

Supporting Information

CO Oxidation over the Polyoxometalates–Supported Single–Atom Catalysts M_1/POM (Fe, Co, Mn, Ru, Rh, Os, Ir, and Pt; $POM = [PW_{12}O_{40}]^{3-}$): A Computational Study for Activation of Surface Oxygen Species

Chun–Guang Liu^{*,†,‡} Li–Long Zhang^{†,‡} and Xue–Mei Chen^{*†}

[†]*College of Chemical Engineering, Northeast Electric Power University, Jilin City, 132012, P. R. China*

[‡]*State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, Ministry of Science and Technology of China, School of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, 15 Yu Cai Road, Guilin, 541004, P. R. China*

Table S1. DFT–derived total energy including electronic and zero-point energies for the clean M_1 /POM with different spin states

M_1 /POM	Spin multiplicity	Total energy (a.u.)	Total energy (kcal mol ⁻¹)	Relative energy (kcal mol ⁻¹)
Fe-PTA	2	-4289.909599	-2691961.172	17.14
	4	-4289.936194	-2691977.861	0.45
	6	-4289.936911	-2691978.311	0.00
Co-PTA	1	-4311.541033	-2705535.114	9.15
	3	-4311.555608	-2705544.26	0.00
	5	-4311.530261	-2705528.354	15.91
Mn-PTA	1	-4270.366699	-2679697.807	56.62
	3	-4270.412632	-2679726.631	27.80
	5	-4270.456933	-2679754.43	0.00
Ru-PTA	2	-4260.297536	-2673379.307	0.00
	4	-4260.294612	-2673377.472	1.83
	6	-4260.273725	-2673364.365	14.94
Rh-PTA	1	-4275.914749	-2683179.264	0.00
	3	-4275.914627	-2683179.188	0.08
	5	-4275.886321	-2683161.425	17.84
Os-PTA	2	-4257.421208	-2671574.382	0.00
	4	-4257.420791	-2671574.121	0.26
	6	-4257.390165	-2671554.902	19.48
Ir-PTA	1	-4271.064353	-2680135.592	1.58
	3	-4271.066863	-2680137.167	0.00
	5	-4271.016521	-2680105.577	31.59
Pt-PTA	2	-4285.506425	-2689198.137	0.00
	4	-4285.475285	-2689178.596	19.54

Table S2. DFT–derived total energy including electronic and zero-point energies for the CO adsorption complexes of M₁/POM with different spin states

M ₁ /POM	Spin multiplicity	Total energy (a.u.)	Total energy (kcal mol ⁻¹)	Relative energy (kcal mol ⁻¹)
Fe-PTA	2	-4516.66	-2834251.40	8.69
	4	-4516.66	-2834250.77	9.31
	6	-4516.68	-2834260.08	0
Co-PTA	1	-4538.30	-2847826.41	0
	3	-4538.27	-2847812.43	13.99
	5	-4538.27	-2847811.94	14.47
Mn-PTA	1	-4497.12	-2821990.48	38.11
	3	-4497.16	-2822013.77	14.82
	5	-4497.19	-2822028.59	0.00
Ru-PTA	2	-4487.09	-2815691.16	0
	4	-4487.05	-2815669.27	21.89
	6	-4487.05	-2815669.28	21.89
Rh-PTA	1	-4502.71	-2825497.53	0
	3	-4502.68	-2825476.85	20.69
	5	-4502.63	-2825444.32	53.21
Os-PTA	2	-4484.27	-2813926.39	0
	4	-4484.21	-2813886.33	40.06
	6	-4484.13	-2813836.30	90.09
Ir-PTA	1	-4497.92	-2822487.82	0
	3	-4497.87	-2822456.82	30.99
	5	-4497.79	-2822406.99	80.82
Pt-PTA	2	-4512.30	-2831514.31	0
	4	-4512.24	-2831476.96	37.35

