Electronic Supplementary Information for

Polymeric tungsten carbide nanoclusters as potential non-noble metal catalysts for CO oxidation

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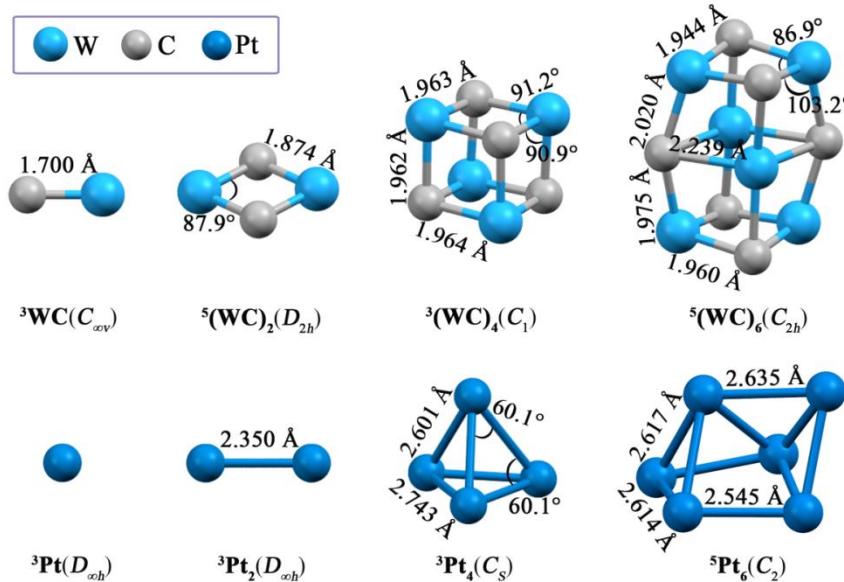E-mail: jlyang@ustc.edu.cn

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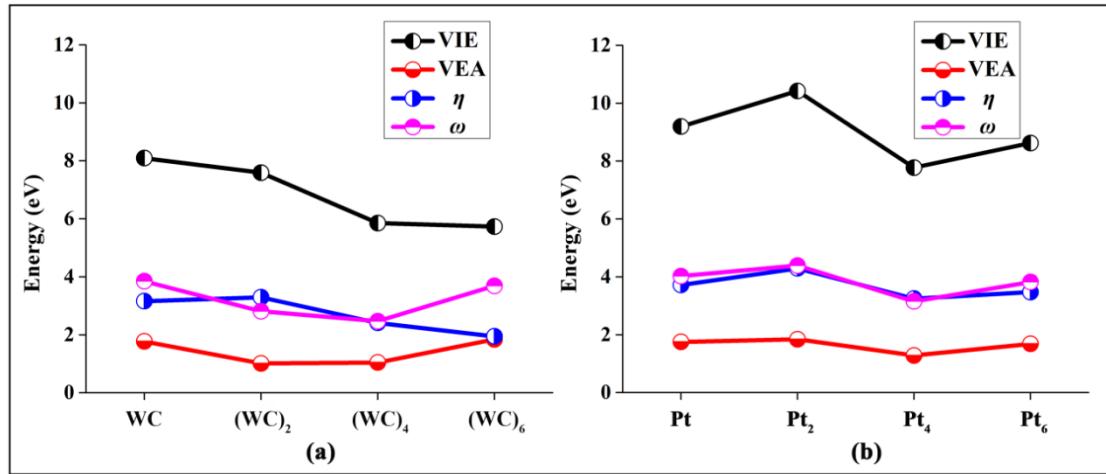
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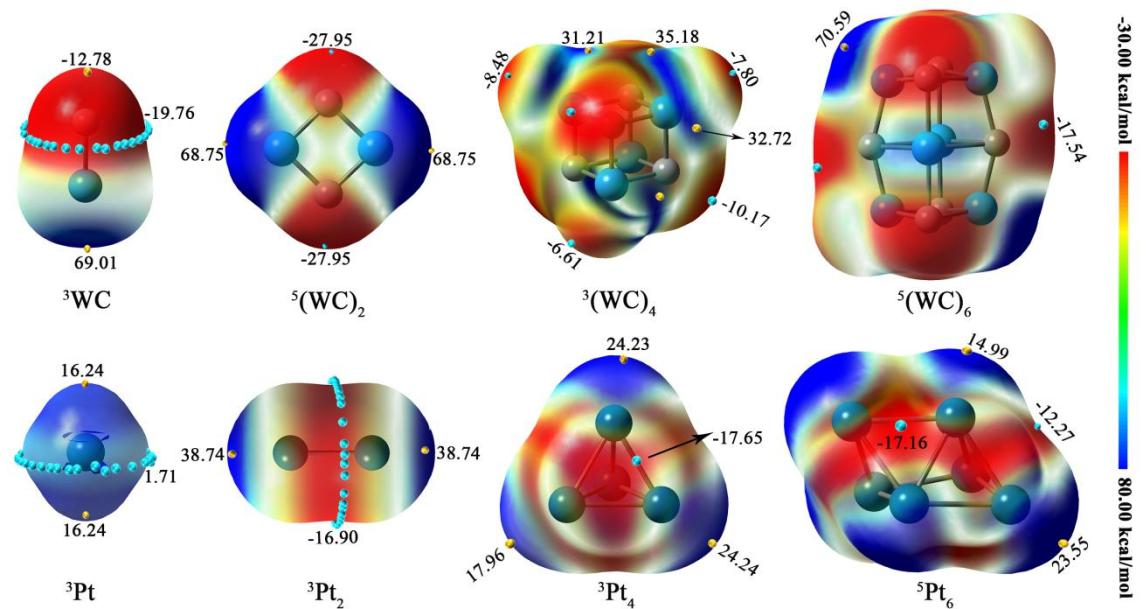
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^3WC

