.0008012528866840	0.2232225601565262	T	F	0.6741038227840549	0.0015222600211322	0.2237739579636964	T
e	0.6650871433171935	0.2491784474251643	0.2236932672455966	T	e	0.6676305514490050	0.2490050864194354	0.2237400557275052	T
F	0.6680487595744868	0.4972927132615190	0.2237333040830697	T	F	0.6668262926266887	0.4935821486995514	0.2240185722189265	T
e	0.6646228235763217	0.7444286133669022	0.2229797120007889	T	e	0.6653586564503351	0.7437169863600098	0.2232726868816830	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1658452105389867	0.1262768806624756	0.1506237248778124	T	F	0.1652104355736983	0.1264981187677792	0.1508624980292749	T
e	0.1694266054535245	0.3737876254366039	0.1477566669668367	T	e	0.1685209792867117	0.3743093474484031	0.1483228796179230	T
F	0.1659931774042929	0.6236587381443028	0.1510791705954334	T	F	0.1660533964374475	0.6245149983855307	0.1506061307690939	T
e	0.1656349125154737	0.8755332356849410	0.1516082436943836	T	e	0.1652075195404844	0.8755307534718373	0.1515342844706459	T
F	0.4995291319952494	0.1254242091737179	0.1508402419354954	T	F	0.5004177162717284	0.1249701440389459	0.1508723828045782	T
e	0.4967611966804284	0.3742034937588226	0.1519556466527995	T	e	0.4961919094981573	0.3744096253402239	0.1520072360938427	T
F	0.4972039452502192	0.6224897709441058	0.1519647970980170	T	F	0.4978717440517595	0.6223525676891207	0.1518732856575588	T
e	0.5006944374071781	0.8752406380584641	0.1515583562033758	T	e	0.5014199082502697	0.8750027528416305	0.1514843494963586	T
F	0.8345729877059783	0.1273473418067477	0.1510116052929527	T	F	0.8350844583169728	0.1271849228011812	0.1509947182422409	T
e	0.8338815285008402	0.3748461363156630	0.1508314295811509	T	e	0.8349693482803821	0.3748461018312138	0.1510451686669510	T
F	0.8349336391957897	0.6232853921757410	0.1514187319945994	T	F	0.8337836188991230	0.6233490627156203	0.1510452761630217	T
e	0.8342520650528006	0.8750013493521476	0.1516449052873513	T	e	0.8339468925573270	0.8753261554425464	0.1516512790159400	T

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	CO+OH+H-t3 (-407.906159; ZPE= 0.623788283)					**TS12 (-406.009071; ZPE= 0.586725)**			
H	0.2605954368890571	0.1228428818778664	0.3411227411853618	T	H	0.2590092575533037	0.1252670558113279	0.3406100541430103	T
H	0.1746269389860196	0.6672579169298395	0.2427147298775519	T	H	0.1617791150125762	0.5368556300327060	0.2966957340807684	T
C	0.1605017204275452	0.3627996196593171	0.2602263861146080	T	C	0.1635004428785072	0.3638129997039421	0.2634364515198585	T
O	0.3495980873274375	0.1240464351642854	0.3091202529304840	T	O	0.3472471260124340	0.1244005719648295	0.3081806934740110	T
O	0.1632944287463003	0.4501340890301437	0.3049530922883133	T	O	0.1609578187548167	0.4308362110026400	0.3223436655013255	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F

F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0012274961801193	0.9985065821242883	0.2233293826856578	T	F	0.9985680790993783	0.9937794342250486	0.2226805178558153	T
e	0.0046961092824144	0.2543025571029511	0.2225073300303558	T	e	0.0054717797176698	0.2579243645578643	0.2237063074671791	T
F	0.9858985599917981	0.4925650566293792	0.2284738867508005	T	F	0.0077958148345180	0.5034243581042753	0.2293383361081644	T
e	-0.0000932751167744	0.7526324703506752	0.2230180600394642	T	e	0.0043176577850707	0.7400155126816456	0.2259997810361998	T
F	0.3414145385452347	0.0096903137331891	0.2321258968849468	T	F	0.3334627666347005	0.0101416036747821	0.2311327005136955	T
e	0.3251199167170435	0.2455126767006342	0.2346271918978225	T	e	0.3248691993432017	0.2479519429885007	0.2347538914111972	T
F	0.3361321799512778	0.4892898860952810	0.2279562504158530	T	F	0.3225275283137884	0.4919963079379085	0.2272109805231438	T
e	0.3356517551684710	0.7673353574400791	0.2249003324857518	T	e	0.3317952893824780	0.7507789323356741	0.2249792196327206	T
F	0.6675698803379702	-0.0089225467327992	0.2240573907037938	T	F	0.6675586783702012	0.9991857656644493	0.2225819709806994	T
e	0.6674319192286368	0.2481444319132930	0.2235401099927487	T	e	0.6682380636111246	0.2498465142268375	0.2232184768832606	T
F	0.6653116241528045	0.5053718744918665	0.2248254096878982	T	F	0.6694405011655203	0.4985910108979906	0.2239804527745465	T
e	0.6593176034511495	0.7437025687681263	0.2254484849225401	T	e	0.6648357697092108	0.7457812056292044	0.2227438046821274	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1673534073956683	0.1236622183815317	0.1504179432209758	T	F	0.1660536601962916	0.1240150050384896	0.1505723132358694	T
e	0.1690251267893497	0.3755897700083519	0.1492911749726540	T	e	0.1680166111943943	0.3746353650270824	0.1495479156970214	T
F	0.1685476680861474	0.6256708329239024	0.1533420755070564	T	F	0.1683612423135406	0.6248073641655829	0.1503562664471410	T
e	0.1679778893445741	0.8789637853441736	0.1507131236435898	T	e	0.1683790632461525	0.8755403617460730	0.1516145648143116	T
F	0.5005304862469766	0.1251125952018372	0.1501583702065227	T	F	0.4988742179620659	0.1259542869412803	0.1502752353589151	T
e	0.5001812123340377	0.3726992248282410	0.1516624460395976	T	e	0.4984789381080829	0.3740084127539510	0.1522339408786070	T
F	0.4965451349614468	0.6242716573662587	0.1515152140783977	T	F	0.4969911522347535	0.6221775004108214	0.1523034788585474	T
e	0.4998192954024308	0.8760122194475956	0.1504429949628336	T	e	0.4980227753367278	0.8753240795037543	0.1519019722020969	T
F	0.8327981362486604	0.1240905279611874	0.1513448452794702	T	F	0.8350557635413590	0.1253713795030361	0.1513961817180507	T
e	0.8308636780477719	0.3746259566549386	0.1506485549503911	T	e	0.8337490316137280	0.3756932502275058	0.1509327254384610	T
F	0.8334904257751418	0.6250646183222467	0.1512584129073135	T	F	0.8346251800616677	0.6233924108098324	0.1517930364712418	T
e	0.8328197734584986	0.8733526502101618	0.1511021094098846	T	e	0.8335264495432878	0.8730700527909784	0.1513704932798686	T
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	COH+OH (-406.909599; ZPE= 0.800257076)		
H	0.2586037431102825 0.1286787591748363 0.3418267575832428 T		
H	0.1731813209403955 0.4542773616016201 0.3646609184247074 T		
C	0.1637863001881463 0.3786431409608068 0.2722128503358362 T		
O	0.3444571577879954 0.1274883547350866 0.3081693017785930 T		
O	0.1589258917754260 0.3744599917470693 0.3460237182423444 T		
F	0.0000000000000000 0.0000000000000000 0.0736297965049744 F		
e	0.0000000000000000 0.2500000000000000 0.0736297965049744 F		
F	0.0000000000000000 0.5000000000000000 0.0736297965049744 F		
e	0.0000000000000000 0.7500000000000000 0.0736297965049744 F		
F	0.3333334028720856 0.0000000000000000 0.0736297965049744 F		
e	0.3333334028720856 0.2500000000000000 0.0736297965049744 F		
F	0.3333334028720856 0.5000000000000000 0.0736297965049744 F		
e	0.3333334028720856 0.7500000000000000 0.0736297965049744 F		
F	0.6666666865348816 0.0000000000000000 0.0736297965049744 F		
e	0.6666666865348816 0.2500000000000000 0.0736297965049744 F		
F	0.6666666865348816 0.5000000000000000 0.0736297965049744 F		
e	0.6666666865348816 0.7500000000000000 0.0736297965049744 F		
F	-0.0020401826234933 0.9982062143392133 0.2225341885178307 T		
e	0.0130571937525574 0.2641660917210321 0.2259472597434459 T		
F	0.0113889589958930 0.4927198046906016 0.2271134769312750 T		
e	0.0023701122905905 0.7437231963629035 0.2241173410383311 T		
F	0.3337820907631588 0.0128940659138168 0.2314672358752503 T		
e	0.3191850921542415 0.2533860938070927 0.2356233620257594 T		
F	0.3200320790256487 0.4866971971038846 0.2265329051918523 T		
e	0.3329495996256478 0.7505030502598882 0.2245416602553976 T		
F	0.6674228300499868 0.0007031850640417 0.2222910003462398 T		
e	0.6677990666344021 0.2502512437415536 0.2238699401455935 T		
F	0.6668332705455743 0.5001804329258761 0.2241524352333260 T		
e	0.6634333423130506 0.7458641329704484 0.2228070957924081 T		
F	0.1666667014360428 0.1250000000000000 0.0000000000000000 F		
e	0.1666667014360428 0.3750000000000000 0.0000000000000000 F		
F	0.1666667014360428 0.6250000000000000 0.0000000000000000 F		
e	0.1666667014360428 0.8750000000000000 0.0000000000000000 F		
F	0.5000001192092896 0.1250000000000000 0.0000000000000000 F		
e	0.5000001192092896 0.3750000000000000 0.0000000000000000 F		

F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F		
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F		
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F		
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F		
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F		
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F		
F	0.1662298273747551	0.1255729938841641	0.1508191610467396	T		
e	0.1684415768138211	0.3744090556505221	0.1462051282671884	T		
F	0.1680610524723510	0.6244069959160417	0.1513192348047283	T		
e	0.1682654811336771	0.8759799979498691	0.1519905871918672	T		
F	0.4985174777810865	0.1266851003830180	0.1503469724604325	T		
e	0.4985696113466068	0.3736041467753493	0.1519910583921533	T		
F	0.4972952224453459	0.6227900416721647	0.1518946135789043	T		
e	0.4979818960526637	0.8762605331480940	0.1519539412021595	T		
F	0.8353275504311112	0.1267403327796322	0.1517182093876833	T		
e	0.8329840749918990	0.3754283134504954	0.1511399277263515	T		
F	0.8348880321357606	0.6233442670663020	0.1516407524976660	T		
e	0.8335098913525761	0.8738009832508414	0.1515546717765875	T		
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Table SX2. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the on the 3O (0.25 ML) pre-covered Fe(100) surface

	3O+CO+H_2O (-432.138626; ZPE= 0.958494341)					**TS13 (-429.732896; ZPE= 0.957362)**			
H	0.5885026457738894	0.5520224535871698	0.3480342285451667	T	H	0.5846062496491609	0.5491901907345025	0.3480090022706838	T
H	0.6441722483117406	0.4223311054010039	0.3640451185731337	T	H	0.6256895552020784	0.4161598741538249	0.3623806759103013	T
C	0.4974165916070409	0.1397662387299553	0.2587177082797520	T	C	0.5106126583141154	0.1401625976509005	0.2704421856663262	T
O	0.1740575766220518	0.3747023564643319	0.2588404139712612	T	O	0.3959104365838576	0.2628654069294894	0.3188260698335498	T
O	0.4914754046676429	0.6327584117571281	0.2602295531364140	T	O	0.4928492305674914	0.6359161180282743	0.2597510626976146	T
O	0.8291963218116419	0.8717332183107989	0.2597188776566496	T	O	0.8287867867004236	0.8701873431247013	0.2594675214247031	T
O	0.4948915106301529	0.0518869334316572	0.3039937336983084	T	O	0.4867190761209192	0.0460783055849152	0.3068788210905974	T
O	0.6787253694137595	0.4977665353575355	0.3449251566582989	T	O	0.6686402147057575	0.4898885378564893	0.3438209337022524	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9957666895344511	0.9966206176217911	0.2270165634633885	T	F	0.9977011341460045	0.9927156712462010	0.2259697209214867	T
e	0.0057545201365104	0.2530342179694766	0.2261266045815691	T	e	0.0051673839497345	0.2479181981928011	0.2243652691077763	T
F	0.0098843678163811	0.5026850930668036	0.2278495172874350	T	F	0.9990298905135048	0.5070234846756341	0.2235372114639821	T
e	-0.0085986943646436	0.7485768576896337	0.2279555164607280	T	e	0.9974662343974819	0.7532906552758485	0.2278883649427462	T
F	0.3313733273171909	0.0023648834132291	0.2273978638808811	T	F	0.3307234699255528	0.0069736763269853	0.2283834266247074	T
e	0.3319968451381287	0.2506890303064590	0.2307560719035102	T	e	0.3289394663594924	0.2599592830680409	0.2337144368766455	T
F	0.3346804097910135	0.4984883744134799	0.2296013400725145	T	F	0.3404138537134122	0.4977953566618182	0.2247802523944462	T
e	0.3283610586522152	0.7462763314126207	0.2253225683740574	T	e	0.3275725643210826	0.7487367108831809	0.2261746946312417	T
F	0.6735608137546314	0.0018069244449741	0.2321991846967469	T	F	0.6778114961525474	0.0025064102249542	0.2311866351469773	T
e	0.6571506491129278	0.2452492804563282	0.2228668674280390	T	e	0.6547872350768956	0.2430857691598990	0.2252361900334838	T
F	0.6798814848436283	0.4990265735040371	0.2301275003095208	T	F	0.6793678012021662	0.4932425428858848	0.2312872675581321	T
e	0.6632438984934254	0.7526193662191599	0.2301412005504260	T	e	0.6631602984226053	0.7515108120831738	0.2307122423320341	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1654572863702609	0.1248460609067517	0.1520449429396876	T	F	0.1653474777578250	0.1253033531403145	0.1511963606542599	T
e	0.1680677936283641	0.3752484263516777	0.1468819374449772	T	e	0.1660903925468380	0.3766398774977902	0.1507338607083120	T
F	0.1659832983929726	0.6256080304414495	0.1512442216352906	T	F	0.1666205075188257	0.6260026285298816	0.1511068796296247	T
e	0.1667144101493639	0.8746875582432577	0.1516691077890266	T	e	0.1683973324861580	0.8754651207110596	0.1516350853045979	T
F	0.4983738875854867	0.1240552348996781	0.1493694340324890	T	F	0.4958341699222994	0.1247162612726544	0.1508803667156693	T
e	0.5007478697446338	0.3770013805150926	0.1518046314300557	T	e	0.5014042217695350	0.3759347212437321	0.1502045824110052	T
F	0.5023594140123264	0.6237509581756430	0.1482947348626741	T	F	0.5029862362699506	0.6242273960622545	0.1483540359714427	T
e	0.4995663136937331	0.8749542647222914	0.1511393227747062	T	e	0.4994626649932561	0.8752901298891573	0.1515963919040176	T
F	0.8351691326226943	0.1255748955147225	0.1518146812728212	T	F	0.8338607557213290	0.1254346395792656	0.1514856410076526	T
e	0.8333080057917773	0.3751387959960082	0.1514994481088106	T	e	0.8333477448018692	0.3739224412864492	0.1516391163359795	T

F	0.8337784552625098	0.6247589619048876	0.1516473660427253	T	F	0.8321103267012625	0.6259191923439600	0.1511547335197924	T
e	0.8316280508632981	0.8749734304572245	0.1470803618620733	T	e	0.8308871942543176	0.8742762423404090	0.1469602612053743	T
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	2O+CO_2+H_2O (-431.068381; ZPE= 1.016565965)					**TS14 (-431.954419; ZPE= 0.84657808)**			
H	0.5444559726123485	0.5214724879534333	0.3452999814921461	T	H	0.5441911354329168	0.6025058398132592	0.3137451767246929	T
H	0.5465707596209983	0.3809533807519841	0.3405552035300623	T	H	0.5612631159377580	0.4517551576574332	0.3522190588890987	T
C	0.5164418807641787	0.1699824962278359	0.2921465270022041	T	C	0.4973985237728385	0.1392462185204757	0.2589520030575589	T
O	0.4842061141935495	0.6419922743958302	0.2590167152517934	T	O	0.1650051243738240	0.3692214243094762	0.2594407092078542	T
O	0.8319747568689426	0.8687055120874058	0.2597598191331061	T	O	0.4990006232510349	0.6900324215172529	0.2841536594209013	T
O	0.6135074583743212	0.4536054976716148	0.3368964634228750	T	O	0.8418604684112866	0.8784779732185325	0.2600070800486325	T
O	0.4368692846581048	0.2465185437833664	0.3292485981754609	T	O	0.4962947810432531	0.0506098576240130	0.3036028833906604	T
O	0.4924353146633333	0.0540570970824605	0.3041783283232604	T	O	0.6183485026041868	0.5133622782064685	0.3276931469302300	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F

e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0043761204220500	0.9945303179135973	0.2265215680077595	T	F	0.0007450728255955	0.9992335583464124	0.2268488784302807	T
e	0.0044728018360640	0.2469014959193376	0.2242732922869682	T	e	0.0016695222362578	0.2510867882580457	0.2263529592035002	T
F	-0.0003407808171808	0.5008617058687473	0.2245137336436115	T	F	0.0016193822146640	0.5023064679292727	0.2282164821465832	T
e	-0.0018270629355183	0.7508011072450255	0.2281724149967396	T	e	0.9956162985594936	0.7504586373088529	0.2270680024252619	T
F	0.3420278416641220	-0.0021357322942365	0.2295622609746777	T	F	0.3318424805035423	0.0034714470784002	0.2268591912873520	T
e	0.3348666309158916	0.2677190705271805	0.2315406627302339	T	e	0.3293802732288675	0.2483156969775380	0.2312056863089093	T
F	0.3332690846494723	0.5091457390669628	0.2240243045107843	T	F	0.3204474854647282	0.4895295660639686	0.2236305091681903	T
e	0.3220895323257184	0.7567827273691082	0.2272859417708450	T	e	0.3343885221504006	0.7503152365317158	0.2277050245976470	T
F	0.6690252661173679	-0.0011225749481259	0.2342677075244113	T	F	0.6766769573021393	0.0034754020331433	0.2322584459936786	T
e	0.6590426843478567	0.2374346221699353	0.2242189041805609	T	e	0.6568214263472320	0.2447111623365854	0.2223711995656259	T
F	0.6785130160022940	0.4830206017843453	0.2316465427071579	T	F	0.6867207109320764	0.4878293927518753	0.2307674507945928	T
e	0.6631116501898727	0.7505420231390381	0.2300874618751536	T	e	0.6671778946655221	0.7638890863423233	0.2337808160538649	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1680618880271038	0.1246248678900071	0.1528973225379739	T	F	0.1655547770031319	0.1251504431435726	0.1515017553118794	T
e	0.1672406298123638	0.3761790062362825	0.1513982223427877	T	e	0.1661254454497076	0.3731929404705813	0.1462479511844416	T
F	0.1649063876495463	0.6269432283773680	0.1508033779671933	T	F	0.1661049324853018	0.6260380909642888	0.1515493828593780	T
e	0.1661257448364901	0.8766856599305372	0.1509385101405269	T	e	0.1675042197952763	0.8747641930521576	0.1511621346628241	T
F	0.4964328501093495	0.1249986680004141	0.1490849730174525	T	F	0.4985351738758386	0.1237561479811023	0.1490572025174262	T
e	0.5009835375573918	0.3760329387934392	0.1505833840582609	T	e	0.5014776780869659	0.3762578646662996	0.1512022528695438	T
F	0.5042232063714081	0.6242226596401166	0.1489289129990446	T	F	0.5024872354943923	0.6226393067637147	0.1522679404809500	T
e	0.5007091793329400	0.8753574253307799	0.1508213280921911	T	e	0.5006483610270624	0.8754730008251712	0.1505747967639599	T
F	0.8342986146949311	0.1241780212781273	0.1513067244451833	T	F	0.8352394752165967	0.1254290312841865	0.1511053084535443	T
e	0.8346741551790541	0.3734592099919077	0.1506114941373235	T	e	0.8351140117566525	0.3730459477103685	0.1500847543614902	T
F	0.8314607825548007	0.6243507278163978	0.1521544165462594	T	F	0.8316164270893520	0.6252864517559434	0.1524878959282472	T
e	0.8308790646760190	0.8744041449316959	0.1472567529759338	T	e	0.8328764056932934	0.8756473440074626	0.1466910605176184	T
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	2O+CO+2OH-t1 (-432.655485; ZPE= 0.98412447)					**TS15 (-431.459793; ZPE= 0.759543)**			
H	0.5110597426735477	0.4342919006021111	0.3388151004145618	T	H	0.5019559016300111	0.6588411252412908	0.3252851439889502	T
H	0.4966102674535950	0.6623719047571320	0.3252309045578881	T	H	0.5847015520080292	0.3770039393223849	0.2816576360675349	T
C	0.4963612478118441	0.1405304529199377	0.2580070474915208	T	C	0.5016279074183643	0.1427883689242429	0.2573324377118128	T
O	0.1643760668645336	0.3675415633599373	0.2587573300988511	T	O	0.1583053971816719	0.3660933517323458	0.2574644687611964	T
O	0.8427077835663412	0.8789956799641371	0.2596687574185144	T	O	0.4952732447911966	0.7392756149439174	0.3058731987202770	T
O	0.4984260781921885	0.0511917562872724	0.3021584999354999	T	O	0.8416843953547412	0.8800780304415344	0.2588202627677981	T
O	0.5077511464410133	0.5034724495222485	0.3086819245097153	T	O	0.4974865244741675	0.0541368670114690	0.3018691737925662	T
O	0.4926124236544714	0.7434252112105393	0.3059537066583279	T	O	0.5082128865771237	0.4835057988966424	0.3011011886129127	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0022199362204482	0.0000521278379476	0.2273537739207760	T	F	0.0030074799024348	0.9993666961817791	0.2268215060718091	T
e	-0.0025719266818009	0.2502106688075778	0.2273579527933860	T	e	0.9937624502960208	0.2466745295348376	0.2274021732251036	T
F	0.0101035263641042	0.4987493321262995	0.2255300097737495	T	F	0.0077369090232694	0.4983851599109854	0.2253975292637569	T
e	0.9919955511134783	0.7503855115952659	0.2257890011384276	T	e	0.9925442832422023	0.7502894426664394	0.2256944614833761	T
F	0.3308938220660650	0.0060369072256330	0.2264590362213947	T	F	0.3344686457033890	0.0056685827946703	0.2262343948836233	T
e	0.3264289852754223	0.2479831927697240	0.2298274681451076	T	e	0.3268310206420827	0.2486940202448158	0.2291328749559325	T
F	0.3423344146279096	0.4911861190126154	0.2325057886886480	T	F	0.3445386851044988	0.4920158178458680	0.2347633427041839	T
e	0.3429139852206850	0.7480261616978835	0.2287248805037935	T	e	0.3434930083560127	0.7438209158939746	0.2293137850369182	T
F	0.6770242538757059	0.0011845571460510	0.2313156174073752	T	F	0.6791050724623319	0.0071011076832550	0.2306719450779990	T
e	0.6600101957902420	0.2436914532340617	0.2223866365333731	T	e	0.6608999942167393	0.2551632658990535	0.2270183467689320	T

F	0.6597208251051430	0.5009630604583444	0.2287298536846548	T	F	0.6618194169497699	0.4919135816795029	0.2300222647051512	T
e	0.6593773493420464	0.7604645202206076	0.2349953593008798	T	e	0.6600848124619566	0.7601556338732659	0.2341261507065381	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1650433528564695	0.1254373507897308	0.1510087416404246	T	F	0.1655018628512399	0.1252629679141385	0.1511332553794142	T
e	0.1679305635992818	0.3751226536162314	0.1467148766199322	T	e	0.1685053778259560	0.3752618241383094	0.1470135312400305	T
F	0.1680755739570863	0.6258411133119808	0.1522892235099450	T	F	0.1676711949385783	0.6255544174431755	0.1523832769930574	T
e	0.1683930631418560	0.8746380821360081	0.1515473639712066	T	e	0.1693404534876111	0.8742615186084800	0.1516929338148663	T
F	0.4989094459976672	0.1240826510182066	0.1488191520634795	T	F	0.5003071828270206	0.1256367357417899	0.1490431113601249	T
e	0.5000829830692115	0.3748759331906902	0.1497546868434234	T	e	0.4991289170099462	0.3744649726644622	0.1486762395435654	T
F	0.5005108183628838	0.6248612367064471	0.1493933117794284	T	F	0.5018786808237400	0.6245179233025625	0.1495073179806990	T
e	0.5000578247620844	0.8753049143741573	0.1498563496097022	T	e	0.4999364449300711	0.8754596373862827	0.1502326853285483	T
F	0.8346971126641660	0.1249786744032854	0.1509482948711078	T	F	0.8339542711843807	0.1260185016545864	0.1504687529093598	T
e	0.8321475294007012	0.3753334267546258	0.1515435310886914	T	e	0.8341912458630082	0.3748335182447688	0.1504891052274098	T
F	0.8323331919012029	0.6242386953668908	0.1524994154132457	T	F	0.8320963809662387	0.6236672202179153	0.1526991946500342	T
e	0.8323605324099037	0.8745215948938440	0.1468072051236285	T	e	0.8314508805169040	0.8749331343832446	0.1468806370474735	T
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	3O+CO+OH+ H-t1 (-432.378515; ZPE= 0.789200898)					**TS16 (-430.596688; ZPE= 0.748472)**			
H	0.4949658090827837	0.6797306304934347	0.3389737962379883	T	H	0.4943221662827381	0.6794406611748071	0.3391110711378474	T
H	0.8255807700836943	0.3463387273774603	0.2408051287020786	T	H	0.8171968739258838	0.3767930871596243	0.2418420493460578	T
C	0.4968520315141728	0.1275537854467821	0.2579828548289786	T	C	0.4985240619787119	0.1232235836212000	0.2550661451193220	T
O	0.1615842162729724	0.3717373270687433	0.2584568826592976	T	O	0.1664864858543270	0.3778470523037676	0.2585983335072481	T
O	0.8395370414535388	0.8782398675331152	0.2595456131016530	T	O	0.4944224922532177	0.7493753088208629	0.3095658261434794	T
O	0.4977882033585290	0.0414503691539762	0.3037818533251989	T	O	0.8423949938904335	0.8765506596830898	0.2596412862644048	T
O	0.4937377556695914	0.7493124871107822	0.3091464882602217	T	O	0.4987501890705455	0.0412931252275609	0.3024865100199767	T
O	0.5087432668199258	0.3963353951562759	0.2591416391365375	T	O	0.5084715999385276	0.2772318567710543	0.2978589391243301	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0005662955162794	-0.0005297767109731	0.2275008305944893	T	F	0.9999896189233688	0.9999685131873695	0.2271926963977175	T
e	0.0045161727080979	0.2484071265854682	0.2261383005116338	T	e	0.0089196026478183	0.2516209910194149	0.2262347064258425	T
F	0.0100179350441684	0.5035511064791321	0.2264571269619502	T	F	0.0089586175424443	0.5067635951683112	0.2279976687563266	T
e	0.9915376666678919	0.7499137576362411	0.2270954171782870	T	e	0.9941894529785573	0.7490226466606374	0.2276405168438277	T
F	0.3291598648398507	0.0035470199709143	0.2259880455767102	T	F	0.3241452765812709	-0.0012393391262802	0.2255090420287713	T
e	0.3325007896259083	0.2485454140624833	0.2341066020238851	T	e	0.3357907659935818	0.2529467776026315	0.2355546422882753	T
F	0.3323152096319160	0.5011966974355049	0.2272451149256685	T	F	0.3269951602031697	0.4957335781943648	0.2237810270326004	T
e	0.3444155944772742	0.7434077584103844	0.2309790736279495	T	e	0.3455091189675645	0.7429683478086152	0.2310105863797079	T
F	0.6768849443491178	0.0003272217529311	0.2302405019385180	T	F	0.6790608293985448	0.9956354571122231	0.2292787382290236	T
e	0.6526011091220227	0.2470756702696024	0.2283713091431288	T	e	0.6604448375299341	0.2506682218089184	0.2286182401724959	T
F	0.6672703588910424	0.5053857728076862	0.2248094933541853	T	F	0.6701563136866291	0.5094988719955209	0.2217408584037788	T
e	0.6607161595715191	0.7529813021876957	0.2358433262375761	T	e	0.6616388335733984	0.7513529438702556	0.2364219679065173	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1655428454286633	0.1256878262116772	0.1515820384828533	T	F	0.1662864366532946	0.1259876798322698	0.1517947187955339	T
e	0.1681008652286869	0.3748566230392912	0.1475802141935481	T	e	0.1666538595218969	0.3738636689472042	0.1466868663215189	T
F	0.1663384231148441	0.6270431504802462	0.1518504694883064	T	F	0.1666980390492186	0.6269533153797771	0.1515222398348630	T
e	0.1685185506618911	0.8737772146357518	0.1516438232137260	T	e	0.1676740972339924	0.8730711853971951	0.1513134235725540	T
F	0.4997837283400611	0.1239891661899016	0.1498234909826297	T	F	0.5005485400242127	0.1247370998755212	0.1510287002167784	T

e	0.4989764348371366	0.3748010023469389	0.1484036513758323	T	e	0.4997295507268605	0.3761878114271910	0.1495226787856904	T
F	0.5008709110487927	0.6252473649416316	0.1495771870805407	T	F	0.5001058435869378	0.6242974497983422	0.1500058750055075	T
e	0.4997403213252058	0.8739482216469497	0.1503640988547310	T	e	0.4999249643052591	0.8736991802284338	0.1504321112861039	T
F	0.8330928115499355	0.1255636035622349	0.1520075050223049	T	F	0.8348435380277416	0.1255004404691186	0.1516915438137763	T
e	0.8336403427940646	0.3751132875427603	0.1521935374191716	T	e	0.8337353863348707	0.3751856158961711	0.1523756838899185	T
F	0.8339295702857258	0.6261195013026677	0.1516386031184292	T	F	0.8341780547476211	0.6270987014889948	0.1511639300241730	T
e	0.8322024798190137	0.8741933344590709	0.1471184136542944	T	e	0.8329096275451982	0.8735696603676293	0.1471083177606677	T
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	2O+CO_2+OH+H (-431.454082; ZPE= 0.823690598)					**3O+CO+OH+ H-t2 (-432.527812; ZPE= 0.801004707)**			
H	0.4913006235570301	0.6835596470463087	0.3410990668512047	T	H	0.4933441321325012	0.6809989887702996	0.3398034440071319	T
H	0.8208315225258515	0.3908635911615038	0.2422685158011689	T	H	0.8322877820066263	0.1655164284884337	0.2422769045674750	T
C	0.4863829338503147	0.1554646152786757	0.2883261120456872	T	C	0.4940397270887923	0.1288464295328061	0.2579516756530913	T
O	0.1694287037839680	0.3732238357716022	0.2584192084580059	T	O	0.1605857609368518	0.3735240090826056	0.2586870427200137	T
O	0.8444604964558626	0.8742934031089725	0.2601386325632402	T	O	0.8375033084325906	0.8738853240949868	0.2589832491068375	T
O	0.4934028671632068	0.7511485493305499	0.3097342296017787	T	O	0.4982782066863952	0.0427845236538833	0.3037858199146420	T

O	0.5794373404445927	0.2264138518153943	0.3219402168162128	T	O	0.4930003419825702	0.7495095565216102	0.3091547426799387	T
O	0.4951401651373052	0.0389208744463824	0.3013579954164900	T	O	0.5192450080629147	0.3948217140587317	0.2591556353199767	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9941134548630486	0.9990744334863817	0.2258979234373182	T	F	0.0008120477867539	0.9885520374795380	0.2243849225686903	T
e	0.0111880073233053	0.2496394632378210	0.2253589182874685	T	e	0.0030599712938908	0.2592039145740849	0.2255745294110345	T
F	0.0028940654310479	0.5035980803078142	0.2290340936613853	T	F	0.0031303847828874	0.5064206026221549	0.2286560597958006	T
e	0.9978363879489858	0.7487286780883902	0.2278022249380082	T	e	0.9967883473170396	0.7446252024461202	0.2280734389194060	T
F	0.3301703003646525	0.0007363017665668	0.2262022792877339	T	F	0.3262085558290830	0.0056355729507091	0.2262438259723604	T
e	0.3331555094863499	0.2487524514931778	0.2334672988096369	T	e	0.3292617794210368	0.2473248774194856	0.2332348624692032	T
F	0.3274664734777169	0.4926822104196181	0.2236109363680732	T	F	0.3348349735722372	0.4974942888687185	0.2265100197137472	T
e	0.3453233227063274	0.7424368337266395	0.2305982034953802	T	e	0.3435859249014749	0.7434742120664318	0.2312621852755653	T
F	0.6652021930307415	-0.0127231744489232	0.2322217593611162	T	F	0.6722780671746090	-0.0025049919731481	0.2299869216034776	T
e	0.6661195445219170	0.2596793824143891	0.2280398496534382	T	e	0.6503891578162027	0.2497969736770291	0.2288718340902045	T
F	0.6730004964599311	0.5134379794921229	0.2225080086953732	T	F	0.6754292954283346	0.5050417307579498	0.2261670609995443	T
e	0.6626291362405274	0.7477031282192848	0.2373603308641475	T	e	0.6604440852670410	0.7501196225587056	0.2357315647880060	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1659431810717060	0.1239321681705051	0.1514183480333719	T	F	0.1638358998929397	0.1252422882586079	0.1519154766179910	T
e	0.1670428222883011	0.3740791765090049	0.1464861015902359	T	e	0.1676545814096257	0.3751066067733625	0.1474413292495173	T
F	0.1665957924523987	0.6253751123999950	0.1518650548532895	T	F	0.1676426818157976	0.6258741796120577	0.1515273338868107	T
e	0.1678635981669390	0.8731156541235640	0.1515652718045926	T	e	0.1694680846310277	0.8725371321588593	0.1513484910452151	T
F	0.5024259777293218	0.1272216740321427	0.1515068749845708	T	F	0.4995032991934260	0.1237580621507192	0.1496435395818705	T
e	0.5000341766347876	0.3760841782684566	0.1503808989320666	T	e	0.4999792429725087	0.3749204714639228	0.1485091629154453	T
F	0.4997554394827646	0.6240237649521125	0.1500287649986823	T	F	0.5011704655434110	0.6247657015660915	0.1496186625145313	T
e	0.4993666110183982	0.8738547634657052	0.1501781196061104	T	e	0.4996648860006236	0.8737195204607772	0.1504626530733796	T
F	0.8319042611572454	0.1248117318444119	0.1521327283578032	T	F	0.8338868236651081	0.1265125889611886	0.1541598674278478	T
e	0.8345671914767607	0.3760223789416218	0.1519672555635453	T	e	0.8332418682573469	0.3764051266706340	0.1507632466904418	T
F	0.8353041132568991	0.6280873221628679	0.1505255876605376	T	F	0.8340671815537442	0.6258161355329175	0.1508208786054969	T
e	0.8316257620105477	0.8732418912867030	0.1472400813118357	T	e	0.8314100439488884	0.8732423951511239	0.1470401808017463	T
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	TS17 (-431.425826; ZPE= 0.799608)					**3O+HCO+OH (-431.715491; ZPE= 0.932951164)**			
H	0.4957360838123672	0.6830143815747178	0.3401729229731613	T	H	0.4944066927579047	0.6826117328424579	0.3393553498502255	T
H	0.6348096719321301	0.1995387061611276	0.3037066079283982	T	H	0.4961119465961519	0.2042255198967974	0.3428708272024282	T
C	0.5122813842946127	0.1397671645263600	0.2646545259954887	T	C	0.5000161170678583	0.1565408209207184	0.2919963472742546	T
O	0.1561268189862661	0.3677945675925377	0.2581955872959940	T	O	0.1548369737938350	0.3708721473802255	0.2590007878007036	T
O	0.8418767711591910	0.8770698270200412	0.2591507642023289	T	O	0.8433008691059642	0.8777520426084389	0.2590969137565421	T
O	0.4967313326212198	0.0410484955828623	0.3014939697742614	T	O	0.4944039457141964	0.7508433436572803	0.3084711627506869	T
O	0.4938753385279083	0.7508807971719607	0.3090399890385581	T	O	0.5114553541995034	0.3943704492867727	0.2601165679915251	T
O	0.5036963119666885	0.4013564151114887	0.2591037577882879	T	O	0.5015075073131102	0.0373036218331463	0.3013405669708888	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F
F	0.0023489361070764	0.9975559843560595	0.2259997907047563	T	F	0.0008840616913041	0.9995683352228748	0.2261832927538252	T
e	0.9991922241622443	0.2467154269173971	0.2273898040812013	T	e	0.0006661953750136	0.2497959517520023	0.2264979709157291	T
F	0.0030988507677415	0.4988805343196590	0.2266158560684652	T	F	0.0019721829754254	0.5004793448703825	0.2273855478768032	T
e	0.9937012876017136	0.7488416136282116	0.2269130352934487	T	e	0.9955949210930234	0.7507018901746803	0.2262672370889134	T
F	0.3332455625874471	0.0048228675673641	0.2258108370761808	T	F	0.3403262695838756	0.0117084873673862	0.2280664645833264	T

e	0.3366750098098727	0.2507529719424359	0.2342016700251209	T
F	0.3297110441050122	0.5050858225749038	0.2276765414642478	T
e	0.3428175901503717	0.7415247064907434	0.2315602332367838	T
F	0.6774131470207166	0.9993532534635510	0.2298277892105582	T
e	0.6581183676020034	0.2501247374774164	0.2271935670722485	T
F	0.6678129136101784	0.5026423170528597	0.2250497693615832	T
e	0.6600870625057438	0.7540224423919811	0.2355372277133067	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1663517394591695	0.1256529480490353	0.1517104179023331	T
e	0.1679960058470420	0.3744142362333518	0.1480892181463563	T
F	0.1650349850875263	0.6266334479255945	0.1515091000364941	T
e	0.1688507444702075	0.8735242811261462	0.1516493502263256	T
F	0.4988790585141011	0.1246063317740035	0.1501955677196773	T
e	0.4990741773129029	0.3749607173041057	0.1485240699913424	T
F	0.5007280750326476	0.6257009495570349	0.1492686466082326	T
e	0.4995156987804954	0.8742366721154431	0.1501791893747430	T
F	0.8331695534136472	0.1260266127941167	0.1515822616627373	T
e	0.8331734121336305	0.3744619005677350	0.1510659383812566	T
F	0.8334243766793195	0.6251382393259799	0.1517508834815466	T
e	0.8318189996215616	0.8739409255327768	0.1468925905426427	T
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e	0.3363739566791662	0.2478920015798232	0.2364835331230663	T
F	0.3316878493212882	0.4969755963513047	0.2271433849611796	T
e	0.3447807669723918	0.7427272974549003	0.2302267382620213	T
F	0.6701280963546891	0.9991888572579968	0.2318973219341281	T
e	0.6452586948900421	0.2434560885629007	0.2294430181356207	T
F	0.6707034716620532	0.5008785148004907	0.2255375662109784	T
e	0.6617486387018237	0.7516564164137014	0.2351753432408823	T
F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F
e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F
F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F
e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F
F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F
e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F
F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F
e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F
F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F
e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F
F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F
e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F
F	0.1661726682358245	0.1253329908672674	0.1515916551866977	T
e	0.1681008340308141	0.3740948766744566	0.1478903726510419	T
F	0.1663858363608988	0.6259818327750873	0.1518574205854048	T
e	0.1705328242430657	0.8749374719001420	0.1522735260865710	T
F	0.4993684658688461	0.1256503147333525	0.1475780362597096	T
e	0.4992752961743175	0.3742285316260608	0.1483697507357833	T
F	0.5011385732783838	0.6245235709726461	0.1495151567241666	T
e	0.4995487404013491	0.8753724044572682	0.1504713439795398	T
F	0.8313701536786392	0.1267880683609816	0.1526445054754706	T
e	0.8333131729118940	0.3742527919020512	0.1509666549072425	T
F	0.8336664131546051	0.6252502313203716	0.1517909643241628	T
e	0.8316882507085874	0.8747516096578302	0.1472301692879580	T
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	TS18 (-431.3930631; ZPE= 0.768849)					**3O+C+O+OH+H (-433.210528; ZPE= 0.790573047)**			
H	0.4881566706596419	0.6821266545604822	0.3409096067977301	T	H	0.4918619632896933	0.6819648127712367	0.3399790745617974	T
H	0.8411112594563910	0.1660775950791450	0.2419401524424251	T	H	0.8250509260861147	0.1611592934628292	0.2427066242915601	T
C	0.5194633234919952	0.1172561014644198	0.2437873468639743	T	C	0.5106839772592217	0.1178066133697636	0.2451832051381063	T
O	0.1560850911287689	0.3778724209752550	0.2589349667327514	T	O	0.1592598995809001	0.3778775252315880	0.2584882911757029	T
O	0.8310653493741286	0.8776133994317470	0.2582245441934776	T	O	0.8326992878389887	0.8818679443813249	0.2572218635661906	T
O	0.3263277232063865	0.1152738262734809	0.3029745265678829	T	O	0.4931330062766194	0.7515732557532162	0.3101796139090412	T
O	0.4904148735553186	0.7503129561303500	0.3100007818445374	T	O	0.5163236376524903	0.3852997432816563	0.2594066545533716	T
O	0.5185566961454365	0.3890574568565945	0.2597564478451950	T	O	0.1548616608068588	0.1128396640370141	0.2590582553982172	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F
F	0.9985962443200589	0.9894621676716997	0.2234568457522134	T	F	0.0030108656655962	0.9946965883986667	0.2311717145160991	T
e	0.0045312160726820	0.2603284976594226	0.2253603277293276	T	e	0.0001189852374336	0.2521226071992193	0.2292405191650358	T
F	0.0018646264370532	0.5069907791262765	0.2286451993486023	T	F	0.0023355606350755	0.5031058456558959	0.2280678380671049	T
e	0.9915738849932257	0.7459696564656443	0.2275636913228665	T	e	0.9889412428904337	0.7496597663250301	0.2261895851349239	T
F	0.3300511949918311	0.0073967048358586	0.2300748273355071	T	F	0.3377167240541427	0.0099523038113834	0.2268515946783676	T
e	0.3322078905422390	0.2438866587827997	0.2399294334362010	T	e	0.3411276638527788	0.2440173309907702	0.2362367594697583	T
F	0.3349401638073707	0.4957870624476712	0.2265164894572134	T	F	0.3331543794678076	0.4959839981848435	0.2261217525034596	T
e	0.3421059889061536	0.7481503699310904	0.2313096144859308	T	e	0.3439778675439787	0.7484669102030631	0.2314510286547396	T
F	0.6669157274676683	0.9962339267904375	0.2283947696022576	T	F	0.6656433117131090	0.0010211277019903	0.2281529543591080	T
e	0.6558431435517982	0.2498323408825460	0.2294622394231815	T	e	0.6554074963695343	0.2479942549979116	0.2301000421645720	T
F	0.6737555134523778	0.5032675102662451	0.2267834485100119	T	F	0.6725927699670391	0.5013256660225742	0.2268200291617549	T
e	0.6572596340021359	0.7493466732206715	0.2360883695789208	T	e	0.6572545232937178	0.7495101230246050	0.2349328751995344	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F