CO*

O	0.55443000	-1.28447100	-0.05449600
O	-1.21957900	-0.05425300	1.26917900
O	-1.22086400	0.05414900	-1.26789600
O	-1.82993900	1.48616300	-3.39610400
W	-2.90683300	1.80378000	-1.79679500
O	-1.49098300	3.01084800	-1.19480800
W	-0.34511600	3.64267800	0.15111500
O	-1.49157700	2.90244600	1.44037500
W	-2.90504800	1.64800400	1.94261600
O	-3.30947600	1.64950700	0.06983000
O	0.55398000	1.28491200	0.05394700
O	-3.69823100	-0.09010300	2.13466700
W	-2.90347800	-1.80514400	1.80001700
O	-1.82564500	-1.48652600	3.39751400
W	-0.51210600	-0.15072200	3.63004900
O	-1.82759100	1.19715100	3.50807700
O	-3.30853100	-1.65083400	-0.06702500
W	-2.90666000	-1.64930700	-1.93952700
O	-1.83056800	-1.19799300	-3.50656700
O	-4.08894400	-2.66473900	-2.59863400
O	-1.49145700	-2.90312200	-1.43978100
W	-0.34344100	-3.64265100	-0.15179900
O	1.16638500	-3.46520200	-1.45793600
W	2.08382800	-1.90661800	-1.84983700
O	2.67819000	0.06128900	-1.45412100
W	2.08386700	2.05474500	-1.68605600
O	1.16448500	3.57404100	-1.16560700
O	-3.70060900	0.08848500	-2.13197500
O	-4.08606500	-2.87152100	2.37234200
O	-1.48854900	-3.01152200	1.19548100
O	-0.66146000	-5.30365300	-0.22112500
O	1.16705400	-3.57339500	1.16457900
W	2.08686100	-2.05447000	1.68434000
O	3.05371300	-2.11458800	-0.08903300
O	3.35718200	-2.61287700	2.67155700
O	0.83591400	-1.39825000	2.87383400
O	2.67924500	-0.06039300	1.45196100
W	2.08525800	1.90840700	1.84741600
O	3.05262800	2.11560700	0.08651100
O	3.35246000	-2.37748900	-2.88356900
O	0.82939000	-1.15538100	-2.97699100
O	-0.18171800	-0.21815600	5.28955800
O	0.83214700	1.15576600	2.97615400

O	-4.08717500	2.66283200	2.60295300
O	-4.09040300	2.86968800	-2.36796400
O	0.83253400	1.39836800	-2.87473200
O	3.35438200	2.38005200	2.88018800
O	1.16572200	3.46572000	1.45698100
O	-0.66388800	5.30351500	0.22092600
O	3.35341800	2.61332300	-2.67415500
P	-0.33122200	0.00003600	0.00017000
W	-0.51698900	0.15092500	-3.62998800
O	-0.18772800	0.21845900	-5.28972600
Pt	4.13845200	0.00049800	-0.00145200
C	5.40709700	-0.05920200	1.45509600
C	5.40672300	0.05991200	-1.45801200
O	6.10360600	-0.09415200	2.35374400
O	6.10356200	0.09428100	-2.35643600

TS1_c

O	-0.53549000	1.29723300	0.15048800
O	1.14392300	-0.21180900	1.30156800
O	1.26996600	0.15177300	-1.21081200
O	1.96181400	-0.88600300	-3.54573900
W	2.94940100	-1.52678500	-1.97779200
O	1.46507300	-2.76933700	-1.68380300
W	0.23954800	-3.60116700	-0.53654500
O	1.32918600	-3.14782500	0.92613400
W	2.75164400	-2.06959800	1.72021900
O	3.25144300	-1.73159800	-0.10241700
O	-0.60194800	-1.24220300	-0.21976600
O	3.58469200	-0.42780800	2.26448000
W	2.86339000	1.35267500	2.21373500
O	1.70000300	0.78381600	3.68274700
W	0.34253400	-0.52039800	3.62062200
O	1.62295500	-1.87325100	3.29936800
O	3.36390600	1.51713300	0.37103800
W	3.04311800	1.89368200	-1.47587900
O	2.03381800	1.77580400	-3.15385600
O	4.28252700	2.97086000	-1.88304700
O	1.64165100	3.06931600	-0.81913500
W	0.44115000	3.60476700	0.53244500
O	-0.99070500	3.70099200	-0.84446000
W	-1.93355800	2.27037000	-1.56542600
O	-2.64357700	0.30494800	-1.54928300
W	-2.04218000	-1.60014100	-2.15822700

O	-1.21070400	-3.22774700	-1.85968100
O	3.79495800	0.19095700	-1.96488200
O	4.04535600	2.25014400	3.02623700
O	1.51997100	2.69141900	1.77869500
O	0.80703000	5.23784900	0.78227000
O	-1.10644300	3.33832200	1.75761100
W	-2.11744600	1.79234700	1.93209500
O	-2.99743600	2.22535300	0.17455700
O	-3.41393900	2.23007200	2.94094700
O	-0.93948000	0.87803900	3.04535500
O	-2.68221800	-0.13706200	1.43036600
W	-2.20190300	-2.14641600	1.39049300
O	-3.14503700	-1.93927200	-0.43506400
O	-3.14304700	2.99667000	-2.51486800
O	-0.66079800	1.70786200	-2.76972300
O	-0.05641000	-0.74063300	5.25093300
O	-0.99146100	-1.68573700	2.70049100
O	3.87105700	-3.23448200	2.22261600
O	4.12994500	-2.51418600	-2.68042600
O	-0.71911700	-0.80583100	-3.15061400
O	-3.54107100	-2.77727600	2.23262600
O	-1.33056000	-3.62461900	0.71410000
O	0.51587400	-5.25506600	-0.76758000
O	-3.26572600	-1.95811700	-3.28273300
P	0.32173500	-0.00272400	0.00524500
W	0.71073900	0.51648200	-3.59431900
O	0.46855300	0.77009500	-5.25049400
Pt	-4.21750600	-0.15820400	-0.29772800
C	-5.70120000	-0.85429900	0.67625000
C	-4.79712700	1.72451300	-0.12457900
O	-6.58812800	-1.29822900	1.23857900
O	-5.52875800	2.61054200	-0.06172800

