Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Being negative can be positive: Metal oxide anions promise a more selective methane to methanol conversion

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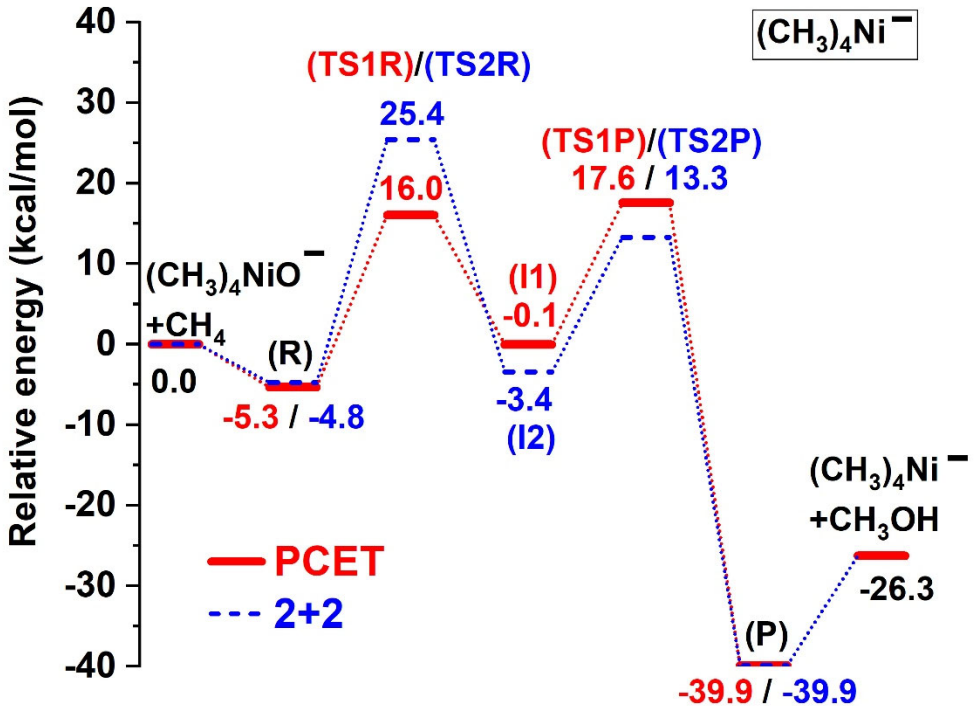

Figure S1. Energy diagram for the reaction $(CH_3)_4NiO^-$ + CH_4 → $(CH_3)_4Ni^-$ + CH_3OH at the MN15/TZ level of theory.

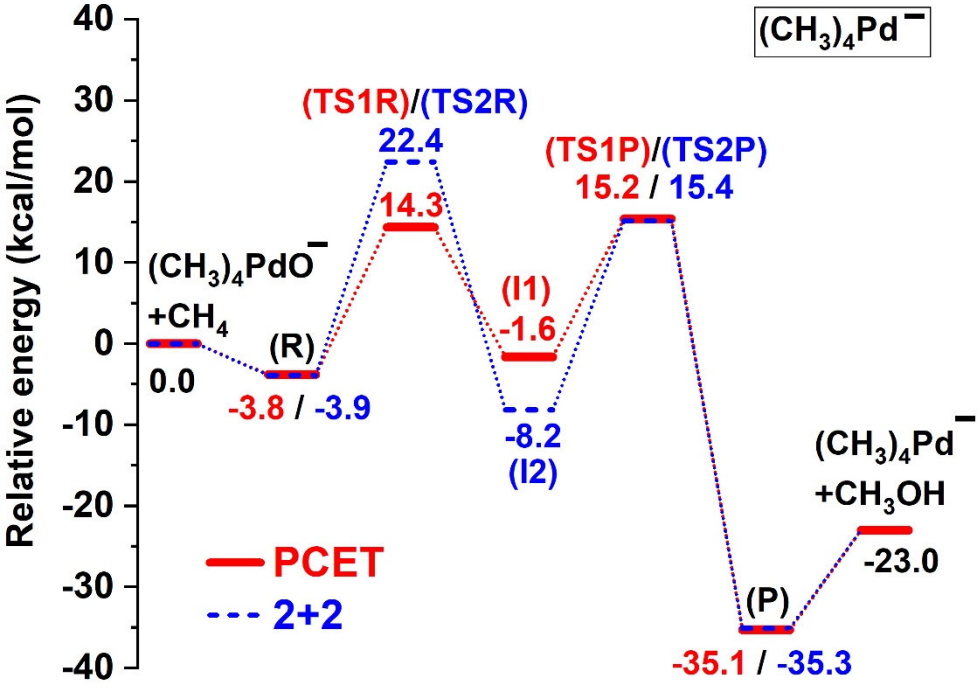

Figure S2. Energy diagram for the reaction $(CH_3)_4PdO^-$ + CH_4 → $(CH_3)_4Pd^-$ + CH_3OH at the MN15/TZ level of theory.

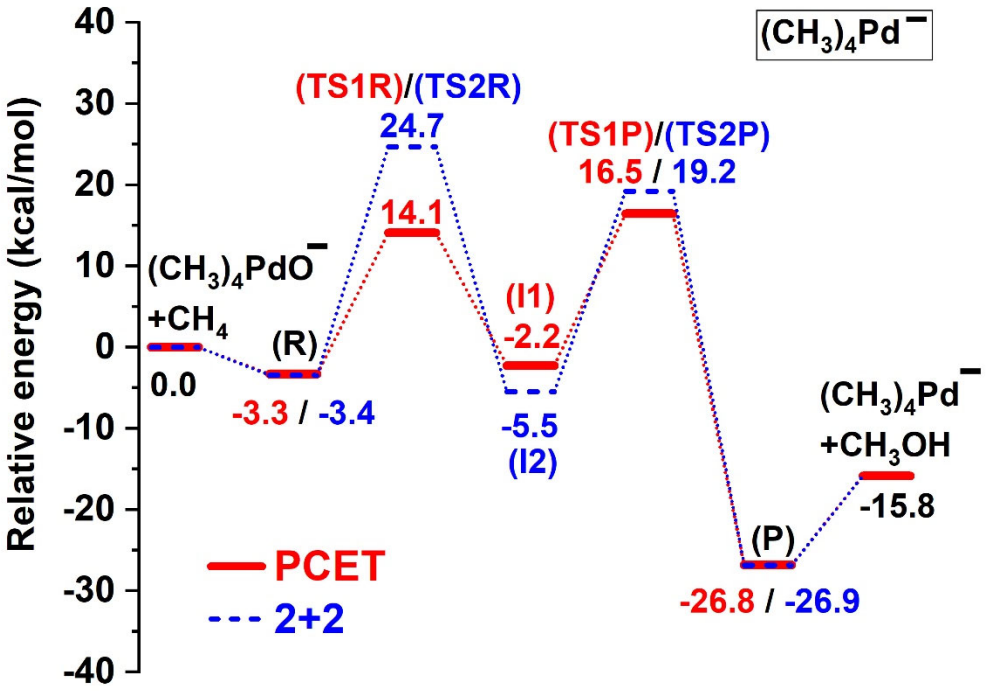

Figure S3. Energy diagram for the reaction $(CH_3)_4PdO^-$ + CH_4 → $(CH_3)_4Pd^-$ + CH_3OH at the CCSD(T)/DZ//MN15/TZ level of theory.

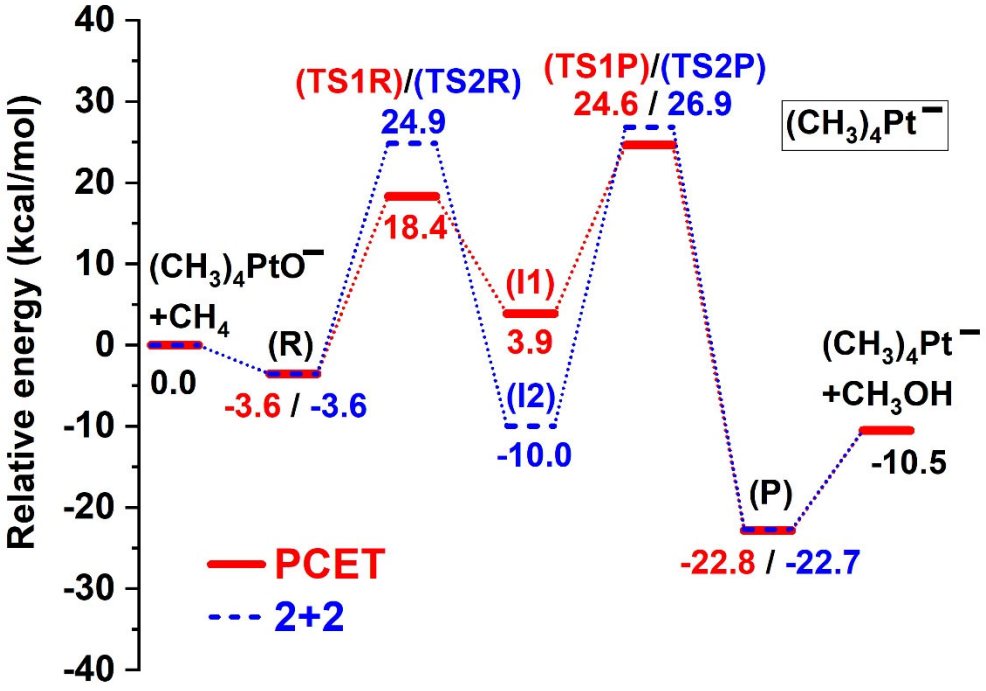

Figure S4. Energy diagram for the reaction $(CH_3)_4PtO^-$ + CH_4 → $(CH_3)_4Pt^-$ + CH_3OH at the MN15/TZ level of theory.

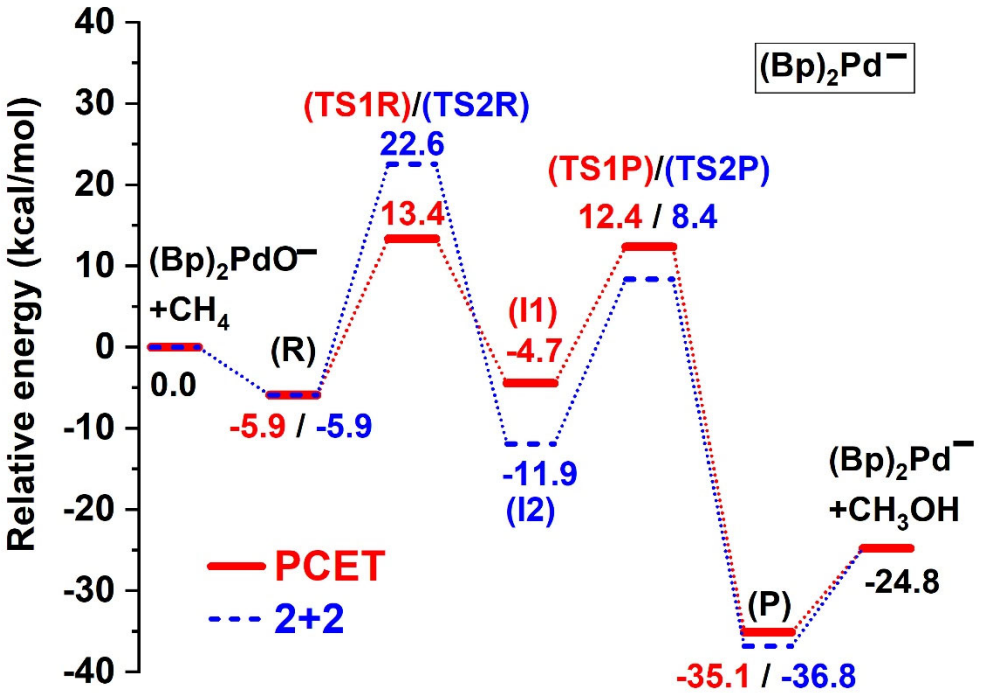

Figure S5. Energy diagram for the reaction $(Bp)_2PdO^- + CH_4 \rightarrow (Bp)_2Pd^- + CH_3OH$ at the MN15/TZ level of theory.

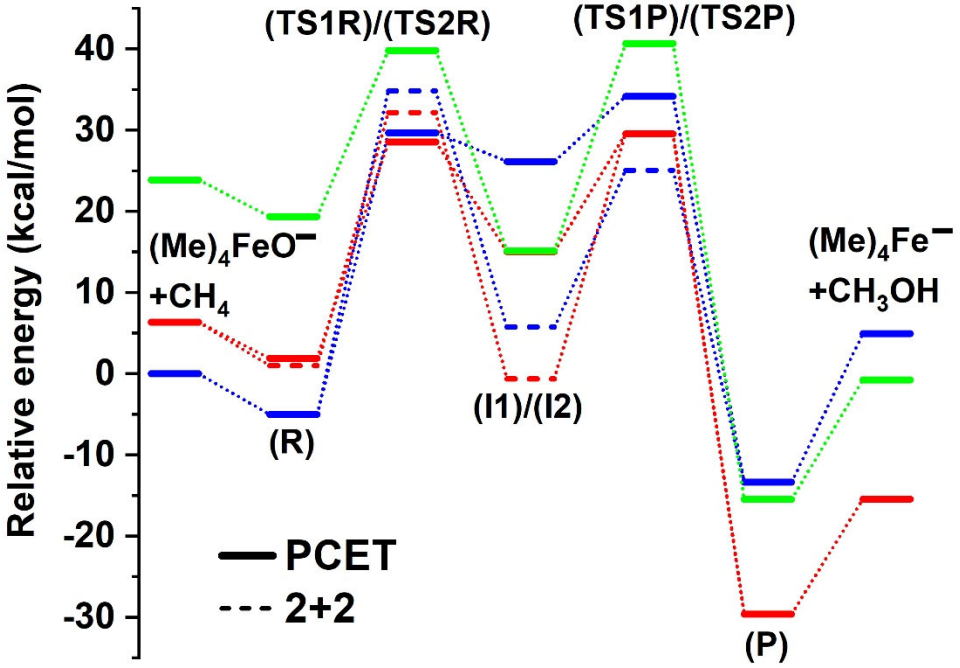

Figure S6. Energy diagram for the reaction $(CH_3)_4FeO^- + CH_4 \rightarrow (CH_3)_4Fe^- + CH_3OH$ at the MN15/TZ level of theory. Blue/red/green correspond to doublet/quartet/sextet spin multiplicities.

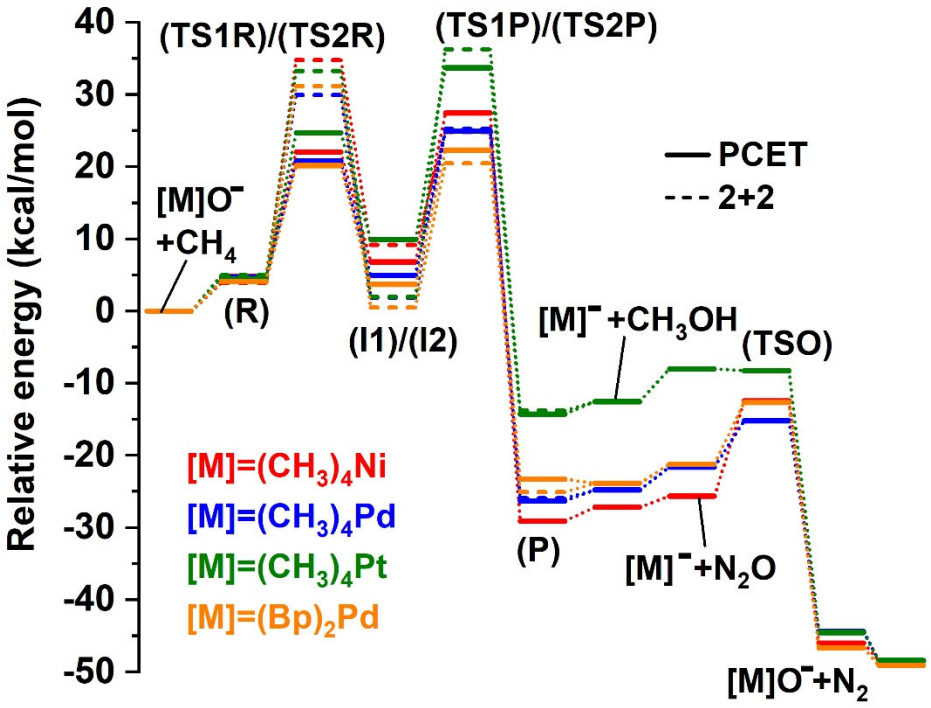

Figure S7. Free energy diagram for the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ facilitated by $[M]O^-$ at the MN15 level of theory.