F	0.1649972484792291	0.1249340370412180	0.1507483626319111	T	F	0.1664203902253319	0.1255115758671215	0.1487304688817463	T
e	0.1688635487127465	0.3747999354571461	0.1477595041421049	T	e	0.1671608125373023	0.3731661369065112	0.1486728104514815	T
F	0.1671818011228786	0.6265357031007258	0.1520334068683109	T	F	0.1667582200286531	0.6269631451440167	0.1525342574489982	T
e	0.1689006352601294	0.8734766715365114	0.1516544496806692	T	e	0.1682974671034904	0.8745627343168453	0.1525808757632488	T
F	0.4986885255949380	0.1244734021385311	0.1461772145836436	T	F	0.5005393784106221	0.1252546626005256	0.1453237402083368	T
e	0.4999998075987841	0.3736678842700091	0.1487685288219056	T	e	0.5006213459572214	0.3738542314360967	0.1483073721262179	T
F	0.5005493464581265	0.6244806258566270	0.1500632484005774	T	F	0.5006936921142648	0.6242609754928118	0.1501181763914596	T
e	0.4993821342965832	0.8747961540884798	0.1509665936864412	T	e	0.4997221267017135	0.8757207729061253	0.1511997002962364	T
F	0.8346333521351862	0.1262483889552980	0.1538472278193151	T	F	0.8339095022357795	0.1249034227375945	0.1526116023660701	T
e	0.8330873821360428	0.3764293175182918	0.1507191872055950	T	e	0.8331732164952965	0.3752030652269969	0.1513439838495236	T
F	0.8324173736625922	0.6256795006627103	0.1512256787317178	T	F	0.8326168597767242	0.6251131591806307	0.1516851167433563	T
e	0.8310914323734505	0.8730426318338269	0.1468649724270262	T	e	0.8317614066960666	0.8746855902421828	0.1473419611810133	T
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	2O+CO+2OH-t2 (-432.340971; ZPE= 0.957150556)					**TS19 (-429.914706; ZPE= 0.920183)**			
H	0.7661644766698784	0.3784753925866487	0.3349567972482722	T	H	0.4944101245124443	0.6823152619385029	0.3376779728293865	T

H	0.4948072470998482	0.6798581915259920	0.3384001418429759	T	H	0.6897005280452706	0.3017317033289652	0.3422877836164690	T
C	0.4930351420142437	0.1368004688098760	0.2582764555955331	T	C	0.5141854095251763	0.1586293627264725	0.2768872847050778	T
O	0.1670968738687786	0.3718579877093629	0.2580659332962583	T	O	0.1658127729459478	0.3724773765819653	0.2589282634364802	T
O	0.8376690622446346	0.8792201600245436	0.2584864832359707	T	O	0.8400752094744153	0.8798394931896755	0.2592716587636992	T
O	0.4955656569550726	0.0479856283096409	0.3026687348540658	T	O	0.4919051512835587	0.7526865649202885	0.3084979871316265	T
O	0.6691242331096512	0.3815625229386657	0.3078190302643153	T	O	0.4889251041963494	0.0580139821619949	0.3067318500798552	T
O	0.4935551072716641	0.7497821473218900	0.3088434066627430	T	O	0.5988751832010595	0.2480628943704814	0.3462992922672566	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0002029075715538	-0.0006545727583428	0.2264502038429264	T	F	0.0014543630394768	0.9979286097319495	0.2258106275737991	T
e	0.0033797775813509	0.2527302308941533	0.2251712754555954	T	e	0.0081045159954244	0.2487804362297406	0.2270715913974680	T
F	0.0091570936678553	0.5067678269316731	0.2261874295231784	T	F	0.9999672773549574	0.5008369019643537	0.2286164133893571	T
e	0.9907803047600663	0.7495228799863580	0.2265804808959905	T	e	0.9927320534050909	0.7490847883240451	0.2272185547648021	T
F	0.3291120234018567	0.0040434321013288	0.2261510363695785	T	F	0.3365865559785951	0.0060850791655668	0.2278581068820818	T
e	0.3275937581807874	0.2472386401973231	0.2303620621158276	T	e	0.3408706058377393	0.2548517512159685	0.2336686980968689	T
F	0.3275107164066947	0.4923707122082114	0.2230514830751671	T	F	0.3218096428582032	0.4961436844465988	0.2235939388649782	T
e	0.3438475058711750	0.7433484294761661	0.2307805777818282	T	e	0.3426826663421481	0.7427872124918233	0.2303583788958435	T
F	0.6743085404124141	0.0049207180589003	0.2304505514891932	T	F	0.6757274444901837	0.0091764521954523	0.2326780198561381	T
e	0.6549581940423690	0.2537899176708502	0.2346442808900740	T	e	0.6619701569403624	0.2492126521034723	0.2280611150475939	T
F	0.6774383652981076	0.4915424048325853	0.2292088293822744	T	F	0.6737869381392119	0.5005837877529017	0.2230305513201987	T
e	0.6578835654591537	0.7508312778531621	0.2342599409803691	T	e	0.6586570741896671	0.7579718293699896	0.2350161350783692	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1650198053077411	0.1251171036386573	0.1511169509419696	T	F	0.1673051821059602	0.1250195601935025	0.1520388790031031	T
e	0.1665017550359521	0.3741435830378951	0.1458978041145864	T	e	0.1670349921637334	0.3732074648148644	0.1469557746698679	T
F	0.1671654938369019	0.6275835108836688	0.1515085412007375	T	F	0.1651039302186955	0.6263387891818452	0.1517963437353452	T
e	0.1684880799206001	0.8739553028879899	0.1516301121702275	T	e	0.1691275062238249	0.8741163962009746	0.1519143635617531	T
F	0.5013866296439715	0.1254878915002750	0.1498837664765394	T	F	0.4997757967324585	0.1261825394600534	0.1496928528508126	T
e	0.5008866911605404	0.3750850903957323	0.1502523948535645	T	e	0.5012895289640386	0.3759332248080182	0.1511456201023059	T
F	0.5019704209925691	0.6224874242231179	0.1508902755386201	T	F	0.5005392838475036	0.6238756441344370	0.1508370088085894	T
e	0.4996637977558385	0.8741971602804155	0.1504531359779501	T	e	0.4999427172244755	0.8757556225950816	0.1508559403925080	T
F	0.8330929705293957	0.1277097692893686	0.1523945746000996	T	F	0.8352661218574169	0.1266388977969378	0.1516155830765247	T
e	0.8342416113467397	0.3741594413060984	0.1497352614043140	T	e	0.8344281420251324	0.3737136842960897	0.1511726825996470	T
F	0.8320533150151848	0.6248137295840888	0.1517690981334565	T	F	0.8328101785325437	0.6261441777646093	0.1519793944136343	T
e	0.8307270061208107	0.8746304135266745	0.1473043236174968	T	e	0.8306180696601314	0.8750852449318568	0.1475937986502298	T
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	2O+COOH+OH (-431.014429; ZPE= 1.030591126)		
H	0.4941640490970320 0.6909695385039237 0.3406814826128820 T		
H	0.6363397616454639 0.2753214949465539 0.3646616193024760 T		
C	0.5518178852562919 0.1590490725745201 0.3033691044688328 T		
O	0.1629675273394668 0.3747306880515213 0.2594438638808348 T		
O	0.8404803549584166 0.8793628957712610 0.2595763923279318 T		
O	0.4919238151565060 0.7578379640613129 0.3088128092150507 T		
O	0.4765155775146035 0.0573464952624948 0.3065203031740003 T		
O	0.5801903239251938 0.2001935558401122 0.3693083858318555 T		
F	0.0000000000000000 0.0000000000000000 0.0736297965049744 F		
e	0.0000000000000000 0.2500000000000000 0.0736297965049744 F		
F	0.0000000000000000 0.5000000000000000 0.0736297965049744 F		
e	0.0000000000000000 0.7500000000000000 0.0736297965049744 F		
F	0.3333334028720856 0.0000000000000000 0.0736297965049744 F		
e	0.3333334028720856 0.2500000000000000 0.0736297965049744 F		
F	0.3333334028720856 0.5000000000000000 0.0736297965049744 F		
e	0.3333334028720856 0.7500000000000000 0.0736297965049744 F		
F	0.6666666865348816 0.0000000000000000 0.0736297965049744 F		
e	0.6666666865348816 0.2500000000000000 0.0736297965049744 F		
F	0.6666666865348816 0.5000000000000000 0.0736297965049744 F		
e	0.6666666865348816 0.7500000000000000 0.0736297965049744 F		

F	0.0001888374362009	0.9979456816920437	0.2256116049009939	T		
e	0.0049472101729998	0.2522426176080264	0.2264055907839482	T		
F	-0.0013768869423438	0.5006134322766906	0.2286834265279518	T		
e	0.9925964028427414	0.7495631588679936	0.2272968989147375	T		
F	0.3417386371302229	0.0050725778744576	0.2271948531871200	T		
e	0.3453884947503836	0.2590013587406623	0.2309541790247080	T		
F	0.3199094480694096	0.4977582269415882	0.2239013383033525	T		
e	0.3432551388416709	0.7427835444589161	0.2307417353005383	T		
F	0.6712923650357118	0.0073324443764738	0.2328774087631395	T		
e	0.6510730339504417	0.2386783791419780	0.2258409946021018	T		
F	0.6762316878626037	0.4963844006533918	0.2233326953445782	T		
e	0.6587630612314417	0.7572316055715322	0.2348525842452153	T		
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F		
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F		
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F		
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F		
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F		
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F		
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F		
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F		
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F		
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F		
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F		
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F		
F	0.1681460222024181	0.1251652058917072	0.1520112435164265	T		
e	0.1664925310807792	0.3736277988385959	0.1467504573302501	T		
F	0.1646503551180309	0.6270742555523297	0.1516109660631750	T		
e	0.1691541825111816	0.8744987652411947	0.1520751686803497	T		
F	0.4985811022764560	0.1249651409411608	0.1474802013953625	T		
e	0.5008165007216380	0.3762109062137536	0.1507093735529282	T		
F	0.5008560443089052	0.6235739454545105	0.1511490814693593	T		
e	0.5003789452451660	0.8756771867718243	0.1504542678551968	T		
F	0.8346646935755018	0.1258226485342006	0.1515561227157792	T		
e	0.8333581484608233	0.3730714813511648	0.1510913358090198	T		
F	0.8322497238049348	0.6259684425343981	0.1518925985775628	T		
e	0.8305714468659704	0.8750436620159933	0.1475952619663637	T		
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Table SX3. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the on the 3OH (0.25 ML) pre-covered Fe(100) surface

	3OH+CO+H_2O (-442.786349; ZPE= 1.919315457)					**TS20 (-442.216207; ZPE= 1.685781)**			
H	0.3251411918103512	0.3045542177646041	0.3529381339816748	T	H	0.4563035385897770	0.2817401397329824	0.3430260015667619	T
H	0.3338794859968821	0.1666095065765474	0.3664354213521451	T	H	0.4021924387987955	0.1415696328356237	0.2891596976278332	T
H	0.2230731394332443	0.8767934460506316	0.3272751151005976	T	H	0.2265492284030742	0.8755230641906192	0.3292062591581911	T
H	0.5622399119472655	0.8760715107314971	0.3304124827935726	T	H	0.5639625585101481	0.8771156846622996	0.3298570609451253	T
H	0.8949106430524137	0.8704570202351455	0.3275413122785689	T	H	0.8937758068430349	0.8736304359815209	0.3264322645331365	T
C	0.1468311027686458	0.3716594543288865	0.2566344536289577	T	C	0.1512913565044950	0.3661748761857393	0.2571639546904237	T
O	0.3828155101736312	0.2313014622922555	0.3409419979546511	T	O	0.5036252752771415	0.2214836274556067	0.3128291197040542	T
O	0.2215327632664583	0.4265901631651763	0.3070044831665988	T	O	0.2284210705431757	0.4220182912054310	0.3056604714189209	T
O	0.3300076825751914	0.8766131817274767	0.3071316941916061	T	O	0.3305700735083967	0.8772914253220838	0.3064503632928261	T
O	0.6653334546423463	0.8747758514805341	0.3070589339600173	T	O	0.6660442467306353	0.8746659678336539	0.3056655502640762	T
O	-0.0007824370635931	0.8746787985043682	0.3052121242601187	T	O	0.9989112148056030	0.8735117227024064	0.3046451497871662	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9885835686689276	0.9949547164891400	0.2286108802190036	T	F	0.0042382546318665	0.9930231493186956	0.2282751696122121	T
e	0.0049542950977080	0.2545151313861588	0.2226872553983738	T	e	0.0023032747108946	0.2532821151263678	0.2230712655083079	T
F	0.9899644355686661	0.4990754368844854	0.2228023149200384	T	F	0.9901983655946484	0.4955193831226024	0.2227372570978378	T
e	0.0106974916230627	0.7552892593848018	0.2282187534222571	T	e	0.0034792416783850	0.7545276453784937	0.2274418591272351	T
F	0.3379035873058444	0.9900552752560955	0.2273901886265148	T	F	0.3299844502019015	0.0038887307538493	0.2333735933630340	T
e	0.3279155222605613	0.2327526509288304	0.2287982098702492	T	e	0.3221063658104849	0.2369465525165407	0.2255600674689805	T
F	0.3391534853576037	0.5097011958821563	0.2284436513945567	T	F	0.3401270802201173	0.5061100352080176	0.2274565656412766	T
e	0.3334609303385002	0.7537113826718836	0.2320011227334015	T	e	0.3361187930682829	0.7588634891030116	0.2303527973987651	T
F	0.6704983095733721	-0.0056322698244927	0.2308720845530450	T	F	0.6644023150178284	0.9899324153130873	0.2271319669226941	T
e	0.6667108437332878	0.2424680331404514	0.2234287859649615	T	e	0.6535900092918159	0.2492243775737444	0.2298919083123278	T
F	0.6647342378652167	0.5096043655405798	0.2239098372871718	T	F	0.6664038772893283	0.5110526555272568	0.2236858512909215	T
e	0.6564368317250926	0.7580116279664626	0.2285979160729825	T	e	0.6584580588265500	0.7550466871292344	0.2292102313350443	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F

e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1650141286473348	0.1205432658762740	0.1512622918699387	T
e	0.1738566632702584	0.3764279904780529	0.1514360673982522	T
F	0.1677450294349951	0.6258319591968097	0.1507565105959567	T
e	0.1666753570059179	0.8752769722588335	0.1478661577348456	T
F	0.4995919761232800	0.1230917335150404	0.1507266347748590	T
e	0.5001954447973007	0.3743113638746612	0.1521515008031605	T
F	0.4997453447039817	0.6277457266136462	0.1506863766571106	T
e	0.5002465273227182	0.8753240483454117	0.1474168377375413	T
F	0.8334852389056117	0.1240050923964089	0.1511017799367763	T
e	0.8298062275717737	0.3746130233263809	0.1511018388635424	T
F	0.8341706959642232	0.6286590637805076	0.1513997826425253	T
e	0.8328154995874275	0.8736004326689442	0.1482484046674378	T
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e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1638541202385225	0.1220890599696006	0.1499626953862967	T
e	0.1702860497919176	0.3774961265033220	0.1502983052157958	T
F	0.1675365241900947	0.6263771963727083	0.1513236772735178	T
e	0.1679879315523801	0.8751686506250353	0.1482247232470712	T
F	0.4994559642109497	0.1232723218500428	0.1501382061055590	T
e	0.5003406739990358	0.3753051504318796	0.1509364090275813	T
F	0.4994485753146962	0.6277321659781034	0.1507381843239212	T
e	0.4983996212947857	0.8760718952930574	0.1479085736450207	T
F	0.8315232461090140	0.1243082019330428	0.1524890968421682	T
e	0.8277970855213681	0.3730984500117298	0.1516370602745594	T
F	0.8345064631150886	0.6274415594329158	0.1510845304326114	T
e	0.8331052250292934	0.8745424433943289	0.1482160281915259	T
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	3OH+CO+OH+H-t1(-443.441329; ZPE= 1.735054946)					**TS21 (-442.585439; ZPE= 1.51066622)**			
H	0.2275736121048268	0.8763901667994676	0.3284321992463842	T	H	0.2273794635764489	0.8771343738226403	0.3280689290384263	T
H	0.5620090823949695	0.8763841714170321	0.3295715030661012	T	H	0.5623399459062836	0.8742713381054993	0.3306202548369213	T
H	0.8947263478758427	0.8710273092151523	0.3276727210972750	T	H	0.8958253829479129	0.8691336489995782	0.3280949319915014	T
H	0.1353608782998050	0.1300514325570423	0.2423782127077350	T	H	0.1697304233660068	0.1276305748289318	0.2413193627191826	T
H	0.4921651310044772	0.3023079609958289	0.3350545557515161	T	H	0.5039695042140349	0.4270748168025267	0.2591296409024679	T
C	0.1477802055134701	0.3742640910981283	0.2575297777975392	T	C	0.1535832503621324	0.3654364973101312	0.2557459443162269	T
O	0.2296209855803802	0.4258998334584048	0.3057826270026174	T	O	0.3325434699451359	0.8741250336586247	0.3063911681321091	T
O	0.3321707400447255	0.8733257337422294	0.3062774190361660	T	O	0.6654640979649867	0.8741615374845021	0.3071627879201675	T
O	0.6654697619913698	0.8737563433000572	0.3064446986671797	T	O	0.9989314748714695	0.8739880217557446	0.3047742316136293	T
O	0.9982502134891854	0.8761449681975605	0.3047351227302682	T	O	0.5024788337228971	0.3064906855437367	0.2780728142870157	T
O	0.4992382233180017	0.2329332081511949	0.3050593861239800	T	O	0.1822556430719339	0.4486818400850801	0.3010223938387744	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9846620758291275	0.9986036319587247	0.2293178277047359	T	F	0.9828220423396424	0.9922118924863255	0.2275352213765625	T
e	0.0086126650985124	0.2546781339419455	0.2238992139911519	T	e	0.0027064587838835	0.2522008123930591	0.2229241570186230	T
F	0.9909350035935088	0.4981218712597065	0.2223760845754894	T	F	0.9930841841140133	0.4974535747470595	0.2243747718095777	T
e	0.0114343397561217	0.7577906747720077	0.2284151462950694	T	e	0.0118980465230148	0.7554462616607811	0.2283584425151592	T
F	0.3388811518070569	0.9862328692944197	0.2264432950554247	T	F	0.3443239132421549	0.9913831898230269	0.2283496774714397	T
e	0.3350502256570095	0.2420622285773150	0.2298373698249095	T	e	0.3282010932626193	0.2392115469300487	0.2311105992992314	T
F	0.3396409926887085	0.5122625529142140	0.2280252816431738	T	F	0.3350372377617779	0.5187291078644259	0.2289413447654595	T
e	0.3315845377242853	0.7510801605252049	0.2319333476478598	T	e	0.3299750263214001	0.7533976269864140	0.2315646781748735	T
F	0.6748584917324019	0.9921727797583245	0.2303727586061161	T	F	0.6683015512349944	0.9948554670559986	0.2322757068830384	T
e	0.6555661471590895	0.2417819184202323	0.2297616469383826	T	e	0.6670210084031931	0.2316443020097735	0.2291596847385337	T
F	0.6638758278678095	0.5112548789111435	0.2227811522096187	T	F	0.6637033247242311	0.5189444293685634	0.2241398154713108	T
e	0.6579510480828880	0.7570863564026934	0.2280495524110343	T	e	0.6609613683929679	0.7594408787410448	0.2278898910290038	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1667417897744685	0.1203503586757704	0.1526103465317886	T	F	0.1646493235488546	0.1187112539402191	0.1517793390205292	T
e	0.1715812527142324	0.3776367198679528	0.1507030728968440	T	e	0.1723621036259950	0.3756477751938445	0.1500811025045312	T
F	0.1669932873595158	0.6259611784081347	0.1503421332318476	T	F	0.1666589785805929	0.6266627635188899	0.1495719021289874	T
e	0.1671106062487669	0.8746024735882341	0.1474849226979666	T	e	0.1671797231635805	0.8751243024381400	0.1477665742513890	T
F	0.5000136819735645	0.1225587763723413	0.1494364090176263	T	F	0.5001320749293235	0.1230190876219847	0.1499571538478978	T

e	0.4997149036577326	0.3751640544842106	0.1510917936593570	T	e	0.5012172064418650	0.3763744530354576	0.1531029314296744	T
F	0.4999787623093928	0.6284831394829755	0.1499417781896558	T	F	0.4993456802878996	0.6299948766589454	0.1501448575907618	T
e	0.5005732383013213	0.8754059481209028	0.1473432882486424	T	e	0.4999658743787135	0.8756187689410857	0.1473759973584025	T
F	0.8313239107273546	0.1257797905031136	0.1508960204411474	T	F	0.8328256989617072	0.1229480838703347	0.1499367451586061	T
e	0.8294352221008475	0.3726093631901553	0.1520438986675821	T	e	0.8291424562677689	0.3735551905079578	0.1524130098653634	T
F	0.8346920722196246	0.6283453502869523	0.1512489494475817	T	F	0.8358008955044963	0.6282068851819641	0.1510221591246441	T
e	0.8340316364117180	0.8736863417852931	0.1480547603663205	T	e	0.8325889605223193	0.8735475122982576	0.1477255275630112	T
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	3OH+CO+O+2H (-443.711536; ZPE= 1.551416623)					**TS22 (-441.303386; ZPE= 1.538549)**			
H	0.2277048993071187	0.8785296759221716	0.3277460203395519	T	H	0.2258209559361422	0.8806238170934606	0.3275874549629788	T
H	0.5606771172077618	0.8746620866410010	0.3284648286764459	T	H	0.5615192453950897	0.8766866247216020	0.3300458771860205	T
H	0.8944984130705600	0.8718034325883826	0.3292487701861003	T	H	0.8942258334376622	0.8704363145388772	0.3276764087475849	T
H	0.1904936711123436	0.1337805767328153	0.2418949929630427	T	H	0.1671538190070955	0.1164081720745145	0.2398242208714026	T
H	0.4743105548093314	0.6275528735987662	0.2440295595334170	T	H	0.4983940508253742	0.6117365885222922	0.2445008085666779	T
C	0.1610393689819050	0.3685023786205411	0.2570384892236047	T	C	0.1614528183818918	0.3651019259428620	0.2701265756869655	T

O	0.3315848570033245	0.8738625159904958	0.3050840058471969	T	O	0.3305025462397955	0.8761696269570582	0.3055548446822885	T
O	0.6655100814785274	0.8773694473538772	0.3065233808420431	T	O	0.6646128924832759	0.8759055170411326	0.3065885434228131	T
O	0.9977736203281830	0.8744114343435018	0.3060007968751596	T	O	0.9975200744850730	0.8748838703416582	0.3044899586077303	T
O	0.1635858407571373	0.4525155731399282	0.3036760456408245	T	O	0.3612657482388087	0.3235296234623113	0.3060322402039070	T
O	0.5133274696323427	0.3634002454685845	0.2574058966959372	T	O	0.1470428659262652	0.4617115158803144	0.3053226652514935	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9863401827928739	0.9907916112890260	0.2274061464598137	T	F	0.9855498111595802	0.9942463337309464	0.2271862848468684	T
e	0.0094331801952831	0.2531857387692719	0.2232411863421147	T	e	0.0197834711919285	0.2543202181921944	0.2251208821534697	T
F	0.9907460803368805	0.5042442777687908	0.2274388160725431	T	F	0.9936463628694777	0.5068685076711453	0.2264309376871926	T
e	0.0079461257376043	0.7542299225186120	0.2308100518278817	T	e	0.0098405948691509	0.7563883296996080	0.2287904227887638	T
F	0.3446864419192616	0.9916864247058386	0.2280440615703961	T	F	0.3446128460927936	0.9928816367428369	0.2276235586482075	T
e	0.3331966338256674	0.2553797130081288	0.2285439234621888	T	e	0.3404324779719011	0.2394487805042191	0.2287890605889675	T
F	0.3388932308936485	0.5022920624120852	0.2291664454406287	T	F	0.3461893412141706	0.4839487592818654	0.2333634489672995	T
e	0.3191800615812199	0.7516025288404966	0.2300225286504117	T	e	0.3206324722832555	0.7558008822823296	0.2305504190553103	T
F	0.6660653817154710	0.9996469110351840	0.2324140026885521	T	F	0.6691362890008399	0.9964094943032422	0.2318549061626847	T
e	0.6684879154039812	0.2411562900444910	0.2272834502180680	T	e	0.6610601429205668	0.2432623077124194	0.2240135328110083	T
F	0.6671561704532283	0.4925554713561154	0.2255740848663355	T	F	0.6725638690917125	0.5092965261128626	0.2221941753533390	T
e	0.6715646573615253	0.7625213724816104	0.2270688896069766	T	e	0.6606864716487829	0.7607174870599869	0.2273896922385367	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1675285015300621	0.1206404787107860	0.1531691947812047	T	F	0.1654284029297020	0.1187480675339710	0.1509770315403312	T
e	0.1682988931632874	0.3770638170572849	0.1490613713305092	T	e	0.1716572837303671	0.3766338769624635	0.1512862292173735	T
F	0.1643237539771898	0.6247645184858099	0.1499510214583264	T	F	0.1671441329870666	0.6242957278530815	0.1504800461610410	T
e	0.1665493454276237	0.8749546527596307	0.1480444207573581	T	e	0.1666864221218738	0.8748103697603794	0.1475403251620939	T
F	0.5006926289405452	0.1244212665529667	0.1507133294849392	T	F	0.5023977807001723	0.1215500524940912	0.1493667823473801	T
e	0.4993415953757109	0.3740528129939263	0.1474886617896627	T	e	0.5030762059321252	0.3727961305312504	0.1494282082747357	T
F	0.5011381853363365	0.6281066124514220	0.1537043742796990	T	F	0.4952532944052631	0.6258953904762805	0.1541320647261450	T
e	0.5002836692231346	0.8756639935738152	0.1478745805584242	T	e	0.4992851506370781	0.8753724664327996	0.1474206328720249	T
F	0.8334292225267950	0.1242388933152490	0.1509848253020287	T	F	0.8329947430904753	0.1258577594872681	0.1512723561203953	T
e	0.8340432083599796	0.3739249208008388	0.1511068726941653	T	e	0.8346493522700420	0.3738915126889628	0.1524991994498534	T
F	0.8324492387568004	0.6265926075027560	0.1517293349103986	T	F	0.8343067847422371	0.6298010757767709	0.1503889188582258	T
e	0.8327093604143294	0.8746976913862322	0.1475757665013888	T	e	0.8319062504350263	0.8746381043486283	0.1477782327439233	T
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	3OH+CO_2+2H (-442.582521; ZPE= 1.605734396)		**TS23 (-442.530016; ZPE= 1.713864)**
H	0.2295998650602976 0.8790352126434891 0.3284992101588091 T	H	0.2246914759336568 0.8760035733253264 0.3282785936451012 T
H	0.5596635024373581 0.8723207870412505 0.3282468887587024 T	H	0.5630410820612302 0.8782900504528083 0.3295804891712402 T
H	0.8943163984210690 0.8750093363010075 0.3299006710253620 T	H	0.8942500638019875 0.8710662308842949 0.3283605795908177 T
H	0.1580376046104340 0.0966470029952353 0.2393803989986213 T	H	0.1191860716282023 0.2352964235027021 0.2914822039637854 T
H	0.5030618456649028 0.6056755032430102 0.2429474594819031 T	H	0.4972037709310127 0.3099962394412869 0.3371657028217029 T
C	0.1528675304577428 0.3432157388414572 0.2874621367400652 T	C	0.1492022440156429 0.3584977354167281 0.2559928898438056 T
O	0.3327419064958541 0.8733791857044741 0.3053034008978959 T	O	0.3295586829604193 0.8755561592816733 0.3062009735128817 T
O	0.6651646403339607 0.8758714530262934 0.3068522865390813 T	O	0.6657629621595984 0.8741629410197338 0.3059834610360130 T
O	0.9970701963176638 0.8755393054084262 0.3061361273742023 T	O	0.9985117193458705 0.8752764458750860 0.3059726235305470 T
O	0.2528707541831041 0.2787025456853318 0.3212416538204841 T	O	0.4994587043468335 0.2413273191034058 0.3064900203792951 T
O	0.1559402073608653 0.4610388071649562 0.3000092782764620 T	O	0.1811204507006799 0.4414648724070706 0.3018736322616913 T
F	0.0000000000000000 0.0000000000000000 0.0736297965049744 F	F	0.0000000000000000 0.0000000000000000 0.0736297965049744 F
e	0.0000000000000000 0.2500000000000000 0.0736297965049744 F	e	0.0000000000000000 0.2500000000000000 0.0736297965049744 F
F	0.0000000000000000 0.5000000000000000 0.0736297965049744 F	F	0.0000000000000000 0.5000000000000000 0.0736297965049744 F
e	0.0000000000000000 0.7500000000000000 0.0736297965049744 F	e	0.0000000000000000 0.7500000000000000 0.0736297965049744 F
F	0.3333334028720856 0.0000000000000000 0.0736297965049744 F	F	0.3333334028720856 0.0000000000000000 0.0736297965049744 F
e	0.3333334028720856 0.2500000000000000 0.0736297965049744 F	e	0.3333334028720856 0.2500000000000000 0.0736297965049744 F
F	0.3333334028720856 0.5000000000000000 0.0736297965049744 F	F	0.3333334028720856 0.5000000000000000 0.0736297965049744 F
e	0.3333334028720856 0.7500000000000000 0.0736297965049744 F	e	0.3333334028720856 0.7500000000000000 0.0736297965049744 F
F	0.6666666865348816 0.0000000000000000 0.0736297965049744 F	F	0.6666666865348816 0.0000000000000000 0.0736297965049744 F
e	0.6666666865348816 0.2500000000000000 0.0736297965049744 F	e	0.6666666865348816 0.2500000000000000 0.0736297965049744 F
F	0.6666666865348816 0.5000000000000000 0.0736297965049744 F	F	0.6666666865348816 0.5000000000000000 0.0736297965049744 F

e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.9896914510771601	0.9918666561797084	0.2264635239605329	T	F	0.9909005938073352	0.9996577859791727	0.2319196950585578	T
e	0.0035976409469904	0.2590647541877451	0.2250922674389181	T	e	0.0077858201172698	0.2437888365631827	0.2230175248521504	T
F	0.9950749568622158	0.5182760703268271	0.2304795024900299	T	F	0.9930148185105163	0.4925354254418783	0.2250906952496683	T
e	-0.0007796138217746	0.7549672081251685	0.2320708157667852	T	e	0.0090795854114541	0.7590630651536314	0.2278817887453067	T
F	0.3463279573012802	0.9923879472910418	0.2283775780006942	T	F	0.3293134844222627	0.9894631881015550	0.2268970596703497	T
e	0.3446491496023637	0.2364239989632617	0.2296367760016092	T	e	0.3383488549113189	0.2432367808558755	0.2306747150703174	T
F	0.3230418737089789	0.5060227456363386	0.2265782947156428	T	F	0.3277094948377119	0.5154435336034566	0.2278394009225688	T
e	0.3162852286049184	0.7582026792654059	0.2277504807447489	T	e	0.3367456500221110	0.7528325526312559	0.2323046162367625	T
F	0.6626506427133680	0.9968587355404230	0.2322259200461428	T	F	0.6763307298454658	0.9919590752813311	0.2290838813265347	T
e	0.6668170133417890	0.2418967874852802	0.2242083823943820	T	e	0.6581855823345627	0.2435240515646475	0.2309533076662096	T
F	0.6697880764254521	0.4987080375423534	0.2214538692502043	T	F	0.6675556835426947	0.5090676101122773	0.2215347555000562	T
e	0.6792487666685004	0.7604002702365122	0.2280685501833187	T	e	0.6551317744056747	0.7559953764481546	0.2286907099928337	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1657723495591606	0.1219544700777436	0.1525200592465747	T	F	0.1671313586137600	0.1211083202277870	0.1504407516857519	T
e	0.1692939543477279	0.3742592495458739	0.1507390854951751	T	e	0.1728920345393152	0.3742886474014258	0.1503908816326669	T
F	0.1636674417231737	0.6262572870673514	0.1494689610318278	T	F	0.1656765627092819	0.6267077077276423	0.1505414449627748	T
e	0.1654021467677817	0.8749674440895941	0.1473640751617072	T	e	0.1663240172680392	0.8749604443204390	0.1474254432601204	T
F	0.5027341385207915	0.1223229943288755	0.1494495679419450	T	F	0.4988124212190000	0.1231184215889610	0.1505962544509361	T
e	0.4988615432513797	0.3736493828500443	0.1515857828954703	T	e	0.4996145340731590	0.3753953553680566	0.1511276176056872	T
F	0.4992676097889044	0.6287665159928950	0.1541685373803711	T	F	0.4990759169721840	0.6270869662613385	0.1504953142257174	T
e	0.5007026465100738	0.8742149803198198	0.1481354578873626	T	e	0.5001105809252825	0.8761539745107738	0.1477791362153956	T
F	0.8329355355846675	0.1242953361423006	0.1507229073747113	T	F	0.8320267997563399	0.1251304541832647	0.1513383782351570	T
e	0.8352804267426687	0.3756397065494291	0.1519307024500304	T	e	0.8298639531721638	0.3727107495330624	0.1515385871597936	T
F	0.8333960143388679	0.6275766250258539	0.1498392968618154	T	F	0.8362967853485148	0.6278649915841753	0.1520071587823594	T
e	0.8325803892970804	0.8757461635645424	0.1474969004455936	T	e	0.8337009091496332	0.8736659691015690	0.1481249059169110	T
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	3OH+HCO+ OH (-442.743773; ZPE= 1.870877682)					**TS24 (-442.828132; ZPE= 1.551649)**			
H	0.2256905753730726	0.8770873875709516	0.3271270562425022	T	H	0.2273725913118908	0.8788452316481807	0.3288479354883504	T
H	0.5627292862105108	0.8778212454182946	0.3291729527033537	T	H	0.5612528148824957	0.8789921728672047	0.3278399219926040	T
H	0.8944475001441391	0.8744942106052588	0.3268208767376909	T	H	0.8957236532030169	0.8718926070902989	0.3294828548070345	T
H	0.4971283120263219	0.3080912590799866	0.3373915883109680	T	H	0.1243137541948316	0.2382134981955496	0.2881259094896385	T
H	0.1166046819948637	0.2904643445083912	0.3429092165061705	T	H	0.4817978343480361	0.6302006709943839	0.2440293273900624	T
C	0.1431957499366265	0.3305603614088835	0.2911436476510056	T	C	0.1461865890582170	0.3599623389913612	0.2562427450105494	T
O	0.3309233227953093	0.8765087615652656	0.3054063727774917	T	O	0.3311768309162437	0.8772435131383974	0.3058872109177977	T
O	0.6654885568142203	0.8750446659834108	0.3055162026796295	T	O	0.6658392557195876	0.8772368331564352	0.3056604223506597	T
O	0.9985014351546484	0.8778135256693171	0.3041877208183089	T	O	0.9995135155413108	0.8759949193444173	0.3066960024552497	T
O	0.4967229666752498	0.2402028611851259	0.3061286647221338	T	O	0.1770892937194895	0.4414555720122626	0.3031734632205489	T
O	0.1884962263841889	0.4457934506591827	0.2991814041607802	T	O	0.5202047265063494	0.3587247291322266	0.2560692426105198	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F
F	0.9911027383693275	0.9981665188510778	0.2277024570796731	T	F	0.9884829820399447	0.9996673100220398	0.2321536406699950	T
e	0.0122029508257094	0.2519629462470696	0.2240432461379456	T	e	-0.0035863727394796	0.2472597098169916	0.2248041137865951	T
F	0.0097956904238323	0.4908951751304513	0.2291092677863188	T	F	0.9935637823111406	0.4951536203192852	0.2249407488730647	T
e	0.0067289614177484	0.7585092152645599	0.2272890116801085	T	e	0.0104266080098643	0.7594433450916049	0.2290054978578232	T
F	0.3329599312887066	0.9920872408358345	0.2268306569037463	T	F	0.3323765285600765	0.9918431152991650	0.2271044036052788	T
e	0.3272103953820972	0.2471589814017016	0.2336219459977716	T	e	0.3370967073475544	0.2505387764421650	0.2255754825931374	T
F	0.3280532920527158	0.5099078503866538	0.2264704027244052	T	F	0.3253500331342870	0.5172939191265264	0.2311935782761331	T
e	0.3376596632858703	0.7548704164129174	0.2304764958720854	T	e	0.3278308066465978	0.7524708358028021	0.2324667366622379	T
F	0.6699790970324948	0.9926715966985441	0.2284404372319497	T	F	0.6777862854052791	0.9986306618984266	0.2309009875290862	T
e	0.6536619555691239	0.2445277424443096	0.2301613564657915	T	e	0.6783290711460606	0.2406796333285794	0.2272284813694784	T
F	0.6694103956428973	0.5081542437191600	0.2213779082082522	T	F	0.6652910577292687	0.4914870617584466	0.2243579527569243	T
e	0.6576597586046777	0.7559166654446776	0.2282048111726170	T	e	0.6640505648819428	0.7611470324010510	0.2270279962808996	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F