CO₂*@ Pt₁-O_{v,c}

O	1.08438100	-0.13196700	0.74453500
O	-1.04192200	1.26598800	0.55387300
O	-1.15368400	-1.27560700	0.29008600
O	-2.47918600	-3.30032900	-0.91400100
W	-3.51935600	-1.66839400	-0.57128800
O	-2.73241400	-0.98097900	-2.21429600
W	-1.90087500	0.40829200	-3.18345800
O	-2.62817900	1.62637900	-1.94355200
W	-3.36451500	2.02582800	-0.18293600
O	-3.76376900	0.16486100	-0.11526300

O	-0.09420400	0.15037200	-1.49544400
O	-3.25738000	2.09222100	1.72336200
W	-1.74735400	1.66140000	2.84919800
O	-0.97012300	3.31667400	2.18437600
W	-0.42851800	3.70074300	0.40396800
O	-2.18665500	3.59815200	-0.19555300
O	-2.20997600	-0.20065000	2.77052800
W	-1.90956600	-2.07023200	2.46142300
O	-1.26807000	-3.61985100	1.46621000
O	-2.50773600	-2.79267400	3.87004500
O	-0.05246600	-1.65047900	2.93915100
W	1.32786800	-0.39263600	3.14772000
O	2.60405800	-1.65280700	2.21920900
W	2.52808000	-2.25721100	0.47395400
O	2.34050800	-1.48966500	-1.29249200
W	0.96736000	-1.46825500	-2.93267400
O	-0.54736600	-0.91804200	-3.84325700
O	-3.43622700	-2.13502400	1.28081100
O	-2.28864900	2.12895800	4.38288900
O	0.06230700	0.99203700	3.21580400
O	1.81733500	-0.58214100	4.75821100
O	2.70734700	0.90216800	2.47590100
W	2.69355600	1.85819100	0.88504500
O	5.35043300	-0.40131200	1.79282900
O	4.18940700	2.67255500	0.94145700
O	1.42713200	3.09172900	1.13080600
O	2.45312700	1.55760100	-0.99646000
W	1.12446900	1.93560100	-2.58723400
O	1.83233700	0.24592800	-3.20681500
O	3.94404900	-3.19307200	0.33370500
O	1.14995800	-3.39311400	0.45044700
O	-0.14257600	5.36878800	0.39078800
O	0.32616800	3.04566900	-1.24707900
O	-4.86589800	2.72790400	-0.51915100
O	-5.07091600	-2.15706300	-1.03399300
O	0.08478600	-2.75483000	-1.84038500
O	2.03306300	3.03276300	-3.50745800
O	-0.43678700	1.70927100	-3.56727800
O	-2.87748500	0.59179600	-4.55286300
O	1.80421000	-2.43021900	-4.05170500
P	-0.30806800	0.00026800	0.03725500
W	-0.74568900	-3.67693000	-0.35538700
O	-0.60398500	-5.32436100	-0.71584900
Pt	3.93611000	-0.13431000	-1.16846400

C	5.54104500	0.79440400	-0.90547500
C	5.18415000	-0.52088500	2.94847100
O	6.54331800	1.32512500	-0.74506700
O	5.03289800	-0.64054400	4.09628900

Pt_I–O_{v,c}

O	-1.01216700	0.06022600	0.98271800
O	1.01092800	-1.33094400	0.28670600
O	1.14897400	1.22475900	0.28203000
O	2.33076400	3.34563100	-0.91259600
W	3.35694700	1.66951900	-0.91184300
O	2.28227800	1.17833800	-2.46670300
W	1.25849300	-0.08474600	-3.41684100
O	2.13567800	-1.44375500	-2.45673900
W	3.14463200	-2.04282100	-0.89381400
O	3.60986200	-0.20582300	-0.70659600
O	-0.23696500	0.01414000	-1.43812800
O	3.35036100	-2.31175100	0.98358600
W	2.05442900	-1.98062200	2.38405500
O	1.13595600	-3.54828400	1.68598300
W	0.29558200	-3.73077400	-0.00817900
O	1.93099500	-3.58740500	-0.88195500
O	2.55761100	-0.12964600	2.42273500
W	2.26777700	1.76685500	2.36818000
O	1.53855300	3.42882600	1.65704200
O	3.11044600	2.31982900	3.72755300
O	0.50372300	1.32337700	3.09730700
W	-0.87217200	0.07126100	3.39338100
O	-2.22495900	1.45390000	2.82426100
W	-2.41060700	2.27188200	1.18337200
O	-2.55598300	1.66590200	-0.64528500
W	-1.46927000	1.79388700	-2.49484100
O	-0.15068600	1.32273800	-3.70077500
O	3.59014000	1.93292800	0.96329200
O	2.82468800	-2.61682000	3.74999600
O	0.35133900	-1.32873500	3.11210300
O	-1.09019800	0.09330300	5.07337700
O	-2.37802200	-1.12591700	2.83232500
W	-2.64418100	-1.92829200	1.18533500
O	-4.13361600	-2.72896300	1.40022900
O	-1.38946500	-3.19330700	1.09134700
O	-2.72053500	-1.40160400	-0.65766400
W	-1.67937900	-1.61997300	-2.48695500