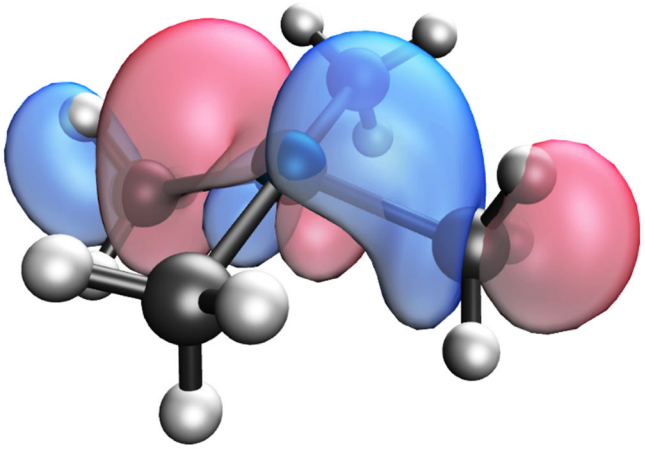

Figure S8. Contour for the singly occupied molecular orbital of $(CH_3)_4Pd^-$.

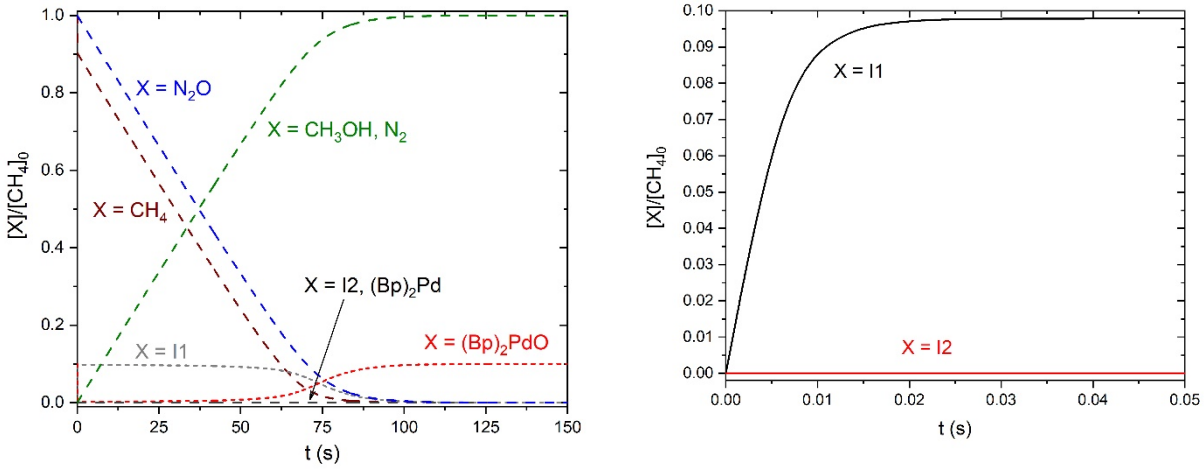

Figure S9. Left: Time evolution for the concentration of the species present in the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ catalyzed by $(Bp)_2PdO^-$. The concentrations are reported with respect to the initial concentration of CH_4, $[CH_4]_0$, which is equal to that of N_2O. Right: Time evolution of intermediates I1 and I2 in the beginning of the reaction. [I2] remains zero throughout the reaction, while [I1] is nearly constant at approximately $[CH_4]_0$ until close to the end of the reaction, where it gradually drops to zero.

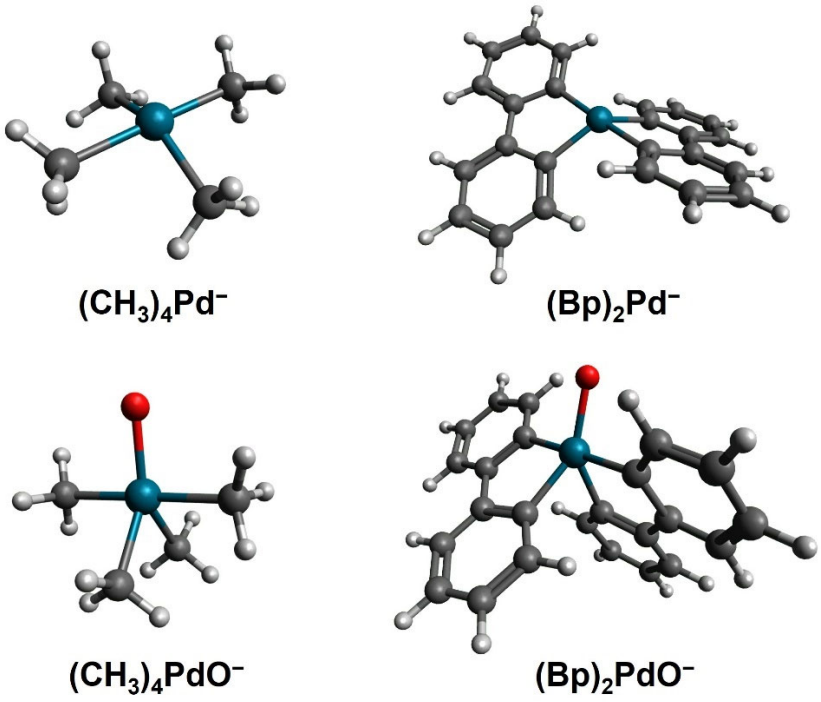

Figure S10. Structures (MN15) of the oxidized and reduced forms of the Pd catalysts.

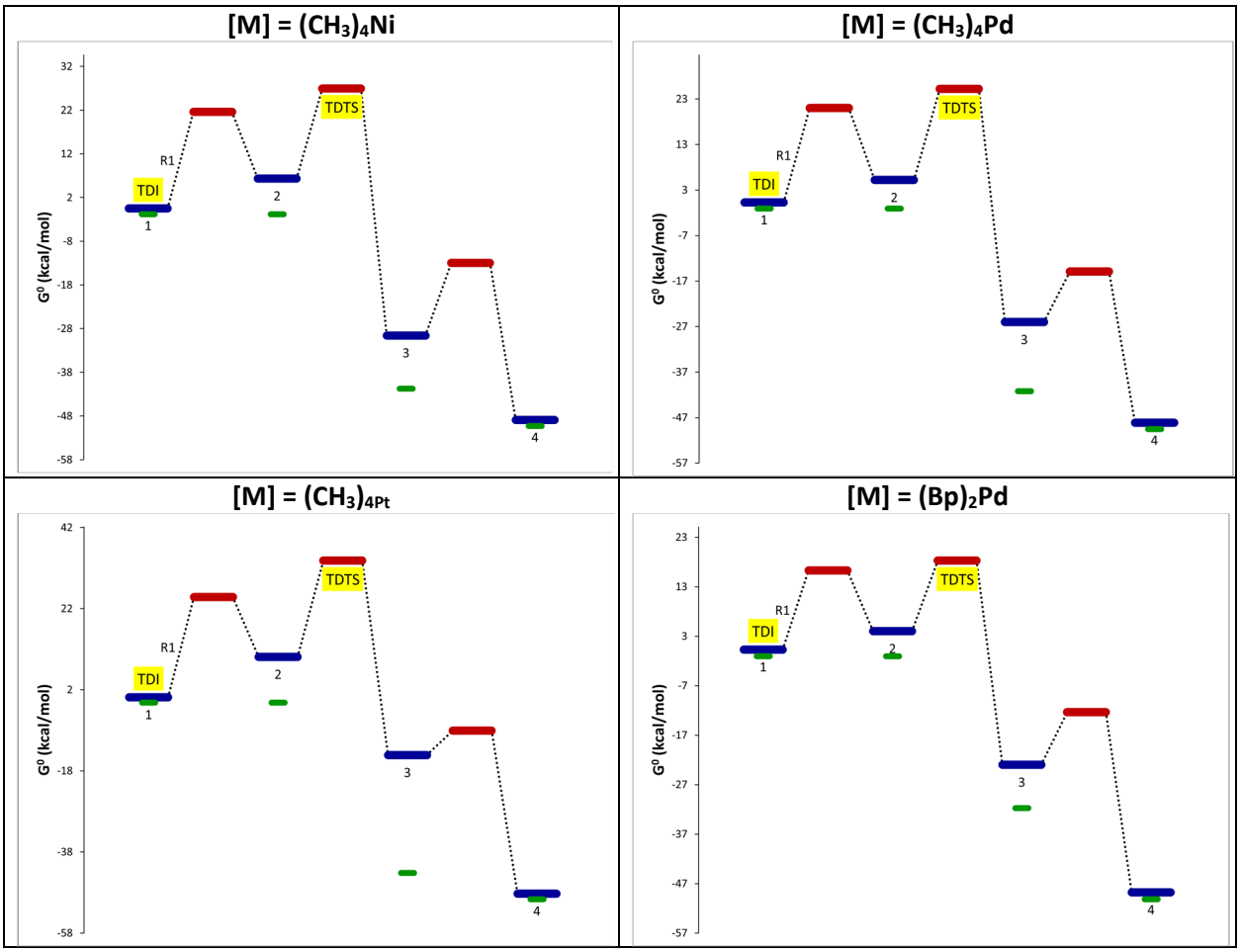

Figure S11. Free energy diagrams showing the TDI/TDTS species for the $[M]O^- + CH_4 + N_2O \rightarrow I1 + N_2O \rightarrow [M]^- + CH_3OH + N_2O \rightarrow [M]O^- + CH_3OH + N_2$.

Table S1. Electronic energies (a.u.) for the lowest lying spin (S) states of the catalytic species considered presently. Adiabatic (EA, eV) and vertical electron affinities (VEA, eV) are reported for the neutral species.

		MN15 [a]				CCSD(T) [b]	
Species	S	$-E_{optg}$ [c]	$-E_{vert}$ [d]	EA	VEA	$-E_{vert}$ [b]	VEA
$(CH_3)_4Ni^-$	$^1/_2$	1668.058424				1666.389759	
$(CH_3)_4Ni$	0	1668.002843	1667.949651	1.512	2.960	1666.292250	2.653
$(CH_3)_4Ni$	1	1667.966854	1667.948204	2.492	2.999	1666.282986	2.905
$(CH_3)_4NiO^-$	$^1/_2$	1743.186788				1741.414060	
$(CH_3)_4NiO$	0	1743.206730	1743.079366	-0.543 [e]	2.923	N/A [f]	
$(CH_3)_4NiO$	1	1743.076477	1743.062008	3.002	3.395	1741.333709	2.186
$(CH_3)_4Pd^-$	$^1/_2$	286.692872				286.094914	
$(CH_3)_4Pd$	0	286.638032	286.598756	1.492	2.561	286.010978	2.284
$(CH_3)_4Pd$	1	286.604351	286.586138	2.409	2.904	285.992145	2.796
$(CH_3)_4PdO^-$	$^1/_2$	361.826440				361.128821	
$(CH_3)_4PdO$	0	361.720034	361.711087	2.895	3.139	361.015418	3.086
$(CH_3)_4PdO$	1	361.714363	361.702844	3.050	3.363	361.008238	3.281
$(CH_3)_4Pt^-$	$^1/_2$	278.770734				278.232031	
$(CH_3)_4Pt$	0	278.711813	278.676698	1.603	2.559	278.145783	2.347
$(CH_3)_4Pt$	1	278.680853	278.651392	2.446	3.247	278.116055	3.156
$(CH_3)_4PtO^-$	$^1/_2$	353.924194				353.286322	
$(CH_3)_4PtO$	0	353.825762	353.799498	2.678	3.393	353.163947	3.330
$(CH_3)_4PtO$	1	353.803981	353.789634	3.271	3.662	N/A [f]	
$(Bp)_2Pd^-$	$^1/_2$	1050.425985				N/A [f]	
$(Bp)_2Pd^-$	$^3/_2$	1050.323041	1050.305382	2.801	3.282	N/A [f]	
$(Bp)_2Pd$	0	1050.338118	1050.304059	2.391	3.318	N/A [f]	
$(Bp)_2Pd$	1	1050.291334	1050.275015	3.664	4.108	N/A [f]	
$(Bp)_2PdO^-$	$^1/_2$	1125.541575				N/A [f]	
$(Bp)_2PdO^-$	$^3/_2$	1125.476728	1125.429601	1.765	3.047	N/A [f]	
$(Bp)_2PdO$	0	1125.395807	1125.385340	3.967	4.251	N/A [f]	
$(Bp)_2PdO$	1	1125.448729	1125.386787	2.526	4.212	N/A [f]	

[a] MN15/TZ for $(CH_3)_4M^{0,-}$ and $(CH_3)_4MO^{0,-}$ species, M=Ni, Pd, Pt; MN15/DZ for $(Bp)_2Pd^{0,-}$ and $(Bp)_2PdO^{0,-}$.

[b] CCSD(T)/DZ//MN15/TZ.

[c] Energies at the optimized geometry of each species.

[d] Energies at the optimized geometry of the doublet state of the corresponding anion.

[e] The geometry optimization for $(CH_3)_4NiO$ [S=0] converged to $(CH_3)_3Ni(OCH_3)$.

[f] Not Available for technical reasons.

Table S2. Relative free energy values for the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ facilitated by $[M]O^-$ at the MN15 level of theory (values used for Figure S7).

[M]	$(CH_3)_4Ni$ [a]	$(CH_3)_4Pd$ [a]	$(CH_3)_4Pt$ [a]	$(Bp)_2Pd$ [b]
$[M]O^- + CH_4$	0.00	0.00	0.00	0.00
R	4.77	4.73	4.48	4.15
TS1R	22.08	20.77	24.71	20.16
I1	6.83	4.92	9.94	3.71
TS1P	27.45	24.96	33.72	22.34
TS2R	34.78	29.94	33.27	31.16
I2	9.17	1.91	1.98	0.51
TS2P	24.80	25.28	36.28	20.48
P	-29.10	-26.30	-14.28	-23.30
$[M]^- + CH_3OH$	-27.17	-24.78	-12.55	-23.87
$[M]^- + N_2O$	-25.63	-21.60	-7.97	-21.21
TSO	-12.46	-15.18	-8.22	-12.66
$[M]O^- + N_2$	-48.43	-48.43	-48.43	-49.09

[a] MN15/TZ; [b] MN15/DZ.

Table S3. Relative electronic energies for the reaction $(CH_3)_4FeO^- + CH_4 \rightarrow (CH_3)_4Fe^- + CH_3OH$ at the MN15/TZ level of theory (values used for Figure S6).

Spin (S)	$^1/_2$	$^3/_2$	$^5/_2$
$(CH_3)_4FeO^- + CH_4$	0.00	6.37	23.89
R	-5.01	0.98	19.38
TS1R	29.70	28.57	39.84
I1	26.16	15.08	15.16
TS1P	34.17	29.53	40.71
TS2R	34.84	32.19	39.84
I2	5.78	-0.62	15.13
TS2P	25.05	29.67	40.71
P	-13.36	-29.58	-15.47
$(CH_3)_4Fe^- + CH_3OH$	4.99	-15.44	-0.74

Table S4. MN15 optimized energies (a.u.) and geometries (Cartesian coordinates in Å) of all intermediates and transition states (see Figure 2 of the manuscript) for the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ catalyzed by $[M]O^-$.