e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F
F	0.1675451201384049	0.1229156662997126	0.1513517387949614	T	F	0.1663850140857017	0.1226652839903001	0.1514440656022781	T
e	0.1692693560374519	0.3739230709104122	0.1473044271749582	T	e	0.1698453317690000	0.3749947565068611	0.1501686506059108	T
F	0.1658529061189658	0.6264316286596979	0.1505652589003404	T	F	0.1642473102817767	0.6266162131697671	0.1500583595603772	T
e	0.1668445900417906	0.8752420601386323	0.1474428745453794	T	e	0.1664439036601356	0.8758040102014177	0.1478141145143710	T
F	0.4979093282469562	0.1245279899490469	0.1503794089041808	T	F	0.4998086458328959	0.1231654664987163	0.1513737309065813	T
e	0.4986346978593388	0.3752337973184466	0.1513565715666000	T	e	0.4976941492596791	0.3749017286976949	0.1480832524525160	T
F	0.4996834945125888	0.6266651126329476	0.1504465289861370	T	F	0.5022340678845503	0.6272060255950507	0.1529052768429543	T
e	0.4998855606961653	0.8757840391589353	0.1473944261647795	T	e	0.4999544789366377	0.8769798994439244	0.1478731470922182	T
F	0.8314480272073053	0.1257551770723855	0.1512730510571631	T	F	0.8339083187582795	0.1230553286681326	0.1494766575202512	T
e	0.8320227706257048	0.3732853350822745	0.1528467926226966	T	e	0.8321423945789299	0.3736691773382178	0.1497315007313482	T
F	0.8376936987875329	0.6265333411586478	0.1522747470969047	T	F	0.8345218757098805	0.6263557210299966	0.1525683545925920	T
e	0.8333658125477506	0.8739777625408914	0.1477832166272973	T	e	0.8339124433508298	0.8742877297976348	0.1483956987794875	T
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	3OH+HCO+O+H (-443.072909; ZPE= 1.680079038)					**3OH+CO+OH+H-t2 (-443.499142; ZPE= 1.747457295)**			
H	0.2271241757239315	0.8804733929392921	0.3273063482330281	T	H	0.2260838447743086	0.8763351500140580	0.3287363791487164	T
H	0.5623861304224776	0.8758489919745119	0.3284412212611292	T	H	0.5627616396283813	0.8736861565194696	0.3300669642527675	T
H	0.8950601550950812	0.8753401546135645	0.3279183445739710	T	H	0.8942318688435869	0.8714627153416485	0.3266089483526091	T
H	0.1320234115603992	0.2834914430328797	0.3435858726110554	T	H	0.8642246268574685	0.1419242808518415	0.2419997026612365	T
H	0.4841298408793875	0.6272769052863916	0.2435374650303922	T	H	0.4885020131335088	0.2998146093812648	0.3357499790270647	T
C	0.1511544880585164	0.3259818380719084	0.2919528303580947	T	C	0.1529863279791776	0.3688973849802626	0.2572221932880673	T
O	0.3319129928747296	0.8759208035210662	0.3053559059854346	T	O	0.2251997995271353	0.4293929675526250	0.3049968697713942	T
O	0.6664831680050141	0.8775024758007194	0.3058300478484792	T	O	0.3305801595286801	0.8755336556888088	0.3064001550600945	T
O	0.9989270183049653	0.8783496438374908	0.3051081591816868	T	O	0.6651586551969744	0.8708712526274829	0.3060956307788789	T
O	0.1683148639817632	0.4460611788879096	0.3000546658543817	T	O	0.9986476825093563	0.8751181080592980	0.3043173083815694	T
O	0.5108492756174766	0.3628949137592827	0.2573701949833002	T	O	0.4979083017556026	0.2322675380015382	0.3044585508291360	T
F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F	F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F	e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F
F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F	F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F	e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F
F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F	F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F
e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F	e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F
F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F	F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F
e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F	e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F
F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F	F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F
e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F	e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F
F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F	F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F
e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F	e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F
F	0.9890957936761727	0.9964790444051180	0.2270697086783797	T	F	0.9945022324022044	0.9957066586519828	0.2277512096067956	T
e	0.0149532127439617	0.2501641003602809	0.2243227062315291	T	e	0.0091993265421382	0.2545411290783716	0.2236845040116762	T
F	0.0095551055644594	0.4978423406399449	0.2283936175244062	T	F	0.9911796429808494	0.4978475094714463	0.2231207913731010	T
e	0.0088412088524831	0.7579306334812973	0.2297566969466124	T	e	0.0109729953727170	0.7560176094482074	0.2281846668905077	T
F	0.3443142607926665	0.9930468588082977	0.2281626704514547	T	F	0.3308418833542586	0.9909857493785589	0.2277545423448562	T
e	0.3258642307478898	0.2555346579498508	0.2308073540992274	T	e	0.3339268443944183	0.2408624152630638	0.2296560820569098	T
F	0.3264872147721337	0.5110825169516742	0.2332634443481091	T	F	0.3405487647999623	0.5126702867149905	0.2279041892565256	T
e	0.3231042841046854	0.7522901571210814	0.2307246063418543	T	e	0.3345256740893752	0.7533487592867311	0.2318577810673802	T
F	0.6661206920841175	0.9996007823024672	0.2315386950220506	T	F	0.6633707002968438	0.9849077496886455	0.2275391072813986	T
e	0.6669482941780693	0.2426830773396133	0.2263144342776842	T	e	0.6534031346683080	0.2478348378758916	0.2287749754072766	T
F	0.6617004874123944	0.4927571576433639	0.2245403962144644	T	F	0.6658215616408611	0.5109616204061971	0.2233582764876941	T
e	0.6699471596990253	0.7616608654887338	0.2262301780071215	T	e	0.6572330720862385	0.7515327930676109	0.2288627462680722	T
F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F
e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F
F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F
e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F
F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F
e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F
F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F
e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F
F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F
e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F
F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F
e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F
F	0.1688219562912640	0.1221011024979159	0.1522552452728385	T	F	0.1671404067967512	0.1225424238250504	0.1510448772436315	T
e	0.1682458446114959	0.3747558820017405	0.1471727989603630	T	e	0.1722889575243989	0.3766599002561597	0.1508813215061620	T
F	0.1645097793320771	0.6252205808544438	0.1500697198030098	T	F	0.1678814329117788	0.6257538527379376	0.1505543751338345	T
e	0.1673988318172983	0.8758123558569483	0.1479594712670161	T	e	0.1665630966882889	0.8749609614362298	0.1476709557252747	T
F	0.4987778716666859	0.1247864920609265	0.1508603600695636	T	F	0.4984612622398525	0.1228848335093726	0.1495104658443753	T
e	0.4966880293258299	0.3749063432287091	0.1480638096404114	T	e	0.4998787750634217	0.3754585669413778	0.1508567576833075	T
F	0.5009666344813030	0.6278578265035876	0.1531042108240825	T	F	0.4998100399291808	0.6277700474572124	0.1497253912950484	T

e	0.5001637169604913	0.8758042126737736	0.1474650678415092	T	e	0.4994011063182813	0.8747667401749459	0.1474217387387064	T
F	0.8327450899399221	0.1250180617219295	0.1506387297893622	T	F	0.8310219262695422	0.1245226480108101	0.1536975403800641	T
e	0.8340454186329042	0.3741743137867569	0.1518598049422551	T	e	0.8298966531276530	0.3743058453734512	0.1512410815046572	T
F	0.8348825113371280	0.6247975989815490	0.1527435051674449	T	F	0.8352583828519036	0.6280458353407466	0.1512381568305974	T
e	0.8333735643201314	0.8747573595156014	0.1477197306923252	T	e	0.8333353562343117	0.8726146637435095	0.1481459693822696	T
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	TS25 (-441.8047077; ZPE= 1.723944)					**3OH+COOH+H (-442.197921; ZPE= 1.803083361)**			
H	0.2261477300312267	0.8726288878796530	0.3286325686559299	T	H	0.2266863933482117	0.8723188847294412	0.3283672991195126	T
H	0.5619857879594004	0.8705840112669683	0.3302175534006582	T	H	0.5602293354180639	0.8720242340299817	0.3287215644757344	T
H	0.8946624975097963	0.8791266849079946	0.3275767555219523	T	H	0.8959201625520115	0.8783991377267700	0.3282098789193461	T
H	0.8513824973206197	0.1513757677999031	0.2416574244747738	T	H	0.8467262446870328	0.1531972977914009	0.2419038790376649	T
H	0.3277965484430727	0.3036181871363923	0.3582820876225357	T	H	0.1534533256173072	0.3432946244556203	0.3982260765617091	T
C	0.1496823902748548	0.3509402465128955	0.2751524359465142	T	C	0.1310304829535032	0.3354556880720586	0.2993639327948436	T
O	0.1771448033589273	0.4538992380346941	0.3020420863876720	T	O	0.3316805736410205	0.8738560436095083	0.3064586239778998	T
O	0.3311022899590368	0.8730635666929082	0.3066965714918560	T	O	0.6642884458838256	0.8752338393085705	0.3061141273314310	T

O	0.6646672651232544	0.8743140850791827	0.3065205456863602	T	O	0.9996248868053437	0.8734521239234033	0.3054492701195720	T
O	0.9988424206083799	0.8755450259149499	0.3050922721704509	T	O	0.1199816705154469	0.2841909105953070	0.3636701242249357	T
O	0.2662045716140754	0.2503430308432868	0.3287751419561829	T	O	0.1872357321138077	0.4457245943911297	0.3033487147181695	T
F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F	F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F	e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F
F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F	F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F	e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F
F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F	F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F
e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F	e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F
F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F	F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F
e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F	e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F
F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F	F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F
e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F	e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F
F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F	F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F
e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F	e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F
F	0.0110946339906289	0.9929535934896772	0.2272664768008548	T	F	0.0136136742517574	0.9914131469787328	0.2280881886573628	T
e	0.0081685609900457	0.2584115910311288	0.2235122526137208	T	e	0.0131735607696823	0.2599020080469903	0.2249524254338649	T
F	0.9884977027277223	0.5008488796605767	0.2259098114844357	T	F	0.0081019761739021	0.4979002480477863	0.2288935682274611	T
e	0.9899465913853358	0.7564887303851437	0.2290353183343611	T	e	-0.0114180592853269	0.7532243521883180	0.2294873925172597	T
F	0.3348180516117237	0.9947189248102278	0.2322847924777200	T	F	0.3346268811142053	0.9968306498980067	0.2324831681364840	T
e	0.3353702793000217	0.2344380744819496	0.2305492732073644	T	e	0.3178627062966415	0.2408009350032869	0.2272273674044353	T
F	0.3278150248953454	0.5115692438699372	0.2263395162230364	T	F	0.3293164028085266	0.5063746251690119	0.2273167831436510	T
e	0.3363046210396923	0.7583201267422226	0.2276185099987082	T	e	0.3358220186463673	0.7584293664685801	0.2273784894368485	T
F	0.6482003764631453	0.9896569642092196	0.2280450043136644	T	F	0.6515928007007622	0.9911122219866779	0.2275123320421589	T
e	0.6651330037958485	0.2430811196365898	0.2215068520548864	T	e	0.6670016069659386	0.2463050492946982	0.2211935909697147	T
F	0.6624120852836626	0.5084387530901257	0.2236838182519837	T	F	0.6643733621409909	0.5082056537626590	0.2231882747569030	T
e	0.6761077397847470	0.7527774966710656	0.2314683625988409	T	e	0.6765641919365241	0.7536680290890987	0.2310764543578551	T
F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F
e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F
F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F
e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F
F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F
e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F
F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F
e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F
F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F
e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F
F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F
e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F
F	0.1680780941833687	0.1233650455630770	0.1502454111779462	T	F	0.1675024381536244	0.1222318534984357	0.1497754033602249	T
e	0.1724850751481405	0.3747605631594014	0.1507622529324896	T	e	0.1694256300600482	0.3754469330847110	0.1471923619708412	T
F	0.1650359149949352	0.6276973317394616	0.1509157629484282	T	F	0.1658502895198170	0.6271355196810582	0.1509666580309350	T
e	0.1668170755183145	0.8745605856872937	0.1478973917684976	T	e	0.1667300584827004	0.8740458810429700	0.1479343032997343	T
F	0.4985637245701028	0.1228836690310559	0.1499325387689464	T	F	0.4970401459216662	0.1248363222173326	0.1512143512174589	T
e	0.4995917720794432	0.3748006290206890	0.1523215261030176	T	e	0.4985397559303359	0.3749308684794674	0.1525132378660365	T
F	0.4996542756283412	0.6280602258718075	0.1509091552500985	T	F	0.4991640659155571	0.6274384458484390	0.1512337080693106	T
e	0.4997802760877428	0.8739073890249475	0.1472174873194520	T	e	0.4995536895584275	0.8743073210824326	0.1476041544474734	T
F	0.8338314563969209	0.1206519173413314	0.1535430013632892	T	F	0.8354112394143731	0.1215208183507020	0.1540546042755528	T
e	0.8308982671600618	0.3757034141901194	0.1509059569993416	T	e	0.8333403612674256	0.3767653407230172	0.1513386394082631	T
F	0.8331755674559796	0.6261856566368315	0.1503467290302427	T	F	0.8346997493445314	0.6245739872138597	0.1510315528666801	T
e	0.8320150153790062	0.8756160349845461	0.1480702678448902	T	e	0.8329402347427313	0.8754308725631855	0.1481727945783330	T
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	TS26 (-442.4965323; ZPE= 1.495067)					**3OH+C+2O+2H (-444.2161407; ZPE= 1.515746032)**			
H	0.2292000096894014	0.8762710608239427	0.3275964217571432	T	H	0.2288776223983869	0.8807789684481633	0.3281636637660112	T
H	0.5629935245907547	0.8729414718602069	0.3268395826608018	T	H	0.5596068050177978	0.8765468084045361	0.3285874311907575	T
H	0.8955383213716439	0.8729402991881209	0.3282832126050163	T	H	0.8934575237934665	0.8762575578639964	0.3295373076628236	T
H	0.1927044152588235	0.1366159492489233	0.2422222701519892	T	H	0.1917147099748746	0.1376913331353489	0.2424314982996170	T
H	0.5072067764837489	0.6245569353472803	0.2435238767468521	T	H	0.5106482845134882	0.6267995674752906	0.2431963142444580	T
C	0.1612991386586071	0.3662609599943024	0.2448297823537785	T	C	0.1576724260383467	0.3691695627130414	0.2449752244729165	T
O	0.1596235574547085	0.5092619835329136	0.3001953825577384	T	O	0.3337852970560450	0.8794199267992655	0.3062250560584309	T
O	0.3325445457193786	0.8769925442423447	0.3042951524662622	T	O	0.6646805426678880	0.8775756951489048	0.3066971215933977	T
O	0.6675586272032116	0.8748930470284658	0.3046362660420175	T	O	0.9968948783080297	0.8779467399706850	0.3064414313772000	T
O	0.9991448100171108	0.8728602538728421	0.3051874429827692	T	O	0.5142355581661985	0.3651002224166017	0.2579102297365768	T
O	0.5190835280311625	0.3625052392169021	0.2576142963300420	T	O	0.1645036214109311	0.6291661468651851	0.2594504714580543	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297999999991	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297999999991	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.0000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.2500000000000000	0.0736297999999991	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334000000008	0.5000000000000000	0.0736297999999991	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334000000008	0.7500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.0000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.2500000000000000	0.0736297999999991	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666667000000004	0.5000000000000000	0.0736297999999991	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666667000000004	0.7500000000000000	0.0736297999999991	F
F	-0.0045077099469204	0.9883462811645578	0.2265900254486111	T	F	0.9855280449091097	0.9901804673793804	0.2275462749519362	T

e	0.0052045679590348	0.2536200733609637	0.2236158573062610	T	e	0.0076928409338501	0.2530019267435474	0.2238494424527645	T
F	0.0036500477976739	0.5019177932730428	0.2310334910294792	T	F	0.0099563808388297	0.4988499683553707	0.2284726025903998	T
e	1.0010633515429981	0.7512431263835787	0.2299650387576325	T	e	0.0032831810008257	0.7516083111683257	0.2311178078779674	T
F	0.3374000774874140	0.0005346834372805	0.2294045537193230	T	F	0.3445583166937149	0.9942217976608405	0.2282968772718339	T
e	0.3333446501478413	0.2573251100326257	0.2300942518387629	T	e	0.3299385488493743	0.2583937021973468	0.2296668390366337	T
F	0.3238415573090942	0.4995082068725302	0.2333716210790471	T	F	0.3219075183919120	0.4941947439713529	0.2340203098376110	T
e	0.3262064904028411	0.7609156311139833	0.2265955119006490	T	e	0.3278247844680959	0.7534767407762213	0.2310649921895950	T
F	0.6622009569820485	0.9941767383326051	0.2289942916728309	T	F	0.6676476182285546	0.0000753383684839	0.2326157519052157	T
e	0.6695776023945057	0.2423747944426476	0.2258714878320278	T	e	0.6668228096105530	0.2418208120054550	0.2266374189887674	T
F	0.6639274152443565	0.4956285010921996	0.2254718507960946	T	F	0.6640933031657963	0.4945352567574929	0.2251289265688539	T
e	0.6768708849238882	0.7542095841323501	0.2277655813888702	T	e	0.6672764184880615	0.7618098634014634	0.2272705107105084	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667000000004	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667000000004	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001000000012	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001000000012	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333334000000008	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333334000000008	0.8750000000000000	0.0000000000000000	F
F	0.1666960207199961	0.1232443000119433	0.1525031899802025	T	F	0.1672642748084088	0.1214461749381326	0.1531551127156504	T
e	0.1676484585661674	0.3772415741223347	0.1453168044223815	T	e	0.1676700877670392	0.3758620816188373	0.1446609624127524	T
F	0.1657796729967304	0.6264454589804002	0.1498554968818239	T	F	0.1669766792912586	0.6248896502416890	0.1476963061186808	T
e	0.1659215905940698	0.8749461015071923	0.1474393657361301	T	e	0.1663479143436691	0.8748332122341755	0.1490381627506661	T
F	0.5006747625947826	0.1251204081245814	0.1510497092672664	T	F	0.5009873441019840	0.1251928757641629	0.1508024137985942	T
e	0.4982364828332532	0.3747306302430619	0.1480083158599341	T	e	0.4980969925603894	0.3745327442701036	0.1479494510387374	T
F	0.4991753865027298	0.6266882763987035	0.1541081141051727	T	F	0.5003986298471067	0.6259722028711144	0.1538058632274873	T
e	0.4993851747391197	0.8757741834378537	0.1480125235316735	T	e	0.4993826765771831	0.8763534206745621	0.1481086109280280	T
F	0.8338255463420720	0.1234170596823722	0.1513744284788013	T	F	0.8329224311038862	0.1248200421865517	0.1509863819190154	T
e	0.8333631818880449	0.3745552435070004	0.1515462546650332	T	e	0.8338570776538597	0.3746207800831950	0.1522520330073081	T
F	0.8342069541784198	0.6237375037415313	0.1517737806935577	T	F	0.8333044649384829	0.6249010026868683	0.1524765478656381	T
e	0.8329815152888740	0.8740531284291230	0.1478196855218646	T	e	0.8322417443448639	0.8743477548752844	0.1481043307967842	T
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Table SX4. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the on the 3H (0.25 ML) pre-covered Fe(100) surface

	3H+CO+H_2O (-418.504788; ZPE= 1.132845108)					**TS27 (-417.620009; ZPE= 1.200031)**			
H	0.2932099841416757	0.2017598222133249	0.3683757248537311	T	H	0.3201816775280342	0.1859301757426666	0.3715721788906441	T
H	0.4390486109356496	0.1345825062648001	0.3369695601927143	T	H	0.4608700996363331	0.1340216193029504	0.3271561785509317	T
H	0.8279748331407427	0.8665271547088611	0.2444030899583497	T	H	0.8393408353177343	0.8520153892577673	0.2435589832933632	T
H	0.8306946642391522	0.3634911744051836	0.2429134753257929	T	H	0.0363196450437143	0.2841459387073662	0.3061858572585872	T
H	0.4989117552464378	0.6196138349949525	0.2441500500994060	T	H	0.5127133379179326	0.6445375272327828	0.2434558334123736	T
C	0.1650242194277394	0.3655642085326178	0.2599269878877835	T	C	0.1414537226677815	0.3477610113732232	0.2691623075871249	T
O	0.3892339679853726	0.2125928055194729	0.3411985132615277	T	O	0.4027540483125787	0.2071385627133167	0.3384846583698198	T
O	0.1672298819093279	0.4518664474013992	0.3055741343164049	T	O	0.1641246141985546	0.4478236067691396	0.3040024863443719	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0110221177924433	0.0073733099783068	0.2238690013522446	T	F	0.0031017548166588	0.0092956162631040	0.2238883838147987	T
e	0.0055860234411121	0.2582378589049503	0.2238717225312898	T	e	-0.0004240457225887	0.2479178270998496	0.2257268442893947	T
F	0.9927352123808226	0.5003254075261436	0.2294354259523255	T	F	0.9913694404519295	0.4956303823329238	0.2294476432637900	T
e	0.9926454082484104	0.7419054770703001	0.2261913496199391	T	e	0.0024638807579597	0.7384699084064859	0.2241180522323687	T
F	0.3364615097048055	0.9924404503099341	0.2246459655027323	T	F	0.3365333612217068	0.9935926193723307	0.2238285727745108	T
e	0.3305767822227855	0.2533506800906252	0.2314154983237615	T	e	0.3255792263477760	0.2538142636418998	0.2320495678072164	T
F	0.3376327137261085	0.4922827873836831	0.2281166535658845	T	F	0.3218078596315255	0.4948252521140212	0.2264366848603336	T
e	0.3199107833029833	0.7526492314844344	0.2240016004774270	T	e	0.3326264929763821	0.7582661318312346	0.2236491955767158	T
F	0.6516489075635967	0.9990112749131390	0.2247703539460192	T	F	0.6518201873067989	0.0107464375383716	0.2241948773602962	T
e	0.6719996470126498	0.2385514399826225	0.2231729196439458	T	e	0.6840183930145456	0.2488995312682195	0.2257460496037184	T
F	0.6652652414736896	0.5118529624923510	0.2241731879330028	T	F	0.6680838642249224	0.5000299298438935	0.2231922209870386	T
e	0.6826222848434250	0.7486550328768948	0.2249460075966292	T	e	0.6753042790207734	0.7510260480255001	0.2232691757178488	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F

e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1683395144457220	0.1258920347056871	0.1513118436388945	T	F	0.1676016145122075	0.1253035491792684	0.1506680084729322	T
e	0.1695026630134697	0.3763509591449005	0.1490251217895685	T	e	0.1679162648886585	0.3743852909481239	0.1495546219592986	T
F	0.1645106183096410	0.6247051085135104	0.1505106305510404	T	F	0.1663542742349083	0.6249766967023146	0.1505837022142582	T
e	0.1652403701084789	0.8750987137189760	0.1506090920167859	T	e	0.1650697538296936	0.8751622835219155	0.1510470167027790	T
F	0.4979844018109091	0.1259674569468908	0.1515424109829846	T	F	0.4966822150271692	0.1291258887740964	0.1517460126104628	T
e	0.5010993439886501	0.3730697001036243	0.1513192146383556	T	e	0.4994162022075951	0.3728492573593717	0.1520518073524340	T
F	0.4971934627205337	0.6265721569911927	0.1529598922227179	T	F	0.4981505913724780	0.6249300688474204	0.1538382161864549	T
e	0.4991500909202497	0.8726985873367081	0.1502554061510855	T	e	0.5015971224307183	0.8755223981620746	0.1501605744936514	T
F	0.8360277828753283	0.1235513242025931	0.1508036057070700	T	F	0.8340636379985393	0.1249209955820055	0.1498646963516929	T
e	0.8298252809963196	0.3756954768561169	0.1520875572369411	T	e	0.8334411315409892	0.3749763377628607	0.1501865896310452	T
F	0.8349993701966090	0.6237944140512303	0.1490499881310283	T	F	0.8352275130551662	0.6227355880942936	0.1503107905921375	T
e	0.8347384815531425	0.8776043803894112	0.1527197378211243	T	e	0.8344666121988166	0.8768215263854937	0.1535167051901347	T
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	2H+HCO+H_2O (-417.733212; ZPE= 1.313550393)					**TS28 (-418.098355; ZPE= 0.92752475)**			
H	0.1181750102548483	0.2957297421810298	0.3463792615787441	T	H	0.3298556069720295	0.1470669181652954	0.3541800824124525	T
H	0.3429437046384784	0.1788204542583754	0.3752725513375730	T	H	0.4811065307131236	0.0719601360477178	0.2882830939610190	T
H	0.4715703012896103	0.1271837778545613	0.3233680350092822	T	H	0.8299903697555020	0.8602573857881740	0.2443452772516128	T
H	0.8366777483491042	0.8480721395818899	0.2434925512948885	T	H	0.8181317489236704	0.3823899937873927	0.2429390542991949	T
H	0.5052119547101827	0.6490157962275034	0.2437566053305833	T	H	0.5174887797653462	0.6246336682778840	0.2441109361184374	T
C	0.1411747484012487	0.3361068188909588	0.2943269215054889	T	C	0.1649199941835901	0.3655910109341900	0.2611246972215396	T
O	0.1643045658318449	0.4558507565885886	0.3019012254232534	T	O	0.4012157715320750	0.1630682357485206	0.3152891267624105	T
O	0.4175182846256609	0.2003727269417878	0.3387151324242506	T	O	0.1645945388427906	0.4535452440516614	0.3054397532121485	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0018963858188929	0.0083895596380867	0.2227197431936749	T	F	0.0009670790255790	0.0070861944524652	0.2233947886153879	T
e	0.0114482765901057	0.2594587608249641	0.2249404833865799	T	e	0.0082279758298372	0.2571310925703618	0.2233822191700772	T
F	0.0014572977580318	0.4987155089258890	0.2318179289790649	T	F	0.9907036841334093	0.4998088995544559	0.2296265652788485	T
e	0.0005009295865754	0.7376258291281298	0.2235358706186903	T	e	0.9986163064816540	0.7416921456025345	0.2248831381442476	T
F	0.3362423690709163	-0.0028350164489283	0.2243162505228158	T	F	0.3432211558290331	0.0000406230574102	0.2275925087602226	T
e	0.3175188601576224	0.2562346791499336	0.2379141151585568	T	e	0.3239905999453963	0.2513504721323477	0.2325186737551435	T
F	0.3209936437255666	0.4906647664518100	0.2272660804691227	T	F	0.3353474013186279	0.4914710621930721	0.2275302412079785	T
e	0.3328364048369651	0.7583317590048354	0.2236043915540838	T	e	0.3219986575517336	0.7600820430551606	0.2238013824287988	T
F	0.6516134347733527	0.0099527051736557	0.2239028751446977	T	F	0.6452518073796591	-0.0013212911482840	0.2283616582226118	T
e	0.6773601210445270	0.2492259605721709	0.2245307895901022	T	e	0.6675866622061636	0.2408266646206163	0.2233637610594445	T
F	0.6744183494865139	0.4925611788893719	0.2234914388792308	T	F	0.6686247243800020	0.5097817598506180	0.2242898563896180	T
e	0.6676891918000495	0.7520965499926051	0.2228580000565992	T	e	0.6799572514831475	0.7453632262702338	0.2249234199295943	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1679701257074236	0.1261596259518788	0.1512957021288442	T	F	0.1669335632771205	0.1248120270030512	0.1510042350143881	T
e	0.1682430182872338	0.3743846379453842	0.1465736060716347	T	e	0.1683838310852765	0.3770598731549172	0.1487319583679370	T
F	0.1668161007476190	0.6239411621337324	0.1504788745936979	T	F	0.1661188850807349	0.6250572425821134	0.1507460386154040	T
e	0.1657357537275678	0.8752468696259434	0.1511920819794319	T	e	0.1654545140219197	0.8771233165299852	0.1508404011135705	T
F	0.4957983287070299	0.1295688952471355	0.1516904635431893	T	F	0.4993618924136910	0.1260714721712184	0.1498126824313671	T
e	0.4979126306015629	0.3727812902048558	0.1520288200314027	T	e	0.4996846110455951	0.3726142864911863	0.1513167730634271	T
F	0.4987534068162814	0.6235533045599236	0.1544346879702187	T	F	0.4967866715804989	0.6260095162892517	0.1533849236757835	T
e	0.5006199969385260	0.8762244911786009	0.1502506990363446	T	e	0.4991335274680175	0.8740220791934351	0.1503796696124390	T
F	0.8343449912429178	0.1260187118819635	0.1503443886430334	T	F	0.8335694858721403	0.1240286722481801	0.1510297432670713	T
e	0.8347304818130024	0.3749569776550565	0.1501796298114400	T	e	0.8296124120159408	0.3749165647168003	0.1521240517478134	T
F	0.8343608381555100	0.6218857985418494	0.1506856642956826	T	F	0.8355815121097794	0.6240131229836309	0.1491023288098503	T
e	0.8345189953130426	0.8758640770893537	0.1538231894143986	T	e	0.8329154972996055	0.8766015502106079	0.1533143810867247	T

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	3H+CO+OH+H (-419.302467; ZPE= 0.977181386)					**TS29 (-418.351574; ZPE= 0.756258)**			
H	0.2581437331153581	0.1260160323790309	0.3412907505366716	T	H	0.1317288647654294	0.1217159608352866	0.2638509551299940	T
H	0.5114129103430735	0.8607709969389131	0.2433781847353022	T	H	0.5020336932839847	0.8703161825968246	0.2423765895269764	T
H	0.8426419278608711	0.8603764402076325	0.2426014891668198	T	H	0.8380545455909764	0.8638055713169525	0.2429137468608909	T
H	0.8157685155864072	0.3825318974080610	0.2430669326352449	T	H	0.8161151953831154	0.3859161037077238	0.2435523572704836	T
H	0.5194602712041930	0.6149183354241752	0.2444178205131723	T	H	0.5189457532617977	0.6165193710256396	0.2439531021158270	T
C	0.1678031582638897	0.3634388869881253	0.2605407820419174	T	C	0.1692200711566135	0.3662665316582672	0.2589523894854232	T
O	0.3465204352862262	0.1223098260195812	0.3090189083430818	T	O	0.2801775876824747	0.1119633691486246	0.2950740388784163	T
O	0.1642690735687475	0.4508195945872671	0.3054425143366486	T	O	0.1647030367093440	0.4511377976150688	0.3053989532432166	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F

e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	-0.0016850859711134	0.9905095666293711	0.2238291039682121	T	F	0.9869380752064421	0.0096802039165274	0.2266766073573895	T
e	0.0120018227482227	0.2538762140036924	0.2230291798165978	T	e	0.0149037430240530	0.2491901764974459	0.2251994161641834	T
F	0.9906959790917761	0.4983806964822955	0.2298982651437500	T	F	0.9907116815322804	0.4958482892967548	0.2295648922187470	T
e	0.0110808830240121	0.7459070504450543	0.2243590570471752	T	e	0.0099179352279768	0.7478561321101965	0.2236396241868661	T
F	0.3198316436355730	0.0096883464211638	0.2314178913282608	T	F	0.3545469115544359	0.0028361427489509	0.2315361885439561	T
e	0.3299161503009639	0.2454808736557696	0.2346528470259484	T	e	0.3297955456025390	0.2435905189155675	0.2357986418262940	T
F	0.3337676147444819	0.4900455552108050	0.2272892653820342	T	F	0.3346159852489921	0.4905806998441290	0.2271451034440220	T
e	0.3313018270794850	0.7660192654641036	0.2242527611337010	T	e	0.3252395999971228	0.7644351197661525	0.2236748092637066	T
F	0.6778821087600332	0.0098528540267540	0.2230608757961499	T	F	0.6770999741053578	0.0063074586813809	0.2247902579776543	T
e	0.6556753729556249	0.2486124182536484	0.2230453511101408	T	e	0.6525361698988683	0.2492486644213978	0.2242473308623366	T
F	0.6789759791024524	0.5080313145075265	0.2248094762112788	T	F	0.6786227780160750	0.5083188775582691	0.2246497906483144	T
e	0.6590127304837653	0.7397877371146452	0.2244104927683623	T	e	0.6652010705256285	0.7391102223950176	0.2236075721621536	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1654467914393322	0.1241037338797214	0.1499818033704478	T	F	0.1664514890047973	0.1225957241098169	0.1501869485958642	T
e	0.1698679621819350	0.3759618938902435	0.1492344004813201	T	e	0.1691830033405321	0.3763043019077250	0.1492211611226312	T
F	0.1677384701549661	0.6250233281087638	0.1513806689341792	T	F	0.1674174764252690	0.6253313461164901	0.1512374741117962	T
e	0.1672869100419370	0.8761154260235375	0.1495804750613052	T	e	0.1666438197182755	0.8787849110868908	0.1507675446384692	T
F	0.4987746871568337	0.1245839384447477	0.1501852053526747	T	F	0.4997608333899551	0.1257477716299745	0.1497555016581036	T
e	0.4986929293796097	0.3731566714356505	0.1507905158111739	T	e	0.4981439171015947	0.3730596231352679	0.1508616682463410	T
F	0.4950539147982025	0.6222953860374071	0.1526697446168681	T	F	0.4961582598837913	0.6222885798229497	0.1526622151161132	T
e	0.4997279160500458	0.8790456777328051	0.1523796406246918	T	e	0.5021580521522819	0.8754301512102028	0.1509510678377688	T
F	0.8360772493483364	0.1263859232508325	0.1507043359318228	T	F	0.8331299963314454	0.1279984578526381	0.1503152012869298	T
e	0.8323492627566478	0.3736279171359087	0.1518417886459088	T	e	0.8321570602331980	0.3723790936086349	0.1523412534380952	T
F	0.8356615886548538	0.6261096472188818	0.1500745745675143	T	F	0.8366284290416128	0.6254944049090432	0.1499875490159280	T
e	0.8317721295792374	0.8731311066971986	0.1519710240961561	T	e	0.8351698739757571	0.8742960579048442	0.1523074746205707	T
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	3H+CO+O+2H (-419.642895; ZPE= 0.860071737)					**TS30 (-417.727654; ZPE= 0.829523)**			
H	0.7828879333895657	0.1263699415544945	0.2442320831041776	T	H	0.7898087421443454	0.1243642372219341	0.2439422846475324	T
H	0.4949572198125377	0.8937675528923660	0.2445818323136106	T	H	0.4931739479241394	0.8912825845116019	0.2441708971343879	T
H	0.8508227403794947	0.8719660370043661	0.2441859455216470	T	H	0.8394252143577858	0.8617349056824829	0.2451852981936888	T
H	0.8006364420860271	0.3902173447331054	0.2431795510522219	T	H	0.7957559244261571	0.3825541403198391	0.2427412415560709	T
H	0.5003928427941751	0.6120494177542540	0.2452697305933263	T	H	0.5189575290368658	0.6199888688830870	0.2448307245413185	T
C	0.1738125319112185	0.3745301710401475	0.2595270975547489	T	C	0.1759753925952497	0.3773768837968227	0.2567248278881870	T
O	0.1711933412915105	0.1042548571213028	0.2595349630558710	T	O	0.1723146804123203	0.2222743186138088	0.2960600269437332	T
O	0.1685106636481662	0.4567327551330522	0.3070878002308161	T	O	0.1632931040325034	0.4550851462892076	0.3055038933496146	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0108521575370920	0.9922583200489401	0.2273577145284230	T	F	0.0161695382003046	0.9861386895888062	0.2252615974506460	T
e	0.0254451867020103	0.2498321256413493	0.2273769252276961	T	e	0.0150823406597295	0.2434472748427329	0.2281538955749740	T
F	0.9970143305470707	0.4981833670929458	0.2280380756722552	T	F	0.9958448266562479	0.5080104447768664	0.2272990389991262	T
e	0.9965762158117889	0.7525382211793685	0.2268919904572990	T	e	0.9973250195166911	0.7528399661572190	0.2278305317359724	T
F	0.3370259044028386	0.9966977107765541	0.2289444223427244	T	F	0.3285135637564117	0.9978840090635736	0.2263670006372920	T
e	0.3312260006548406	0.2507029691550784	0.2303544576779297	T	e	0.3368284889236663	0.2495301836029467	0.2302111958892492	T
F	0.3460326531670061	0.4925954949493550	0.2288812637210573	T	F	0.3522609768505729	0.4959326914574834	0.2281478367652573	T
e	0.3107220965814330	0.7552908653062980	0.2240955188635686	T	e	0.3114014975427664	0.7571484890686853	0.2242558753899203	T
F	0.6441552127073653	0.0089265588840467	0.2258973363982026	T	F	0.6450313282580488	0.0078795303109322	0.2251650855892356	T
e	0.6535341547898054	0.2494197964934594	0.2241910400904312	T	e	0.6579407054597743	0.2478200420286571	0.2238190496202771	T
F	0.6598191303656110	0.5088228003565907	0.2247889128624625	T	F	0.6628684120581393	0.5071474722722685	0.2247475144179102	T
e	0.6909942617041521	0.7420945414979170	0.2247135075550890	T	e	0.6893472930432256	0.7419758073408809	0.2254622227244612	T