$^5(WC)_2$

$^3(WC)_4$

$^5(WC)_6$

^3Pt

$^3Pt_2$

$^3Pt_4$

$^5Pt_6$
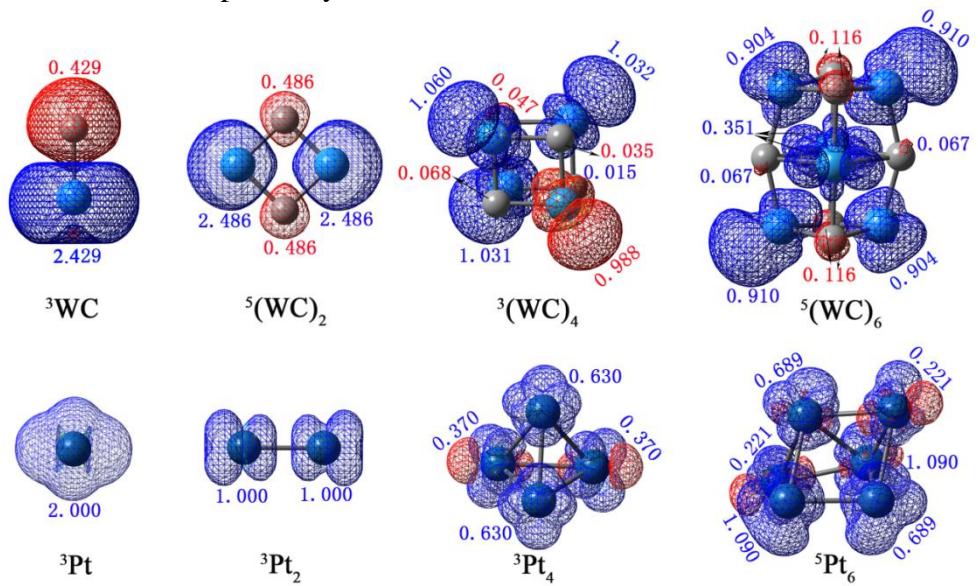
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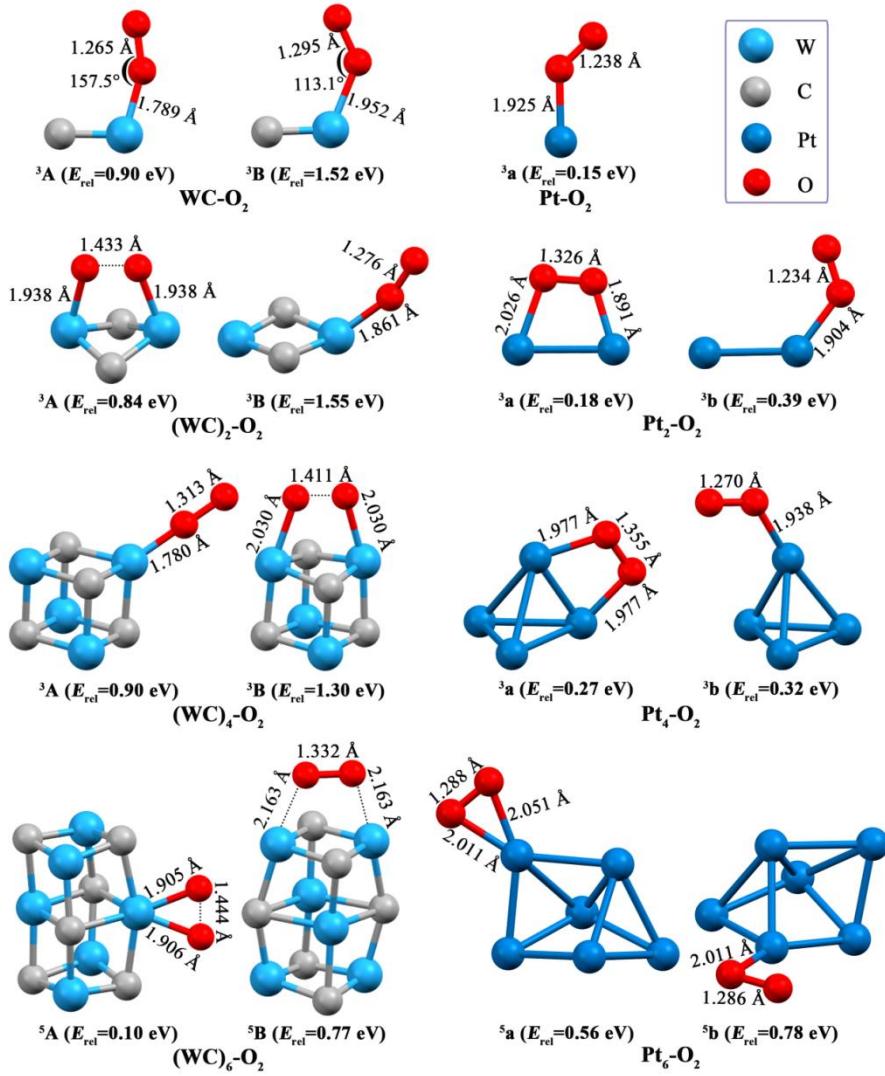
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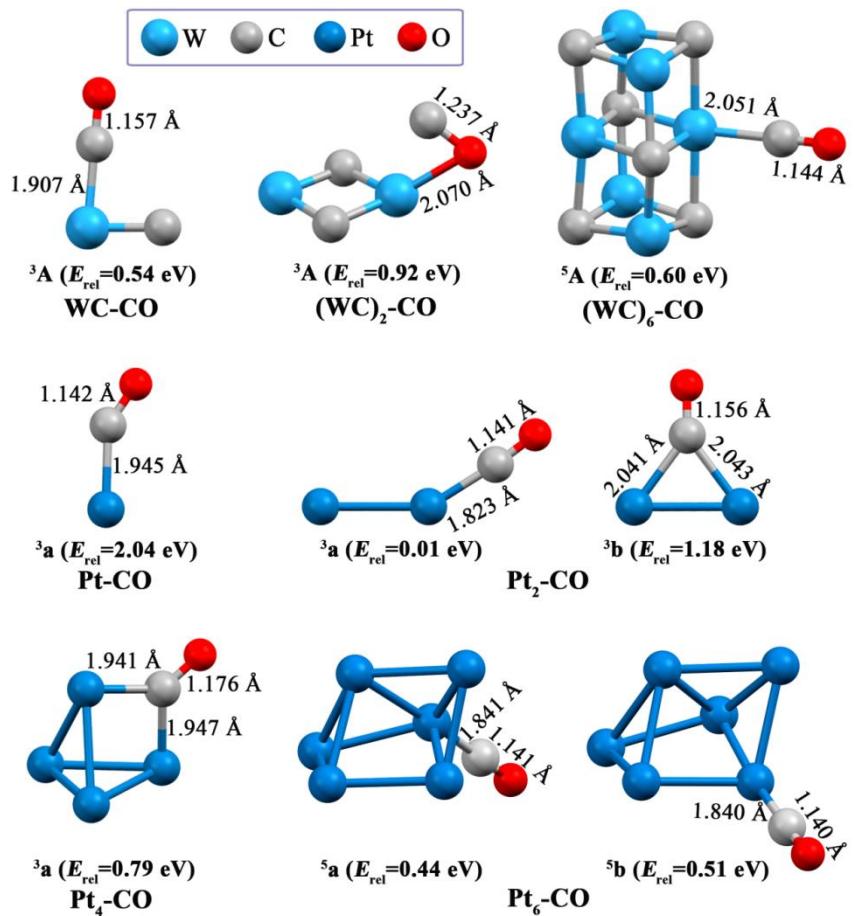
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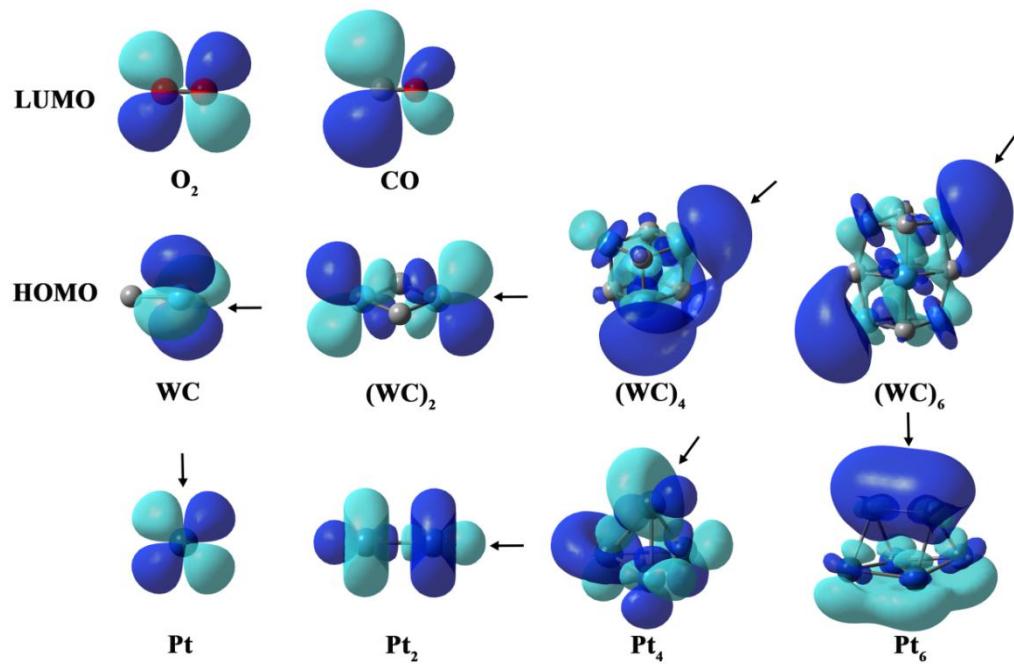
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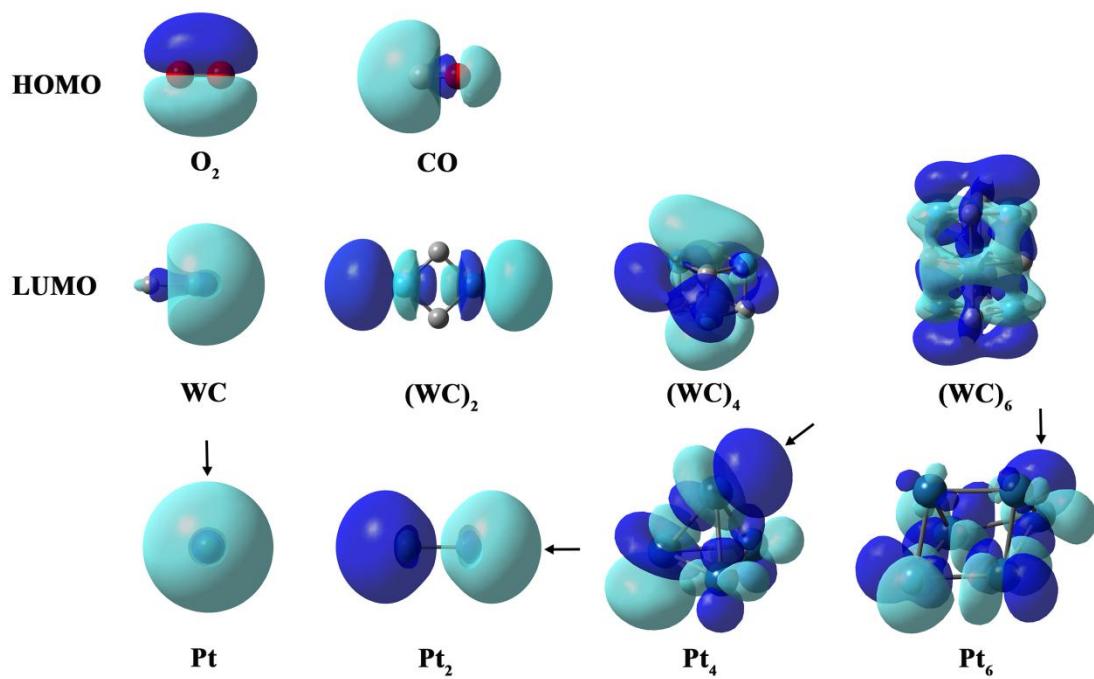