	[M] = $(CH_3)_4Ni$	**[M] = $(CH_3)_4Pd$**	**[M] = $(CH_3)_4Pt$**	**[M] = $(Bp)_2Pd$**
R	-1783.664412	-402.301644	-394.398971	-1166.001044
	C -3.321101 0.062155 0.457264	C -3.568461 0.212493 0.632305	C 3.666845 -0.216668 0.632377	C 0.432923 -3.688959 0.709274
	H -2.523962 0.061666 -0.286678	H -2.749259 0.676145 0.083746	H 2.900359 -0.711849 0.039052	H 0.721023 -3.271399 -0.262649
	H -4.293188 0.121024 -0.031397	H -4.082862 -0.491662 -0.019598	H 4.160293 0.540670 0.025636	H 0.523919 -4.781338 0.689996
	H -3.264602 -0.852783 1.046087	H -3.163453 -0.327714 1.486866	H 3.187853 0.266699 1.482373	H 1.078130 -3.272297 1.492287
	H -3.193389 0.919934 1.116511	H -4.270533 0.970133 0.979232	H 4.401384 -0.939241 0.986725	H -0.605100 -3.404107 0.916676
	O -0.573630 0.163775 -1.671796	O -0.749960 1.284188 -1.224476	O 0.745054 -1.317729 -1.115020	O 0.053150 -1.496549 -2.387146
	Ni 0.362382 0.007627 -0.205687	Pd 0.309218 0.083977 -0.170366	Pt -0.227848 -0.078773 -0.129250	C 0.432402 -0.317400 1.110508
	C 2.185122 -0.074647 0.317694	C 2.045247 -0.967625 -0.119283	C -1.927081 1.077840 -0.150847	C -0.481333 -0.557205 2.138429
	C 0.256006 -0.182688 1.691723	C 0.288975 -0.884803 1.609175	C -0.210258 0.952075 1.645925	H -1.549309 -0.584988 1.922928
	C 0.163759 -1.953156 -0.390866	C -0.779802 -1.560451 -0.940517	C 0.918689 1.528771 -0.911433	C -0.030482 -0.776137 3.444688
	H 0.955305 -2.476425 0.157024	H -0.141816 -2.450127 -0.984429	H 0.288010 2.412778 -1.059118	H -0.753201 -0.972520 4.238371
	H 0.170426 -2.258134 -1.438985	H -1.173277 -1.344366 -1.936430	H 1.394630 1.274394 -1.862027	C 1.336903 -0.739177 3.732945
	H -0.804638 -2.218010 0.047927	H -1.620443 -1.771036 -0.271223	H 1.707601 1.797540 -0.200198	H 1.689253 -0.911859 4.751097
	C 0.401062 1.984310 -0.112851	C 1.406936 1.713198 0.613035	C -1.440572 -1.597543 0.719963	C 2.250525 -0.479789 2.710383
	H 1.032306 2.352266 -0.926488	H 2.234374 1.938274 -0.067501	H -2.271067 -1.826975 0.043579	H 3.318953 -0.460783 2.933649
	H 0.804977 2.326554 0.845836	H 1.823550 1.455567 1.592981	H -1.866375 -1.259847 1.671444	Pd 0.000283 -0.373963 -0.854002
	H -0.609891 2.377151 -0.249919	H 0.781410 2.603571 0.706183	H -0.883832 -2.521734 0.893697	C 2.035171 -0.044165 -1.004550
	H 0.548482 -1.168812 2.054460	H 0.225825 -1.966461 1.491218	H -0.111299 2.030264 1.498206	C 2.705121 -0.036223 0.239133
	H -0.831888 -0.067674 1.754957	H -0.643813 -0.500397 2.030541	H 0.681744 0.583540 2.162702	C 4.089785 0.172370 0.310706
	H 0.745995 0.598359 2.273822	H 1.128372 -0.618548 2.251482	H -1.087121 0.756435 2.268164	H 4.603171 0.177707 1.275127
	H 2.583879 -0.076191 -0.702530	H 2.443390 -0.743753 -1.112380	H -2.371309 0.890138 -1.132940	C 4.823338 0.376879 -0.860515
	H 2.483046 -0.985070 0.837274	H 1.897415 -2.042424 -0.012440	H -1.724974 2.147360 -0.053469	C 4.173695 0.360890 -2.100120
	H 2.530400 0.806548 0.857908	H 2.729382 -0.600508 0.646124	H -2.639924 0.779116 0.621951	H 4.750039 0.512205 -3.015965
				H 5.900687 0.545253 -0.808291
				C 2.790524 0.144122 -2.167466
				H 2.293508 0.113636 -3.139997
				C 1.817056 -0.263884 1.394170
				C -2.028887 -0.692062 -0.644266
				C -2.733475 -1.878332 -0.876896
				H -2.194512 -2.760224 -1.233515
				C -4.117933 -1.945123 -0.666092
				H -4.656042 -2.878495 -0.847704
				C -4.817240 -0.814647 -0.228355
				H -5.895300 -0.866694 -0.064438
				C -4.132688 0.382623 -0.002714
				H -4.684985 1.262719 0.335357
				C -0.510231 1.439779 -0.143913
				C -1.904190 1.635821 0.004008
				C -2.383358 2.919738 0.299929

				H -3.458340 3.082722 0.400501 C -1.506304 3.995185 0.450251 C -0.131223 3.791661 0.305241 H 0.562315 4.626309 0.422994 H -1.893715 4.989824 0.676988 C 0.365643 2.515372 0.015945 H 1.440387 2.359296 -0.080181 C -2.747262 0.443618 -0.207719
TS1R	-1783.630372 C -3.474888 0.065700 -0.000078 H -2.191120 0.580970 0.000121 H -4.065481 0.976314 0.000114 H -3.558637 -0.520709 -0.907846 H -3.558820 -0.521230 0.907336 O -1.177341 1.086264 0.000115 Ni 0.319268 0.058025 0.000027 C 1.591087 -0.671763 -1.196262 C 1.591407 -0.671805 1.195963 C -0.687573 -1.636638 0.000172 H -0.046089 -2.524555 0.000296 H -1.327260 -1.651015 -0.887877 H -1.327338 -1.650819 0.888165 C 1.260132 1.793684 0.000013 H 0.938569 2.344541 -0.887607 H 2.351071 1.689250 -0.000536 H 0.939448 2.343936 0.888333 H 1.685180 -1.756996 1.159974 H 1.064146 -0.370730 2.108274 H 2.573202 -0.200664 1.160382 H 1.063960 -0.369990 -2.108418 H 1.684282 -1.757018 -1.160728 H 2.573133 -0.201159 -1.160519	-402.272698 C -3.592110 0.048304 -0.013659 H -2.381583 0.668592 0.008828 H -3.687440 -0.344712 -1.019587 H -3.537380 -0.720737 0.747578 H -4.280999 0.855623 0.213589 O -1.372494 1.208382 0.033379 Pd 0.249314 0.063537 -0.001907 C 1.665038 -0.700940 -1.219730 C 1.565327 -0.807392 1.251865 C -0.812194 -1.762838 -0.053763 H -0.139046 -2.614412 -0.208784 H -1.555981 -1.749319 -0.856476 H -1.340212 -1.906006 0.895580 C 1.331773 1.871591 0.019643 H 1.364679 2.265598 -1.001727 H 2.360484 1.728230 0.371106 H 0.822104 2.600452 0.654029 H 1.575891 -1.892031 1.147547 H 1.140866 -0.525634 2.218476 H 2.573265 -0.404736 1.156176 H 1.235229 -0.479098 -2.199858 H 1.795304 -1.777239 -1.106322 H 2.619302 -0.186687 -1.105620	-394.364064 C -3.665056 0.055053 -0.012221 H -2.410137 0.651026 0.003858 H -3.769325 -0.334957 -1.017845 H -3.621268 -0.709604 0.753392 H -4.317735 0.890921 0.216163 O -1.408192 1.178004 0.027977 Pt 0.183364 0.051658 0.000929 C 1.598257 -0.732080 -1.235738 C 1.519663 -0.841041 1.247826 C -0.893055 -1.767022 -0.048931 H -0.226800 -2.624461 -0.210433 H -1.643806 -1.769202 -0.847520 H -1.423769 -1.933968 0.896816 C 1.294582 1.849802 0.021294 H 1.393456 2.236795 -1.000164 H 2.307380 1.693359 0.414662 H 0.800409 2.621042 0.619365 H 1.535355 -1.927360 1.129161 H 1.159814 -0.597466 2.251810 H 2.535478 -0.454693 1.133660 H 1.224473 -0.530921 -2.244172 H 1.726358 -1.811106 -1.115771 H 2.566947 -0.241040 -1.112638	-1165.970354 C -1.656079 -0.953366 1.402119 C -0.306244 -0.570904 1.225685 C 0.672481 -1.001402 2.121841 H 1.713567 -0.718207 1.971764 C 0.313759 -1.800522 3.214093 H 1.083825 -2.130165 3.913747 C -1.017844 -2.178847 3.405447 H -1.294710 -2.801639 4.257583 C -1.992946 -1.756272 2.501031 H -3.034537 -2.045542 2.654538 H 4.824991 -0.830746 -0.643819 C 4.217244 -0.004877 -0.266111 C 2.821375 -0.024630 -0.396995 C 4.841460 1.081127 0.353538 H 5.927754 1.097505 0.462543 C 2.032239 1.042148 0.088348 C 4.071039 2.149037 0.828528 C 2.676291 2.128839 0.688679 H 4.562726 3.001063 1.304629 H 2.073929 2.970844 1.037979 H -4.410477 -1.462018 1.029434 C -3.955958 -0.786861 0.300513 C -2.600018 -0.442193 0.393914 C -4.732060 -0.272910 -0.740946 H -5.786921 -0.541436 -0.821861 C -2.003425 0.440682 -0.533492 C -4.149475 0.581587 -1.684966 C -2.797686 0.933309 -1.575988 H -4.754394 0.976024 -2.504732 H -2.360861 1.617572 -2.308372 H -0.273803 -3.771160 -2.682694 C 0.377477 -3.025541 -2.222679 C -0.186483 -1.926271 -1.562573 H -1.271241 -1.830979 -1.508248 C 1.765254 -3.170419 -2.286030 H 2.206451 -4.026868 -2.798859 C 0.629511 -0.957378 -0.972927 C 2.586744 -2.211814 -1.689735

				C 2.037702 -1.103998 -1.029132 H 3.671651 -2.320538 -1.748577 O -0.136775 2.751728 -0.211848 Pd 0.001743 0.793369 -0.194280 C -2.420368 3.749930 -0.030857 H -2.185161 4.680955 0.490575 H -2.818485 3.890727 -1.037980 H -2.982240 3.026783 0.563471 H -1.221961 3.198294 -0.187275
I1	-1783.655992 C -3.280724 0.079384 0.659239 H -1.146305 -0.285159 -1.968702 H -3.110835 -0.816593 1.233759 H -2.518076 0.427695 -0.024958 H -4.209068 0.612612 0.783133 O -0.801435 0.520687 -1.570241 Ni 0.327167 0.026804 -0.172362 C 2.143595 -0.374251 0.122825 C 0.362279 -0.253325 1.699004 C -0.103657 -1.876304 -0.502039 H 0.424471 -2.585069 0.147690 H 0.134399 -2.117948 -1.546228 H -1.184391 -2.012322 -0.358632 C 0.637934 1.943557 0.087785 H 0.977253 2.341142 -0.872943 H 1.354033 2.198739 0.877702 H -0.338329 2.384076 0.316941 H 0.582610 -1.278983 1.995747 H -0.699154 -0.031539 1.863703 H 0.976742 0.448180 2.262932 H 2.434239 -0.293609 -0.931048 H 2.333754 -1.382778 0.489251 H 2.682889 0.361172 0.718826	-402.298101 C -3.402641 0.097865 0.836056 H -1.439087 0.379337 -1.918746 H -3.224473 -0.908430 1.177677 H -2.672981 0.583770 0.203202 H -4.304230 0.604296 1.139310 O -0.979310 1.048268 -1.399737 Pd 0.283700 0.054655 -0.172257 C 2.129818 -0.709878 0.099495 C 0.235430 -0.683824 1.696194 C -0.479936 -1.787333 -0.881352 H 0.078647 -2.652008 -0.502063 H -0.454784 -1.815043 -1.977886 H -1.526219 -1.890456 -0.566183 C 1.012292 1.905569 0.490613 H 1.789288 2.244148 -0.204424 H 1.446547 1.856609 1.496623 H 0.194676 2.630719 0.473799 H 0.302624 -1.771416 1.703310 H -0.760299 -0.361540 2.012087 H 0.993981 -0.248150 2.345816 H 2.569535 -0.548798 -0.888817 H 2.121916 -1.775600 0.331050 H 2.699348 -0.162099 0.850924	-394.387091 C -3.509343 0.086797 0.845137 H -1.428749 0.545289 -1.896544 H -3.319165 -0.933620 1.132510 H -2.762945 0.625437 0.281363 H -4.434248 0.556482 1.136091 O -0.950598 1.153574 -1.321874 Pt 0.212567 0.050189 -0.124347 C 2.050943 -0.783953 0.104925 C 0.138682 -0.844178 1.692186 C -0.611009 -1.713306 -0.959351 H 0.022456 -2.592429 -0.779338 H -0.757409 -1.633551 -2.046088 H -1.594428 -1.928924 -0.518469 C 0.995192 1.832339 0.669654 H 1.867976 2.157179 0.088183 H 1.324804 1.715914 1.711243 H 0.252973 2.636001 0.624728 H 0.220144 -1.932090 1.621997 H -0.852336 -0.583488 2.078247 H 0.897840 -0.470865 2.384324 H 2.568461 -0.573279 -0.836378 H 2.016694 -1.867141 0.252648 H 2.615670 -0.330433 0.924220	-1165.998762 C 1.704672 0.704845 1.359796 C 0.349790 0.332618 1.197115 C -0.567621 0.554464 2.225575 H -1.613273 0.279838 2.090874 C -0.145264 1.134308 3.427308 H -0.868952 1.301557 4.226997 C 1.191586 1.503244 3.601069 H 1.519355 1.955964 4.538197 C 2.106909 1.286746 2.570696 H 3.153703 1.562246 2.712230 H -4.932616 0.716341 -0.180784 C -4.266880 -0.139009 -0.040931 C -2.887127 -0.016448 -0.256743 C -4.799031 -1.369420 0.354396 H -5.872076 -1.469462 0.529800 C -2.023242 -1.120408 -0.081515 C -3.954667 -2.474777 0.515809 C -2.576801 -2.349447 0.289628 H -4.377094 -3.438115 0.812427 H -1.919318 -3.216926 0.384617 H 4.450122 1.241508 0.978612 C 3.958542 0.712543 0.158975 C 2.594885 0.398797 0.225910 C 4.704973 0.335477 -0.961856 H 5.767788 0.577369 -1.017919 C 1.949025 -0.295902 -0.823364 C 4.083917 -0.351597 -2.010546 C 2.717606 -0.662143 -1.935349 H 4.666403 -0.645845 -2.886660 H 2.249676 -1.204088 -2.762796 H -0.081532 4.262392 -1.889048 C -0.675082 3.409169 -1.555246 C -0.033899 2.218340 -1.190516 H 1.053859 2.154178 -1.231919 C -2.066846 3.507475 -1.483326 H -2.567366 4.435659 -1.764550 C -0.779360 1.115917 -0.767370

				C -2.816096 2.411282 -1.050588 C -2.190251 1.210674 -0.688034 H -3.904673 2.485463 -1.006142 O 0.202578 -2.607510 -1.017121 Pd -0.038144 -0.724401 -0.448533 C 3.201464 -2.935129 0.895610 H 3.573037 -3.838216 1.369212 H 3.895658 -2.240127 0.432202 H 2.134983 -2.729665 0.874513 H 1.119102 -2.737244 -1.299391
TS1P	-1783.627895 H -2.600177 -1.040547 0.826133 H -3.773559 -0.025330 -0.160373 C -2.890711 -0.069119 0.459086 O -1.498653 0.114816 -0.825806 H -2.710424 0.767831 1.119200 H -1.613313 1.051700 -1.033963 Ni 0.309722 0.002246 -0.192407 C 2.192331 -0.117304 -0.294069 C 0.181000 -1.952172 -0.342545 H 0.444600 -2.211944 -1.376123 H -0.853300 -2.267259 -0.167990 H 0.848456 -2.493699 0.335844 H 2.712581 0.668859 0.254652 H 2.339575 0.032074 -1.371280 H 2.574148 -1.096550 -0.001986 C 0.626147 -0.065128 1.713423 H -0.412628 -0.116370 2.055139 H 1.109477 0.847281 2.063157 H 1.180086 -0.950352 2.023630 C 0.383571 1.988292 -0.200837 H 1.303631 2.397243 0.231021 H -0.460993 2.353783 0.403145 H 0.274827 2.394452 -1.216720	-402.270986 H -2.672439 -1.077560 0.886995 H -3.950273 -0.064965 0.037461 C -3.009133 -0.104628 0.565158 O -1.734888 0.106337 -0.825373 H -2.781668 0.722848 1.222787 H -1.850073 1.045315 -1.028173 Pd 0.267519 0.004839 -0.211720 C 2.272008 -0.114310 -0.135972 C 0.179959 -2.092275 -0.297050 H 0.601384 -2.437461 -1.248799 H -0.863255 -2.421743 -0.247523 H 0.745906 -2.562206 0.515648 H 2.709511 0.702302 0.441351 H 2.589017 -0.029579 -1.179885 H 2.601758 -1.073245 0.267745 C 0.537727 -0.033550 1.817596 H -0.487804 -0.085193 2.187473 H 1.028427 0.885090 2.135320 H 1.106485 -0.912800 2.115018 C 0.324567 2.124889 -0.168941 H 1.219477 2.496670 0.343704 H -0.553897 2.492213 0.381116 H 0.299906 2.566271 -1.172901	-394.354034 H -2.768545 -1.048163 0.880179 H -4.017049 -0.017147 0.015629 C -3.084620 -0.067719 0.558949 O -1.795807 0.158308 -0.762504 H -2.881003 0.742412 1.245726 H -1.898887 1.098025 -0.973791 Pt 0.207855 0.006311 -0.162671 C 2.220733 -0.145781 -0.014482 C 0.061385 -2.087546 -0.298738 H 0.469453 -2.449236 -1.251539 H -0.983376 -2.419436 -0.250394 H 0.617122 -2.593486 0.502491 H 2.651580 0.659384 0.590426 H 2.642114 -0.075253 -1.023191 H 2.527370 -1.104576 0.416762 C 0.386487 -0.110604 1.873155 H -0.633819 -0.116868 2.264851 H 0.929559 0.756889 2.252691 H 0.900828 -1.029168 2.161160 C 0.335797 2.119497 -0.090655 H 1.040988 2.451202 0.683783 H -0.635418 2.584558 0.143889 H 0.674164 2.555047 -1.039675	-1165.971902 C 1.820062 0.194755 1.510370 C 0.449923 -0.053734 1.275213 C -0.463346 -0.039874 2.328051 H -1.523939 -0.208744 2.136132 C -0.017300 0.197652 3.635544 H -0.734145 0.203045 4.459003 C 1.337528 0.433958 3.883246 H 1.683968 0.620471 4.901227 C 2.248070 0.433603 2.824523 H 3.306348 0.614422 3.024524 H -4.783940 1.144601 -0.081682 C -4.190574 0.227346 -0.106232 C -2.807313 0.280424 -0.323719 C -4.823320 -1.003213 0.094372 H -5.900387 -1.044020 0.267403 C -2.025586 -0.902272 -0.365767 C -4.066967 -2.179341 0.086095 C -2.683972 -2.119147 -0.140668 H -4.554472 -3.141671 0.259335 H -2.116093 -3.056981 -0.123344 H 4.589727 0.653959 1.246238 C 4.070631 0.397817 0.319542 C 2.690690 0.150677 0.319648 C 4.793623 0.313216 -0.873104 H 5.867417 0.509953 -0.877735 C 2.008183 -0.185483 -0.873208 C 4.136807 -0.033978 -2.058887 C 2.758122 -0.289953 -2.051019 H 4.703535 -0.111459 -2.989985 H 2.262337 -0.583695 -2.979467 H 0.312707 4.608105 -0.919428 C -0.344130 3.743640 -0.803307 C 0.206643 2.458483 -0.733139 H 1.288566 2.332037 -0.786029 C -1.728493 3.921912 -0.719578 H -2.158452 4.923703 -0.773175