F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1677127610989924	0.1234807137924949	0.1473700192923235	T
e	0.1691717174693876	0.3779063118536636	0.1494825076880073	T
F	0.1653893442608552	0.6248689252393308	0.1503727610989476	T
e	0.1663560544667249	0.8754856756764304	0.1485999519134578	T
F	0.4958278120283744	0.1263444368416549	0.1496310652259255	T
e	0.5002087642153940	0.3737456612017747	0.1501540747151756	T
F	0.4981176169759867	0.6271350807496985	0.1528498221159504	T
e	0.5001715327864789	0.8724327478370405	0.1522590999778152	T
F	0.8348505195643076	0.1242733256145454	0.1540803768664976	T
e	0.8345386495978311	0.3737360080837990	0.1538547071464497	T
F	0.8378255687215885	0.6227313270611327	0.1493596877428247	T
e	0.8332241517630173	0.8763392151789848	0.1513714646457986	T
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F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1674181045731530	0.1224109641956373	0.1489023447120770	T
e	0.1669424325112773	0.3757352628097403	0.1516636481515302	T
F	0.1662061725098270	0.6250793584959111	0.1507255111678293	T
e	0.1669552067105075	0.8742936563758629	0.1474493210590184	T
F	0.4964921721876003	0.1265655004744490	0.1497879022740940	T
e	0.5009288623614586	0.3733201877163606	0.1500857287863484	T
F	0.4986943927575612	0.6275753682913112	0.1525377607149263	T
e	0.4999247700597950	0.8734357198450754	0.1520552558702431	T
F	0.8355858281694636	0.1234915476890746	0.1536982243100664	T
e	0.8347125206480345	0.3748204999739911	0.1536505791825754	T
F	0.8367037703849565	0.6247550028692078	0.1489090940808555	T
e	0.8322778023248567	0.8765628732220069	0.1511630429150778	T
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	3H+CO_2+2H (-418.645018; ZPE= 0.927860091)					**TS31 (-418.3946626; ZPE= 0.766656)**			
H	0.7859776357751516	0.1172035867868054	0.2429657822361253	T	H	0.5263897095065879	0.8681417528711377	0.2421931840777590	T
H	0.4928356133200884	0.8847015356596035	0.2448739538782284	T	H	0.7968992487853249	0.1318191983895378	0.2433062548490479	T
H	0.8281789324157139	0.8639332444548106	0.2445381442399898	T	H	0.8472554681858188	0.8785159572372568	0.2440937153856109	T
H	0.7961889964529462	0.3664155817496129	0.2428315281998237	T	H	0.8040579889610241	0.3888500458512147	0.2429654255603002	T
H	0.5496699111016148	0.6238358323817581	0.2438540733122215	T	H	0.5076470035719192	0.6171838148425572	0.2449682578218820	T
C	0.1575313561871128	0.3382485409896119	0.2931727427002463	T	C	0.1706097318094642	0.3722208679525884	0.2465867244028183	T
O	0.2589919185036471	0.2766361401191732	0.3279184799459997	T	O	0.1618353960330718	0.5127894770631388	0.2994715698815552	T
O	0.1587854306992810	0.4568311715942808	0.3029301548959548	T	O	0.1632985638363262	0.1053325885173633	0.2597043123567883	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0134810473371683	0.0046756201580536	0.2230467873933306	T	F	0.0023876093063320	0.9921731995678382	0.2288134686024191	T
e	0.0178606698915075	0.2595087713899252	0.2264668741748412	T	e	0.0186384035923866	0.2508983502742012	0.2278540173481221	T
F	0.0005448066010934	0.5172517520894687	0.2330950670346694	T	F	0.0020488618575638	0.4973282407742150	0.2323415541074789	T
e	0.9928806198943864	0.7491975207738063	0.2269979701229835	T	e	0.9993351587378332	0.7509455342842040	0.2247925813723960	T
F	0.3398293062987918	0.0012990323231061	0.2272925747950753	T	F	0.3274883811428863	0.0001149037526599	0.2254321762670055	T
e	0.3359756340507898	0.2330717265591101	0.2337767244035306	T	e	0.3293518697112807	0.2508026227304436	0.2301831980199293	T
F	0.3238028503908188	0.4971166095899822	0.2267053813751715	T	F	0.3240348293920847	0.4982217089798598	0.2311920498792690	T
e	0.3118322007355662	0.7580211801474636	0.2238154721988291	T	e	0.3413385936109963	0.7605926909924784	0.2239649135856187	T
F	0.6452379874234239	-0.0021503694782837	0.2260120044084214	T	F	0.6780498730698830	0.0028082692620946	0.2240898507478986	T
e	0.6518317304729371	0.2451195236596563	0.2234364502472792	T	e	0.6454689251532852	0.2497426201694216	0.2245430922871085	T
F	0.6748023138820847	0.4983366060862318	0.2235037932449865	T	F	0.6628907263848266	0.5040286230693284	0.2249823128812914	T
e	0.6881503574584528	0.7452175772467557	0.2254063993697330	T	e	0.6711742556389824	0.7333206032321529	0.2250063887880447	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1679317729526174	0.1255433187463038	0.1502076983560726	T	F	0.1669545974043558	0.1250784973786732	0.1475343403956575	T
e	0.1694906531875010	0.3743956849664274	0.1491900281997666	T	e	0.1674061109165675	0.3764389486044800	0.1455763352207688	T
F	0.1662528271068841	0.6253930403654370	0.1503070528988576	T	F	0.1661744789128263	0.6258384456741324	0.1506695107703105	T
e	0.1645677376861339	0.8767886951249179	0.1492091966356306	T	e	0.1677100190198242	0.8739828165967364	0.1501759917782280	T
F	0.4990326477253051	0.1247364559198787	0.1487657451671731	T	F	0.4985215904233504	0.1241718730683791	0.1511193495042875	T
e	0.4971561851492437	0.3738316325627012	0.1514552022009873	T	e	0.4965846062364099	0.3749491857422341	0.1509293780315376	T
F	0.4979069232629268	0.6248222940018235	0.1547325795584114	T	F	0.4962098330953535	0.6226988629151881	0.1519050758603381	T

e	0.4981715341961803	0.8719550204549029	0.1511582038794150	T	e	0.5027550548587524	0.8778717453169970	0.1522960512924717	T
F	0.8348831962006316	0.1248985327577225	0.1534183014547820	T	F	0.8349066671173845	0.1265597565852514	0.1527026785983143	T
e	0.8363147945314562	0.3748927099893758	0.1532367653114029	T	e	0.8337561239216397	0.3742372873466039	0.1536735182361761	T
F	0.8352802087542980	0.6238317698173929	0.1485750607393020	T	F	0.8359825414314574	0.6226755808967710	0.1502392072340588	T
e	0.8346058916880410	0.8771632006860485	0.1515376917436255	T	e	0.8335708397511518	0.8727524395571402	0.1514724715428042	T
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	3H+C+2O+2H (-420.502291; ZPE= 0.855620213)					**TS32 (-418.459898; ZPE= 1.026813)**			
H	0.7918251388452880	0.1232961062069968	0.2440438770908529	T	H	0.2601700332933716	0.1260150279872532	0.3424890696713759	T
H	0.4826800764015152	0.8884430907145527	0.2445807363302303	T	H	0.5075911506819820	0.8659464508802993	0.2427398130368267	T
H	0.8497728387920946	0.8645720932285438	0.2442787665457892	T	H	0.8302700924559762	0.8422504174233920	0.2428826589691883	T
H	0.7888522346127754	0.3849009816132274	0.2434610862849208	T	H	0.0352762560441587	0.2819368506099615	0.3048840953589616	T
H	0.5044307314309663	0.6126476857560256	0.2449626632031011	T	H	0.5217443044164704	0.6235314710199202	0.2441054907763494	T
C	0.1738441421918584	0.3764752734030088	0.2452752248455608	T	C	0.1435074993013616	0.3455079936512851	0.2683413100706117	T
O	0.1695859026044172	0.1075708960684405	0.2596594579187926	T	O	0.3466407713950928	0.1248204108923571	0.3091179023434374	T
O	0.1577383046603864	0.6443390365655803	0.2596910998176105	T	O	0.1664588300409324	0.4452453590732756	0.3033060452745623	T

F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0089276999932133	0.9921025188200737	0.2278762596961927	T	F	0.0157061104288712	0.0077897923609164	0.2233055164469809	T
e	0.0232459436447697	0.2521936223278991	0.2284464742958243	T	e	0.9985112091844144	0.2491284261939522	0.2240271598731845	T
F	0.0180784976933244	0.4996920578766185	0.2288094175235674	T	F	0.9925526228175716	0.4942474009112582	0.2293271235114559	T
e	0.9945379605862291	0.7532356978230491	0.2292368133666625	T	e	0.0016425063940790	0.7433540917095544	0.2230520992770628	T
F	0.3354945789872748	-0.0017572467168874	0.2295607586214503	T	F	0.3330104762158565	0.0064130871639111	0.2341110280655288	T
e	0.3284510021898659	0.2515921712684546	0.2291025311589546	T	e	0.3249250079817063	0.2450850872924348	0.2334096466138826	T
F	0.3293698843528653	0.4990300974008547	0.2301901752947118	T	F	0.3265919342780969	0.4905999121268508	0.2265470759734861	T
e	0.3214453538886751	0.7587409922621663	0.2279588052570471	T	e	0.3301403345475633	0.7657014884633249	0.2240410350616065	T
F	0.6417860080815316	0.0099222567302547	0.2254246259082584	T	F	0.6550937744869880	0.0093063563411211	0.2216725830672898	T
e	0.6678069710222742	0.2501087098754817	0.2229968596486968	T	e	0.6771536659259149	0.2515307364826783	0.2244472587135196	T
F	0.6457968844432087	0.4987691134964971	0.2250656441957390	T	F	0.6737232352415946	0.5052713271956938	0.2244416490329517	T
e	0.6884526697264174	0.7371068268005754	0.2251697337234324	T	e	0.6695581636091059	0.7379648497571558	0.2243275929751967	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F	F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F	e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F	F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F	e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F	F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F	e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1675721232218375	0.1244462107306924	0.1477867422513015	T	F	0.1680671282845988	0.1253193360371271	0.1484563132910033	T
e	0.1688946775413070	0.3757312193095180	0.1448671848051169	T	e	0.1687334984725893	0.3742205763494122	0.1493181344790657	T
F	0.1676078517623113	0.6255094868518600	0.1480646480031231	T	F	0.1677439433731842	0.6256383489560136	0.1512724271111154	T
e	0.1665568654254821	0.8752714503184343	0.1494241677346136	T	e	0.1667767865162519	0.8765679706047785	0.1503387739113063	T
F	0.4966892823791292	0.1277335576374901	0.1497501962262256	T	F	0.4977266167827728	0.1282385150737380	0.1492608079980045	T
e	0.4971561314147567	0.3731852663652731	0.1508361972112317	T	e	0.4995980728441813	0.3722285507722480	0.1519328163109615	T
F	0.4986531062267194	0.6269350244809039	0.1521330115336962	T	F	0.4953731042856300	0.6234283187866192	0.1526163269015954	T
e	0.5001781762557559	0.8737424265896794	0.1522037756485954	T	e	0.4996760993139164	0.8772797411483167	0.1513593464363600	T
F	0.8354284258438740	0.1240415715967983	0.1536288619609684	T	F	0.8336339601514744	0.1246090866460194	0.1503027486200111	T
e	0.8371839124518721	0.3768330140628960	0.1549780773970823	T	e	0.8331810261098569	0.3754134439576196	0.1501093835689165	T
F	0.8373320187696256	0.6213129736098558	0.1501116341765875	T	F	0.8367129666446267	0.6231616192087744	0.1499551524065452	T
e	0.8322004060775473	0.8757709770754774	0.1520131862966760	T	e	0.8342578665163426	0.8770453052922280	0.1539214430134215	T
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	3H+HCO+OH (-418.602057; ZPE= 1.14478608)					**TS33 (-417.524706; ZPE= 0.999802)**			
H	0.2779840377885458	0.1199221383584996	0.3479011522023521	T	H	0.2506522429806258	0.1859607191702008	0.3516213519415382	T
H	0.1249300729680081	0.2923841361688695	0.3464121080501173	T	H	0.4912197922089777	0.8863181848318910	0.2443794720966908	T
H	0.5060247611028327	0.8643119237329743	0.2425834355965191	T	H	0.8357631470094152	0.8551473743499100	0.2440106187831964	T
H	0.8290111696447608	0.8391324522880674	0.2428236243121262	T	H	0.8032973204822660	0.3788254184254283	0.2435121632531602	T
H	0.5273397167003421	0.6182554792050905	0.2437035270424277	T	H	0.5314892071536494	0.6246656897128285	0.2442891756219730	T
C	0.1463445517407382	0.3329322188251418	0.2943191677258449	T	C	0.1710647058507697	0.3400023672993150	0.2803391249827858	T
O	0.3544406307836280	0.1229995540698497	0.3101069156032475	T	O	0.3052951824822486	0.2581270990229606	0.3377228432690098	T
O	0.1692154902100536	0.4527207741767961	0.3017820897205149	T	O	0.1710102264524282	0.4458187075284975	0.3067207101164836	T
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F	F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F	e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F	F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F	e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F	F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F	e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F
F	0.0125865318833458	0.0083649647125576	0.2222411367353608	T	F	0.0013987452095993	0.0030144191432904	0.2229748719080281	T
e	0.0079735996290601	0.2606649106049796	0.2250092187841828	T	e	0.0182179165288184	0.2532489641128266	0.2258996074069452	T
F	0.0037112382523342	0.4961052467658936	0.2322604908160608	T	F	0.0039044465539182	0.5045075882331937	0.2321800214688846	T
e	0.0005970829269391	0.7412888421750659	0.2230682875298263	T	e	0.9969488971735365	0.7433182416600977	0.2257721042230084	T
F	0.3341744411722129	0.0077187931001856	0.2338129048821960	T	F	0.3408870041782701	0.9991826206120836	0.2250900096673966	T
e	0.3133792265385914	0.2467087254006811	0.2376077825313042	T	e	0.3384135497272132	0.2451094292801618	0.2340892377521252	T
F	0.3236731755885269	0.4888708294620863	0.2272247896552231	T	F	0.3292305101935072	0.4866937484409099	0.2283599339470148	T

e	0.3280236816414038	0.7640078348166198	0.2232476932356139	T
F	0.6558057427220424	0.0096094204714088	0.2212408860703063	T
e	0.6680058426458590	0.2512026134388360	0.2245115308323929	T
F	0.6782320920769936	0.4997950358209803	0.2246543150146699	T
e	0.6670619022608339	0.7374709092656276	0.2235798919394634	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1674479611302457	0.1262350634063801	0.1492791221714051	T
e	0.1684169797999359	0.3743827812619793	0.1468109651900316	T
F	0.1678963713258882	0.6246633714866249	0.1508989256259233	T
e	0.1663176690336822	0.8770968359142889	0.1503968812954583	T
F	0.4964294865717505	0.1283367134041419	0.1492999216406274	T
e	0.4972966743544188	0.3717911089725789	0.1521635433750683	T
F	0.4954091493269184	0.6217568936783041	0.1530025017041583	T
e	0.4997016320102000	0.8767334101972705	0.1515388259979202	T
F	0.8337649160159254	0.1259675851477604	0.1509197172958029	T
e	0.8334607552593193	0.3751719959523505	0.1506925606956722	T
F	0.8365632586602494	0.6219955769156524	0.1503586946858601	T
e	0.8344065170863463	0.8763044322500417	0.1541946269054562	T
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e	0.3162572761790900	0.7587719352721944	0.2237178560443649	T
F	0.6487499931106757	0.0092973814844884	0.2250030738215723	T
e	0.6632559061345410	0.2456813245719240	0.2235243192241316	T
F	0.6647715207719356	0.5036085522957946	0.2236381407251379	T
e	0.6864742815841004	0.7402473129992503	0.2249374297662814	T
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F
F	0.1674482706909425	0.1242896375452087	0.1511455813776956	T
e	0.1686056820272145	0.3741795595930891	0.1483228845359810	T
F	0.1675715678051107	0.6239913957446553	0.1511431062839215	T
e	0.1644423786083112	0.8764605055037048	0.1498679415174109	T
F	0.4979733985098513	0.1276912156902965	0.1493263462323047	T
e	0.4985700846973432	0.3732561760219167	0.1505931610398843	T
F	0.4966462816789797	0.6247052142827429	0.1538490733458971	T
e	0.5000706186491775	0.8730205561370442	0.1516184435510198	T
F	0.8338469145104901	0.1249137447667954	0.1514688075288660	T
e	0.8351013919610502	0.3745832525190256	0.1537523410402877	T
F	0.8364821471227558	0.6221207294908137	0.1493177217924342	T
e	0.8332326777327154	0.8763371670298408	0.1525050595635897	T
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	3H+COOH+H (-418.075425; ZPE= 1.111156512)						
H	0.4875079570878737	0.8936201241718594	0.2444128200352496	T			
H	0.2844564223163572	0.2140403184844773	0.3661838194854858	T			
H	0.8315683940905870	0.8540823183975955	0.2445246452618164	T			
H	0.7885190548925376	0.3768795019408857	0.2437049066901196	T			
H	0.5254825513358425	0.6238432697742574	0.2447072987760648	T			
C	0.2181603674302190	0.3346347629301075	0.3041295406825495	T			
O	0.1512951100287482	0.4402517524995581	0.3061760155085327	T			
O	0.2369640530319294	0.2925625628715844	0.3703958300894653	T			
F	0.0000000000000000	0.0000000000000000	0.0736297965049744	F			
e	0.0000000000000000	0.2500000000000000	0.0736297965049744	F			
F	0.0000000000000000	0.5000000000000000	0.0736297965049744	F			
e	0.0000000000000000	0.7500000000000000	0.0736297965049744	F			
F	0.3333334028720856	0.0000000000000000	0.0736297965049744	F			
e	0.3333334028720856	0.2500000000000000	0.0736297965049744	F			
F	0.3333334028720856	0.5000000000000000	0.0736297965049744	F			
e	0.3333334028720856	0.7500000000000000	0.0736297965049744	F			
F	0.6666666865348816	0.0000000000000000	0.0736297965049744	F			
e	0.6666666865348816	0.2500000000000000	0.0736297965049744	F			
F	0.6666666865348816	0.5000000000000000	0.0736297965049744	F			
e	0.6666666865348816	0.7500000000000000	0.0736297965049744	F			
F	0.0061873754540582	0.0039019939241761	0.2234222846460042	T			
e	0.0239290293391932	0.2416141365979782	0.2273111239404529	T			
F	0.0164949161505139	0.5046336739497355	0.2289101751258387	T			
e	0.9933186553884665	0.7464431461431748	0.2251923409428901	T			
F	0.3417683959752280	0.0122271624172269	0.2262568152264088	T			
e	0.3226635857781322	0.2537457080816334	0.2281462556668914	T			
F	0.3340738786007941	0.4836800969126447	0.2305672376868446	T			
e	0.3187504985409504	0.7567331143938062	0.2231193438275400	T			
F	0.6501726900910454	0.0084297657624190	0.2253374692313938	T			
e	0.6526883607473207	0.2480951690446329	0.2244653757665098	T			
F	0.6552873450654392	0.5010544841900094	0.2239719864480446	T			
e	0.6853509230794640	0.7373640045029537	0.2250193341051143	T			
F	0.1666667014360428	0.1250000000000000	0.0000000000000000	F			
e	0.1666667014360428	0.3750000000000000	0.0000000000000000	F			
F	0.1666667014360428	0.6250000000000000	0.0000000000000000	F			
e	0.1666667014360428	0.8750000000000000	0.0000000000000000	F			
F	0.5000001192092896	0.1250000000000000	0.0000000000000000	F			
e	0.5000001192092896	0.3750000000000000	0.0000000000000000	F			
F	0.5000001192092896	0.6250000000000000	0.0000000000000000	F			
e	0.5000001192092896	0.8750000000000000	0.0000000000000000	F			
F	0.8333333730697632	0.1250000000000000	0.0000000000000000	F			
e	0.8333333730697632	0.3750000000000000	0.0000000000000000	F			
F	0.8333333730697632	0.6250000000000000	0.0000000000000000	F			
e	0.8333333730697632	0.8750000000000000	0.0000000000000000	F			
F	0.1684450699238382	0.1235467274177547	0.1495031730162742	T			
e	0.1663656593283742	0.3752642169248611	0.1470931996297618	T			

F	0.1687753885234259	0.6246491063356655	0.1508564041603370	T		
e	0.1661007436928891	0.8764227902575922	0.1501578377651583	T		
F	0.4988454587904594	0.1283233844498092	0.1491527422172027	T		
e	0.4978793156344028	0.3738436737822610	0.1496296796869213	T		
F	0.4961081569940049	0.6249586141255654	0.1533828422955969	T		
e	0.4983860396646603	0.8741239807625861	0.1524838365623456	T		
F	0.8340009577967926	0.1259114214688237	0.1522690641781320	T		
e	0.8365581057844933	0.3745819645113219	0.1550704884321492	T		
F	0.8371686524527542	0.6207549460196957	0.1496652056103306	T		
e	0.8326034092754039	0.8766516445436671	0.1528289745146820	T		
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Table SX5. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the Fe(111) surface

	CO+H_2O (-445.627769; ZPE= 0.846961575)		**TS1’ (-444.882101; ZPE= 0.663456)**

H	0.1802940239839802	0.3992902202984180	0.3211865830850085	T	H	0.2454245649575941	0.3640525733459606	0.3308865423730872	T
H	0.2954823749729250	0.2590246636449791	0.3329014581265109	T	H	0.1645049076962452	0.2070305404654013	0.2439522381071831	T
C	0.9613525806309001	0.5180374861793365	0.2552209666758224	T	C	0.8948396674466642	0.5452620872356378	0.2623434531016237	T
O	0.2757640729417282	0.3448621965466331	0.3182741065677671	T	O	0.3182658133541050	0.3643664521051871	0.3085693345872160	T
O	0.0090386107628999	0.4926339577996722	0.3139681447093359	T	O	0.8992074662630868	0.5395117985925574	0.3249889544878199	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1111187095776227	0.1105399398330145	0.1314554493878538	T	e	0.1109242733771718	0.1107638971285389	0.1302931735731101	T
F	0.1127846247793072	0.4435279611781930	0.1301784244364575	T	F	0.1132670925435955	0.4439022420477267	0.1304052887007305	T
e	0.1111646710138601	0.7781556155328702	0.1313434774311721	T	e	0.1113445833375734	0.7773252498834391	0.1311509309191651	T
F	0.4446242895150272	0.1113448870848092	0.1311414643368352	T	F	0.4445065317092920	0.1120217885801544	0.1305498498912290	T
e	0.4445741583821539	0.4440035176116225	0.1308950909535965	T	e	0.4441506510148476	0.4439413459118313	0.1303430116849477	T
F	0.4444168961883841	0.7777456472607589	0.1312412032015657	T	F	0.4441132048535770	0.7781099861124681	0.1317982914246717	T
e	0.7763068618741289	0.1117324124724966	0.1313263966250083	T	e	0.7767875031206611	0.1118146595937858	0.1315748337041194	T
F	0.7774977021177668	0.4439523498024618	0.1312167911541064	T	F	0.7774899885840572	0.4431614574853036	0.1304924699687795	T
e	0.7774824996703682	0.7785760558466341	0.1313273952061905	T	e	0.7767224830454563	0.7791102521551309	0.1308945256472586	T
F	0.9987409706653855	0.0006572420171864	0.2100390365684519	T	F	0.9984820914753899	0.0002673417078545	0.2100541634893530	T
e	-0.0006217830977911	0.3300137563636066	0.2100725457558825	T	e	0.0066479189275047	0.3305602951209171	0.2117036998470379	T
F	-0.0005413685141733	0.6696547863106341	0.2102097243138514	T	F	0.9967497958510585	0.6662422816169858	0.2097904992844727	T
e	0.3339881007878404	-0.0003023984843396	0.2097336410620617	T	e	0.3313502181688524	0.0034120332318326	0.2104921891907239	T
F	0.3293299371970674	0.3350774034644501	0.2135763168529563	T	F	0.3303054462345568	0.3359201749827319	0.2150691006620344	T
e	0.3339237349388275	0.6654461382244328	0.2098900406437842	T	e	0.3347880780222128	0.6670264299267612	0.2098134732827071	T
F	0.6674433678235376	-0.0003205959816561	0.2102535534163937	T	F	0.6669781732732141	0.9988356457588307	0.2101301899729396	T
e	0.6672354884415153	0.3329008512478015	0.2102798389469496	T	e	0.6681535256844509	0.3328161807850942	0.2101754808611285	T
F	0.6695650942905427	0.6651890012550964	0.2100430438691770	T	F	0.6682662137979786	0.6661235533694214	0.2095160783404120	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2223816243853144	0.2216397708866461	0.1683699035212037	T	e	0.2231015124527879	0.2234881849985865	0.1693048974918908	T
F	0.2223825999701447	0.5554847379344151	0.1682463699505612	T	F	0.2224991139349065	0.5548744601436735	0.1696577502777276	T
e	0.2223735632231320	0.8885553171357419	0.1694498045788373	T	e	0.2216186670366953	0.8893721097179271	0.1690158024691526	T
F	0.5535471899231723	0.2233054259199213	0.1692974955758828	T	F	0.5533278147502164	0.2233236837712826	0.1694101433877856	T
e	0.5558819664878999	0.5554179731172700	0.1688609420873185	T	e	0.5559340065822725	0.5549129738025258	0.1683949102193188	T
F	0.5559340777051001	0.8886281078831687	0.1689796653803719	T	F	0.5541003597526792	0.8896585595503272	0.1688108769727016	T
e	0.8884650714439615	0.2219374297149504	0.1683452410417421	T	e	0.8900978922225824	0.2224051931325127	0.1689397789677447	T
F	0.8892957716610930	0.5553254419513362	0.1708141264558763	T	F	0.8894902608902072	0.5537107904092451	0.1698553889112488	T
e	0.8887578418376579	0.8892363775871326	0.1684373350350947	T	e	0.8889543052136663	0.8884075099654910	0.1685380036024011	T
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	CO+OH+H-t1 (-445.962472; ZPE= 0.683775521)					**TS2' (-445.041396; ZPE= 0.492596)**			
H	0.2161306005742842	0.5525614025163946	0.3061436225453362	T	H	0.2812252782959042	0.2045498134832330	0.2458136379135008	T
H	0.2436746567256490	0.2399628218673086	0.2494197104195009	T	H	0.2561658018748480	0.5864683152771385	0.2493083908924384	T
C	0.8824251187864489	0.5562751337455644	0.2619277039720024	T	C	0.8804850473380545	0.5584130414927905	0.2619212380434713	T
O	0.1833810479771636	0.5210049074261912	0.2688884198731820	T	O	0.1915385833428940	0.5199648801306859	0.2607186576301792	T
O	0.8783344441563419	0.5571705829452670	0.3246084760836470	T	O	0.8755981526596810	0.5595777967790758	0.3245811767368787	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F

e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1102621053527665	0.1115121246472772	0.1309484502633585	T	e	0.1099129010055325	0.1115038706457929	0.1307767730399100	T
F	0.1115878214902166	0.4443122310166370	0.1271303522591015	T	F	0.1108092194147291	0.4439074742179486	0.1265333249398265	T
e	0.1112964600075093	0.7777962443970889	0.1310026791856318	T	e	0.1110480606575643	0.7786525418814308	0.1309045805589469	T
F	0.4447946618342669	0.1118676734269690	0.1307690420343900	T	F	0.4446052529608900	0.1125725083551202	0.1302369599872700	T
e	0.4451285500470327	0.4436311184088231	0.1302063579750782	T	e	0.4465313083851358	0.4427128378093522	0.1297936367422066	T
F	0.4451338830992731	0.7784773481721462	0.1317107842789577	T	F	0.4446742110975166	0.7783032434323900	0.1322246681160360	T
e	0.7762255706534452	0.1108425050327388	0.1331516270057307	T	e	0.7762394491906474	0.1100746372144954	0.1336737153615073	T
F	0.7776419736857829	0.4433870809800953	0.1301570073734317	T	F	0.7775130399321991	0.4432758245002111	0.1299898752553287	T
e	0.7777560407238137	0.7787926104116434	0.1308369390816833	T	e	0.7781526095328878	0.7787254696912302	0.1307147152695223	T
F	0.9983654914699661	0.0005895306474422	0.2100653100684934	T	F	0.9982192237529680	1.0005884470172368	0.2104021488423759	T
e	0.0044817647548418	0.3332782756316677	0.2101080091076444	T	e	0.0016774170749365	0.3345628233426166	0.2097763837680419	T
F	0.0101072697096154	0.6535136699079312	0.2146719970622824	T	F	0.0159697050126401	0.6450529621602815	0.2159545739511073	T
e	0.3310458543996219	0.0057869439852940	0.2101535011486221	T	e	0.3302364752981488	0.0075845262347607	0.2106130919439824	T
F	0.3143405472902361	0.3396772930804919	0.2168890712276939	T	F	0.3042243792898624	0.3445882820835043	0.2202168959330643	T
e	0.3379511012762950	0.6705981740954802	0.2089434603947077	T	e	0.3384031990446776	0.6713389830054831	0.2111122991654802	T
F	0.6678049722893026	0.0007222600982959	0.2102226768677638	T	F	0.6688422858134101	0.0008740235827836	0.2100561296869407	T
e	0.6664583990276627	0.3322244704179025	0.2101104117743214	T	e	0.6671064305106416	0.3315666565311999	0.2103742015276150	T
F	0.6675974617145375	0.6663901276455981	0.2097938219622014	T	F	0.6653015691986565	0.6670313156104785	0.2099926047773081	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2220863593546587	0.2228995093506909	0.1670296036044732	T	e	0.2210918508238495	0.2234379851359742	0.1669029713566974	T
F	0.2254256938576369	0.5557063885206911	0.1694265468801585	T	F	0.2283379077977616	0.5570124425883631	0.1669760824600610	T
e	0.2216114665638937	0.8909615166720568	0.1689021532297703	T	e	0.2215310156971477	0.8913888766499651	0.1692790859001620	T
F	0.5483107220047798	0.2256207274646036	0.1711678123178739	T	F	0.5475486326280193	0.2260473490415860	0.1715647877423897	T
e	0.5570776476652562	0.5545200071077143	0.1682436491981723	T	e	0.5569366303156656	0.5540055875753761	0.1683440192680549	T
F	0.5556203275759478	0.8899144206386602	0.1689265594099156	T	F	0.5555310059349725	0.8905469348298438	0.1688937198475683	T
e	0.8893505697645377	0.2228910044061332	0.1691932709179918	T	e	0.8890769475060732	0.2224347027322600	0.1688543991428568	T
F	0.8896962931346074	0.5551805862355306	0.1693548349161112	T	F	0.8885698181753441	0.5557592139350720	0.1693036907351197	T
e	0.8917168915168724	0.8836096502943844	0.1704724591174207	T	e	0.8928964799602024	0.8816413306424333	0.1711534369820107	T
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	CO+O+2H (-445.863043; ZPE= 0.574560706)					**TS3’ (-444.194343; ZPE= 0.545474)**			
H	0.2443846283055777	0.1627725994448519	0.2487541733060596	T	H	0.2513314251464410	0.1663275746900270	0.2486800336423836	T
H	0.2647177586493161	0.6060806644542526	0.2477026009377454	T	H	0.2717641865927856	0.5861634375877168	0.2511946520029796	T
C	0.8739729136134285	0.5493671248274874	0.2613920919866776	T	C	0.9282701994493551	0.5182812196118108	0.2636023926337506	T
O	0.1587472925402563	0.4873627130257510	0.2261411292530930	T	O	0.0668575000842370	0.5460619584269422	0.2705547690511025	T
O	0.8676538811176132	0.5474649572242196	0.3239344727821650	T	O	0.9042924416699499	0.4913577937825291	0.3203988939514879	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1093068312868121	0.1110153537130382	0.1297747893558548	T	e	0.1104934046300607	0.1107025500587497	0.1305580331035195	T
F	0.1132068316989174	0.4453637418196205	0.1318792048954518	T	F	0.1115071952547903	0.4430515608744647	0.1284831826957226	T
e	0.1103700272976883	0.7794337363228555	0.1312516666985381	T	e	0.1106924615280384	0.7771351654040746	0.1321294991124856	T
F	0.4450491807379466	0.1110397219683569	0.1310119130934794	T	F	0.4456028235514011	0.1107582221526111	0.1308695635478449	T
e	0.4459995251383784	0.4432095403557857	0.1309388151035639	T	e	0.4422827617893877	0.4454331495356971	0.1315381690943168	T
F	0.4450265047277949	0.7785703372802761	0.1315182259224203	T	F	0.4449568885537974	0.7780219033339983	0.1308021338345847	T

e	0.7770156997701909	0.1102192402035402	0.1322671925461835	T	e	0.7767810721024312	0.1116775135373960	0.1311597232317767	T
F	0.7769783903711616	0.4423048165297991	0.1293950780112701	T	F	0.7778828137213324	0.4438303993637664	0.1301167439399653	T
e	0.7769638889154187	0.7791321213111846	0.1313537531805204	T	e	0.7759383782125993	0.7797023825831235	0.1309187409960332	T
F	0.9970619388868341	0.0009352094485274	0.2104286973949783	T	F	0.0003155275347572	0.9995482439536889	0.2099385531040196	T
e	0.0002998602447620	0.3308278631144411	0.2105854107532262	T	e	0.0027682663389022	0.3286385735893820	0.2114921349282107	T
F	-0.0001427870506706	0.6592728225391503	0.2105177730110669	T	F	0.9861404553796278	0.6731327719657479	0.2109099761464271	T
e	0.3312535763667729	0.0041722892252771	0.2112275625103637	T	e	0.3298859763093232	0.0065259174070297	0.2110763297713527	T
F	0.3272625395511611	0.3312629909533997	0.2108973915756881	T	F	0.3340925854801315	0.3264631371502823	0.2114080253623184	T
e	0.3423270878001287	0.6744785505152029	0.2112998237734436	T	e	0.3349795916695739	0.6667001822440058	0.2099763936682413	T
F	0.6667241218387163	0.0005537082098412	0.2107257833986321	T	F	0.6681176345649467	0.9984982224010285	0.2105870339707655	T
e	0.6669355858036179	0.3309544779120552	0.2103476469512753	T	e	0.6668691355233634	0.3325358613805597	0.2099512390853777	T
F	0.6626849214121202	0.6681730135929737	0.2108129149557378	T	F	0.6682420473770124	0.6661650097539137	0.2099264052543476	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2209995479264146	0.2189162880581899	0.1683887367736216	T	e	0.2217821858618877	0.2213124681502883	0.1680404860262722	T
F	0.2308314845238486	0.5640416297909959	0.1720711832403257	T	F	0.2194176321993268	0.5556981800783157	0.1760620708463412	T
e	0.2214405731845216	0.8913976504689087	0.1686691614862776	T	e	0.2236917535915662	0.8887227264455501	0.1688651003127910	T
F	0.5528684552438088	0.2225739339174387	0.1690412199383449	T	F	0.5546147824637613	0.2224982231703449	0.1686460523817346	T
e	0.5571095086540162	0.5543116348696732	0.1678121831722144	T	e	0.5560990163618520	0.5553855916107487	0.1684594091047087	T
F	0.5547093423192594	0.8898819387174054	0.1690168897870389	T	F	0.5539510240782752	0.8896405891092412	0.1692561603026266	T
e	0.8886549967260304	0.2217172901133814	0.1682864301808015	T	e	0.8890960479269856	0.2219221699172791	0.1682896045338937	T
F	0.8842334731726065	0.5541388043676687	0.1690873667073213	T	F	0.8873249779469260	0.5545425602511588	0.1687998254562765	T
e	0.8896855309112198	0.8858442266727483	0.1693048159475538	T	e	0.8878979070895817	0.8899012895725520	0.1679885765200022	T
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	CO_2+2H (-445.907402; ZPE= 0.581526514)					**TS4' (-444.844669; ZPE= 0.462799)**			
H	0.2611814942597917	0.1633145684967229	0.2484624298985213	T	H	0.2478639899526902	0.1619074318333306	0.2483861575941008	T
H	0.2608782486589711	0.5750631623188598	0.2484828112347911	T	H	0.2610082710296167	0.6091964451645031	0.2479000119017056	T
C	0.9305266935620879	0.5346475727244389	0.2714297312008446	T	C	0.7844532940073087	0.7205979241011001	0.2168358282975971	T
O	0.9516034227098810	0.6184454853653328	0.3020467991627729	T	O	0.1483217713881469	0.4938231589412554	0.2275870216278863	T
O	0.9519827794944540	0.4297124288621234	0.3021191783128880	T	O	0.8382986093674057	0.8314344968084247	0.2518094371657735	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1105473596180708	0.1112535240227705	0.1310774783863725	T	e	0.1097023887515325	0.1110620414887114	0.1292736914223866	T
F	0.1114137788559134	0.4442235017148719	0.1288113809288867	T	F	0.1114208811886667	0.4465242796860845	0.1332187314490582	T
e	0.1106251072623193	0.7780841058050190	0.1310640998954317	T	e	0.1108289433305972	0.7795923470476109	0.1308912757445558	T
F	0.4450841486405409	0.1108644498025315	0.1304128001168603	T	F	0.4463978762628398	0.1094363041152407	0.1326076885218482	T
e	0.4451084874299266	0.4440053330994709	0.1303945971798890	T	e	0.4453434684884923	0.4432187383267878	0.1319857827648444	T
F	0.4446544810595589	0.7776103660138632	0.1306397148213567	T	F	0.4454799920231802	0.7783377862397056	0.1309299629679937	T
e	0.7775258171063071	0.1112514407919238	0.1312270678184859	T	e	0.7764939914771344	0.1105292483029414	0.1321069508644839	T
F	0.7780542797428910	0.4446986241578354	0.1308549167352070	T	F	0.7775821799648175	0.4432707037346470	0.1309235816180153	T
e	0.7780907923378462	0.7771790306554611	0.1307926265222364	T	e	0.7783299880908543	0.7779511203390038	0.1228775020464673	T
F	-0.0000648840897673	-0.0000040281036172	0.2098195183299938	T	F	0.9991047973809706	0.0011656013995644	0.2098854561948621	T
e	-0.0027807130034192	0.3350429288250280	0.2136469119761875	T	e	-0.0014928035628370	0.3317780754487314	0.2093104396561690	T
F	-0.0026487078770895	0.6676955411961417	0.2136514941929298	T	F	0.9920417582415504	0.6650376857844909	0.2191244786931908	T
e	0.3300918015550874	0.0070607816911899	0.2103101016915065	T	e	0.3342180523988161	0.0037224383294882	0.2104837000825818	T
F	0.3302864375262579	0.3348056389899431	0.2102039256084677	T	F	0.3263808585555443	0.3332537595277861	0.2114094535393567	T
e	0.3299552272375673	0.6626758191953929	0.2103961616344936	T	e	0.3433555414491992	0.6728060906565374	0.2116633533815483	T
F	0.6669936627483000	-0.0002449841224907	0.2099495536414457	T	F	0.6718434283285684	-0.0031434594389519	0.2148050245330677	T