O	-2.43301900	0.13621100	-2.78477900
O	-3.79554600	3.24372900	1.38089900
O	-1.01388700	3.37735800	1.04961500
O	-0.04059600	-5.38298700	-0.15233700
O	-0.70927600	-2.88157900	-1.42110400
O	4.54685800	-2.72516200	-1.54852800
O	4.82843400	2.17953300	-1.57128900
O	-0.37373700	2.94107700	-1.43950700
O	-2.76703100	-2.59614700	-3.34740000
O	-0.30036900	-1.31392200	-3.68723800
O	1.98603500	-0.13020500	-4.94393300
O	-2.44750700	2.88534300	-3.34902900
P	0.23627000	-0.00764200	0.04394400
W	0.72822900	3.69273100	-0.03740000
O	0.59231300	5.37125300	-0.20468900
Pt	-4.13905300	0.32510200	-0.34081900
C	-5.70249100	-0.58969900	0.12957500
O	-6.68469400	-1.10846900	0.41041700

CO@*O_{v,c}**

O	0.75148700	0.00002100	-1.14119900
O	-1.22003100	-1.28302000	-0.17213600
O	-1.22031700	1.28280700	-0.17255300
O	-2.09542000	3.47549400	1.12589600
W	-3.20275100	1.85911300	1.27209600
O	-1.96162900	1.31336300	2.68248700
W	-0.88749700	0.00061100	3.49659600
O	-1.96142900	-1.31227900	2.68280700
W	-3.20260900	-1.85899400	1.27257000
O	-3.58987900	0.00006700	1.12904200
O	0.31845100	0.00029400	1.35431700
O	-3.66420400	-2.12905300	-0.55996600
W	-2.53644700	-1.87649700	-2.11640300
O	-1.63684100	-3.50374800	-1.52437600
W	-0.60581000	-3.73968600	0.04686300
O	-2.09485700	-3.47518200	1.12751100
O	-2.93820500	-0.00066800	-2.11334900
W	-2.53698800	1.87537400	-2.11693900
O	-1.63716200	3.50281600	-1.52596300
O	-3.50874800	2.46755600	-3.36992600
O	-0.89997000	1.32855800	-3.04980600
W	0.37060700	-0.00056300	-3.46993300
O	1.86555700	1.29062000	-3.07765200

W	2.26526100	2.15382900	-1.49437300
O	2.62279800	1.47711900	0.22722100
W	1.79365100	1.70879800	2.18936300
O	0.62751900	1.32534900	3.57292400
O	-3.66453700	2.12837000	-0.56080500
O	-3.50815100	-2.46933100	-3.36912500
O	-0.89957900	-1.33014600	-3.04919600
O	0.40843300	-0.00097800	-5.16486500
O	1.86581800	-1.29151400	-3.07700900
W	2.26557000	-2.15435500	-1.49363500
O	3.70255000	-2.99815500	-1.86106200
O	0.97437800	-3.36534600	-1.25517500
O	2.62322100	-1.47646700	0.22751000
W	1.79391100	-1.70757300	2.19002900
O	2.69269300	0.00069100	2.38428700
O	3.70230800	2.99742200	-1.86202300
O	0.97410000	3.36496800	-1.25648300
O	-0.36941900	-5.40945200	0.18830500
O	0.62834100	-2.91676000	1.28980400
O	-4.54258800	-2.45654200	2.11458200
O	-4.54282800	2.45684500	2.11381800
O	0.62776100	2.91751600	1.28879100
O	2.95433000	-2.74015200	2.87684200
O	0.62773200	-1.32385900	3.57346700
O	-1.39892800	0.00082600	5.10984000
O	2.95391100	2.74178700	2.87583300
P	-0.35402600	0.00001000	-0.05145900
W	-0.60627400	3.73964400	0.04528600
O	-0.37010900	5.40950800	0.18593300
Pt	4.41356300	0.00010600	0.19497600
C	5.62613400	-1.49088000	0.02781400
O	6.53710500	-2.17901400	-0.08328500
C	5.62555100	1.49171300	0.02916200
O	6.53586400	2.18076300	-0.08159900