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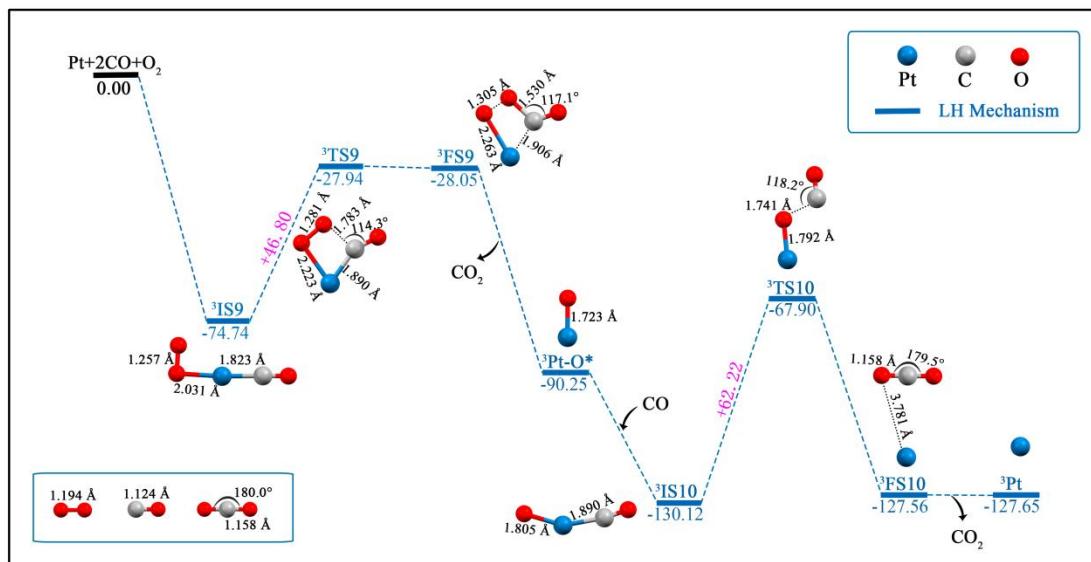
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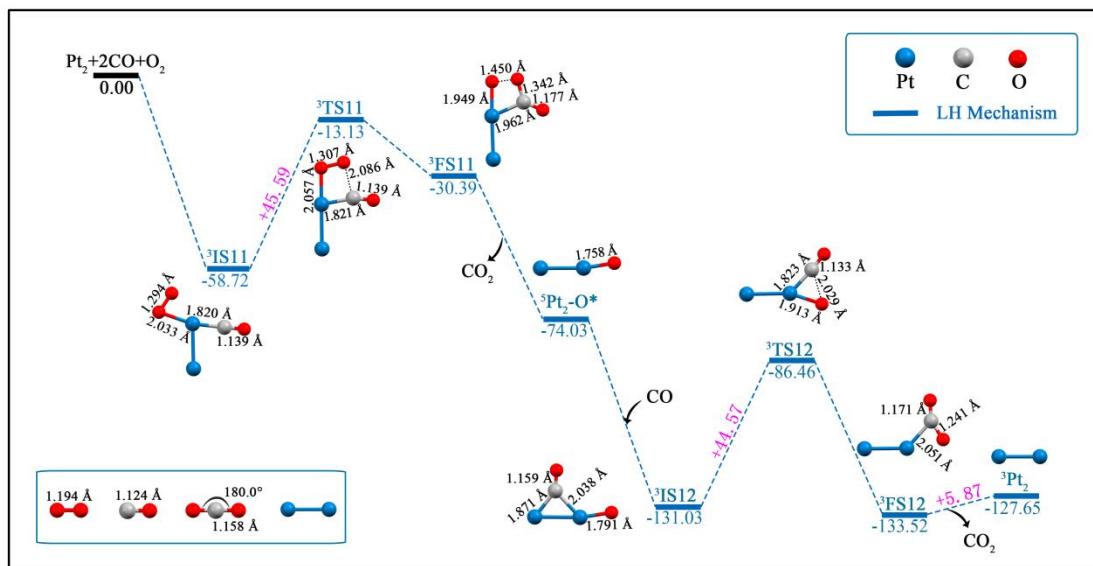
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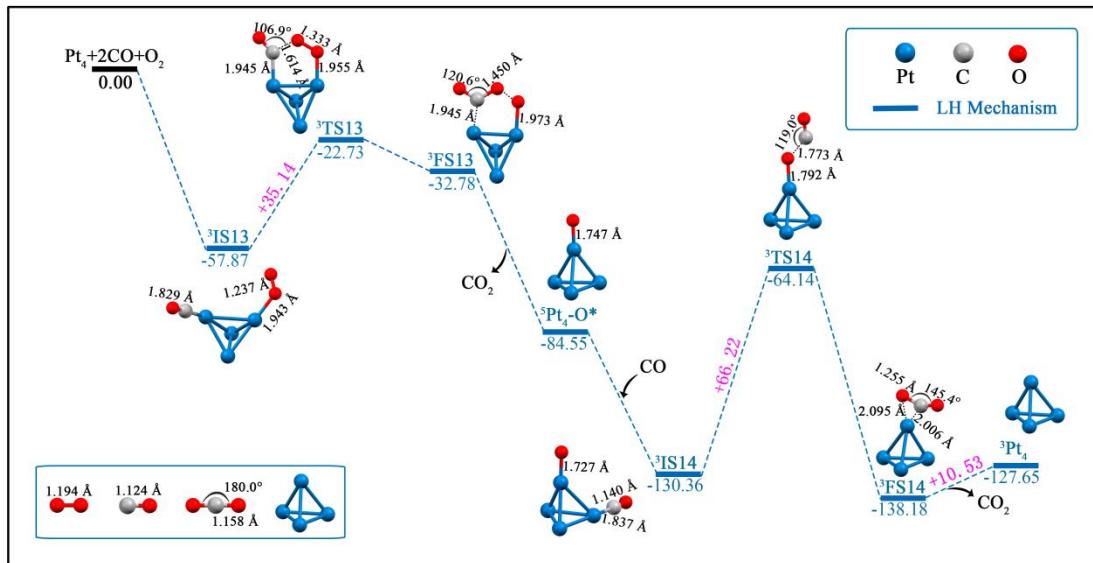
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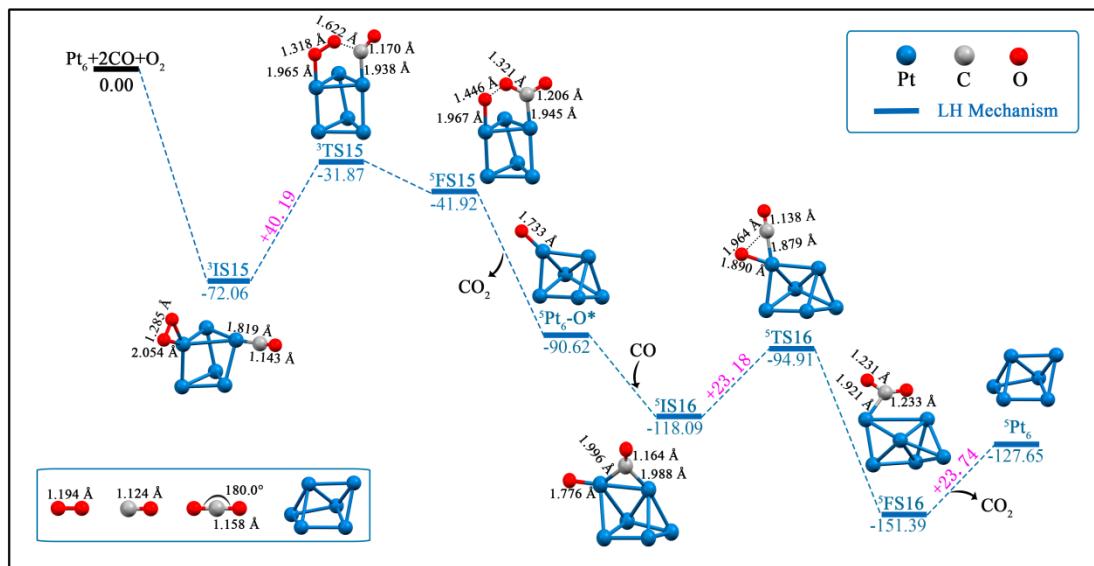
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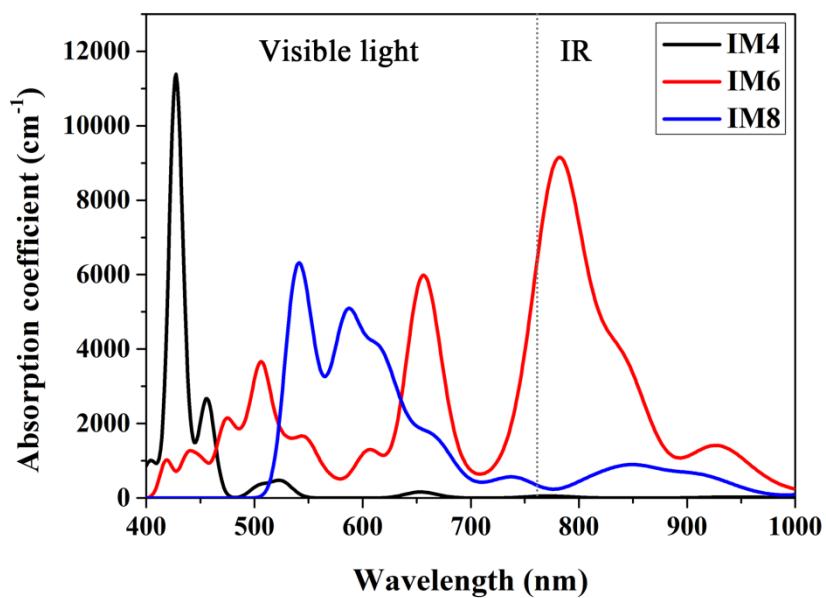