				C -0.618285 1.336055 -0.597355 C -2.558254 2.810777 -0.560781 C -2.021082 1.517153 -0.493991 H -3.639099 2.952263 -0.492719 Pd -0.006565 -0.560575 -0.641063 O 0.354564 -2.441774 -1.344857 H 2.018364 -2.903053 0.217860 C 1.126034 -3.521498 0.176357 H 0.347487 -3.330834 0.912218 H 1.220797 -4.527655 -0.224049 H -0.511413 -2.867651 -1.441816
TS2R	-1783.615430 C 2.082042 -0.119709 0.678894 H 1.572857 -0.162206 -0.655147 H 2.648868 -1.057222 0.664913 H 2.766686 0.729536 0.578433 H 1.601063 -0.044462 1.653444 O 0.899548 -0.210491 -1.657965 Ni -0.061987 0.002224 -0.046738 C -1.790898 0.017125 -0.861736 C -1.022165 0.268677 1.597942 C 0.185802 1.981539 -0.106766 H -0.776062 2.482178 -0.232338 H 0.864254 2.257137 -0.915849 H 0.626652 2.258621 0.854184 C -0.184163 -1.966994 0.213517 H -1.224420 -2.296876 0.202021 H 0.257016 -2.156547 1.195317 H 0.387376 -2.489722 -0.555099 H -0.279408 0.452249 2.379646 H -1.609827 -0.615431 1.855005 H -1.681899 1.136320 1.527931 H -1.560007 -0.364787 -1.856420 H -2.174880 1.036220 -0.908913 H -2.502730 -0.627191 -0.345860	-402.259842 C 2.162665 -0.127680 0.850493 H 1.803016 -0.166274 -0.555003 H 2.738974 -1.057311 0.901776 H 2.840512 0.731910 0.834570 H 1.585098 -0.060593 1.776935 O 1.246810 -0.190856 -1.631035 Pd -0.043311 -0.000651 -0.037105 C -1.807346 0.112291 -1.017208 C -1.187667 0.176947 1.631875 C 0.131277 2.112313 -0.041934 H -0.859289 2.568911 -0.108047 H 0.753163 2.457058 -0.870226 H 0.599211 2.395734 0.905018 C -0.296771 -2.097603 0.115973 H -1.282551 -2.319383 0.531137 H 0.477097 -2.504320 0.772682 H -0.206687 -2.551446 -0.873093 H -1.495731 1.214719 1.773426 H -0.586472 -0.146382 2.485934 H -2.073238 -0.457139 1.563263 H -1.521284 0.200925 -2.066713 H -2.375482 0.986805 -0.698393 H -2.391462 -0.794025 -0.853350	-394.353657 C 2.202053 -0.173684 0.768372 H 1.823283 -0.123437 -0.587534 H 2.760518 -1.114097 0.759217 H 2.887241 0.678357 0.793076 H 1.638751 -0.151244 1.707002 O 1.159242 -0.059014 -1.648110 Pt -0.025168 0.004765 -0.037399 C -1.809100 0.153495 -0.993470 C -1.091091 0.026156 1.724491 C 0.074233 2.118310 0.126605 H -0.925579 2.527804 0.295828 H 0.498316 2.578187 -0.769211 H 0.702296 2.380452 0.984734 C -0.284363 -2.098791 0.050529 H -1.271152 -2.331630 0.460463 H 0.475229 -2.543707 0.702105 H -0.199366 -2.549027 -0.941583 H -1.151143 1.031037 2.153524 H -0.615658 -0.633691 2.459082 H -2.112160 -0.339106 1.572029 H -1.585525 0.226187 -2.061264 H -2.360106 1.041471 -0.674226 H -2.426197 -0.730045 -0.810443	-1165.955696 C 0.436547 -2.135628 -2.116350 H 0.077832 -0.846805 -2.633462 H -0.298585 -2.651634 -2.754023 H 1.445900 -2.254963 -2.531988 H 0.413663 -2.645695 -1.141427 O -0.200694 0.337229 -2.818590 C 0.437469 -0.975264 0.995553 C -0.477816 -1.540823 1.888352 H -1.538591 -1.569373 1.638893 C -0.045648 -2.075383 3.109307 H -0.773896 -2.515744 3.793110 C 1.307883 -2.042750 3.453400 H 1.643997 -2.458424 4.404954 C 2.228516 -1.471509 2.573711 H 3.286198 -1.444489 2.843565 Pd 0.012796 -0.245812 -0.824368 C 2.038939 0.128396 -0.815296 C 2.699464 -0.308483 0.353539 C 4.082036 -0.125063 0.501004 H 4.592092 -0.463366 1.405872 C 4.818044 0.495673 -0.511001 C 4.172387 0.929349 -1.674240 H 4.747424 1.414404 -2.466386 H 5.893623 0.640966 -0.394336 C 2.791319 0.741958 -1.823539 H 2.294839 1.084086 -2.735025 C 1.808618 -0.934147 1.348685 C -2.029179 -0.588008 -0.653652 C -2.758108 -1.701788 -1.080764 H -2.250049 -2.522528 -1.592846 C -4.139384 -1.794456 -0.855535 H -4.691431 -2.674937 -1.192334 C -4.811641 -0.758922 -0.199731 H -5.886730 -0.827131 -0.023318 C -4.100857 0.364183 0.231407

				H -4.630916 1.169233 0.745334 C -0.480820 1.425487 0.183116 C -1.863044 1.573401 0.443775 C -2.326412 2.737428 1.073619 H -3.393460 2.861091 1.269758 C -1.437369 3.744854 1.451885 C -0.071289 3.590148 1.203855 H 0.631156 4.371503 1.500763 H -1.808673 4.647363 1.940657 C 0.404470 2.431742 0.575179 H 1.473810 2.321734 0.392247 C -2.719332 0.451976 0.010331
I2	-1783.661386 C 1.557224 0.665959 -1.074378 H 2.191583 1.346998 -0.508744 H 2.124710 -0.183341 -1.454278 H 1.051536 1.191455 -1.887336 O 0.099417 -1.770573 -0.721894 H 1.029851 -2.016248 -0.755436 Ni -0.003061 -0.017996 -0.024142 C -0.204843 1.819143 0.553868 C -1.469760 -0.542510 1.234923 H -1.008723 -0.337596 2.202302 H -1.589943 -1.606891 1.046246 H -2.403419 0.005869 1.130397 H -0.248690 2.461305 -0.332115 H 0.648146 2.130650 1.163969 H -1.126012 1.959442 1.126553 C 1.517508 -0.450542 1.226725 H 1.039607 -1.178784 1.882034 H 1.824029 0.445342 1.766437 H 2.368705 -0.901393 0.715972 C -1.594386 0.254417 -1.177931 H -2.250728 1.056009 -0.842860 H -2.110452 -0.697573 -1.273106 H -1.084287 0.514420 -2.108159	-402.308596 C -1.693446 0.072133 -1.287115 H -0.858118 -2.362466 -0.272739 H -1.259910 -0.061730 -2.280590 H -2.389137 -0.736655 -1.058446 H -2.186386 1.040222 -1.199641 O 0.046450 -2.068409 -0.120548 Pd 0.000933 -0.023472 -0.012983 C 1.612736 -0.105452 1.361822 C 0.034024 2.019390 0.015572 C -1.578456 0.031446 1.411306 H -1.094083 0.365526 2.328423 H -1.936517 -0.993960 1.497790 H -2.374361 0.712221 1.116185 C 1.679533 0.084904 -1.302244 H 2.285812 0.965626 -1.101426 H 1.194491 0.146481 -2.278036 H 2.233245 -0.843094 -1.184931 H -0.864313 2.421409 0.492773 H 0.070557 2.381738 -1.016876 H 0.916344 2.389879 0.545143 H 1.995951 -1.121020 1.282808 H 1.142183 0.069860 2.330500 H 2.383382 0.638416 1.164624	-394.409174 C -0.001481 -2.063665 0.342862 H -0.426512 -2.244515 1.328978 H -0.633404 -2.496332 -0.434972 H 1.017230 -2.445990 0.282056 O -0.871465 0.000134 -1.874801 H -1.825034 0.001191 -1.729703 Pt -0.004651 0.000006 -0.062679 C 1.012130 -0.001149 1.741353 C 0.006234 2.063992 0.340809 H -0.418783 2.247602 1.326428 H -0.623533 2.498199 -0.437931 H 1.026398 2.442452 0.280250 H 1.651992 -0.883560 1.830064 H 0.309751 -0.000403 2.582388 H 1.654088 0.879721 1.830173 C -1.945066 0.003914 0.807985 H -2.511972 0.892351 0.499711 H -1.897514 0.005368 1.903946 H -2.514722 -0.883608 0.502159 C 1.893706 -0.003396 -0.973956 H 2.479228 0.877903 -0.682018 H 1.779972 -0.000798 -2.062681 H 2.474145 -0.889308 -0.685837	-1166.010620 C 0.402723 -2.160510 1.578947 H -1.178125 -2.659196 -1.383888 H 0.202463 -3.137771 1.132829 H 1.445568 -2.007151 1.861115 H -0.310597 -1.850674 2.344553 O -0.235753 -2.440547 -1.367936 C 0.532440 0.534437 1.219696 C -0.325954 1.186004 2.110167 H -1.396345 0.972021 2.082876 C 0.170478 2.116685 3.031217 H -0.514217 2.617308 3.718938 C 1.537472 2.408903 3.068181 H 1.925357 3.135609 3.784262 C 2.403915 1.765168 2.182821 H 3.472131 1.990536 2.215034 Pd -0.000720 -0.885501 -0.124595 C 2.012875 -0.830737 -0.502167 C 2.744550 0.082877 0.290728 C 4.130441 0.221211 0.121122 H 4.697738 0.928421 0.731237 C 4.794970 -0.549468 -0.836277 C 4.076778 -1.460807 -1.621003 H 4.601502 -2.063385 -2.366540 H 5.873214 -0.441796 -0.970843 C 2.692727 -1.600586 -1.450451 H 2.124178 -2.312228 -2.054069 C 1.917149 0.829251 1.258591 C -2.046250 -0.880115 0.255980 C -2.790608 -1.841182 0.952325 H -2.283334 -2.699126 1.403943 C -4.182541 -1.734818 1.090454 H -4.739016 -2.497065 1.641042 C -4.860580 -0.652345 0.522172 H -5.943155 -0.563400 0.630160

				C -4.145126 0.311644 -0.192910 H -4.679991 1.149552 -0.646118 C -0.526233 0.850792 -1.099028 C -1.906550 1.137537 -1.086275 C -2.364720 2.257107 -1.798195 H -3.431590 2.489505 -1.813871 C -1.472426 3.075783 -2.491890 C -0.104207 2.786993 -2.477797 H 0.597025 3.427869 -3.015632 H -1.842673 3.943439 -3.040663 C 0.373185 1.678449 -1.767712 H 1.441750 1.462218 -1.741380 C -2.754968 0.196517 -0.331718
TS2P	-1783.634730 C 1.947389 -0.172585 -0.722814 H 1.255104 -0.077766 -1.568022 H 2.651948 0.649967 -0.707522 H 2.395537 -1.154452 -0.675884 O 1.546611 -0.118377 1.054693 H 1.672028 0.818284 1.258117 Ni -0.111444 0.005027 0.004885 C -1.421547 0.079104 -1.382219 C -1.533268 0.052267 1.391667 H -1.913837 1.068269 1.507512 H -0.988340 -0.275103 2.281010 H -2.338653 -0.642722 1.151186 H -0.867139 0.087148 -2.331858 H -2.015121 0.993534 -1.314339 H -2.079654 -0.792177 -1.365909 C 0.072027 1.993433 -0.147558 H 0.812504 2.431856 0.545006 H -0.882816 2.494432 0.041651 H 0.390075 2.257856 -1.167021 C -0.191575 -1.959792 -0.109750 H -1.182577 -2.347474 0.144230 H 0.549176 -2.375348 0.583284 H 0.051151 -2.284598 -1.131721	-402.271396 C 2.260348 -0.205601 -0.694013 H 1.631213 -0.077359 -1.579149 H 3.105448 0.472827 -0.715532 H 2.516841 -1.238061 -0.509898 O 1.789892 0.214777 0.993308 H 1.842189 1.181425 1.000426 Pd -0.105602 -0.006231 -0.022101 C -1.593343 -0.268880 -1.358226 C -1.678245 0.198286 1.367991 H -2.240826 1.101254 1.130607 H -1.163013 0.289121 2.326079 H -2.312886 -0.687294 1.340624 H -1.131131 -0.353970 -2.347916 H -2.273542 0.584761 -1.351460 H -2.148398 -1.183521 -1.142054 C -0.110596 2.102646 -0.306948 H 0.049873 2.602706 0.659677 H -1.072617 2.451199 -0.698051 H 0.676327 2.442568 -0.995295 C -0.031348 -2.092782 0.198930 H -0.993819 -2.506678 0.518417 H 0.731389 -2.349479 0.943438 H 0.240619 -2.563100 -0.756109	-394.350474 C 2.478490 -0.146631 -0.660332 H 2.026784 0.330901 -1.526160 H 3.445896 0.273360 -0.404229 H 2.452449 -1.226013 -0.690610 O 1.797775 0.186898 0.967343 H 1.905209 1.145165 1.065949 Pt -0.096197 -0.006060 -0.042946 C -1.708314 -0.231528 -1.240124 C -1.509512 0.153105 1.466745 H -2.126019 1.040581 1.304770 H -0.942202 0.249146 2.396713 H -2.136824 -0.740830 1.497337 H -1.387880 -0.309944 -2.285602 H -2.390417 0.621789 -1.160147 H -2.265372 -1.140546 -0.989509 C -0.130333 2.101965 -0.263135 H 0.194006 2.598889 0.666012 H -1.142415 2.469986 -0.476150 H 0.523437 2.472945 -1.065447 C 0.012101 -2.096686 0.150732 H -0.931170 -2.528671 0.510925 H 0.803998 -2.381505 0.855731 H 0.237074 -2.579139 -0.811858	-1165.978273 C -1.912481 1.081273 -1.200399 C -0.527344 0.807489 -1.208189 C 0.334850 1.586100 -1.980000 H 1.408527 1.385166 -1.967795 C -0.171130 2.627604 -2.769879 H 0.507698 3.231938 -3.375910 C -1.543308 2.895842 -2.778458 H -1.939523 3.707516 -3.391597 C -2.407270 2.127047 -1.995352 H -3.477137 2.347911 -2.006823 H 4.699477 1.057638 0.787642 C 4.143747 0.331214 0.189380 C 2.762580 0.169763 0.368153 C 4.821557 -0.439404 -0.759711 H 5.897016 -0.313380 -0.900163 C 2.035506 -0.768920 -0.403824 C 4.116143 -1.371752 -1.529689 C 2.734583 -1.530911 -1.349192 H 4.645741 -1.972982 -2.272970 H 2.188501 -2.259603 -1.955541 H -4.676921 1.103590 -0.739972 C -4.130609 0.331473 -0.193296 C -2.741289 0.210704 -0.335131 C -4.835255 -0.535478 0.647848 H -5.916983 -0.434953 0.755837 C -2.020287 -0.788006 0.371279 C -4.146950 -1.528905 1.348150 C -2.755728 -1.647217 1.201401 H -4.690833 -2.208628 2.008612 H -2.239531 -2.428820 1.769512 H -0.537466 2.726514 3.737125 C 0.156727 2.219009 3.063868 C -0.325472 1.258644 2.165057