[CO*+O₂*]_c

O	0.51445500	-0.07058500	1.32915700
O	-1.07217700	1.39721200	-0.02319600
O	-1.38534200	-1.13657800	-0.00509800
O	-2.29774800	-3.24253900	-1.43102600
W	-3.13296600	-1.52271600	-1.83702600
O	-1.55501500	-1.20469900	-2.97283100
W	-0.19011200	-0.09092900	-3.57922000

O	-1.18793000	1.40846300	-2.98577200
W	-2.59273900	2.17098300	-1.87768700
O	-3.25290000	0.37706900	-1.79481000
O	0.58848600	-0.09119900	-1.20802300
O	-3.42046100	2.55580200	-0.19186700
W	-2.76613500	2.18572500	1.58667700
O	-1.50337700	3.67291100	1.24282100
W	-0.14924100	3.72273700	-0.04064900
O	-1.36905500	3.64578400	-1.45508100
O	-3.41801000	0.40087500	1.47664000
W	-3.24648700	-1.51046300	1.62003500
O	-2.43125300	-3.23656500	1.24295100
O	-4.54781200	-1.94242700	2.61132700
O	-1.84175700	-1.11789700	2.88206600
W	-0.50646200	0.02516400	3.60422900
O	0.74415300	-1.47014800	3.52082100
W	1.61295600	-2.22526500	2.01569700
O	2.29827200	-1.93422700	0.25657400
W	1.90017800	-2.08798900	-1.65772700
O	1.16160500	-1.49837900	-3.28512800
O	-4.00631300	-1.66364200	-0.15912600
O	-3.90579200	2.95370700	2.57489200
O	-1.47629000	1.47609700	2.84678300
O	-0.88290300	0.09818000	5.25311200
O	1.12461000	1.17373800	3.52416400
W	2.13485900	1.61082600	2.02864600
O	3.50795000	2.35888000	2.70013900
O	1.10300300	2.93873400	1.34801300
O	2.87913400	1.19131700	0.19928600
W	2.30214400	1.49895100	-1.84697700
O	3.11667100	-0.38840000	-1.78272800
O	2.69156400	-3.33904900	2.70555400
O	0.22338500	-3.23384300	1.39977100
O	0.35413000	5.33930400	-0.05159400
O	1.18286300	2.80785400	-1.19993900
O	-3.62919900	2.90711600	-2.99438400
O	-4.33328800	-1.96527600	-2.94409300
O	0.42565900	-3.12535800	-1.18062500
O	3.69888200	2.34283700	-2.34040600
O	1.44993100	1.10151300	-3.41182500
O	-0.38357400	-0.09739200	-5.26157300
O	3.08599400	-3.20562800	-2.14734100
P	-0.35884000	0.02254700	0.02753200
W	-1.10228700	-3.64327100	-0.04410500

O	-1.05478600	-5.33471300	-0.06569200
Pt	4.49776700	0.00390800	-0.31234800
C	5.68599000	0.67130500	1.04501600
O	6.45156600	1.13578900	1.75128100
C	5.79645800	-1.13932400	-1.08833700
O	6.54246000	-1.84287200	-1.58733400
O	4.18279100	-0.66819800	2.52243400
O	2.89587900	-0.44013800	2.37795000

TS2_c

O	0.59624800	-0.18707200	1.27351300
O	-1.15452500	1.32467700	0.20350400
O	-1.29906400	-1.20895300	-0.09687700
O	-2.14286400	-3.16711900	-1.75879900
W	-3.11700900	-1.47682800	-1.88690000
O	-1.64277300	-0.88505800	-3.04082200
W	-0.40069300	0.41041800	-3.56290900
O	-1.46964600	1.72460500	-2.72782800
W	-2.85697100	2.21859200	-1.44974700
O	-3.37627500	0.38641500	-1.57529200
O	0.51438200	0.12389800	-1.25633100
O	-3.58668700	2.32423900	0.31303000
W	-2.78462800	1.78264000	1.98839500
O	-1.65404300	3.38485100	1.76522900
W	-0.39349200	3.70518600	0.41577700
O	-1.69769100	3.71367500	-0.91562300
O	-3.32199200	-0.02061000	1.67227100
W	-3.02154800	-1.91581400	1.54671000
O	-2.11417100	-3.51882900	0.90115800
O	-4.23055700	-2.56967200	2.53297300
O	-1.57561400	-1.59239700	2.78364500
W	-0.27815600	-0.45722500	3.58311200
O	1.05601500	-1.84928300	3.24389100
W	1.86409900	-2.34977900	1.61606000
O	2.42059800	-1.72163100	-0.09825400
W	1.93433000	-1.64758500	-2.05902900
O	1.04589700	-0.95605200	-3.54912400
O	-3.87244100	-1.90045100	-0.19662700
O	-3.90959400	2.32663800	3.12949600
O	-1.38041800	1.00756600	3.07747300
O	-0.55736800	-0.62098500	5.24445800
O	1.27702500	0.78638600	3.55751700
W	2.11932100	1.54237200	2.06971400