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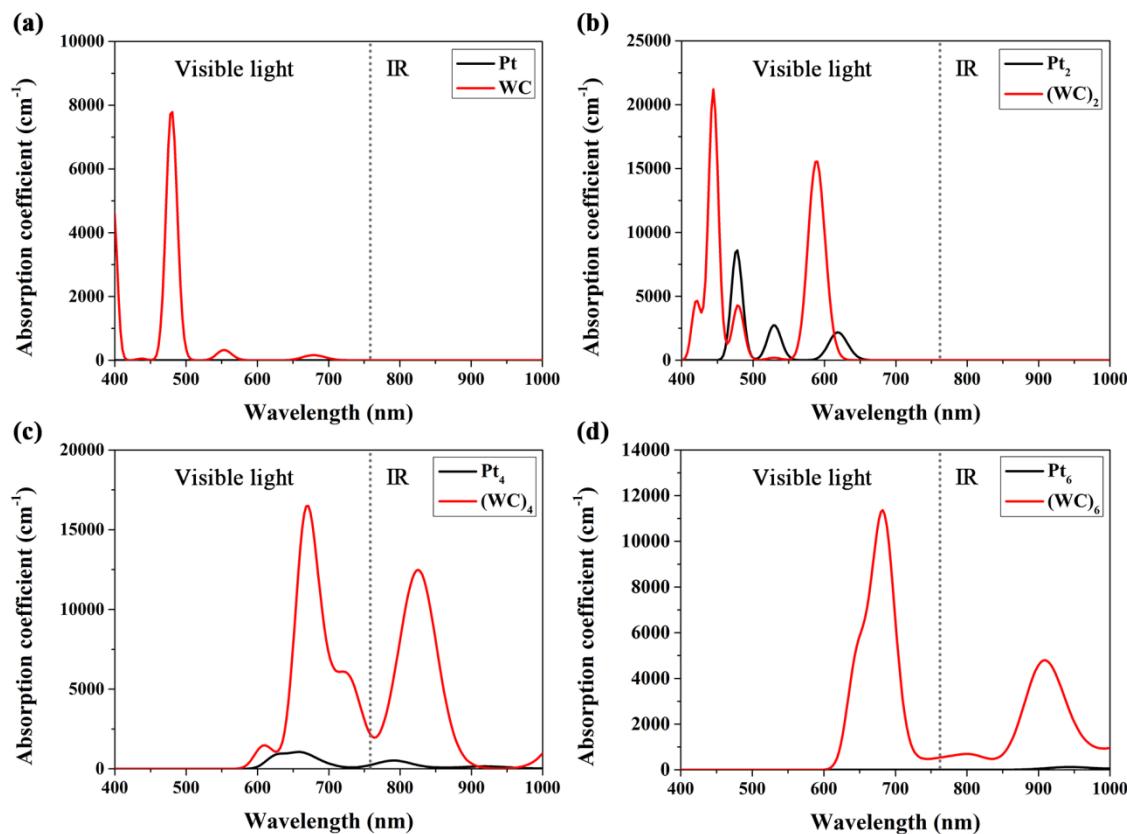
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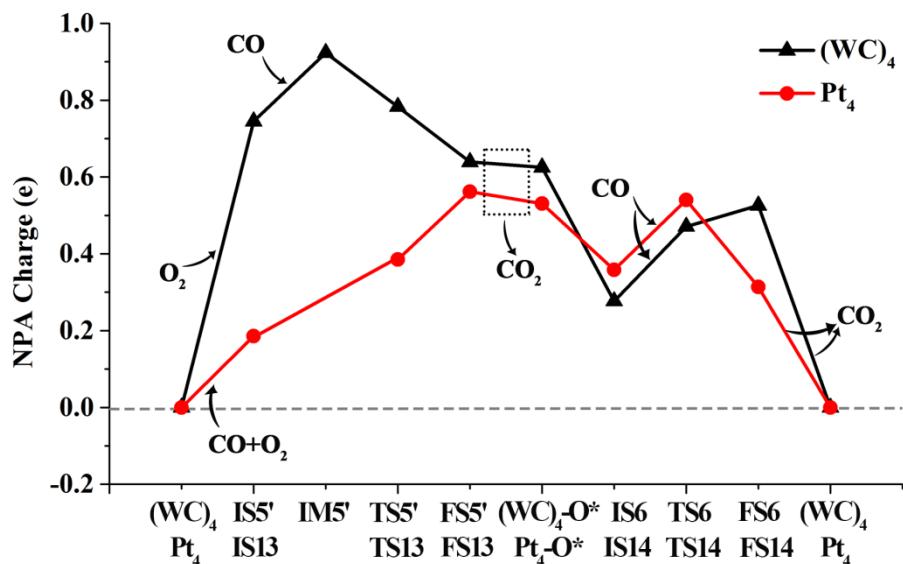
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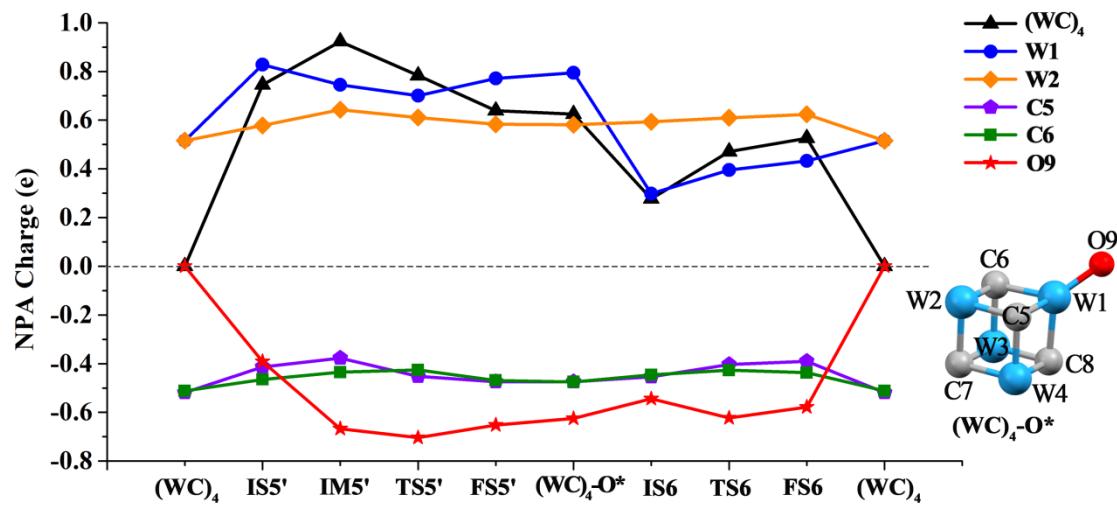
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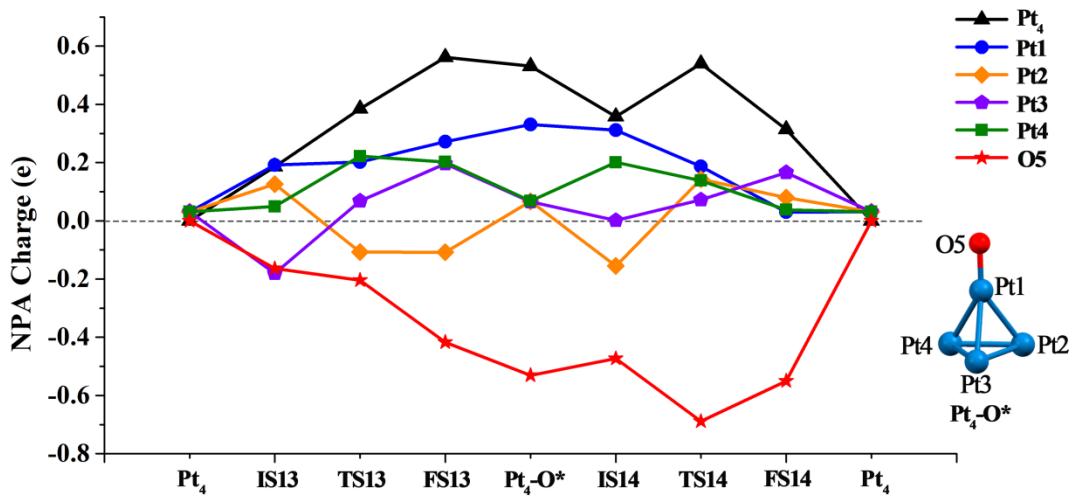