e	0.6669924151352017	0.3331400861089516	0.2099776664791829	T	e	0.6655189331688509	0.3330537855177664	0.2101852199247347	T
F	0.6718468622400450	0.6640193695710245	0.2098668349305660	T	F	0.6638074909087869	0.6653422309312579	0.2125465257637364	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2207155873737748	0.2236771155889173	0.1690147660235928	T	e	0.2212722488255620	0.2193799338122767	0.1681747648613184	T
F	0.2207937792614678	0.5554259492527477	0.1689772344056170	T	F	0.2268321793604029	0.5652866908167196	0.1724130045058705	T
e	0.2238375458655241	0.8880171287131912	0.1693099425246422	T	e	0.2229327536065381	0.8906699194780975	0.1686735449633272	T
F	0.5549785461471720	0.2224860265955317	0.1687212796170069	T	F	0.5543106813195819	0.2196809682939033	0.1699278335336114	T
e	0.5549148119369465	0.5562727409914012	0.1690792505612916	T	e	0.5570534995586660	0.5545695659733201	0.1675308782869135	T
F	0.5549779743295261	0.8886716607986267	0.1690248474927225	T	F	0.5611124385045817	0.8850369600695459	0.1708918292795261	T
e	0.8893095807148765	0.2227360393356728	0.1685118765176036	T	e	0.8880004194161286	0.2219396143817513	0.1682259135348552	T
F	0.8915782151926624	0.5541890267484827	0.1701120186657133	T	F	0.8849206233708501	0.5566331261757100	0.1686616083036659	T
e	0.8893198565988556	0.8879584006992570	0.1684370056410161	T	e	0.8911106712782785	0.8872043336537705	0.1700232012196467	T
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	C+2O+2H (-445.960563; ZPE= 0.490404842)					**TS5' (-444.96705; ZPE= 0.669729)**			
H	0.2411556228713248	0.1638629869665988	0.2484215991108357	T	H	0.9497987463720270	0.6453510765300002	0.3448362950559605	T
H	0.2564957798499694	0.6186974904988934	0.2477047250608651	T	H	0.2488997763970195	0.2503020340811940	0.2496036845205782	T
C	0.8188484186955284	0.6904808493379190	0.2231124007039998	T	C	0.8662400974479144	0.5681480529178886	0.2632378382946234	T
O	0.1574578142279210	0.4899886135987914	0.2297437939259379	T	O	0.9924960410158959	0.5902094958010241	0.3044123415151661	T
O	0.8328505678982415	0.0010401210027808	0.2374818673922565	T	O	0.7799511022393930	0.5997105473743174	0.3071273821184016	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1093025328403389	0.1101597859062578	0.1298967505821131	T	e	0.1108358242904813	0.1112746679566527	0.1309678563880469	T
F	0.1144093180135778	0.4436543453709159	0.1322193917073050	T	F	0.1122132510676777	0.4444415217059410	0.1295578856031469	T
e	0.1116040190911448	0.7794875195755366	0.1298313346747021	T	e	0.1112190164720870	0.7770290351779370	0.1315837527384012	T
F	0.4458235398132635	0.1103693567991454	0.1314468456742994	T	F	0.4450253743214705	0.1108387312706223	0.1306962405679651	T
e	0.4440731069821782	0.4474946775665958	0.1316290844445865	T	e	0.4448799968504464	0.4440841802734236	0.1310267137807511	T
F	0.4447962767721733	0.7803097891762820	0.1317144258865018	T	F	0.4454908894210983	0.7773364257622832	0.1313150200676070	T
e	0.7767150050373288	0.1110051967246554	0.1314747439927109	T	e	0.7778957569880246	0.1108099975055132	0.1317166184073754	T
F	0.7755873975626543	0.4431904046062256	0.1290870976934322	T	F	0.7774288163423566	0.4443415116113661	0.1302411676238495	T
e	0.7774834790186046	0.7753690206830280	0.1303544018695565	T	e	0.7779008764308590	0.7783851627196607	0.1299500942286057	T
F	0.9877540591585454	0.0061141755449943	0.2124939376733860	T	F	1.0001158292056325	0.9997846683924932	0.2095759622030764	T
e	0.0043535385551404	0.3248469311483534	0.2102130333688937	T	e	0.9995060045166524	0.3389557667366229	0.2107236932017545	T
F	0.9920250701486195	0.6494655159280017	0.2162527885121007	T	F	0.0027574492234934	0.6625576598257572	0.2146933829928366	T
e	0.3306901564917245	0.0038994860324660	0.2109224337951050	T	e	0.3327957425456425	0.0031421935391256	0.2097670281719425	T
F	0.3264583501787713	0.3325219498754752	0.2115900920586725	T	F	0.3290675175348053	0.3294742988449310	0.2110732614122630	T
e	0.3438872052041830	0.6768856944587581	0.2125984756478827	T	e	0.3340633185277554	0.6657460238481666	0.2095014635029774	T
F	0.6674140146661183	0.0137559079902579	0.2130451087219064	T	F	0.6674089157352366	0.9994047141377236	0.2101417814156789	T
e	0.6624338665530992	0.3381568738411719	0.2094532674745492	T	e	0.6664263894271374	0.3331789924280775	0.2099206691112780	T
F	0.6721412380370485	0.6705922336418414	0.2142256646760411	T	F	0.6674180953647975	0.6664798068065481	0.2131357774367259	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F

e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2227294381155568	0.2180185508747296	0.1677088238429449	T	e	0.2210448151560332	0.2228449700803043	0.1688928650956784	T
F	0.2278778989216854	0.5667779738566181	0.1729665324273751	T	F	0.2224727779833360	0.5542901107993063	0.1686763070687731	T
e	0.2186135566137559	0.8926455636924834	0.1694447178821129	T	e	0.2230330217932489	0.8890468611409674	0.1689458433416863	T
F	0.5500696546124300	0.2266779598342466	0.1677039612418010	T	F	0.5540466308537992	0.2227435536671495	0.1692825030736936	T
e	0.5580122943283168	0.5585431616665456	0.1680151256956947	T	e	0.5563679924399189	0.5558745533694264	0.1686357321150815	T
F	0.5568045026088934	0.8910355512565764	0.1710840034519009	T	F	0.5563200307685955	0.8881096477334709	0.1686863282028561	T
e	0.8876405518586443	0.2241208416091963	0.1676875086460216	T	e	0.8896349533275555	0.2234193915027856	0.1692881788953295	T
F	0.8888507165082759	0.5437535658734842	0.1659959068673404	T	F	0.8903169735551170	0.5550461072743228	0.1675648394686567	T
e	0.8965580716819717	0.8704430805645175	0.1706007015520286	T	e	0.8902861902631460	0.8860788957102371	0.1692411641558120	T
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	COOH+H (-445.20797; ZPE= 0.734589228)					**TS6' (-444.069883; ZPE= 0.542812)**			
H	0.2504032407863626	0.2500651938968528	0.2499826247860802	T	H	0.2473970608857684	0.2527105045713764	0.2496217262285159	T
H	0.9203023495734149	0.6384466721837314	0.3505878692538769	T	H	0.9333896375629944	0.7273434355584190	0.2875914557787505	T
C	0.8695841545874861	0.5765781805924985	0.2678024659746847	T	C	0.8701886964156387	0.5847292910611696	0.2690484511550236	T
O	0.9622773504051455	0.5929619552469731	0.3069032229267166	T	O	0.9556223565480836	0.6103566312576584	0.3018197484328788	T
O	0.7670011443370196	0.6081552570917540	0.3025659342556469	T	O	0.7662005390382842	0.6114291399836825	0.3021182634190626	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1108769166470515	0.1110573191794773	0.1308694806656518	T	e	0.1109972745465468	0.1112240702429124	0.1305659390881258	T
F	0.1108424464422506	0.4448351896000971	0.1303489492436095	T	F	0.1111443989145313	0.4438791741831669	0.1294506759130563	T
e	0.1112461509834337	0.7771696024355659	0.1315452587571856	T	e	0.1104811884594198	0.7774698624935966	0.1315454007057440	T
F	0.4449184101656376	0.1108591693897627	0.1307293408323265	T	F	0.4448139413710329	0.1104723957447671	0.1309289881402316	T
e	0.4448142821416236	0.4438988731499405	0.1310599007651854	T	e	0.4452402573968884	0.4440347350922815	0.1310159851816586	T
F	0.4450658940769497	0.7773036385325833	0.1311903886006157	T	F	0.4454021393231364	0.7771020659555675	0.1311742040096240	T
e	0.7773647165709753	0.1114579632649978	0.1314356248259381	T	e	0.7785862315880016	0.1094217627319510	0.1321457464264971	T
F	0.7775666090283148	0.4445027761451892	0.1302472078349683	T	F	0.7778066782182342	0.4445838073108474	0.1302724403880630	T
e	0.7774720394772636	0.7783257572740413	0.1300408260608610	T	e	0.7778627670114350	0.7776577850281513	0.1299890648653507	T
F	0.9994755082078663	0.0000217517724603	0.2096312192755405	T	F	0.0000199401605591	0.0000673147595116	0.2094709248022817	T
e	-0.0005018271325568	0.3373285559348385	0.2104117456690208	T	e	0.0001625205296843	0.3379128692935213	0.2107933890338948	T
F	0.0010505940468833	0.6665560460894232	0.2121271610986594	T	F	0.0029453496900690	0.6617851552830712	0.2101869114130455	T
e	0.3320972664074531	0.0027063007255842	0.2098385656521114	T	e	0.3325477945735700	0.0024504417234772	0.2097919612133101	T
F	0.3292736988921288	0.3294662884277763	0.2110988652159963	T	F	0.3292314828707861	0.3299218915592874	0.2108354214246547	T
e	0.3333292887463309	0.6651438763127256	0.2096169165227366	T	e	0.3338192364044830	0.6659534900178795	0.2094552298017562	T
F	0.6670435113496397	-0.0006364918266980	0.2102284343444527	T	F	0.6647483420686551	0.9999619220332936	0.2103588543276952	T
e	0.6664845444988697	0.3332841890412851	0.2099363454511113	T	e	0.6668590908455043	0.3323641489083521	0.2097064169343025	T
F	0.6660708574367841	0.6659286013789889	0.2126782340180371	T	F	0.6694379244142036	0.6634215758107417	0.2137730064277054	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F

e	0.2211021728387570	0.2227537854519180	0.1692646794461149	T	e	0.2210771151686724	0.2225770871688762	0.1691285018995244	T
F	0.2225213121064903	0.5539450841263034	0.1686950051325894	T	F	0.2226926498944162	0.5540530290643627	0.1683586692818265	T
e	0.2228067298226914	0.8888124616247618	0.1690268529557085	T	e	0.2227060076348432	0.8891540905550034	0.1686499030647536	T
F	0.5540198164410193	0.2227134023918096	0.1693817845279424	T	F	0.5542822414098377	0.2222804312316502	0.1691602977906426	T
e	0.5560217730140899	0.5558179360091813	0.1684165236597433	T	e	0.5567370504726279	0.5557254834658579	0.1687237145141824	T
F	0.5559950867451285	0.8879203843555692	0.1686817468169863	T	F	0.5564072784447825	0.8867652544589223	0.1688154072130721	T
e	0.8893795117646703	0.2231817836255602	0.1690410240477191	T	e	0.8897079623622443	0.2232480477397679	0.1690441150771647	T
F	0.8892619298046865	0.5551757254589829	0.1691818384090810	T	F	0.8892317300735978	0.5547966751734159	0.1690211789517493	T
e	0.8891043709697034	0.8880601270933530	0.1686226904531599	T	e	0.8904431779373894	0.8839973442262979	0.1725187346571685	T
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	TS7' (-445.080877; ZPE= 0.685209)					**HCO+OH (-445.229609; ZPE= 0.755589641)**			
H	0.5894213638962247	0.5218457797771777	0.3069758428796180	T	H	0.2648127457607286	0.4401441305483950	0.2946769684993664	T
H	0.3905070437174379	0.3737787709475804	0.2765352531703864	T	H	0.6596078069484845	0.4790471762665581	0.3001513018407609	T
C	0.2991749136509459	0.4923530241948407	0.2594459555697460	T	C	0.2618541258289700	0.5246751865017245	0.2623988662570067	T
O	0.5573668201793586	0.4904417242702488	0.2694912686526179	T	O	0.2946439929423703	0.5927356816540988	0.2998784167124107	T
O	0.2949017534200187	0.5701784997638801	0.3047632205061842	T	O	0.5978264812604129	0.4671153088221122	0.2727583049720124	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1111412889429594	0.1098211851356820	0.1325233836462152	T	e	0.1116412150700696	0.1109748953152667	0.1315101720569327	T
F	0.1096937343488866	0.4434218637709049	0.1296177072051753	T	F	0.1104402062206650	0.4436081234109363	0.1299469752786882	T
e	0.1108354778604560	0.7783753022370050	0.1303528300264535	T	e	0.1104916969697571	0.7781400223006657	0.1304992886447618	T
F	0.4437763554148034	0.1119983258324174	0.1305915623588879	T	F	0.4429718870958269	0.1118677048151123	0.1306374203973445	T
e	0.4453992411400894	0.4446223742252330	0.1272286804114417	T	e	0.4461850567392239	0.4448071310529551	0.1283996179243720	T
F	0.4437759027883331	0.7775611820161424	0.1306534293105878	T	F	0.4449090358562310	0.7754762794713301	0.1322111719319962	T
e	0.7754762317454860	0.1127866553323212	0.1324039703486331	T	e	0.7777234987757535	0.1110212812241380	0.1318213780595305	T
F	0.7769280231118677	0.4448236331342226	0.1300813587540379	T	F	0.7771835827036214	0.4448231082167205	0.1293702233968559	T
e	0.7780277602969319	0.7778968479876248	0.1307796382733109	T	e	0.7779626937099468	0.7780991452672168	0.1310322250942626	T
F	0.9990182633081404	0.0013127425614028	0.2096570818057196	T	F	0.9988238360885201	0.0004983003872332	0.2100296903458800	T
e	0.0012460457813779	0.3311193028935005	0.2099447279286620	T	e	0.9998074318652208	0.3326182566200247	0.2099309710303984	T
F	0.0005861264233245	0.6657298085424248	0.2085580750242752	T	F	0.0061800913326812	0.6622919906952069	0.2095623652836035	T
e	0.3310428923641359	0.0004184478143840	0.2095908583274136	T	e	0.3314819574635997	0.0007725288877832	0.2097463247517478	T
F	0.3241197873965938	0.3433641731304115	0.2106591395026984	T	F	0.3319409569305650	0.3380961853077847	0.2117073450885858	T
e	0.3288681586832594	0.6582548738155420	0.2174300048021693	T	e	0.3255126523118235	0.6687343444149650	0.2142481633439424	T
F	0.6669236501670225	0.0010271079001027	0.2094004376647099	T	F	0.6675628841522325	0.0026370830479479	0.2096180759097063	T
e	0.6658478625055939	0.3331445993664932	0.2138988098625514	T	e	0.6736935874357218	0.3147095291293540	0.2151310217345654	T
F	0.6692649132043182	0.6716239147539435	0.2084282048296444	T	F	0.6686956251850009	0.6736481920839718	0.2089159110527306	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2232222847477946	0.2233539605761155	0.1688696309888985	T	e	0.2230646610524354	0.2235321492390548	0.1693877043835544	T
F	0.2210453404483297	0.5556402021710207	0.1662742412911260	T	F	0.2225839940974885	0.5542405466933411	0.1671181375503533	T
e	0.2241472466503659	0.8833379837238563	0.1700870044157054	T	e	0.2227392779485055	0.8867682606512044	0.1688899642978579	T
F	0.5501805730231683	0.2259802638964966	0.1714646904546380	T	F	0.5526454645069251	0.2231317894246971	0.1677227952907517	T
e	0.5541195142354074	0.5578334334529481	0.1719132994646571	T	e	0.5566018629402533	0.5528901011842309	0.1764638070033300	T
F	0.5542576342232497	0.8906432989424800	0.1682502070495627	T	F	0.5544016430542317	0.8909811556946644	0.1683238283794976	T
e	0.8859885817807762	0.2238801803874680	0.1690301409234081	T	e	0.8887089535290730	0.2223475814043851	0.1682479309112052	T
F	0.8894568054560612	0.5543345889173620	0.1681837317041392	T	F	0.8894725267774571	0.5551927677941448	0.1684668519521242	T
e	0.8890640979988660	0.8888226145869988	0.1685519226367300	T	e	0.8899017558407566	0.8872263201288418	0.1690261294665525	T
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	CO+OH+H-t2 (-446.023419; ZPE= 0.697901768)					**TS8′ (-444.339748; ZPE= 0.562099)**			
H	0.2240822517150723	0.5384813245187927	0.3064707858368445	T	H	0.8013330602298809	0.3602944240150588	0.2652097353397060	T
H	0.9317385403958479	0.2349571230578884	0.2490484179741849	T	H	0.2179571130049255	0.5472688682344072	0.3061184965356569	T
C	0.8859501887082639	0.5535160192180855	0.2618631985034459	T	C	0.8302333343348245	0.5150590448402035	0.2440208690029834	T
O	0.1907689395243072	0.5094267245473573	0.2682438502705191	T	O	0.8300504895809392	0.4456195643969902	0.2952781271304218	T
O	0.8828737489638974	0.5539817681167719	0.3245657487817442	T	O	0.1851655075537646	0.5154335421903192	0.2689946782469458	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F

e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1112269701925912	0.1111440937160803	0.1302474108175051	T	e	0.1088539168215690	0.1131565046663153	0.1315903566036219	T
F	0.1121080980886889	0.4431934255248484	0.1271675106182318	T	F	0.1114768425374935	0.4440570360066608	0.1273424332071524	T
e	0.1111909227195364	0.7782398559841176	0.1307756612655370	T	e	0.1107093915218210	0.7785004216089578	0.1302214899558496	T
F	0.4436620604488370	0.1120674949577804	0.1317307657783330	T	F	0.4445912698328183	0.1126610466627533	0.1321653624691977	T
e	0.4451065989840343	0.4439093496807593	0.1299363051208628	T	e	0.4458562414366419	0.4440017604387507	0.1301249119309331	T
F	0.4451638902013638	0.7784349354984680	0.1315016658414171	T	F	0.4447196732779262	0.7783276517726078	0.1314839022861582	T
e	0.7764668450190608	0.1105457815183270	0.1324115516319989	T	e	0.7764535883309259	0.1115677813516159	0.1333355133952625	T
F	0.7771895681933478	0.4436940440862753	0.1300778561644772	T	F	0.7780198565473972	0.4448799661063780	0.1303265102196397	T
e	0.7779663371906039	0.7785094602992666	0.1308900215126316	T	e	0.7772794702652155	0.7789177849665109	0.1307047337853255	T
F	0.9978931226632107	0.0027008328181629	0.2102860512553604	T	F	0.9973588625185177	0.0013252275019592	0.2095659724919461	T
e	-0.0055373661670144	0.3317630109778634	0.2116501150181462	T	e	0.0016178944810975	0.3346941507726421	0.2114884077161008	T
F	0.0103321110024919	0.6534007886141010	0.2137155092048159	T	F	0.0119098395281190	0.6537646860112490	0.2135398770759606	T
e	0.3343741101507021	0.0009256050688282	0.2099112697701821	T	e	0.3337829451564231	0.0011644417611087	0.2094053159582239	T
F	0.3194682421081657	0.3416895327682123	0.2142248787471996	T	F	0.3193630276588107	0.3436285006107142	0.2147477837038115	T
e	0.3381515190578626	0.6715820482305223	0.2091529244673135	T	e	0.3383545910466434	0.6712724958024682	0.2090644716150007	T
F	0.6676235273365329	0.0003695550090166	0.2100862504274366	T	F	0.6662771014460219	0.0007013563348616	0.2099362029657978	T
e	0.6687244396447399	0.3318235783275834	0.2100107203939542	T	e	0.6691360873801284	0.3351406858774771	0.2141110675978078	T
F	0.6687834139918992	0.6650908055020101	0.2100236636465593	T	F	0.6683406202162923	0.6668829416047588	0.2116739899129763	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2197958534266182	0.2235054354054898	0.1684830061202110	T	e	0.2210999391849466	0.2240384685997693	0.1678721040034252	T
F	0.2249114362932516	0.5572790387395338	0.1690128298820508	T	F	0.2255077633571610	0.5571495336613735	0.1686653986357763	T
e	0.2212946441637559	0.8908646329453652	0.1685939710051629	T	e	0.2207787462040674	0.8908180643938667	0.1684112067800205	T
F	0.5505128881514441	0.2249604269772522	0.1705166664086534	T	F	0.5508868435386458	0.2264541042288886	0.1712735566841602	T
e	0.5568106793272170	0.5547023750987634	0.1681576191708586	T	e	0.5579241785475638	0.5545498384616760	0.1691056431887635	T
F	0.5566092836542026	0.8887407305008992	0.1688133559920091	T	F	0.5565907592025714	0.8883007460622411	0.1684840858292912	T
e	0.8891367352108027	0.2221074048796175	0.1689645252928707	T	e	0.8857917958946061	0.2260101823898754	0.1723106711633637	T
F	0.8902015623378015	0.5539446421741102	0.1692630070123259	T	F	0.8920546306371117	0.5578696480403151	0.1681086347825817	T
e	0.8919791625305590	0.8842886538393312	0.1705641350234172	T	e	0.8905570868019262	0.8844446728653436	0.1703110412639523	T
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	COH+OH (-444.740679; ZPE= 0.787938081)		
H	0.7643032954205196 0.4241713358164461 0.3015451544386392 T		
H	0.2169468582830051 0.5491318035755440 0.3061480124808504 T		
C	0.8227126770160977 0.4909620455365846 0.2263530770351556 T		
O	0.8123364512633575 0.4709652099992130 0.2977768814137137 T		
O	0.1836946041498586 0.5170610021514893 0.2693600481472269 T		
F	0.2222221940755844 0.2222221940755844 0.0428677015006542 F		
e	0.2222221940755844 0.5555555820465088 0.0428677015006542 F		
F	0.2222221940755844 0.8888888955116272 0.0428677015006542 F		
e	0.5555555820465088 0.2222221940755844 0.0428677015006542 F		
F	0.5555555820465088 0.5555555820465088 0.0428677015006542 F		
e	0.5555555820465088 0.8888888955116272 0.0428677015006542 F		
F	0.8888888955116272 0.2222221940755844 0.0428677015006542 F		
e	0.8888888955116272 0.5555555820465088 0.0428677015006542 F		
F	0.8888888955116272 0.8888888955116272 0.0428677015006542 F		
e	0.1100727562627844 0.1120218906012968 0.1313237346640975 T		
F	0.1128381976635940 0.4431993890647695 0.1277803643245816 T		
e	0.1106020626202688 0.7785671320996990 0.1301284384616757 T		
F	0.4433096883735710 0.1114223768202007 0.1314895554523937 T		

e	0.4445852698917160	0.4438002157458563	0.1300756580410861	T		
F	0.4448770668073136	0.7778698262997222	0.1316975802201986	T		
e	0.7765225782611072	0.1095470141209068	0.1326585756527081	T		
F	0.7784128886901500	0.4442263505228666	0.1355509032447701	T		
e	0.7773269656623840	0.7793980295207317	0.1314563457375184	T		
F	0.9978309758856667	0.0008494688600286	0.2101615896974561	T		
e	0.0004397251789484	0.3349617785332730	0.2098098068210011	T		
F	0.0119292579861761	0.6535646763829804	0.2147497208687370	T		
e	0.3335812996175323	0.0010060289256205	0.2098695652990396	T		
F	0.3183387178503246	0.3433353605333494	0.2151962006686330	T		
e	0.3382838632069785	0.6712913878946215	0.2094856433792554	T		
F	0.6646319661678696	0.0002996843357913	0.2102072310713431	T		
e	0.6617343975051431	0.3277486976064868	0.2093701533268194	T		
F	0.6677337115963298	0.6669978665169874	0.2097750316550372	T		
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F		
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F		
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F		
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F		
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F		
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F		
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F		
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F		
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F		
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F		
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F		
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F		
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F		
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F		
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F		
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F		
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F		
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F		
e	0.2213689926300944	0.2233049262320910	0.1678346026283420	T		
F	0.2250021070789258	0.5575029360596124	0.1688779095085906	T		
e	0.2209599348084056	0.8905879034724765	0.1685985062996564	T		
F	0.5484584659452030	0.2236716834865876	0.1696315408545798	T		
e	0.5560016878836587	0.5538083266918208	0.1692728956808079	T		
F	0.5559762073878826	0.8884724672774185	0.1681847299414077	T		
e	0.8877386213260509	0.2213697366270484	0.1696719820273028	T		
F	0.8953759154894818	0.5613413641815677	0.1679272897594430	T		
e	0.8909094204363762	0.8838053627779157	0.1709545100966054	T		
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Table SX6. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the 3O pre-covered Fe(111) surface

	3O+CO+H_2O (-469.677551; ZPE= 0.995699112)					**TS9' (-467.7613718; ZPE= 0.899803)**			
H	0.6385716026954383	0.5841093806248502	0.3366266159515903	T	H	0.6455542813719588	0.5858445662404421	0.3374671562754834	T
H	0.7559817370857134	0.4798130042355578	0.2901450819305951	T	H	0.7595713081355193	0.4792940971254969	0.2899746976990435	T
C	0.2283808929644422	0.8851405250330473	0.2631407897576784	T	C	0.3493351883061639	0.8183067624502807	0.2324120309151487	T
O	0.4940401920287052	0.3423932482725612	0.2339045621966459	T	O	0.4954161733514173	0.3426783601695927	0.2332709243967673	T
O	0.1619696869346244	0.3440960514305823	0.2340191808955693	T	O	0.1645032544861841	0.3420838699833557	0.2326291094440971	T
O	0.8271643872289252	0.3447313440863207	0.2421697839726878	T	O	0.8273179604102552	0.3441559820038345	0.2413850095088375	T
O	0.7113775632936953	0.5717849112693442	0.3082862089615377	T	O	0.7177392538385343	0.5711456916772080	0.3078084201504284	T
O	0.2334161622166366	0.8823472001526155	0.3258896129813904	T	O	0.1985834756347390	0.9464927162862647	0.2584986040423642	T
F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1099958141679937	0.1120431915751480	0.1304303029701300	T	e	0.1101662649430817	0.1131900843850728	0.1279898916194446	T
F	0.1104639714752415	0.4449303222608326	0.1325324258663252	T	F	0.1121056148981177	0.4436300573404404	0.1334272441890663	T
e	0.1097049976580074	0.7789932240355704	0.1295204209376721	T	e	0.1096371603020606	0.7778270973021515	0.1289380500866816	T
F	0.4449517844646213	0.1097838631692572	0.1301398527559996	T	F	0.4449552282519496	0.1095878166847085	0.1301382039593944	T
e	0.4441904855049489	0.4443108910840645	0.1340025622835444	T	e	0.4442830910702625	0.4448594055141981	0.1339232686946735	T
F	0.4451612153251293	0.7785974791205731	0.1294693801921903	T	F	0.4432942391226020	0.7802224523627750	0.1302445878085071	T
e	0.7784691927318239	0.1112179404549520	0.1302919070755203	T	e	0.7798510071546521	0.1105870851549308	0.1303946411355518	T
F	0.7776138588163539	0.4458308631693467	0.1304922242008195	T	F	0.7784743517992999	0.4447787263469415	0.1308158559323750	T

e	0.7769672495459402	0.7790162846984576	0.1297425891518377	T	e	0.7759255670097157	0.7808644281061796	0.1310371283240647	T
F	0.0035861769846649	-0.0049164502182181	0.2104170534551434	T	F	0.0136634582606204	0.9934989187600701	0.2150922162742748	T
e	0.9981289051370774	0.3387573766282228	0.2176888733699061	T	e	0.9996405618252957	0.3373709905748780	0.2168573913371133	T
F	0.9972865283646931	0.6723447795726611	0.2097802720614586	T	F	0.9977587463648044	0.6721797366641840	0.2094860122933986	T
e	0.3355413145927815	0.9944862223932068	0.2105369051913911	T	e	0.3300908657241141	0.9875506079243556	0.2171334183976077	T
F	0.3294086908562399	0.3404788063377976	0.2169874369657711	T	F	0.3309625668984950	0.3407795697270865	0.2166644163767426	T
e	0.3313147751776542	0.6695378840137701	0.2097276709434696	T	e	0.3375251039498122	0.6707411272319919	0.2123702792906544	T
F	0.6712035265643106	0.9913994864930765	0.2108759330139182	T	F	0.6716436487333296	0.9914455169517642	0.2101273571478146	T
e	0.6624194354194538	0.3386686608169189	0.2169836076143554	T	e	0.6627804835884978	0.3397327566435105	0.2166525803057145	T
F	0.6657299017246555	0.6678197912851953	0.2127118207219111	T	F	0.6704934114685177	0.6677137573023592	0.2122620382637755	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F	e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F	F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F	e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F	F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F	e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F	F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F	e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F	F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F	e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F	F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F	e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F	F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F	e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F	F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F	e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F	F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F	e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F	F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2268946263353567	0.2132645276882079	0.1686390719111375	T	e	0.2293626282088660	0.2082566505817424	0.1694253510187676	T
F	0.2195950705652902	0.5596333209385962	0.1672392386720850	T	F	0.2203681823180458	0.5603368610273460	0.1676769273749142	T
e	0.2222725862275255	0.8889467922094549	0.1703416752825652	T	e	0.2161327242776986	0.8888708627609262	0.1620028213976764	T
F	0.5611543788671651	0.2106207999470932	0.1690338652557162	T	F	0.5618657768834601	0.2107216459307440	0.1685813558453227	T
e	0.5542641779024199	0.5588891253371938	0.1668735532283938	T	e	0.5549667780393459	0.5596944213012919	0.1672515486082063	T
F	0.5559566088443361	0.8880519686058728	0.1679997590939739	T	F	0.5511064585675285	0.8905776723016231	0.1699874115162363	T
e	0.8905550582359832	0.2184413321512731	0.1704867286921153	T	e	0.8934180909796644	0.2153573020880649	0.1710154572038363	T
F	0.8868236221771989	0.5593257972689029	0.1672110452276467	T	F	0.8876242269809099	0.5587746027895872	0.1666677204890490	T
e	0.8887090095487135	0.8898357405442676	0.1675561961673521	T	e	0.8912728302829812	0.8916300943798724	0.1688835075903007	T
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	3O+C+O+H_2O (-469.3747092; ZPE= 0.905607842)					**TS10' (-469.567458; ZPE= 0.874684)**			
H	0.6624734094010334	0.5776431992946918	0.3435557565316735	T	H	0.6624137393423642	0.5781315677372165	0.3376595800694590	T
H	0.7687388964935188	0.4741993937677756	0.2913686810882817	T	H	0.7751504899990901	0.4424661857418065	0.2782896109379851	T
C	0.4707291646530954	0.7679314292169506	0.2188597715449532	T	C	0.2255022090828385	0.8871356089087250	0.2627709363115848	T
O	0.4939953733313535	0.3464131528864776	0.2323031507268971	T	O	0.4920172517289680	0.3416405866581496	0.2340856525459258	T
O	0.1640342590650181	0.3417742074503549	0.2329165611143998	T	O	0.1653427480310473	0.3427997124802872	0.2345106349575673	T
O	0.8288196821781247	0.3453223361203276	0.2412696233452936	T	O	0.8266947326017773	0.3383535206429005	0.2535292871641645	T
O	0.7313896303313308	0.5642671130988431	0.3116419565596228	T	O	0.7216817586688310	0.5579993861297635	0.2986677674540926	T
O	0.1660916781974819	-0.0117819224347012	0.2438159542238863	T	O	0.2288813540576981	0.8850642609219931	0.3255160254163618	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221940755844	0.2222221940755844	0.0428677015006542	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221940755844	0.5555555820465088	0.0428677015006542	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221940755844	0.8888888955116272	0.0428677015006542	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555820465088	0.2222221940755844	0.0428677015006542	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555820465088	0.5555555820465088	0.0428677015006542	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555820465088	0.8888888955116272	0.0428677015006542	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888955116272	0.2222221940755844	0.0428677015006542	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888955116272	0.5555555820465088	0.0428677015006542	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888955116272	0.8888888955116272	0.0428677015006542	F
e	0.1097654245156872	0.1133236714429445	0.1289212365952334	T	e	0.1086010760149940	0.1130736293732426	0.1306376467926748	T
F	0.1126415143181549	0.4449117009207966	0.1346675616580023	T	F	0.1105487694256727	0.4447757143857934	0.1322832981602225	T
e	0.1078048627458593	0.7790403472954062	0.1285614540178572	T	e	0.1096293183200843	0.7790153505278917	0.1294356743244972	T
F	0.4468921635481347	0.1064799121887987	0.1310895978400698	T	F	0.4454366792636977	0.1086975822361131	0.1301971373593721	T
e	0.4444598909746669	0.4460764550881174	0.1342511455135897	T	e	0.4443868265218782	0.4442212796510771	0.1339467037906513	T
F	0.4436469110571826	0.7794299105295154	0.1209682859565413	T	F	0.4453726473769712	0.7781197214585689	0.1295329260479857	T
e	0.7787403847744663	0.1104527584839883	0.1303475153589407	T	e	0.7790127565715254	0.1121640032094588	0.1305177915425538	T
F	0.7768097862509469	0.4472201736122183	0.1304954552243111	T	F	0.7771479989191867	0.4469578297666965	0.1273207700509627	T
e	0.7743290109874887	0.7810073775485575	0.1311853120447972	T	e	0.7771801168317377	0.7785802228457105	0.1298422367002025	T
F	0.0060288596333929	0.0015742775239551	0.2133554546193476	T	F	0.0021085976270505	0.9979383218451019	0.2097746659185226	T
e	0.9985031132046565	0.3404612345158654	0.2160261747415681	T	e	1.0010484107061179	0.3373184667159032	0.2182867484436286	T
F	0.9968716169650602	0.6720369333674072	0.2090832145359081	T	F	0.9973683245446111	0.6727325726493714	0.2096711236895876	T
e	0.3370225470890975	0.9643596904628650	0.2188739610136679	T	e	0.3352472144150579	0.9940599451648837	0.2102862265452476	T
F	0.3308839559436519	0.3399358837130018	0.2159011483666343	T	F	0.3296003864580316	0.3400747989738574	0.2170036768487461	T
e	0.3468691640329453	0.6848983405846136	0.2144654210093844	T	e	0.3308694163771762	0.6702049892263963	0.2094990201408626	T