				H -1.393124 1.035911 2.140896 C 1.518650 2.532761 3.096612 H 1.894043 3.283610 3.794431 C 0.544925 0.586298 1.298126 C 2.395758 1.883632 2.225275 C 1.925843 0.916248 1.326065 H 3.459215 2.132651 2.247084 Pd 0.022679 -0.814182 -0.028327 H 1.246369 -3.487147 0.299055 O -0.245911 -2.622208 -1.114718 C 0.248453 -3.160174 0.580766 H 0.236737 -2.580228 1.515077 H -1.212867 -2.717491 -1.094198 H -0.508073 -3.945204 0.597320
P	-1783.719458 C 2.357586 -1.015945 -0.356261 H 1.776605 -1.541465 0.407846 H 1.753380 -0.992451 -1.269945 H 3.271486 -1.577932 -0.554681 O 2.733061 0.277137 0.058408 H 1.924942 0.812588 0.119592 Ni -0.578563 0.073407 0.032494 C -1.412185 -0.057437 -1.729232 C -0.656780 0.479999 1.936423 H -0.870228 1.532874 2.135330 H 0.372434 0.270726 2.263696 H -1.334548 -0.168633 2.495775 H -1.712778 0.913753 -2.130211 H -2.243379 -0.765588 -1.762842 H -0.600349 -0.451882 -2.357029 C 0.023658 1.912241 -0.373314 H 0.684588 2.380777 0.370811 H -0.899562 2.501899 -0.385177 H 0.486797 2.003720 -1.364514 C -1.089112 -1.780047 0.397614 H -2.168347 -1.820835 0.579772 H -0.580007 -2.177485 1.284750 H -0.864761 -2.425434 -0.461664	-402.351453 C -2.869707 -0.758737 -0.388731 H -2.094342 -1.420789 -0.790346 H -2.805873 -0.798606 0.704483 H -3.847517 -1.132777 -0.696383 O -2.740684 0.555490 -0.871138 H -1.890298 0.895691 -0.539530 Pd 0.480280 0.016323 0.034818 C 0.327069 -1.323164 1.605826 C 1.698573 1.472742 -0.778485 H 1.792386 2.318873 -0.100214 H 1.121643 1.751755 -1.666744 H 2.664182 1.058951 -1.062943 H 0.184075 -0.796301 2.547923 H 1.191489 -1.984310 1.629521 H -0.572983 -1.884550 1.333627 C -0.511361 1.491403 1.198098 H -0.777550 2.411418 0.658336 H 0.200974 1.778844 1.981183 H -1.416275 1.125198 1.704208 C 1.510634 -1.443335 -1.062851 H 2.510320 -1.581056 -0.631972 H 1.639324 -1.154702 -2.113655 H 1.001775 -2.415897 -1.033193	-394.429452 C -3.118060 -0.670603 -0.383371 H -2.452047 -1.436017 -0.796733 H -2.991378 -0.674761 0.705054 H -4.149896 -0.937607 -0.617465 O -2.866305 0.597336 -0.933800 H -1.960870 0.843126 -0.670324 Pt 0.387165 0.005983 0.031772 C 0.069108 -1.397102 1.506711 C 1.619384 1.482907 -0.697984 H 1.703348 2.330488 -0.016430 H 1.090859 1.803366 -1.606757 H 2.602722 1.099801 -0.974364 H -0.170491 -0.944507 2.470494 H 0.913614 -2.082296 1.595693 H -0.801282 -1.959282 1.141553 C -0.615737 1.454460 1.208433 H -0.842845 2.392636 0.682163 H 0.045261 1.720164 2.044876 H -1.555742 1.097341 1.653890 C 1.435257 -1.431257 -1.089262 H 2.420913 -1.609034 -0.635980 H 1.615711 -1.116090 -2.125705 H 0.923984 -2.403129 -1.124908	-1166.050307 C -2.523996 -0.364618 -0.822017 C -1.209160 -0.898583 -0.812883 C -0.940634 -2.081719 -1.509112 H 0.076475 -2.474286 -1.535494 C -1.974561 -2.779944 -2.153867 H -1.757804 -3.712292 -2.678424 C -3.279647 -2.283275 -2.114303 H -4.088021 -2.829134 -2.603552 C -3.549239 -1.078316 -1.457564 H -4.569858 -0.690267 -1.449417 H 5.134416 -0.901155 -0.020568 C 4.155816 -1.351365 0.164017 C 2.989427 -0.581668 0.074442 C 4.076443 -2.706386 0.500780 H 4.985154 -3.307099 0.574657 C 1.709733 -1.149331 0.303438 C 2.828024 -3.285154 0.747215 C 1.662993 -2.509815 0.646573 H 2.761818 -4.341382 1.018616 H 0.695788 -2.987669 0.839363 H -4.819925 1.204531 -0.434652 C -3.900746 1.624089 -0.018581 C -2.684748 0.939851 -0.142722 C -3.949149 2.852877 0.646340 H -4.896260 3.386853 0.744539 C -1.476863 1.467030 0.386978 C -2.777223 3.389708 1.186803 C -1.563391 2.699170 1.054580 H -2.809839 4.347210 1.712410 H -0.659536 3.139752 1.487424 H 2.494929 4.615875 -1.205304 C 2.623657 3.566582 -0.931323

				C 1.505388 2.787818 -0.597046 H 0.509537 3.232197 -0.623137 C 3.899143 2.997199 -0.918077 H 4.770657 3.600460 -1.179524 C 1.659294 1.448581 -0.230409 C 4.058407 1.648441 -0.584777 C 2.949115 0.859229 -0.253540 H 5.057604 1.207065 -0.594658 Pd 0.141576 0.184648 0.262199 H -0.784712 -1.568543 2.254579 O -2.106470 -3.037242 1.557852 C -1.835826 -1.894019 2.346905 H -2.482019 -1.043410 2.080014 H -1.969578 -2.802306 0.626423 H -2.023129 -2.170556 3.391624
TSOR	-1852.606444 Ni 0.701447 0.026890 0.000543 C 1.063369 1.944245 -0.000292 C 0.588732 0.018403 -1.963357 C 1.367848 -1.810029 0.000082 C 0.585773 0.019349 1.964345 H 0.148609 -0.915199 2.341207 H -0.001646 0.868428 2.338863 H 1.600121 0.105171 2.369770 H 1.587025 2.276585 -0.900153 H 1.585846 2.276608 0.900275 H 0.055844 2.380829 -0.000791 H 0.000166 0.866073 -2.339273 H 0.154744 -0.917197 -2.341297 H 1.603642 0.106783 -2.366911 H 1.933946 -2.054976 0.902467 H 1.944521 -2.049281 -0.897108 H 0.448712 -2.411095 -0.007597 O -2.499349 0.996128 -0.001805 N -2.254619 -1.290766 0.000112 N -2.365608 -0.178731 -0.000809	-471.237875 Pd 0.616744 0.002989 0.046311 C 0.620607 1.859697 0.950217 C 1.698828 0.786102 -1.578312 C 1.655353 -1.775491 -0.121739 C -0.448806 -0.782093 1.694973 H -0.825319 -1.796881 1.504860 H -1.298482 -0.149729 1.992104 H 0.224217 -0.840665 2.560026 H 1.448904 2.470051 0.594093 H 0.613980 1.760624 2.034359 H -0.337578 2.256115 0.595843 H 1.276191 1.731170 -1.944582 H 1.753521 0.085164 -2.421951 H 2.727355 0.990553 -1.253467 H 1.728293 -2.275622 0.842524 H 2.628491 -1.621276 -0.584905 H 0.990984 -2.330725 -0.793528 O -2.871286 1.005304 -0.159802 N -2.621970 -1.170209 -0.861969 N -2.733230 -0.113790 -0.516332	-463.318556 O -1.655388 0.732080 0.025014 C 1.846480 -0.380140 -1.198985 C 1.738413 -0.461235 1.283927 C -0.319058 -1.998730 -0.056002 H 0.547728 -2.672062 -0.103558 H -0.955457 -2.206416 -0.923722 H -0.903979 -2.265261 0.831884 C 0.839645 2.056889 0.008322 H 0.762720 2.479787 -1.001300 H 1.877372 2.191982 0.340746 H 0.188645 2.651301 0.657858 H 2.055976 -1.499771 1.174313 H 1.280650 -0.324944 2.267281 H 2.605663 0.196233 1.197181 H 1.449909 -0.275560 -2.212924 H 2.227218 -1.395507 -1.069216 H 2.660998 0.333893 -1.058790 N -3.834476 0.111149 -0.007624 N -2.709436 -0.177535 0.005323 Pt 0.264361 0.026842 -0.006504	-1234.931139 C 2.280608 1.170726 -0.990179 C 0.925861 1.497319 -0.725794 C 0.426328 2.737808 -1.132590 H -0.625072 2.978157 -0.971521 C 1.266445 3.677612 -1.747851 H 0.867479 4.647456 -2.052678 C 2.610217 3.370169 -1.974300 H 3.265941 4.099275 -2.454124 C 3.111741 2.120324 -1.599408 H 4.159485 1.881683 -1.795275 H -5.281382 0.174069 0.186252 C -4.393501 0.756561 0.444544 C -3.112412 0.257965 0.176722 C -4.547446 2.005423 1.054353 H -5.545700 2.393419 1.266720 C -1.945329 0.999660 0.496807 C -3.414372 2.750097 1.393525 C -2.135326 2.246905 1.112400 H -3.527746 3.724019 1.876143 H -1.263001 2.851213 1.381365 H 4.806275 -0.059951 -1.062976 C 4.001095 -0.682968 -0.666351 C 2.691942 -0.191856 -0.591437 C 4.293366 -1.971755 -0.209784 H 5.315582 -2.352041 -0.257051 C 1.630034 -0.982423 -0.080213 C 3.268974 -2.767069 0.312871 C 1.956524 -2.273151 0.366465 H 3.492548 -3.773207 0.675775 H 1.169601 -2.911486 0.780910 H -1.784313 -4.391921 -2.173018

				C -2.079562 -3.461414 -1.683401 C -1.098227 -2.574521 -1.215526 H -0.043438 -2.815346 -1.352393 C -3.432178 -3.150723 -1.525848 H -4.198284 -3.837977 -1.890092 C -1.462879 -1.387749 -0.575196 C -3.805391 -1.950194 -0.913894 C -2.834713 -1.053673 -0.447027 H -4.865557 -1.708188 -0.810367 Pd -0.166446 0.013369 0.141371 O 1.195978 -0.929217 3.343170 N 2.172825 -0.345209 2.996914 N 3.103674 0.211087 2.678878
TSO	-1852.589337 O 1.309020 0.701473 -0.000011 C -1.843483 -0.358129 1.189486 C -1.843518 -0.358157 -1.189446 C 0.115681 -1.855076 -0.000008 H -0.724874 -2.557423 -0.000019 H 0.736158 -2.028561 0.884768 H 0.736188 -2.028564 -0.884763 C -0.910353 1.943199 -0.000013 H -0.459464 2.397861 0.886963 H -1.990251 2.128461 0.000019 H -0.459532 2.397823 -0.887045 H -2.203971 -1.385170 -1.156657 H -1.244308 -0.197124 -2.092881 H -2.674115 0.345287 -1.160383 H -1.244274 -0.196965 2.092899 H -2.203857 -1.385173 1.156795 H -2.674132 0.345251 1.160373 N 3.604495 0.154825 0.000009 N 2.532367 -0.230283 0.000000 Ni -0.433347 0.030346 -0.000006	-471.231451 O -1.531962 0.798084 -0.027099 C 1.756374 -0.485691 -1.320212 C 1.968587 -0.393419 1.150085 C -0.252194 -1.975938 0.088122 H 0.597923 -2.665366 0.155844 H -0.829610 -2.211607 -0.811359 H -0.906161 -2.129903 0.952017 C 0.985179 2.049593 -0.003530 H 0.301455 2.645918 -0.613230 H 2.007068 2.159050 -0.385461 H 0.958235 2.437544 1.020963 H 2.326969 -1.413182 1.013305 H 1.549361 -0.276934 2.152822 H 2.776415 0.321723 0.997660 H 1.210600 -0.307467 -2.248942 H 2.031445 -1.535498 -1.235610 H 2.637798 0.151433 -1.271172 N -3.807041 0.132757 0.006494 N -2.716911 -0.192011 -0.008302 Pd 0.359004 0.036676 0.022083	-463.317997 O 1.613943 0.762190 -0.022812 C -1.827993 -0.398057 1.217152 C -1.755808 -0.483312 -1.265294 C 0.341070 -1.990897 0.050365 H -0.517230 -2.674847 0.097426 H 0.978898 -2.190004 0.919055 H 0.928897 -2.249274 -0.838089 C -0.874068 2.050705 -0.009194 H -0.800407 2.472851 1.000726 H -1.916225 2.162781 -0.336008 H -0.240067 2.659804 -0.661654 H -2.058904 -1.525869 -1.150044 H -1.317685 -0.343433 -2.257303 H -2.631558 0.161645 -1.167288 H -1.420456 -0.286951 2.226012 H -2.198015 -1.418284 1.093614 H -2.653421 0.305274 1.086313 N 3.852992 0.134889 0.005585 N 2.757326 -0.196862 0.000941 Pt -0.264574 0.028102 0.002127	-1234.919040 C 1.967849 1.125229 1.140083 C 0.565849 0.954495 1.038713 C -0.290189 1.838678 1.698477 H -1.369983 1.723253 1.610906 C 0.232607 2.880671 2.475219 H -0.447748 3.561009 2.990424 C 1.614120 3.052179 2.583928 H 2.021797 3.864667 3.187665 C 2.472923 2.176335 1.917565 H 3.553073 2.303220 2.012667 H -4.384120 1.665132 -0.968544 C -3.953174 0.907213 -0.310097 C -2.603047 0.547532 -0.422459 C -4.753054 0.301558 0.660945 H -5.803670 0.580909 0.758554 C -2.030557 -0.436045 0.414744 C -4.199573 -0.664160 1.509705 C -2.853406 -1.029988 1.379696 H -4.823228 -1.138374 2.270925 H -2.446316 -1.800569 2.038665 H 4.766578 0.962070 0.781239 C 4.187563 0.158220 0.320398 C 2.790497 0.128834 0.428964 C 4.849464 -0.850136 -0.385283 H 5.936982 -0.828494 -0.478127 C 2.036506 -0.908873 -0.162209 C 4.114963 -1.889595 -0.967043 C 2.718272 -1.919321 -0.848033 H 4.635232 -2.681533 -1.511082 H 2.149937 -2.744179 -1.284060 H 1.138635 2.529137 -3.722104 C 0.357256 2.142936 -3.065501 C 0.698667 1.254741 -2.037778

				H 1.737413 0.960910 -1.895030 C -0.970831 2.536420 -3.245408 H -1.234653 3.228357 -4.046766 C -0.296302 0.751608 -1.200285 C -1.960904 2.039604 -2.396469 C -1.642894 1.146602 -1.363694 H -3.000209 2.339379 -2.543984 N -1.491379 -4.603681 0.043771 N -1.392727 -3.459398 0.096016 O -0.041895 -2.739991 0.007353 Pd -0.004814 -0.731127 0.103832
TSOP	-1852.637716 O -0.577697 0.192100 -1.569024 C 2.347874 -0.114361 0.161056 C 0.536280 -0.196140 1.700170 C 0.251797 -1.949927 -0.395792 H 1.061293 -2.489476 0.108146 H 0.212583 -2.233807 -1.449416 H -0.700689 -2.215318 0.074702 C 0.581468 1.983377 -0.106771 H 1.191088 2.324224 -0.948604 H 1.042478 2.310673 0.831320 H -0.418470 2.414396 -0.200567 H 0.838288 -1.191814 2.026680 H -0.538013 -0.057294 1.869203 H 1.094420 0.568967 2.240611 H 2.659199 -0.124446 -0.888872 H 2.670989 -1.029887 0.656183 H 2.753709 0.760799 0.668420 N -3.015364 0.604802 0.376363 N -3.142856 -0.479537 0.333451 Ni 0.484204 0.007558 -0.198439	-471.275858 O -0.779366 1.234736 -1.119289 C 2.180524 -0.914258 -0.275973 C 0.603576 -0.863410 1.620080 C -0.678002 -1.607504 -0.837122 H 0.011191 -2.394398 -1.162662 H -1.340125 -1.341349 -1.665045 H -1.285752 -2.003624 -0.016537 C 1.524105 1.753622 0.497271 H 2.260367 2.010657 -0.271020 H 2.057457 1.517732 1.424619 H 0.876123 2.617570 0.660068 H 0.594527 -1.948778 1.522683 H -0.310289 -0.526394 2.116402 H 1.480045 -0.538545 2.180568 H 2.479223 -0.675235 -1.299996 H 2.075895 -1.993313 -0.162795 H 2.920333 -0.528576 0.425873 N -3.013007 0.168444 0.934754 N -3.616547 0.116043 0.025472 Pd 0.413948 0.080962 -0.164021	-463.373306 O 0.814054 -1.213608 -1.069358 C -2.077370 0.974015 -0.235179 C -0.479332 0.895393 1.673281 C 0.773658 1.631047 -0.795252 H 0.086033 2.429983 -1.094468 H 1.426638 1.397751 -1.640838 H 1.398465 2.019696 0.017046 C -1.475316 -1.693039 0.583997 H -2.239537 -1.951163 -0.157138 H -1.988191 -1.418046 1.512473 H -0.871880 -2.585318 0.768480 H -0.482064 1.982953 1.567519 H 0.419778 0.596606 2.221324 H -1.362648 0.590329 2.239507 H -2.457343 0.765726 -1.239942 H -1.947438 2.053271 -0.124160 H -2.810934 0.627492 0.497379 N 3.162680 -0.167554 0.955559 N 3.700746 -0.126527 0.005445 Pt -0.309963 -0.071620 -0.129493	-1234.968563 C -1.723246 0.314797 -1.413009 C -0.360365 0.016702 -1.176588 C 0.526878 -0.090690 -2.249035 H 1.578947 -0.307943 -2.066020 C 0.069705 0.083490 -3.560379 H 0.771028 -0.007011 -4.391686 C -1.274835 0.376187 -3.804691 H -1.631006 0.511719 -4.827168 C -2.161913 0.489084 -2.733417 H -3.215201 0.702145 -2.925693 H 4.896686 0.863655 -0.125487 C 4.255398 -0.009792 0.015061 C 2.879829 0.142521 0.238951 C 4.815313 -1.289142 -0.032144 H 5.885305 -1.411063 -0.211209 C 2.045831 -0.983579 0.420663 C 4.001346 -2.412284 0.153434 C 2.627369 -2.255666 0.383679 H 4.441788 -3.411780 0.122752 H 1.999702 -3.136049 0.542293 H -4.447910 1.005039 -1.143570 C -3.945009 0.717864 -0.217223 C -2.589354 0.360579 -0.221059 C -4.663040 0.707850 0.981179 H -5.717614 0.989626 0.988951 C -1.933746 -0.014643 0.973045 C -4.028215 0.328695 2.169279 C -2.674803 -0.036213 2.159651 H -4.593858 0.310978 3.103867 H -2.192212 -0.351433 3.087747 H 0.020811 4.674297 0.597630 C 0.624314 3.768337 0.516611 C -0.002729 2.516741 0.522018 H -1.088545 2.454713 0.596816 C 2.014019 3.858373 0.400237