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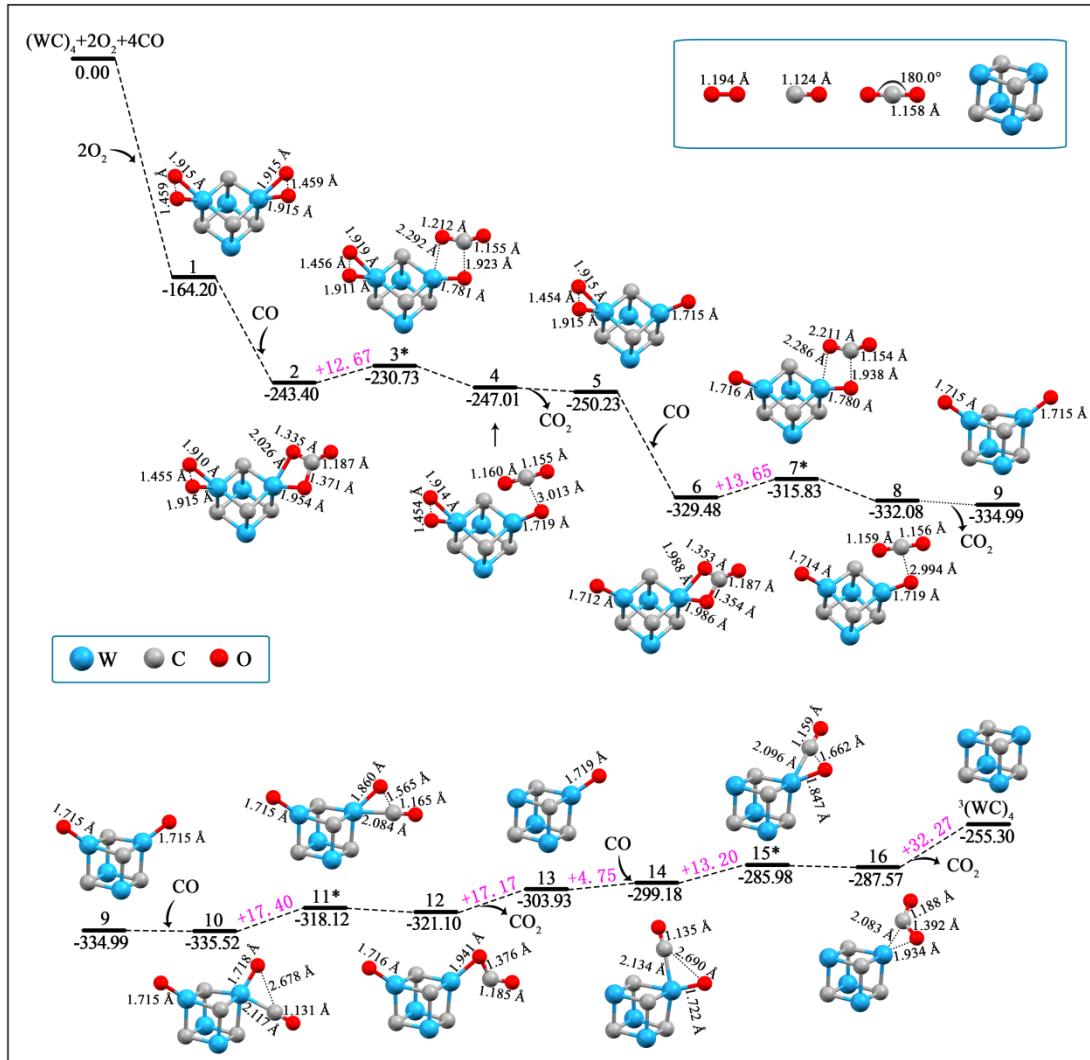
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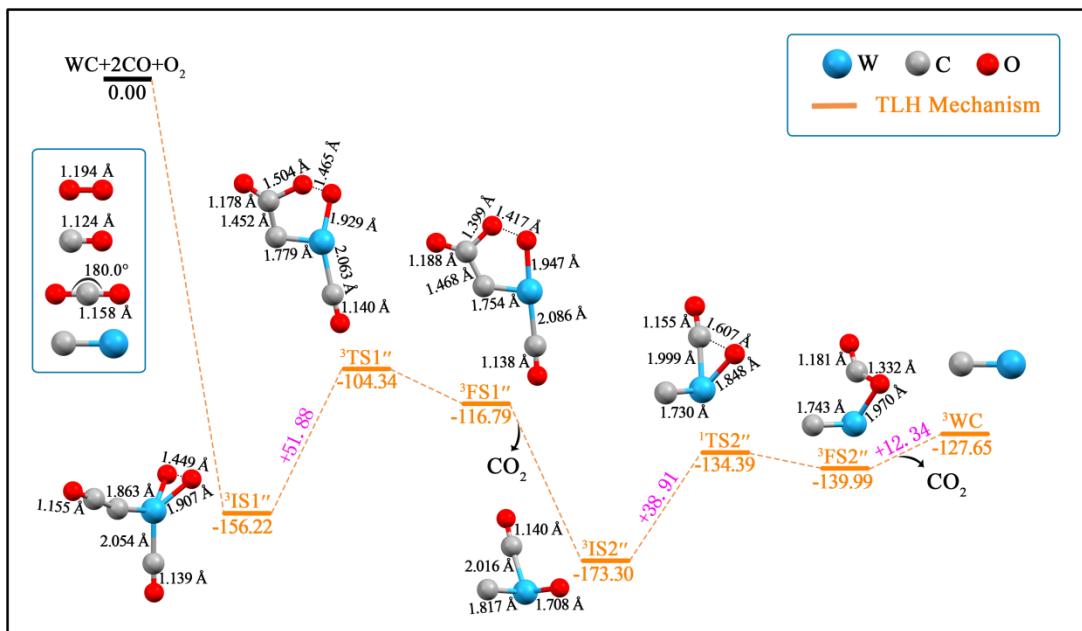
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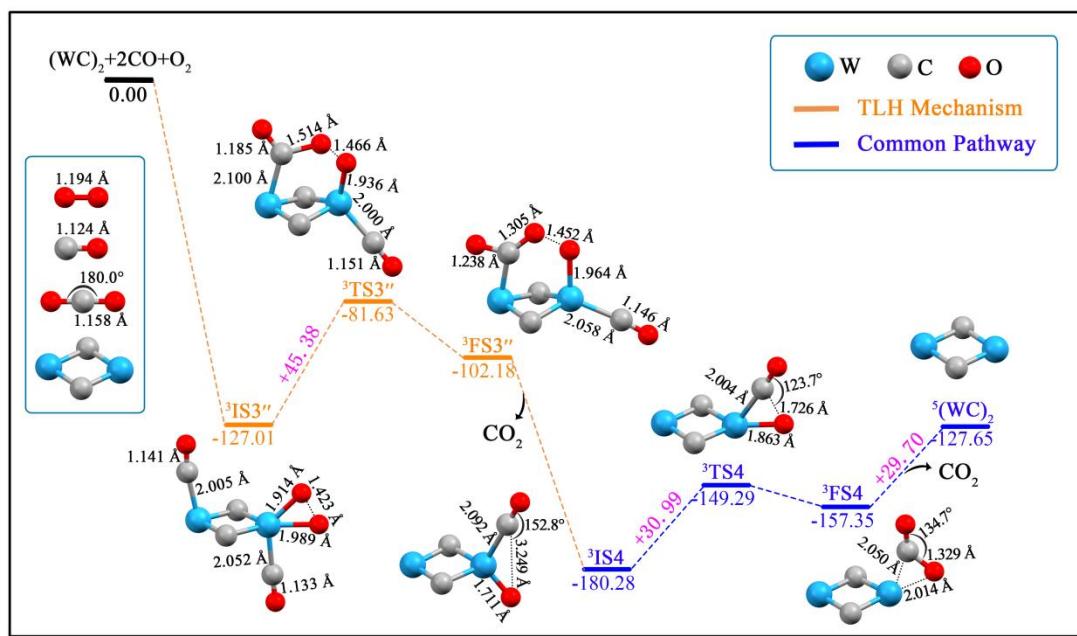
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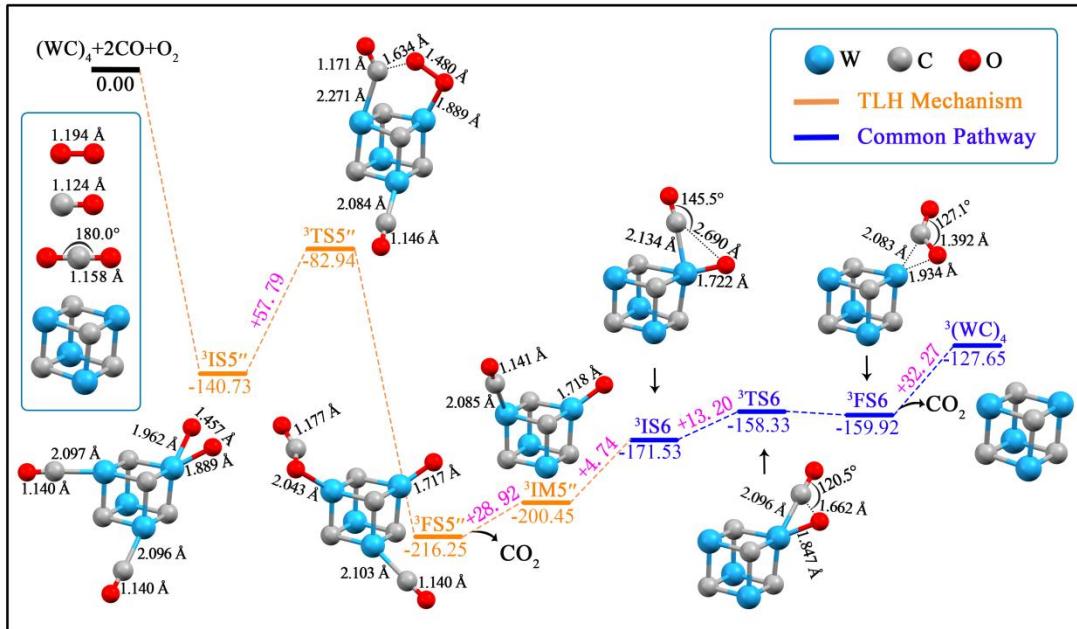
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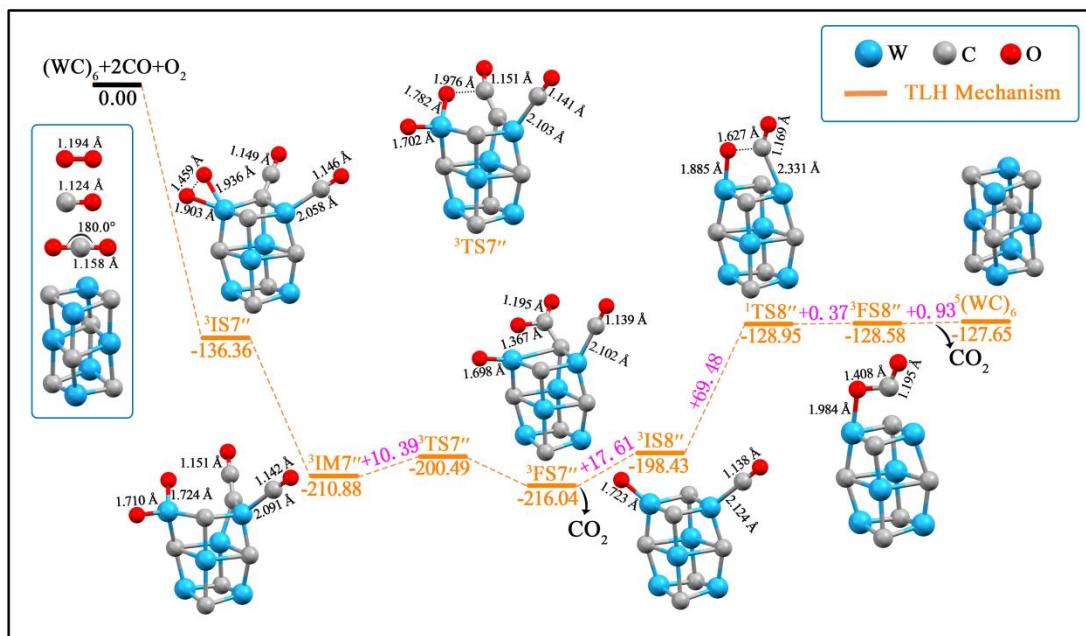
3. Cartesian Coordinates