F	0.6679473440977393	0.9893063244868429	0.2100875893589950	T
e	0.6607920913791137	0.3439050074189578	0.2161664306073859	T
F	0.6593377682726493	0.6716227353548395	0.2193195952110454	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2329449040930205	0.2039988334003655	0.1713433575144941	T
F	0.2230954651815919	0.5642663203156890	0.1698371959557826	T
e	0.2194282826695268	0.8837592837604897	0.1639995277598551	T
F	0.5610888632539134	0.2108881318611852	0.1690685903422934	T
e	0.5538991340514110	0.5660101509858675	0.1684311352029778	T
F	0.5505049976674036	0.8830928927684265	0.1715055222056837	T
e	0.8891245588146616	0.2201513875385936	0.1694014249358486	T
F	0.8843495857761053	0.5613561210470476	0.1673232725943481	T
e	0.8889369401960877	0.8914305968344520	0.1689240262545872	T
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F	0.6718869774745512	0.9909859377752210	0.2107005233638487	T
e	0.6609379538149770	0.3369316271354205	0.2181163104566559	T
F	0.6694624847163655	0.6612549725456019	0.2135333590177776	T
e	0.1111110970377922	0.1111110970377922	0.0000000000000000	F
F	0.1111110970377922	0.4444443881511688	0.0000000000000000	F
e	0.1111110970377922	0.7777777910232544	0.0000000000000000	F
F	0.4444443881511688	0.1111110970377922	0.0000000000000000	F
e	0.4444443881511688	0.4444443881511688	0.0000000000000000	F
F	0.4444443881511688	0.7777777910232544	0.0000000000000000	F
e	0.7777777910232544	0.1111110970377922	0.0000000000000000	F
F	0.7777777910232544	0.4444443881511688	0.0000000000000000	F
e	0.7777777910232544	0.7777777910232544	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857352986931801	F
e	0.0000000000000000	0.3333333134651184	0.0857352986931801	F
F	0.0000000000000000	0.6666666865348816	0.0857352986931801	F
e	0.3333333134651184	0.0000000000000000	0.0857352986931801	F
F	0.3333333134651184	0.3333333134651184	0.0857352986931801	F
e	0.3333333134651184	0.6666666865348816	0.0857352986931801	F
F	0.6666666865348816	0.0000000000000000	0.0857352986931801	F
e	0.6666666865348816	0.3333333134651184	0.0857352986931801	F
F	0.6666666865348816	0.6666666865348816	0.0857352986931801	F
e	0.2270102081610660	0.2129883050749811	0.1684930921527296	T
F	0.2195955276487051	0.5596277166584096	0.1672963092196398	T
e	0.2215752871965602	0.8894238636949245	0.1699707445971835	T
F	0.5613039798319249	0.2102571463932859	0.1688939065008091	T
e	0.5553494682043957	0.5575634463841401	0.1670672824737555	T
F	0.5567390663733056	0.8863352993392855	0.1686153687509245	T
e	0.8872886426924871	0.2252586561425587	0.1717677047781069	T
F	0.8874524741947434	0.5579430104833304	0.1670400067829452	T
e	0.8888309331026816	0.8901712816057687	0.1673679881210605	T
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	2O+CO+2OH-t1 (-469.711412; ZPE= 1.00357901)					**2O+CO+2OH-t2 (-469.739542; ZPE= 1.006016462)**			
H	0.8139782371000457	0.4021376476597351	0.2827942729405340	T	H	0.8005557912011581	0.3756144393693442	0.2828673320602412	T
H	0.6585382571649188	0.6010295439929436	0.3401246810489267	T	H	0.5277673369534651	0.8188108971306383	0.3021248778850374	T
C	0.2202067509489062	0.8915920480053584	0.2625855709758672	T	C	0.2363419237912514	0.8810313091124041	0.2621421241370805	T
O	0.4911211470673961	0.3338495590888548	0.2375845004181494	T	O	0.4829919645706081	0.3416119922622393	0.2342732845100945	T
O	0.1729599870367563	0.3429099308856774	0.2339723372989956	T	O	0.1756391812007502	0.3316428962491865	0.2395592167265490	T
O	0.2204854434347963	0.8917070422914312	0.3253062899400443	T	O	0.2473672022969367	0.8750669749765254	0.3247504335953467	T
O	0.6998060309619453	0.5593212010276259	0.2963122771572230	T	O	0.8019996349677329	0.2952894236767819	0.2716252953536378	T
O	0.8848456861289717	0.3153362092495866	0.2666094874883592	T	O	0.6005400321285024	0.8059035868713932	0.2734170287333366	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1063102176282217	0.1151757180019590	0.1312394120654204	T	e	0.1062262831767305	0.1142845574935112	0.1309282615582558	T
F	0.1112427743134193	0.4449527907874445	0.1314591079246171	T	F	0.1106984888132716	0.4472081100231418	0.1287651948555422	T
e	0.1097544612396489	0.7788632184138390	0.1295526585805473	T	e	0.1101105159744159	0.7778743447333432	0.1293628917984937	T
F	0.4466522118131394	0.1065713365228366	0.1293776905247309	T	F	0.4466371674270901	0.1064448645677365	0.1298659104034436	T
e	0.4431217986461012	0.4457235828800499	0.1312222250246043	T	e	0.4430644816930500	0.4448177309085617	0.1325351483561146	T
F	0.4454946400728775	0.7774324089444249	0.1296735848248393	T	F	0.4458929610422254	0.7773359021065835	0.1282423404944641	T
e	0.7799422123539258	0.1131837330948143	0.1314381851506524	T	e	0.7796785025943617	0.1133669432918106	0.1305652301240615	T
F	0.7768839459392595	0.4463276132254154	0.1261745961502779	T	F	0.7785578807123040	0.4456082854679752	0.1285884021340820	T
e	0.7777800475154720	0.7773271695523633	0.1301709233921358	T	e	0.7767852404763308	0.7784917141941298	0.1288414369367557	T
F	-0.0007519082256516	0.0000238738625358	0.2096840787253515	T	F	0.0034901737521173	0.9974322595839331	0.2096602661860276	T
e	0.0152442700207745	0.3369995404548566	0.2210030909435986	T	e	0.0131057832870822	0.3409820042672111	0.2135558275660367	T
F	0.9969778480588368	0.6727564691489694	0.2097077971051910	T	F	0.9962295344058827	0.6715871978773951	0.2097533274187571	T
e	0.3354937944284038	0.9933584761489439	0.2100350018262739	T	e	0.3266146988390352	0.0010662577329646	0.2086242556680166	T
F	0.3324030844995170	0.3390886973348055	0.2169896523509438	T	F	0.3278936917247807	0.3378703316035429	0.2175014996492083	T
e	0.3303090741455509	0.6712633780945614	0.2092800764776854	T	e	0.3341178810268983	0.6679709038790754	0.2098571239079005	T
F	0.6729764531497712	0.9902706370970954	0.2103095857698940	T	F	0.6734873221058890	0.9949913231032941	0.2101875795123148	T
e	0.6499329563901538	0.3361031538230147	0.2134044422384269	T	e	0.6449408049111652	0.3401894234840624	0.2212562747478079	T
F	0.6718755236751555	0.6568083082708153	0.2144302418181053	T	F	0.6748318072738686	0.6527061581732330	0.2148706577041834	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F

e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2301825261261891	0.2119152126219589	0.1675211128854654	T	e	0.2283658092078661	0.2149847513393295	0.1661588279053614	T
F	0.2200878534995037	0.5593753132304551	0.1677264703966797	T	F	0.2193871403366297	0.5589629230034576	0.1681028351543736	T
e	0.2202899234111109	0.8905603715265921	0.1697637583801018	T	e	0.2216425904603432	0.8881226010098475	0.1696698859436331	T
F	0.5593985574149589	0.2096792085991026	0.1677833940644625	T	F	0.5588757153031417	0.2110479552173444	0.1676801795071940	T
e	0.5560627501842959	0.5566896006823396	0.1677183614218388	T	e	0.5574088651824005	0.5547963437699307	0.1676152386316130	T
F	0.5576279817215338	0.8844119140644690	0.1690639755218866	T	F	0.5561060326524629	0.8854167604219696	0.1752351638537141	T
e	0.8840852904082501	0.2322006954860305	0.1765657244776673	T	e	0.8842905798796942	0.2295859157960915	0.1768941385887908	T
F	0.8886225480266930	0.5555020092159674	0.1677376601675307	T	F	0.8879448096543509	0.5567461947316042	0.1671420482241047	T
e	0.8891191772658884	0.8899124645196981	0.1671315725104277	T	e	0.8894498353916084	0.8898684420471573	0.1668852181346068	T
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	TS11' (-468.870561; ZPE= 0.775179)					**3O+CO+OH+ H (-469.979745; ZPE= 0.861745801)**			
H	0.7917123391333791	0.4190527912456826	0.2598452274419679	T	H	0.8217349422704904	0.3800975650458638	0.2817431565582306	T
H	0.4886686139501475	0.7294027927647775	0.2250537892150685	T	H	0.4977783182690101	0.5719996746366092	0.2468468025271297	T
C	0.2162705708260025	0.8891983956581224	0.2621988577108162	T	C	0.2074590260011595	0.8842037400323255	0.2614712370746103	T
O	0.4903338963169512	0.3412990860399007	0.2350246048709601	T	O	0.4932202042577772	0.3264107684183490	0.2407427419669724	T
O	0.1699722873301638	0.3403476540581316	0.2353464127490406	T	O	0.1738647626057120	0.3422411836748264	0.2334318365459003	T
O	0.2172483414413679	0.8878880196029248	0.3249250271391915	T	O	0.1996835027830249	0.8819217858841158	0.3238576944437994	T
O	0.8238203238210423	0.3251355215494565	0.2637152096960841	T	O	0.8987485856313698	0.2980188774913787	0.2709475764225299	T
O	0.5076063773335098	0.8257440653687950	0.2484181678534731	T	O	0.5105939306490774	0.8399705482993335	0.2441634511448335	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1088463258786356	0.1129610899094398	0.1318707126960508	T	e	0.1078510978923208	0.1136622600118990	0.1313839219622461	T
F	0.1111089524119854	0.4441522731326129	0.1328553570099477	T	F	0.1101511014215425	0.4451037998979684	0.1331786791717929	T
e	0.1102969582500889	0.7779142377276972	0.1292577879823971	T	e	0.1106589845983684	0.7776090908617035	0.1289158197593201	T
F	0.4449005810641591	0.1103544139956392	0.1302170580522017	T	F	0.4452053650867596	0.1099187802910916	0.1284794011194046	T
e	0.4445210605273543	0.4456536950466162	0.1335660756963584	T	e	0.4417362201310374	0.4459443409273490	0.1284373166384978	T
F	0.4438141991020261	0.7769022178136019	0.1249577903722912	T	F	0.4444725627916528	0.7770690817219211	0.1270048367845298	T
e	0.7791420583973677	0.1131270048204650	0.1307272853081781	T	e	0.7797892752693738	0.1130328398421776	0.1310591349061540	T
F	0.7765309827695014	0.4479621782013926	0.1271598260395493	T	F	0.7762329163340836	0.4465187720341988	0.1283462643057612	T
e	0.7785637912582548	0.7770714164134560	0.1303152262376520	T	e	0.7788399927608889	0.7766592477480638	0.1290882304491728	T
F	0.0009165297229656	0.9995501192999436	0.2098265042822766	T	F	-0.0024986643520637	-0.0008690645144219	0.2099975246018959	T
e	0.0073375874631529	0.3360145561120657	0.2183487576084161	T	e	0.0153192162480329	0.3367207419150725	0.2206458341485676	T
F	0.9957955305140879	0.6714178785002385	0.2095083246426960	T	F	0.9968734704954706	0.6706174587778112	0.2093393424735587	T
e	0.3416962886042852	0.9867500296483103	0.2133204866220379	T	e	0.3438899010844485	0.9825974986713719	0.2125790886751230	T
F	0.3307990214026992	0.3391408932147323	0.2174409947808530	T	F	0.3340159235562474	0.3374909047955414	0.2175049984291592	T
e	0.3329034403367621	0.6703222757037327	0.2106689013041034	T	e	0.3386530560566229	0.6680202031169749	0.2105122654037125	T
F	0.6730141824162054	0.9960680882767863	0.2101504873555106	T	F	0.6752973499431100	0.9967498114823600	0.2095217354705016	T
e	0.6572143292743999	0.3387333595904851	0.2197833321910016	T	e	0.6458613208260218	0.3402448496143562	0.2132433821130357	T
F	0.6697633899808582	0.6680082033001388	0.2141671586430378	T	F	0.6531830917356088	0.6740682268981234	0.2132357283729618	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F

F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2291775472347069	0.2094890948261871	0.1696452098874307	T
F	0.2202112475358079	0.5594168631950669	0.1676620302265816	T
e	0.2203054546586212	0.8892077814319415	0.1693393550761772	T
F	0.5603116744464897	0.2129611504274487	0.1682171582921900	T
e	0.5557066728813251	0.5599485295793857	0.1694321839799314	T
F	0.5590636763418990	0.8901646818669814	0.1688764099595013	T
e	0.8862331358037878	0.2276575491763681	0.1724976795772947	T
F	0.8867282249323039	0.5556340770739078	0.1680160379613029	T
e	0.8895903157215003	0.8899255949150352	0.1672443677563057	T
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F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2317239072179559	0.2079772496902936	0.1689557782850347	T
F	0.2216032368002658	0.5590665654532079	0.1684275680356708	T
e	0.2198051740243640	0.8890828931798126	0.1690270230956896	T
F	0.5580247223891081	0.2133172956574720	0.1667429381659173	T
e	0.5561022498935040	0.5554397186292026	0.1674591957439524	T
F	0.5616581223067533	0.8929461948669850	0.1671630924410092	T
e	0.8850346543357743	0.2299796205269881	0.1764066889376575	T
F	0.8834956398214620	0.5569988094525565	0.1693738231651404	T
e	0.8901867779897722	0.8884608926314093	0.1666490282313222	T
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	TS12' (-468.307688; ZPE= 0.786322)					**2O+CO_2+OH+H (-469.642281; ZPE= 0.903417693)**			
H	0.7911441879510929	0.4176457059436949	0.2628046433587522	T	H	0.8182275523453053	0.3834447646570301	0.2821104142090222	T
H	0.5559500324292821	0.5998326404132417	0.2475748661446941	T	H	0.5992803346161740	0.5735817491738097	0.2486164733169470	T
C	0.3083306497806003	0.8493282371073038	0.2573073915262269	T	C	0.2607393417685867	0.8683052743761063	0.2708870791772678	T
O	0.4888103746560081	0.3391023042390914	0.2346718554369613	T	O	0.4915280046384187	0.3316752293281446	0.2374962322481259	T
O	0.1682561331218176	0.3427411448846333	0.2347612453043046	T	O	0.1734333136198422	0.3421011339515334	0.2331542069359280	T
O	0.2941080865217936	0.8129562693579854	0.3147754152100187	T	O	0.8950502714689139	0.3019330488671246	0.2701250980357623	T
O	0.8519940038504631	0.3238315856336726	0.2641069911268633	T	O	0.2841433047490070	0.9508019988231406	0.3013386835873976	T
O	0.4450797327899080	0.8681373795121329	0.2552964165219256	T	O	0.2791317334903580	0.7645303371888632	0.3016698123196661	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1062219974945643	0.1144655730787339	0.1303399034899060	T	e	0.1079815861751120	0.1123987760230681	0.1305068893555588	T
F	0.1075671243845363	0.4486971328080420	0.1323877337670946	T	F	0.1109237798397592	0.4450845978618830	0.1317575951128847	T
e	0.1117092878975516	0.7790639402812921	0.1295163966277280	T	e	0.1113518999900621	0.7793734145649884	0.1293575767173877	T
F	0.4441969730636680	0.1087599163643329	0.1307294031295703	T	F	0.4456427574446644	0.1078355063699325	0.1294759331882032	T
e	0.4428814308090104	0.4450449094541705	0.1326334048767377	T	e	0.4420390195285371	0.4471819715878029	0.1308432757874819	T
F	0.4440969251948234	0.7769993138683743	0.1267357465646737	T	F	0.4441849296547180	0.7783110506889190	0.1287638811635277	T
e	0.7791832665690832	0.1118770513873713	0.1302349681495180	T	e	0.7800742622027074	0.1128948463615287	0.1307985146613935	T
F	0.7768585073842377	0.4466495135038582	0.1267416883483306	T	F	0.7770990341073730	0.4452855098336009	0.1276345280415271	T
e	0.7725621874856154	0.7805128704116038	0.1322463460320267	T	e	0.7773354111325032	0.7782971956982399	0.1304688273880609	T
F	0.0016462520604203	0.9991679655583871	0.2086709067175838	T	F	0.0038855094999502	0.9966498600854693	0.2097967802346060	T
e	0.0052281255649355	0.3352523940127229	0.2204916294855070	T	e	0.0142706213789881	0.3379958093192757	0.2205665310031463	T
F	0.9936914575008969	0.6721494523318375	0.2095652900732181	T	F	0.9955702003737779	0.6725045137755415	0.2093515104774284	T
e	0.3146209681705363	0.0128726810066792	0.2097320941637904	T	e	0.3311477351272020	-0.0029067889642140	0.2129373843395141	T
F	0.3289111336518227	0.3412993417367750	0.2173184383848933	T	F	0.3331737364008036	0.3377192577680623	0.2168492798949473	T
e	0.3381537188257346	0.6669541721122526	0.2144640682647355	T	e	0.3288331097383931	0.6695020249161211	0.2133794958031524	T
F	0.6727958312783082	0.9921938507532234	0.2101647284862723	T	F	0.6718105194387104	0.9920380003451121	0.2097911558323834	T
e	0.6551523394949181	0.3366823103686534	0.2161155955985207	T	e	0.6464987253958354	0.3401160029809513	0.2124923900687782	T
F	0.6613009160800533	0.6604295650251966	0.2131828114165266	T	F	0.6656353595630746	0.6629498864190061	0.2107548794868721	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F

e	0.2223740210807885	0.2200294280919642	0.1659533131230025	T
F	0.2197832958357885	0.5618122671386705	0.1681526584170572	T
e	0.2219656416936313	0.8895443595642769	0.1686983486925416	T
F	0.5603142520188139	0.2106111814801503	0.1682241857715936	T
e	0.5559008709192279	0.5547117296844136	0.1668504076500990	T
F	0.5473750424984608	0.8891237522740744	0.1764523635163978	T
e	0.8849446962798503	0.2277210065603031	0.1722086386482656	T
F	0.8830300995777886	0.5578516269026345	0.1689502677039947	T
e	0.8896989106257397	0.8891998845745269	0.1671362959300517	T
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e	0.2299722181590128	0.2114101729254130	0.1671535508419760	T
F	0.2204230495447406	0.5596596094537344	0.1676877585171663	T
e	0.2231210388236667	0.8884479013643679	0.1694022674163328	T
F	0.5593948131207336	0.2104799175668549	0.1669862594059572	T
e	0.5548411443437269	0.5578232794145273	0.1685685846664699	T
F	0.5543275982189100	0.8877798786574539	0.1688779460246849	T
e	0.8859683137683728	0.2290421202843202	0.1760514354092811	T
F	0.8874640867220784	0.5555377882140842	0.1681269153302392	T
e	0.8897629471930836	0.8900558209449081	0.1672089777126944	T
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	TS13' (-468.686027; ZPE= 0.811426)					**3O+HCO+OH (-469.18889; ZPE= 0.930170662)**			
H	0.7909160357442869	0.4198398925290320	0.2606713232019837	T	H	0.8015893071860246	0.3708898084622410	0.2847773486614119	T
H	0.3730046670889717	0.7116832355778249	0.2802529836643490	T	H	0.1665438390695183	0.8421200762986573	0.3017615892603615	T
C	0.2635675369229817	0.8625362551657272	0.2604260974239492	T	C	0.1963793472981618	0.8964415583624165	0.2657663939198144	T
O	0.4896846190158361	0.3409385794786778	0.2344999565037778	T	O	0.4813856953980690	0.3426374043538036	0.2335092574426915	T
O	0.1692667586353684	0.3399909802685905	0.2341560116385938	T	O	0.1739974269137574	0.3328886451559105	0.2353130027201029	T
O	0.2629715672219121	0.9200337532540229	0.3134497519851396	T	O	0.8016558806699354	0.2920056275969610	0.2717665489403579	T
O	0.8305138629645247	0.3248451992719118	0.2636135684169281	T	O	0.5169374296234240	0.8307187397002116	0.2432273792217021	T
O	0.5182103141083076	0.8353802476354968	0.2446084546546765	T	O	0.2470859247186870	0.9571904598271596	0.2981306771526765	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1094688271481533	0.1121571413264774	0.1309317093788717	T	e	0.1081661012006690	0.1123341436588454	0.1302127426359328	T
F	0.1095903511116385	0.4450274235286672	0.1336736442954479	T	F	0.1105580753492770	0.4455605473079455	0.1313628625248305	T
e	0.1097586540238831	0.7779644936592719	0.1282240611891703	T	e	0.1103274235069262	0.7780267839049092	0.1285341452719277	T
F	0.4443250913550432	0.1108056868759628	0.1296889174759942	T	F	0.4451152761989527	0.1088405621291745	0.1287270912755387	T
e	0.4434060577874622	0.4457495423093541	0.1337682988752719	T	e	0.4426745329390050	0.4451207805006138	0.1320543354785537	T
F	0.4448389126586881	0.7774719935563286	0.1265192133223003	T	F	0.4442983500826121	0.7775859295110673	0.1272322638281272	T
e	0.7796668482525400	0.1123597420319174	0.1305152789350111	T	e	0.7797261854669025	0.1130967320048224	0.1300311248093302	T
F	0.7746755450421565	0.4484391990977076	0.1274658578199584	T	F	0.7778937445799164	0.4451636243583637	0.1292806437413896	T
e	0.7785427076137568	0.7773265519413629	0.1291736873894005	T	e	0.7777915390046578	0.7784710989216499	0.1295822775648454	T
F	0.0033484711061559	0.9973994514139600	0.2090044429307097	T	F	0.0129192045328952	0.9925417443273046	0.2112369779513047	T
e	0.0061719285468575	0.3354792670948245	0.2177791369863671	T	e	0.0117978318238259	0.3393456293119590	0.2114596940082349	T
F	0.9955227906065729	0.6702111460457086	0.2092644085743019	T	F	0.9949762462837205	0.6709313084560878	0.2089824899481535	T
e	0.3427748800821324	0.9852145096009283	0.2172343987331625	T	e	0.3383881109403341	0.9799874768221941	0.2202621806836697	T
F	0.3306359164170812	0.3384622202241446	0.2169046368373384	T	F	0.3278485489841758	0.3375931098840579	0.2160750176812688	T
e	0.3238162404414964	0.6798746008048998	0.2107610550202594	T	e	0.3288586430772718	0.6757589789395292	0.2098927025067479	T
F	0.6742877245938619	0.9965207658087539	0.2096879538907312	T	F	0.6748639021503192	-0.0028675214839943	0.2094937362158055	T
e	0.6588339222554968	0.3358245143545222	0.2197962519053873	T	e	0.6447234683823936	0.3388384725073789	0.2209782956468524	T
F	0.6564234696229085	0.6737479997557538	0.2130668957558142	T	F	0.6570903481816183	0.6700642169902788	0.2127890407297789	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2297510606120877	0.2075407696526336	0.1696904219209251	T	e	0.2332710269444932	0.2030390210487972	0.1691811176614922	T
F	0.2197199846389519	0.5603932755723815	0.1679633764638988	T	F	0.2194787784618634	0.5600590816464697	0.1683856674425307	T
e	0.2202509557538828	0.8900184453872789	0.1663505553019458	T	e	0.2217267440512890	0.8881027734769162	0.1662072544692061	T
F	0.5603330375220200	0.2130036545692360	0.1676965172920636	T	F	0.5582491624649311	0.2122198207595328	0.1669884741172128	T
e	0.5519830360616609	0.5586422724754037	0.1703700867806391	T	e	0.5558703689690903	0.5542510235874073	0.1675861354079713	T
F	0.5599391988488585	0.8938554165930279	0.1669815344567346	T	F	0.5590651129579984	0.8939507458073396	0.1679433734996587	T
e	0.8869874657898421	0.2266109952560078	0.1722173201004599	T	e	0.8859146516815812	0.2267926863804235	0.1774301975516384	T

F	0.8825678468813858	0.5579901977383995	0.1688525826230773	T	F	0.8831270315780704	0.5586197577123378	0.1682464168430849	T
e	0.8902194547366656	0.8888960072675458	0.1670170819280060	T	e	0.8913885678571466	0.8903782743666713	0.1675072692460939	T
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	TS14' (-468.580264; ZPE= 0.952104)					**2O+COOH+OH (-468.856838; ZPE= 1.047824505)**			
H	0.7921257835335187	0.4173685750431392	0.2612648755757682	T	H	0.8237533564974963	0.3779079657175236	0.2820781684610456	T
H	0.2640953744557688	0.9848140414979920	0.3440141114283810	T	H	0.2466247836778619	0.9785351782500131	0.3485948006947517	T
C	0.1949108574774630	0.8957012120410197	0.2631121434850907	T	C	0.2008079423383120	0.9072380318498877	0.2675435932132095	T
O	0.4896261865698120	0.3395124204445498	0.2349375006648474	T	O	0.4930028947019566	0.3304655275344244	0.2385513185759060	T
O	0.1679948595279335	0.3410628987544361	0.2338300150637317	T	O	0.1751177714741431	0.3419550828497185	0.2339440968058527	T

O	0.1051933716289968	0.9268719411368653	0.3050890932389946	T	O	0.9019940056858652	0.2968208104459216	0.2712022297340956	T
O	0.8580460891642936	0.3248411667894679	0.2640785537408348	T	O	0.2911699075333204	0.9290915142493785	0.3063183791841654	T
O	0.3129056822262969	0.9262983300843750	0.3057832631196940	T	O	0.0996362842463215	0.9349478045279851	0.3026344099408654	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1082551398066482	0.1130640761841895	0.1301520319459341	T	e	0.1072750837764965	0.1136667741982455	0.1300635428306793	T
F	0.1107963986338747	0.4440841860653056	0.1329475071446642	T	F	0.1112147387398083	0.4454579754709621	0.1316967074111016	T
e	0.1098863370054293	0.7791618650518184	0.1286952416191463	T	e	0.1107297442057991	0.7789589998790956	0.1293065546503379	T
F	0.4447755429365585	0.1089531903842772	0.1300531020806427	T	F	0.4462534865374846	0.1076586669082200	0.1292771575241982	T
e	0.4439566708021742	0.4451968553329056	0.1337927442885388	T	e	0.4425215352831512	0.4464697368376009	0.1305066225520359	T
F	0.4450330781063646	0.7784108894196312	0.1291837540652493	T	F	0.4441351150276170	0.7784767393313599	0.1297946352190845	T
e	0.7794907836243344	0.1123311207805951	0.1309227072332856	T	e	0.7801696888540610	0.1126045885079372	0.1311141778289807	T
F	0.7759879775510569	0.4475161127591190	0.1263620387406356	T	F	0.7766366334014115	0.4454830800595939	0.1281428426744409	T
e	0.7772007870692478	0.7783359054124217	0.1302424412123278	T	e	0.7778729226182794	0.7773618698160077	0.1302798294382740	T
F	0.9977120232195319	0.0011631583710501	0.2125651593346433	T	F	-0.0016699851055342	-0.0020765289731220	0.2129993794649445	T
e	0.0060920696308438	0.3359193491137069	0.2200597240266957	T	e	0.0164964683867568	0.3372773506795354	0.2204334346794839	T
F	0.9962114543698850	0.6715924717861038	0.2093340641619333	T	F	0.9965808627132939	0.6715824621975258	0.2093831098644909	T
e	0.3356523686675547	0.9902512206335083	0.2157361623367011	T	e	0.3359980805280112	0.9948337504874391	0.2119799902293784	T
F	0.3303230111454581	0.3382662811408160	0.2165779620963682	T	F	0.3343402488661323	0.3372257591306300	0.2166542256584540	T
e	0.3292201041400465	0.6775005579117264	0.2097684451436257	T	e	0.3306056137154587	0.6750858901143665	0.2098007287421002	T
F	0.6715056129159473	0.9923410471090247	0.2103714596350598	T	F	0.6720217208512479	0.9915417562327554	0.2100463563358011	T
e	0.6552452264054608	0.3364321190343970	0.2165942332587319	T	e	0.6469271681654233	0.3392065196214461	0.2126194852817549	T
F	0.6655128447531569	0.6685112406778727	0.2103233553075378	T	F	0.6678397133759404	0.6656099942571326	0.2103527022815992	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2291386005103879	0.2084879194461930	0.1692649099879369	T	e	0.2304273397908987	0.2112236192822165	0.1673930163522364	T
F	0.2200018907711914	0.5603436927726744	0.1678771589822836	T	F	0.2209168119213797	0.5596877231715122	0.1682534230808562	T
e	0.2212236940609208	0.8899301052903384	0.1668339429344310	T	e	0.2207348707603857	0.8900860685505309	0.1684228016878558	T
F	0.5603610179798435	0.2103958997002664	0.1682150459008669	T	F	0.5595517160296006	0.2101451658918874	0.1672407967299339	T
e	0.5565175364131726	0.5570057657815348	0.1682123867418459	T	e	0.5556830487754346	0.5572788349656462	0.1678736904616279	T
F	0.5540378826676480	0.8895577420226501	0.1679745368437377	T	F	0.5556173235363648	0.8879665419948500	0.1680399077754106	T
e	0.8857664885662458	0.2276204311232688	0.1723124376282158	T	e	0.8861236194507297	0.2286232361295568	0.1764132009310562	T
F	0.8867057998373801	0.5562544723363921	0.1681787379832236	T	F	0.8883866220776990	0.5546739932485348	0.1682467938560038	T
e	0.8890617870454647	0.8902239708584330	0.1671853928810194	T	e	0.8894121223214196	0.8898292064020793	0.1669553829908613	T
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Table SX7. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the 3OH pre-covered Fe(111) surface

	3OH+CO+H_2O (-480.600002; ZPE= 1.885576251)					**TS15' (-479.0430434; ZPE= 1.878088)**			
H	0.5416514740257601	0.2215952382186925	0.2935412440296908	T	H	0.5372045281412646	0.2293108202362186	0.2930760718554347	T
H	0.3341180293999463	0.3537376121714973	0.3456053759169495	T	H	0.3309646164196455	0.3682594303210159	0.3437770058247817	T
H	0.3131842771847942	0.1823596693371660	0.2942424317626042	T	H	0.3287383821417241	0.9461341936070975	0.3451788046486376	T
H	0.5246067210440407	0.7022926494413959	0.3164584179988247	T	H	0.5194285405769992	0.6921405971131601	0.3182339956086173	T
H	0.6614858538176057	0.5847398450893392	0.3377023719704914	T	H	0.6576423910327011	0.5826974270449479	0.3373193472864567	T
C	0.3379927192596249	0.8333451890890275	0.2436125080365395	T	C	0.2560240113746569	0.8578075227339405	0.2635820118489079	T
O	0.3749586057163912	0.2900989157396767	0.3086978731193668	T	O	0.3753627399018214	0.3015007970664704	0.3088354228025731	T
O	0.6230537301435826	0.1835178799032113	0.2652305323780831	T	O	0.6196543651867705	0.1887784122364490	0.2649789582371609	T
O	0.2627313186925522	0.1483983505870944	0.2697641746309310	T	O	0.2684742702882740	0.9870703213813878	0.3063720195984693	T

O	0.6203369358694201	0.6698058790163237	0.3163817857837006	T	O	0.6099607243286403	0.6705666237465732	0.3194454586971629	T
O	0.3725243767886127	0.7562861998231399	0.2963152818681122	T	O	0.3000879134499824	0.7667604102588761	0.3061768608550632	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F	F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1112023321346601	0.1122606193619296	0.1294742646059465	T	e	0.1111144155495729	0.1114640021834295	0.1302000085848196	T
F	0.1129406397449680	0.4421887553383188	0.1313830734488298	T	F	0.1103892595671196	0.4443840802435656	0.1313404233851459	T
e	0.1105294676342920	0.7784425377357519	0.1297790999086589	T	e	0.1113545654398303	0.7772056565418175	0.1305717121907373	T
F	0.4438258470937149	0.1107339629813548	0.1269474689120033	T	F	0.4427921758223713	0.1109098650640519	0.1291216356497789	T
e	0.4438500826591245	0.4456480494347111	0.1303048051344071	T	e	0.4435072622695064	0.4450782641224793	0.1296851945475428	T
F	0.4468294145861916	0.7763084597503287	0.1329631741522663	T	F	0.4474391981249060	0.7764631515850868	0.1310012295210874	T
e	0.7795995090442783	0.1098537601491008	0.1268259502250455	T	e	0.7793470179947456	0.1102451463181017	0.1272990393954182	T
F	0.7779046127078804	0.4438869297627424	0.1307868699185867	T	F	0.7781541162573598	0.4434887988311361	0.1305954782870542	T
e	0.7761700014800368	0.7799071499143805	0.1315905750459958	T	e	0.7765759662788793	0.7791361037967826	0.1310338508849249	T
F	0.0013318849576850	0.0006613388988641	0.2086225274290620	T	F	0.0063376930545272	0.9965082350406158	0.2096688984980118	T
e	0.9970842424654206	0.3360234595919426	0.2093098763669555	T	e	0.9988376310544591	0.3337579693469945	0.2091723387981776	T
F	-0.0011082876777532	0.6661408249978571	0.2094566423572382	T	F	0.9987841235188529	0.6670984419800581	0.2092523461286916	T
e	0.3309801678884368	-0.0097902465186117	0.2201336220052311	T	e	0.3317568286473386	0.0011729892322089	0.2142692386013735	T
F	0.3309506504464654	0.3468810401900684	0.2142970563098772	T	F	0.3251858830575580	0.3372907733961571	0.2154038478470794	T
e	0.3372483763604078	0.6638099421259319	0.2128544707177646	T	e	0.3370224260884396	0.6607350690869114	0.2114470008168094	T
F	0.6693800874407830	0.0102485297192968	0.2142122443227410	T	F	0.6683019286243354	0.0134871005581323	0.2140490094491670	T
e	0.6691585865503865	0.3148340356437203	0.2139257618369351	T	e	0.6678236005018700	0.3158328672914348	0.2140784432845802	T
F	0.6701429060294123	0.6651802923565872	0.2124599240975434	T	F	0.6612245206215921	0.6691686331913475	0.2122929750695726	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2251204781382349	0.2189294598083819	0.1738168357292988	T	e	0.2229373695241262	0.2212821683992023	0.1681481655402713	T
F	0.2217114129026027	0.5579085999816428	0.1676266288316151	T	F	0.2228351073148764	0.5542009573840533	0.1681365799909348	T
e	0.2207592994108411	0.8883748785680950	0.1674960466630130	T	e	0.2239526618898021	0.8882150062189669	0.1694396581086520	T
F	0.5517686779870068	0.2226798280471756	0.1656250248240776	T	F	0.5500475102385564	0.2241587085930864	0.1656895520898784	T
e	0.5603611435911103	0.5485776927956212	0.1698458430179186	T	e	0.5591945219031571	0.5488210036019994	0.1692990563107870	T
F	0.5541146890546449	0.8930872597734522	0.1712917200355229	T	F	0.5557102862026546	0.8928343565187721	0.1701630695441257	T
e	0.8879825981923923	0.2226070845338332	0.1677025449479863	T	e	0.8880512126320315	0.2213624905754320	0.1685179488272443	T
F	0.8880578001034946	0.5560304173830627	0.1673893200315793	T	F	0.8859954124995031	0.5570999290441326	0.1685343499093386	T
e	0.8886689052608808	0.8895466204136386	0.1683390086775458	T	e	0.8882047081513025	0.8901308075831258	0.1684039940685551	T
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	2OH+COOH+ H_2O (-479.356184; ZPE= 1.934584991)		**TS16' (-479.789173; ZPE= 1.69482)**
H	0.5361457508093065 0.2325975500399685 0.2928110814995397 T	H	0.5421583284074551 0.2219149771448627 0.2930725904093858 T
H	0.3368980712600194 0.3848611261797606 0.3395846134555083 T	H	0.3357643476169324 0.3532091015517819 0.3457137732712193 T
H	0.5018210966085928 0.7001570119727211 0.3132158320923045 T	H	0.3117338781619274 0.1849898534447928 0.2943878915716134 T
H	0.6373847693227854 0.5842384468013414 0.3339956450531635 T	H	0.5418293053138167 0.7132513676640766 0.3231266222146987 T
H	0.3102064352738478 0.9373282387382345 0.3520014181246600 T	H	0.6011141037654982 0.5878766550440758 0.2593598507074414 T
C	0.2704674738700713 0.8700960781231462 0.2673341719341981 T	C	0.3212005161124998 0.8427596745310806 0.2487668251612707 T
O	0.3739884898468548 0.3092750012111335 0.3096029200677836 T	O	0.3753539155514975 0.2900510586989044 0.3084597274132295 T
O	0.6192593378094343 0.1904283224036249 0.2653095257332617 T	O	0.6232224225038637 0.1844638806210956 0.2644732421320098 T
O	0.5953051960547230 0.6719479082562517 0.3159432048837582 T	O	0.2607014428970948 0.1518969360233624 0.2696556347867750 T
O	0.2604517242983911 0.9736157621362859 0.3085841990876506 T	O	0.6313529926581666 0.6528198653666505 0.3098977487278519 T
O	0.3308513381394529 0.7608338628400144 0.3001772375041714 T	O	0.3543680342080807 0.7669904044305309 0.3000872325976203 T
F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F	F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F
e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F	e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F