O	3.51025200	2.24246200	2.75818200
O	0.99231600	2.89327500	1.69506600
O	2.73711900	1.31017900	0.21307100
W	2.11080200	1.87960100	-1.75151100
O	3.00981400	0.09418600	-2.01648000
O	3.09170900	-3.42777100	2.08251400
O	0.54093400	-3.39033400	0.94283600
O	-0.00987300	5.34570000	0.57725700
O	0.93537700	3.01390200	-0.86492200
O	-4.01185900	3.01111000	-2.39794800
O	-4.34898700	-1.86422900	-2.97908100
O	0.57619100	-2.85282600	-1.59037500
O	3.41294400	2.88756600	-2.17591100
O	1.16690900	1.66374200	-3.30974000
O	-0.69933300	0.61004600	-5.21686100
O	3.15360200	-2.62805100	-2.72344000
P	-0.35278100	0.00936800	0.03490700
W	-0.84850900	-3.65651200	-0.49801100
O	-0.69136900	-5.31993400	-0.76397500
Pt	4.38716300	0.15386300	-0.37578300
C	5.35285000	0.17319700	1.36826400
O	6.41344900	0.43874100	1.78866800
C	5.83515700	-0.70888800	-1.18416300
O	6.71608400	-1.21541400	-1.70865100
O	4.43150700	-0.63453400	2.38906100
O	3.11460400	-0.52296800	2.17065400

[CO*-O₂*]

O	0.65258300	0.71001700	1.03176100
O	-1.25927600	1.08245300	-0.61260600
O	-1.17474400	-1.05231600	0.77374600
O	-1.82880200	-3.65783300	0.82327200
W	-2.96836300	-2.51812900	-0.29061800
O	-1.60905600	-2.70650800	-1.67940400
W	-0.52607900	-1.96732500	-3.02682300
O	-1.69680500	-0.50151600	-3.11141200
W	-3.09357700	0.61159800	-2.31920900
O	-3.42222100	-0.90269500	-1.20658000
O	0.47999200	-0.68615600	-1.10250800
O	-3.78418100	1.78412300	-0.98725300
W	-2.90448800	2.50051700	0.58116200
O	-1.91645800	3.62702500	-0.69596600
W	-0.71088100	3.06376100	-2.02248500

O	-2.04810800	2.15070000	-2.95171800
O	-3.28300600	0.87826300	1.52442200
W	-2.78749000	-0.62439900	2.60732800
O	-1.70257100	-2.19514700	3.08203200
O	-3.90211400	-0.57757700	3.87928000
O	-1.35468900	0.50361500	3.23671800
W	-0.17425500	1.98120000	3.04495300
O	1.28984400	0.76993100	3.57784600
W	2.15472300	-0.52294400	2.53924200
O	2.65129900	-1.24574900	0.73951300
W	2.01705700	-2.52835100	-0.78612900
O	1.02001100	-2.99350700	-2.27303000
O	-3.64879500	-1.80786100	1.34315700
O	-4.06067200	3.58215500	1.17735300
O	-1.43837500	2.69776800	1.82082300
O	-0.41114600	2.88736800	4.45384500
O	1.21208000	3.02081300	2.11045900
W	2.03418900	2.64385900	0.46895600
O	3.31014900	3.76347900	0.41497000
O	0.76081600	3.29323000	-0.63799700
O	2.66463300	1.28946900	-0.89215100
W	1.91637800	0.43259900	-2.70184200
O	2.91773800	-1.09974000	-1.87729100
O	3.49970700	-0.96715300	3.47744400
O	0.94924700	-1.86899100	2.72630400
O	-0.46408200	4.44488800	-2.96898800
O	0.65382800	1.79257400	-2.67798600
O	-4.34233500	0.54300400	-3.45774100
O	-4.17705300	-3.59702800	-0.77591100
O	0.82898200	-3.14762900	0.50577800
O	3.11301900	0.98833500	-3.77248600
O	0.93698500	-0.77988800	-3.69954600
O	-0.90101400	-2.87451600	-4.40520100
O	3.30396800	-3.64195200	-0.75460000
P	-0.33837900	0.01289500	0.02412600
W	-0.47368100	-3.11209200	1.99386600
O	-0.13224700	-4.52439600	2.86175600
Pt	4.23671400	-0.04368600	-0.46260400
C	5.26006600	1.07635300	0.90918200
O	6.42765900	1.32601900	0.87046100
C	5.63260100	-1.31618200	-0.34904000
O	6.46866700	-2.09103900	-0.30480300
O	4.49621700	1.51278100	1.94502000
O	3.10465200	1.22011700	1.69655500