				H 2.503251 4.833817 0.394111 C 0.756305 1.348528 0.426386 C 2.774933 2.692916 0.295384 C 2.164170 1.430895 0.306120 H 3.861782 2.763927 0.218240 N -1.684049 -3.114761 -1.033148 N -2.552666 -3.063794 -0.350431 Pd 0.054841 -0.518859 0.716260 O -0.140944 -1.967068 1.931324

Table S5. Harmonic frequencies (cm^{-1}) of all intermediates and transition states (see Figure 2 of the manuscript) for the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ catalyzed by $[M]O^-$. Negative values indicate imaginary frequencies.

	[M] = $(CH_3)_4Ni$	[M] = $(CH_3)_4Pd$	[M] = $(CH_3)_4Pt$	[M] = $(Bp)_2Pd$
R	-7	24	19	-32
	59	53	48	39
	84	71	71	44
	91	88	83	48
	96	93	93	54
	123	107	96	72
	133	115	116	88
	151	132	129	90
	159	137	135	100
	184	171	149	108
	214	182	192	127
	232	185	195	135
	236	213	222	150
	260	217	231	155
	275	251	249	164
	291	286	288	173
	318	306	328	182
	478	467	479	203
	511	485	533	207
	553	517	560	235
	579	568	586	271
	588	572	637	276
	621	639	706	291
	690	698	753	303
	703	727	784	335
	720	749	803	365
	767	755	824	368
	805	837	866	415
	836	847	875	417
	841	848	877	438
	1101	1116	1169	452
	1113	1130	1185	468
	1158	1184	1228	473
	1201	1222	1263	495
	1282	1287	1289	495
	1330	1326	1321	548
	1339	1334	1334	577
	1417	1425	1432	580
	1419	1425	1434	601
	1425	1430	1438	601

	1428	1435	1442	639
	1437	1439	1446	642
	1444	1443	1451	651
	1445	1449	1457	655
	1454	1452	1460	723
	1541	1539	1537	726
	1543	1542	1541	729
	2993	2999	2997	730
	2999	3002	3000	736
	3010	3024	3005	738
	3014	3027	3010	750
	3028	3036	3041	751
	3065	3067	3057	797
	3077	3070	3059	799
	3092	3094	3073	863
	3096	3095	3080	867
	3100	3105	3081	875
	3105	3113	3084	877
	3116	3122	3085	942
	3125	3129	3092	944
	3142	3144	3146	948
	3143	3150	3153	951
	3144	3154	3165	966
				972
				975
				976
				977
				977
				1021
				1032
				1042
				1043
				1061
				1062
				1071
				1072
				1115
				1117
				1120
				1123
				1138
				1138
				1143
				1145
				1232
				1233
				1255

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	47	78	75	41
	81	87	88	42
	109	94	93	48
	129	101	122	79
	138	131	131	87
	190	162	163	95
	236	183	188	103
	245	194	197	128
	256	230	235	136
	264	238	236	144
	295	250	249	163
	295	279	275	172
	329	301	323	189
	388	392	410	201
	393	396	415	209
	479	462	479	233
	502	488	533	270
	541	509	548	280
	574	575	585	293
	584	582	600	302
	601	592	616	334
	602	604	668	363
	689	697	742	368
	697	710	763	406
	719	754	804	417
	776	764	831	419
	794	840	873	428
	834	850	886	450
	843	854	889	453
	1024	1029	1048	469
	1087	1088	1105	472
	1102	1116	1135	496
	1105	1122	1170	499
	1109	1129	1183	532
	1151	1188	1235	579
	1197	1226	1270	581
	1410	1408	1406	600
	1412	1415	1413	601
	1415	1423	1431	619
	1422	1426	1434	640
	1423	1430	1437	642
	1432	1434	1440	652
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	1438	1444	1449	724

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	1456	1452	1459	729
	2992	2988	2978	732
	2996	2993	2984	736
	3006	3027	3007	738
	3011	3031	3011	750
	3068	3056	3034	751
	3075	3059	3037	796
	3081	3077	3052	800
	3087	3084	3070	862
	3097	3093	3075	869
	3099	3109	3082	875
	3105	3117	3084	880
	3122	3125	3088	940
	3125	3132	3089	947
	3208	3208	3215	951
	3218	3221	3229	955
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I1	23 63 67 89 99	35 55 63 78 80	38 50 60 75 88	31 41 42 53 65

	119	93	95	76
	129	112	106	87
	142	124	120	96
	184	170	154	107
	237	188	187	123
	247	203	192	125
	250	209	198	137
	263	219	217	159
	270	234	227	164
	281	239	247	173
	297	266	258	186
	319	302	324	203
	468	460	476	213
	498	478	522	216
	509	498	543	234
	529	502	544	276
	577	574	602	279
	583	588	611	293
	585	603	622	308
	645	638	672	335
	680	677	719	364
	689	705	765	369
	702	749	795	418
	773	759	830	419
	802	793	861	444
	821	840	875	455
	830	847	885	469
	847	855	899	473
	1097	1118	1177	497
	1106	1127	1184	498
	1156	1187	1235	536
	1201	1225	1269	551
	1377	1379	1380	581
	1411	1411	1406	581
	1416	1422	1430	601
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	1420	1428	1435	637
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	1437	1442	1446	652
	1447	1445	1454	658
	1454	1451	1457	726
	2967	2976	2963	728
	2986	2988	2974	731
	3003	3021	3000	732
	3009	3029	3006	738
	3039	3045	3016	739

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	3064	3051	3024	752
	3087	3088	3059	800
	3094	3102	3068	802
	3098	3108	3074	841
	3103	3116	3077	866
	3119	3119	3084	869
	3125	3131	3125	879
	3270	3277	3292	881
	3293	3296	3302	943
	3856	3853	3846	945
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				967
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TS1P	-917 69 86 107 117 139 150 152 200 206 236	-839 57 72 88 94 108 128 153 184 189 205	-838 44 57 83 89 101 138 155 184 195 208	-767 29 36 41 45 58 80 86 114 125 129

	247	212	217	138
	269	219	226	160
	283	251	239	181
	315	257	264	186
	406	386	402	197
	461	448	470	211
	494	485	531	225
	504	495	536	271
	555	568	604	280
	560	575	611	289
	624	607	654	295
	640	642	678	329
	664	664	717	359
	669	693	746	366
	680	706	755	415
	712	729	797	418
	735	748	808	435
	755	785	836	448
	758	794	841	453
	824	837	877	466
	873	847	895	470
	901	904	944	497
	1091	1114	1177	502
	1104	1127	1189	563
	1110	1143	1206	580
	1169	1205	1257	582
	1400	1402	1405	598
	1408	1409	1412	600
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	2953	2967	2946	733
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	2996	3015	2992	736
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	3047	3048	3023	750
	3052	3049	3025	777
	3068	3067	3036	801
	3083	3090	3053	804
	3108	3105	3056	858
	3113	3126	3104	864

	3128	3138	3108	867
	3132	3148	3123	878
	3271	3269	3264	879
	3290	3287	3282	940
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TS2R	-1659 57 126 137 154 165 194 199 214 250 258 262 285 308 319 393 477	-1627 41 50 114 123 126 150 169 175 203 209 240 249 274 294 354 451	-1729 66 79 115 135 138 151 174 191 209 214 241 255 263 306 435 476	-1503 35 38 41 74 82 94 107 125 126 131 165 191 196 203 206 235

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	542	512	541	276
	545	524	569	289
	557	560	573	291
	572	574	599	331
	611	594	608	334
	678	669	730	362
	725	713	765	368
	737	738	788	373
	754	764	812	419
	770	789	843	419
	807	821	854	455
	820	830	860	458
	831	839	878	467
	1043	979	1096	472
	1083	1101	1162	494
	1111	1126	1166	503
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	1197	1213	1256	582
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	1447	1444	1453	658
	1450	1449	1454	729
	1455	1453	1460	730
	1719	1684	1719	735
	3003	3006	2997	737
	3013	3013	3004	740
	3016	3015	3006	742
	3018	3021	3011	750
	3034	3030	3015	751
	3073	3082	3053	802
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	3096	3092	3071	867
	3105	3095	3072	870
	3107	3099	3081	875
	3116	3104	3085	882
	3118	3106	3089	884
	3127	3109	3091	946
	3134	3120	3094	949
	3143	3126	3097	958
				960

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				1635 1636 1643 1645 1682 3033 3116 3149 3174 3174 3181 3181 3184 3185 3192 3193 3195 3196 3208 3209 3210 3211 3220 3223
I2	76 126 156 184 198 220 227 248 255 271 272 286 293 314 322 381 434 452 460 497 549 589 665	46 63 106 142 145 153 181 182 195 207 222 235 248 259 270 364 413 463 470 482 550 610 667	73 88 105 125 133 177 203 213 224 229 237 243 244 336 434 454 478 516 526 542 581 715 719	35 43 47 81 84 94 118 122 132 151 165 177 189 190 213 225 241 273 287 288 303 329 342

	690	681	736	365
	700	711	762	378
	734	720	783	416
	749	731	794	417
	760	744	799	429
	778	749	806	450
	792	776	844	461
	800	790	887	466
	824	822	895	474
	985	952	1122	495
	1062	1062	1136	507
	1078	1087	1179	522
	1105	1107	1187	580
	1186	1194	1257	583
	1413	1410	1421	599
	1416	1413	1424	603
	1417	1418	1428	624
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	3172	3173	3138	948
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				979
				987

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TS2P	-765 67 113 142 149 162 173 210 232 249 254 273 292 295 322 417 449 461 494 556 593 647 659 682 695 716 729 753 767	-842 80 92 102 116 140 147 155 175 186 192 200 222 246 264 389 432 440 486 554 598 633 672 676 696 710 720 734 771	-941 67 82 93 95 134 139 145 184 195 196 201 219 237 245 402 464 474 535 604 647 661 684 731 759 771 777 789 806	-768 32 37 38 60 83 86 114 124 135 155 166 186 194 197 219 226 260 266 285 288 306 325 356 366 413 419 433 447

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	841	825	878	462
	968	970	922	472
	1028	1060	1104	499
	1113	1121	1158	503
	1135	1125	1183	581
	1144	1128	1186	583
	1173	1191	1253	601
	1405	1399	1400	602
	1409	1415	1423	624
	1415	1421	1425	642
	1415	1423	1429	645
	1423	1427	1433	656
	1426	1431	1437	688
	1438	1435	1442	721
	1441	1439	1445	725
	1444	1440	1447	734
	1452	1447	1453	735
	2921	2958	2943	736
	2966	2973	2961	737
	2972	3005	2989	745
	2992	3011	2993	751
	3010	3022	3002	752
	3012	3032	3010	802
	3040	3038	3022	803
	3055	3051	3031	806
	3063	3061	3046	866
	3072	3081	3053	869
	3097	3105	3079	878
	3114	3127	3095	879
	3120	3135	3098	942
	3160	3145	3150	945
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P	46 57 83 107 130 145 153 157 190 198 211 228 239 279 293 451 480 486 512 536 555 580 625 655 669 728 734 756 1082 1088 1090 1117 1124 1136 1167	39 56 74 80 106 119 130 139 146 158 175 178 189 192 215 439 462 479 494 524 538 589 600 661 684 711 719 722 1038 1058 1081 1124 1127 1136 1170	32 57 71 87 102 120 127 143 149 166 169 183 188 197 209 463 501 529 535 544 571 649 683 722 748 776 776 786 1080 1124 1126 1134 1169 1180 1188	31 32 39 45 47 80 90 93 110 117 134 145 152 158 161 185 195 213 245 251 283 286 317 351 359 411 418 423 438 456 459 466 476 496 581

	1382	1388	1390	586
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	1409	1401	1404	602
	1427	1425	1431	629
	1431	1426	1433	636
	1434	1431	1436	646
	1440	1436	1440	652
	1443	1437	1443	721
	1453	1445	1445	727
	1460	1455	1455	727
	1482	1469	1469	734
	1491	1496	1496	738
	2964	2963	2961	740
	2976	2974	2966	747
	2979	3010	2989	748
	2985	3016	2994	805
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	3035	3032	3011	875
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	3058	3038	3019	892
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	3065	3100	3075	953
	3069	3112	3078	960
	3096	3114	3099	961
	3098	3147	3110	965
	3103	3150	3114	969
	3717	3665	3660	978
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				3207 3208 3212 3219 3221 3812
TSOR	42 46 51 78 94 126 148 157 184 189 196 204 239 261 456 486 500 509 550 565 608 629 629 638 653 721 722 744 1078 1083 1105 1115 1356 1409 1410 1422 1425 1430 1431 1439 1441	27 38 50 80 88 104 119 137 141 144 173 180 188 190 453 463 479 493 517 585 587 608 629 657 682 707 716 719 1032 1051 1117 1120 1356 1399 1400 1424 1425 1431 1434 1436 1440	31 61 75 81 117 128 156 187 214 222 234 247 264 314 335 488 541 586 610 626 653 663 743 765 812 835 878 895 899 1184 1197 1242 1279 1430 1432 1434 1435 1440 1449 1453 1459	13 17 29 34 41 46 72 86 97 103 115 143 152 161 183 195 212 244 250 282 286 316 351 359 416 422 435 454 457 464 478 496 580 586 592 600 601 602 628 635 645

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	2966	2960	2976	720
	2970	2969	2981	725
	2989	3013	3014	727
	2995	3016	3021	733
	3026	3017	3033	736
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	3053	3030	3060	748
	3065	3108	3085	804
	3068	3111	3094	810
	3091	3145	3096	868
	3093	3146	3103	872
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				944
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TSO	-645 53 73 87 131 139 141 182 238	-639 25 55 77 92 112 126 146 188	-528 39 58 72 80 116 132 163 189	-597 25 41 46 50 61 82 87 98

	254	209	217	118
	257	229	226	125
	274	234	236	137
	292	240	253	165
	293	274	267	175
	330	294	318	184
	349	318	335	204
	490	474	487	212
	519	496	540	232
	574	577	608	264
	583	581	615	278
	588	593	631	289
	614	598	658	293
	691	699	743	337
	695	712	765	351
	723	757	811	364
	784	769	834	371
	806	844	877	417
	840	853	893	418
	851	858	897	445
	1111	1127	1182	453
	1122	1139	1194	468
	1160	1192	1241	472
	1208	1231	1277	495
	1411	1423	1430	498
	1419	1424	1433	579
	1423	1427	1435	580
	1429	1429	1436	598
	1434	1434	1441	601
	1435	1443	1449	603
	1451	1445	1454	640
	1457	1453	1459	641
	1955	1960	1918	652
	2992	2989	2977	657
	2997	2994	2982	724
	3009	3029	3013	727
	3014	3040	3018	730
	3070	3056	3035	731
	3072	3063	3038	738
	3085	3079	3053	739
	3090	3088	3062	750
	3105	3113	3084	751
	3112	3129	3092	796
	3133	3131	3093	800
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				878

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TSOP	17 30 66 69 76 99 115 139 146 222 232 237 258 271 291 314 478 509 550 577 591 625 689 705	38 45 51 72 77 93 101 108 139 185 188 217 227 250 288 307 467 485 519 568 572 642 699 729	33 44 51 71 77 82 91 127 139 194 196 225 235 248 288 326 478 533 561 585 638 708 753 786	9 24 35 39 44 53 75 84 86 87 93 121 129 153 163 181 202 204 234 271 276 292 303 335

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	767	756	826	368
	798	839	869	417
	832	845	872	417
	836	848	876	440
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	1114	1131	1186	469
	1155	1184	1228	471
	1199	1222	1263	495
	1417	1424	1432	497
	1420	1427	1435	548
	1426	1432	1440	580
	1428	1435	1442	580
	1438	1439	1446	601
	1445	1447	1454	601
	1446	1449	1457	639
	1453	1453	1460	642
	2472	2472	2471	651
	2994	2997	2995	656
	2998	3001	2999	725
	3007	3024	3006	727
	3013	3027	3011	730
	3068	3065	3054	731
	3076	3067	3057	737
	3093	3090	3075	739
	3096	3095	3078	750
	3098	3106	3081	752
	3104	3114	3084	799
	3116	3123	3085	801
	3124	3130	3093	865
				868
				878
				879
				944
				944
				953
				954
				966
				971
				977
				977
				980
				980
				1020
				1032
				1042
				1043

				1061 1062 1072 1074 1115 1117 1121 1123 1138 1138 1144 1144 1232 1233 1256 1259 1308 1308 1326 1330 1347 1348 1432 1433 1442 1444 1463 1465 1499 1500 1613 1614 1619 1620 1637 1638 1644 1646 2467 3173 3174 3181 3182 3186 3188 3194 3196

				3197 3199 3208 3209 3213 3214 3225 3229

Table S6. MN15 optimized energies (a.u.) and geometries (Cartesian coordinates in Å) of all intermediates and transition states (see Figure 2 of the manuscript) for the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ catalyzed by $(CH_3)_4FeO^-$.