F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1117272365118576	0.1101074726033460	0.1307846589992686	T	e	0.1108933801679913	0.1126345829173400	0.1293166173552447	T
F	0.1097752541981927	0.4455574182661904	0.1313292705251378	T	F	0.1130157784225817	0.4426218384775535	0.1314197059016098	T
e	0.1116786227462861	0.7778581359299539	0.1312224644057794	T	e	0.1106390164713805	0.7784809749770166	0.1295410348339084	T
F	0.4431954567930345	0.1115343355554260	0.1292476714411588	T	F	0.4438685161198862	0.1110711386861302	0.1269253941456449	T
e	0.4431798578596657	0.4451212618708966	0.1292401333604860	T	e	0.4440832333094527	0.4464414054583986	0.1307920618918584	T
F	0.4472449524635104	0.7767860909071336	0.1305873727023246	T	F	0.4472428963385666	0.7767791348346565	0.1318525943604824	T
e	0.7792170098022961	0.1102392287646291	0.1272770223381191	T	e	0.7796444693380589	0.1101135940866959	0.1267228531726779	T
F	0.7780693653652028	0.4434900262766290	0.1307431100661738	T	F	0.7779338445302831	0.4441382395476325	0.1305062476804607	T
e	0.7775881860502035	0.7784319414310052	0.1305635210597618	T	e	0.7752738589913846	0.7801408056671122	0.1315705045695739	T
F	0.0045623522920125	-0.0036283680181820	0.2093888321614379	T	F	0.0019969572704530	0.0002213526038881	0.2083942869724917	T
e	0.9990364078997026	0.3338911358901843	0.2091127423130169	T	e	0.9973277116519449	0.3357360836032428	0.2094601118162278	T
F	0.9990472988487874	0.6673530915439003	0.2092859168832724	T	F	0.9987442569631018	0.6659897582224948	0.2093749801864329	T
e	0.3360042059216103	0.0042304042588627	0.2112800730408552	T	e	0.3258494244239262	0.9935030597927420	0.2200974700651892	T
F	0.3239199209795748	0.3369608677076905	0.2156562856305975	T	F	0.3314472316590863	0.3467664590218237	0.2142028856078035	T
e	0.3361236486885805	0.6634631041506210	0.2109324844881812	T	e	0.3392359772296590	0.6644111564502748	0.2139333598260133	T
F	0.6678266244151346	0.0145375440858516	0.2142323707348740	T	F	0.6695278751503205	0.0104513896074497	0.2140899235548811	T
e	0.6688589831557414	0.3152838547583304	0.2139568063849552	T	e	0.6670071955974973	0.3208672060721630	0.2145241068989793	T
F	0.6588655104718406	0.6695825870121382	0.2125509126903675	T	F	0.6686879798190289	0.6686479227942297	0.2143808865781610	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777777999999955	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2219804532444853	0.2230419840129747	0.1673067736575193	T	e	0.2246700478557845	0.2196045235944187	0.1733985938369180	T
F	0.2231289568687642	0.5546500518402604	0.1684045043186462	T	F	0.2223909572206641	0.5583115263885241	0.1678976700563813	T
e	0.2247280700863175	0.8889229507413717	0.1715046333416530	T	e	0.2214513252991926	0.8881139607817683	0.1666619539705212	T
F	0.5496922470966067	0.2249459258308852	0.1657788148583923	T	F	0.5522266632119003	0.2235321581415824	0.1656886283705095	T
e	0.5585583223214018	0.5487391137518911	0.1688360901529291	T	e	0.5612318706330269	0.5515477822050256	0.1708910023223922	T
F	0.5584020995802714	0.8920134194116189	0.1694987042451941	T	F	0.5527537662190660	0.8938491612966630	0.1718123082973241	T
e	0.8883691888230956	0.2212514757834884	0.1685640917299579	T	e	0.8876327871361879	0.2229524604095150	0.1676516373061789	T
F	0.8852433112154030	0.5575425891207711	0.1689051503186600	T	F	0.8875848923894915	0.5563888104492078	0.1674172707073164	T
e	0.8876707647901585	0.8900746179390741	0.1683141450238134	T	e	0.8887045186860003	0.8894333978287551	0.1681314937968178	T
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	3OH+CO+OH+H (-480.79561; ZPE= 1.726487607)		**TS17' (-479.945273; ZPE= 1.552771)**
H	0.5407049129070491 0.2278475909712067 0.2927023029478824 T	H	0.5414077514526489 0.2272799916708340 0.2929815289967093 T
H	0.3352601943423384 0.3554949632671266 0.3452535156024146 T	H	0.3365009785596238 0.3554118073818525 0.3451817057180063 T
H	0.3014163602339854 0.1875727582485322 0.2971425175779485 T	H	0.3054173935560567 0.1820304187318944 0.2971355320521971 T
H	0.5737285214001385 0.8654585047479899 0.3071964261660084 T	H	0.5989423989374649 0.9117562780206784 0.2504626709300425 T
H	0.6904083576206295 0.4601685996964998 0.2181956993977964 T	H	0.6892538314228061 0.4632734471245689 0.2188905402181785 T
C	0.2877414051986905 0.8449257867036739 0.2580545418234671 T	C	0.2923411505984100 0.8445574862300294 0.2584652747349131 T
O	0.3744379943440306 0.2896439478346809 0.3092496302923617 T	O	0.3754466507198495 0.2900666893230786 0.3089027289601777 T
O	0.6222087455053316 0.1914506415168246 0.2644367233686981 T	O	0.6231277466436210 0.1899639339202221 0.2647108956319409 T
O	0.2529771859152977 0.1518851851472805 0.2724272956251070 T	O	0.2585100578014250 0.1462094964480938 0.2711617474428347 T
O	0.3165542757818302 0.7661448639298917 0.3065679605470648 T	O	0.3186221891732244 0.7642242163561285 0.3060612672540399 T
O	0.5376617192249391 0.8374033140464860 0.2699520789878906 T	O	0.5373033359398653 0.8439878822239398 0.2594516440428424 T
F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F	F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F
e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F	e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F
F	0.2222221999999974 0.8888888999999978 0.0428677000000022 F	F	0.2222221999999974 0.8888888999999978 0.0428677000000022 F
e	0.5555555999999982 0.2222221999999974 0.0428677000000022 F	e	0.5555555999999982 0.2222221999999974 0.0428677000000022 F
F	0.5555555999999982 0.5555555999999982 0.0428677000000022 F	F	0.5555555999999982 0.5555555999999982 0.0428677000000022 F
e	0.5555555999999982 0.8888888999999978 0.0428677000000022 F	e	0.5555555999999982 0.8888888999999978 0.0428677000000022 F

F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1115812822483580	0.1116743536317906	0.1290448567695072	T	e	0.1115838139278223	0.1114295773364188	0.1288776029877760	T
F	0.1126519030987192	0.4411340691983143	0.1323519834898913	T	F	0.1123864488121455	0.4410673726780463	0.1324888417439011	T
e	0.1113534687664479	0.7779446630043595	0.1297860327430845	T	e	0.1109036817901515	0.7783843258846667	0.1304329009448442	T
F	0.4444865725798453	0.1115491055611219	0.1262428265619759	T	F	0.4437142401921568	0.1126652241565754	0.1268548079218731	T
e	0.4424112873941088	0.4464102787619701	0.1301308565959376	T	e	0.4422584247323438	0.4461951202003591	0.1300085550818091	T
F	0.4466675009330960	0.7768283091871674	0.1277478530464867	T	F	0.4461953806548081	0.7757072902077112	0.1268728735806262	T
e	0.7802449763184657	0.1107436849287950	0.1267357300375755	T	e	0.7794261904170499	0.1100475415507191	0.1265916705973321	T
F	0.7780995256789303	0.4436206940824715	0.1338401989731152	T	F	0.7777597028357530	0.4441291202238616	0.1341250670888780	T
e	0.7765426463002105	0.7796911367513423	0.1316948320364128	T	e	0.7782010143347724	0.7785477581299416	0.1309012876897458	T
F	0.0063989212825097	-0.0026407754129566	0.2092824440612414	T	F	0.0057928477342367	0.9966184061387754	0.2094895439788078	T
e	0.0012514534274168	0.3340902638416701	0.2099765333547789	T	e	0.9989933631212226	0.3351113232235071	0.2096677843020945	T
F	0.9986023178320341	0.6670289542487263	0.2095513229683902	T	F	0.9992395728301848	0.6673283982268644	0.2097075653418295	T
e	0.3309636977096294	0.9798251502171267	0.2308957521419554	T	e	0.3439494545049626	0.9708757046507058	0.2318818341158463	T
F	0.3305268977733187	0.3449333409558172	0.2146191889971668	T	F	0.3308781573656347	0.3445104465776765	0.2145065836327838	T
e	0.3357269567194987	0.6630683726389106	0.2139046129467542	T	e	0.3351433068315646	0.6632824869321694	0.2139833500113866	T
F	0.6725808322223604	0.0163499273974013	0.2129538472768840	T	F	0.6651402050425926	0.0166362727283418	0.2163389911989745	T
e	0.6641534646113529	0.3239488018772558	0.2158375689161690	T	e	0.6648791928630094	0.3235362746083399	0.2159260077769720	T
F	0.6576432950875638	0.6745091018042676	0.2135292148310477	T	F	0.6538365777917952	0.6741127626691207	0.2144294048093844	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777777999999955	0.0000000000000000	F	e	0.7777778000000026	0.7777777999999955	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2288232157135753	0.2130354835807478	0.1747646345818185	T	e	0.2281011347765310	0.2126344664148214	0.1755155863891857	T
F	0.2214651939418682	0.5570835245254353	0.1675794384251696	T	F	0.2214925704781155	0.5569222473732639	0.1674693072102481	T
e	0.2246268047359347	0.8874485743700633	0.1675062417015818	T	e	0.2252541687066440	0.8879752184819037	0.1678757064014674	T
F	0.5518173571509275	0.2252938428655834	0.1651267862400674	T	F	0.5517564157908512	0.2253416459856662	0.1655917895216964	T
e	0.5559897876826674	0.5526313780346546	0.1692850167053754	T	e	0.5554883512815244	0.5520175038449754	0.1693377425797195	T
F	0.5538946057479177	0.8966000893592982	0.1719141880416672	T	F	0.5576427995489538	0.8968211576333291	0.1674913243032179	T
e	0.8886466083726299	0.2215659657052269	0.1687908325816432	T	e	0.8884566109067996	0.2208809979991027	0.1686151406267118	T
F	0.8860579082150747	0.5569663810400008	0.1689040874133141	T	F	0.8853513992096970	0.5577931309365963	0.1692591991392193	T
e	0.8897039776424320	0.8898396932946983	0.1679450459622131	T	e	0.8872817806363381	0.8910030884629190	0.1688711268801338	T
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	3OH+CO+O+2H-t1 (-481.066468; ZPE= 1.605172429)					**TS18' (-479.918748; ZPE= 1.578928)**			
H	0.5395264953801913	0.2269123031910306	0.2938344682062515	T	H	0.5420811940886436	0.2297958717732164	0.2933261788365514	T
H	0.3325941230273439	0.3523295120875406	0.3451190649763731	T	H	0.3378485303284563	0.3577931937722006	0.3453931858485995	T
H	0.2942484205860400	0.1855902465978316	0.2951243747399132	T	H	0.2930302273586763	0.1986835550412865	0.2966013912928081	T
H	0.6892576784957556	0.4603280983232012	0.2194631803111732	T	H	0.6341184034025293	0.9082977795866841	0.2447574419122676	T
H	0.7180010177389825	0.8591720444735443	0.2131557002624000	T	H	0.6907511895902683	0.4606510211277633	0.2189517868421436	T
C	0.2042715473246758	0.8765540805662553	0.2615176319372778	T	C	0.3474010559424647	0.8210083704353157	0.2492333219408664	T
O	0.3719116947850006	0.2873655721460359	0.3086850510573221	T	O	0.3749730152735287	0.2921326160677603	0.3091730961624727	T
O	0.6220620279432298	0.1909707655360481	0.2665711672294070	T	O	0.6242596692325328	0.1931452216949125	0.2656063314697736	T
O	0.2464460451724041	0.1502741414435015	0.2694236508172443	T	O	0.2418914533924650	0.1661799677079500	0.2715781949080130	T
O	0.1955640983124139	0.8687603198824593	0.3236259877080055	T	O	0.3499820612120814	0.7502630975209111	0.2990229383713643	T
O	0.5016051384107656	0.8208489287585217	0.2321076106292687	T	O	0.4912591891190061	0.8104576292440155	0.2392168802857813	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1106344517205650	0.1117974478861426	0.1286527123722148	T	e	0.1117739151063460	0.1114194882745000	0.1299442650459357	T

F	0.1124596738328795	0.4415461682220490	0.1313617612317237	T	F	0.1120059571494366	0.4429284610428028	0.1310043505727338	T
e	0.1090829725118649	0.7778077516128307	0.1295847494789194	T	e	0.1107511240818576	0.7789262039006197	0.1299457015934326	T
F	0.4437242202155724	0.1125270466626401	0.1284465219952574	T	F	0.4442118251383997	0.1119351052657843	0.1278041510777699	T
e	0.4426432026074859	0.4449987092617577	0.1296099438771988	T	e	0.4420086203149431	0.4459371354369778	0.1296541893004206	T
F	0.4462155072336476	0.7777861209913199	0.1332254457524895	T	F	0.4459695118529804	0.7767169627459521	0.1286707352047319	T
e	0.7791011584436526	0.1101960837556672	0.1275198832632643	T	e	0.7795222295051016	0.1101441809200870	0.1266437406474526	T
F	0.7780559099462347	0.4434915247872847	0.1336542131292280	T	F	0.7786033830135324	0.4434150957298071	0.1333420019110653	T
e	0.7810568326906245	0.7758498067310070	0.1310596158673941	T	e	0.7775605546507998	0.7790262045769001	0.1322035673703324	T
F	0.9988249502326854	0.0014560408084126	0.2100588598084109	T	F	0.0017689389914313	0.0014044808501575	0.2091081462782645	T
e	0.9984085590210049	0.3338319229336932	0.2102778553444312	T	e	0.0012098143097491	0.3334082947682864	0.2103087632363445	T
F	0.0034728280006060	0.6624531184468946	0.2098989443797349	T	F	0.9980990305619624	0.6676814398866509	0.2096926411197177	T
e	0.3453056999015412	0.9849749996763859	0.2214056547292692	T	e	0.3219701524153489	0.9997496181672988	0.2264412730490074	T
F	0.3289642099590626	0.3437046554924520	0.2145223551652437	T	F	0.3315075666282499	0.3470605883034170	0.2146292900322364	T
e	0.3324392287444277	0.6641502516856678	0.2099491294389673	T	e	0.3362318167078686	0.6606282370217916	0.2125128305303643	T
F	0.6708244224684697	0.0207219765481789	0.2177899780776595	T	F	0.6686404590435112	0.0195143160960584	0.2181832670691968	T
e	0.6656041268760228	0.3218964993032747	0.2170594559746238	T	e	0.6659372906133993	0.3229399122806214	0.2165213171650295	T
F	0.6623297506745198	0.6647735942300874	0.2107417602600312	T	F	0.6651943569356115	0.6635337923975433	0.2114856493357333	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777777999999955	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2252257249163870	0.2176463137279468	0.1731605402550196	T	e	0.2256125234964173	0.2203827534060817	0.1721065654081017	T
F	0.2217222290411985	0.5556300608212916	0.1669868102386184	T	F	0.2202773491882798	0.5577632892720360	0.1669854437397904	T
e	0.2208887180632437	0.8890943234911283	0.1697792525302681	T	e	0.2244644847042277	0.8877424246763163	0.1690459491436711	T
F	0.5509932840792379	0.2260537935479112	0.1659854679836864	T	F	0.5521931071052826	0.2254081451253080	0.1656393792494958	T
e	0.5560534788525906	0.5483566420283604	0.1692809052961724	T	e	0.5569460186888462	0.5480642418919719	0.1690288546935541	T
F	0.5677707925647159	0.8994983677742575	0.1722508364342192	T	F	0.5566749946417291	0.8977440552137135	0.1739363826475345	T
e	0.8876318217131637	0.2216423864632009	0.1681375544775726	T	e	0.8878830256374020	0.2221661712897511	0.1682360444919554	T
F	0.8887176327252826	0.5543469673641280	0.1684076144145041	T	F	0.8882102114400178	0.5555717042416434	0.1682736975815566	T
e	0.8876843031122063	0.8895381857585449	0.1694272786675025	T	e	0.8872926756384352	0.8913351417544032	0.1689509505357068	T
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	3OH+CO_2+2H (-480.551292; ZPE= 1.625139016)					**TS19' (-479.9194876; ZPE= 1.514532)**			
H	0.5401983850777496	0.2257518692985455	0.2921452065761030	T	H	0.5382720460141533	0.2263823015214325	0.2931442564559381	T
H	0.3384559796633782	0.3765187377609706	0.3410243945657297	T	H	0.3303071539289819	0.3522292139694099	0.3442574132576536	T
H	0.2188744935541690	0.2470989545373020	0.2963484487125662	T	H	0.2924849668106303	0.1844692741581435	0.2946634739474976	T
H	0.6911646658620652	0.4574291414648912	0.2181410094692010	T	H	0.6877984537456856	0.4592630720794406	0.2202009730267442	T
H	0.6352003359679339	0.8798298203414403	0.2426236417372252	T	H	0.7109058564252211	0.8587226479520390	0.2134014726920142	T
C	0.2725922624255990	0.8517162249234949	0.2727871449662354	T	C	0.1495171048330445	0.8029211970598593	0.2195336332165071	T
O	0.3658844106417457	0.3039244069766309	0.3093322957313446	T	O	0.3706343294401872	0.2869919249524741	0.3080175458947197	T
O	0.6219582213151389	0.1864586513035676	0.2641561068073610	T	O	0.6209440325040068	0.1900994655870554	0.2659666741695423	T
O	0.1775524575754607	0.2119574401042286	0.2658520114848777	T	O	0.2441790934962780	0.1491863525288679	0.2694429393157209	T
O	0.2996116165966169	0.9293347958278685	0.3045527099747168	T	O	-0.0012165353216546	0.8188334866447851	0.2518809242452476	T
O	0.2863561839327479	0.7482878492886680	0.3021443973147342	T	O	0.4976646514099182	0.8202497693904168	0.2319521771038375	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1118087984927249	0.1089269685995270	0.1287335824671295	T	e	0.1095889295539495	0.1123203212382199	0.1287294939893419	T
F	0.1113719253548166	0.4443769535993940	0.1290982233357618	T	F	0.1116820038723762	0.4423758030486911	0.1321303850567196	T
e	0.1110849663396294	0.7791926308555469	0.1307395715151723	T	e	0.1114776738328779	0.7789020140693300	0.1238937986857042	T
F	0.4439615140595805	0.1108066583831719	0.1291290240559823	T	F	0.4428916634014215	0.1127800026823512	0.1286336855374276	T
e	0.4437731014872284	0.4451430782292859	0.1304568879889864	T	e	0.4429545350900938	0.4452685003451675	0.1288626446916692	T

F	0.4453816401649080	0.7781118135326139	0.1301846731612748	T	F	0.4455274831464525	0.7769534223181093	0.1340043338152462	T
e	0.7794941666432690	0.1098043899146369	0.1267618714685817	T	e	0.7794718349593722	0.1104529926624972	0.1271734899517803	T
F	0.7792161956224966	0.4430239507299422	0.1340097326545278	T	F	0.7778928509230558	0.4428609608570772	0.1345202270760996	T
e	0.7779104652106501	0.7780616543413565	0.1316912850096094	T	e	0.7808299578866960	0.7761074255793211	0.1312450603817280	T
F	0.0052491116706209	0.9970886485265733	0.2094893356598325	T	F	0.0054014518952341	0.9897106680472992	0.2135249831539628	T
e	0.0109676841658696	0.3234274176876023	0.2131777442261833	T	e	0.9955176354360697	0.3371467529495303	0.2104043580002850	T
F	0.9994429508328005	0.6686854284657785	0.2097060158119261	T	F	0.0062671019350070	0.6628901139654425	0.2136425539934338	T
e	0.3200630162429707	0.0101762235927639	0.2190467424672320	T	e	0.3472544332108137	0.9860043571105640	0.2212250492992847	T
F	0.3346137036580571	0.3406516423489802	0.2134467016276511	T	F	0.3278233436744170	0.3433336529613051	0.2138821941177476	T
e	0.3335413984022420	0.6622595299680261	0.2120469129460657	T	e	0.3223692831072886	0.6703565208622742	0.2110011184190884	T
F	0.6607388989865568	0.0098409449946934	0.2186891836130819	T	F	0.6668682355424036	0.0204899654094910	0.2164006755974483	T
e	0.6643930582682850	0.3219479642547116	0.2156423936085104	T	e	0.6655931324757141	0.3209789136638383	0.2170658685497774	T
F	0.6650190409977278	0.6729101160772205	0.2097109708600081	T	F	0.6625048084552198	0.6644006871798989	0.2111602006472052	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2252137605713460	0.2237173445773601	0.1668481623763453	T	e	0.2241615237420447	0.2181467797818060	0.1732583730631982	T
F	0.2215558044300845	0.5560158434568769	0.1671416082064286	T	F	0.2218508099892242	0.5563329243543367	0.1673232818960615	T
e	0.2267061283310903	0.8862040291021186	0.1715766215628244	T	e	0.2220208683353561	0.8936038822648031	0.1688402034504895	T
F	0.5537291050627283	0.2217007003981420	0.1654851148207070	T	F	0.5508977634309078	0.2265151637848121	0.1655163342146382	T
e	0.5562779801067024	0.5527761311517952	0.1700443976963570	T	e	0.5546884104870654	0.5486473726269279	0.1700515643217155	T
F	0.5524976971685485	0.8943627967110754	0.1704663830799056	T	F	0.5660506671904816	0.8975485598784959	0.1712693642765010	T
e	0.8888324657636110	0.2212529833440799	0.1689920126642347	T	e	0.8896886977159914	0.2176260199155442	0.1694045829392097	T
F	0.8918008844360260	0.5525154100673659	0.1693126776099576	T	F	0.8893460064689007	0.5563982453653165	0.1689314532475277	T
e	0.8856799097027538	0.8917678078805434	0.1690967416696755	T	e	0.8854085732553030	0.8901908913638026	0.1711769641592499	T
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	3OH+C+2O+2H (-480.744768; ZPE= 1.573617953)		**3OH+CO+O+2H-t2 (-481.2072751; ZPE= 1.601222209)**
H	0.5392903769631419 0.2269990117602803 0.2933936578145641 T	H	0.5406734214522274 0.2281280838073131 0.2939780467521672 T
H	0.3307217922800826 0.3536911272347472 0.3450934920619639 T	H	0.3296356747459813 0.3549567397382300 0.3449216873872888 T
H	0.2932936459119431 0.1860851106920476 0.2949970603716528 T	H	0.2928519714468738 0.1880352482150976 0.2951897905336917 T
H	0.6875492474665919 0.4595407973024231 0.2200263842169567 T	H	0.6914585933266328 0.4566037335644696 0.2187700646314943 T
H	0.7006173107965707 0.8573145399107390 0.2118455557002548 T	H	-0.0750120183254862 0.8323583190574843 0.2485189600824500 T
C	0.1595874732041234 0.8234154570213457 0.2204652788239617 T	C	0.2149219879418695 0.8694365461935951 0.2611762637553032 T
O	0.3698476659873159 0.2886572346927224 0.3086519606228083 T	O	0.3695726064449918 0.2896114277254189 0.3087231603300842 T
O	0.6213834664142039 0.1905634880166861 0.2658767344320974 T	O	0.6224177643184802 0.1918879666032102 0.2663352868375614 T
O	0.2459960171721498 0.1497717999092481 0.2695535867769064 T	O	0.2456252979064130 0.1520969756086590 0.2693577762403790 T
O	0.4992049102772046 0.8205120964757880 0.2322021789744245 T	O	0.2136941067528355 0.8553360388120845 0.3232261398552175 T
O	-0.0752767117427900 0.7982395914777444 0.2559002129338075 T	O	0.5076303430421939 0.8262153496540755 0.2359992338357071 T
F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F	F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F
e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F	e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F
F	0.2222221999999974 0.8888888999999978 0.0428677000000022 F	F	0.2222221999999974 0.8888888999999978 0.0428677000000022 F
e	0.5555555999999982 0.2222221999999974 0.0428677000000022 F	e	0.5555555999999982 0.2222221999999974 0.0428677000000022 F
F	0.5555555999999982 0.5555555999999982 0.0428677000000022 F	F	0.5555555999999982 0.5555555999999982 0.0428677000000022 F
e	0.5555555999999982 0.8888888999999978 0.0428677000000022 F	e	0.5555555999999982 0.8888888999999978 0.0428677000000022 F
F	0.8888888999999978 0.2222221999999974 0.0428677000000022 F	F	0.8888888999999978 0.2222221999999974 0.0428677000000022 F
e	0.8888888999999978 0.5555555999999982 0.0428677000000022 F	e	0.8888888999999978 0.5555555999999982 0.0428677000000022 F
F	0.8888888999999978 0.8888888999999978 0.0428677000000022 F	F	0.8888888999999978 0.8888888999999978 0.0428677000000022 F
e	0.1089368622070335 0.1140976409150994 0.1279186505208276 T	e	0.1107798801002443 0.1116467075451669 0.1286749372841317 T
F	0.1125635091333628 0.4413946422467059 0.1312504142287211 T	F	0.1121811320817365 0.4418875503119267 0.1314883737392862 T
e	0.1116367953567259 0.7794006306266786 0.1293533005033930 T	e	0.1106327609639678 0.7771803652537439 0.1291169470922459 T
F	0.4428792047847157 0.1129795438475839 0.1287232781693455 T	F	0.4431325969318167 0.1124157519568365 0.1280118461796085 T
e	0.4424857254338385 0.4456216891839471 0.1291923067346617 T	e	0.4427274870883816 0.4448923129483883 0.1300380562146027 T
F	0.4469869529400980 0.7760873670729819 0.1331592395707626 T	F	0.4461489249144885 0.7769406865746604 0.1320969229068855 T
e	0.7807787116451265 0.1089348991954276 0.1280198709295458 T	e	0.7793957966173833 0.1105797489720453 0.1271664671386439 T
F	0.7767228585385635 0.4415885907804413 0.1341087116928208 T	F	0.7784359304448812 0.4437099829857744 0.1339949142405144 T
e	0.7792762766695932 0.7768258335825263 0.1285867948991117 T	e	0.7793570835617702 0.7773054805088390 0.1305014826812278 T

F	0.0085710864273183	-0.0115928062045176	0.2119792610675565	T	F	-0.0006537115938855	-0.0008456219752231	0.2102045826032526	T
e	0.9963502720348500	0.3379274019911210	0.2104363864975035	T	e	0.9982408167511818	0.3355762319453344	0.2099543617676419	T
F	0.0068852982766504	0.6425504257737810	0.2152201217576120	T	F	-0.0026721437035152	0.6729387893400745	0.2112942004568598	T
e	0.3501138709116413	0.9866993491336444	0.2214286940160814	T	e	0.3442531517937704	0.9856781277383332	0.2219459532247307	T
F	0.3257847552085432	0.3450265644068062	0.2146584781378437	T	F	0.3282984027444616	0.3442706170474569	0.2144122519809237	T
e	0.3224636915842307	0.6724945979735112	0.2120117528048678	T	e	0.3336663631533771	0.6628196201849539	0.2100184224401171	T
F	0.6669753156389483	0.0191597534555970	0.2154703179347691	T	F	0.6727439226725781	0.0161228178469921	0.2147978477349831	T
e	0.6652001794442993	0.3207739786915231	0.2174238099223505	T	e	0.6654640532020707	0.3211233226929134	0.2173542779702136	T
F	0.6625230632680881	0.6642506980673132	0.2112156669076592	T	F	0.6623790256411611	0.6686251081286392	0.2111732212513922	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2240871856937749	0.2178932004184199	0.1733508487165221	T	e	0.2250116222939928	0.2177442552813210	0.1730070589707033	T
F	0.2210118500450984	0.5570506896034538	0.1676286570041594	T	F	0.2201695405239782	0.5563644863179376	0.1675124306509159	T
e	0.2274771282785615	0.8977505158293189	0.1655953390414619	T	e	0.2216083861286925	0.8891400821080203	0.1694264309546128	T
F	0.5509960407759942	0.2261072721916039	0.1655442643247314	T	F	0.5513946048718976	0.2251294875456605	0.1659600117574049	T
e	0.5540040108858284	0.5490789622230910	0.1702102795423968	T	e	0.5568984669337863	0.5485197210100151	0.1695170933584103	T
F	0.5643375923013894	0.8968242163475743	0.1696080507863710	T	F	0.5648272609900562	0.8987141350251974	0.1699616524420436	T
e	0.8893704790167123	0.2180083482674464	0.1696432763488661	T	e	0.8882803934679099	0.2208248653523565	0.1686409649461358	T
F	0.8865867737689795	0.5547494604444112	0.1668922676124321	T	F	0.8888965348022903	0.5566975616773526	0.1688571333043268	T
e	0.8900857249636176	0.8840349106596224	0.1744811672115565	T	e	0.8887686576317965	0.8893855957578209	0.1684328404941518	T
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	TS20' (-480.0787168; ZPE= 1.586166)					**3OH+HCO+O+H (-480.1798478; ZPE= 1.696686195)**			
H	0.5405665864007165	0.2280797928849891	0.2935533632594238	T	H	0.5416981390471286	0.2281675276994178	0.2943087053259853	T
H	0.3307462499490038	0.3543376495426286	0.3447308016360895	T	H	0.3330879026574196	0.3587079751326966	0.3456872544721716	T
H	0.2926633007565849	0.1879959557604981	0.2947435412406850	T	H	0.2950133904177582	0.1955084407485899	0.2955048388745531	T
H	0.6918043021487909	0.4563372005662838	0.2180397236203973	T	H	0.6920154600627658	0.4559184600219760	0.2181540787933605	T
H	0.0577568186212442	0.8958885742500013	0.2743581310021457	T	H	0.1656714281567986	0.8148877109054591	0.2932838990007708	T
C	0.1745872300207792	0.9035731865227786	0.2648541134919567	T	C	0.2130571497090772	0.8623425988496083	0.2645107925131028	T
O	0.3704326866279637	0.2891495485328978	0.3084342406815689	T	O	0.3723455884708681	0.2929608124310628	0.3096476952687305	T
O	0.6222383261885597	0.1920281921508389	0.2657624885188172	T	O	0.6232868743287637	0.1912103395761192	0.2663242258885502	T
O	0.2457012295704901	0.1523116374317044	0.2685168359794702	T	O	0.2472254631722066	0.1607181015837514	0.2692075742566826	T
O	0.2228005397910860	0.9004504752164840	0.3215036107385136	T	O	0.5066698290519894	0.8226872308268025	0.2332393458338856	T
O	0.5074055149601542	0.8239104756951775	0.2350263228229410	T	O	0.2664672048892459	0.9091440777858870	0.3048225980375827	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1104517156780450	0.1121485296809605	0.1279778397037187	T	e	0.1117162716013053	0.1111226060152964	0.1286832458344707	T
F	0.1126736210269460	0.4419848382290762	0.1315274195834922	T	F	0.1126378189611845	0.4415967703038921	0.1315637189455253	T
e	0.1110952165162915	0.7763838947379683	0.1283217475655688	T	e	0.1097137837669835	0.7774491109630486	0.1286169008642278	T
F	0.4431860194424949	0.1127263543756837	0.1278974610740736	T	F	0.4437607725998172	0.1129672140614574	0.1274247564925149	T
e	0.4427325222033869	0.4449927977786738	0.1295378710729601	T	e	0.4423381780228196	0.4455723888840940	0.1296831195654484	T
F	0.4458993573318997	0.7775482679501514	0.1333941975472583	T	F	0.4463200942644853	0.7780785274601030	0.1332204073401556	T
e	0.7800306033957015	0.1097787890361229	0.1272531910849671	T	e	0.7793892471349869	0.1103460399994809	0.1269765678071642	T
F	0.7780586479087014	0.4429271170751124	0.1338636358384386	T	F	0.7779658946791750	0.4430456823846607	0.1339137396176557	T
e	0.7804226832554427	0.7780969258922839	0.1312401148031961	T	e	0.7783568986527012	0.7782393280993009	0.1313248855393854	T
F	0.0099412018908020	0.9951243309129447	0.2097816522836437	T	F	0.0085084796910540	-0.0041324231495695	0.2098465361601050	T
e	0.9984310587078257	0.3347653098892523	0.2098399370392707	T	e	0.0011062467338061	0.3334494582444429	0.2096689003647327	T
F	0.9999070554690190	0.6641397035001170	0.2098722557597403	T	F	-0.0015020692401708	0.6659545401596038	0.2095471015208130	T
e	0.3456382289238094	0.9838038511567202	0.2231050516135497	T	e	0.3363704762989164	0.9829467397041834	0.2316214879827124	T

F	0.3292264590515608	0.3429688241417129	0.2140081589671368	T	F	0.3304918726079129	0.3459236423091688	0.2148304796038487	T
e	0.3312672705505254	0.6687124678745097	0.2098921282633113	T	e	0.3287566207981221	0.6681045830317867	0.2108214896335214	T
F	0.6721622783846196	0.0170844431399603	0.2145198842232679	T	F	0.6708136239051150	0.0179880381393125	0.2145646395642429	T
e	0.6649807693731429	0.3218849277743572	0.2167334234518663	T	e	0.6658303345060744	0.3210257478618557	0.2168815530430521	T
F	0.6638435695273490	0.6680189263000014	0.2105536035442950	T	F	0.6635265418699395	0.6676483916166160	0.2102062903042966	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2251161451145573	0.2175121386407280	0.1726870319851954	T	e	0.2271416003457874	0.2161241662775256	0.1726605039680407	T
F	0.2218163052739424	0.5561337482514493	0.1676624401055559	T	F	0.2206372468314569	0.5568204196041874	0.1674196577863618	T
e	0.2225017275898417	0.8894665747894995	0.1680342595680974	T	e	0.2218228096894069	0.8878006467856924	0.1669349309825046	T
F	0.5515607936240496	0.2254001304305096	0.1656172167302259	T	F	0.5510329350957639	0.2262593539408456	0.1657461510235065	T
e	0.5558978463696325	0.5490611335013746	0.1697477491423693	T	e	0.5552312331779260	0.5494496999865259	0.1702899654310205	T
F	0.5651811954973549	0.8987613282787645	0.1702319456567369	T	F	0.5619722085036994	0.9013304303029420	0.1708905691517990	T
e	0.8889887418467799	0.2193362320694964	0.1691731199081944	T	e	0.8889440284210773	0.2203123133812587	0.1690457859874612	T
F	0.8884281408552201	0.5552434773931657	0.1679756066196819	T	F	0.8883194942665944	0.5550261394809647	0.1680925006353893	T
e	0.8916357876669562	0.8899833386978984	0.1705345947763401	T	e	0.8888170073706327	0.8901042687090179	0.1684351429664578	T
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	TS21' (-479.230504; ZPE= 1.725651)					**3OH+COOH+H (-479.877485; ZPE= 1.791795919)**			
H	0.5419228952517489	0.2269651984300665	0.2926124035157429	T	H	0.5389584769950462	0.2284338898148052	0.2931697197237826	T
H	0.3381823271827096	0.3594040528070033	0.3452100965301304	T	H	0.3279652980239800	0.3792351912681290	0.3411595123370798	T
H	0.2709914679856726	0.2178527677725901	0.2921465346659641	T	H	0.2233942913501293	0.2487210921225342	0.2946532289203031	T
H	0.3982710865155548	0.8758992877452029	0.3491352072485814	T	H	0.6899361815488281	0.4589349590517858	0.2191372150714794	T
H	0.6910276587569847	0.4581360062325112	0.2190821565597244	T	H	0.3124582698618593	0.8968274125596422	0.3521418040648019	T
C	0.2694108574308325	0.8323922764954652	0.2675729165364585	T	C	0.2437572694125243	0.8580470266969698	0.2686266131262767	T
O	0.3734589910512590	0.2928566721886978	0.3093987011251405	T	O	0.3569574852415220	0.3056212736268019	0.3100490849683586	T
O	0.6233758203452454	0.1898842793451113	0.2643595898678729	T	O	0.6200494344017619	0.1906172740661521	0.2652727540597100	T
O	0.2191809680454081	0.1885644324349982	0.2650327290751968	T	O	0.1818274439790152	0.2107229559507423	0.2662316804838704	T
O	0.2829072456625026	0.7480687108321166	0.3094129982404995	T	O	0.2665026772643597	0.9428873173552234	0.3093607387270199	T
O	0.3568075742071214	0.9070537668797430	0.3037392377824220	T	O	0.2685304138788203	0.7550681583305494	0.3016005789145381	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1126252603763292	0.1095494259066778	0.1299154441400638	T	e	0.1107090335401565	0.1102798380207075	0.1287211612308143	T
F	0.1123346349611235	0.4434307399948327	0.1292662716654920	T	F	0.1112309826720121	0.4447519982315635	0.1291396390934181	T
e	0.1122216574112490	0.7792929821940704	0.1304899780851734	T	e	0.1106957735724456	0.7786821924623522	0.1293999078217141	T
F	0.4453579700106201	0.1105783728878298	0.1281560001465618	T	F	0.4447516711738019	0.1105153297239470	0.1288406558284463	T
e	0.4439569737609541	0.4452458515717703	0.1300340224403788	T	e	0.4430788471216875	0.4457453351105058	0.1302809157846275	T
F	0.4460045877700833	0.7781219339907438	0.1303125459765203	T	F	0.4457574909502763	0.7777877989017367	0.1310547933531106	T
e	0.7802040792810503	0.1104709765370420	0.1269297728985084	T	e	0.7796204251175678	0.1106170561016065	0.1271532060936100	T
F	0.7800711590722176	0.4420062932855118	0.1331147624846272	T	F	0.7797428397866765	0.4420289557294628	0.1336868675196873	T
e	0.7784539838487227	0.7779168438160076	0.1325613272802163	T	e	0.7765551172253264	0.7783821286860431	0.1330146343087968	T
F	0.0069126884626675	0.9980564490774145	0.2102045281143564	T	F	0.0067451455844759	0.9967010539969381	0.2099438013884331	T
e	0.0158312570721166	0.3210095635143438	0.2121714447836308	T	e	0.0129096371429291	0.3219844041749640	0.2137492377801929	T
F	0.9994871079627458	0.6673311830043039	0.2094515851526764	T	F	0.9975052983337753	0.6681141520857549	0.2092777316559209	T
e	0.3349679380558057	0.0056320287683067	0.2202659111567114	T	e	0.3214581936776975	0.0122532625682808	0.2157191927400936	T
F	0.3348668464122214	0.3454479542134038	0.2143365828647866	T	F	0.3324747728259244	0.3427425404556460	0.2137209712755576	T
e	0.3407729543505160	0.6539598441870694	0.2125193053186223	T	e	0.3364391946209707	0.6615059715246748	0.2116272739210077	T
F	0.6692793100093315	0.0132756394580042	0.2138345174675032	T	F	0.6673757978471914	0.0128621515390818	0.2139076813137508	T
e	0.6646732772947741	0.3235952999134831	0.2166378006289089	T	e	0.6637849639933566	0.3233695478142009	0.2166289746031605	T

F	0.6687101037316318	0.6686674874693432	0.2090057399597675	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777777999999955	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2276901671863154	0.2229190535234709	0.1661946289572900	T
F	0.2212118238523728	0.5565124802637245	0.1666033729830292	T
e	0.2275052803539988	0.8860984320549090	0.1733376990450547	T
F	0.5534624898974619	0.2242857582747131	0.1652623203404751	T
e	0.5585404728603933	0.5511106166634252	0.1691093237374170	T
F	0.5558961602898536	0.8931225933076440	0.1699214444165017	T
e	0.8893409171405999	0.2213489094958512	0.1691852298889482	T
F	0.8927774777861101	0.5513080151987370	0.1689919601616278	T
e	0.8892322224726059	0.8907649426080158	0.1684612546385030	T
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F	0.6678642356361729	0.6678550855404539	0.2092224100688876	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2254000424743812	0.2239802269070067	0.1662437385184791	T
F	0.2210605635555695	0.5567374917085869	0.1672111792130691	T
e	0.2235552795910101	0.8880441385682417	0.1698330802492629	T
F	0.5524592908765007	0.2246356575733821	0.1655181562579203	T
e	0.5569386977971177	0.5515132387973725	0.1695314013340803	T
F	0.5525866389039655	0.8937809713856428	0.1713558946089985	T
e	0.8888061753536706	0.2212128534524258	0.1696541694181863	T
F	0.8922601220731698	0.5509818314862360	0.1692184155364494	T
e	0.8879782360014299	0.8909086755523730	0.1684155635706172	T
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e		e	
F		F	
e		e	
F		F	
e		e	
F		F	
e		e	
F		F	
e		e	