(1) $(WC)_n$ and Pt_n (n = 1, 2, 4, and 6) species

WC

W	0.00000000	0.00000000	0.12751900
C	0.00000000	0.00000000	-1.57273500

$(WC)_2$

W	0.00000000	0.00000000	1.34862800
W	0.00000000	0.00000000	-1.34862800
C	0.00000000	1.30101800	0.00000000
C	0.00000000	-1.30101800	0.00000000

$(WC)_4$

W	-0.57997000	-0.75030100	-1.42672200
W	1.72108100	-0.03125100	0.00924200
C	0.53397700	-1.59552900	-0.04996000
C	0.58456700	0.82729700	-1.34419500
W	-0.59670300	-0.84235400	1.36730700
W	-0.54422100	1.62386600	0.05016000
C	0.56747900	0.73722100	1.40270200
C	-1.68833300	0.03150700	-0.00836700

$(WC)_6$

W	-1.38476700	1.89679500	0.00000000
W	0.00000000	0.00000000	1.22726900
C	-1.87177100	-0.06317700	0.00000000
C	0.00000000	2.11035800	1.34768400
W	1.41717800	1.98557100	0.00000000
W	0.00000000	0.00000000	-1.22726900
C	0.00000000	2.11035800	-1.34768400
C	1.87177100	0.06317700	0.00000000
W	-1.41717800	-1.98557100	0.00000000
W	1.38476700	-1.89679500	0.00000000
C	0.00000000	-2.11035800	-1.34768400
C	0.00000000	-2.11035800	1.34768400

Pt_2

Pt	0.00000000	0.00000000	1.17506500
Pt	0.00000000	0.00000000	-1.17506500

Pt_4

Pt	0.52478900	-0.72581200	1.37158700
Pt	0.52478900	-0.72581200	-1.37158700

| Pt | 0.52478900 | 1.48489300 | 0.00000000 |
| Pt | -1.57436700 | -0.03327000 | 0.00000000 |

Pt$_6$

Pt	-1.15669200	-0.53057400	1.50781300
Pt	-1.15669200	0.55054800	-0.89228200
Pt	1.15669200	0.53057400	1.50781300
Pt	0.99537100	2.04647500	-0.61553100
Pt	-0.99537100	-2.04647500	-0.61553100
Pt	1.15669200	-0.55054800	-0.89228200

(2) X$_n$-O$_2$ and X$_n$-CO (X = WC and Pt, n = 1, 2, 4, and 6) structures

WC-O$_2$

W	0.22246500	-0.16208200	-0.03106300
C	1.20302500	1.26690800	0.24774600
O	-1.47320500	0.50062400	-0.63447500
O	-1.48686200	0.04844900	0.73599600

WC-CO

W	-0.43038900	-0.09210100	-0.00009900
C	0.24848800	1.52944100	0.00001700
C	1.51169700	-0.15507600	0.00324000
O	2.66095600	-0.17883700	-0.00152900

(WC)$_2$-O$_2$

W	1.06625200	-0.00005500	0.00093800
W	-1.62397300	0.00002500	-0.00029200
C	-0.36978200	-1.31680600	-0.00015500
C	-0.36967500	1.31679300	-0.00009700
O	2.85477000	0.00018100	-0.71079900
O	2.85874900	0.00010100	0.70501200

(WC)$_2$-CO

W	-1.52231100	0.20983500	0.00003500
W	1.06041300	-0.48311700	-0.00006900
C	-0.27435900	-0.15423300	1.30812800
C	-0.27438600	-0.15298100	-1.30818700
C	2.34777500	1.00279200	-0.00016600
O	2.92328000	2.00617600	0.00048400

(WC)$_4$-O$_2$

W	-0.83480300	1.50593000	-0.46533000
W	-0.69502900	-1.22868300	-1.06019200
C	-1.89742900	-0.09269300	-0.00375700

C	0.35088900	0.36914100	-1.53651500
W	-0.75165300	-0.36829800	1.52706200
W	1.61487300	0.11405400	-0.01843200
C	0.42273200	-1.49885100	0.49224700
C	0.33379300	1.20197300	1.06497000
O	3.32334600	-0.79132300	0.29778000
O	3.43532000	0.59387300	-0.15423500

$(WC)_4$-CO

W	0.90485100	-0.67931500	1.39621600
W	-1.53045500	-0.29181100	0.00372200
C	-0.05115500	-1.67542600	0.01642300
C	-0.49893700	0.70112500	1.37860000
W	0.90317500	-0.70638100	-1.38359800
W	0.45599100	1.68625900	-0.01646900
C	-0.50064800	0.67421600	-1.39112200
C	1.84729400	0.31272000	-0.00403600
C	-3.55808800	-0.07466000	0.00109400
O	-4.71429600	-0.03442900	0.00047700

$(WC)_6$-O_2

W	2.22201100	-0.91293000	0.00351200
W	-0.11529000	0.07129900	-1.27125700
C	0.23567500	-1.53004300	0.00566600
C	1.89983500	0.51428200	-1.36461400
W	1.44148500	1.84259600	-0.01077400
W	-0.13658200	0.15680700	1.26181000
C	1.90339900	0.48563400	1.34361800
C	-0.55621000	1.91751200	0.01323300
W	-1.78047000	-1.73396100	0.00527500
W	-2.32452900	0.99276100	-0.00586400
C	-2.16861200	-0.41782300	1.36313300
C	-2.15010200	-0.44840500	-1.36921200
O	3.06868000	-2.61036800	0.38653800
O	3.97205700	-1.63378700	-0.22041100

$(WC)_6$-CO

W	2.24349400	0.71205600	0.00003700
W	-0.13237700	-0.06181600	1.20403800
C	0.48295800	1.68559000	0.00003800
C	1.86355500	-0.68626100	1.34808300
W	1.26665100	-1.97432600	0.00001600
W	-0.13236400	-0.06183400	-1.20405100
C	1.86359600	-0.68623700	-1.34801600

C	-0.73136100	-1.85310400	-0.00004700
W	-1.56800400	1.82433400	0.00001600
W	-2.45391100	-0.83261200	-0.00002900
C	-2.17034200	0.57117600	-1.33979700
C	-2.17037100	0.57115100	1.33978900
C	3.93781600	1.87259900	-0.00011900
O	4.87583100	2.54014100	-0.00020000