	S = 1/2			S = 3/2			S = 5/2		
R	-1538.971235			-1538.961688			-1538.932369		
	C	-3.586112	0.215284	-0.188493	C	-3.175323	0.000012	-0.335303	C	3.499136	-0.085700	-0.172818
	H	-2.596832	-0.006925	-0.585912	H	-2.427346	0.000007	-1.125965	H	2.561425	-0.148757	-0.724073
	H	-4.345036	0.040832	-0.950467	H	-3.031880	0.884229	0.283018	H	3.780961	-1.076455	0.181148
	H	-3.780781	-0.425405	0.670618	H	-4.179380	-0.000024	-0.759417	H	4.288132	0.311174	-0.811133
	H	-3.620222	1.255944	0.129968	H	-3.031836	-0.884162	0.283068	H	3.356008	0.567935	0.686109
	O	-0.397714	-0.477623	-1.452321	O	0.127796	-0.000011	-1.738815	O	0.295280	-0.024321	-1.622400
	Fe	0.425622	-0.021299	-0.181881	Fe	0.303111	-0.000002	-0.101817	Fe	-0.490802	0.022435	0.032221
	C	2.204642	-0.823294	0.114071	C	2.284712	0.000008	-0.045091	C	-2.478492	0.559082	0.141845
	C	-0.481947	1.019730	1.242048	C	-0.446224	0.000001	1.810131	C	0.578824	-0.540990	1.705316
	C	-0.251644	-1.619725	0.777699	C	0.323219	-2.015255	0.145886	C	0.157544	1.933624	0.009703
	H	0.179362	-1.614675	1.782915	H	0.747952	-2.323882	1.104476	H	-0.167766	2.308351	0.983860
	H	0.057523	-2.517584	0.242104	H	0.856580	-2.476953	-0.687239	H	-0.324914	2.474306	-0.801390
	H	-1.340057	-1.584625	0.843686	H	-0.729894	-2.314771	0.111174	H	1.241676	1.963086	-0.078766
	C	1.547906	1.647540	-0.268041	C	0.323233	2.015250	0.145879	C	-0.931153	-1.894434	-0.419787
	H	2.322585	1.724691	0.498523	H	0.747986	2.323876	1.104461	H	-1.439771	-2.248628	0.479881
	H	0.936252	2.553889	-0.247255	H	-0.729881	2.314767	0.111190	H	-0.014564	-2.451325	-0.599331
	H	2.040694	1.563166	-1.242950	H	0.856578	2.476947	-0.687256	H	-1.591066	-1.920132	-1.283911
	H	-1.293254	0.449041	1.698831	H	-1.029284	-0.893980	2.052181	H	1.097200	0.304790	2.166463
	H	-0.874416	1.947742	0.821138	H	-1.029261	0.893994	2.052190	H	1.310892	-1.317179	1.467685
	H	0.260145	1.274403	2.003770	H	0.448530	-0.000015	2.445392	H	-0.141633	-0.951876	2.421904
	H	2.166963	-1.892454	-0.102908	H	2.632779	-0.900437	-0.539971	H	-2.851918	0.757017	-0.866295
	H	2.404076	-0.684066	1.180710	H	2.504626	0.000042	1.021468	H	-2.597011	1.461200	0.748983
	H	3.001462	-0.346429	-0.458999	H	2.632777	0.900423	-0.540027	H	-3.064189	-0.251732	0.584770
TS1R	-1538.915918			-1538.917731			-1538.899770		
	C	3.358251	0.136582	0.042026	C	3.513544	0.134473	0.000032	C	2.987164	-0.055266	0.020531
	H	2.064797	0.716563	-0.039176	H	2.148908	0.633721	-0.000149	H	2.010836	0.788061	-0.052835
	H	3.640457	0.309157	1.074345	H	4.059153	1.072165	-0.002305	H	3.552044	0.099397	-0.893797
	H	3.248657	-0.909065	-0.219838	H	3.608834	-0.444624	0.910837	H	3.525593	0.225662	0.920558
	H	3.912868	0.725913	-0.679502	H	3.607874	-0.448682	-0.908270	H	2.527480	-1.035231	0.082034
	O	1.052601	1.181826	-0.102482	O	1.143607	1.092739	-0.000265	O	0.994112	1.429213	-0.113730
	Fe	-0.388133	0.118372	-0.022357	Fe	-0.328096	0.064960	-0.000003	Fe	-0.307754	0.063780	-0.015203
	C	0.234736	-1.191052	1.299180	C	-1.583809	-0.712455	1.313182	C	-1.671739	1.593034	-0.087277
	C	-2.176957	-0.811619	0.073097	C	-1.583711	-0.712721	-1.313112	C	-1.963256	-1.056624	0.065742
	C	0.128091	-1.274001	-1.305197	C	0.738280	-1.655761	0.000137	C	0.226903	-0.797982	1.798446
	H	-0.284004	-0.863377	-2.233596	H	0.132950	-2.568104	0.001244	H	-0.603472	-0.728485	2.506723
	H	-0.276198	-2.266414	-1.111728	H	1.386925	-1.649005	0.883385	H	1.103082	-0.291103	2.209155
	H	1.217473	-1.300684	-1.365467	H	1.384699	-1.649812	-0.884769	H	0.457260	-1.856227	1.632073
	C	-1.556700	1.776178	0.013990	C	-1.380595	1.801389	-0.000017	C	0.236266	-1.065320	-1.666995
	H	-1.038679	2.605853	-0.471886	H	-1.075874	2.367640	0.885496	H	-0.574862	-1.069393	-2.400392

	H -1.602881 1.987897 1.090331	H -2.468410 1.672384 -0.001283	H 0.425620 -2.096399 -1.348492
	H -2.578933 1.680993 -0.358146	H -1.073867 2.369560 -0.883578	H 1.138478 -0.649673 -2.121455
	H -2.089781 -1.892961 0.224052	H -1.633333 -1.799390 -1.268849	H -1.635694 -2.090701 0.176463
	H -2.720485 -0.624925 -0.859370	H -1.068195 -0.395303 -2.228937	H -2.523474 -0.927679 -0.859627
	H -2.772036 -0.382737 0.887068	H -2.574277 -0.263480 -1.269410	H -2.561853 -0.747021 0.921808
	H 1.323974 -1.140034 1.354308	H -1.067045 -0.396998 2.228984	H -2.150627 1.647927 0.893449
	H -0.100115 -2.218001 1.154101	H -1.635299 -1.798984 1.267780	H -2.426970 1.427650 -0.857966
	H -0.199005 -0.776977 2.217070	H -2.573660 -0.261499 1.270705	H -1.106778 2.504171 -0.285272
I1	-1538.921564	-1538.939217	-1538.939092
	C -3.610244 -0.175780 0.119182	C 3.546167 0.028677 0.390034	C 3.552391 0.032603 0.387246
	H -0.478797 -1.538118 -1.575570	H -0.046636 -0.028022 2.417712	H -0.041856 -0.008774 2.418150
	H -3.633121 -0.123410 1.194895	H 3.620070 0.461214 -0.593852	H 3.617737 0.430491 -0.611780
	H -2.666353 -0.272874 -0.398098	H 2.587311 -0.021285 0.886387	H 2.595135 -0.014256 0.887045
	H -4.535724 -0.106246 -0.428603	H 4.433931 -0.365684 0.857197	H 4.446609 -0.332731 0.865529
	O -0.634946 -0.593784 -1.461882	O 0.510288 -0.067940 1.636680	O 0.513074 -0.059699 1.636362
	Fe 0.436182 0.020840 -0.110370	Fe -0.415261 -0.013188 -0.013217	Fe -0.415373 -0.013485 -0.012226
	C 1.341739 -1.786977 0.114625	C -2.149296 -1.090203 0.212359	C -2.152301 -1.086163 0.215615
	C -0.249987 1.903961 -0.277129	C 0.685242 1.134076 -1.315179	C 0.678058 1.124281 -1.329663
	C -0.446331 -0.164794 1.635213	C 0.327986 -1.627956 -1.011431	C 0.326063 -1.636699 -0.998110
	H 0.362111 -0.103555 2.367624	H 0.012928 -1.638565 -2.057352	H -0.004761 -1.664789 -2.038850
	H -0.905542 -1.154023 1.683651	H 0.006749 -2.543318 -0.511862	H 0.015641 -2.545164 -0.479462
	H -1.185413 0.615919 1.814793	H 1.416215 -1.541613 -0.961599	H 1.414474 -1.546807 -0.965816
	C 2.248972 0.829583 0.073615	C -1.601964 1.646029 0.141064	C -1.597546 1.648683 0.139635
	H 3.046071 0.156365 -0.248485	H -2.129432 1.588962 1.096841	H -2.122171 1.596052 1.097293
	H 2.326802 0.972253 1.157419	H -2.334656 1.667274 -0.669542	H -2.332702 1.670450 -0.668692
	H 2.341064 1.802641 -0.412261	H -0.988392 2.548167 0.107797	H -0.981073 2.548741 0.102266
	H -1.344645 1.860524 -0.272675	H 1.433454 0.563810 -1.868179	H 1.420099 0.549890 -1.886624
	H 0.088269 2.291074 -1.244615	H 1.179859 1.863252 -0.666343	H 1.179528 1.856834 -0.690158
	H 0.095363 2.569345 0.520669	H 0.034457 1.667482 -2.011244	H 0.021482 1.654607 -2.022685
	H 0.580171 -2.571560 0.219980	H -1.896331 -2.065985 0.632509	H -1.904519 -2.063898 0.634229
	H 2.011012 -1.834224 0.980646	H -2.602931 -1.235889 -0.772045	H -2.607389 -1.228226 -0.768711
	H 1.932687 -1.991647 -0.787730	H -2.860939 -0.577133 0.862694	H -2.861124 -0.570438 0.866915
TS1P	-1538.908794	-1538.916194	-1538.898385
	H 2.758154 0.097720 1.192764	H -3.014654 0.941512 -0.608454	C 3.255219 -0.186253 -0.003581
	H 3.237236 0.768975 -0.442601	H -3.887772 -0.400754 0.314630	H 3.625483 -0.710042 0.864522
	C 3.047319 -0.096587 0.170320	C -3.237310 -0.104668 -0.491039	H 3.627140 -0.506618 -0.964468
	O 1.396209 -0.605701 -0.607164	O -1.423307 -0.467068 0.400145	H 3.048087 0.864002 0.113770
	H 3.681983 -0.954849 -0.001536	H -3.167928 -0.741375 -1.357220	O 1.446403 -0.732891 -0.073561
	H 1.390269 -1.554049 -0.429396	H -1.431977 -1.432345 0.447993	H 1.417129 -1.699512 -0.082940
	Fe -0.338430 0.013970 -0.179396	Fe 0.379037 0.026826 -0.021331	Fe -0.403570 0.033966 -0.018782
	C -2.229983 0.563574 -0.298617	C 1.000977 -0.072869 1.870073	C -1.387554 0.418651 1.774255
	C 0.245615 1.933622 -0.407530	C -0.018530 1.994132 0.230109	C -1.465846 0.457672 -1.751254
	H 0.381783 2.165566 -1.474867	H -0.795277 2.118424 0.993778	H -1.657404 -0.440081 -2.343350
	H 1.221328 2.043932 0.082654	H -0.364873 2.433605 -0.715445	H -0.964784 1.212841 -2.360243
	H -0.435736 2.675710 0.022560	H 0.876446 2.541805 0.544991	H -2.419659 0.861127 -1.393060
	H -2.932030 -0.218916 -0.003279	H 2.044265 0.231463 1.748362	H -0.700386 0.127990 2.574459
	H -2.364111 0.777592 -1.370356	H 0.938520 -1.091862 2.250327	H -2.298921 -0.179383 1.848468

	H -2.432568 1.479929 0.260379 C -0.405323 0.135638 1.753050 H 0.502308 -0.394398 2.068191 H -1.283746 -0.363507 2.164289 H -0.360616 1.176068 2.078783 C -1.023895 -1.922159 -0.206153 H -1.767592 -2.101105 0.579412 H -0.250091 -2.701771 -0.099549 H -1.519463 -2.099025 -1.172265	H 0.460041 0.635619 2.494137 C 1.560849 0.545026 -1.558665 H 0.840250 0.488345 -2.387947 H 2.370830 -0.158940 -1.767993 H 1.944198 1.567627 -1.515079 C 0.943473 -1.906900 -0.355921 H 2.015373 -1.999268 -0.146147 H 0.785259 -2.196215 -1.403385 H 0.422030 -2.626906 0.293548	H -1.620925 1.480920 1.870331 C -1.074376 -1.923969 0.042205 H -0.697357 -2.494788 -0.811710 H -2.163082 -1.861411 -0.023448 H -0.795249 -2.413644 0.978981 C 0.458759 1.907909 0.047185 H -0.341183 2.649272 -0.009937 H 1.125074 2.010658 -0.814250 H 1.020431 2.034633 0.976826
TS2R	-1538.907741 C 2.254202 0.285002 0.306425 H 1.582632 -0.500058 -0.713966 H 2.956430 -0.490046 0.634389 H 2.795278 1.037853 -0.276730 H 1.867472 0.771258 1.201673 O 0.717452 -1.009512 -1.375597 Fe -0.022861 -0.059396 -0.169111 C -1.872093 -0.396303 -0.744715 C -0.752283 0.866136 1.576663 C -0.183477 1.852722 -0.644756 H -1.210403 2.208891 -0.692942 H 0.251423 1.785089 -1.647056 H 0.423115 2.492165 -0.004209 C -0.145168 -1.582799 1.130023 H -1.180074 -1.763974 1.411866 H 0.455886 -1.324896 2.001905 H 0.271822 -2.439885 0.605037 H 0.115215 1.142148 2.186110 H -1.365735 0.172379 2.155431 H -1.340999 1.769791 1.400530 H -2.004406 0.116645 -1.700394 H -2.598185 -0.032369 -0.015813 H -1.971792 -1.473133 -0.886022	-1538.911960 C 2.019092 -0.800413 0.592676 H 1.441023 -0.704166 -0.688895 H 2.154206 -1.879391 0.706416 H 2.970918 -0.314162 0.360129 H 1.661599 -0.396980 1.540848 O 0.672066 -0.461509 -1.643479 Fe -0.065047 0.055704 -0.143784 C -1.915665 0.118855 -0.841506 C -0.804749 0.833202 1.599802 C 0.869209 1.875492 -0.180432 H 0.103830 2.574397 -0.534567 H 1.688838 1.826053 -0.896586 H 1.221470 2.199084 0.800148 C -0.705643 -1.747554 0.602184 H -1.782690 -1.787154 0.758549 H -0.188994 -1.883673 1.553396 H -0.388482 -2.497151 -0.123128 H 0.008876 0.868352 2.330804 H -1.617227 0.217789 1.994858 H -1.165143 1.852843 1.437857 H -2.005916 -0.697709 -1.552161 H -1.869095 1.082209 -1.356375 H -2.691987 0.105950 -0.081406	
I2	-1538.954041 C 1.694762 0.286141 -1.053044 H 2.119770 1.284459 -0.956879 H 2.455860 -0.483698 -0.922596 H 1.231148 0.173710 -2.045570 O 0.342818 -1.922232 -0.042105 H 1.279438 -2.040626 0.150609 Fe -0.014127 -0.074820 -0.106385 C -0.423376 1.836843 -0.591585 C -1.311016 0.298689 1.446294 H -0.852484 1.086990 2.043253 H -1.294954 -0.658226 1.970650 H -2.324570 0.572729 1.166019 H -0.281070 1.931689 -1.676349	-1538.964244 C 1.477287 -1.426805 0.198299 H 1.912920 -1.690285 -0.765734 H 2.243036 -1.038813 0.871424 H 0.998517 -2.301996 0.647973 O 0.385805 0.689120 1.803377 H 1.300412 0.990991 1.790110 Fe 0.011770 -0.006643 0.089787 C -0.598018 -1.253003 -1.405615 C -1.121491 1.453806 -0.828752 H -0.751829 1.695644 -1.826633 H -1.005693 2.315189 -0.167364 H -2.169622 1.153762 -0.877505 H -0.646694 -2.286346 -1.060557	