TS3_c

O	0.60116100	0.59078600	1.11580000
O	-1.25230700	1.14349100	-0.52995700
O	-1.21363400	-1.12384000	0.63322900
O	-1.87752100	-3.70541900	0.42224700
W	-2.97642800	-2.45338000	-0.60366600
O	-1.58907800	-2.50998000	-1.97790000
W	-0.47128900	-1.64309700	-3.21880600
O	-1.62520400	-0.16242300	-3.17446800
W	-3.03378400	0.87675500	-2.30054100
O	-3.39739500	-0.74710700	-1.36535500
O	0.49172600	-0.57889800	-1.15535400
O	-3.75499700	1.90982600	-0.86875300
W	-2.90648900	2.45471600	0.78190200
O	-1.87891700	3.69732000	-0.34512200
W	-0.64261300	3.26517300	-1.69115600
O	-1.96832600	2.46706100	-2.74161500
O	-3.31490500	0.74755600	1.54574100
W	-2.86311100	-0.86529000	2.47490100
O	-1.79606100	-2.48033000	2.81645800
O	-4.00882100	-0.93663100	3.71760300
O	-1.43193000	0.17722600	3.25204400
W	-0.23723300	1.65087100	3.23602200
O	1.21879600	0.38908200	3.66084600
W	2.11052400	-0.78136700	2.49929900
O	2.61772100	-1.36222600	0.64443300
W	2.00627900	-2.47764300	-0.97944200
O	1.05176200	-2.75547800	-2.54264300
O	-3.69932400	-1.90166100	1.07593500
O	-4.06578300	3.48038900	1.46445400
O	-1.46393100	2.50654800	2.06406400
O	-0.49897000	2.40749100	4.72653500
O	1.18411800	2.77174300	2.44280100
W	2.05214500	2.53041600	0.80341200
O	3.33944700	3.64014800	0.87265400
O	0.79559400	3.28775300	-0.27196700
O	2.68138800	1.34616500	-0.73841700
W	1.97233000	0.71092100	-2.60791000
O	2.94939000	-0.94029500	-1.92176600
O	3.42898300	-1.34710200	3.41328100
O	0.86919200	-2.12504400	2.51676200
O	-0.36597500	4.74011200	-2.47356900

O	0.71535900	2.05976100	-2.49127500
O	-4.25490300	0.94033700	-3.46923000
O	-4.18126300	-3.46646600	-1.22225600
O	0.78075500	-3.21814700	0.19725500
O	3.19329800	1.34799400	-3.60236700
O	1.02044300	-0.41490200	-3.73168200
O	-0.82421200	-2.39635500	-4.69250000
O	3.28053200	-3.60361900	-1.04528500
P	-0.35541000	0.00450100	0.01202200
W	-0.54089200	-3.28763000	1.67292300
O	-0.22393800	-4.77932400	2.40687700
Pt	4.23775800	-0.03669600	-0.39631000
C	5.39711700	1.13181200	0.98061900
O	6.48430900	1.43422400	0.55882500
C	5.61302800	-1.33427200	-0.33957700
O	6.42904100	-2.13263300	-0.33394100
O	4.79243900	1.31817900	2.07820300
O	3.01026600	0.96675800	1.81090200

CO₂*+Pt₁

O	0.54908100	0.11573900	-1.28952000
O	-1.03569100	-1.38123400	-0.00020500
O	-1.37504600	1.14122500	0.00021000
O	-2.30583100	3.22358200	1.33776200
W	-3.14148800	1.50850700	1.72569700
O	-1.64908900	1.16201900	2.95768700
W	-0.35507900	0.00027400	3.64242500
O	-1.29525000	-1.46589700	2.95698100
W	-2.63309400	-2.20574000	1.72566100
O	-3.27036100	-0.39881200	1.65665900
O	0.54893500	0.11518300	1.28970500
O	-3.39471500	-2.55690900	-0.00085000
W	-2.63311600	-2.20483900	-1.72702300
O	-1.37106000	-3.63321700	-1.33809300
W	-0.03111700	-3.64085600	-0.00095500
O	-1.37122400	-3.63403200	1.33609000
O	-3.26985100	-0.39789200	-1.65725400
W	-3.14120300	1.50953700	-1.72536400
O	-2.30563800	3.22434700	-1.33638800
O	-4.39401700	1.94995200	-2.77316000
O	-1.64857500	1.16360300	-2.95725500
W	-0.35467900	0.00193700	-3.64240200
O	1.00675200	1.47486900	-3.51069000