Pt-O$_2$

Pt	0.00000000	0.37536700	0.00000000
O	0.50070100	-1.45531600	0.00000000
O	-0.50070100	-2.20451400	0.00000000

Pt-CO

Pt	0.00000000	0.00000000	0.36734200
C	0.00000000	0.00000000	-1.39277500
O	0.00000000	0.00000000	-2.53700500

Pt$_2$-O$_2$

Pt	0.91374600	-0.05340700	0.00002100
Pt	-1.49002600	0.02005900	-0.00000900
O	2.69209200	0.78593900	-0.00003100
O	2.92663900	-0.46080200	-0.00008100

Pt$_2$-CO

Pt	0.94668100	-0.00003200	0.00032800
Pt	-1.56273100	0.00001600	-0.00054200
C	2.78072100	0.00008300	0.00097500
O	3.92094800	0.00009200	0.00135100

Pt$_4$-O$_2$

Pt	0.54055400	-1.27806300	0.79890600
Pt	-1.51140000	0.00003500	-0.09106100
Pt	1.11017400	0.00007000	-1.35512300
Pt	0.54058100	1.27795700	0.79903300
O	-3.31456300	0.64250900	-0.73965200
O	-3.31454100	-0.64250700	-0.73995300

Pt$_4$-CO

Pt	1.00134900	-1.35746100	0.16409000
Pt	1.00418900	0.88788600	-1.04185500
Pt	0.11527400	0.74010500	1.37279600
Pt	-1.42862300	-0.26938000	-0.48361500
C	-3.22088600	-0.08710900	-0.19527300

O	-4.33317400	0.05411700	0.03515500

Pt$_6$-O$_2$

Pt	-0.87098100	0.96853200	-1.27967900
Pt	-0.15932500	-1.44219000	-0.54495200
Pt	1.20018100	1.78213500	0.08208800
Pt	2.13441200	-0.60274300	-0.07464200
Pt	-2.44741100	-0.28690300	0.32094400
Pt	-0.19407600	0.15300200	1.53749100
O	1.02273600	-3.01486000	-0.28803400
O	2.26496300	-2.56050100	-0.11415800

Pt$_6$-CO

Pt	-0.58417500	0.46251400	-1.52736000
Pt	-0.12644200	-1.57793000	0.00058700
Pt	0.91691800	1.88457400	-0.00013300
Pt	2.22017700	-0.38327600	0.00006700
Pt	-2.49909200	-0.42260700	-0.00033800
Pt	-0.58507900	0.46349200	1.52707700
C	3.27394000	-1.85358400	-0.00034200
O	3.95706500	-2.77078900	0.00123800

(3) Transition states involved in the CO oxidation mechanism

TS1

O	0.58853900	2.08175300	-0.40496400
O	-0.39307200	1.54977800	0.45845600
C	2.21706000	1.06153000	0.03693200
O	3.13523700	1.77592400	0.04285000
W	-0.16110500	-0.16326600	-0.25702600
C	1.62637600	-0.19670600	0.06433100

TS1'

W	-0.13854000	-0.13054500	-0.05975100
C	1.04186900	1.27557200	0.03952700
O	-1.27137700	0.20185600	-1.46636800
O	-1.02683800	-0.04398900	1.40921400
C	-1.60639600	1.62367000	-2.36913900
O	-2.32513900	1.53627700	-3.26461700

TS1''

O	0.79896400	1.98644700	-0.33604000
O	-0.31590200	1.65425000	0.55427700
C	2.03673900	1.14976500	-0.01466300
O	3.06995200	1.72170200	0.04371700

W	-0.21877300	-0.11892100	-0.27941800
C	1.55249100	-0.22112200	-0.03364600
C	-0.94725900	-2.04236400	-0.52514900
O	-1.39210300	-3.10241500	-0.54763300

TS2

W	0.05062100	0.33937100	0.04534600
C	0.90928700	-1.24494200	-0.00337100
O	-1.49490100	-0.68595700	-0.01866000
C	-0.38256000	-1.89193300	-0.04933300
O	-0.84379000	-2.98201300	-0.10031000

TS2''

O	-0.88464400	1.03099200	0.77333900
W	0.43659700	0.07228200	-0.11711200
C	0.89119100	-1.39684900	0.78959700
C	-1.53896500	-0.21927500	-0.14611800
O	-2.66804800	-0.48751000	-0.17266400

TS3

W	0.31277300	1.25964400	-0.02664000
W	-1.19955700	-0.94117000	0.02851000
C	-0.56867100	0.32447600	1.32715200
C	-0.58709900	0.26961400	-1.32892400
C	2.21058400	0.34798500	-0.02044600
O	3.34874300	0.17756800	-0.02455000
O	0.29784100	-2.02291600	0.03863300
O	1.57891800	-1.68636300	0.02324000

TS3'

W	1.02213300	0.04102500	0.04501500
W	-1.66731500	-0.01638500	0.21522500
C	-0.41764600	1.33719000	0.06300200
C	-0.34827800	-1.30978400	0.27181000
O	3.13197700	0.15316500	0.68752000
O	1.94026600	-0.05684200	-1.50121000
C	3.58676100	0.07208600	-0.45381800
O	4.47902300	0.03536500	-1.19840900

TS3''

W	-0.72259700	-0.14283200	-0.05493100
W	1.89216700	0.44011600	-0.00165000
C	0.51497300	0.50957900	1.26169100
C	0.68343500	0.37814200	-1.37315500

C	1.69751300	-1.66448000	-0.00415900
O	2.57577200	-2.46972200	0.03932900
C	-2.23355400	1.19231400	-0.02220200
O	-3.07466800	1.98876800	-0.00637600
O	-0.76907700	-2.00421600	0.57578800
O	0.34116300	-2.20762100	-0.36829100

TS4

W	0.86358700	-0.01606500	0.33956600
W	-1.60474300	-0.00607100	-0.79604400
C	-0.43480500	-1.34142400	-0.24635500
C	-0.41734000	1.31975500	-0.26056500
O	2.51189700	-0.02211700	1.23651900
C	1.12980700	-0.00692200	2.33649200
O	1.22846900	-0.00157200	3.48829400

TS5

W	-0.28222400	-1.26753500	-1.35528700
W	-0.96595500	1.18853700	-0.02187000
C	0.27588000	0.65495700	-1.41998300
C	-1.60805800	-0.77564200	0.00868600
W	1.63126000	0.49743400	-0.00762500
W	-0.28523400	-1.22367900	1.39092900
C	0.27250000	0.69975200	1.39561200
C	1.07570200	-1.57528700	0.02460600
C	-1.12202100	3.35095000	-0.06218900
O	-1.31132200	4.48114100	-0.08397000
O	2.02811000	2.37804600	-0.03668600
O	1.03225100	3.30265300	-0.05235400

TS5'

W	0.00531600	0.60197400	0.01457900
W	-0.41140600	-2.08909200	-0.69847200
C	-1.41485000	-0.72270600	0.32514600
C	1.00613000	-0.76722000	-0.98660300
W	-0.55528900	-1.29919800	2.01350000
W	1.97770400	-1.38691700	0.69789900
C	0.43558700	-2.65732700	0.98682800
C	0.86345000	0.01145200	1.68556800
O	3.66838600	-1.98494700	0.95335000
O	3.67851200	0.29322500	0.32743500
C	4.59430300	-0.47489000	0.59262900
O	5.74649000	-0.66499100	0.71339900

TS5''

W	-0.21580000	-1.35747200	-1.32438000
W	-0.88867300	1.08668300	0.08838000
C	0.13939900	0.57128900	-1.50200900
C	-1.38632700	-0.99554700	0.21046700
W	1.69392900	0.51463300	-0.29079700
W	0.14006800	-1.24805700	1.42069100
C	0.53125400	0.67954000	1.34186300
C	1.37227000	-1.51461500	-0.18571800
C	0.15189200	3.10123400	-0.22716100
O	-0.22505200	4.20178300	-0.45508100
O	2.71114300	2.12854900	-0.07006000
O	1.68933000	3.07292800	-0.58649100
C	-0.80424500	-2.11499200	3.07415900
O	-1.29801600	-2.63302700	3.97863700

TS6 (15*)

W	-1.51430700	0.16293400	0.35164700
W	-1.42118300	2.82480300	1.30206700
C	-2.73485700	1.71796900	0.32493700
C	-0.20743100	1.27179800	1.30930800
W	-1.99376600	2.32812600	-1.40230800
W	0.69223300	1.83585600	-0.42200500
C	-0.71062200	3.40689100	-0.41370900
C	-0.77135100	0.78194800	-1.35753800
O	2.47421300	1.38694600	-0.71405600
C	2.32477700	3.05435200	-0.98399900
O	3.25492600	3.68488600	-1.29155900