Table SX8. Coordinates of all atoms of the IS, TS and FS as well as the total energies (eV) and the zero-point energy (ZPE/eV) in the reaction of CO+H_2O on the 3H pre-covered Fe(111) surface

	3H+CO+H_2O (-457.343969; ZPE= 1.276381703)					**TS22' (-456.578034; ZPE= 1.269276)**			
H	0.2706019280530796	0.2289348357387974	0.2477363394595701	T	H	0.3105008598494510	0.9801108653556098	0.2929494675032293	T
H	0.5881636311502263	0.2480395324459647	0.2494232887091993	T	H	0.5827741696985436	0.2518994125572521	0.2490115722302549	T
H	0.9190269792987873	0.2486843091317814	0.2491922107024319	T	H	0.9170986598356593	0.2507071672622875	0.2494282946776505	T
H	0.5142954746306000	0.7359508445460679	0.3213870078869070	T	H	0.5147496223451076	0.7119423520880424	0.3163407199366990	T
H	0.6329870980088474	0.5987458456653049	0.3372209264094495	T	H	0.6480691171538920	0.5916970722665809	0.3393395616616060	T
C	0.2960480948501278	0.8524483943397066	0.2545022695214817	T	C	0.3210593994855676	0.8616657037700629	0.2504184997056732	T
O	0.6098771339377795	0.6829977546271058	0.3182623343109822	T	O	0.6108702571021347	0.6752796836076701	0.3164992451606370	T
O	0.3436236758229343	0.8286332974497952	0.3132882791062672	T	O	0.3589771244148930	0.7705240834384373	0.2957528537761849	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1114327611608000	0.1113356664196968	0.1305881661317252	T	e	0.1115094388660226	0.1122679150831499	0.1304105312765485	T
F	0.1091683898487262	0.4457799200066579	0.1306972938277943	T	F	0.1116304322022651	0.4444245427113160	0.1320514215301565	T
e	0.1111893229234829	0.7771721550302345	0.1311327500585729	T	e	0.1114028952396345	0.7771775917665014	0.1309651600127600	T
F	0.4453805070453743	0.1108413534124121	0.1302609801493483	T	F	0.4432869686399616	0.1109535174370855	0.1313928505236656	T
e	0.4442397950027200	0.4446249025259305	0.1311868233949706	T	e	0.4433041281704784	0.4461523344008324	0.1308914515593369	T
F	0.4463265700704090	0.7769444079679847	0.1301295864598280	T	F	0.4447433037462726	0.7776683380813246	0.1302013135969561	T
e	0.7783820605861229	0.1104280891933276	0.1306351436338209	T	e	0.7784649132553292	0.1103962402879818	0.1304417086377645	T
F	0.7775624214499968	0.4454362023620885	0.1302925173779251	T	F	0.7772816358595883	0.4453946599399004	0.1306485352433062	T
e	0.7781190842771664	0.7772436685764245	0.1311366562958799	T	e	0.7776544813336757	0.7774991919962331	0.1312785056015777	T
F	0.0017264059701447	0.0016640607382544	0.2099640926068088	T	F	0.0005061461629363	0.0017016068136121	0.2094925084768816	T
e	-0.0012447021945468	0.3279481693113964	0.2105214786813571	T	e	0.9968978880111945	0.3293948052301491	0.2107782998753769	T
F	0.0007136447739068	0.6659404981426464	0.2099356145306476	T	F	0.0001921671472803	0.6657342203501416	0.2096535825220087	T
e	0.3298768770388972	0.0078759850202432	0.2111927727498953	T	e	0.3329066902023619	0.9984910146176523	0.2137369045172710	T
F	0.3318861136681108	0.3295538247887844	0.2108669657330710	T	F	0.3359436811484497	0.3315327607979852	0.2098197286193314	T
e	0.3327614374737542	0.6633976138112743	0.2096563703858131	T	e	0.3330380527214707	0.6710326066853800	0.2139372033631672	T
F	0.6659718174577910	0.0021940085967805	0.2098679908572976	T	F	0.6647740010254667	0.0021623487243270	0.2095453109185989	T
e	0.6658803212094940	0.3281076234044865	0.2104461504575687	T	e	0.6651718021328251	0.3282403385753389	0.2102370202607853	T
F	0.6630431488766730	0.6687931482913909	0.2132632754986276	T	F	0.6673241822588745	0.6654567127163662	0.2130760060469784	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F

F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2211433252406535	0.2238024699959264	0.1685240443551021	T
F	0.2225238954943329	0.5538356770861033	0.1684332560932646	T
e	0.2229637322937385	0.8891662057404944	0.1703743317454940	T
F	0.5548902980382915	0.2227070408929196	0.1694442617251723	T
e	0.5568059918981052	0.5538019088935399	0.1685671386297327	T
F	0.5553717578895548	0.8899306032258643	0.1683961527926055	T
e	0.8879293439155094	0.2230098171797490	0.1688784336614374	T
F	0.8877610087192878	0.5550664760923811	0.1694125785479958	T
e	0.8896502096835878	0.8891824796772142	0.1689181400944041	T
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F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2224097353222854	0.2210779574439189	0.1699238277933767	T
F	0.2238018503496834	0.5564652349029939	0.1695621978413137	T
e	0.2203961646651099	0.8904466744657545	0.1678045979100256	T
F	0.5557816682218132	0.2225740273537260	0.1685392347151409	T
e	0.5558139785938307	0.5545586066292240	0.1682927586423563	T
F	0.5538082571392561	0.8897243196053255	0.1696586346467582	T
e	0.8876879017630445	0.2228848244625905	0.1691266003744089	T
F	0.8886029999134802	0.5545489708418203	0.1688727957179231	T
e	0.8894764117166918	0.8890909230894781	0.1689756508148214	T
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	2H+HCO+H_2O (-456.709057; ZPE= 1.36391622)					**TS23' (-456.616492; ZPE= 1.070115)**			
H	0.5830585564402758	0.2518012992945505	0.2494975297868743	T	H	0.2732266859350850	0.2251253440100897	0.2471931306124485	T
H	0.9174393593056386	0.2522651409314525	0.2498084127575379	T	H	0.5878590797645524	0.2495997681493537	0.2491089356713175	T
H	0.5050616816272301	0.7132111746716744	0.3133124538171412	T	H	0.9167737457723474	0.2501887871077149	0.2488032094906927	T
H	0.6394787602128623	0.5980126152055143	0.3396982513208938	T	H	0.5342145776656264	0.7443002468465905	0.3229917213909358	T
H	0.2776409891023771	0.9624767735334434	0.2933479861484401	T	H	0.5744140333965287	0.6141186789339109	0.2598168678648906	T
C	0.2968877222547802	0.8736333089504865	0.2581439119132502	T	C	0.2800164737821082	0.8656827452466279	0.2575851328505061	T
O	0.6009147632359507	0.6801324661510316	0.3152119026018440	T	O	0.6167047964372216	0.6692272873856444	0.3100872183074689	T
O	0.3512996593022755	0.7664072305104125	0.2951874744592423	T	O	0.3185280844683800	0.8528451515620952	0.3172121493611574	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1111901622474552	0.1117845723188862	0.1304134795772513	T	e	0.1112634716472386	0.1114728356632239	0.1305094303694791	T
F	0.1106690440917230	0.4455484721376978	0.1318017107809211	T	F	0.1095774563489921	0.4461746234643055	0.1309249070574161	T
e	0.1116859235413858	0.7774952735294288	0.1311442027273549	T	e	0.1113289077687215	0.7769523837429633	0.1311236087958718	T
F	0.4438059824878445	0.1113446453916528	0.1314737707921943	T	F	0.4454924884095860	0.1114056576669199	0.1303278710432565	T
e	0.4433656747358810	0.4457318353986730	0.1308891549624200	T	e	0.4449303501452391	0.4454282615938851	0.1315762264327172	T
F	0.4454166563599541	0.7770899254853688	0.1292275628032824	T	F	0.4464648203419699	0.7773788005802392	0.1296274587703219	T
e	0.7784389626906092	0.1104937344343567	0.1304849340617823	T	e	0.7783940635352807	0.1106160170623621	0.1305269903393491	T
F	0.7774407687178851	0.4452014212585034	0.1307126262108211	T	F	0.7773633690882776	0.4457643310265481	0.1299773582384323	T
e	0.7779578779387335	0.7773072378203926	0.1311101519938483	T	e	0.7778584471521124	0.7772823173278194	0.1311483180203880	T
F	0.0030854372324961	-0.0001795629027274	0.2096229614883538	T	F	0.0024412673666820	0.0013630880435365	0.2097272410705947	T
e	0.9974102147562114	0.3293398282873481	0.2105522334922503	T	e	0.9985391944620140	0.3280557876303436	0.2105912085306544	T
F	0.0002208232651953	0.6665001439878124	0.2097417337538043	T	F	0.0004760523670226	0.6656566753432602	0.2098501161767228	T
e	0.3333025347798013	0.0011371419342817	0.2120586718858281	T	e	0.3291682456436466	0.0095273882259889	0.2113349547115600	T
F	0.3349280819881724	0.3311660097275165	0.2097815085565678	T	F	0.3325273170299375	0.3290846812856394	0.2109522757895546	T
e	0.3332195862571176	0.6699840347351506	0.2133127243457017	T	e	0.3356382837027342	0.6638096943208788	0.2103191856076296	T
F	0.6656577841674680	0.0016548832238748	0.2094768785720900	T	F	0.6656273637036416	0.0024405777589139	0.2097909714679889	T
e	0.6651160517442183	0.3279531814602881	0.2104712698542164	T	e	0.6651015307760345	0.3316293364448092	0.2111492146337839	T
F	0.6635976742948593	0.6679969691377724	0.2130631639743455	T	F	0.6647997441744231	0.6728249730224384	0.2148089333417244	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F

e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2216544547316235	0.2222462862972271	0.1688854598267638	T	e	0.2208546158777948	0.2243131792029122	0.1682249315861867	T
F	0.2235767669190332	0.5564622981517724	0.1694631807865162	T	F	0.2236850115207953	0.5539587646920241	0.1688748273515643	T
e	0.2219330319549197	0.8903416618232197	0.1687846070284464	T	e	0.2238422254020992	0.8886676619288095	0.1698857798716360	T
F	0.5556502848037470	0.2226208188200164	0.1689883282100488	T	F	0.5553252063090633	0.2236640886169210	0.1694081511785039	T
e	0.5555583932783212	0.5544261052077569	0.1681287371655165	T	e	0.5581458270316580	0.5566960238895793	0.1702644733838348	T
F	0.5547038128356350	0.8895985305089809	0.1686857707942753	T	F	0.5549902415558027	0.8904525460375298	0.1684944151703364	T
e	0.8878714332084735	0.2224378338888592	0.1696408419629353	T	e	0.8875196173069272	0.2232782641676750	0.1686139531671765	T
F	0.8877624103750851	0.5551765980694318	0.1693436356068287	T	F	0.8876649973379824	0.5551888866144747	0.1693292113696534	T
e	0.8896256459094252	0.8892673225456610	0.1688740692620183	T	e	0.8897049178824167	0.8892783400919351	0.1688307449949771	T
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	3H+CO+OH+H (-457.683337; ZPE= 1.102597321)					**TS24' (-456.637314; ZPE= 0.945358)**			
H	0.2581568206582399	0.2479786845749889	0.2500110892305413	T	H	0.2709294795289323	0.2327403294348403	0.2486387234394205	T
H	0.6050195217824627	0.2331532570692436	0.2478737907115598	T	H	0.5939870531456076	0.2423165417972591	0.2488112564471795	T
H	0.9197428111174112	0.2493807455273619	0.2490326516883114	T	H	0.9179077149730686	0.2494262945823184	0.2489594529532526	T
H	0.5580483295256563	0.8734079423351749	0.3061986937545708	T	H	0.5914615161709642	0.9148311143205331	0.2500163561952091	T
H	0.6411847878153298	0.4995337960128972	0.2386070669657492	T	H	0.5959254273123148	0.5553801373677553	0.2482030947594023	T
C	0.2189085425944076	0.8851538299251589	0.2616611765186039	T	C	0.2548980514235260	0.8634101558074918	0.2607015593972203	T
O	0.2166555181690901	0.8830026481332476	0.3243124477893425	T	O	0.5312672384173407	0.8437004693303174	0.2568804266967972	T
O	0.5234056128317821	0.8446032401759060	0.2685572283206279	T	O	0.2770099994335228	0.8447504848227418	0.3220659429817920	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F	e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F	F	0.8888888999999978	0.2222221999999974	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1116349759575829	0.1117181762103614	0.1306347818491647	T	e	0.1121043801949628	0.1109288935584955	0.1313284564589056	T
F	0.1092516668850312	0.4446516304254189	0.1318224695763304	T	F	0.1088123727645994	0.4449783820828127	0.1321102574073633	T
e	0.1110608853611180	0.7765816736197372	0.1300550700674316	T	e	0.1113039069095746	0.7766485932523423	0.1307815307665713	T
F	0.4454479128840139	0.1108155701648836	0.1305499965463332	T	F	0.4450561362211445	0.1117204204617263	0.1300962470494435	T
e	0.4426562470904328	0.4456374430380876	0.1308693690630692	T	e	0.4429396364762008	0.4450469286840412	0.1307752063472484	T
F	0.4450954068252775	0.7769754930147323	0.1270221057853035	T	F	0.4449387919644353	0.7765215974904034	0.1266320692084463	T
e	0.7790761356752267	0.1114679743571694	0.1308360949789782	T	e	0.7785221666112264	0.1103348629643189	0.1306094050047742	T
F	0.7784155985350028	0.4456204656862883	0.1303404113429688	T	F	0.7779930071347916	0.4461411835098556	0.1304867601080456	T
e	0.7790756893995829	0.7762305445282115	0.1306354167041758	T	e	0.7799907209552631	0.7762324689233564	0.1296733660446157	T
F	0.0000169289336881	0.0027248319735060	0.2098909530225338	T	F	0.0012184151590650	0.0012053726705551	0.2099946103633266	T
e	0.9995827945854574	0.3280347806166790	0.2107689532574658	T	e	0.9982379062447876	0.3281830479928860	0.2107278711859951	T
F	-0.0003182409586765	0.6659309529625786	0.2100378873153622	T	F	0.0009008948626000	0.6651612208269999	0.2101208654783230	T
e	0.3420058608303643	0.9897623986774062	0.2143005776722204	T	e	0.3413422211971503	0.9938456562883918	0.2141213063484952	T
F	0.3315343370752716	0.3298650552018308	0.2104981904880179	T	F	0.3318623397153995	0.3296504985713528	0.2111197135591891	T
e	0.3360292576612852	0.6658258460250848	0.2093296361351231	T	e	0.3378651055166568	0.6612133781462733	0.2103951434628064	T
F	0.6685760346137252	0.0080905865706772	0.2090040048983705	T	F	0.6679154182672035	0.0080223684063206	0.2117557932992077	T
e	0.6621851051574558	0.3361601868413378	0.2136004955873722	T	e	0.6627942096288089	0.3345322834557466	0.2119115997219806	T
F	0.6496778244706477	0.6717216222623954	0.2169393074594397	T	F	0.6467110865187830	0.6700434378684075	0.2180586961549086	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F

F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2243971603317390	0.2184401122418083	0.1708266903519977	T	e	0.2235270659842618	0.2195121205708808	0.1699855465446300	T
F	0.2223955864155621	0.5545897781311038	0.1688882030213765	T	F	0.2228451578128066	0.5540083351003011	0.1687140935642456	T
e	0.2232006170094268	0.8888891451711400	0.1691873471453749	T	e	0.2244318382775884	0.8881134704937169	0.1695511309611804	T
F	0.5550469629170468	0.2258574345004802	0.1689540243639964	T	F	0.5549465433984295	0.2247634917481979	0.1691093354654039	T
e	0.5560453227082005	0.5544839762321483	0.1670968719072896	T	e	0.5561446838739669	0.5535943921930069	0.1669408236850025	T
F	0.5589393793516635	0.8892001004554568	0.1694332507886841	T	F	0.5616876682016693	0.8913455062010901	0.1671111462463417	T
e	0.8873226292745037	0.2240332600586538	0.1689077526440751	T	e	0.8873298949786426	0.2231083294083419	0.1687046159281304	T
F	0.8842707924444803	0.5564786569882647	0.1711800701492419	T	F	0.8836343444626721	0.5572061362730882	0.1712185649082390	T
e	0.8902000740158689	0.8886887112393949	0.1683410693347543	T	e	0.8896766284194836	0.8887542733386999	0.1689179009846244	T
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Fe					Fe				
	3H+CO+O+2H (-457.60707; ZPE= 1.000639708)					**TS25' (-456.534714; ZPE= 0.916242)**			
H	0.2556028556437771	0.2448885498331591	0.2490306147126021	T	H	0.2728721292040685	0.2178442322447285	0.2467545508674920	T
H	0.6315260543024298	0.1910542640711131	0.2434258672002389	T	H	0.5994844416156914	0.2362726930077500	0.2484953317905769	T
H	0.9225424043889292	0.2419895749468472	0.2492671903832481	T	H	0.9152290243681048	0.2516611204271329	0.2495083527761438	T
H	0.5969062260925962	0.4927105236449497	0.2479625466230704	T	H	0.6194647262585607	0.5309378715903040	0.2444980360066847	T
H	0.6090131981941889	0.9322969361386054	0.2473259007527133	T	H	0.6112986695792049	0.9248777467043744	0.2482347313853135	T
C	0.2084174870521395	0.8747521812481988	0.2609138126219790	T	C	0.3345523697087058	0.8283169119412315	0.2485492892642735	T
O	0.2026291422884909	0.8664475182296736	0.3231396566459768	T	O	0.4822313378771134	0.8197620433370642	0.2368494888370557	T
O	0.4923466831926657	0.8229288735232817	0.2263216815071759	T	O	0.3405848760884442	0.7618743671932235	0.3003106648175917	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F	e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F	F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1112480883687973	0.1116448020637580	0.1309544206663834	T	e	0.1101964034961934	0.1123592122800248	0.1312662484646954	T
F	0.1094402927153430	0.4444241516193597	0.1311908835370393	T	F	0.1085837281215580	0.4460601248196083	0.1314285948865492	T
e	0.1099982661621027	0.7758996399823107	0.1297889405042310	T	e	0.1125832175114440	0.7769654075236220	0.1300924492473244	T
F	0.4442834828346978	0.1123576197257293	0.1308964470229770	T	F	0.4452996675462792	0.1116648556165313	0.1306696142786724	T
e	0.4418824215729222	0.4454028008949639	0.1301613176442845	T	e	0.4416138371889505	0.4453603879612091	0.1301356771512569	T
F	0.4470770195984378	0.7784409834805038	0.1321170628657038	T	F	0.4455217578356459	0.7770965076166734	0.1281447231003209	T
e	0.7790986153169636	0.1108953952293978	0.1298904152392268	T	e	0.7789990897844304	0.1115467416756288	0.1299207845192595	T
F	0.7785087031458158	0.4448816562134708	0.1306350059801064	T	F	0.7787038334933652	0.4447268939923903	0.1302119856239990	T
e	0.7799223670095820	0.7764028512433172	0.1313162545991772	T	e	0.7783372109170176	0.7777863139730603	0.1316497343024797	T
F	-0.0034698341142369	0.0046399608291727	0.2109362626396575	T	F	0.9993930012484143	0.0049736818718545	0.2095299407450763	T
e	0.9982497870767183	0.3268931961370275	0.2118077894178987	T	e	0.9977604470294070	0.3290873645847944	0.2116411001143483	T
F	-0.0008865655951962	0.6655349610060588	0.2101595636250179	T	F	0.9994970189720117	0.6654213417857836	0.2098396771472549	T
e	0.3330548823060058	-0.0039825531357521	0.2112336274188415	T	e	0.3231868547151835	0.0106025821364308	0.2143430321571996	T
F	0.3288000184909617	0.3301635048879759	0.2109103558699781	T	F	0.3304156496953838	0.3286056168507649	0.2111743605399474	T
e	0.3342835316763482	0.6623881805034650	0.2100376186619039	T	e	0.3373125615140556	0.6603042713481683	0.2126676159997617	T
F	0.6716938694830571	0.0177490081313861	0.2144897904894918	T	F	0.6703564094181597	0.0100597545247520	0.2111913997791884	T
e	0.6638787445929646	0.3321633626511885	0.2131759554069458	T	e	0.6629555883331766	0.3350122313006539	0.2136580056260851	T
F	0.6593973520533832	0.6642138020722070	0.2115722046915331	T	F	0.6570762102834319	0.6601543732176651	0.2134090083010578	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2215781369304179	0.2207017010004333	0.1692113270369543	T	e	0.2205111349365256	0.2233458645569757	0.1675575250655881	T
F	0.2216329659935028	0.5539372503134872	0.1685211613580505	T	F	0.2224215082674985	0.5544043143230265	0.1687147635188843	T
e	0.2185817992788378	0.8880354590939957	0.1690263300568910	T	e	0.2216059833152242	0.8898050175251132	0.1687291753227166	T
F	0.5533174039802810	0.2263869036903208	0.1682530418722626	T	F	0.5552456923525918	0.2255963661475259	0.1688515012297394	T
e	0.5564525298118264	0.5496991260914018	0.1684801004321906	T	e	0.5562338980115944	0.5495003509150962	0.1668877844395334	T
F	0.5660523755244355	0.8980166175477782	0.1723173332970745	T	F	0.5582348743772553	0.8945207596267897	0.1734603358574774	T

e	0.8872741008982477	0.2235370811643723	0.1685241537982834	T	e	0.8863662007695660	0.2247406264823480	0.1691046753213493	T
F	0.8873157127668406	0.5539677477499334	0.1696565742169268	T	F	0.8856025850972099	0.5554625346101502	0.1699350700414191	T
e	0.8889355239029773	0.8899374235503674	0.1687321838250452	T	e	0.8907270528786041	0.8892991759764796	0.1685510471754533	T
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	3H+CO_2+2H (-457.52692; ZPE= 1.04917501)					**TS26’ (-456.821112; ZPE= 0.914499)**			
H	0.2579612309969076	0.2467317040283228	0.2476979504396317	T	H	0.2472721720713159	0.2562004267623940	0.2486290916272883	T
H	0.5847302060942959	0.2518032424154714	0.2485857823440731	T	H	0.6221297666273031	0.1793279676053435	0.2452277583527274	T
H	0.9191528193788953	0.2494143227724555	0.2487955160395501	T	H	0.9164875029064991	0.2506325794753779	0.2501190482757437	T
H	0.5959023835459845	0.5776384071029855	0.2475819564636859	T	H	0.5148643344805744	0.5551983391636747	0.2497182466339009	T

H	0.5872317276108943	0.9170517293510995	0.2484370968761579	T	H	0.7071001855772348	0.8547054091836978	0.2141172140192451	T
C	0.2630598109398450	0.8670607796122672	0.2713310614898499	T	C	0.1722970774433698	0.7524886401638420	0.2082652223855840	T
O	0.2834291150703430	0.9505023008554040	0.3025896551664287	T	O	0.0087255469948381	0.8282357057773970	0.2522849789866203	T
O	0.2830479075507681	0.7620967972861247	0.3013283007604400	T	O	0.4909929916964003	0.8330138542354706	0.2326662098669494	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F
e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F	e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F	F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F	e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F	F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F	e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F	F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1122314368079561	0.1099496037735080	0.1302858415137411	T	e	0.1126793142855252	0.1073534749052193	0.1322744201043745	T
F	0.1104556663771475	0.4452465331286138	0.1305867429749344	T	F	0.1100958316457801	0.4471629512492639	0.1328591224398853	T
e	0.1116202319294811	0.7781335694339068	0.1308382388896305	T	e	0.1045852367665921	0.7806216436375011	0.1188816244136540	T
F	0.4444962388398545	0.1109216229745468	0.1301143867771429	T	F	0.4424365287201659	0.1134880883700364	0.1305056989929201	T
e	0.4437800126876137	0.4456245011575831	0.1308598498184279	T	e	0.4420026815108933	0.4464768514442101	0.1306811393045794	T
F	0.4450456840751376	0.7777263160549772	0.1291972950758421	T	F	0.4441007959688776	0.7777719574238032	0.1324998859272007	T
e	0.7784405863410842	0.1107297314811918	0.1302194025055285	T	e	0.7793976319454836	0.1108807643339778	0.1310011716148429	T
F	0.7781153839320971	0.4447177458094444	0.1299701094456386	T	F	0.7801171040662515	0.4444856608054333	0.1324471856596460	T
e	0.7784957477349097	0.7774542060678800	0.1309143592261411	T	e	0.7809014603205945	0.7762588511003125	0.1324563388771870	T
F	0.0033092519471850	0.0006887422608013	0.2101181980986437	T	F	0.0011338187337806	0.9926371250116198	0.2179293523712888	T
e	0.9995105375818674	0.3277445050693477	0.2105115200696972	T	e	0.9977631339947410	0.3283160261156946	0.2119581179549128	T
F	-0.0000297726013934	0.6668419392679178	0.2099157184769798	T	F	0.0025957083799360	0.6720908928673730	0.2159860308143060	T
e	0.3290101698799624	0.0027379724213555	0.2146392129818246	T	e	0.3338239980369995	0.9925282097548224	0.2114092568866061	T
F	0.3332934139916107	0.3289024808772038	0.2103347063998816	T	F	0.3259947079033717	0.3350313710168660	0.2096322518900399	T
e	0.3309581440933129	0.6662441415990311	0.2133484026505795	T	e	0.3548619243118436	0.6499723343587062	0.2211872670472101	T
F	0.6620966093341867	-0.0011541338599721	0.2103824141503143	T	F	0.6646990243276587	0.0178988395078450	0.2131831271623386	T
e	0.6642177690115780	0.3312779768116155	0.2109431349905748	T	e	0.6658880913282033	0.3310816462586881	0.2109649135957690	T
F	0.6626289580204436	0.6670483169215263	0.2104383863553690	T	F	0.6549003016039181	0.6686973015380336	0.2119369797844469	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F	e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F	F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F	e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F	F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F	e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F	F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F	e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F	F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F	e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F	F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F	e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F	F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F	e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F	F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F	e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F	F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F	e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F	F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2221564649538391	0.2221585767180436	0.1685981793939623	T	e	0.2208714262019190	0.2209652675352646	0.1696531844226322	T
F	0.2232529581882967	0.5549007405086521	0.1684815462812463	T	F	0.2211746384458238	0.5670926487570215	0.1710633636455394	T
e	0.2246148939840205	0.8881411904649755	0.1700532930738227	T	e	0.2190001218925776	0.8797599499467456	0.1703506998690679	T
F	0.5560416589056679	0.2222600619249460	0.1689487753475847	T	F	0.5526295872261685	0.2262939773866015	0.1676579752231556	T
e	0.5553288723752223	0.5555073955965291	0.1690453469406966	T	e	0.5587636966571958	0.5493369843501513	0.1673131789255884	T
F	0.5541959372810119	0.8893905548739884	0.1690368278850578	T	F	0.5636089388925088	0.8982807133024870	0.1703818414982308	T
e	0.8881086369404469	0.2226476478414952	0.1688988294095979	T	e	0.8913129974746964	0.2180252106794053	0.1700582340059322	T
F	0.8886708937960175	0.5548075953218611	0.1693299710762237	T	F	0.8887153439913843	0.5567510445254210	0.1713797419829193	T
e	0.8885214076370171	0.8903294067937061	0.1690806267442823	T	e	0.8878327079450850	0.8909853945478527	0.1710166386855542	T
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	3H+C+2O+2H (-457.4827401; ZPE= 0.967796278)					**TS27' (-456.333791; ZPE= 1.119415)**			
H	0.2415559506085192	0.2635388176997278	0.2489685741576341	T	H	0.2594318251558628	0.2453616498832043	0.2473109607114881	T
H	0.6170609199658834	0.1760484637008406	0.2465527467761018	T	H	0.5879560544828834	0.2481665633985077	0.2487953521406325	T
H	0.9114694854883366	0.2640037978746556	0.2500828714831109	T	H	0.9173886326584964	0.2503174940246504	0.2491755239101683	T
H	0.5351402500064754	0.5710259680710897	0.2506710206645136	T	H	0.5908445543197947	0.5786265313983310	0.2479105586123095	T
H	0.7033618370320697	0.8512790065848401	0.2120044375454622	T	H	0.3839665254895602	0.9017990611076702	0.3474718359958912	T
C	0.1927787120306803	0.7451880729004884	0.2080539327232617	T	C	0.2719482053102817	0.8403436194958602	0.2653381851234968	T
O	0.4911546585241095	0.8341005777752416	0.2343998526397499	T	O	0.3566949058433218	0.9190325649422058	0.2986884472411892	T
O	0.9344751262925413	0.8381175735788181	0.2602112114370946	T	O	0.2855075288052089	0.7592976420899077	0.3092007565178921	T
F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F	F	0.2222221999999974	0.2222221999999974	0.0428677000000022	F
e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F	e	0.2222221999999974	0.5555555999999982	0.0428677000000022	F
F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F	F	0.2222221999999974	0.8888888999999978	0.0428677000000022	F

e	0.5555555999999982	0.2222221999999974	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1149549860224751	0.1060604164717531	0.1309636868236463	T
F	0.1109727831670913	0.4483608689969059	0.1336745931836504	T
e	0.1054942333978231	0.7791243052639594	0.1202261454806449	T
F	0.4423241141948283	0.1135748504277040	0.1307257199486790	T
e	0.4427554054035309	0.4465208484065245	0.1317131199201031	T
F	0.4461398382946891	0.7760707610223930	0.1313470191150579	T
e	0.7777013784088554	0.1122745206525619	0.1271691773775320	T
F	0.7832589312206462	0.4407656587990080	0.1316189713596329	T
e	0.7780884024715552	0.7762000294263720	0.1306456739850072	T
F	0.0436791627609869	-0.0956457913680716	0.2328833609725466	T
e	-0.0011029876588139	0.3305525942539745	0.2112614502293773	T
F	-0.0041462216270786	0.6718450979812377	0.2156989750014296	T
e	0.3319490178837080	-0.0113138880344391	0.2125609468658308	T
F	0.3248707601746762	0.3369677502547515	0.2103196500867302	T
e	0.3702305241413901	0.6404064620964068	0.2216464220756333	T
F	0.6651477519195342	0.0157135931087680	0.2126634619638761	T
e	0.6682134034325000	0.3285298053396145	0.2103384821137992	T
F	0.6553273139206237	0.6681511473341620	0.2128845184410501	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2212071315729937	0.2209834317867752	0.1702019402203669	T
F	0.2225970766520651	0.5675255601848658	0.1727523757292818	T
e	0.2252644215178488	0.8781925914291590	0.1685958413594942	T
F	0.5529006741291861	0.2255388751479430	0.1679954304254190	T
e	0.5652315984381565	0.5465054954528513	0.1660780700447927	T
F	0.5614663569173549	0.8976561313698128	0.1700655594692410	T
e	0.8951196229180239	0.2124618466456803	0.1714956246818321	T
F	0.8874008911271419	0.5568736810195088	0.1703903360092560	T
e	0.8829850600526391	0.8933759138849328	0.1672274383351988	T
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e	0.5555555999999982	0.2222222000000045	0.0428677000000022	F
F	0.5555555999999982	0.5555555999999982	0.0428677000000022	F
e	0.5555555999999982	0.8888888999999978	0.0428677000000022	F
F	0.8888888999999978	0.2222222000000045	0.0428677000000022	F
e	0.8888888999999978	0.5555555999999982	0.0428677000000022	F
F	0.8888888999999978	0.8888888999999978	0.0428677000000022	F
e	0.1124443364789722	0.1107303361606079	0.1310798437448532	T
F	0.1097315403857503	0.4461107674902370	0.1301107109095717	T
e	0.1129579292566555	0.7780568423895300	0.1312296325651310	T
F	0.4452377080841731	0.1112453482311168	0.1302814553080031	T
e	0.4440042714748982	0.4450210715201738	0.1307089886006396	T
F	0.4453703545242830	0.7777377430675195	0.1292220738349117	T
e	0.7787155605074818	0.1107909110187785	0.1301103550375848	T
F	0.7787517196753156	0.4441109632938469	0.1300992707776158	T
e	0.7785689509437274	0.7776451525640946	0.1315935813350997	T
F	0.0044031613770077	0.0011861637031481	0.2101360259000624	T
e	0.9987982302442827	0.3276928022161410	0.2109494057392611	T
F	0.0009423311605729	0.6666815518374364	0.2096674779294238	T
e	0.3349400443397312	0.0106569204835325	0.2133700663066717	T
F	0.3339210479682639	0.3303234104947876	0.2108285719620066	T
e	0.3386437238160211	0.6574944914420766	0.2127523790639242	T
F	0.6666609524781935	0.0031750312547677	0.2094828546688629	T
e	0.6643587279108293	0.3320701695147668	0.2114323801343292	T
F	0.6642804218805313	0.6628788927875002	0.2101207160284471	T
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F
e	0.2209106757410314	0.2255043180974230	0.1681192709709872	T
F	0.2234598879433417	0.5541738347552109	0.1680109403422832	T
e	0.2262058810659324	0.8883194574085891	0.1715960059401944	T
F	0.5558138631435712	0.2236457508989790	0.1688791436508656	T
e	0.5570180962598933	0.5536700874332903	0.1682139756619971	T
F	0.5564824921397664	0.8889911641111922	0.1685796127083400	T
e	0.8880233302070791	0.2224824145883100	0.1689159862142839	T
F	0.8886427939185154	0.5547398570737775	0.1695803811814818	T
e	0.8907151308341327	0.8898776410048785	0.1688058410650471	T
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	3H+COOH+H (-456.872737; ZPE= 1.186777896)		
H	0.2574008461719730 0.2465940987956897 0.2483498959623854 T		
H	0.5873777196154989 0.2484905060230139 0.2489784533104850 T		
H	0.9176846570376324 0.2510649945432681 0.2493664558141206 T		
H	0.5934205122069227 0.5776709718028430 0.2484028617541146 T		
H	0.3120169117313755 0.9153869902357659 0.3502251865016759 T		
C	0.2460610790290305 0.8674809337829270 0.2681263143846029 T		
O	0.2646817882282479 0.9586059051505459 0.3071472838319830 T		
O	0.2758937679233912 0.7653215175121302 0.3026785590622081 T		
F	0.2222221999999974 0.2222221999999974 0.0428677000000022 F		
e	0.2222221999999974 0.5555555999999982 0.0428677000000022 F		
F	0.2222221999999974 0.8888888999999978 0.0428677000000022 F		
e	0.5555555999999982 0.2222222000000045 0.0428677000000022 F		
F	0.5555555999999982 0.5555555999999982 0.0428677000000022 F		
e	0.5555555999999982 0.8888888999999978 0.0428677000000022 F		
F	0.8888888999999978 0.2222222000000045 0.0428677000000022 F		
e	0.8888888999999978 0.5555555999999982 0.0428677000000022 F		
F	0.8888888999999978 0.8888888999999978 0.0428677000000022 F		
e	0.1117910599301666 0.1108138348818206 0.1304114218087191 T		

F	0.1101334327297297	0.4454510401446229	0.1303972860513849	T		
e	0.1113697144671671	0.7777144952370207	0.1304216545810120	T		
F	0.4450728490744219	0.1105832173818698	0.1305503435796852	T		
e	0.4437343892394013	0.4454043888231097	0.1309009737788115	T		
F	0.4449151726415499	0.7777125152532945	0.1299579600403254	T		
e	0.7785780700223670	0.1105645060664699	0.1304271645198504	T		
F	0.7783895447831238	0.4445066922313758	0.1300070819006283	T		
e	0.7784838645822426	0.7774557575633552	0.1314669282031488	T		
F	0.0043743398919159	0.0000314263594662	0.2102785022905516	T		
e	0.9990090902781629	0.3278273933530195	0.2106326987765223	T		
F	0.0000859284831629	0.6667937445021713	0.2097823619183162	T		
e	0.3321578135882158	0.0039432650806148	0.2124371497601546	T		
F	0.3327900674564678	0.3291949066250873	0.2103547641824891	T		
e	0.3350178758918965	0.6630722824026566	0.2130150853593201	T		
F	0.6654753938545886	0.0018855087521125	0.2096406292854594	T		
e	0.6643702806395309	0.3309052755108334	0.2112033404707738	T		
F	0.6635349423695668	0.6638672870866776	0.2104496676196748	T		
e	0.1111111000000022	0.1111111000000022	0.0000000000000000	F		
F	0.1111111000000022	0.4444444000000018	0.0000000000000000	F		
e	0.1111111000000022	0.7777778000000026	0.0000000000000000	F		
F	0.4444444000000018	0.1111111000000022	0.0000000000000000	F		
e	0.4444444000000018	0.4444444000000018	0.0000000000000000	F		
F	0.4444444000000018	0.7777778000000026	0.0000000000000000	F		
e	0.7777778000000026	0.1111111000000022	0.0000000000000000	F		
F	0.7777778000000026	0.4444444000000018	0.0000000000000000	F		
e	0.7777778000000026	0.7777778000000026	0.0000000000000000	F		
F	0.0000000000000000	0.0000000000000000	0.0857353000000032	F		
e	0.0000000000000000	0.3333332999999996	0.0857353000000032	F		
F	0.0000000000000000	0.6666667000000004	0.0857353000000032	F		
e	0.3333332999999996	0.0000000000000000	0.0857353000000032	F		
F	0.3333332999999996	0.3333332999999996	0.0857353000000032	F		
e	0.3333332999999996	0.6666667000000004	0.0857353000000032	F		
F	0.6666667000000004	0.0000000000000000	0.0857353000000032	F		
e	0.6666667000000004	0.3333332999999996	0.0857353000000032	F		
F	0.6666667000000004	0.6666667000000004	0.0857353000000032	F		
e	0.2217510376621227	0.2231547253665265	0.1687174537862589	T		
F	0.2232723427315918	0.5547589881812521	0.1684729063798542	T		
e	0.2226932111602185	0.8893184961543463	0.1694829627927021	T		
F	0.5553760719237560	0.2233024087008978	0.1690143610390828	T		
e	0.5560539802893669	0.5542441185601035	0.1689220493349942	T		
F	0.5555846703688423	0.8884987097898168	0.1688401691110962	T		
e	0.8881072765006609	0.2223144263886858	0.1692352589956220	T		
F	0.8887556769421806	0.5546347300018754	0.1694923564768504	T		
e	0.8898393679342974	0.8897640239839755	0.1689538016675323	T		
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