W	1.80141600	2.10025200	-1.96566700
O	2.27490400	1.95885100	0.00072300
W	1.80122700	2.09928100	1.96705000
O	1.00632200	1.47301000	3.51172600
O	-3.96906700	1.65003800	0.00011300
O	-3.72368800	-2.96500600	-2.77346800
O	-1.29498300	-1.46448600	-2.95798300
O	-0.66943100	-0.03795500	-5.30485000
O	1.34048700	-1.09102400	-3.52898900
W	2.27796000	-1.45501800	-1.99197200
O	3.66934900	-2.29284100	-2.50099800
O	1.18605400	-2.78179100	-1.30721000
O	2.73672000	-1.11863000	-0.00009600
W	2.27764900	-1.45599600	1.99155200
O	3.10279600	0.44404100	2.00662600
O	2.93172000	3.25413700	-2.49500400
O	0.38430700	3.09994700	-1.31542400
O	0.50302300	-5.24649300	-0.00141000
O	1.18585700	-2.78248500	1.30592300
O	-3.72374600	-2.96647300	2.77163600
O	-4.39447600	1.94851100	2.77345300
O	0.38409000	3.09920400	1.31729600
O	3.66896600	-2.29406900	2.50032900
O	1.34000700	-1.09288900	3.52862700
O	-0.67007600	-0.04057600	5.30480400
O	2.93134200	3.25296200	2.49722400
P	-0.32786200	-0.00226700	0.00002300
W	-1.01892000	3.59200200	0.00090800
O	-0.93678700	5.28229100	0.00141500
Pt	3.92210600	0.48766300	0.00035100
C	5.21218700	-2.67466900	0.00012700
O	4.77834800	-3.75212100	-0.00056900
C	5.19880100	1.89843700	-0.00032400
O	5.98601000	2.72573100	-0.00289700
O	5.65802900	-1.58416700	0.00080700
O	3.10309200	0.44505300	-2.00596800
Pt₁			
O	0.64674100	1.28812200	0.06125100
O	-1.02610900	0.00168100	-1.34175700
O	-1.21782700	-0.00135300	1.19552700
O	-2.01429100	-1.34168200	3.33219300
W	-2.95602500	-1.72770800	1.67352200

O	-1.49111900	-2.95966600	1.23024500
W	-0.26809400	-3.64108000	-0.00820700
O	-1.29190700	-2.95428600	-1.41503200
W	-2.67995400	-1.72373800	-2.06502200
O	-3.20092700	-1.65726400	-0.22378000
O	0.64635800	-1.28845800	0.05820100
O	-3.46191900	0.00284500	-2.36630400
W	-2.68012300	1.72869800	-2.06056900
O	-1.51406100	1.34004000	-3.56844600
W	-0.17639700	0.00471100	-3.66437000
O	-1.51379400	-1.33134200	-3.57151000
O	-3.20149700	1.65745500	-0.21963400
W	-2.95604200	1.72352100	1.67785600
O	-2.01450900	1.33332000	3.33562600
O	-4.18019900	2.76869100	2.19753700
O	-1.49104400	2.95606700	1.23741300
W	-0.26804200	3.64109900	0.00078300
O	1.17096100	3.52022700	1.40674100
W	2.01260000	1.98453100	1.97285200
O	2.53240800	-0.00207600	1.72568800
W	2.01278100	-1.98927500	1.96808600
O	1.17120800	-3.52346000	1.39843500
O	-3.77336600	-0.00239300	1.86527600
O	-3.81557100	2.77631400	-2.74953700
O	-1.29173100	2.95688400	-1.40761900
O	-0.58486600	5.30333400	-0.02415900
O	1.36812800	3.51986600	-1.16891800
W	2.26893200	1.97987700	-1.62351400
O	3.21997800	1.99617600	0.26572100
O	3.61176600	2.51301800	-2.51817000
O	1.08756300	1.33003700	-2.89598500
O	2.68913500	0.00185400	-1.42631200
W	2.26892500	-1.97571700	-1.62849400
O	3.22001800	-1.99672800	0.26082000
O	3.17921200	2.52192900	3.08287400
O	0.66493200	1.30238000	3.03678300
O	0.25041900	0.00667500	-5.30172800
O	1.08764900	-1.32275700	-2.89940100
O	-3.81556200	-2.76964000	-2.75630300
O	-4.18014600	-2.77431800	2.19039900
O	0.66519200	-1.30933300	3.03385100
O	3.61162300	-2.50686600	-2.52453900
O	1.36829500	-3.51675100	-1.17740700
O	-0.58403200	-5.30341000	-0.03743700

O	3.17947500	-2.52937600	3.07669900
P	-0.23778400	0.00006700	-0.00604900
W	-0.70773100	-0.00449600	3.61968100
O	-0.52002300	-0.00683300	5.30141000
Pt	3.98201800	-0.00047100	0.36094800
C	5.53081500	0.00048600	-0.74398600
O	6.48131000	0.00127100	-1.37769900