TS7

W	-1.38788300	2.03822600	0.01150600
W	0.00195900	-0.08221300	1.19415000
C	-1.87435000	-0.04700500	-0.01633500
C	0.01330100	1.98989300	1.39116300
W	1.37174000	2.07009500	0.01383400
W	0.00344400	-0.04946200	-1.22678600
C	0.01520900	2.02737800	-1.36687700
C	1.86618000	0.06496300	-0.01415100
W	-1.42228200	-2.05534300	-0.04402600
W	1.46649000	-1.99030800	-0.04122800
C	0.02394900	-2.18260700	-1.37258900
C	0.02220600	-2.21855900	1.28256200
O	-1.39186800	3.96194000	0.03835000
O	-0.18376700	4.60641000	0.05137200

C	1.97742800	4.17352900	0.04423700
O	2.36544500	5.24950500	0.06121900

TS7'

W	-2.50323400	0.63654200	0.09550000
W	-0.13943300	-0.07263400	-1.34906300
C	-0.80634700	1.65812600	-0.12852900
C	-2.01850000	-0.95250000	-1.24286000
W	-1.37078200	-2.06516100	0.15877100
W	0.01049700	0.10936300	1.21779600
C	-1.86962800	-0.75578000	1.47155500
C	0.60531400	-1.64024100	0.01365500
W	1.19155400	1.98045900	-0.28282500
W	2.36368200	-0.66241700	-0.16101100
C	2.01043600	0.78338600	1.09578300
C	1.85983300	0.58864200	-1.56146400
O	-3.97959000	1.55656000	0.56499800
O	-5.43965900	2.73015900	-1.16583200
C	-4.48697100	2.05776000	-1.20795600
O	-3.59701500	1.46863900	-1.79648100

TS7''

W	1.98203800	-1.64689000	-0.39723500
W	-0.36696700	-0.12181700	-1.15082800
C	0.02242300	-1.77744200	0.24349000
C	1.71359900	0.13805700	-1.40728500
W	1.46538700	1.64562600	-0.20628800
W	-0.17638300	0.13019300	1.28347600
C	1.78320000	0.68003200	1.55817500
C	-0.57251800	1.78892400	-0.21345500
W	-2.04373700	-1.60954400	0.38299400
W	-2.48807000	1.14155100	0.11872900
C	-2.32959800	-0.12232300	1.60882100
C	-2.53959700	-0.42939500	-1.06039100
O	3.20108800	-1.43201800	0.90731000
O	2.33503700	-2.95538800	-1.45928700
C	3.22603400	2.80404800	-0.38717800
O	4.17153500	3.44022200	-0.52860100
C	2.92717200	0.15056800	2.11022300
O	3.79735900	0.10607900	2.87521500

TS8

W	-2.33847500	-0.83111200	-0.00440900
W	-0.03071500	0.18670300	1.29772100

C	-0.54090600	-1.65587500	0.12704900
C	-1.98120800	0.85067100	1.26535700
W	-1.52707200	2.00046400	-0.18785800
W	0.03292300	-0.03233800	-1.26961200
C	-1.91203100	0.64849400	-1.47871100
C	0.49026200	1.78799300	-0.10160100
W	1.47675000	-1.74934800	0.19952300
W	2.35212300	0.98900500	0.00130900
C	2.10472900	-0.49449300	-1.23001600
C	2.03846900	-0.27006100	1.43792800
O	-3.78281200	-2.01465000	-0.11543500
C	-3.47186300	-1.80556200	1.46021600
O	-4.08982800	-2.34077300	2.29472600

TS8''

W	-1.95898600	1.34448300	0.00042500
W	0.24797900	-0.00749300	-1.24956800
C	0.09937700	1.85216100	0.00039900
C	-1.77486100	-0.01949100	-1.40485600
W	-1.79352100	-1.37273300	-0.00050800
W	0.24803300	-0.00909900	1.24971500
C	-1.77491700	-0.02058400	1.40476100
C	0.29789100	-1.82457700	-0.00031800
W	2.13406800	1.43989800	0.00023800
W	2.28035400	-1.37644200	-0.00030100
C	2.40789400	0.06027100	1.35216800
C	2.40798500	0.06084900	-1.35219700
O	-3.83585600	1.10047800	0.00033200
C	-4.00332200	-0.56989200	-0.00031000
O	-5.12000100	-0.92671500	-0.00008200

TS9

Pt	0.04641200	-0.33832700	-0.00550600
C	-0.84297800	1.34396700	-0.00269700
O	-1.80109700	2.00038400	-0.00439300
O	0.68428500	2.26752900	0.00652500
O	1.55930500	1.32113400	0.00648200

TS10

Pt	-0.21861700	-0.00970100	0.28420300
O	0.09142800	-0.00002600	-1.50255800
C	1.72454000	-0.50395900	-1.96425800
O	1.88928800	-0.92745400	-3.01841600

TS11

Pt	0.76412500	-0.38491100	0.00024300
Pt	-1.67456000	0.08319700	-0.00015300
C	1.48869400	1.30123100	0.00049400
O	1.60381900	2.44424200	0.00041100
O	2.80479700	-0.83512600	-0.00012100
O	3.35160500	0.35666800	-0.00154400

TS12

Pt	0.85346300	-0.35224700	0.00390500
Pt	-1.54475600	0.13092700	-0.00171700
O	2.70705000	-0.77972600	-0.02132500
C	1.97420800	1.11639000	0.00135500
O	2.55240300	2.10031200	-0.00102800

TS13

Pt	-0.59769600	-1.19172800	-0.99080100
Pt	-0.87731500	0.87512000	0.68584800
Pt	1.31652800	0.55304100	-0.59797100
Pt	0.73859000	-1.27112000	1.16370000
O	0.43392300	3.24249800	-0.66129300
O	1.48580100	2.45168300	-0.86662800
C	-1.15354500	2.61673600	-0.13310800
O	-1.92368500	3.44374100	-0.41768200

TS14

Pt	-0.74489000	1.37199900	0.65097400
Pt	1.45077200	-0.07362800	0.41574100
Pt	-0.38812800	-0.10734400	-1.42728900
Pt	-0.90583700	-1.18145400	0.85528000
O	3.26948400	-0.19297700	0.12661600
C	3.80643500	-0.34616100	-1.74613500
O	4.92423100	-0.37344500	-1.98371400

TS15

Pt	-1.22171100	0.12673200	1.49902400
Pt	-1.59922600	1.34104400	-0.73167400
Pt	1.28083100	-0.37274200	1.59454500
Pt	1.02819100	1.28986400	-0.46001800
Pt	-1.64542900	-1.21962200	-0.65080900
Pt	0.88759900	-1.30451900	-0.87869800
C	2.93555300	1.26136400	-0.64249800
O	3.86699900	1.95245900	-0.55761900
O	3.53507200	-0.24039400	-1.22025800

| O | 2.77628100 | -1.30046300 | -1.37086000 |

TS16

Pt	0.18963400	0.02796900	1.55149800
Pt	0.27568500	-1.63074600	-0.50833000
Pt	-0.78647000	1.95933300	0.12513200
Pt	-1.97549400	-0.36297400	-0.08014600
Pt	2.47663100	-0.34474900	0.33897700
Pt	0.87214700	0.74346500	-1.38579300
O	-3.80651500	0.10501800	-0.37370500
C	-3.25940800	-1.74899000	-0.04964800
O	-4.00722800	-2.61818000	0.00789900

3*

W	0.02356800	-1.29461100	-1.31816700
W	1.55053000	0.62553800	0.22549100
C	1.30444700	-1.37318200	0.18884400
C	0.13564100	0.56094300	-1.41088500
W	-0.14113500	-1.25938600	1.52546600
W	-1.35181300	0.83919400	-0.01064500
C	0.02810400	0.63421700	1.54124800
C	-1.43650500	-1.15927300	0.00503100
O	-2.76711400	2.03437300	0.53709800
O	-2.55434000	2.07892600	-0.90440000
O	3.13497600	1.21632200	0.83536700
O	2.28555200	2.42185000	-1.03617300
C	3.33115600	2.64792500	-0.45001400
O	4.32582200	3.21929000	-0.25823400

7*

W	-0.71818700	-0.97418000	1.50228900
W	-0.93609500	1.40046700	-0.08602600
C	-1.84842200	-0.42334200	-0.03948100
C	0.21969800	0.68195400	1.50268500
W	-0.54860400	-1.14306000	-1.32712300
W	1.61812300	0.01495000	0.21568900
C	0.28920200	0.52320800	-1.45278100
C	0.57745500	-1.70666700	0.21746700
O	3.05566400	1.21648700	-1.13721800
O	3.28906100	-0.04253900	0.87673700
O	-1.67900600	2.96105200	-0.22757600
C	4.08882400	1.05806000	-0.50928300
O	5.22430700	1.19268300	-0.29917500

11*

W	-0.10569300	-1.04752200	1.44929600
W	-1.32162700	1.23639600	0.19735000
C	-1.73847800	-0.75558800	0.37238100
C	0.34893000	0.80127500	1.33255600
W	-0.75495900	-1.13191300	-1.30140500
W	1.42394600	0.54212400	-0.37619800
C	-0.36171800	0.69834500	-1.53480800
C	0.85301100	-1.43682500	-0.22546500
O	3.01289300	1.43646800	-0.78857100
O	-2.40801800	2.56775200	0.42418300
C	3.41626500	0.23800800	0.20680900
O	4.52120300	0.04533400	0.53714500