	H 0.270004 2.528490 -0.099260 H -1.450429 2.132151 -0.357416 C 1.395179 0.260952 1.383185 H 0.941872 -0.262058 2.224778 H 1.421553 1.337059 1.557730 H 2.400330 -0.121904 1.208122 C -1.744316 -0.650391 -0.849455 H -2.526134 0.105134 -0.932696 H -2.104058 -1.573522 -0.397319 H -1.328926 -0.882618 -1.842591	H 0.161157 -1.154967 -2.183722 H -1.568983 -0.930806 -1.778118 C 1.482056 1.119584 -0.841371 H 1.270082 2.187525 -0.763395 H 1.497116 0.828663 -1.895636 H 2.455186 0.896990 -0.393418 C -1.749854 -0.564324 0.927006 H -2.543391 -0.847251 0.237683 H -2.036639 0.277350 1.555146 H -1.447910 -1.411443 1.550866	
TS2P	-1538.923340 C 1.575727 -0.198277 -1.037010 H 0.684089 -0.010423 -1.729958 H 2.294218 0.607359 -1.153924 H 1.985767 -1.184112 -1.226194 O 1.707687 -0.337974 0.854296 H 1.890496 0.575802 1.112484 Fe -0.072994 0.005617 -0.081382 C -1.878866 0.405600 -0.830612 C -0.864522 -0.094785 1.709738 H -0.690785 0.845051 2.240458 H -0.376305 -0.918708 2.232127 H -1.934281 -0.286866 1.619788 H -1.781201 0.667196 -1.891338 H -2.312598 1.260260 -0.306369 H -2.544233 -0.455949 -0.737438 C 0.221302 2.051320 -0.086680 H 1.232075 2.342521 0.249903 H -0.504513 2.570378 0.549608 H 0.105398 2.442891 -1.107009 C -0.443733 -1.972657 -0.330556 H -1.369727 -2.295875 0.156885 H 0.401813 -2.509923 0.118210 H -0.503310 -2.239066 -1.394933	-1538.915966 C 2.019964 0.141474 0.622753 H 1.392312 0.151155 1.516198 H 2.659906 -0.730219 0.589532 H 2.508079 1.086452 0.441115 O 1.471257 -0.018096 -1.184748 H 1.582067 -0.969115 -1.319853 Fe -0.171359 0.011551 -0.056406 C -1.321704 0.059315 1.543517 C -1.699546 -0.146721 -1.394450 H -2.186813 -1.122710 -1.331008 H -1.237186 -0.020406 -2.380282 H -2.436483 0.644989 -1.232963 H -0.657485 0.126826 2.417252 H -1.925034 -0.847578 1.634471 H -1.963691 0.943718 1.534707 C 0.110174 -1.995431 0.356142 H 0.862881 -2.512735 -0.264198 H -0.846880 -2.505747 0.208730 H 0.401521 -2.140555 1.405612 C -0.017280 2.028177 0.097630 H -0.999202 2.459929 -0.122681 H 0.717197 2.417493 -0.617049 H 0.264441 2.342051 1.111416	
P	-1538.984537 C -1.923926 0.018512 -1.389865 H -1.270142 0.899853 -1.393905 H -1.294391 -0.871785 -1.505093 H -2.593273 0.082640 -2.248331 O -2.715249 -0.044066 -0.227193 H -2.103927 -0.057169 0.525804 Fe 0.617271 0.005668 0.238118 C 1.703552 -1.297177 -0.894436 C -0.322427 1.371772 1.438320 H -0.908405 0.940303 2.258558 H -0.970833 2.048829 0.869089 H 0.464520 1.996582 1.880500	-1539.010394 C 2.051679 -0.668625 -1.115676 H 1.480998 -1.485749 -0.661341 H 1.348242 -0.028143 -1.662822 H 2.755004 -1.093770 -1.832371 O 2.789994 0.057677 -0.161143 H 2.150098 0.530724 0.393638 Fe -0.665682 0.082376 0.186987 C -1.609340 1.013746 -1.347132 C -0.125149 -0.753808 1.950327 H -0.035849 -0.036025 2.774291 H 0.878583 -1.171728 1.782295 H -0.767636 -1.586868 2.258569	-1538.988336 C -2.686601 0.677730 -0.018639 H -2.066309 1.088607 0.781860 H -2.282920 1.046411 -0.966340 H -3.707948 1.044433 0.095975 O -2.730249 -0.728320 0.023238 H -1.811070 -1.038433 0.004771 Fe 0.724007 -0.022792 -0.000433 C 0.459548 2.037811 -0.013044 C 2.757757 -0.281596 -0.016570 H 3.143979 0.201025 -0.920137 H 3.069032 -1.329614 -0.001789 H 3.164142 0.231473 0.860881

H 1.977654 -2.207056 -0.349506	H -1.789327 2.083192 -1.184527	H 1.429251 2.523649 -0.163706
H 2.607093 -0.841392 -1.311643	H -2.541154 0.528313 -1.660119	H 0.045122 2.387229 0.939612
H 1.070787 -1.606617 -1.738002	H -0.910938 0.932308 -2.192648	H -0.212569 2.355900 -0.817559
C -0.169591 -1.630036 1.179536	C 0.292195 1.819377 0.654649	C -0.034619 -0.897289 -1.725084
H -1.023555 -1.443143 1.840864	H 1.082474 1.806750 1.419426	H -0.274595 -1.960648 -1.610727
H 0.638113 -2.043580 1.798192	H -0.545168 2.373188 1.103376	H 0.785696 -0.818359 -2.448340
H -0.447779 -2.413552 0.464817	H 0.630075 2.411869 -0.204013	H -0.909635 -0.396542 -2.150982
C 1.469084 1.564229 -0.768201	C -1.320314 -1.703400 -0.491561	C -0.005054 -0.853246 1.757320
H 2.468702 1.728101 -0.344761	H -2.357826 -1.777894 -0.138091	H 0.818349 -0.744282 2.473061
H 0.914742 2.505454 -0.683658	H -0.776049 -2.564622 -0.085872	H -0.234039 -1.921817 1.674284
H 1.603486 1.323895 -1.828569	H -1.348165 -1.768467 -1.585965	H -0.884852 -0.350356 2.170583

Table S7. Harmonic frequencies (cm^{-1}) of all intermediates and transition states (see Figure 2 of the manuscript) for the reaction $CH_4 + N_2O \rightarrow CH_3OH + N_2$ catalyzed by $(CH_3)_4FeO^-$. Negative values indicate imaginary frequencies.

	S = 1/2	S = 3/2	S = 5/2
R	53	24	34
	63	67	61
	77	80	74
	86	94	90
	99	102	97
	125	117	114
	147	117	126
	162	137	139
	183	149	152
	197	183	160
	216	201	168
	226	205	173
	262	235	189
	275	235	197
	321	278	220
	325	281	228
	367	306	235
	444	450	446
	530	487	468
	549	492	486
	558	493	499
	633	566	511
	656	590	534
	690	627	570
	724	686	588
	737	691	601
	778	711	603
	805	715	641
	817	761	650
	999	901	732
	1118	1070	1047
	1134	1090	1062
	1142	1097	1075
	1180	1134	1094
	1286	1294	1287
	1331	1311	1326
	1334	1331	1335
	1412	1408	1406
	1420	1416	1407
	1426	1417	1417

	1430	1423	1420
	1443	1423	1422
	1445	1435	1425
	1451	1437	1427
	1465	1447	1433
	1542	1535	1539
	1543	1538	1542
	2999	2990	3000
	3016	3004	3009
	3017	3009	3035
	3024	3042	3036
	3038	3059	3041
	3073	3069	3072
	3088	3073	3086
	3093	3083	3092
	3095	3084	3095
	3105	3107	3133
	3106	3107	3136
	3108	3145	3142
	3125	3159	3151
	3144	3164	3153
	3151	3177	3165
	3162	3197	3166
TS1R	-1759	-1760	-1832
	36	45	45
	65	65	60
	100	105	85
	110	116	97
	121	133	114
	146	144	131
	168	183	164
	182	188	166
	204	194	184
	221	222	203
	245	225	210
	261	264	243
	274	278	258
	331	290	304
	376	398	385
	401	407	419
	427	460	456
	471	481	460
	506	495	472
	520	511	513
	543	541	517
	557	552	552
	570	568	578

	605	578	583
	609	658	592
	664	668	616
	716	688	626
	746	728	686
	751	741	695
	789	751	715
	990	1034	1048
	1051	1076	1056
	1092	1088	1068
	1107	1095	1097
	1117	1102	1124
	1125	1121	1137
	1158	1142	1217
	1404	1399	1410
	1407	1404	1411
	1412	1404	1412
	1415	1408	1418
	1416	1414	1420
	1419	1420	1424
	1427	1425	1429
	1428	1425	1431
	1441	1435	1441
	1442	1438	1443
	2987	2990	3001
	2994	2995	3004
	3002	2998	3021
	3009	3001	3043
	3056	3067	3077
	3061	3070	3078
	3069	3071	3080
	3086	3083	3102
	3092	3083	3104
	3099	3103	3107
	3105	3106	3126
	3122	3142	3133
	3132	3143	3140
	3217	3214	3197
	3221	3223	3217
I1	42	31	28
	51	48	47
	65	69	63
	74	94	94
	123	104	102
	126	106	105
	138	135	134
	151	142	140

	181	155	154
	192	166	165
	198	174	174
	218	182	183
	242	194	194
	255	214	214
	260	231	232
	268	243	240
	275	283	281
	449	318	318
	472	431	431
	492	481	481
	500	496	496
	508	515	515
	556	535	536
	587	537	537
	608	593	593
	620	605	606
	631	637	637
	645	649	649
	655	656	657
	692	658	659
	719	682	682
	755	691	691
	800	731	731
	1086	1070	1070
	1096	1094	1094
	1109	1097	1097
	1139	1128	1128
	1380	1379	1379
	1407	1411	1411
	1409	1414	1414
	1414	1416	1417
	1421	1421	1421
	1424	1426	1426
	1428	1426	1427
	1432	1432	1432
	1437	1439	1439
	1440	1445	1445
	2971	3013	3013
	2992	3015	3015
	3009	3017	3017
	3027	3022	3023
	3037	3092	3091
	3057	3097	3098
	3070	3099	3099
	3074	3102	3103

	3086	3104	3105
	3107	3108	3108
	3113	3111	3111
	3114	3112	3112
	3125	3117	3117
	3284	3282	3282
	3298	3297	3297
	3848	3910	3911
TS1P	-1476	-665	-856
	29	50	31
	84	54	47
	93	81	66
	100	93	73
	121	137	78
	136	139	87
	148	158	119
	168	174	153
	189	180	174
	205	219	185
	217	226	191
	237	236	207
	263	243	262
	300	263	292
	425	369	325
	449	430	351
	460	450	429
	493	472	452
	501	486	464
	537	507	492
	557	536	503
	608	557	542
	618	569	570
	649	585	583
	651	599	586
	664	609	590
	681	635	594
	700	686	632
	718	699	648
	742	732	699
	884	787	880
	920	829	919
	1091	1058	1030
	1106	1091	1040
	1116	1102	1054
	1138	1118	1082
	1399	1396	1400
	1405	1403	1409

	1408	1405	1410
	1412	1405	1415
	1417	1421	1417
	1418	1422	1420
	1425	1427	1425
	1432	1432	1426
	1434	1437	1430
	1444	1440	1434
	2924	2953	3005
	2958	2974	3008
	2965	2978	3010
	2990	3017	3013
	2995	3024	3084
	3031	3040	3089
	3036	3049	3094
	3054	3055	3094
	3062	3062	3099
	3083	3088	3104
	3096	3118	3108
	3112	3147	3109
	3127	3150	3140
	3268	3308	3287
	3293	3316	3312
	3845	3832	3802
TS2R	-1661	-1818	
	62	89	
	74	141	
	102	157	
	118	166	
	135	184	
	169	207	
	185	221	
	217	229	
	248	242	
	262	260	
	284	265	
	304	280	
	332	299	
	383	315	
	437	445	
	458	472	
	501	495	
	516	506	
	535	514	
	539	549	
	589	611	
	685	628	

	701 711 731 753 766 771 823 861 1095 1107 1120 1129 1136 1189 1417 1421 1422 1427 1431 1437 1440 1447 1457 1473 1867 3003 3005 3021 3022 3046 3072 3077 3087 3107 3116 3122 3134 3143 3144 3154	653 667 702 712 740 777 786 797 1084 1092 1108 1123 1138 1153 1413 1416 1421 1422 1426 1433 1440 1441 1447 1457 1795 3005 3013 3017 3035 3038 3082 3087 3097 3100 3122 3128 3133 3138 3144 3182	
I2	84 142 175 184 207 225 231	95 124 149 171 189 210 229	

	254	231	
	276	235	
	289	261	
	293	267	
	312	298	
	320	303	
	371	329	
	397	336	
	411	432	
	461	441	
	464	469	
	473	502	
	508	509	
	533	544	
	617	637	
	634	645	
	665	663	
	678	681	
	710	696	
	752	719	
	761	728	
	774	744	
	803	765	
	814	779	
	826	804	
	1055	1080	
	1095	1092	
	1110	1103	
	1128	1108	
	1164	1152	
	1401	1413	
	1409	1417	
	1420	1421	
	1422	1424	
	1426	1425	
	1427	1430	
	1435	1433	
	1448	1447	
	1455	1450	
	1458	1453	
	2964	3006	
	2973	3015	
	2981	3021	
	3031	3023	
	3036	3034	
	3047	3084	
	3065	3103	

	3080	3105	
	3084	3111	
	3123	3117	
	3131	3119	
	3133	3122	
	3140	3128	
	3140	3135	
	3151	3154	
	3841	3865	
TS2P	-613	-693	
	62	44	
	129	107	
	142	138	
	161	145	
	192	180	
	212	193	
	221	209	
	226	210	
	237	220	
	248	224	
	266	248	
	283	275	
	395	301	
	420	314	
	443	425	
	476	434	
	501	465	
	518	477	
	521	516	
	551	566	
	598	571	
	624	592	
	648	616	
	683	623	
	711	640	
	720	665	
	744	703	
	748	752	
	787	772	
	867	807	
	919	911	
	1099	1041	
	1115	1100	
	1121	1119	
	1149	1125	
	1282	1150	
	1318	1404	

	1415	1406	
	1419	1408	
	1421	1411	
	1424	1415	
	1433	1423	
	1434	1428	
	1437	1431	
	1439	1439	
	1446	1444	
	2528	2927	
	2926	2975	
	2969	2976	
	2995	2996	
	3005	3006	
	3020	3045	
	3037	3054	
	3047	3058	
	3057	3065	
	3069	3067	
	3093	3080	
	3103	3091	
	3117	3096	
	3122	3189	
	3193	3263	
	3826	3813	
P	44	50	56
	50	71	77
	77	89	86
	93	92	93
	111	128	103
	116	140	110
	124	145	125
	154	153	128
	165	164	146
	187	183	152
	188	202	171
	202	213	182
	206	218	184
	233	259	204
	284	275	205
	412	437	396
	444	456	443
	478	470	453
	503	499	455
	510	507	462
	547	526	474
	558	536	484

	592	564	516
	611	576	529
	652	675	542
	664	688	546
	670	726	571
	698	728	577
	1076	1079	1031
	1109	1110	1060
	1118	1116	1077
	1127	1122	1082
	1128	1128	1093
	1144	1141	1125
	1159	1161	1172
	1385	1386	1389
	1416	1412	1412
	1422	1414	1415
	1424	1418	1418
	1429	1425	1420
	1431	1431	1421
	1435	1432	1425
	1438	1439	1427
	1442	1445	1431
	1453	1455	1461
	1477	1481	1475
	1501	1499	1494
	2980	2961	2993
	2981	2973	2995
	2984	2976	2997
	2987	2978	3004
	3008	3009	3032
	3036	3014	3059
	3041	3031	3060
	3043	3032	3065
	3046	3038	3073
	3049	3043	3076
	3053	3046	3077
	3054	3052	3079
	3059	3053	3086
	3070	3061	3088
	3108	3109	3104
	3758	3746	3756